Full wwPDB EM Validation Report ⓘ

Dec 11, 2024 – 06:03 pm GMT

PDB ID	:	9G93
EMDB ID	:	EMD-45459
Title	:	CryoET structure of the in vitro grown Bacillus anthracis Sap S-layer
Authors	:	Sogues, A.; Leigh, K.; Van der Verren, S.; Kudryashev, M.; Pak, A.; Halingstad, E.V.; Cecil, A.J.; Fioravanti, A.; Remaut, H.
Deposited on	:	2024-07-24
Resolution	:	7.20 Å(reported)

This is a Full wwPDB EM 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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

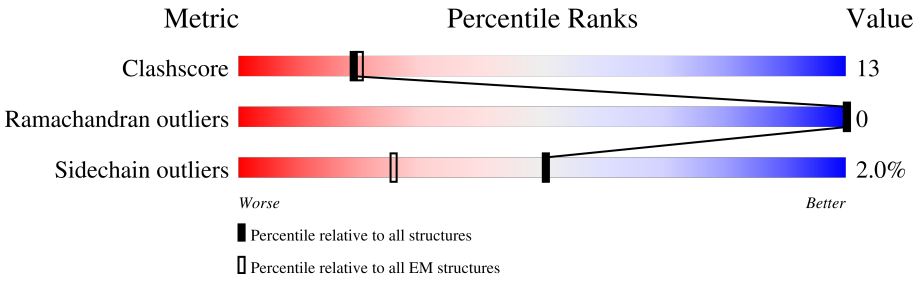
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	814	62% 11% 27%
1	B	814	63% 9% 27%
1	C	814	63% 10% 27%
1	D	814	64% 9% 27%
1	E	814	62% 11% 27%
1	F	814	62% 10% 27%
1	G	814	29% 5% 66%
1	I	814	39% 7% 54%
1	J	814	28% 6% 66%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	814	
1	L	814	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 37178 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 S-layer protein sap.

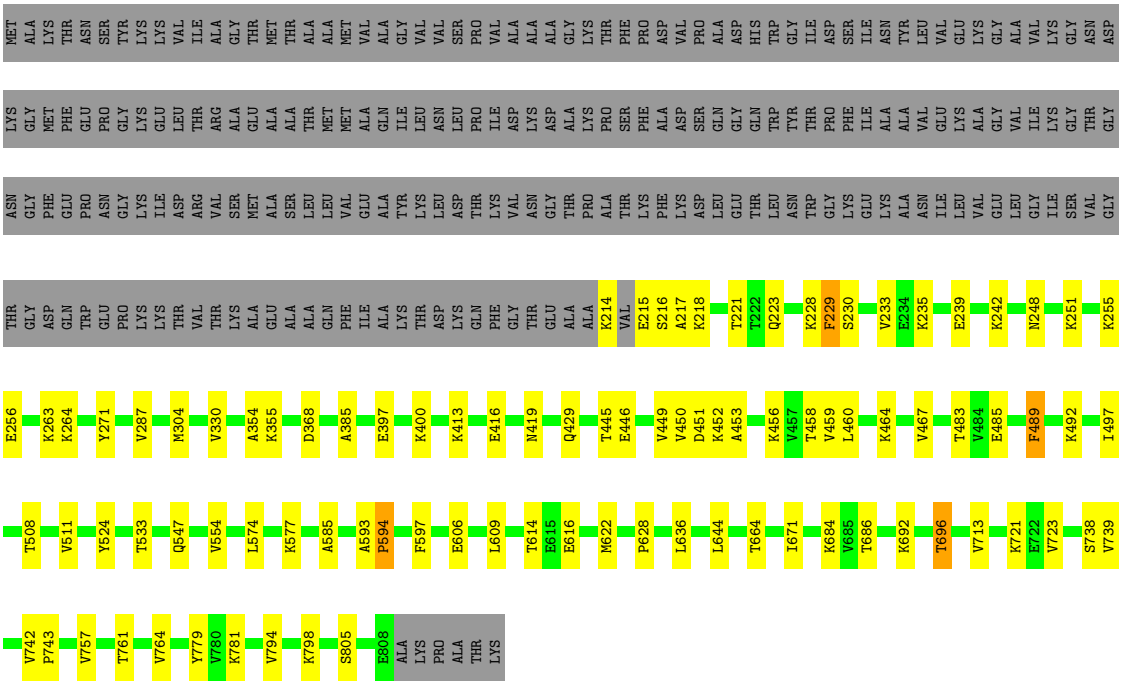
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	B	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	C	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	D	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	E	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	F	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	G	278	Total	C	N	O	S	0	0
			2097	1315	343	438	1		
1	I	376	Total	C	N	O	S	0	0
			2804	1761	458	584	1		
1	J	277	Total	C	N	O	S	0	0
			2088	1310	341	436	1		
1	L	88	Total	C	N	O	S	0	0
			649	406	103	139	1		
1	K	376	Total	C	N	O	S	0	0
			2804	1761	458	584	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

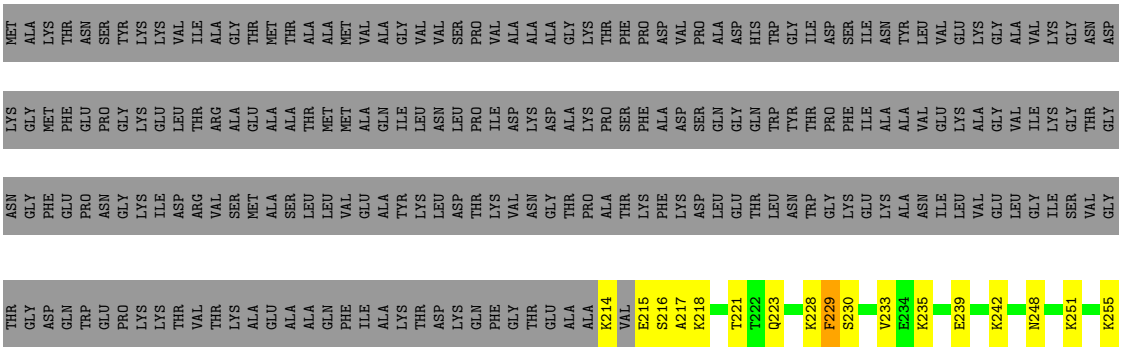
• Molecule 1: S-layer protein sap

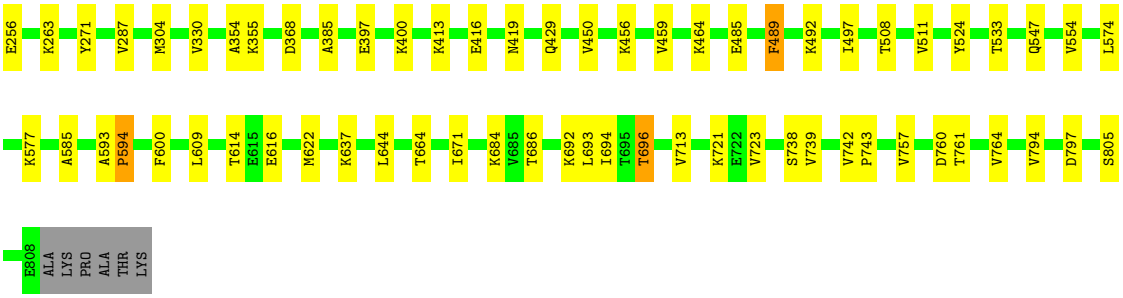
Chain A:



• Molecule 1: S-layer protein sap

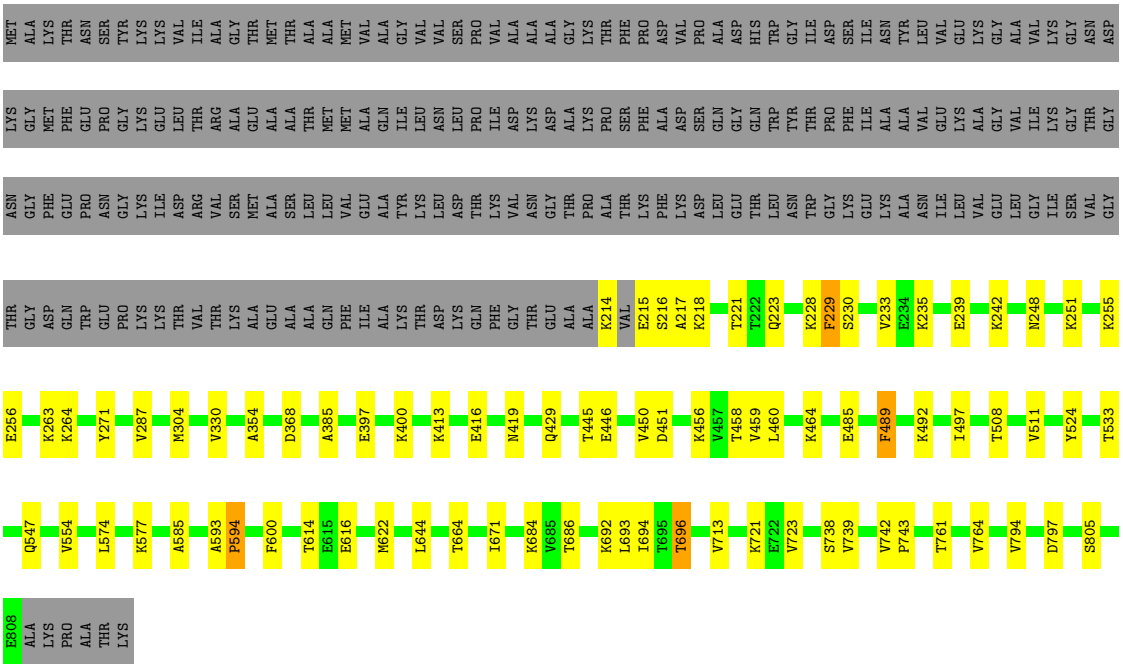
Chain B:





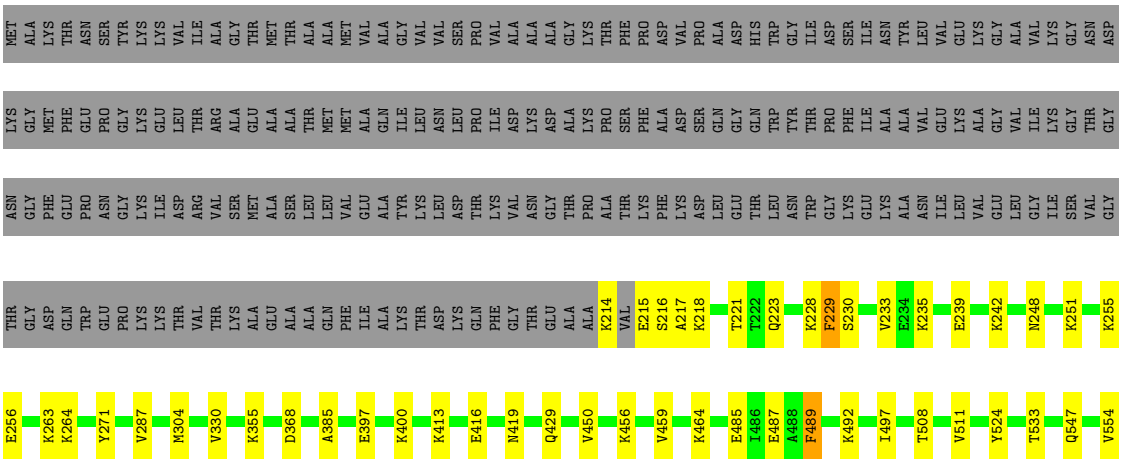
• Molecule 1: S-layer protein sap

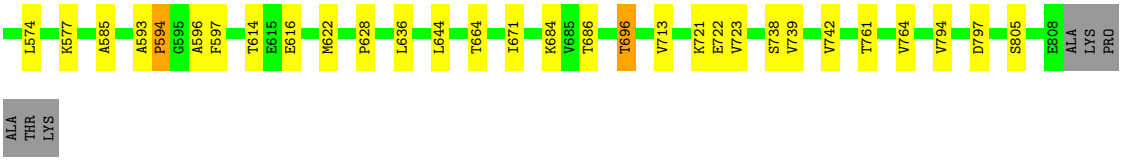
Chain C:



• Molecule 1: S-layer protein sap

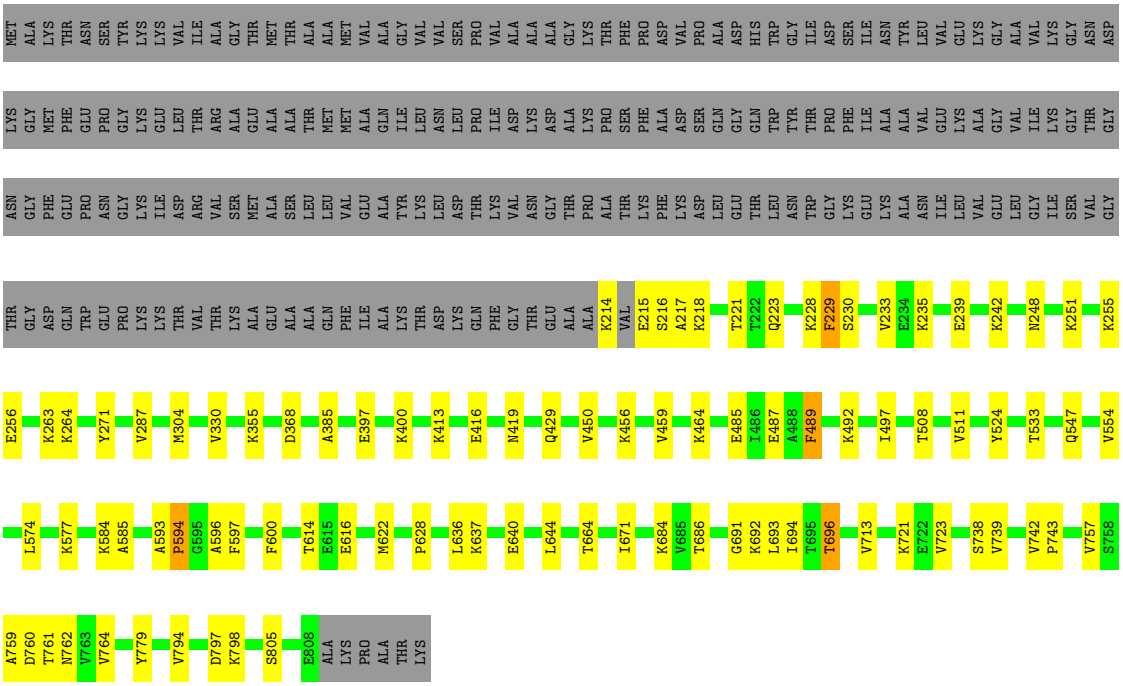
Chain D:





