



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:59 AM UTC

PDB ID : 2Y7H / pdb_00002y7h
EMDB ID : EMD-1534
Title : Atomic model of the DNA-bound methylase complex from the Type I restriction-modification enzyme EcoKI (M2S1). Based on fitting into EM map 1534.
Authors : Kennaway, C.K.; Obarska-Kosinska, A.; White, J.H.; Tuszyńska, I.; Cooper, L.P.; Bujnicki, J.M.; Trinick, J.; Dryden, D.T.F.
Deposited on : 2011-01-31
Resolution : 18.00 Å (reported)
Based on initial models : 1YF2, 2AR0, 1S7Z

This is a Full wwPDB EM Validation Report for a publicly released PDB 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:

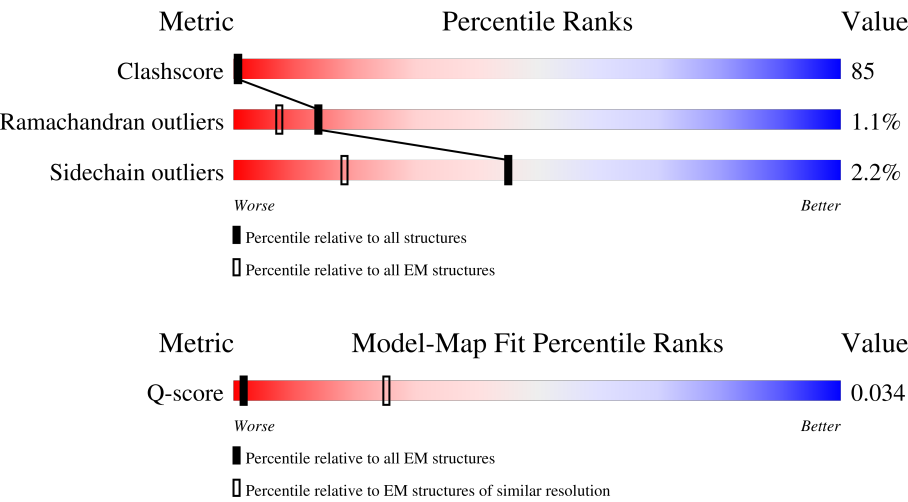
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 18.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	24 (17.50 - 18.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	52% 23%65%12%
2	B	529	47% 35%59%6%
2	C	529	47% 34%60%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	20	
4	E	20	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SAM	B	530	-	-	X	-
5	SAM	C	530	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12846 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 TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	464	Total	C	N	O	S	0	0
			3622	2298	644	671	9		

- Molecule 2 is a protein called TYPE I RESTRICTION ENZYME ECOKI M PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	529	Total	C	N	O	S	0	0
			4175	2612	730	816	17		
2	C	529	Total	C	N	O	S	0	0
			4175	2612	730	816	17		

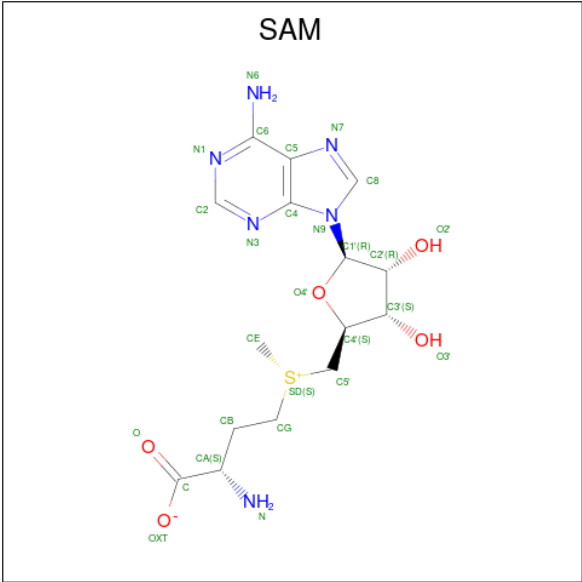
- Molecule 3 is a DNA chain called 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*A
P*CP*GP *TP*GP*CP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	20	Total	C	N	O	P	0	0
			409	194	76	119	20		

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*A
P*CP*GP *TP*TP*GP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	20	Total	C	N	O	P	0	0
			411	195	75	121	20		

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

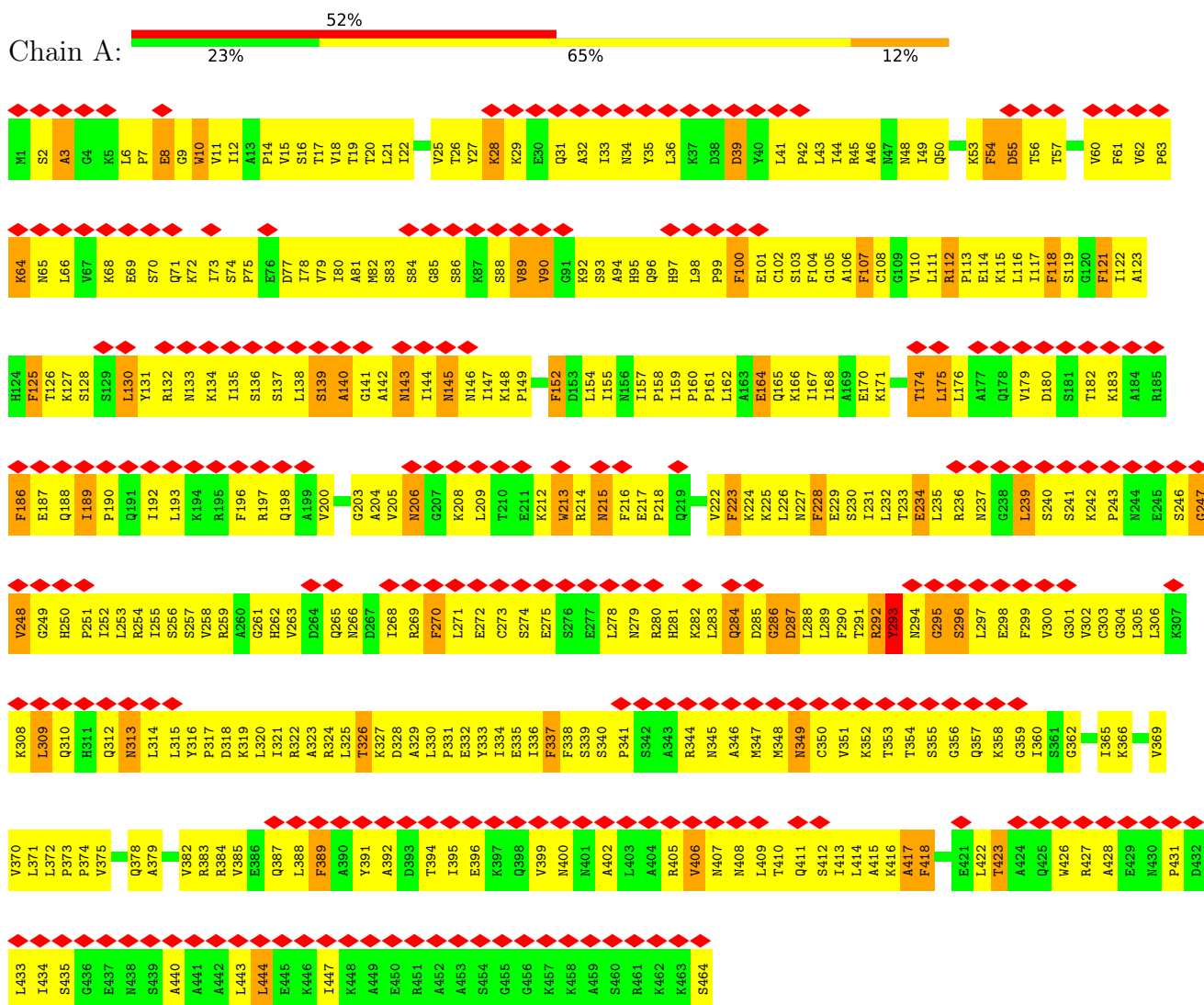


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	S	0
			27	15	6	5	1	
5	C	1	Total	C	N	O	S	0
			27	15	6	5	1	

3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: TYPE-1 RESTRICTION ENZYME ECOKI SPECIFICITY PROTEIN

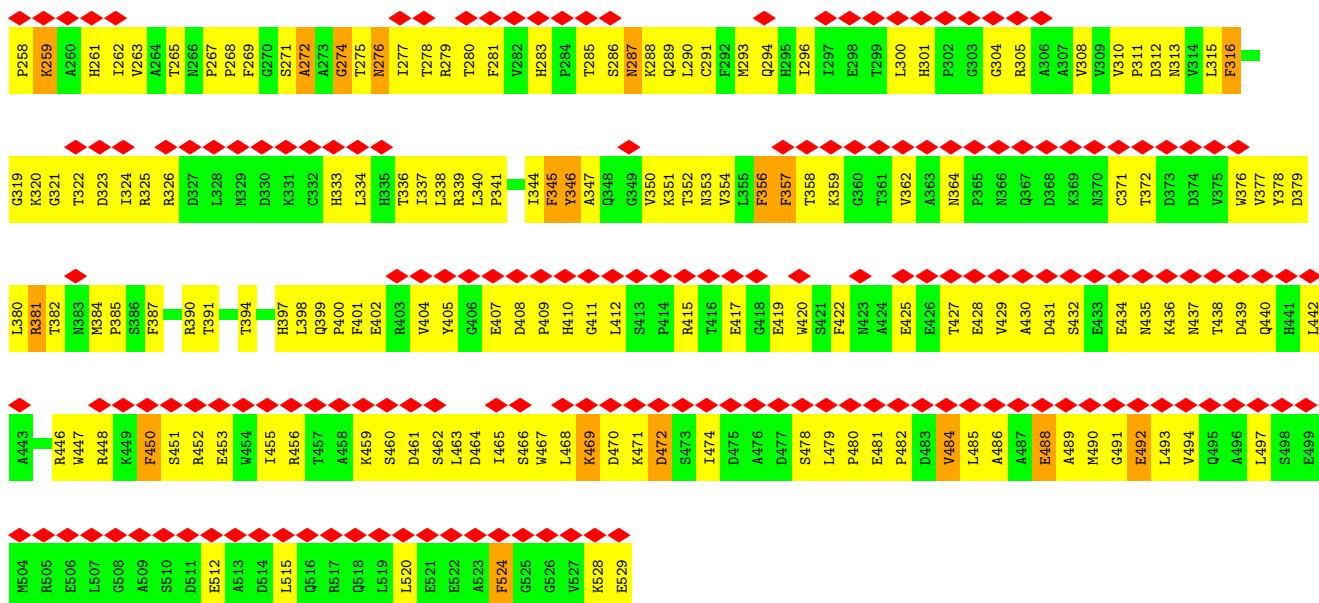


• Molecule 2: TYPE I RESTRICTION ENZYME ECOKI M PROTEIN





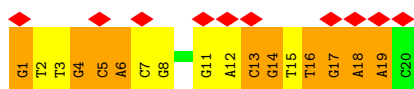
D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	A211	F212	I213	G214	L215	E216	L217	V218	P219	G220	T221	R222	R223	L224	A225	L226	M227	N228	C229	L230	L231	H232	D233	I234	E235	G236	N237	L238	D239	H240	G241	G242	A243	I244	R245	L246	G247	N248	T249	G251	S252	D253	G254	E255	N256	L257
Q136	R137	N138	A139	N140	E141	T142	K143	S144	G145	A146	G147	Q148	Y149	F150	T151	P152	A153	P154	L155	I156	Y157	T158	L159	L160	H161	L162	K163	K164	P165	Q166	P167	R168	E169	V170	L171	Q172	D173	G177	T178	A179	G180	F181	L182	I183	E184	A185	R187	Y188	V189	K190	S191	L192	L193	L194	D195	L196	D197	
M1	N2	N3	M4	D5	L6	V7	A8	K9	L10	G14	L17	R18	D19	G20	G21	V22	S23	Y24	Q25	N26	Y27	V28	N29	E30	L31	I32	A33	S33	L34	L35	K38	K39	E42	T43	G44	Q45	E46	A47	E48	R55	W56	D57	D58	L59	K60	S61	R62	I63	E66	Q67	L68	Q69	F70	Y71	L135			