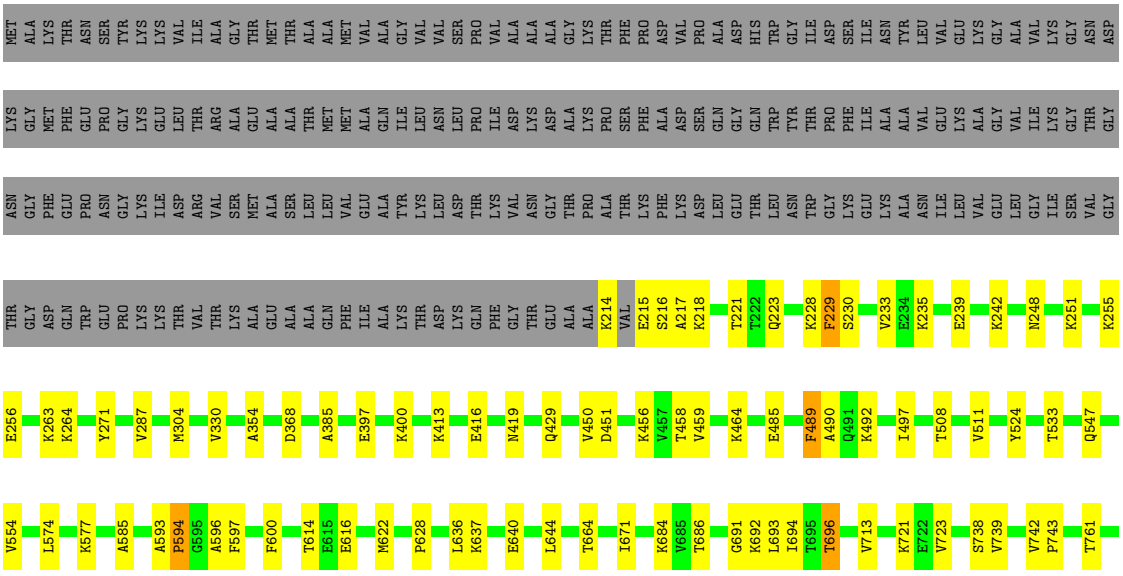
• Molecule 1: S-layer protein sap

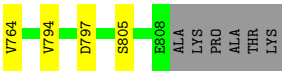
Chain E:



• Molecule 1: S-layer protein sap

Chain F:



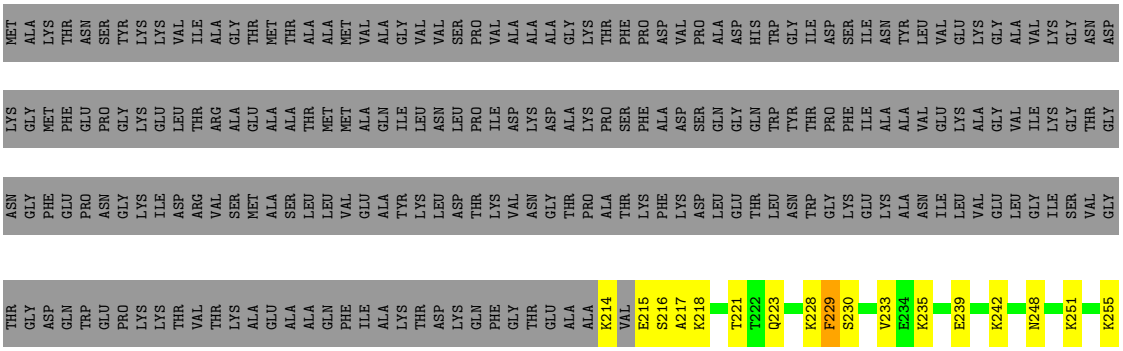


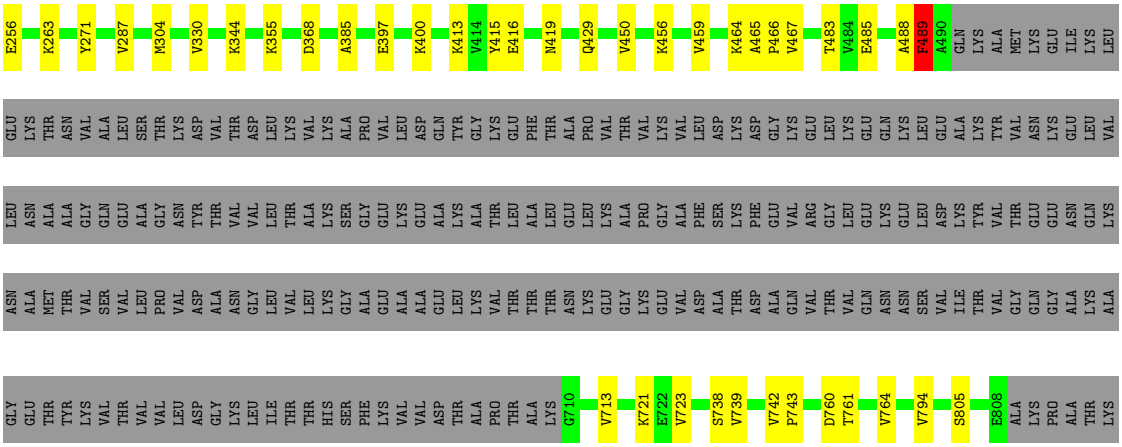
• Molecule 1: S-layer protein sap

Chain G:

• Molecule 1: S-layer protein sap

Chain I:



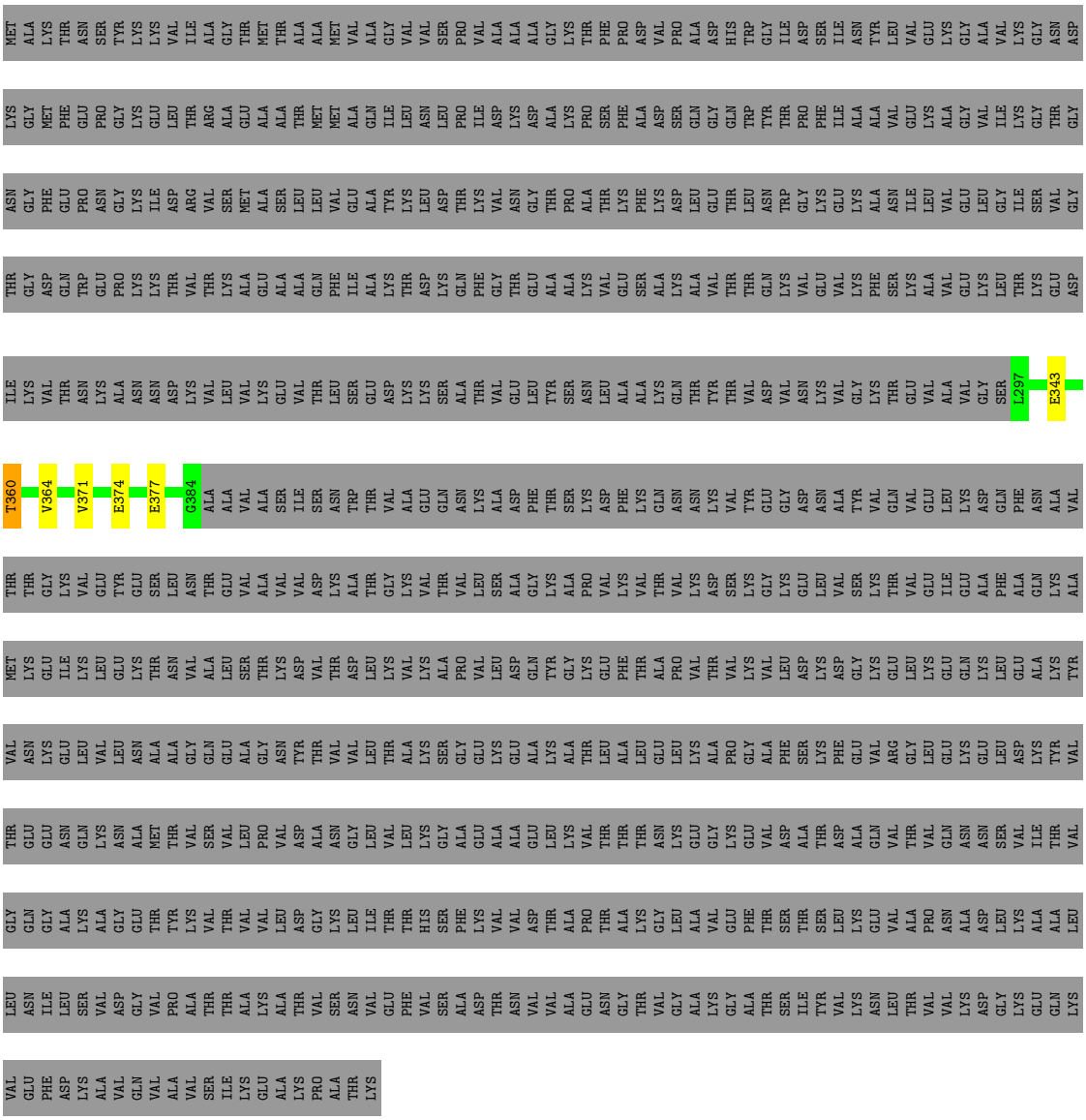


• Molecule 1: S-layer protein sap

Chain J:

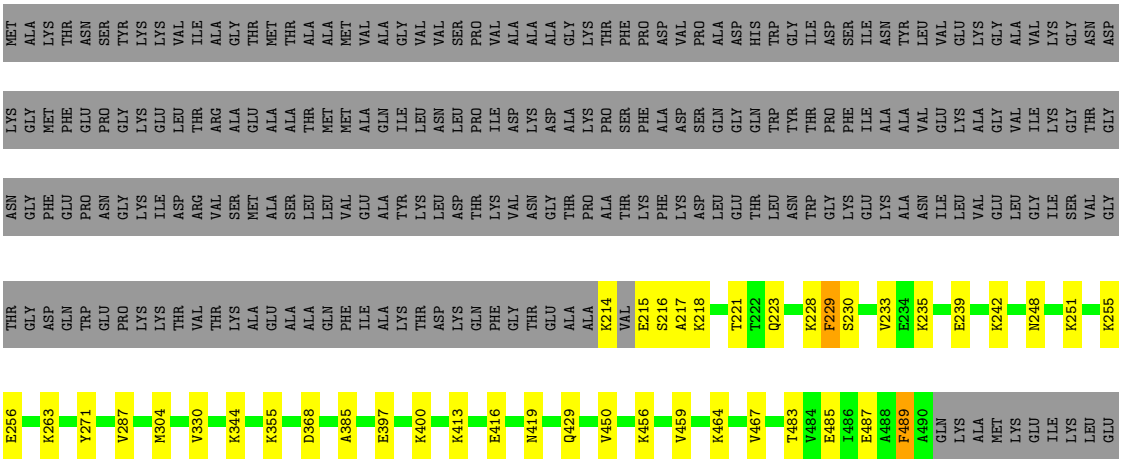
• Molecule 1: S-layer protein sap

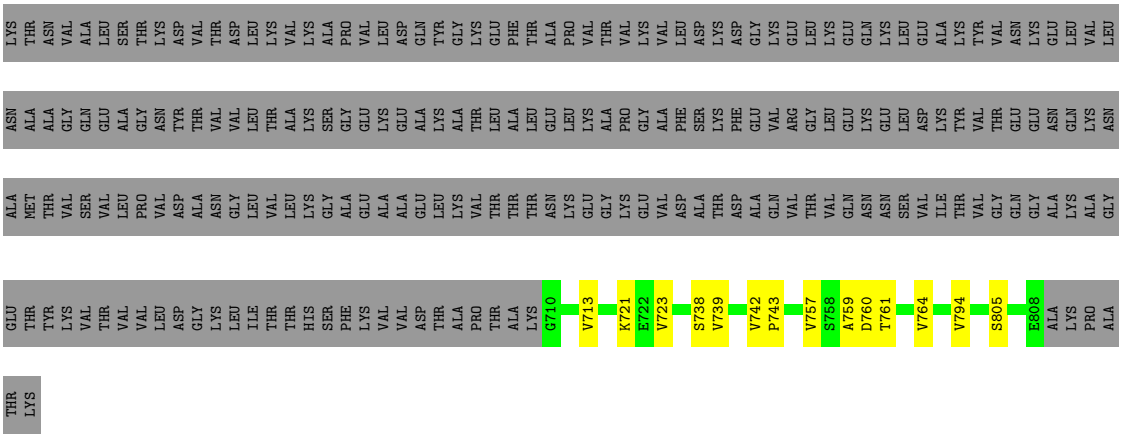
Chain L:



• Molecule 1: S-layer protein sap

Chain K:




LYS THR ASN VAL ALA LEU SER THR LYS ASP VAL THR ASP LEU LYS VAL LYS ALA PRO VAL LEU ASP GLN TYR GLY LYS GLU PHE THR ALA PRO VAL THR VAL LYS VAL LEU ASP LYS ASP GLY LYS GLU LEU LYS GLU GLN LYS LEU GLU ALA LYS TYR VAL ASN LYS GLU LEU VAL LEU
ASN ALA ALA GLY GLN GLU ALA GLY ASN TYR THR VAL VAL LEU THR ALA LYS SER GLY GLU LYS GLU ALA LYS ALA THR LEU ALA LEU GLU GLU LEU LYS ALA PRO GLY GLU ALA PHE SER LYS PHE GLU VAL ARG GLY LEU GLU LYS GLU LEU ASP LYS TYR VAL THR GLU GLU ASN GLN LYS ASN
ALA MET THR VAL SER VAL LEU PRO VAL ASP ALA ASN GLY LEU VAL ALA ALA GLU LEU LYS GLY ALA GLU ALA ALA GLU LEU LYS VAL THR THR THR ASN LYS GLU GLY LYS GLU VAL ASP ALA THR ASP ALA GLN VAL THR VAL GLN ASN ASN ASN SER VAL ILE THR VAL GLY GLN GLY ALA LYS ALA GLY
GLU THR TYR LYS VAL THR VAL VAL LEU ASP GLY LYS LEU ILE THR THR HIS SER PHE LYS VAL VAL ASP THR ALA PRO THR ALA LYS G710 V713 K721 E722 V723 S738 V739 V742 P743 V757 S758 A759 D760 T761 V764 V794 S805 E808 ALA LYS PRO ALA
THR LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	10126	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	156	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	1/4495 (0.0%)	0.63	3/6079 (0.0%)
1	B	0.44	1/4495 (0.0%)	0.63	3/6079 (0.0%)
1	C	0.44	1/4495 (0.0%)	0.63	3/6079 (0.0%)
1	D	0.44	2/4495 (0.0%)	0.62	2/6079 (0.0%)
1	E	0.45	2/4495 (0.0%)	0.62	2/6079 (0.0%)
1	F	0.44	1/4495 (0.0%)	0.62	2/6079 (0.0%)
1	G	0.49	3/2115 (0.1%)	0.65	3/2857 (0.1%)
1	I	0.48	3/2827 (0.1%)	0.63	2/3825 (0.1%)
1	J	0.49	3/2106 (0.1%)	0.66	4/2845 (0.1%)
1	K	0.46	2/2827 (0.1%)	0.62	1/3825 (0.0%)
1	L	0.48	0/654	0.58	0/884
All	All	0.45	19/37499 (0.1%)	0.63	25/50710 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	488	ALA	C-N	7.92	1.52	1.34
1	J	488	ALA	C-N	7.92	1.52	1.34
1	G	488	ALA	C-N	7.90	1.52	1.34
1	K	487	GLU	C-N	-7.16	1.17	1.34
1	E	487	GLU	C-N	-6.16	1.19	1.34
1	G	489	PHE	C-N	-5.99	1.20	1.34
1	J	489	PHE	C-N	-5.97	1.20	1.34
1	I	489	PHE	C-N	-5.96	1.20	1.34
1	D	487	GLU	C-N	-5.62	1.21	1.34
1	F	304	MET	CG-SD	5.14	1.94	1.81
1	I	304	MET	CG-SD	5.13	1.94	1.81
1	K	304	MET	CG-SD	5.13	1.94	1.81
1	E	304	MET	CG-SD	5.13	1.94	1.81
1	D	304	MET	CG-SD	5.12	1.94	1.81
1	A	304	MET	CG-SD	5.12	1.94	1.81
1	G	304	MET	CG-SD	5.12	1.94	1.81
1	C	304	MET	CG-SD	5.11	1.94	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	304	MET	CG-SD	5.11	1.94	1.81
1	B	304	MET	CG-SD	5.09	1.94	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	594	PRO	O-C-N	-7.91	109.75	123.20
1	A	594	PRO	O-C-N	-7.89	109.79	123.20
1	B	594	PRO	O-C-N	-7.82	109.91	123.20
1	F	594	PRO	O-C-N	-7.05	111.21	123.20
1	D	594	PRO	O-C-N	-6.83	111.60	123.20
1	E	594	PRO	O-C-N	-6.82	111.61	123.20
1	J	467	VAL	CB-CA-C	6.23	123.23	111.40
1	G	467	VAL	CB-CA-C	5.90	122.61	111.40
1	C	594	PRO	CA-C-N	5.52	127.24	116.20
1	I	489	PHE	O-C-N	-5.49	113.91	122.70
1	A	594	PRO	CA-C-N	5.49	127.18	116.20
1	J	489	PHE	O-C-N	-5.48	113.93	122.70
1	G	489	PHE	O-C-N	-5.44	114.00	122.70
1	B	594	PRO	CA-C-N	5.43	127.05	116.20
1	J	467	VAL	N-CA-C	-5.34	96.58	111.00
1	A	368	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	368	ASP	CB-CG-OD2	5.22	123.00	118.30
1	K	368	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	368	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	368	ASP	CB-CG-OD2	5.20	122.98	118.30
1	F	368	ASP	CB-CG-OD2	5.18	122.97	118.30
1	I	368	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	368	ASP	CB-CG-OD2	5.17	122.95	118.30
1	J	368	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	368	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4456	0	4624	180	0
1	B	4456	0	4624	110	0
1	C	4456	0	4624	134	0
1	D	4456	0	4624	88	0
1	E	4456	0	4624	210	0
1	F	4456	0	4624	157	0
1	G	2097	0	2157	37	0
1	I	2804	0	2891	86	0
1	J	2088	0	2149	54	0
1	K	2804	0	2891	81	0
1	L	649	0	663	4	0
All	All	37178	0	38495	950	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 13.