• Molecule 3: 5'-D(*GP*TP*TP*CP*AP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*GP*CP*AP*AP*C)-3'



• Molecule 4: 5'-D(*GP*TP*TP*GP*CP*AP*CP*GP*TP*CP*GP*AP*CP*GP *TP*TP*GP*AP*AP*C)-3'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	17807	Depositor
Resolution determination method	Not provided	
CTF correction method	FILTERED AT FIRST ZERO	Depositor
Microscope	JEOL 1200EX	Depositor
Voltage (kV)	80	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	275	Depositor
Maximum defocus (nm)	870	Depositor
Magnification	39500	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	13.363	Depositor
Minimum map value	-3.137	Depositor
Average map value	-0.105	Depositor
Map value standard deviation	2.517	Depositor
Recommended contour level	6.41	Depositor
Map size ($\text{\AA}$)	150, 150, 150	wwPDB
Map dimensions	48, 48, 48	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	3.125, 3.125, 3.125	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	1.42	2/3685 (0.1%)	1.55	46/4968 (0.9%)
2	B	1.36	0/4262	1.56	36/5773 (0.6%)
2	C	1.35	0/4262	1.54	37/5773 (0.6%)
3	D	1.66	4/458 (0.9%)	2.33	37/704 (5.3%)
4	E	1.69	5/460 (1.1%)	2.28	33/708 (4.7%)
All	All	1.40	11/13127 (0.1%)	1.62	189/17926 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
3	D	1	1
All	All	1	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ARG	C-N	23.11	1.68	1.33
1	A	295	GLY	C-N	-11.13	1.18	1.33
4	E	5	DC	O3'-P	8.73	1.74	1.61
3	D	5	DA	O3'-P	7.49	1.72	1.61
4	E	11	DG	O3'-P	6.10	1.70	1.61
3	D	16	DG	O3'-P	5.91	1.70	1.61
3	D	17	DC	O3'-P	5.45	1.69	1.61
3	D	15	DT	O3'-P	5.40	1.69	1.61
4	E	16	DT	O3'-P	5.30	1.69	1.61
4	E	17	DG	O3'-P	5.16	1.68	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	7	DC	O3'-P	5.05	1.68	1.61

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	470	ASP	O-C-N	-23.06	95.26	122.93
2	B	90	PHE	CA-CB-CG	-13.27	100.53	113.80
2	C	90	PHE	CA-CB-CG	-13.24	100.56	113.80
1	A	292	ARG	O-C-N	-10.44	110.82	122.09
1	A	39	ASP	CA-CB-CG	-10.34	102.26	112.60
2	B	450	PHE	CA-CB-CG	-8.19	105.61	113.80
1	A	90	VAL	N-CA-C	7.97	118.52	110.23
2	C	450	PHE	CA-CB-CG	-7.87	105.94	113.80
2	C	469	LYS	CA-C-N	-7.41	112.92	122.77
2	C	469	LYS	C-N-CA	-7.41	112.92	122.77
1	A	107	PHE	CA-CB-CG	-7.37	106.43	113.80
2	C	422	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	309	LEU	N-CA-C	-7.33	98.43	109.94
1	A	349	ASN	CA-CB-CG	-7.33	105.27	112.60
2	B	422	PHE	CA-CB-CG	-7.28	106.52	113.80
1	A	247	GLY	N-CA-C	-7.28	104.32	112.33
2	B	356	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	223	PHE	CA-CB-CG	-7.14	106.66	113.80
2	C	19	ASP	CA-CB-CG	-7.11	105.49	112.60
2	B	19	ASP	CA-CB-CG	-7.05	105.55	112.60
2	C	356	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	189	ILE	N-CA-CB	7.00	114.91	110.50
2	B	212	PHE	CA-CB-CG	-6.99	106.81	113.80
1	A	389	PHE	CA-CB-CG	-6.99	106.81	113.80
2	C	212	PHE	CA-CB-CG	-6.98	106.82	113.80
1	A	89	VAL	N-CA-C	6.97	121.58	113.42
1	A	164	GLU	CB-CG-CD	-6.85	100.95	112.60
4	E	4	DG	C4-C5-N7	-6.59	100.91	110.80
2	C	116	TYR	CA-C-N	-6.59	112.72	122.41
2	C	116	TYR	C-N-CA	-6.59	112.72	122.41
1	A	39	ASP	CA-C-N	6.58	129.64	120.29
1	A	39	ASP	C-N-CA	6.58	129.64	120.29
2	B	116	TYR	CA-C-N	-6.57	112.75	122.41
2	B	116	TYR	C-N-CA	-6.57	112.75	122.41
4	E	16	DT	O3'-P-O5'	6.56	113.84	104.00
3	D	14	DG	C5'-C4'-C3'	-6.51	105.13	114.90
2	C	345	PHE	CA-CB-CG	-6.47	107.33	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	PHE	CA-CB-CG	-6.46	107.34	113.80
3	D	1	DG	C4-C5-N7	-6.46	101.12	110.80
2	C	127	PHE	CA-CB-CG	-6.45	107.35	113.80
4	E	8	DG	C4-C5-N7	-6.45	101.12	110.80
4	E	17	DG	C4-C5-N7	-6.45	101.13	110.80
1	A	174	THR	CA-CB-CG2	-6.44	99.56	110.50
1	A	143	ASN	CA-C-N	-6.43	114.71	123.14
1	A	143	ASN	C-N-CA	-6.43	114.71	123.14
1	A	140	ALA	N-CA-C	-6.41	104.29	111.28
4	E	11	DG	C4-C5-N7	-6.41	101.18	110.80
2	B	381	ARG	N-CA-C	6.41	118.06	111.14
3	D	11	DG	N3-C4-C5	-6.39	118.81	128.40
3	D	8	DG	C4-C5-N7	-6.39	101.22	110.80
2	B	345	PHE	CA-CB-CG	-6.37	107.43	113.80
2	C	381	ARG	N-CA-C	6.37	118.01	111.14
4	E	1	DG	C4-C5-N7	-6.37	101.25	110.80
4	E	14	DG	C4-C5-N7	-6.36	101.27	110.80
1	A	100	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	423	THR	CB-CA-C	-6.33	100.94	110.88
3	D	16	DG	C4-C5-N7	-6.33	101.31	110.80
2	B	240	HIS	CA-CB-CG	-6.31	107.49	113.80
2	C	241	GLY	N-CA-C	-6.30	106.41	113.79
2	B	241	GLY	N-CA-C	-6.28	106.44	113.79
3	D	16	DG	N3-C4-C5	-6.28	118.98	128.40
3	D	11	DG	C4-C5-N7	-6.27	101.40	110.80
4	E	14	DG	N3-C4-C5	-6.25	119.02	128.40
2	C	387	PHE	CA-CB-CG	-6.25	107.55	113.80
2	B	387	PHE	CA-CB-CG	-6.23	107.57	113.80
2	C	117	ASN	CA-CB-CG	-6.22	106.38	112.60
4	E	17	DG	O3'-P-O5'	6.22	113.32	104.00
2	B	117	ASN	CA-CB-CG	-6.20	106.40	112.60
4	E	11	DG	N3-C4-C5	-6.17	119.14	128.40
4	E	4	DG	N3-C4-C5	-6.16	119.16	128.40
2	C	240	HIS	CA-CB-CG	-6.13	107.67	113.80
3	D	1	DG	N3-C4-C5	-6.12	119.21	128.40
4	E	8	DG	N3-C4-C5	-6.10	119.25	128.40
3	D	14	DG	N3-C4-C5	-6.06	119.31	128.40
4	E	1	DG	N3-C4-C5	-6.05	119.32	128.40
3	D	8	DG	N3-C4-C5	-6.03	119.36	128.40
3	D	17	DC	O3'-P-O5'	6.02	113.03	104.00
1	A	175	LEU	CB-CA-C	-6.01	100.81	110.79
2	B	44	GLY	N-CA-C	-6.00	107.55	114.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	44	GLY	N-CA-C	-6.00	107.55	114.69
3	D	16	DG	O3'-P-O5'	6.00	113.00	104.00
3	D	14	DG	C4-C5-N7	-6.00	101.81	110.80
2	B	115	TRP	N-CA-C	-5.99	106.03	113.15
2	C	316	PHE	CA-CB-CG	-5.98	107.82	113.80
4	E	17	DG	N3-C4-C5	-5.97	119.44	128.40
2	C	115	TRP	N-CA-C	-5.94	106.08	113.15
3	D	14	DG	C2-N3-C4	5.90	120.65	111.80
3	D	14	DG	C5-C6-O6	-5.86	119.51	128.30
1	A	152	PHE	CA-CB-CG	-5.84	107.96	113.80
2	C	232	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	130	LEU	N-CA-C	-5.78	104.97	111.28
2	B	232	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	64	LYS	N-CA-C	-5.75	105.01	111.28
2	B	145	GLY	N-CA-C	-5.75	107.38	115.32
1	A	286	GLY	N-CA-C	-5.75	107.31	115.30
4	E	17	DG	C6-C5-N7	5.74	138.71	130.10
4	E	13	DC	O3'-P-O5'	5.71	112.57	104.00
4	E	14	DG	C2-N3-C4	5.71	120.36	111.80
1	A	417	ALA	N-CA-C	-5.71	105.15	111.71
4	E	6	DA	C2-N3-C4	5.70	119.35	110.80
3	D	1	DG	C2-N3-C4	5.70	120.34	111.80
3	D	16	DG	C2-N3-C4	5.70	120.34	111.80
4	E	11	DG	C2-N3-C4	5.68	120.32	111.80
2	C	145	GLY	N-CA-C	-5.68	107.49	115.32
1	A	54	PHE	CA-CB-CG	-5.67	108.13	113.80
2	C	364	ASN	CA-CB-CG	-5.67	106.93	112.60
1	A	125	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	418	PHE	CA-C-N	-5.65	113.04	122.64
1	A	418	PHE	C-N-CA	-5.65	113.04	122.64
4	E	8	DG	C2-N3-C4	5.64	120.26	111.80
3	D	11	DG	C2-N3-C4	5.64	120.26	111.80
4	E	17	DG	C2-N3-C4	5.64	120.25	111.80
1	A	55	ASP	CA-CB-CG	-5.63	106.97	112.60
3	D	1	DG	C6-C5-N7	5.63	138.55	130.10
4	E	1	DG	C2-N3-C4	5.62	120.24	111.80
4	E	4	DG	C6-C5-N7	5.62	138.53	130.10
3	D	8	DG	C6-C5-N7	5.62	138.52	130.10
2	B	364	ASN	CA-CB-CG	-5.61	106.99	112.60
3	D	14	DG	C6-C5-N7	5.60	138.50	130.10
4	E	8	DG	C6-C5-N7	5.59	138.49	130.10
4	E	4	DG	C2-N3-C4	5.59	120.18	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	DG	C2-N3-C4	5.58	120.17	111.80
4	E	1	DG	C6-C5-N7	5.58	138.47	130.10
2	C	140	ASN	CA-CB-CG	-5.58	107.02	112.60
2	B	29	ASN	CA-CB-CG	-5.57	107.03	112.60
4	E	11	DG	C6-C5-N7	5.56	138.44	130.10
2	B	140	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	270	PHE	CA-CB-CG	-5.55	108.25	113.80
2	B	195	ASP	CA-CB-CG	-5.54	107.06	112.60
2	C	29	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	287	ASP	CA-CB-CG	-5.54	107.06	112.60
2	C	195	ASP	CA-CB-CG	-5.52	107.08	112.60
2	C	21	GLY	N-CA-C	-5.49	107.44	114.85
2	B	209	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	418	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	400	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	121	PHE	CA-CB-CG	-5.45	108.35	113.80
2	B	21	GLY	N-CA-C	-5.45	107.49	114.85
3	D	6	DA	C2-N3-C4	5.43	118.94	110.80
1	A	186	PHE	CA-CB-CG	-5.42	108.38	113.80
2	C	209	HIS	CA-CB-CG	-5.41	108.39	113.80
4	E	6	DA	N3-C4-C5	-5.41	118.79	126.90
2	C	181	PHE	CA-CB-CG	-5.40	108.40	113.80
2	B	181	PHE	CA-CB-CG	-5.40	108.40	113.80
2	C	276	ASN	CA-CB-CG	-5.38	107.22	112.60
4	E	14	DG	C6-C5-N7	5.36	138.15	130.10
2	B	276	ASN	CA-CB-CG	-5.35	107.25	112.60
3	D	16	DG	C6-C5-N7	5.35	138.12	130.10
3	D	5	DA	C5'-C4'-O4'	-5.34	101.39	109.40
2	C	411	GLY	N-CA-C	-5.34	107.90	115.43
1	A	3	ALA	N-CA-C	-5.33	105.47	111.28
2	B	411	GLY	N-CA-C	-5.31	107.94	115.43
1	A	118	PHE	CA-CB-CG	-5.30	108.50	113.80
3	D	6	DA	N1-C2-N3	-5.30	121.05	129.00
1	A	337	PHE	CA-CB-CG	-5.26	108.54	113.80
4	E	6	DA	N1-C2-N3	-5.25	121.13	129.00
1	A	213	TRP	N-CA-C	-5.24	105.46	111.07
1	A	206	ASN	CA-CB-CG	-5.22	107.38	112.60
2	B	197	ASP	CA-CB-CG	-5.21	107.39	112.60
3	D	11	DG	C5-C6-O6	-5.20	120.50	128.30
3	D	18	DA	C2-N3-C4	5.19	118.59	110.80
2	C	197	ASP	CA-CB-CG	-5.19	107.41	112.60
3	D	19	DA	C2-N3-C4	5.18	118.57	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	256	ASN	CA-CB-CG	-5.17	107.43	112.60
4	E	18	DA	C2-N3-C4	5.17	118.56	110.80
3	D	13	DC	O3'-P-O5'	5.17	111.75	104.00
1	A	408	ASN	CA-CB-CG	-5.16	107.44	112.60
2	B	256	ASN	CA-CB-CG	-5.16	107.44	112.60
3	D	6	DA	N3-C4-C5	-5.15	119.18	126.90
1	A	406	VAL	CB-CA-C	-5.14	105.20	112.14
2	B	461	ASP	CA-CB-CG	-5.14	107.46	112.60
3	D	11	DG	C6-C5-N7	5.12	137.78	130.10
4	E	19	DA	C2-N3-C4	5.12	118.47	110.80
1	A	228	PHE	CA-CB-CG	-5.10	108.70	113.80
2	B	97	ILE	CB-CA-C	-5.10	105.79	111.35
3	D	18	DA	N3-C4-C5	-5.10	119.25	126.90
2	C	357	PHE	CA-CB-CG	-5.10	108.70	113.80
2	C	461	ASP	CA-CB-CG	-5.10	107.50	112.60
3	D	5	DA	C2-N3-C4	5.09	118.44	110.80
2	C	97	ILE	CB-CA-C	-5.09	105.80	111.35
3	D	11	DG	O3'-P-O5'	5.09	111.63	104.00
2	B	357	PHE	CA-CB-CG	-5.08	108.72	113.80
2	B	524	PHE	CA-CB-CG	-5.06	108.74	113.80
2	C	524	PHE	CA-CB-CG	-5.06	108.74	113.80
4	E	18	DA	N3-C4-C5	-5.05	119.33	126.90
3	D	10	DC	O3'-P-O5'	5.04	111.57	104.00
2	B	82	ASP	CA-CB-CG	-5.03	107.57	112.60
3	D	8	DG	C5-C6-O6	-5.03	120.76	128.30
1	A	293	TYR	CA-CB-CG	-5.02	104.86	113.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	15	DT	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	TYR	Sidechain
2	B	470	ASP	Mainchain
3	D	18	DA	Sidechain