All (950) 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:F:239:GLU:CB	1:F:742:VAL:CG1	1.77	1.62
1:B:239:GLU:CB	1:B:742:VAL:CG1	1.77	1.61
1:K:239:GLU:CB	1:K:742:VAL:CG1	1.77	1.60
1:I:239:GLU:CB	1:I:742:VAL:CG1	1.77	1.59
1:C:239:GLU:CB	1:C:742:VAL:CG1	1.77	1.58
1:B:239:GLU:CB	1:B:742:VAL:HG11	1.32	1.57
1:A:239:GLU:CB	1:A:742:VAL:CG1	1.77	1.56
1:E:239:GLU:CB	1:E:742:VAL:HG11	1.31	1.56
1:E:239:GLU:CB	1:E:742:VAL:CG1	1.77	1.54
1:A:239:GLU:CB	1:A:742:VAL:HG11	1.31	1.52
1:F:239:GLU:CB	1:F:742:VAL:HG11	1.32	1.49
1:K:239:GLU:CB	1:K:742:VAL:HG11	1.31	1.48
1:I:239:GLU:CB	1:I:742:VAL:HG11	1.31	1.48
1:C:239:GLU:CB	1:C:742:VAL:HG11	1.32	1.45
1:A:458:THR:CB	1:E:757:VAL:HG11	1.57	1.34
1:B:239:GLU:HB3	1:B:742:VAL:CG1	0.85	1.32
1:E:692:LYS:HE3	1:F:600:PHE:CE1	1.64	1.32
1:A:239:GLU:HB3	1:A:742:VAL:CG1	0.85	1.32
1:C:239:GLU:HB3	1:C:742:VAL:CG1	0.85	1.32
1:F:239:GLU:HB3	1:F:742:VAL:CG1	0.85	1.32
1:E:239:GLU:HB3	1:E:742:VAL:CG1	0.85	1.31
1:I:239:GLU:HB3	1:I:742:VAL:CG1	0.85	1.31
1:K:239:GLU:HB3	1:K:742:VAL:CG1	0.85	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ALA:HB1	1:E:762:ASN:ND2	1.46	1.29
1:B:239:GLU:O	1:B:742:VAL:HG12	1.33	1.29
1:C:239:GLU:O	1:C:742:VAL:HG12	1.33	1.28
1:A:239:GLU:O	1:A:742:VAL:HG12	1.33	1.28
1:K:239:GLU:O	1:K:742:VAL:HG12	1.33	1.26
1:E:239:GLU:O	1:E:742:VAL:HG12	1.33	1.26
1:I:239:GLU:O	1:I:742:VAL:HG12	1.33	1.25
1:A:451:ASP:HA	1:E:759:ALA:O	1.35	1.23
1:A:449:VAL:HG21	1:E:779:TYR:CD1	1.73	1.23
1:E:600:PHE:CE1	1:F:692:LYS:HE3	1.72	1.23
1:A:239:GLU:C	1:A:742:VAL:HG12	1.60	1.22
1:B:239:GLU:C	1:B:742:VAL:HG12	1.60	1.22
1:F:239:GLU:O	1:F:742:VAL:HG12	1.33	1.22
1:A:451:ASP:OD1	1:E:760:ASP:CA	1.88	1.21
1:E:239:GLU:C	1:E:742:VAL:HG12	1.60	1.21
1:C:239:GLU:C	1:C:742:VAL:HG12	1.60	1.21
1:A:451:ASP:OD1	1:E:760:ASP:HA	1.07	1.21
1:F:239:GLU:C	1:F:742:VAL:HG12	1.60	1.20
1:I:239:GLU:C	1:I:742:VAL:HG12	1.60	1.20
1:K:239:GLU:C	1:K:742:VAL:HG12	1.60	1.20
1:C:693:LEU:O	1:D:597:PHE:N	1.76	1.19
1:E:693:LEU:CD2	1:F:596:ALA:HA	1.76	1.15
1:E:596:ALA:HA	1:F:693:LEU:HD23	1.26	1.11
1:C:242:LYS:HG2	1:C:743:PRO:HD3	1.10	1.09
1:A:458:THR:CG2	1:E:757:VAL:HG11	1.82	1.09
1:E:242:LYS:HG2	1:E:743:PRO:HD3	1.10	1.09
1:E:693:LEU:HD23	1:F:596:ALA:HA	1.25	1.09
1:F:242:LYS:HG2	1:F:743:PRO:HD3	1.10	1.08
1:F:239:GLU:CB	1:F:742:VAL:HG12	1.60	1.08
1:K:242:LYS:HG2	1:K:743:PRO:HD3	1.10	1.08
1:A:449:VAL:HG13	1:E:759:ALA:HB2	1.35	1.07
1:A:451:ASP:CG	1:E:761:THR:H	1.57	1.07
1:A:458:THR:HB	1:E:757:VAL:HG11	1.16	1.07
1:A:242:LYS:HG2	1:A:743:PRO:HD3	1.10	1.07
1:B:242:LYS:HG2	1:B:743:PRO:HD3	1.10	1.07
1:I:242:LYS:HG2	1:I:743:PRO:HD3	1.10	1.07
1:A:242:LYS:CG	1:A:743:PRO:HD3	1.86	1.06
1:B:242:LYS:CG	1:B:743:PRO:HD3	1.86	1.06
1:A:239:GLU:CA	1:A:742:VAL:HG12	1.86	1.06
1:C:242:LYS:CG	1:C:743:PRO:HD3	1.86	1.06
1:F:242:LYS:CG	1:F:743:PRO:HD3	1.86	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:GLU:CB	1:K:742:VAL:HG12	1.60	1.05
1:E:242:LYS:CG	1:E:743:PRO:HD3	1.86	1.05
1:E:600:PHE:CE2	1:F:600:PHE:CE2	2.44	1.05
1:B:492:LYS:CD	1:B:524:TYR:HE2	1.70	1.05
1:B:239:GLU:CA	1:B:742:VAL:HG12	1.86	1.04
1:C:239:GLU:CA	1:C:742:VAL:HG12	1.86	1.04
1:I:239:GLU:CA	1:I:742:VAL:HG12	1.86	1.04
1:C:492:LYS:CD	1:C:524:TYR:HE2	1.69	1.04
1:K:239:GLU:CA	1:K:742:VAL:HG12	1.86	1.04
1:A:239:GLU:CB	1:A:742:VAL:HG12	1.60	1.04
1:A:458:THR:HG21	1:E:757:VAL:CG1	1.87	1.04
1:E:596:ALA:HA	1:F:693:LEU:CD2	1.87	1.04
1:A:492:LYS:CD	1:A:524:TYR:HE2	1.70	1.04
1:B:239:GLU:CB	1:B:742:VAL:HG12	1.60	1.04
1:E:239:GLU:CA	1:E:742:VAL:HG12	1.86	1.04
1:F:492:LYS:CD	1:F:524:TYR:HE2	1.69	1.04
1:K:242:LYS:CG	1:K:743:PRO:HD3	1.86	1.04
1:A:458:THR:CB	1:E:757:VAL:CG1	2.36	1.03
1:D:492:LYS:CD	1:D:524:TYR:HE2	1.70	1.03
1:I:242:LYS:CG	1:I:743:PRO:HD3	1.86	1.03
1:A:492:LYS:CD	1:A:524:TYR:CE2	2.41	1.03
1:E:492:LYS:CD	1:E:524:TYR:HE2	1.70	1.03
1:C:492:LYS:CD	1:C:524:TYR:CE2	2.41	1.03
1:A:458:THR:HG21	1:E:757:VAL:CG2	1.89	1.03
1:B:492:LYS:CD	1:B:524:TYR:CE2	2.41	1.03
1:C:239:GLU:CB	1:C:742:VAL:HG12	1.60	1.03
1:F:239:GLU:CA	1:F:742:VAL:HG12	1.86	1.02
1:F:492:LYS:CD	1:F:524:TYR:CE2	2.41	1.02
1:C:692:LYS:HA	1:D:636:LEU:HD23	1.40	1.02
1:D:492:LYS:CD	1:D:524:TYR:CE2	2.41	1.02
1:E:492:LYS:CD	1:E:524:TYR:CE2	2.41	1.02
1:E:692:LYS:CE	1:F:600:PHE:HE1	1.71	1.02
1:B:239:GLU:CG	1:B:742:VAL:HG11	1.90	1.01
1:E:692:LYS:CE	1:F:600:PHE:CE1	2.44	1.01
1:F:239:GLU:CG	1:F:742:VAL:HG11	1.90	1.01
1:K:239:GLU:CG	1:K:742:VAL:HG11	1.90	1.01
1:A:239:GLU:CG	1:A:742:VAL:HG11	1.90	1.00
1:E:239:GLU:CB	1:E:742:VAL:HG12	1.60	1.00
1:I:239:GLU:CB	1:I:742:VAL:HG12	1.60	1.00
1:I:239:GLU:CG	1:I:742:VAL:HG11	1.90	1.00
1:E:239:GLU:CG	1:E:742:VAL:HG11	1.90	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASP:HA	1:E:759:ALA:C	1.81	1.00
1:C:239:GLU:CG	1:C:742:VAL:HG11	1.90	0.99
1:D:239:GLU:HB3	1:D:742:VAL:HG12	1.44	0.99
1:I:242:LYS:HG2	1:I:743:PRO:CD	1.93	0.99
1:C:242:LYS:HG2	1:C:743:PRO:CD	1.93	0.98
1:F:242:LYS:HG2	1:F:743:PRO:CD	1.93	0.98
1:K:242:LYS:HG2	1:K:743:PRO:CD	1.93	0.98
1:B:242:LYS:HG2	1:B:743:PRO:CD	1.93	0.98
1:E:692:LYS:HE3	1:F:600:PHE:CZ	1.98	0.98
1:E:242:LYS:HG2	1:E:743:PRO:CD	1.93	0.98
1:K:239:GLU:O	1:K:742:VAL:CG1	2.10	0.97
1:A:242:LYS:HG2	1:A:743:PRO:CD	1.93	0.97
1:I:239:GLU:O	1:I:742:VAL:CG1	2.10	0.97
1:B:239:GLU:O	1:B:742:VAL:CG1	2.10	0.97
1:K:221:THR:HG22	1:K:223:GLN:H	1.30	0.96
1:J:221:THR:HG22	1:J:223:GLN:H	1.30	0.96
1:A:221:THR:HG22	1:A:223:GLN:H	1.30	0.96
1:A:453:ALA:CB	1:E:762:ASN:ND2	2.27	0.96
1:I:221:THR:HG22	1:I:223:GLN:H	1.30	0.96
1:D:492:LYS:HD3	1:D:524:TYR:CE2	2.01	0.96
1:F:239:GLU:O	1:F:742:VAL:CG1	2.10	0.96
1:D:221:THR:HG22	1:D:223:GLN:H	1.30	0.95
1:B:221:THR:HG22	1:B:223:GLN:H	1.30	0.95
1:F:492:LYS:HD3	1:F:524:TYR:CE2	2.01	0.95
1:C:492:LYS:HD3	1:C:524:TYR:CE2	2.01	0.95
1:A:239:GLU:O	1:A:742:VAL:CG1	2.10	0.94
1:C:221:THR:HG22	1:C:223:GLN:H	1.30	0.94
1:B:492:LYS:HD3	1:B:524:TYR:CE2	2.01	0.94
1:E:221:THR:HG22	1:E:223:GLN:H	1.30	0.94
1:C:239:GLU:O	1:C:742:VAL:CG1	2.10	0.94
1:E:492:LYS:HD3	1:E:524:TYR:CE2	2.01	0.94
1:F:221:THR:HG22	1:F:223:GLN:H	1.30	0.94
1:E:692:LYS:HD2	1:F:628:PRO:HB3	1.50	0.94
1:E:600:PHE:HE1	1:F:692:LYS:CE	1.79	0.94
1:G:221:THR:HG22	1:G:223:GLN:H	1.30	0.94
1:A:453:ALA:CB	1:E:762:ASN:HD22	1.81	0.93
1:J:451:ASP:OD1	1:K:760:ASP:HA	1.68	0.93
1:A:492:LYS:HD3	1:A:524:TYR:CE2	2.01	0.93
1:A:451:ASP:CA	1:E:759:ALA:O	2.18	0.92
1:A:453:ALA:HB1	1:E:762:ASN:HD22	1.15	0.92
1:E:600:PHE:CZ	1:F:692:LYS:HE3	2.05	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:691:GLY:HA3	1:F:637:LYS:NZ	1.85	0.91
1:A:458:THR:CG2	1:E:757:VAL:CG1	2.46	0.91
1:D:239:GLU:HB3	1:D:742:VAL:CG1	2.01	0.91
1:E:600:PHE:CE1	1:F:692:LYS:CE	2.52	0.91
1:E:600:PHE:HE1	1:F:692:LYS:HE3	1.16	0.91
1:G:413:LYS:HB3	1:G:489:PHE:CZ	2.06	0.91
1:I:413:LYS:HB3	1:I:489:PHE:CZ	2.06	0.91
1:E:239:GLU:O	1:E:742:VAL:CG1	2.10	0.91
1:J:413:LYS:HB3	1:J:489:PHE:CZ	2.06	0.90
1:G:385:ALA:HA	1:G:429:GLN:HE22	1.37	0.90
1:C:692:LYS:CA	1:D:636:LEU:HD23	2.02	0.89
1:E:600:PHE:CE2	1:F:600:PHE:HE2	1.90	0.88
1:E:692:LYS:HE3	1:F:600:PHE:HE1	1.09	0.88
1:E:692:LYS:CD	1:F:628:PRO:HB3	2.04	0.88
1:A:449:VAL:CG2	1:E:779:TYR:CD1	2.57	0.87
1:E:600:PHE:CZ	1:F:600:PHE:HE2	1.92	0.87
1:A:449:VAL:CG2	1:E:779:TYR:CE1	2.57	0.86
1:E:600:PHE:CZ	1:F:600:PHE:CE2	2.62	0.86
1:A:449:VAL:CG1	1:E:759:ALA:HB2	2.06	0.85
1:E:600:PHE:CE2	1:F:600:PHE:CZ	2.64	0.85
1:B:492:LYS:HD2	1:B:524:TYR:CD2	2.12	0.85
1:F:492:LYS:HD2	1:F:524:TYR:CD2	2.12	0.85
1:D:492:LYS:HD2	1:D:524:TYR:CD2	2.12	0.85
1:D:739:VAL:O	1:D:742:VAL:HG22	1.77	0.85
1:E:492:LYS:HD2	1:E:524:TYR:CD2	2.12	0.85
1:K:739:VAL:O	1:K:742:VAL:HG22	1.77	0.85
1:I:413:LYS:HB3	1:I:489:PHE:CE1	2.12	0.85
1:I:739:VAL:O	1:I:742:VAL:HG22	1.77	0.85
1:A:492:LYS:HD2	1:A:524:TYR:CD2	2.12	0.85
1:E:637:LYS:HZ2	1:F:691:GLY:HA3	1.42	0.85
1:E:600:PHE:HE2	1:F:600:PHE:CZ	1.95	0.85
1:G:413:LYS:HB3	1:G:489:PHE:CE1	2.12	0.84
1:B:739:VAL:O	1:B:742:VAL:HG22	1.76	0.84
1:C:492:LYS:HD2	1:C:524:TYR:CD2	2.12	0.84
1:F:739:VAL:O	1:F:742:VAL:HG22	1.76	0.84
1:J:413:LYS:HB3	1:J:489:PHE:CE1	2.12	0.84
1:E:628:PRO:HB3	1:F:692:LYS:HD2	1.57	0.84
1:C:739:VAL:O	1:C:742:VAL:HG22	1.77	0.84
1:E:248:ASN:HA	1:E:721:LYS:HG3	1.60	0.84
1:E:637:LYS:NZ	1:F:691:GLY:HA3	1.92	0.84
1:B:492:LYS:HD2	1:B:524:TYR:CE2	2.13	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASP:CG	1:E:760:ASP:HA	1.99	0.84
1:A:458:THR:HB	1:E:757:VAL:CG1	2.03	0.84
1:E:492:LYS:HD2	1:E:524:TYR:CE2	2.13	0.84
1:E:600:PHE:HE2	1:F:600:PHE:CE2	1.90	0.83
1:A:492:LYS:HD2	1:A:524:TYR:CE2	2.13	0.83
1:A:739:VAL:O	1:A:742:VAL:HG22	1.77	0.83
1:F:248:ASN:HA	1:F:721:LYS:HG3	1.60	0.83
1:F:492:LYS:HD2	1:F:524:TYR:CE2	2.12	0.83
1:B:248:ASN:HA	1:B:721:LYS:HG3	1.60	0.83
1:A:248:ASN:HA	1:A:721:LYS:HG3	1.60	0.83
1:C:248:ASN:HA	1:C:721:LYS:HG3	1.60	0.83
1:K:248:ASN:HA	1:K:721:LYS:HG3	1.60	0.83
1:E:739:VAL:O	1:E:742:VAL:HG22	1.76	0.82
1:D:492:LYS:HD2	1:D:524:TYR:CE2	2.13	0.82
1:I:248:ASN:HA	1:I:721:LYS:HG3	1.60	0.82
1:C:492:LYS:HD2	1:C:524:TYR:CE2	2.13	0.82
1:E:693:LEU:HD23	1:F:596:ALA:CA	2.09	0.82
1:A:597:PHE:N	1:B:693:LEU:O	2.12	0.82
1:A:458:THR:HG21	1:E:757:VAL:HG21	1.62	0.81
1:A:451:ASP:CG	1:E:761:THR:N	2.34	0.81
1:E:692:LYS:CD	1:F:600:PHE:HE1	1.94	0.81
1:A:449:VAL:HG21	1:E:779:TYR:CE1	2.14	0.81
1:E:492:LYS:HD3	1:E:524:TYR:HE2	1.42	0.81
1:J:385:ALA:HA	1:J:429:GLN:HE22	1.45	0.81
1:A:248:ASN:O	1:A:721:LYS:HB2	1.82	0.80
1:C:248:ASN:O	1:C:721:LYS:HB2	1.82	0.80
1:F:248:ASN:O	1:F:721:LYS:HB2	1.82	0.80
1:B:248:ASN:O	1:B:721:LYS:HB2	1.82	0.80
1:K:248:ASN:O	1:K:721:LYS:HB2	1.82	0.79
1:I:248:ASN:O	1:I:721:LYS:HB2	1.82	0.79
1:E:628:PRO:HB3	1:F:692:LYS:CD	2.13	0.79
1:A:458:THR:CG2	1:E:757:VAL:HG21	2.13	0.78
1:A:449:VAL:HG22	1:E:779:TYR:CE1	2.18	0.77
1:E:248:ASN:O	1:E:721:LYS:HB2	1.82	0.77
1:B:492:LYS:HD3	1:B:524:TYR:HE2	1.42	0.77
1:E:239:GLU:CG	1:E:742:VAL:CG1	2.58	0.77
1:C:692:LYS:HB3	1:D:636:LEU:CD2	2.14	0.77
1:D:492:LYS:HD3	1:D:524:TYR:HE2	1.42	0.77
1:A:449:VAL:HG12	1:E:759:ALA:HA	1.68	0.76
1:C:694:ILE:HD13	1:D:597:PHE:HB3	1.68	0.75
1:A:239:GLU:CG	1:A:742:VAL:CG1	2.58	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:PHE:CE2	1:D:597:PHE:CE2	2.75	0.75
1:B:761:THR:OG1	1:F:451:ASP:OD2	2.04	0.74
1:E:691:GLY:HA3	1:F:637:LYS:HZ3	1.48	0.74
1:E:600:PHE:HE1	1:F:692:LYS:CD	1.99	0.74
1:K:251:LYS:HZ3	1:K:743:PRO:HG3	1.51	0.74
1:B:239:GLU:CG	1:B:742:VAL:CG1	2.58	0.74
1:A:251:LYS:HZ3	1:A:743:PRO:HG3	1.52	0.73
1:F:251:LYS:HZ3	1:F:743:PRO:HG3	1.51	0.73
1:I:489:PHE:CD1	1:I:489:PHE:N	2.53	0.73
1:E:693:LEU:CG	1:F:596:ALA:HA	2.19	0.73
1:E:693:LEU:H	1:F:636:LEU:HD23	1.52	0.72
1:A:248:ASN:HB2	1:A:721:LYS:HB2	1.72	0.72
1:B:248:ASN:HB2	1:B:721:LYS:HB2	1.72	0.72
1:C:693:LEU:HG	1:D:596:ALA:HA	1.71	0.72