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	3622	0	3738	1051	0
2	B	4175	0	4050	577	0
2	C	4175	0	4050	594	0
3	D	409	0	225	91	0
4	E	411	0	226	78	0
5	B	27	0	22	28	0
5	C	27	0	22	30	0
All	All	12846	0	12333	2141	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 85.

All (2141) 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:A:292:ARG:C	1:A:293:TYR:N	1.68	1.48
1:A:209:LEU:HB2	1:A:216:PHE:CZ	1.60	1.36
1:A:3:ALA:O	2:B:488:GLU:HG3	1.22	1.28
1:A:412:SER:HB2	2:B:495:GLN:CG	1.68	1.23
2:C:512:GLU:HB2	2:C:515:LEU:HD23	1.20	1.17
1:A:3:ALA:O	2:B:488:GLU:CG	1.93	1.15
1:A:193:LEU:HG	1:A:388:LEU:HD13	1.19	1.14
1:A:70:SER:HB2	3:D:2:DT:C7	1.76	1.14
1:A:234:GLU:HG3	4:E:2:DT:H3'	1.20	1.14
1:A:412:SER:HB2	2:B:495:GLN:CD	1.73	1.13
2:B:512:GLU:HB2	2:B:515:LEU:HD23	1.20	1.13
2:C:440:GLN:HB2	2:C:484:VAL:HG21	1.30	1.13
1:A:209:LEU:CB	1:A:216:PHE:CZ	2.32	1.12
1:A:415:ALA:HB2	2:B:492:GLU:CG	1.80	1.12
1:A:412:SER:HB2	2:B:495:GLN:HG3	1.21	1.11
1:A:6:LEU:HD21	1:A:10:TRP:HB2	1.26	1.10
1:A:325:LEU:HD13	1:A:329:ALA:HB3	1.32	1.10
1:A:189:ILE:HG23	1:A:190:PRO:HD3	1.33	1.10
2:B:269:PHE:HB2	3:D:6:DA:C8	1.88	1.09
2:C:139:ALA:HB1	2:C:150:PHE:HB2	1.29	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:PHE:HB2	4:E:6:DA:C8	1.87	1.08
1:A:265:GLN:HG3	1:A:269:ARG:HH21	1.12	1.08
1:A:234:GLU:HG3	4:E:2:DT:C3'	1.83	1.07
2:B:93:VAL:HG12	2:B:223:ARG:HD3	1.32	1.07
2:C:122:LYS:HD3	2:C:124:ARG:HE	1.13	1.07
1:A:143:ASN:HB2	2:B:313:ASN:HA	1.11	1.06
1:A:279:ASN:O	4:E:1:DG:P	2.13	1.06
2:B:139:ALA:HB1	2:B:150:PHE:HB2	1.29	1.06
2:B:122:LYS:HD3	2:B:124:ARG:HE	1.13	1.06
2:C:163:LEU:HD11	2:C:262:ILE:HD13	1.34	1.06
2:B:440:GLN:HB2	2:B:484:VAL:HG21	1.31	1.06
2:C:440:GLN:HB2	2:C:484:VAL:CG2	1.84	1.06
1:A:75:PRO:HG2	1:A:111:LEU:HD21	1.38	1.05
1:A:294:ASN:ND2	3:D:13:DC:H2''	1.69	1.05
1:A:175:LEU:HG	1:A:406:VAL:HG22	1.38	1.05
1:A:289:LEU:HD11	1:A:320:LEU:HD11	1.37	1.05
2:C:93:VAL:HG12	2:C:223:ARG:HD3	1.33	1.05
1:A:139:SER:HB2	2:B:466:SER:HB3	1.33	1.05
1:A:25:VAL:HG13	1:A:71:GLN:HA	1.37	1.05
1:A:294:ASN:HD21	3:D:13:DC:H2''	0.88	1.04
1:A:355:SER:HB3	2:C:316:PHE:HE1	1.22	1.04
2:B:440:GLN:HB2	2:B:484:VAL:CG2	1.85	1.04
5:C:530:SAM:CE	4:E:6:DA:N6	2.19	1.04
1:A:239:LEU:HD22	1:A:241:SER:H	1.18	1.03
1:A:160:PRO:HG2	1:A:165:GLN:HG2	1.35	1.03
2:B:350:VAL:CG1	3:D:6:DA:H4'	1.88	1.02
1:A:83:SER:HA	1:A:147:ILE:HG22	1.41	1.02
1:A:292:ARG:NH1	4:E:3:DT:H73	1.72	1.02
1:A:415:ALA:HB2	2:B:492:GLU:HG3	1.40	1.02
1:A:252:ILE:HG13	1:A:317:PRO:HD3	1.41	1.02
1:A:292:ARG:HH12	4:E:3:DT:H73	0.87	1.01
1:A:71:GLN:HG2	1:A:102:CYS:HB3	1.41	1.01
1:A:428:ALA:HB1	1:A:433:LEU:HD12	1.39	1.01
1:A:412:SER:CB	2:B:495:GLN:HG3	1.90	1.00
2:B:285:THR:HG22	2:B:287:ASN:H	1.22	1.00
5:B:530:SAM:CE	3:D:6:DA:N6	2.25	1.00
1:A:209:LEU:HB2	1:A:216:PHE:HZ	1.23	1.00
2:C:24:TYR:HA	2:C:27:TYR:CE2	1.97	1.00
2:B:24:TYR:HA	2:B:27:TYR:CE2	1.97	1.00
5:C:530:SAM:HE3	4:E:6:DA:N6	1.76	0.99
2:C:285:THR:HG22	2:C:287:ASN:H	1.22	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:H	1:A:28:LYS:HD3	1.27	0.99
1:A:196:PHE:CZ	1:A:384:ARG:HD2	1.97	0.99
1:A:209:LEU:HB2	1:A:216:PHE:CE2	1.98	0.99
2:C:276:ASN:HD22	2:C:278:THR:HG23	1.26	0.99
3:D:12:DA:H2''	3:D:13:DC:H5'	1.45	0.99
1:A:70:SER:HB2	3:D:2:DT:H72	1.43	0.98
1:A:85:GLY:HA2	4:E:14:DG:C8	1.99	0.98
1:A:62:VAL:HG12	1:A:64:LYS:H	1.28	0.98
1:A:355:SER:HB3	2:C:316:PHE:CE1	1.99	0.98
2:C:220:GLY:HA2	2:C:223:ARG:HE	1.27	0.98
2:B:220:GLY:HA2	2:B:223:ARG:HE	1.28	0.97
1:A:39:ASP:HB3	1:A:60:VAL:HG12	1.42	0.97
1:A:70:SER:HB2	3:D:2:DT:H71	1.45	0.97
2:C:430:ALA:HB2	2:C:469:LYS:HG3	1.46	0.97
2:B:276:ASN:HD22	2:B:278:THR:HG23	1.26	0.97
1:A:251:PRO:HA	1:A:269:ARG:HG2	1.45	0.97
1:A:234:GLU:CG	4:E:2:DT:H3'	1.95	0.97
1:A:283:LEU:HD22	1:A:322:ARG:HD2	1.46	0.97
2:B:448:ARG:HD3	2:B:467:TRP:CE2	2.01	0.96
1:A:283:LEU:HD11	1:A:316:TYR:CE1	2.00	0.96
2:C:128:GLY:HA3	2:C:231:LEU:HD22	1.46	0.96
1:A:215:ASN:HD21	2:C:492:GLU:CB	1.77	0.96
1:A:293:TYR:HB2	1:A:319:LYS:HD2	1.47	0.96
2:C:448:ARG:HD3	2:C:467:TRP:CE2	2.01	0.96
1:A:196:PHE:CZ	1:A:200:VAL:HG21	2.00	0.96
1:A:209:LEU:HD22	1:A:216:PHE:HE2	1.26	0.96
2:C:93:VAL:HG12	2:C:223:ARG:CD	1.96	0.95
1:A:143:ASN:CB	2:B:313:ASN:HA	1.95	0.95
2:C:28:VAL:HB	2:C:131:TYR:CZ	2.02	0.95
2:C:39:MET:HE2	2:C:39:MET:HA	1.49	0.95
1:A:19:THR:HG21	1:A:22:ILE:HD11	1.49	0.95
2:C:269:PHE:CD1	4:E:6:DA:C5	2.54	0.95
1:A:334:ILE:HG12	1:A:338:PHE:CE2	2.01	0.95
2:C:84:LYS:HA	2:C:87:GLN:HG2	1.49	0.94
2:B:39:MET:HA	2:B:39:MET:HE2	1.49	0.94
2:B:93:VAL:HG12	2:B:223:ARG:CD	1.96	0.94
1:A:142:ALA:CA	2:B:312:ASP:HB3	1.98	0.94
2:C:322:THR:HA	2:C:325:ARG:HE	1.33	0.94
1:A:271:LEU:HD22	1:A:273:CYS:H	1.30	0.94
2:B:128:GLY:HA3	2:B:231:LEU:HD22	1.46	0.94
1:A:209:LEU:CB	1:A:216:PHE:CE2	2.50	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:VAL:HB	2:B:131:TYR:CZ	2.02	0.94
2:C:257:LEU:HD12	2:C:258:PRO:HD2	1.47	0.94
2:B:257:LEU:HD12	2:B:258:PRO:HD2	1.47	0.94
1:A:223:PHE:CE1	1:A:369:VAL:HG13	2.04	0.93
2:B:250:LEU:HD13	2:B:277:ILE:HG12	1.50	0.93
1:A:427:ARG:HB3	1:A:447:ILE:HD12	1.50	0.93
2:C:268:PRO:HG3	5:C:530:SAM:C8	1.97	0.93
1:A:142:ALA:HA	2:B:312:ASP:HB3	1.50	0.93
2:B:268:PRO:HG3	5:B:530:SAM:C8	1.99	0.93
2:B:350:VAL:HG12	3:D:6:DA:H4'	1.46	0.93
1:A:325:LEU:HD13	1:A:329:ALA:CB	1.98	0.93
1:A:319:LYS:HE3	3:D:15:DT:H4'	1.49	0.92
2:C:440:GLN:CG	2:C:484:VAL:HB	1.98	0.92
1:A:212:LYS:HE3	1:A:223:PHE:HB2	1.49	0.92
2:B:84:LYS:HA	2:B:87:GLN:HG2	1.49	0.92
1:A:215:ASN:OD1	2:C:489:ALA:HA	1.70	0.92
1:A:212:LYS:CE	1:A:223:PHE:HB2	1.99	0.92
1:A:290:PHE:HB3	1:A:321:ILE:CG2	1.98	0.92
2:B:20:GLY:HA2	2:B:102:GLN:HG3	1.51	0.92
2:B:440:GLN:CG	2:B:484:VAL:HB	1.99	0.92
1:A:428:ALA:CB	1:A:433:LEU:HD12	1.98	0.91
2:B:149:TYR:HD1	5:B:530:SAM:HO3'	0.92	0.91
2:C:106:LEU:CD2	2:C:110:MET:HE3	1.99	0.91
1:A:90:VAL:HG13	1:A:132:ARG:HD2	1.49	0.91
1:A:168:ILE:CD1	1:A:417:ALA:HB1	2.00	0.91
1:A:232:LEU:CG	1:A:321:ILE:HD11	2.01	0.91
2:B:106:LEU:CD2	2:B:110:MET:HE3	1.99	0.91
2:C:71:TYR:CE2	2:C:75:LEU:HD11	2.06	0.91
2:B:71:TYR:CE2	2:B:75:LEU:HD11	2.06	0.91
2:B:1:MET:CE	2:B:129:ASP:HA	2.00	0.90
2:C:20:GLY:HA2	2:C:102:GLN:HG3	1.51	0.90
4:E:12:DA:H2''	4:E:13:DC:H5''	1.53	0.90
2:C:250:LEU:HD13	2:C:277:ILE:HG12	1.50	0.90
1:A:71:GLN:CG	1:A:102:CYS:HB3	2.01	0.90
1:A:112:ARG:HB2	1:A:117:ILE:HG23	1.50	0.90
1:A:168:ILE:HG23	1:A:413:ILE:CD1	2.00	0.90
1:A:280:ARG:HB2	1:A:315:LEU:HD11	1.51	0.90
1:A:248:VAL:HG11	1:A:269:ARG:CB	2.01	0.90
1:A:348:MET:SD	2:C:469:LYS:HG2	2.12	0.90
2:B:1:MET:HE2	2:B:132:GLU:HG3	1.53	0.90
2:B:84:LYS:HA	2:B:87:GLN:CG	2.01	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD22	1:A:216:PHE:CE2	2.07	0.89
1:A:285:ASP:HB3	1:A:308:LYS:HG2	1.55	0.89
1:A:294:ASN:HA	3:D:14:DG:C8	2.07	0.89
2:B:269:PHE:CD1	3:D:6:DA:C5	2.61	0.89
2:C:84:LYS:HA	2:C:87:GLN:CG	2.01	0.89
2:C:439:ASP:HA	2:C:485:LEU:CD2	2.02	0.89
2:B:6:LEU:HB3	2:B:130:MET:SD	2.13	0.89
2:C:394:THR:H	2:C:397:HIS:HD2	1.20	0.89
2:B:439:ASP:HA	2:B:485:LEU:CD2	2.02	0.89
1:A:168:ILE:HG23	1:A:413:ILE:HD11	1.52	0.89
2:B:394:THR:H	2:B:397:HIS:HD2	1.20	0.89
2:B:215:LEU:HD13	2:B:245:ARG:HE	1.38	0.88
2:B:217:LEU:HD22	2:B:275:THR:HG22	1.55	0.88
1:A:300:VAL:HG13	1:A:344:ARG:HD2	1.55	0.88
1:A:32:ALA:HB3	1:A:35:TYR:CD2	2.08	0.88
1:A:75:PRO:HA	1:A:100:PHE:CD2	2.08	0.88
1:A:426:TRP:CZ2	1:A:444:LEU:HG	2.08	0.88
1:A:196:PHE:CE1	1:A:384:ARG:HD2	2.09	0.88
1:A:352:LYS:HE2	2:C:468:LEU:H	1.39	0.88
2:B:115:TRP:HH2	2:B:122:LYS:HE2	1.39	0.88
1:A:248:VAL:HG13	1:A:270:PHE:C	1.98	0.88
2:C:217:LEU:HD22	2:C:275:THR:HG22	1.55	0.88
2:C:6:LEU:HB3	2:C:130:MET:SD	2.13	0.87
2:C:149:TYR:HA	5:C:530:SAM:SD	2.14	0.87
2:C:217:LEU:HD22	2:C:275:THR:CG2	2.03	0.87
1:A:215:ASN:ND2	1:A:216:PHE:H	1.71	0.87
1:A:215:ASN:HD21	2:C:492:GLU:HB2	1.40	0.87
2:B:217:LEU:HD22	2:B:275:THR:CG2	2.03	0.87
2:C:115:TRP:HH2	2:C:122:LYS:HE2	1.39	0.87
2:B:149:TYR:HA	5:B:530:SAM:SD	2.15	0.86
1:A:415:ALA:HB2	2:B:492:GLU:HG2	1.57	0.86
2:C:3:ASN:HD22	2:C:7:VAL:HG11	1.39	0.86
2:C:220:GLY:HA2	2:C:223:ARG:NE	1.90	0.86
1:A:326:THR:HG23	1:A:327:LYS:H	1.38	0.86
2:B:440:GLN:HG2	2:B:484:VAL:HB	1.57	0.86
2:C:283:HIS:H	2:C:294:GLN:HE22	1.24	0.86
1:A:39:ASP:HB2	1:A:62:VAL:CG2	2.06	0.86
1:A:143:ASN:HB2	2:B:313:ASN:CA	2.02	0.86
1:A:85:GLY:HA2	4:E:14:DG:H8	1.38	0.86
1:A:320:LEU:HD23	1:A:321:ILE:N	1.90	0.86
2:C:440:GLN:HG2	2:C:484:VAL:HB	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:DA:H2''	3:D:13:DC:C5'	2.06	0.86
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.56	0.86
2:C:84:LYS:HD3	2:C:87:GLN:HG2	1.58	0.86
2:C:207:GLN:HA	2:C:211:ALA:HB2	1.58	0.86
1:A:292:ARG:HH12	4:E:3:DT:C7	1.81	0.86
2:B:6:LEU:HB2	2:B:117:ASN:CG	2.01	0.86
2:B:24:TYR:HB3	2:B:138:ASN:HD21	1.41	0.86
1:A:232:LEU:HD23	1:A:233:THR:N	1.91	0.85
1:A:215:ASN:ND2	2:C:492:GLU:HB2	1.89	0.85
1:A:215:ASN:ND2	1:A:216:PHE:N	2.23	0.85
1:A:46:ALA:HB1	1:A:82:MET:HE3	1.57	0.85
1:A:46:ALA:HA	1:A:107:PHE:CZ	2.11	0.85
1:A:280:ARG:CB	1:A:315:LEU:HD11	2.06	0.85
1:A:428:ALA:HB2	1:A:443:LEU:HD21	1.57	0.85
1:A:303:CYS:SG	1:A:335:GLU:HG3	2.16	0.85
2:B:220:GLY:HA2	2:B:223:ARG:NE	1.91	0.85
5:B:530:SAM:HE1	3:D:6:DA:N6	1.91	0.85
2:C:6:LEU:HB2	2:C:117:ASN:CG	2.01	0.85
1:A:49:ILE:HG13	1:A:107:PHE:HE2	1.40	0.85
1:A:433:LEU:HD13	1:A:443:LEU:HD13	1.58	0.85
2:B:222:ARG:NH1	2:B:226:LEU:HD11	1.91	0.85
1:A:6:LEU:HD23	1:A:7:PRO:N	1.90	0.85
2:C:350:VAL:HG12	4:E:6:DA:H4'	1.59	0.85
1:A:252:ILE:CG2	1:A:268:ILE:HG23	2.06	0.85
1:A:299:PHE:CE2	1:A:347:MET:HG2	2.12	0.85
5:B:530:SAM:HE3	3:D:6:DA:H61	1.42	0.84
2:C:215:LEU:HD13	2:C:245:ARG:HE	1.38	0.84
1:A:118:PHE:CZ	1:A:166:LYS:HE3	2.12	0.84
2:B:207:GLN:HA	2:B:211:ALA:HB2	1.58	0.84
2:C:222:ARG:NH1	2:C:226:LEU:HD11	1.91	0.84
1:A:133:ASN:HD21	2:B:430:ALA:HA	1.39	0.84
2:C:122:LYS:HD3	2:C:124:ARG:NE	1.93	0.84
2:C:148:GLN:O	5:C:530:SAM:HE1	1.77	0.84
2:B:84:LYS:HD3	2:B:87:GLN:HG2	1.58	0.84
2:B:115:TRP:CH2	2:B:122:LYS:HE2	2.12	0.84
2:C:24:TYR:HB3	2:C:138:ASN:HD21	1.41	0.84
1:A:235:LEU:HD23	1:A:236:ARG:N	1.92	0.84
1:A:282:LYS:C	1:A:283:LEU:HD23	2.02	0.84
2:C:70:PHE:CE2	2:C:74:MET:HE3	2.12	0.84
2:C:163:LEU:CD1	2:C:262:ILE:HD13	2.06	0.84
1:A:77:ASP:HA	1:A:95:HIS:NE2	1.91	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:481:GLU:HB2	2:B:482:PRO:HD3	1.60	0.84
1:A:143:ASN:HD21	3:D:5:DA:P	2.01	0.84
2:B:1:MET:HE2	2:B:132:GLU:CG	2.07	0.84
1:A:208:LYS:C	1:A:209:LEU:HD12	2.03	0.84
1:A:290:PHE:HB3	1:A:321:ILE:HG23	1.58	0.84
2:B:339:ARG:HD3	2:B:381:ARG:NH2	1.93	0.84
1:A:75:PRO:HA	1:A:100:PHE:CE2	2.12	0.83
2:B:439:ASP:HA	2:B:485:LEU:HD22	1.60	0.83
2:C:115:TRP:CH2	2:C:122:LYS:HE2	2.12	0.83
1:A:73:ILE:CG2	1:A:100:PHE:HB3	2.07	0.83
1:A:289:LEU:HD11	1:A:320:LEU:CD1	2.08	0.83
2:C:149:TYR:HD1	5:C:530:SAM:O3'	1.60	0.83
1:A:39:ASP:OD1	1:A:62:VAL:HA	1.78	0.83
2:C:38:LYS:HD3	2:C:56:TRP:CZ2	2.13	0.83
1:A:196:PHE:CE2	1:A:200:VAL:HG21	2.12	0.83
1:A:254:ARG:NH2	1:A:256:SER:HB2	1.93	0.83
5:C:530:SAM:HE3	4:E:6:DA:H61	1.41	0.83
1:A:236:ARG:HA	1:A:318:ASP:OD2	1.78	0.83
2:B:38:LYS:HD3	2:B:56:TRP:CZ2	2.13	0.83
2:B:148:GLN:O	5:B:530:SAM:HE1	1.78	0.83
1:A:348:MET:HB3	2:C:469:LYS:NZ	1.94	0.83
2:B:122:LYS:HD3	2:B:124:ARG:NE	1.93	0.83
2:B:3:ASN:HD22	2:B:7:VAL:HG11	1.41	0.83
2:C:439:ASP:HA	2:C:485:LEU:HD22	1.58	0.83
1:A:348:MET:HB3	2:C:469:LYS:HZ2	1.44	0.83
2:C:106:LEU:HD21	2:C:110:MET:HE3	1.61	0.83
2:C:319:GLY:O	2:C:322:THR:HG22	1.77	0.83
1:A:70:SER:OG	3:D:1:DG:H2'	1.79	0.83
1:A:315:LEU:HD23	1:A:316:TYR:N	1.93	0.83
4:E:1:DG:C8	4:E:2:DT:H72	2.14	0.83
1:A:3:ALA:C	2:B:488:GLU:HG3	2.03	0.82
1:A:391:TYR:O	1:A:394:THR:HG22	1.79	0.82
1:A:415:ALA:CB	2:B:492:GLU:CG	2.57	0.82
2:B:431:ASP:OD2	2:B:488:GLU:HB3	1.79	0.82
1:A:3:ALA:O	2:B:488:GLU:CD	2.21	0.82
2:B:70:PHE:CE2	2:B:74:MET:HE3	2.14	0.82
1:A:10:TRP:CE2	1:A:418:PHE:HA	2.15	0.82