1:I:239:GLU:CG	1:I:742:VAL:CG1	2.58	0.72
1:E:248:ASN:HB2	1:E:721:LYS:HB2	1.71	0.71
1:G:489:PHE:N	1:G:489:PHE:CD1	2.53	0.71
1:K:239:GLU:HB3	1:K:742:VAL:HG12	1.00	0.71
1:A:449:VAL:HG13	1:E:759:ALA:CB	2.15	0.71
1:A:451:ASP:OD2	1:E:761:THR:OG1	2.01	0.71
1:B:385:ALA:HA	1:B:429:GLN:HE22	1.56	0.71
1:I:385:ALA:HA	1:I:429:GLN:HE22	1.56	0.71
1:J:489:PHE:CD1	1:J:489:PHE:N	2.53	0.71
1:I:239:GLU:HB3	1:I:742:VAL:HG12	1.00	0.71
1:F:248:ASN:HB2	1:F:721:LYS:HB2	1.71	0.71
1:F:492:LYS:HD3	1:F:524:TYR:HE2	1.42	0.71
1:D:385:ALA:HA	1:D:429:GLN:HE22	1.56	0.70
1:E:596:ALA:CA	1:F:693:LEU:HD23	2.15	0.70
1:K:248:ASN:HB2	1:K:721:LYS:HB2	1.72	0.70
1:C:248:ASN:HB2	1:C:721:LYS:HB2	1.72	0.70
1:E:385:ALA:HA	1:E:429:GLN:HE22	1.56	0.70
1:I:248:ASN:HB2	1:I:721:LYS:HB2	1.72	0.70
1:K:239:GLU:CG	1:K:742:VAL:CG1	2.58	0.70
1:E:251:LYS:HZ3	1:E:743:PRO:HG3	1.57	0.70
1:C:239:GLU:CG	1:C:742:VAL:CG1	2.58	0.70
1:C:692:LYS:HD3	1:D:628:PRO:CB	2.22	0.70
1:F:385:ALA:HA	1:F:429:GLN:HE22	1.56	0.70
1:K:385:ALA:HA	1:K:429:GLN:HE22	1.56	0.70
1:A:451:ASP:OD1	1:E:761:THR:N	2.25	0.69
1:C:385:ALA:HA	1:C:429:GLN:HE22	1.56	0.69
1:A:385:ALA:HA	1:A:429:GLN:HE22	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LYS:HZ3	1:B:743:PRO:HG3	1.56	0.69
1:F:239:GLU:CG	1:F:742:VAL:CG1	2.58	0.69
1:A:636:LEU:HD23	1:B:692:LYS:HA	1.73	0.68
1:F:492:LYS:CG	1:F:524:TYR:HE2	2.07	0.68
1:A:492:LYS:CG	1:A:524:TYR:HE2	2.07	0.68
1:E:693:LEU:CD2	1:F:596:ALA:CA	2.66	0.68
1:B:239:GLU:HB3	1:B:742:VAL:HG11	0.68	0.68
1:B:492:LYS:CG	1:B:524:TYR:HE2	2.07	0.68
1:A:239:GLU:HB3	1:A:742:VAL:HG11	0.67	0.67
1:C:692:LYS:CB	1:D:636:LEU:HD23	2.25	0.67
1:A:492:LYS:HD3	1:A:524:TYR:HE2	1.42	0.67
1:E:239:GLU:HB3	1:E:742:VAL:HG11	0.67	0.67
1:I:251:LYS:HZ3	1:I:743:PRO:HG3	1.60	0.67
1:D:492:LYS:CG	1:D:524:TYR:HE2	2.07	0.67
1:F:239:GLU:HB3	1:F:742:VAL:HG11	0.67	0.67
1:C:492:LYS:CG	1:C:524:TYR:HE2	2.07	0.67
1:D:492:LYS:CD	1:D:524:TYR:CD2	2.76	0.67
1:G:415:TYR:HA	1:G:489:PHE:O	1.95	0.67
1:I:239:GLU:HB3	1:I:742:VAL:HG11	0.67	0.67
1:E:492:LYS:CG	1:E:524:TYR:HE2	2.07	0.67
1:I:415:TYR:HA	1:I:489:PHE:O	1.95	0.67
1:J:415:TYR:HA	1:J:489:PHE:O	1.95	0.67
1:B:757:VAL:HG11	1:F:458:THR:HB	1.77	0.66
1:K:239:GLU:HB3	1:K:742:VAL:HG11	0.67	0.66
1:E:492:LYS:CD	1:E:524:TYR:CD2	2.76	0.66
1:J:458:THR:HG21	1:K:757:VAL:HG21	1.76	0.66
1:C:239:GLU:HB3	1:C:742:VAL:HG11	0.67	0.66
1:B:492:LYS:CD	1:B:524:TYR:CD2	2.76	0.65
1:E:692:LYS:CD	1:F:600:PHE:CE1	2.76	0.65
1:F:492:LYS:CD	1:F:524:TYR:CD2	2.76	0.65
1:C:692:LYS:HB3	1:D:636:LEU:HD22	1.79	0.65
1:C:694:ILE:O	1:D:596:ALA:HB1	1.97	0.65
1:A:460:LEU:HD11	1:E:779:TYR:CG	2.31	0.65
1:E:251:LYS:NZ	1:E:743:PRO:HG3	2.12	0.65
1:A:449:VAL:CG1	1:E:759:ALA:CB	2.72	0.65
1:A:251:LYS:NZ	1:A:743:PRO:HG3	2.12	0.64
1:B:251:LYS:NZ	1:B:743:PRO:HG3	2.12	0.64
1:F:251:LYS:NZ	1:F:743:PRO:HG3	2.12	0.64
1:C:492:LYS:CD	1:C:524:TYR:CD2	2.76	0.64
1:J:310:VAL:HG22	1:J:430:PHE:CZ	2.32	0.64
1:C:251:LYS:NZ	1:C:743:PRO:HG3	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:691:GLY:HA3	1:F:637:LYS:HZ2	1.61	0.64
1:A:451:ASP:OD1	1:E:760:ASP:C	2.35	0.64
1:I:251:LYS:NZ	1:I:743:PRO:HG3	2.12	0.64
1:A:458:THR:HG21	1:E:757:VAL:CB	2.27	0.63
1:I:413:LYS:HD2	1:I:489:PHE:CZ	2.34	0.63
1:G:413:LYS:HD2	1:G:489:PHE:CZ	2.34	0.63
1:K:251:LYS:NZ	1:K:743:PRO:HG3	2.12	0.63
1:J:413:LYS:HD2	1:J:489:PHE:CZ	2.34	0.63
1:E:640:GLU:OE2	1:F:692:LYS:HD3	1.99	0.63
1:I:713:VAL:HG22	1:I:794:VAL:HG21	1.81	0.63
1:E:600:PHE:CE1	1:F:692:LYS:CD	2.82	0.62
1:K:713:VAL:HG22	1:K:794:VAL:HG21	1.81	0.62
1:A:458:THR:CG2	1:E:757:VAL:CG2	2.69	0.62
1:C:693:LEU:CG	1:D:596:ALA:HA	2.29	0.62
1:D:713:VAL:CG2	1:D:794:VAL:HG21	2.30	0.62
1:D:713:VAL:HG22	1:D:794:VAL:HG21	1.81	0.62
1:A:451:ASP:OD2	1:E:761:THR:N	2.25	0.62
1:C:492:LYS:HD2	1:C:524:TYR:HD2	1.65	0.62
1:F:239:GLU:HG2	1:F:742:VAL:HG11	1.80	0.62
1:A:449:VAL:CG1	1:E:759:ALA:CA	2.78	0.62
1:A:761:THR:N	1:C:451:ASP:OD1	2.30	0.62
1:A:492:LYS:CD	1:A:524:TYR:CD2	2.76	0.62
1:K:713:VAL:CG2	1:K:794:VAL:HG21	2.30	0.62
1:C:713:VAL:CG2	1:C:794:VAL:HG21	2.29	0.62
1:C:713:VAL:HG22	1:C:794:VAL:HG21	1.80	0.62
1:F:713:VAL:HG22	1:F:794:VAL:HG21	1.80	0.62
1:F:713:VAL:CG2	1:F:794:VAL:HG21	2.30	0.62
1:B:713:VAL:CG2	1:B:794:VAL:HG21	2.30	0.62
1:E:242:LYS:HA	1:E:251:LYS:NZ	2.15	0.62
1:A:713:VAL:CG2	1:A:794:VAL:HG21	2.30	0.61
1:B:713:VAL:HG22	1:B:794:VAL:HG21	1.81	0.61
1:G:489:PHE:N	1:G:489:PHE:HD1	1.97	0.61
1:K:242:LYS:HA	1:K:251:LYS:NZ	2.15	0.61
1:B:492:LYS:HD2	1:B:524:TYR:HD2	1.65	0.61
1:G:242:LYS:HA	1:G:251:LYS:NZ	2.15	0.61
1:I:242:LYS:HA	1:I:251:LYS:NZ	2.15	0.61
1:A:757:VAL:HG11	1:C:458:THR:HB	1.82	0.61
1:B:242:LYS:HA	1:B:251:LYS:NZ	2.15	0.61
1:E:239:GLU:HG2	1:E:742:VAL:HG11	1.80	0.61
1:I:489:PHE:N	1:I:489:PHE:HD1	1.97	0.61
1:J:489:PHE:N	1:J:489:PHE:HD1	1.97	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:HA	1:A:251:LYS:NZ	2.15	0.61
1:C:242:LYS:HA	1:C:251:LYS:NZ	2.15	0.61
1:E:713:VAL:HG22	1:E:794:VAL:HG21	1.81	0.61
1:A:798:LYS:HE2	1:C:446:GLU:CG	2.30	0.61
1:E:713:VAL:CG2	1:E:794:VAL:HG21	2.30	0.61
1:D:242:LYS:HA	1:D:251:LYS:NZ	2.15	0.61
1:F:242:LYS:HA	1:F:251:LYS:NZ	2.15	0.61
1:I:713:VAL:CG2	1:I:794:VAL:HG21	2.30	0.61
1:J:242:LYS:HA	1:J:251:LYS:NZ	2.15	0.61
1:F:248:ASN:HA	1:F:721:LYS:CG	2.31	0.60
1:A:713:VAL:HG22	1:A:794:VAL:HG21	1.81	0.60
1:C:248:ASN:HA	1:C:721:LYS:CG	2.31	0.60
1:I:239:GLU:CB	1:I:742:VAL:CB	2.75	0.60
1:A:458:THR:HG21	1:E:757:VAL:HG13	1.80	0.60
1:A:597:PHE:CE2	1:B:600:PHE:CE2	2.89	0.60
1:E:248:ASN:HA	1:E:721:LYS:CG	2.31	0.60
1:I:489:PHE:HD1	1:I:489:PHE:H	1.51	0.59
1:C:239:GLU:HG2	1:C:742:VAL:HG11	1.80	0.59
1:C:692:LYS:CD	1:D:628:PRO:CB	2.80	0.59
1:A:458:THR:OG1	1:E:757:VAL:CG1	2.49	0.59
1:B:228:LYS:HD3	1:B:229:PHE:N	2.18	0.59
1:I:413:LYS:HB3	1:I:489:PHE:HZ	1.65	0.59
1:A:450:VAL:O	1:E:759:ALA:O	2.20	0.59
1:C:239:GLU:CB	1:C:742:VAL:CB	2.76	0.59
1:G:489:PHE:HD1	1:G:489:PHE:H	1.51	0.59
1:J:489:PHE:HD1	1:J:489:PHE:H	1.51	0.59
1:F:239:GLU:CB	1:F:742:VAL:CB	2.76	0.59
1:F:492:LYS:HD2	1:F:524:TYR:HD2	1.65	0.59
1:K:228:LYS:HD3	1:K:229:PHE:N	2.18	0.59
1:A:228:LYS:HD3	1:A:229:PHE:N	2.18	0.59
1:F:228:LYS:HD3	1:F:229:PHE:N	2.18	0.59
1:A:492:LYS:HD2	1:A:524:TYR:HD2	1.65	0.58
1:J:228:LYS:HD3	1:J:229:PHE:N	2.18	0.58
1:A:248:ASN:HA	1:A:721:LYS:CG	2.31	0.58
1:C:228:LYS:HD3	1:C:229:PHE:N	2.18	0.58
1:B:239:GLU:CB	1:B:742:VAL:CB	2.76	0.58
1:E:600:PHE:CZ	1:F:600:PHE:CZ	2.89	0.58
1:E:692:LYS:CD	1:F:628:PRO:CB	2.80	0.58
1:C:600:PHE:HE2	1:D:597:PHE:CE2	2.18	0.58
1:D:214:LYS:HB2	1:D:230:SER:HB3	1.86	0.58
1:A:214:LYS:HB2	1:A:230:SER:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HB3	1:E:760:ASP:OD2	2.03	0.58
1:E:692:LYS:HD3	1:F:640:GLU:OE2	2.03	0.58
1:B:248:ASN:HA	1:B:721:LYS:CG	2.31	0.58
1:C:214:LYS:HB2	1:C:230:SER:HB3	1.86	0.58
1:C:547:GLN:O	1:C:547:GLN:HG3	2.04	0.58
1:I:228:LYS:HD3	1:I:229:PHE:N	2.18	0.58
1:B:214:LYS:HB2	1:B:230:SER:HB3	1.86	0.58
1:E:228:LYS:HD3	1:E:229:PHE:N	2.18	0.58
1:I:248:ASN:HB2	1:I:721:LYS:CB	2.34	0.58
1:A:547:GLN:O	1:A:547:GLN:HG3	2.04	0.57
1:D:228:LYS:HD3	1:D:229:PHE:N	2.18	0.57
1:F:214:LYS:HB2	1:F:230:SER:HB3	1.86	0.57
1:G:228:LYS:HD3	1:G:229:PHE:N	2.18	0.57
1:K:248:ASN:HB2	1:K:721:LYS:CB	2.34	0.57
1:A:458:THR:HG21	1:E:757:VAL:HG22	1.81	0.57
1:E:214:LYS:HB2	1:E:230:SER:HB3	1.86	0.57
1:F:248:ASN:HB2	1:F:721:LYS:CB	2.34	0.57
1:G:214:LYS:HB2	1:G:230:SER:HB3	1.86	0.57
1:K:248:ASN:HA	1:K:721:LYS:CG	2.31	0.57
1:D:547:GLN:HG3	1:D:547:GLN:O	2.04	0.57
1:I:248:ASN:HA	1:I:721:LYS:CG	2.31	0.57
1:F:248:ASN:CB	1:F:721:LYS:HB2	2.35	0.57
1:F:547:GLN:HG3	1:F:547:GLN:O	2.04	0.57
1:I:239:GLU:HG2	1:I:742:VAL:HG11	1.80	0.57
1:K:739:VAL:O	1:K:742:VAL:CG2	2.51	0.57
1:C:248:ASN:CB	1:C:721:LYS:HB2	2.35	0.57
1:C:248:ASN:HB2	1:C:721:LYS:CB	2.34	0.57
1:D:239:GLU:HB3	1:D:742:VAL:HG11	1.86	0.57
1:E:547:GLN:O	1:E:547:GLN:HG3	2.04	0.57
1:E:636:LEU:HD23	1:F:693:LEU:H	1.68	0.57
1:I:214:LYS:HB2	1:I:230:SER:HB3	1.86	0.57
1:J:453:ALA:HB2	1:K:760:ASP:OD1	2.05	0.57
1:K:239:GLU:CB	1:K:742:VAL:CB	2.76	0.57
1:B:547:GLN:O	1:B:547:GLN:HG3	2.04	0.57
1:J:468:LYS:NZ	1:J:470:THR:CG2	2.67	0.57
1:B:239:GLU:HG2	1:B:742:VAL:HG11	1.80	0.57
1:D:739:VAL:O	1:D:742:VAL:CG2	2.51	0.57
1:I:248:ASN:CB	1:I:721:LYS:HB2	2.35	0.57
1:A:248:ASN:HB2	1:A:721:LYS:CB	2.34	0.56
1:A:248:ASN:CB	1:A:721:LYS:HB2	2.35	0.56
1:B:248:ASN:CB	1:B:721:LYS:HB2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:VAL:O	1:E:742:VAL:CG2	2.51	0.56
1:K:248:ASN:CB	1:K:721:LYS:HB2	2.35	0.56
1:B:221:THR:HG22	1:B:223:GLN:N	2.13	0.56
1:E:248:ASN:HB2	1:E:721:LYS:CB	2.34	0.56
1:J:214:LYS:HB2	1:J:230:SER:HB3	1.86	0.56
1:C:492:LYS:HD3	1:C:524:TYR:HE2	1.42	0.56
1:K:214:LYS:HB2	1:K:230:SER:HB3	1.86	0.56
1:K:239:GLU:HG2	1:K:742:VAL:HG11	1.80	0.56
1:A:239:GLU:HG3	1:A:742:VAL:HB	1.88	0.56
1:A:757:VAL:CG2	1:C:458:THR:HG21	2.35	0.56
1:B:239:GLU:HG3	1:B:742:VAL:HB	1.88	0.56
1:E:239:GLU:CB	1:E:742:VAL:CB	2.76	0.56
1:E:596:ALA:HA	1:F:693:LEU:CG	2.34	0.56
1:B:248:ASN:HB2	1:B:721:LYS:CB	2.34	0.56
1:J:451:ASP:OD1	1:K:760:ASP:CA	2.51	0.56
1:J:390:ILE:HD13	1:J:469:VAL:HG23	1.87	0.56
1:L:364:VAL:HG12	1:L:374:GLU:HG2	1.87	0.56
1:A:239:GLU:HG2	1:A:742:VAL:HG11	1.80	0.56
1:B:739:VAL:O	1:B:742:VAL:CG2	2.51	0.56
1:C:242:LYS:HB3	1:C:251:LYS:HZ3	1.71	0.56
1:F:239:GLU:HG3	1:F:742:VAL:HB	1.88	0.56
1:A:739:VAL:O	1:A:742:VAL:CG2	2.51	0.55
1:C:239:GLU:HG3	1:C:742:VAL:HB	1.88	0.55
1:E:239:GLU:HG3	1:E:742:VAL:HB	1.88	0.55
1:A:248:ASN:CA	1:A:721:LYS:HB2	2.37	0.55
1:C:248:ASN:CA	1:C:721:LYS:HB2	2.37	0.55
1:F:248:ASN:CA	1:F:721:LYS:HB2	2.37	0.55
1:F:739:VAL:O	1:F:742:VAL:CG2	2.51	0.55
1:K:221:THR:HG22	1:K:223:GLN:N	2.13	0.55
1:I:248:ASN:CA	1:I:721:LYS:HB2	2.37	0.55
1:K:248:ASN:CA	1:K:721:LYS:HB2	2.37	0.55
1:E:248:ASN:CA	1:E:721:LYS:HB2	2.37	0.55
1:E:694:ILE:HA	1:F:597:PHE:HB3	1.86	0.55
1:E:492:LYS:HD2	1:E:524:TYR:HD2	1.65	0.55
1:I:239:GLU:HG3	1:I:742:VAL:HB	1.88	0.55
1:A:492:LYS:HG2	1:A:524:TYR:HE2	1.72	0.55
1:C:739:VAL:O	1:C:742:VAL:CG2	2.51	0.55
1:A:453:ALA:HB2	1:E:760:ASP:OD1	2.07	0.55
1:E:492:LYS:HG2	1:E:524:TYR:HE2	1.72	0.55
1:K:239:GLU:HG3	1:K:742:VAL:HB	1.88	0.55
1:C:694:ILE:CD1	1:D:597:PHE:HB3	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:LYS:HG2	1:F:628:PRO:HG3	1.89	0.54
1:D:492:LYS:HD2	1:D:524:TYR:HD2	1.65	0.54
1:D:492:LYS:HG2	1:D:524:TYR:HE2	1.72	0.54
1:G:221:THR:HG22	1:G:223:GLN:N	2.13	0.54
1:B:492:LYS:HG2	1:B:524:TYR:HE2	1.72	0.54
1:E:248:ASN:CB	1:E:721:LYS:HB2	2.35	0.54
1:A:628:PRO:CB	1:B:692:LYS:HD3	2.38	0.54
1:F:492:LYS:HG2	1:F:524:TYR:HE2	1.72	0.54
1:B:248:ASN:CA	1:B:721:LYS:HB2	2.37	0.54
1:C:693:LEU:HG	1:D:596:ALA:CA	2.36	0.54
1:A:239:GLU:CB	1:A:742:VAL:CB	2.76	0.54
1:A:453:ALA:CB	1:E:760:ASP:OD1	2.56	0.54
1:C:492:LYS:HG2	1:C:524:TYR:HE2	1.72	0.54