1:A:253:LEU:HD11	1:A:263:VAL:HG21	1.59	0.82
2:B:283:HIS:H	2:B:294:GLN:HE22	1.24	0.82
2:C:442:LEU:HG	2:C:448:ARG:NH1	1.94	0.82
1:A:142:ALA:CB	2:B:312:ASP:HB3	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:HG3	1:A:111:LEU:HD11	1.60	0.82
1:A:83:SER:HA	1:A:147:ILE:CG2	2.08	0.82
1:A:10:TRP:CH2	1:A:161:PRO:HD2	2.15	0.82
2:B:1:MET:HE1	2:B:129:ASP:HA	1.61	0.82
2:C:478:SER:C	2:C:479:LEU:HD12	2.05	0.82
2:C:480:PRO:HG3	2:C:520:LEU:HD21	1.62	0.82
2:C:481:GLU:HB2	2:C:482:PRO:HD3	1.60	0.82
1:A:25:VAL:CG1	1:A:71:GLN:HA	2.10	0.82
1:A:6:LEU:HD21	1:A:10:TRP:CB	2.10	0.81
1:A:10:TRP:CZ2	1:A:161:PRO:HD2	2.15	0.81
1:A:270:PHE:HD2	1:A:274:SER:HB3	1.44	0.81
2:B:372:THR:O	2:B:452:ARG:HD2	1.81	0.81
2:B:442:LEU:HG	2:B:448:ARG:NH1	1.95	0.81
1:A:25:VAL:HG11	1:A:71:GLN:HG3	1.62	0.81
2:C:372:THR:O	2:C:452:ARG:HD2	1.80	0.81
2:C:431:ASP:OD2	2:C:488:GLU:HB3	1.79	0.81
5:B:530:SAM:HE3	3:D:6:DA:N6	1.93	0.81
1:A:45:ARG:HA	1:A:104:PHE:CE1	2.14	0.81
1:A:46:ALA:HB1	1:A:82:MET:CE	2.09	0.81
1:A:285:ASP:CB	1:A:308:LYS:HG2	2.11	0.81
2:B:106:LEU:HD21	2:B:110:MET:HE3	1.61	0.81
1:A:270:PHE:CE2	1:A:275:GLU:HB3	2.15	0.81
1:A:319:LYS:HD2	3:D:15:DT:OP2	1.80	0.81
1:A:42:PRO:HB3	1:A:57:THR:HG21	1.63	0.81
2:C:3:ASN:ND2	2:C:7:VAL:HG11	1.96	0.81
1:A:6:LEU:HD13	1:A:12:ILE:HD11	1.62	0.80
1:A:39:ASP:HB2	1:A:62:VAL:HG23	1.61	0.80
1:A:179:VAL:O	1:A:182:THR:HG22	1.81	0.80
1:A:235:LEU:HD23	1:A:236:ARG:H	1.45	0.80
1:A:215:ASN:HD22	1:A:216:PHE:N	1.79	0.80
1:A:223:PHE:HE1	1:A:369:VAL:HG13	1.45	0.80
1:A:225:LYS:HB2	1:A:228:PHE:CE1	2.16	0.80
2:B:91:HIS:HB3	2:B:222:ARG:NH2	1.95	0.80
1:A:283:LEU:HD22	1:A:322:ARG:CD	2.10	0.80
1:A:352:LYS:CG	2:C:466:SER:HB3	2.12	0.80
2:C:32:ALA:HB1	2:C:227:MET:SD	2.22	0.80
2:C:91:HIS:HB3	2:C:222:ARG:NH2	1.95	0.80
1:A:294:ASN:HB2	3:D:14:DG:H5"	1.62	0.80
2:B:480:PRO:HG3	2:B:520:LEU:HD21	1.62	0.80
1:A:50:GLN:HG3	4:E:14:DG:OP1	1.82	0.80
1:A:352:LYS:CD	2:C:466:SER:HB3	2.10	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:SER:C	2:B:479:LEU:HD12	2.05	0.80
2:C:350:VAL:CG1	4:E:6:DA:H4'	2.12	0.80
1:A:250:HIS:HE1	1:A:282:LYS:HE3	1.47	0.80
1:A:281:HIS:O	1:A:315:LEU:HG	1.79	0.80
1:A:314:LEU:HD23	1:A:315:LEU:N	1.97	0.80
1:A:296:SER:OG	1:A:300:VAL:HB	1.82	0.80
2:B:32:ALA:HB1	2:B:227:MET:SD	2.22	0.79
2:C:122:LYS:NZ	2:C:124:ARG:HG2	1.97	0.79
2:C:471:LYS:HD2	2:C:472:ASP:H	1.47	0.79
1:A:188:GLN:HE22	1:A:192:ILE:HG13	1.47	0.79
1:A:112:ARG:HB2	1:A:117:ILE:CG2	2.11	0.79
2:B:471:LYS:HD2	2:B:472:ASP:H	1.47	0.79
1:A:189:ILE:CG2	1:A:190:PRO:HD3	2.13	0.79
1:A:319:LYS:CE	3:D:15:DT:H4'	2.12	0.79
2:C:480:PRO:O	2:C:484:VAL:HG13	1.83	0.79
1:A:209:LEU:CD2	1:A:216:PHE:CE2	2.66	0.79
1:A:131:TYR:CZ	1:A:135:ILE:HD11	2.18	0.79
1:A:239:LEU:CD2	1:A:241:SER:H	1.96	0.79
1:A:248:VAL:HG11	1:A:269:ARG:HB3	1.65	0.79
1:A:160:PRO:HG2	1:A:165:GLN:CG	2.13	0.79
1:A:248:VAL:HG12	1:A:250:HIS:H	1.49	0.78
2:C:149:TYR:HD1	5:C:530:SAM:HO3'	0.79	0.78
2:C:163:LEU:HD11	2:C:262:ILE:CD1	2.11	0.78
1:A:26:THR:CG2	1:A:70:SER:HB3	2.13	0.78
1:A:373:PRO:HG2	1:A:378:GLN:HG2	1.65	0.78
2:B:122:LYS:NZ	2:B:124:ARG:HG2	1.97	0.78
2:B:480:PRO:O	2:B:484:VAL:HG13	1.83	0.78
2:C:322:THR:HB	2:C:325:ARG:HH21	1.49	0.78
1:A:49:ILE:HD12	1:A:82:MET:HG3	1.66	0.78
1:A:374:PRO:O	1:A:378:GLN:HG3	1.83	0.78
2:B:394:THR:H	2:B:397:HIS:CD2	2.01	0.78
1:A:283:LEU:HD11	1:A:316:TYR:CD1	2.19	0.78
2:C:3:ASN:HB2	2:C:7:VAL:HB	1.65	0.78
1:A:78:ILE:HA	1:A:112:ARG:HH12	1.47	0.78
1:A:164:GLU:HG3	1:A:423:THR:HA	1.65	0.78
1:A:434:ILE:O	1:A:440:ALA:HB2	1.84	0.78
2:B:146:ALA:O	2:B:149:TYR:HD2	1.65	0.78
2:C:394:THR:H	2:C:397:HIS:CD2	2.01	0.78
1:A:294:ASN:HD21	3:D:13:DC:C2'	1.84	0.78
2:B:6:LEU:HB3	2:B:130:MET:HE3	1.65	0.78
2:B:481:GLU:O	2:B:485:LEU:HG	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:CG	1:A:149:PRO:HD2	2.13	0.78
1:A:247:GLY:O	1:A:271:LEU:HB2	1.83	0.78
1:A:41:LEU:HD23	1:A:42:PRO:N	1.98	0.77
2:B:3:ASN:ND2	2:B:7:VAL:HG11	1.98	0.77
5:C:530:SAM:HE1	4:E:6:DA:N6	1.99	0.77
2:C:200:ASP:O	2:C:204:GLN:HG3	1.85	0.77
2:C:481:GLU:O	2:C:485:LEU:HG	1.84	0.77
1:A:236:ARG:HD2	4:E:2:DT:O4	1.83	0.77
1:A:289:LEU:CD1	1:A:320:LEU:HD21	2.15	0.77
2:B:268:PRO:HG3	5:B:530:SAM:H8	1.64	0.77
2:C:83:LYS:H	2:C:83:LYS:HD3	1.50	0.77
1:A:35:TYR:CD1	1:A:65:ASN:HA	2.20	0.77
1:A:46:ALA:HA	1:A:107:PHE:CE1	2.19	0.77
2:B:384:MET:HB3	2:B:385:PRO:HD2	1.67	0.77
4:E:16:DT:H2''	4:E:17:DG:C8	2.18	0.77
2:B:1:MET:HE2	2:B:132:GLU:CB	2.15	0.77
2:B:149:TYR:HD1	5:B:530:SAM:O3'	1.66	0.77
2:B:200:ASP:O	2:B:204:GLN:HG3	1.84	0.77
2:B:334:LEU:HD12	2:B:356:PHE:O	1.85	0.77
1:A:141:GLY:HA2	2:B:464:ASP:OD2	1.85	0.77
1:A:271:LEU:HD23	1:A:272:GLU:N	1.99	0.77
1:A:283:LEU:CD2	1:A:322:ARG:HD2	2.15	0.77
1:A:392:ALA:O	1:A:395:ILE:HG22	1.85	0.77
1:A:285:ASP:CG	1:A:308:LYS:HG2	2.10	0.77
2:B:83:LYS:HD3	2:B:83:LYS:H	1.50	0.77
1:A:253:LEU:HD22	1:A:320:LEU:CD1	2.15	0.77
1:A:289:LEU:CD1	1:A:320:LEU:HD11	2.12	0.77
1:A:299:PHE:CZ	1:A:347:MET:HE2	2.19	0.77
1:A:10:TRP:NE1	1:A:418:PHE:HA	2.00	0.76
1:A:70:SER:CB	3:D:2:DT:H72	2.14	0.76
1:A:271:LEU:CD2	1:A:273:CYS:H	1.97	0.76
2:C:6:LEU:HB3	2:C:130:MET:HE3	1.66	0.76
2:C:490:MET:O	2:C:494:VAL:HG23	1.85	0.76
1:A:46:ALA:CB	4:E:14:DG:H5'	2.15	0.76
2:C:268:PRO:HG3	5:C:530:SAM:H8	1.66	0.76
2:B:179:ALA:O	2:B:183:ILE:HD13	1.85	0.76
2:C:9:LYS:NZ	2:C:113:LEU:HB2	2.01	0.76
1:A:39:ASP:HB3	1:A:60:VAL:CG1	2.15	0.76
1:A:426:TRP:CE2	1:A:444:LEU:HG	2.21	0.76
2:B:490:MET:O	2:B:494:VAL:HG23	1.85	0.76
1:A:232:LEU:HG	1:A:321:ILE:HD11	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LEU:HD23	2:B:113:LEU:O	1.86	0.76
2:B:350:VAL:HG11	3:D:6:DA:C4'	2.16	0.76
2:C:20:GLY:CA	2:C:102:GLN:HG3	2.15	0.76
2:C:384:MET:HB3	2:C:385:PRO:HD2	1.67	0.76
2:C:512:GLU:HB2	2:C:515:LEU:CD2	2.11	0.76
1:A:10:TRP:CE2	1:A:160:PRO:HA	2.21	0.76
1:A:168:ILE:HD13	1:A:417:ALA:HB1	1.66	0.76
2:B:271:SER:O	2:B:288:LYS:HG3	1.86	0.76