1:I:739:VAL:O	1:I:742:VAL:CG2	2.51	0.54
1:J:221:THR:HG22	1:J:223:GLN:N	2.13	0.53
1:C:692:LYS:HD3	1:D:628:PRO:HB3	1.90	0.53
1:K:413:LYS:HD2	1:K:489:PHE:HZ	1.74	0.53
1:F:508:THR:HG22	1:F:594:PRO:HD3	1.91	0.53
1:C:508:THR:HG22	1:C:594:PRO:HD3	1.91	0.53
1:C:251:LYS:HZ3	1:C:743:PRO:HG3	1.72	0.53
1:C:692:LYS:CB	1:D:636:LEU:CD2	2.82	0.53
1:D:508:THR:HG22	1:D:594:PRO:HD3	1.91	0.53
1:E:413:LYS:HD2	1:E:489:PHE:HZ	1.73	0.53
1:J:310:VAL:CG2	1:J:430:PHE:CZ	2.92	0.53
1:A:449:VAL:CG1	1:E:759:ALA:HA	2.33	0.53
1:E:692:LYS:CE	1:F:600:PHE:CZ	2.81	0.53
1:E:508:THR:HG22	1:E:594:PRO:HD3	1.91	0.53
1:D:413:LYS:HD2	1:D:489:PHE:HZ	1.74	0.52
1:C:600:PHE:CD2	1:D:597:PHE:CE2	2.97	0.52
1:G:413:LYS:HB3	1:G:489:PHE:HZ	1.65	0.52
1:B:508:THR:HG22	1:B:594:PRO:HD3	1.91	0.52
1:A:508:THR:HG22	1:A:594:PRO:HD3	1.91	0.52
1:D:614:THR:HG23	1:D:616:GLU:H	1.75	0.52
1:F:614:THR:HG23	1:F:616:GLU:H	1.75	0.52
1:F:239:GLU:O	1:F:742:VAL:HA	2.10	0.52
1:A:413:LYS:HD2	1:A:489:PHE:HZ	1.75	0.52
1:A:723:VAL:HG12	1:A:805:SER:O	2.10	0.52
1:B:614:THR:HG23	1:B:616:GLU:H	1.75	0.52
1:A:614:THR:HG23	1:A:616:GLU:H	1.75	0.52
1:B:239:GLU:O	1:B:742:VAL:HA	2.10	0.52
1:C:614:THR:HG23	1:C:616:GLU:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:LYS:HG2	1:F:628:PRO:CG	2.40	0.52
1:J:310:VAL:HG22	1:J:430:PHE:CE1	2.45	0.52
1:J:458:THR:HG21	1:K:757:VAL:CG2	2.40	0.52
1:K:723:VAL:HG12	1:K:805:SER:O	2.10	0.52
1:B:723:VAL:HG12	1:B:805:SER:O	2.10	0.52
1:E:614:THR:HG23	1:E:616:GLU:H	1.75	0.52
1:J:413:LYS:HB3	1:J:489:PHE:HZ	1.66	0.52
1:K:239:GLU:O	1:K:742:VAL:HA	2.10	0.52
1:C:723:VAL:HG12	1:C:805:SER:O	2.10	0.51
1:D:248:ASN:HA	1:D:721:LYS:HD3	1.91	0.51
1:C:413:LYS:HD2	1:C:489:PHE:HZ	1.75	0.51
1:A:239:GLU:O	1:A:742:VAL:HA	2.10	0.51
1:D:723:VAL:HG12	1:D:805:SER:O	2.10	0.51
1:F:723:VAL:HG12	1:F:805:SER:O	2.10	0.51
1:J:458:THR:HB	1:K:757:VAL:HG11	1.92	0.51
1:E:628:PRO:CB	1:F:692:LYS:CD	2.88	0.51
1:I:723:VAL:HG12	1:I:805:SER:O	2.10	0.51
1:A:239:GLU:CG	1:A:742:VAL:CB	2.89	0.51
1:B:239:GLU:CG	1:B:742:VAL:CB	2.89	0.51
1:E:596:ALA:CA	1:F:693:LEU:CD2	2.77	0.51
1:I:239:GLU:O	1:I:742:VAL:HA	2.10	0.51
1:E:723:VAL:HG12	1:E:805:SER:O	2.10	0.51
1:C:239:GLU:O	1:C:742:VAL:HA	2.10	0.51
1:C:242:LYS:HG2	1:C:743:PRO:CG	2.41	0.51
1:E:239:GLU:CG	1:E:742:VAL:CB	2.89	0.51
1:A:458:THR:HG22	1:E:757:VAL:HG21	1.90	0.50
1:C:239:GLU:CG	1:C:742:VAL:CB	2.89	0.50
1:A:239:GLU:HB3	1:A:742:VAL:HG12	1.00	0.50
1:E:239:GLU:O	1:E:742:VAL:HA	2.10	0.50
1:F:242:LYS:HG2	1:F:743:PRO:CG	2.41	0.50
1:I:239:GLU:CG	1:I:742:VAL:CB	2.89	0.50
1:K:239:GLU:CG	1:K:742:VAL:CB	2.89	0.50
1:I:221:THR:HG22	1:I:223:GLN:N	2.13	0.50
1:K:242:LYS:HG2	1:K:743:PRO:CG	2.41	0.50
1:A:533:THR:OG1	1:A:577:LYS:NZ	2.38	0.50
1:B:413:LYS:HD2	1:B:489:PHE:HZ	1.76	0.50
1:E:242:LYS:HG2	1:E:743:PRO:CG	2.41	0.50
1:I:242:LYS:HG2	1:I:743:PRO:CG	2.41	0.50
1:I:413:LYS:HD2	1:I:489:PHE:HZ	1.76	0.50
1:C:242:LYS:HA	1:C:251:LYS:HZ1	1.76	0.50
1:E:497:ILE:HD11	1:E:574:LEU:HD23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:GLU:CG	1:F:742:VAL:CB	2.89	0.50
1:C:497:ILE:HD11	1:C:574:LEU:HD23	1.94	0.49
1:A:242:LYS:HG2	1:A:743:PRO:CG	2.41	0.49
1:A:761:THR:CG2	1:C:451:ASP:OD2	2.59	0.49
1:F:497:ILE:HD11	1:F:574:LEU:HD23	1.94	0.49
1:A:636:LEU:HD23	1:B:692:LYS:CA	2.41	0.49
1:A:757:VAL:HG21	1:C:458:THR:HG21	1.93	0.49
1:A:221:THR:HG22	1:A:223:GLN:N	2.13	0.49
1:B:622:MET:HG3	1:B:671:ILE:HB	1.95	0.49
1:D:221:THR:HG22	1:D:223:GLN:N	2.13	0.49
1:E:221:THR:HG22	1:E:223:GLN:N	2.13	0.49
1:B:251:LYS:HE2	1:B:743:PRO:CB	2.43	0.49
1:D:497:ILE:HD11	1:D:574:LEU:HD23	1.94	0.49
1:J:310:VAL:CG2	1:J:430:PHE:CE1	2.96	0.49
1:B:242:LYS:HG2	1:B:743:PRO:CG	2.41	0.49
1:C:693:LEU:CB	1:D:596:ALA:HA	2.43	0.49
1:E:622:MET:HG3	1:E:671:ILE:HB	1.95	0.49
1:F:251:LYS:HE2	1:F:743:PRO:CB	2.43	0.49
1:E:693:LEU:HG	1:F:596:ALA:HA	1.94	0.49
1:A:622:MET:HG3	1:A:671:ILE:HB	1.95	0.49
1:E:251:LYS:HE2	1:E:743:PRO:CB	2.43	0.49
1:E:600:PHE:CZ	1:F:692:LYS:CE	2.87	0.49
1:F:622:MET:HG3	1:F:671:ILE:HB	1.95	0.49
1:B:242:LYS:HA	1:B:251:LYS:HZ1	1.77	0.49
1:C:251:LYS:HE2	1:C:743:PRO:CB	2.43	0.49
1:C:622:MET:HG3	1:C:671:ILE:HB	1.95	0.49
1:D:622:MET:HG3	1:D:671:ILE:HB	1.95	0.49
1:A:445:THR:HB	1:E:779:TYR:OH	2.13	0.48
1:F:242:LYS:HA	1:F:251:LYS:HZ1	1.78	0.48
1:F:248:ASN:CB	1:F:721:LYS:CB	2.91	0.48
1:C:248:ASN:CB	1:C:721:LYS:CB	2.91	0.48
1:E:242:LYS:HA	1:E:251:LYS:HZ1	1.77	0.48
1:F:533:THR:OG1	1:F:577:LYS:NZ	2.38	0.48
1:I:251:LYS:HE2	1:I:743:PRO:CB	2.43	0.48
1:B:497:ILE:HD11	1:B:574:LEU:HD23	1.94	0.48
1:C:248:ASN:HA	1:C:721:LYS:CB	2.44	0.48
1:C:248:ASN:CA	1:C:721:LYS:CB	2.91	0.48
1:E:248:ASN:CB	1:E:721:LYS:CB	2.91	0.48
1:F:221:THR:HG22	1:F:223:GLN:N	2.13	0.48
1:A:251:LYS:HE2	1:A:743:PRO:CB	2.43	0.48
1:F:248:ASN:HA	1:F:721:LYS:CB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:LYS:HA	1:I:251:LYS:HZ1	1.77	0.48
1:A:248:ASN:CB	1:A:721:LYS:CB	2.91	0.48
1:D:533:THR:OG1	1:D:577:LYS:NZ	2.38	0.48
1:F:248:ASN:CA	1:F:721:LYS:CB	2.91	0.48
1:I:248:ASN:CB	1:I:721:LYS:CB	2.91	0.48
1:E:248:ASN:CA	1:E:721:LYS:CB	2.91	0.48
1:F:413:LYS:HD2	1:F:489:PHE:HZ	1.78	0.48
1:I:248:ASN:HA	1:I:721:LYS:CB	2.44	0.48
1:A:761:THR:OG1	1:C:451:ASP:OD2	2.14	0.48
1:B:248:ASN:CB	1:B:721:LYS:CB	2.91	0.48
1:J:452:LYS:N	1:K:759:ALA:O	2.33	0.48
1:J:385:ALA:HA	1:J:429:GLN:NE2	2.22	0.48
1:K:248:ASN:CB	1:K:721:LYS:CB	2.91	0.48
1:C:221:THR:HG22	1:C:223:GLN:N	2.13	0.48
1:A:452:LYS:N	1:E:759:ALA:O	2.46	0.47
1:K:248:ASN:HA	1:K:721:LYS:CB	2.44	0.47
1:K:248:ASN:CA	1:K:721:LYS:CB	2.91	0.47
1:A:497:ILE:HD11	1:A:574:LEU:HD23	1.94	0.47
1:K:242:LYS:HA	1:K:251:LYS:HZ1	1.78	0.47
1:B:239:GLU:HB3	1:B:742:VAL:HG12	1.00	0.47
1:G:413:LYS:HD2	1:G:489:PHE:HZ	1.76	0.47
1:I:242:LYS:HB3	1:I:251:LYS:HZ3	1.79	0.47
1:I:248:ASN:CA	1:I:721:LYS:CB	2.91	0.47
1:A:248:ASN:HA	1:A:721:LYS:CB	2.44	0.47
1:A:248:ASN:CA	1:A:721:LYS:CB	2.91	0.47
1:A:692:LYS:HG2	1:B:637:LYS:HD3	1.96	0.47
1:B:248:ASN:CA	1:B:721:LYS:CB	2.91	0.47
1:E:248:ASN:HA	1:E:721:LYS:CB	2.44	0.47
1:K:251:LYS:HE2	1:K:743:PRO:CB	2.43	0.47
1:A:397:GLU:HG2	1:A:419:ASN:HB3	1.97	0.47
1:B:397:GLU:HG2	1:B:419:ASN:HB3	1.97	0.47
1:G:242:LYS:HA	1:G:251:LYS:HZ1	1.80	0.47
1:C:692:LYS:CD	1:D:628:PRO:HB2	2.44	0.47
1:A:242:LYS:HA	1:A:251:LYS:HZ1	1.78	0.47
1:A:508:THR:HG22	1:A:593:ALA:HA	1.97	0.47
1:B:248:ASN:HA	1:B:721:LYS:CB	2.44	0.47
1:D:397:GLU:HG2	1:D:419:ASN:HB3	1.97	0.47
1:E:397:GLU:HG2	1:E:419:ASN:HB3	1.97	0.47
1:J:413:LYS:HD2	1:J:489:PHE:HZ	1.76	0.47
1:A:446:GLU:HG2	1:E:798:LYS:HE2	1.96	0.47
1:L:360:THR:HG23	1:L:377:GLU:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:LYS:HA	1:J:251:LYS:HZ1	1.80	0.47
1:J:468:LYS:HZ2	1:J:470:THR:CG2	2.28	0.47
1:K:397:GLU:HG2	1:K:419:ASN:HB3	1.97	0.47
1:A:761:THR:HG23	1:C:451:ASP:OD2	2.15	0.46
1:B:508:THR:HG22	1:B:593:ALA:HA	1.97	0.46
1:E:691:GLY:CA	1:F:637:LYS:HZ3	2.25	0.46
1:I:397:GLU:HG2	1:I:419:ASN:HB3	1.97	0.46
1:A:460:LEU:HD11	1:E:779:TYR:CB	2.45	0.46
1:A:606:GLU:H	1:A:622:MET:HE3	1.81	0.46
1:I:242:LYS:HB3	1:I:251:LYS:NZ	2.31	0.46
1:C:239:GLU:O	1:C:742:VAL:CA	2.64	0.46
1:E:508:THR:HG22	1:E:593:ALA:HA	1.97	0.46
1:E:637:LYS:HZ3	1:F:691:GLY:HA3	1.79	0.46
1:E:692:LYS:HD3	1:F:628:PRO:HB3	1.95	0.46
1:F:239:GLU:O	1:F:742:VAL:CA	2.64	0.46
1:F:242:LYS:HB3	1:F:251:LYS:NZ	2.31	0.46
1:F:397:GLU:HG2	1:F:419:ASN:HB3	1.97	0.46
1:A:239:GLU:O	1:A:742:VAL:CA	2.64	0.46
1:B:239:GLU:CG	1:B:742:VAL:HB	2.46	0.46
1:C:397:GLU:HG2	1:C:419:ASN:HB3	1.97	0.46
1:E:239:GLU:CG	1:E:742:VAL:HB	2.46	0.46
1:J:397:GLU:HG2	1:J:419:ASN:HB3	1.97	0.46
1:K:239:GLU:O	1:K:742:VAL:CA	2.64	0.46
1:A:242:LYS:HB3	1:A:251:LYS:NZ	2.31	0.46
1:A:355:LYS:HB2	1:A:355:LYS:HE3	1.73	0.46
1:A:458:THR:OG1	1:E:757:VAL:HG13	2.15	0.46
1:B:239:GLU:O	1:B:742:VAL:CA	2.64	0.46
1:C:214:LYS:N	1:C:230:SER:HG	2.14	0.46
1:F:508:THR:HG22	1:F:593:ALA:HA	1.97	0.46
1:C:242:LYS:HB3	1:C:251:LYS:NZ	2.31	0.46
1:E:214:LYS:N	1:E:230:SER:HG	2.14	0.46
1:F:214:LYS:N	1:F:230:SER:HG	2.14	0.46
1:B:242:LYS:HB3	1:B:251:LYS:NZ	2.31	0.46
1:B:761:THR:N	1:F:451:ASP:OD1	2.40	0.46
1:D:508:THR:HG22	1:D:593:ALA:HA	1.97	0.46
1:E:239:GLU:O	1:E:742:VAL:CA	2.64	0.46
1:I:239:GLU:CG	1:I:742:VAL:HB	2.46	0.46
1:E:242:LYS:HB3	1:E:251:LYS:HZ3	1.81	0.46
1:G:214:LYS:N	1:G:230:SER:HG	2.14	0.46
1:J:439:GLU:HB2	1:J:470:THR:OG1	2.16	0.46
1:G:397:GLU:HG2	1:G:419:ASN:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:THR:OG1	1:B:577:LYS:NZ	2.38	0.45
1:C:508:THR:HG22	1:C:593:ALA:HA	1.97	0.45
1:D:214:LYS:N	1:D:230:SER:HG	2.14	0.45
1:E:242:LYS:HB3	1:E:251:LYS:NZ	2.31	0.45
1:G:242:LYS:HB3	1:G:251:LYS:NZ	2.31	0.45
1:I:239:GLU:O	1:I:742:VAL:CA	2.64	0.45
1:J:214:LYS:N	1:J:230:SER:HG	2.14	0.45
1:A:597:PHE:CE2	1:B:600:PHE:HE2	2.31	0.45
1:B:242:LYS:HB3	1:B:251:LYS:HZ3	1.82	0.45
1:K:239:GLU:CG	1:K:742:VAL:HB	2.46	0.45
1:K:242:LYS:HB3	1:K:251:LYS:NZ	2.31	0.45
1:A:233:VAL:O	1:A:263:LYS:HB3	2.17	0.45
1:A:239:GLU:CG	1:A:742:VAL:HB	2.46	0.45
1:C:255:LYS:HA	1:C:271:TYR:CE2	2.52	0.45
1:E:533:THR:OG1	1:E:577:LYS:NZ	2.38	0.45
1:I:233:VAL:O	1:I:263:LYS:HB3	2.17	0.45
1:J:242:LYS:HB3	1:J:251:LYS:NZ	2.31	0.45
1:K:255:LYS:HA	1:K:271:TYR:CE2	2.52	0.45
1:A:400:LYS:HB3	1:A:400:LYS:HE2	1.69	0.45
1:A:449:VAL:HG22	1:E:779:TYR:CZ	2.50	0.45
1:A:453:ALA:HB2	1:E:762:ASN:HB2	1.99	0.45
1:A:597:PHE:HB3	1:B:694:ILE:HD13	1.97	0.45
1:C:233:VAL:O	1:C:263:LYS:HB3	2.17	0.45
1:F:255:LYS:HA	1:F:271:TYR:CE2	2.52	0.45
1:A:449:VAL:HG21	1:E:779:TYR:CG	2.41	0.45
1:E:233:VAL:O	1:E:263:LYS:HB3	2.17	0.45
1:G:400:LYS:HE2	1:G:400:LYS:HB3	1.69	0.45
1:D:233:VAL:O	1:D:263:LYS:HB3	2.17	0.45
1:F:239:GLU:CG	1:F:742:VAL:HB	2.46	0.45
1:G:397:GLU:HB2	1:G:400:LYS:HD3	1.99	0.45
1:J:255:LYS:HA	1:J:271:TYR:CE2	2.52	0.45
1:A:798:LYS:HE2	1:C:446:GLU:CD	2.37	0.45
1:B:255:LYS:HG2	1:B:256:GLU:HG3	1.99	0.45
1:E:239:GLU:CA	1:E:742:VAL:CG1	2.60	0.45
1:G:255:LYS:HA	1:G:271:TYR:CE2	2.52	0.45
1:J:458:THR:CB	1:K:757:VAL:HG11	2.47	0.45
1:D:229:PHE:CD1	1:D:287:VAL:HG11	2.52	0.45
1:G:233:VAL:O	1:G:263:LYS:HB3	2.17	0.45
1:I:239:GLU:CA	1:I:742:VAL:CG1	2.60	0.45
1:A:214:LYS:N	1:A:230:SER:HG	2.14	0.45
1:A:255:LYS:HG2	1:A:256:GLU:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:VAL:HG22	1:C:458:THR:HG21	1.99	0.45
1:C:693:LEU:HB3	1:D:596:ALA:HA	1.99	0.45
1:D:397:GLU:HB2	1:D:400:LYS:HD3	1.99	0.45
1:I:214:LYS:N	1:I:230:SER:HG	2.14	0.45
1:I:229:PHE:CD1	1:I:287:VAL:HG11	2.52	0.45
1:L:343:GLU:H	1:L:343:GLU:CD	2.19	0.45
1:K:229:PHE:CD1	1:K:287:VAL:HG11	2.52	0.45
1:A:229:PHE:CD1	1:A:287:VAL:HG11	2.52	0.44
1:B:229:PHE:CD1	1:B:287:VAL:HG11	2.52	0.44
1:D:242:LYS:HB3	1:D:251:LYS:NZ	2.31	0.44
1:E:255:LYS:HG2	1:E:256:GLU:HG3	1.99	0.44
1:F:255:LYS:HG2	1:F:256:GLU:HG3	1.99	0.44
1:I:415:TYR:CZ	1:I:489:PHE:CE1	3.05	0.44
1:K:214:LYS:N	1:K:230:SER:HG	2.14	0.44
1:A:255:LYS:HA	1:A:271:TYR:CE2	2.52	0.44
1:A:397:GLU:HB2	1:A:400:LYS:HD3	1.99	0.44
1:A:636:LEU:CD2	1:B:692:LYS:HB3	2.47	0.44
1:B:255:LYS:HA	1:B:271:TYR:CE2	2.52	0.44
1:B:497:ILE:HG23	1:B:585:ALA:HB2	2.00	0.44
1:C:239:GLU:CG	1:C:742:VAL:HB	2.46	0.44
1:I:400:LYS:HB3	1:I:400:LYS:HE2	1.69	0.44
1:J:415:TYR:CZ	1:J:489:PHE:CE1	3.05	0.44
1:A:497:ILE:HG23	1:A:585:ALA:HB2	2.00	0.44
1:E:229:PHE:CD1	1:E:287:VAL:HG11	2.52	0.44
1:J:397:GLU:HB2	1:J:400:LYS:HD3	1.99	0.44
1:G:229:PHE:CD1	1:G:287:VAL:HG11	2.52	0.44
1:G:415:TYR:CZ	1:G:489:PHE:CE1	3.05	0.44
1:B:214:LYS:N	1:B:230:SER:HG	2.14	0.44
1:B:233:VAL:O	1:B:263:LYS:HB3	2.17	0.44
1:C:692:LYS:HD3	1:D:628:PRO:CG	2.47	0.44
1:D:239:GLU:O	1:D:742:VAL:HG12	2.18	0.44
1:E:597:PHE:HB3	1:F:694:ILE:HA	1.98	0.44
1:F:233:VAL:O	1:F:263:LYS:HB3	2.17	0.44
1:J:233:VAL:O	1:J:263:LYS:HB3	2.17	0.44
1:K:397:GLU:HB2	1:K:400:LYS:HD3	1.99	0.44
1:K:761:THR:HA	1:K:764:VAL:O	2.18	0.44
1:C:255:LYS:HG2	1:C:256:GLU:HG3	1.99	0.44
1:E:255:LYS:HA	1:E:271:TYR:CE2	2.52	0.44
1:I:255:LYS:HA	1:I:271:TYR:CE2	2.52	0.44
1:J:255:LYS:HG2	1:J:256:GLU:HG3	1.99	0.44
1:K:255:LYS:HG2	1:K:256:GLU:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PRO:CB	1:B:692:LYS:CD	2.96	0.44
1:A:628:PRO:HB3	1:B:692:LYS:HD3	2.00	0.44
1:F:497:ILE:HG23	1:F:585:ALA:HB2	2.00	0.44
1:I:397:GLU:HB2	1:I:400:LYS:HD3	1.99	0.44
1:J:229:PHE:CD1	1:J:287:VAL:HG11	2.52	0.44
1:B:761:THR:HA	1:B:764:VAL:O	2.18	0.44
1:D:242:LYS:HA	1:D:251:LYS:HZ1	1.81	0.44
1:D:761:THR:HA	1:D:764:VAL:O	2.18	0.44
1:E:397:GLU:HB2	1:E:400:LYS:HD3	1.99	0.44
1:I:761:THR:HA	1:I:764:VAL:O	2.18	0.44
1:C:761:THR:HA	1:C:764:VAL:O	2.18	0.44
1:I:255:LYS:HG2	1:I:256:GLU:HG3	1.99	0.44
1:K:233:VAL:O	1:K:263:LYS:HB3	2.17	0.44
1:A:416:GLU:HG3	1:A:459:VAL:HG22	2.00	0.43
1:B:416:GLU:HG3	1:B:459:VAL:HG22	2.00	0.43
1:C:229:PHE:CD1	1:C:287:VAL:HG11	2.52	0.43
1:D:255:LYS:HA	1:D:271:TYR:CE2	2.52	0.43
1:B:355:LYS:HB2	1:B:355:LYS:HE3	1.73	0.43
1:B:397:GLU:HB2	1:B:400:LYS:HD3	1.99	0.43
1:E:355:LYS:HB2	1:E:355:LYS:HE3	1.73	0.43
1:A:761:THR:HA	1:A:764:VAL:O	2.18	0.43
1:C:497:ILE:HG23	1:C:585:ALA:HB2	2.00	0.43
1:D:497:ILE:HG23	1:D:585:ALA:HB2	2.00	0.43
1:E:497:ILE:HG23	1:E:585:ALA:HB2	2.00	0.43
1:F:761:THR:HA	1:F:764:VAL:O	2.18	0.43
1:G:255:LYS:HG2	1:G:256:GLU:HG3	1.99	0.43
1:D:255:LYS:HG2	1:D:256:GLU:HG3	1.99	0.43
1:D:400:LYS:HB3	1:D:400:LYS:HE2	1.69	0.43
1:F:229:PHE:CD1	1:F:287:VAL:HG11	2.52	0.43
1:I:416:GLU:HG3	1:I:459:VAL:HG22	2.00	0.43
1:B:228:LYS:HD3	1:B:228:LYS:C	2.39	0.43
1:K:228:LYS:HD3	1:K:228:LYS:C	2.39	0.43
1:K:248:ASN:C	1:K:721:LYS:HB2	2.38	0.43
1:A:248:ASN:C	1:A:721:LYS:HB2	2.38	0.43
1:B:450:VAL:HA	1:B:456:LYS:O	2.19	0.43
1:C:416:GLU:HG3	1:C:459:VAL:HG22	2.01	0.43
1:D:416:GLU:HG3	1:D:459:VAL:HG22	2.01	0.43
1:I:464:LYS:HD3	1:I:485:GLU:OE1	2.19	0.43
1:K:239:GLU:CA	1:K:742:VAL:CG1	2.60	0.43
1:K:450:VAL:HA	1:K:456:LYS:O	2.19	0.43
1:C:450:VAL:HA	1:C:456:LYS:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:VAL:HA	1:D:456:LYS:O	2.19	0.43
1:D:721:LYS:HG2	1:D:722:GLU:HG3	2.00	0.43
1:E:450:VAL:HA	1:E:456:LYS:O	2.19	0.43
1:E:761:THR:HA	1:E:764:VAL:O	2.18	0.43
1:F:416:GLU:HG3	1:F:459:VAL:HG22	2.00	0.43
1:F:450:VAL:HA	1:F:456:LYS:O	2.19	0.43
1:J:464:LYS:HD3	1:J:485:GLU:OE1	2.19	0.43
1:C:228:LYS:HD3	1:C:228:LYS:C	2.39	0.43
1:F:228:LYS:HD3	1:F:228:LYS:C	2.39	0.43
1:I:228:LYS:HD3	1:I:228:LYS:C	2.39	0.43
1:I:242:LYS:CA	1:I:251:LYS:NZ	2.81	0.43
1:J:451:ASP:HA	1:K:759:ALA:O	2.18	0.43
1:K:416:GLU:HG3	1:K:459:VAL:HG22	2.00	0.43
1:K:464:LYS:HD3	1:K:485:GLU:OE1	2.19	0.43
1:A:684:LYS:HD2	1:A:696:THR:HG21	2.01	0.43
1:D:355:LYS:HB2	1:D:355:LYS:HE3	1.73	0.43
1:F:397:GLU:HB2	1:F:400:LYS:HD3	1.99	0.43
1:F:464:LYS:HD3	1:F:485:GLU:OE1	2.19	0.43
1:A:450:VAL:HA	1:A:456:LYS:O	2.19	0.43
1:C:397:GLU:HB2	1:C:400:LYS:HD3	1.99	0.43
1:C:464:LYS:HD3	1:C:485:GLU:OE1	2.19	0.43
1:C:692:LYS:CD	1:D:628:PRO:HB3	2.47	0.43
1:C:692:LYS:HD2	1:D:628:PRO:HB2	2.01	0.43
1:E:416:GLU:HG3	1:E:459:VAL:HG22	2.00	0.43
1:E:628:PRO:HG3	1:F:692:LYS:HG2	1.99	0.43
1:F:264:LYS:HB2	1:F:264:LYS:HE3	1.78	0.43
1:B:248:ASN:C	1:B:721:LYS:HB2	2.38	0.42
1:B:464:LYS:HD3	1:B:485:GLU:OE1	2.19	0.42
1:C:693:LEU:HG	1:D:596:ALA:CB	2.49	0.42
1:G:464:LYS:HD3	1:G:485:GLU:OE1	2.19	0.42
1:A:798:LYS:NZ	1:C:446:GLU:HG3	2.35	0.42
1:B:684:LYS:HD2	1:B:696:THR:HG21	2.01	0.42
1:E:600:PHE:CE2	1:F:600:PHE:HZ	2.32	0.42
1:E:691:GLY:O	1:F:637:LYS:HD2	2.19	0.42
1:G:465:ALA:HA	1:G:466:PRO:HD3	1.94	0.42
1:A:781:LYS:HD3	1:C:460:LEU:CD2	2.50	0.42
1:K:242:LYS:CA	1:K:251:LYS:NZ	2.81	0.42
1:A:228:LYS:HD3	1:A:228:LYS:C	2.39	0.42
1:J:416:GLU:HG3	1:J:459:VAL:HG22	2.00	0.42
1:B:644:LEU:HD13	1:B:671:ILE:HD11	2.02	0.42
1:C:600:PHE:CD2	1:D:597:PHE:CD2	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:LYS:HD2	1:C:696:THR:HG21	2.01	0.42
1:D:217:ALA:C	1:D:218:LYS:HD2	2.40	0.42
1:G:217:ALA:C	1:G:218:LYS:HD2	2.40	0.42
1:B:217:ALA:C	1:B:218:LYS:HD2	2.40	0.42
1:E:228:LYS:HD3	1:E:228:LYS:C	2.39	0.42
1:I:217:ALA:C	1:I:218:LYS:HD2	2.40	0.42
1:I:248:ASN:C	1:I:721:LYS:HB2	2.38	0.42
1:J:228:LYS:HD3	1:J:228:LYS:C	2.39	0.42
1:A:644:LEU:HD13	1:A:671:ILE:HD11	2.02	0.42
1:F:248:ASN:C	1:F:721:LYS:HB2	2.38	0.42
1:F:400:LYS:HB3	1:F:400:LYS:HE2	1.69	0.42
1:G:228:LYS:HD3	1:G:228:LYS:C	2.39	0.42
1:G:310:VAL:HG22	1:G:430:PHE:CZ	2.54	0.42
1:J:400:LYS:HB3	1:J:400:LYS:HE2	1.69	0.42
1:A:464:LYS:HD3	1:A:485:GLU:OE1	2.19	0.42
1:A:798:LYS:HE2	1:C:446:GLU:OE1	2.19	0.42
1:C:533:THR:OG1	1:C:577:LYS:NZ	2.38	0.42
1:D:242:LYS:CA	1:D:251:LYS:NZ	2.81	0.42
1:K:217:ALA:C	1:K:218:LYS:HD2	2.40	0.42
1:E:684:LYS:HD2	1:E:696:THR:HG21	2.01	0.42
1:E:713:VAL:HA	1:E:738:SER:O	2.20	0.42
1:F:684:LYS:HD2	1:F:696:THR:HG21	2.01	0.42
1:G:242:LYS:CA	1:G:251:LYS:NZ	2.81	0.42
1:I:450:VAL:HA	1:I:456:LYS:O	2.19	0.42
1:J:217:ALA:C	1:J:218:LYS:HD2	2.40	0.42
1:K:467:VAL:O	1:K:483:THR:HA	2.20	0.42
1:A:467:VAL:O	1:A:483:THR:HA	2.20	0.42
1:C:217:ALA:C	1:C:218:LYS:HD2	2.40	0.42
1:C:248:ASN:C	1:C:721:LYS:HB2	2.38	0.42
1:D:464:LYS:HD3	1:D:485:GLU:OE1	2.19	0.42
1:E:221:THR:HG23	1:E:330:VAL:HG23	2.02	0.42
1:E:242:LYS:CA	1:E:251:LYS:NZ	2.81	0.42
1:E:584:LYS:HE3	1:E:584:LYS:HB3	1.91	0.42
1:G:450:VAL:HA	1:G:456:LYS:O	2.19	0.42
1:B:242:LYS:CA	1:B:251:LYS:NZ	2.81	0.41
1:D:221:THR:HG23	1:D:330:VAL:HG23	2.02	0.41
1:D:713:VAL:HG21	1:D:794:VAL:HG21	2.02	0.41
1:J:450:VAL:HA	1:J:456:LYS:O	2.19	0.41
1:K:355:LYS:HB2	1:K:355:LYS:HE3	1.73	0.41
1:B:713:VAL:HA	1:B:738:SER:O	2.20	0.41
1:F:713:VAL:HA	1:F:738:SER:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:416:GLU:HG3	1:G:459:VAL:HG22	2.00	0.41
1:I:713:VAL:HA	1:I:738:SER:O	2.20	0.41
1:L:371:VAL:HG11	1:L:374:GLU:HG3	2.02	0.41
1:A:217:ALA:C	1:A:218:LYS:HD2	2.40	0.41
1:C:644:LEU:HD13	1:C:671:ILE:HD11	2.02	0.41
1:D:228:LYS:HD3	1:D:228:LYS:C	2.39	0.41
1:E:464:LYS:HD3	1:E:485:GLU:OE1	2.19	0.41
1:F:217:ALA:C	1:F:218:LYS:HD2	2.40	0.41
1:I:713:VAL:HG21	1:I:794:VAL:HG21	2.02	0.41
1:D:264:LYS:HE3	1:D:264:LYS:HB2	1.78	0.41
1:E:217:ALA:C	1:E:218:LYS:HD2	2.40	0.41
1:E:797:ASP:N	1:E:797:ASP:OD1	2.54	0.41
1:F:242:LYS:HB3	1:F:251:LYS:HZ3	1.86	0.41
1:F:797:ASP:N	1:F:797:ASP:OD1	2.54	0.41
1:I:465:ALA:HA	1:I:466:PRO:HD3	1.94	0.41
1:I:467:VAL:O	1:I:483:THR:HA	2.20	0.41
1:K:713:VAL:HA	1:K:738:SER:O	2.20	0.41
1:A:242:LYS:HB3	1:A:251:LYS:HZ3	1.85	0.41
1:A:460:LEU:HD11	1:E:779:TYR:CD2	2.55	0.41
1:A:713:VAL:HA	1:A:738:SER:O	2.20	0.41
1:C:221:THR:HG23	1:C:330:VAL:HG23	2.02	0.41
1:C:713:VAL:HA	1:C:738:SER:O	2.20	0.41
1:C:713:VAL:HG21	1:C:794:VAL:HG21	2.02	0.41
1:D:684:LYS:HD2	1:D:696:THR:HG21	2.01	0.41
1:E:644:LEU:HD13	1:E:671:ILE:HD11	2.02	0.41
1:A:597:PHE:CE2	1:B:600:PHE:CD2	3.09	0.41
1:C:264:LYS:HB2	1:C:264:LYS:HE3	1.78	0.41
1:F:489:PHE:HB2	1:F:490:ALA:H	1.76	0.41
1:F:644:LEU:HD13	1:F:671:ILE:HD11	2.02	0.41
1:I:221:THR:HG23	1:I:330:VAL:HG23	2.02	0.41
1:J:465:ALA:HA	1:J:466:PRO:HD3	1.94	0.41
1:K:221:THR:HG23	1:K:330:VAL:HG23	2.02	0.41
1:A:242:LYS:CA	1:A:251:LYS:NZ	2.81	0.41
1:B:713:VAL:HG21	1:B:794:VAL:HG21	2.02	0.41
1:D:644:LEU:HD13	1:D:671:ILE:HD11	2.02	0.41
1:E:248:ASN:C	1:E:721:LYS:HB2	2.38	0.41
1:E:264:LYS:HB2	1:E:264:LYS:HE3	1.78	0.41
1:G:415:TYR:CZ	1:G:489:PHE:CZ	3.09	0.41
1:A:354:ALA:HB1	1:G:344:LYS:HE2	2.03	0.41
1:F:221:THR:HG23	1:F:330:VAL:HG23	2.02	0.41
1:I:355:LYS:HB2	1:I:355:LYS:HE3	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:HG23	1:A:330:VAL:HG23	2.02	0.41
1:A:757:VAL:HG21	1:C:458:THR:CG2	2.51	0.41
1:A:779:TYR:CE2	1:C:445:THR:HB	2.56	0.41
1:B:354:ALA:HB1	1:J:344:LYS:HE2	2.03	0.41
1:B:609:LEU:HD23	1:B:609:LEU:HA	1.93	0.41
1:B:757:VAL:CG2	1:F:458:THR:HG21	2.51	0.41
1:B:760:ASP:HA	1:F:451:ASP:OD1	2.21	0.41
1:C:797:ASP:OD1	1:C:797:ASP:N	2.54	0.41
1:D:797:ASP:N	1:D:797:ASP:OD1	2.54	0.41
1:F:242:LYS:CA	1:F:251:LYS:NZ	2.81	0.41
1:A:264:LYS:HB2	1:A:264:LYS:HE3	1.78	0.41
1:D:713:VAL:HA	1:D:738:SER:O	2.20	0.41
1:G:451:ASP:OD1	1:I:760:ASP:HA	2.20	0.41
1:J:242:LYS:CA	1:J:251:LYS:NZ	2.81	0.41
1:J:415:TYR:CZ	1:J:489:PHE:CZ	3.09	0.41
1:B:797:ASP:N	1:B:797:ASP:OD1	2.54	0.40
1:C:354:ALA:HB1	1:I:344:LYS:HE2	2.03	0.40
1:F:354:ALA:HB1	1:K:344:LYS:HE2	2.03	0.40
1:K:242:LYS:HB3	1:K:251:LYS:HZ3	1.85	0.40
1:C:242:LYS:CA	1:C:251:LYS:NZ	2.82	0.40
1:J:264:LYS:HB2	1:J:264:LYS:HE3	1.78	0.40
1:B:221:THR:HG23	1:B:330:VAL:HG23	2.02	0.40
1:I:415:TYR:CZ	1:I:489:PHE:CZ	3.09	0.40
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.93	0.40
1:C:400:LYS:HB3	1:C:400:LYS:HE2	1.69	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	593/814 (73%)	572 (96%)	21 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	C	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	D	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	E	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	F	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	G	276/814 (34%)	269 (98%)	7 (2%)	0	100	100
1	I	372/814 (46%)	364 (98%)	8 (2%)	0	100	100
1	J	275/814 (34%)	268 (98%)	7 (2%)	0	100	100
1	K	372/814 (46%)	364 (98%)	8 (2%)	0	100	100
1	L	86/814 (11%)	81 (94%)	5 (6%)	0	100	100
All	All	4939/8954 (55%)	4778 (97%)	161 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	B	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	C	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	D	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	E	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	F	491/659 (74%)	481 (98%)	10 (2%)	50	68
1	G	233/659 (35%)	227 (97%)	6 (3%)	41	59
1	I	311/659 (47%)	306 (98%)	5 (2%)	58	73
1	J	232/659 (35%)	227 (98%)	5 (2%)	47	65
1	K	311/659 (47%)	306 (98%)	5 (2%)	58	73
1	L	71/659 (11%)	70 (99%)	1 (1%)	62	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4104/7249 (57%)	4022 (98%)	82 (2%)	50 68