2:C:271:SER:O	2:C:288:LYS:HG3	1.86	0.76
1:A:35:TYR:HB3	1:A:65:ASN:OD1	1.85	0.76
2:C:71:TYR:HE2	2:C:95:THR:HB	1.50	0.76
1:A:270:PHE:CZ	1:A:315:LEU:HD13	2.20	0.75
1:A:25:VAL:HG12	1:A:26:THR:H	1.48	0.75
1:A:225:LYS:HB2	1:A:228:PHE:CD1	2.20	0.75
2:B:1:MET:HE2	2:B:132:GLU:HB2	1.66	0.75
2:B:6:LEU:HB3	2:B:130:MET:CE	2.16	0.75
1:A:352:LYS:CE	2:C:468:LEU:H	1.99	0.75
1:A:427:ARG:HB3	1:A:447:ILE:CD1	2.14	0.75
2:B:1:MET:HE3	2:B:129:ASP:HA	1.68	0.75
1:A:78:ILE:HD12	1:A:111:LEU:HD21	1.68	0.75
1:A:133:ASN:ND2	2:B:430:ALA:HA	2.02	0.75
2:B:222:ARG:CD	2:B:246:LEU:HB2	2.17	0.75
2:C:113:LEU:O	2:C:113:LEU:HD23	1.86	0.75
1:A:294:ASN:O	1:A:358:LYS:HD2	1.86	0.75
2:C:131:TYR:OH	2:C:224:LEU:HG	1.87	0.75
1:A:90:VAL:HG13	1:A:132:ARG:CD	2.16	0.75
2:B:71:TYR:HE2	2:B:95:THR:HB	1.52	0.75
2:C:6:LEU:HB3	2:C:130:MET:CE	2.17	0.75
2:C:100:PRO:O	2:C:103:ILE:HG22	1.86	0.75
2:C:471:LYS:CD	2:C:472:ASP:H	2.00	0.75
1:A:42:PRO:HB2	1:A:101:GLU:OE2	1.87	0.75
1:A:333:TYR:O	1:A:336:ILE:HG22	1.87	0.75
2:B:305:ARG:HD3	2:B:410:HIS:CE1	2.22	0.75
2:C:1:MET:SD	2:C:132:GLU:HB2	2.26	0.75
1:A:139:SER:HB2	2:B:466:SER:CB	2.16	0.75
2:B:20:GLY:CA	2:B:102:GLN:HG3	2.15	0.75
2:B:128:GLY:HA3	2:B:231:LEU:CD2	2.18	0.74
1:A:137:SER:HB3	2:B:432:SER:HB3	1.69	0.74
2:B:9:LYS:NZ	2:B:113:LEU:HB2	2.01	0.74
1:A:239:LEU:HD22	1:A:241:SER:N	1.98	0.74
2:C:305:ARG:HD3	2:C:410:HIS:CE1	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:HZ	1:A:166:LYS:HE3	1.52	0.74
1:A:253:LEU:O	1:A:317:PRO:HD2	1.87	0.74
2:B:6:LEU:HB2	2:B:117:ASN:CB	2.18	0.74
2:B:91:HIS:HB3	2:B:222:ARG:HH21	1.51	0.74
2:C:179:ALA:O	2:C:183:ILE:HD13	1.85	0.74
3:D:16:DG:H2''	3:D:17:DC:C5	2.22	0.74
1:A:148:LYS:HG3	1:A:149:PRO:HD2	1.69	0.74
2:C:334:LEU:HD12	2:C:356:PHE:O	1.86	0.74
1:A:19:THR:HG21	1:A:22:ILE:CD1	2.17	0.74
1:A:176:LEU:O	1:A:179:VAL:HG22	1.86	0.74
1:A:371:LEU:HD23	1:A:371:LEU:H	1.52	0.74
4:E:12:DA:H2''	4:E:13:DC:C5'	2.17	0.74
1:A:49:ILE:HG23	1:A:94:ALA:HB2	1.69	0.74
1:A:234:GLU:O	4:E:2:DT:OP2	2.06	0.74
1:A:272:GLU:O	1:A:275:GLU:HG2	1.87	0.74
1:A:309:LEU:CD2	1:A:310:GLN:H	2.01	0.74
2:C:222:ARG:CD	2:C:246:LEU:HB2	2.17	0.74
1:A:255:ILE:HD13	3:D:14:DG:H5'	1.69	0.73
1:A:319:LYS:HG3	3:D:15:DT:OP1	1.88	0.73
1:A:334:ILE:HG12	1:A:338:PHE:HE2	1.53	0.73
2:B:131:TYR:OH	2:B:224:LEU:HG	1.87	0.73
2:C:91:HIS:HB3	2:C:222:ARG:HH21	1.51	0.73
1:A:252:ILE:CD1	1:A:315:LEU:HD22	2.18	0.73
1:A:253:LEU:CD1	1:A:263:VAL:HG21	2.18	0.73
2:C:24:TYR:CD2	2:C:27:TYR:HE2	2.06	0.73
1:A:112:ARG:HD2	1:A:119:SER:OG	1.88	0.73
1:A:142:ALA:HB1	2:B:312:ASP:HB3	1.70	0.73
1:A:133:ASN:OD1	2:B:431:ASP:HB2	1.89	0.73
1:A:285:ASP:HB3	1:A:308:LYS:CG	2.17	0.73
1:A:26:THR:CG2	1:A:69:GLU:HG2	2.18	0.73
1:A:62:VAL:HG12	1:A:64:LYS:N	2.04	0.73
1:A:250:HIS:O	1:A:269:ARG:HB3	1.88	0.73
1:A:415:ALA:CB	2:B:492:GLU:HG3	2.17	0.73
2:B:6:LEU:HB2	2:B:117:ASN:HB2	1.70	0.73
2:B:24:TYR:CD2	2:B:27:TYR:HE2	2.06	0.73
2:B:100:PRO:O	2:B:103:ILE:HG22	1.86	0.73
2:B:350:VAL:CG1	3:D:6:DA:C4'	2.65	0.73
2:B:471:LYS:CD	2:B:472:ASP:H	2.00	0.73
1:A:123:ALA:O	1:A:126:THR:HG22	1.89	0.73
1:A:84:SER:HA	1:A:146:ASN:HD22	1.52	0.73
2:B:435:ASN:HD21	2:B:467:TRP:HB2	1.52	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:HB3	1:A:35:TYR:CE2	2.22	0.73
1:A:175:LEU:CG	1:A:406:VAL:HG22	2.16	0.73
1:A:407:ASN:O	1:A:410:THR:HG22	1.88	0.73
1:A:45:ARG:HA	1:A:104:PHE:HE1	1.53	0.73
1:A:186:PHE:HD1	1:A:395:ILE:HG21	1.53	0.73
2:B:512:GLU:HB2	2:B:515:LEU:CD2	2.10	0.73
2:C:263:VAL:HG23	2:C:300:LEU:HD21	1.71	0.73
2:C:275:THR:HG21	5:C:530:SAM:N6	2.04	0.73
1:A:154:LEU:HD23	1:A:154:LEU:O	1.89	0.72
1:A:271:LEU:HD23	1:A:272:GLU:H	1.53	0.72
2:C:6:LEU:HB2	2:C:117:ASN:CB	2.19	0.72
2:B:275:THR:HG21	5:B:530:SAM:N6	2.05	0.72
2:C:128:GLY:HA3	2:C:231:LEU:CD2	2.17	0.72
1:A:196:PHE:CE1	1:A:200:VAL:HG21	2.23	0.72
2:C:220:GLY:O	2:C:224:LEU:HD13	1.89	0.72
1:A:6:LEU:HD13	1:A:12:ILE:CD1	2.18	0.72
1:A:349:ASN:HD21	2:C:467:TRP:HA	1.53	0.72
2:B:220:GLY:O	2:B:224:LEU:HD13	1.89	0.72
2:C:69:GLN:O	2:C:72:ARG:HG2	1.88	0.72
2:C:149:TYR:CD1	5:C:530:SAM:O3'	2.38	0.72
2:B:433:GLU:HA	2:B:436:LYS:HB2	1.72	0.72
1:A:35:TYR:HB3	1:A:65:ASN:CG	2.14	0.72
2:B:263:VAL:HG23	2:B:300:LEU:HD21	1.71	0.72
1:A:111:LEU:HD22	1:A:112:ARG:HH22	1.55	0.72
1:A:231:ILE:O	1:A:323:ALA:HA	1.90	0.72
2:B:362:VAL:HG21	2:B:412:LEU:HD11	1.71	0.72
2:C:146:ALA:O	2:C:149:TYR:HD2	1.71	0.72
1:A:78:ILE:HG13	1:A:111:LEU:HD23	1.70	0.72
1:A:253:LEU:HD22	1:A:320:LEU:HD12	1.72	0.72
1:A:257:SER:HB2	1:A:266:ASN:ND2	2.05	0.71
1:A:330:LEU:HD22	1:A:333:TYR:H	1.54	0.71
1:A:339:SER:HA	1:A:344:ARG:NH2	2.05	0.71
2:B:92:ASN:CB	2:B:219:PRO:HB3	2.20	0.71
2:C:39:MET:HE2	2:C:39:MET:CA	2.20	0.71
2:C:276:ASN:ND2	2:C:278:THR:HG23	2.04	0.71
1:A:331:PRO:O	1:A:334:ILE:HG22	1.90	0.71
1:A:293:TYR:CB	1:A:319:LYS:HD2	2.20	0.71
1:A:315:LEU:HD23	1:A:316:TYR:H	1.53	0.71
1:A:330:LEU:CD1	1:A:379:ALA:HA	2.20	0.71
2:C:92:ASN:CB	2:C:219:PRO:HB3	2.20	0.71
2:C:362:VAL:HG21	2:C:412:LEU:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:CB	2:B:432:SER:HB3	2.20	0.71
1:A:288:LEU:HD11	1:A:303:CYS:SG	2.31	0.71
2:B:350:VAL:HG11	3:D:6:DA:H4'	1.71	0.71
2:C:90:PHE:HA	2:C:93:VAL:HG11	1.73	0.71
1:A:388:LEU:HD23	1:A:388:LEU:O	1.90	0.71
1:A:119:SER:O	1:A:122:ILE:HG22	1.91	0.71
1:A:353:THR:HG23	2:C:351:LYS:CE	2.20	0.71
2:C:322:THR:HA	2:C:325:ARG:NE	2.03	0.71
1:A:29:LYS:HE3	1:A:31:GLN:HB3	1.72	0.71
1:A:197:ARG:HD3	1:A:341:PRO:HD2	1.71	0.71
1:A:28:LYS:HG3	1:A:65:ASN:OD1	1.90	0.71
1:A:253:LEU:HB2	1:A:314:LEU:HD11	1.73	0.71
1:A:289:LEU:HD12	1:A:320:LEU:HD21	1.73	0.71
2:B:399:GLN:O	2:B:402:GLU:HG2	1.90	0.71
2:B:439:ASP:HA	2:B:485:LEU:HD23	1.73	0.71
2:C:399:GLN:HB2	2:C:400:PRO:HD3	1.72	0.71
1:A:15:VAL:HG23	1:A:155:ILE:HG23	1.71	0.71
1:A:111:LEU:HD22	1:A:112:ARG:NH2	2.05	0.71
1:A:295:GLY:HA3	1:A:358:LYS:HA	1.71	0.71
1:A:357:GLN:OE1	1:A:358:LYS:HG2	1.91	0.71