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	GLU
1	A	216	SER
1	A	229	PHE
1	A	235	LYS
1	A	489	PHE
1	A	511	VAL
1	A	554	VAL
1	A	664	THR
1	A	686	THR
1	A	696	THR
1	B	215	GLU
1	B	216	SER
1	B	229	PHE
1	B	235	LYS
1	B	489	PHE
1	B	511	VAL
1	B	554	VAL
1	B	664	THR
1	B	686	THR
1	B	696	THR
1	C	215	GLU
1	C	216	SER
1	C	229	PHE
1	C	235	LYS
1	C	489	PHE
1	C	511	VAL
1	C	554	VAL
1	C	664	THR
1	C	686	THR
1	C	696	THR
1	D	215	GLU
1	D	216	SER
1	D	229	PHE
1	D	235	LYS
1	D	489	PHE
1	D	511	VAL
1	D	554	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	664	THR
1	D	686	THR
1	D	696	THR
1	E	215	GLU
1	E	216	SER
1	E	229	PHE
1	E	235	LYS
1	E	489	PHE
1	E	511	VAL
1	E	554	VAL
1	E	664	THR
1	E	686	THR
1	E	696	THR
1	F	215	GLU
1	F	216	SER
1	F	229	PHE
1	F	235	LYS
1	F	489	PHE
1	F	511	VAL
1	F	554	VAL
1	F	664	THR
1	F	686	THR
1	F	696	THR
1	G	215	GLU
1	G	216	SER
1	G	229	PHE
1	G	235	LYS
1	G	489	PHE
1	G	491	GLN
1	I	215	GLU
1	I	216	SER
1	I	229	PHE
1	I	235	LYS
1	I	489	PHE
1	J	215	GLU
1	J	216	SER
1	J	229	PHE
1	J	235	LYS
1	J	489	PHE
1	L	360	THR
1	K	215	GLU
1	K	216	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	229	PHE
1	K	235	LYS
1	K	489	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	762	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	I	1
1	J	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	E	1
1	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	489:PHE	C	490:ALA	N	1.20
1	I	489:PHE	C	490:ALA	N	1.20
1	J	489:PHE	C	490:ALA	N	1.20
1	E	487:GLU	C	488:ALA	N	1.19
1	K	487:GLU	C	488:ALA	N	1.17