2:B:245:ARG:NH2	2:B:253:ASP:HB3	2.06	0.71
1:A:35:TYR:HD1	1:A:65:ASN:HA	1.53	0.70
1:A:212:LYS:HB3	1:A:215:ASN:O	1.91	0.70
1:A:319:LYS:CD	3:D:15:DT:OP2	2.39	0.70
2:C:170:VAL:H	2:C:261:HIS:HD2	1.39	0.70
2:B:3:ASN:HB2	2:B:7:VAL:HB	1.73	0.70
2:C:6:LEU:HB2	2:C:117:ASN:HB2	1.72	0.70
1:A:270:PHE:CZ	1:A:275:GLU:HB3	2.26	0.70
1:A:319:LYS:HG3	3:D:15:DT:P	2.31	0.70
2:B:90:PHE:HA	2:B:93:VAL:HG11	1.73	0.70
2:C:5:ASP:CB	2:C:116:TYR:HE2	2.05	0.70
1:A:198:GLN:C	1:A:198:GLN:OE1	2.33	0.70
1:A:294:ASN:ND2	3:D:14:DG:H8	1.88	0.70
2:B:39:MET:HE2	2:B:39:MET:CA	2.19	0.70
2:B:350:VAL:HG11	3:D:6:DA:C1'	2.22	0.70
1:A:78:ILE:HG22	1:A:96:GLN:HG2	1.74	0.70
1:A:144:ILE:CG2	1:A:146:ASN:H	2.05	0.70
1:A:193:LEU:HG	1:A:388:LEU:CD1	2.11	0.70
1:A:232:LEU:CD2	1:A:321:ILE:HD11	2.22	0.70
2:B:69:GLN:OE1	2:C:76:VAL:HG13	1.92	0.70
2:C:321:GLY:O	2:C:325:ARG:HG3	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NE	1:A:340:SER:HA	2.07	0.70
1:A:293:TYR:CD1	1:A:319:LYS:HD3	2.26	0.70
2:B:5:ASP:CB	2:B:116:TYR:HE2	2.05	0.70
2:B:399:GLN:HB2	2:B:400:PRO:HD3	1.72	0.70
1:A:252:ILE:HA	1:A:315:LEU:O	1.92	0.69
2:C:245:ARG:NH2	2:C:253:ASP:HB3	2.06	0.69
2:C:399:GLN:O	2:C:402:GLU:HG2	1.90	0.69
2:B:147:GLY:HA3	2:B:346:TYR:CG	2.28	0.69
1:A:348:MET:HE1	2:C:470:ASP:H	1.56	0.69
1:A:282:LYS:O	1:A:283:LEU:HD23	1.92	0.69
2:B:28:VAL:HB	2:B:131:TYR:CE1	2.27	0.69
2:B:90:PHE:C	2:B:93:VAL:HG13	2.17	0.69
1:A:20:THR:CG2	1:A:111:LEU:HB2	2.23	0.69
2:B:339:ARG:HD3	2:B:381:ARG:CZ	2.23	0.69
2:C:6:LEU:CB	2:C:130:MET:HE3	2.22	0.69
1:A:28:LYS:HD3	1:A:28:LYS:N	2.04	0.69
1:A:144:ILE:HG12	2:B:316:PHE:CZ	2.26	0.69
1:A:175:LEU:HD13	1:A:175:LEU:O	1.92	0.69
1:A:209:LEU:HB3	1:A:216:PHE:CZ	2.27	0.69
2:C:90:PHE:C	2:C:93:VAL:HG13	2.17	0.69
2:C:149:TYR:O	5:C:530:SAM:HB2	1.93	0.69
2:C:222:ARG:HD3	2:C:246:LEU:HB2	1.75	0.69
2:C:269:PHE:CB	4:E:6:DA:C8	2.73	0.69
1:A:270:PHE:CE1	1:A:315:LEU:HD13	2.28	0.69
1:A:345:ASN:HA	2:C:469:LYS:CE	2.22	0.69
1:A:352:LYS:HE3	2:C:466:SER:HB3	1.75	0.69
1:A:362:GLY:O	1:A:365:ILE:HG22	1.93	0.69
2:B:170:VAL:H	2:B:261:HIS:HD2	1.39	0.69
2:C:257:LEU:CD1	2:C:258:PRO:HD2	2.21	0.69
1:A:341:PRO:HA	1:A:344:ARG:HG2	1.75	0.69
2:B:6:LEU:CB	2:B:130:MET:HE3	2.22	0.69
2:B:146:ALA:O	2:B:149:TYR:CD2	2.45	0.69
1:A:70:SER:OG	3:D:1:DG:H3'	1.93	0.69
1:A:282:LYS:HE2	1:A:313:ASN:CG	2.18	0.69
1:A:349:ASN:HB2	2:C:431:ASP:N	2.08	0.69
2:B:222:ARG:HD3	2:B:246:LEU:HB2	1.74	0.69
2:B:440:GLN:C	2:B:440:GLN:OE1	2.36	0.69
2:C:110:MET:O	2:C:113:LEU:HD22	1.93	0.69
1:A:39:ASP:CB	1:A:60:VAL:HG12	2.20	0.68
2:C:147:GLY:HA3	2:C:346:TYR:CG	2.27	0.68
1:A:14:PRO:O	1:A:17:THR:HG22	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:O	1:A:193:LEU:HD23	1.92	0.68
1:A:250:HIS:CE1	1:A:282:LYS:HE3	2.28	0.68
1:A:44:ILE:HG12	1:A:102:CYS:O	1.93	0.68
1:A:80:ILE:CD1	1:A:107:PHE:HD2	2.06	0.68
2:C:135:LEU:O	2:C:135:LEU:HD23	1.93	0.68
1:A:49:ILE:HG13	1:A:107:PHE:CE2	2.27	0.68
1:A:75:PRO:CG	1:A:111:LEU:HD11	2.24	0.68
1:A:118:PHE:HZ	1:A:162:LEU:HD11	1.57	0.68
1:A:270:PHE:CD2	1:A:274:SER:HB3	2.27	0.68
1:A:345:ASN:HA	2:C:469:LYS:HE2	1.76	0.68
2:B:28:VAL:HG23	2:B:224:LEU:HD21	1.75	0.68
1:A:75:PRO:HG2	1:A:111:LEU:CD2	2.21	0.68
1:A:255:ILE:HG21	3:D:14:DG:H5'	1.76	0.68
2:B:110:MET:O	2:B:113:LEU:HD22	1.93	0.68
2:C:440:GLN:OE1	2:C:440:GLN:O	2.12	0.68
1:A:198:GLN:OE1	1:A:198:GLN:O	2.12	0.68
1:A:412:SER:CB	2:B:495:GLN:CD	2.62	0.68
2:B:135:LEU:HD23	2:B:135:LEU:O	1.93	0.68
2:C:28:VAL:HB	2:C:131:TYR:CE1	2.27	0.68
1:A:46:ALA:CB	1:A:82:MET:HE3	2.23	0.68
2:C:28:VAL:HG23	2:C:224:LEU:HD21	1.75	0.68
1:A:232:LEU:HD21	1:A:321:ILE:HD11	1.76	0.68
1:A:73:ILE:HG23	1:A:100:PHE:HB3	1.75	0.68
1:A:283:LEU:HD11	1:A:316:TYR:HE1	1.55	0.68
1:A:79:VAL:HB	1:A:110:VAL:CG1	2.24	0.68
2:B:276:ASN:ND2	2:B:278:THR:HG23	2.04	0.68
5:B:530:SAM:CE	3:D:6:DA:H61	1.96	0.68
2:C:9:LYS:HZ1	2:C:113:LEU:HB2	1.59	0.68
1:A:25:VAL:O	1:A:105:GLY:HA2	1.93	0.67
1:A:236:ARG:HG2	1:A:237:ASN:N	2.09	0.67
1:A:292:ARG:HB3	1:A:319:LYS:O	1.93	0.67
2:B:1:MET:CE	2:B:132:GLU:HB2	2.24	0.67
2:C:440:GLN:OE1	2:C:440:GLN:C	2.36	0.67
1:A:164:GLU:O	1:A:167:ILE:HG22	1.94	0.67
1:A:252:ILE:HG22	1:A:268:ILE:O	1.95	0.67
1:A:347:MET:HE1	1:A:360:ILE:HD12	1.77	0.67
2:B:149:TYR:O	5:B:530:SAM:HB2	1.94	0.67
5:C:530:SAM:CE	4:E:6:DA:H62	2.07	0.67
1:A:130:LEU:HD23	1:A:130:LEU:O	1.95	0.67
1:A:293:TYR:O	1:A:294:ASN:HB3	1.95	0.67
2:C:269:PHE:HB3	4:E:6:DA:H5''	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:439:ASP:HA	2:C:485:LEU:HD23	1.75	0.67
1:A:209:LEU:CD2	1:A:216:PHE:HE2	2.00	0.67
1:A:9:GLY:C	1:A:10:TRP:HE3	2.02	0.67
2:B:218:VAL:HG12	2:B:220:GLY:H	1.60	0.67
2:C:322:THR:CB	2:C:325:ARG:HH21	2.07	0.67
1:A:25:VAL:HG12	1:A:26:THR:N	2.10	0.67
1:A:193:LEU:CG	1:A:388:LEU:HD13	2.12	0.67
2:B:380:LEU:O	2:B:384:MET:HG3	1.95	0.67
2:B:481:GLU:O	2:B:484:VAL:HG22	1.95	0.67
1:A:284:GLN:CD	1:A:322:ARG:HH22	2.03	0.66
2:B:440:GLN:OE1	2:B:440:GLN:O	2.12	0.66
2:C:22:VAL:HG22	2:C:96:THR:OG1	1.95	0.66
3:D:17:DC:H2''	3:D:18:DA:N7	2.10	0.66
1:A:152:PHE:O	1:A:155:ILE:HG22	1.94	0.66
1:A:232:LEU:CD1	1:A:321:ILE:HD11	2.25	0.66
1:A:349:ASN:HB3	2:C:432:SER:HB3	1.76	0.66
3:D:16:DG:H2''	3:D:17:DC:C6	2.31	0.66
1:A:25:VAL:CG1	1:A:71:GLN:HG3	2.24	0.66
1:A:316:TYR:CD2	1:A:320:LEU:HB3	2.30	0.66
2:C:486:ALA:HB3	2:C:489:ALA:CB	2.26	0.66
1:A:77:ASP:HA	1:A:95:HIS:CE1	2.30	0.66
2:C:380:LEU:O	2:C:384:MET:HG3	1.94	0.66
2:C:486:ALA:HB1	2:C:488:GLU:OE2	1.95	0.66
2:B:339:ARG:HA	2:B:353:ASN:HD22	1.59	0.66
2:B:486:ALA:HB1	2:B:488:GLU:OE2	1.95	0.66
1:A:112:ARG:CB	1:A:117:ILE:HG23	2.24	0.66
1:A:204:ALA:HB3	1:A:218:PRO:HG3	1.76	0.66
1:A:248:VAL:HG12	1:A:249:GLY:N	2.11	0.66
1:A:352:LYS:CE	2:C:466:SER:HB3	2.25	0.66
2:B:257:LEU:CD1	2:B:258:PRO:HD2	2.21	0.66
1:A:142:ALA:HB1	2:B:312:ASP:O	1.96	0.66
1:A:353:THR:C	2:C:351:LYS:HE2	2.21	0.66
1:A:233:THR:CG2	1:A:322:ARG:HB3	2.26	0.66
1:A:28:LYS:HZ1	1:A:43:LEU:HD21	1.61	0.66
2:B:350:VAL:HG11	3:D:6:DA:H1'	1.78	0.66
1:A:372:LEU:HD13	1:A:373:PRO:O	1.96	0.65
2:C:344:ILE:HG13	2:C:345:PHE:CD1	2.31	0.65
2:C:481:GLU:O	2:C:484:VAL:HG22	1.95	0.65
1:A:196:PHE:O	1:A:200:VAL:HG23	1.95	0.65
1:A:289:LEU:HD21	1:A:320:LEU:HD11	1.78	0.65
1:A:345:ASN:HA	2:C:469:LYS:NZ	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:CD2	1:A:270:PHE:HE1	2.14	0.65
1:A:282:LYS:HE2	1:A:313:ASN:OD1	1.96	0.65
2:C:6:LEU:HG	2:C:10:LEU:CD1	2.26	0.65
2:C:163:LEU:HG	2:C:262:ILE:HG21	1.79	0.65
1:A:230:SER:OG	1:A:323:ALA:HB1	1.96	0.65
1:A:305:LEU:HD23	1:A:306:LEU:N	2.11	0.65
1:A:352:LYS:HG3	2:C:466:SER:HB3	1.77	0.65
2:B:344:ILE:HG13	2:B:345:PHE:CD1	2.32	0.65
2:C:24:TYR:HB3	2:C:138:ASN:ND2	2.10	0.65
1:A:46:ALA:HB1	4:E:14:DG:H5'	1.76	0.65
2:C:339:ARG:HA	2:C:353:ASN:HD22	1.62	0.65
2:C:380:LEU:CD2	2:C:384:MET:HE2	2.27	0.65
2:B:22:VAL:HG22	2:B:96:THR:OG1	1.95	0.65
2:B:269:PHE:CD2	2:B:311:PRO:HB3	2.31	0.65
2:C:5:ASP:HB3	2:C:116:TYR:HE2	1.61	0.65
2:C:71:TYR:CE2	2:C:95:THR:HB	2.31	0.65
2:C:269:PHE:HB2	4:E:6:DA:N9	2.10	0.65
1:A:10:TRP:HE3	1:A:10:TRP:N	1.93	0.65
1:A:44:ILE:HD11	1:A:103:SER:HB2	1.79	0.65
1:A:265:GLN:HG3	1:A:269:ARG:NH2	1.98	0.65
2:C:218:VAL:HG12	2:C:220:GLY:H	1.60	0.65
1:A:410:THR:O	1:A:413:ILE:HG22	1.96	0.65
2:C:89:VAL:CG1	2:C:227:MET:HE2	2.27	0.65
1:A:20:THR:O	1:A:21:LEU:HD23	1.97	0.65
1:A:299:PHE:CE2	1:A:347:MET:HE2	2.32	0.65
1:A:355:SER:H	2:C:312:ASP:CB	2.10	0.65
2:B:448:ARG:HD3	2:B:467:TRP:CD2	2.32	0.65
1:A:39:ASP:HB2	1:A:62:VAL:HG22	1.78	0.64
1:A:236:ARG:HA	1:A:318:ASP:CG	2.22	0.64
1:A:61:PHE:CZ	1:A:66:LEU:HA	2.32	0.64
2:B:24:TYR:HB3	2:B:138:ASN:ND2	2.10	0.64
2:C:28:VAL:CG2	2:C:224:LEU:HD21	2.27	0.64
1:A:70:SER:OG	3:D:1:DG:C2'	2.45	0.64
1:A:140:ALA:HB1	2:B:351:LYS:NZ	2.13	0.64
1:A:164:GLU:HG3	1:A:423:THR:CA	2.27	0.64
1:A:357:GLN:CD	1:A:358:LYS:HG2	2.23	0.64
2:B:5:ASP:HB3	2:B:116:TYR:HE2	1.61	0.64
2:B:89:VAL:CG1	2:B:227:MET:HE2	2.27	0.64
2:B:29:ASN:HD22	2:B:224:LEU:CD1	2.11	0.64
2:C:269:PHE:CE1	4:E:6:DA:C6	2.85	0.64
2:C:442:LEU:HG	2:C:448:ARG:HH12	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLY:O	1:A:263:VAL:HG13	1.98	0.64
1:A:300:VAL:HG12	1:A:301:GLY:N	2.12	0.64
1:A:330:LEU:HD23	1:A:332:GLU:H	1.62	0.64
2:B:229:CYS:HB3	2:B:234:ILE:HB	1.80	0.64
2:B:269:PHE:CE1	3:D:6:DA:C6	2.85	0.64
2:C:216:GLU:O	2:C:246:LEU:HD22	1.98	0.64
1:A:214:ARG:HD2	1:A:369:VAL:CG1	2.28	0.64
1:A:248:VAL:HG11	1:A:269:ARG:HB2	1.79	0.64
2:B:269:PHE:CB	3:D:6:DA:C8	2.76	0.64
2:C:6:LEU:HD23	2:C:130:MET:CB	2.27	0.64
2:C:229:CYS:HB3	2:C:234:ILE:HB	1.80	0.64
1:A:286:GLY:HA2	1:A:305:LEU:HD21	1.79	0.64
2:C:263:VAL:HG23	2:C:300:LEU:CD2	2.28	0.64
1:A:28:LYS:HB2	1:A:65:ASN:HD21	1.63	0.63
1:A:413:ILE:HG12	1:A:417:ALA:HB2	1.80	0.63
1:A:35:TYR:HE1	1:A:68:LYS:HD2	1.63	0.63
1:A:44:ILE:HG22	1:A:54:PHE:CZ	2.33	0.63
1:A:70:SER:CB	3:D:2:DT:C7	2.66	0.63
1:A:300:VAL:HG12	1:A:301:GLY:H	1.63	0.63
2:C:448:ARG:HD3	2:C:467:TRP:CD2	2.33	0.63
1:A:426:TRP:CE3	1:A:447:ILE:HB	2.33	0.63
2:B:6:LEU:HD23	2:B:130:MET:CB	2.28	0.63
2:B:216:GLU:O	2:B:246:LEU:HD22	1.98	0.63
2:C:29:ASN:HD22	2:C:224:LEU:CD1	2.11	0.63
1:A:15:VAL:O	1:A:19:THR:HG22	1.99	0.63
1:A:175:LEU:HG	1:A:406:VAL:CG2	2.24	0.63
1:A:232:LEU:HD12	1:A:365:ILE:HG21	1.80	0.63
1:A:265:GLN:HG2	1:A:266:ASN:N	2.13	0.63
2:B:304:GLY:O	2:B:358:THR:HG23	1.99	0.63
2:C:123:SER:HB3	2:C:126:ASP:CG	2.23	0.63
2:B:92:ASN:HB3	2:B:219:PRO:HB3	1.81	0.63
2:C:304:GLY:O	2:C:358:THR:HG23	1.99	0.63
2:C:486:ALA:HB3	2:C:489:ALA:HB3	1.80	0.63
1:A:115:LYS:O	1:A:162:LEU:HD23	1.99	0.63
1:A:253:LEU:HD23	1:A:254:ARG:O	1.99	0.63
2:B:28:VAL:CG2	2:B:224:LEU:HD21	2.28	0.63
2:B:24:TYR:HA	2:B:27:TYR:CD2	2.34	0.63
2:C:68:LEU:HD23	2:C:68:LEU:O	1.99	0.63
2:B:71:TYR:CE2	2:B:95:THR:HB	2.33	0.62
2:B:68:LEU:O	2:B:68:LEU:HD23	1.99	0.62
2:B:123:SER:HB3	2:B:126:ASP:CG	2.23	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:VAL:CG2	2:C:300:LEU:HD21	2.30	0.62
1:A:41:LEU:HD23	1:A:42:PRO:CD	2.28	0.62
1:A:188:GLN:NE2	1:A:192:ILE:HG13	2.14	0.62
2:B:84:LYS:HA	2:B:87:GLN:HG3	1.81	0.62
2:C:84:LYS:HA	2:C:87:GLN:HG3	1.82	0.62
2:C:146:ALA:O	2:C:149:TYR:CD2	2.52	0.62
1:A:326:THR:HG23	1:A:327:LYS:N	2.13	0.62
1:A:371:LEU:H	1:A:371:LEU:CD2	2.12	0.62
3:D:2:DT:H2''	3:D:3:DT:H72	1.80	0.62
1:A:78:ILE:HA	1:A:112:ARG:NH1	2.13	0.62
1:A:232:LEU:HD11	1:A:321:ILE:HD11	1.81	0.62
2:B:263:VAL:HG23	2:B:300:LEU:CD2	2.28	0.62
2:B:83:LYS:HD3	2:B:83:LYS:N	2.14	0.62
2:C:55:ARG:NE	2:C:57:ASP:HB2	2.15	0.62
1:A:28:LYS:NZ	1:A:43:LEU:HD21	2.15	0.62
1:A:294:ASN:CB	3:D:14:DG:H5''	2.29	0.62
1:A:383:ARG:O	1:A:387:GLN:HG2	2.00	0.62
1:A:131:TYR:CE2	1:A:135:ILE:HD11	2.33	0.62
2:B:149:TYR:O	5:B:530:SAM:CB	2.47	0.62
1:A:125:PHE:HE1	1:A:418:PHE:HZ	1.47	0.61
1:A:333:TYR:HA	1:A:382:VAL:HG22	1.81	0.61
2:B:263:VAL:CG2	2:B:300:LEU:HD21	2.30	0.61
2:C:24:TYR:HA	2:C:27:TYR:CD2	2.34	0.61
2:C:83:LYS:HD3	2:C:83:LYS:N	2.14	0.61
1:A:12:ILE:HD12	1:A:12:ILE:N	2.15	0.61
1:A:157:ILE:O	1:A:157:ILE:HD12	1.99	0.61
1:A:214:ARG:HD2	1:A:369:VAL:HG11	1.82	0.61
2:B:322:THR:HA	2:B:325:ARG:NH2	2.16	0.61
2:C:92:ASN:HB2	2:C:219:PRO:HB3	1.82	0.61
1:A:248:VAL:HG13	1:A:270:PHE:O	2.00	0.61
1:A:274:SER:O	1:A:278:LEU:HD23	2.00	0.61
1:A:319:LYS:HE3	3:D:15:DT:C4'	2.27	0.61
2:B:249:THR:O	2:B:254:GLY:HA3	2.01	0.61
2:B:380:LEU:CD2	2:B:384:MET:HE2	2.30	0.61
2:C:38:LYS:HB2	2:C:56:TRP:CZ3	2.35	0.61
2:C:92:ASN:HB3	2:C:219:PRO:HB3	1.81	0.61
1:A:35:TYR:HD1	1:A:65:ASN:CA	2.13	0.61
1:A:186:PHE:CD1	1:A:395:ILE:HG21	2.35	0.61
1:A:234:GLU:CB	4:E:2:DT:H3'	2.30	0.61
1:A:330:LEU:HD23	1:A:331:PRO:HD2	1.81	0.61
2:C:227:MET:O	2:C:231:LEU:HD13	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:CA	4:E:14:DG:C8	2.80	0.61
1:A:427:ARG:O	1:A:447:ILE:HD11	2.00	0.61
1:A:217:GLU:CG	1:A:218:PRO:HD2	2.30	0.61
1:A:314:LEU:HD23	1:A:314:LEU:C	2.25	0.61
2:B:92:ASN:HB2	2:B:219:PRO:HB3	1.82	0.61
2:C:215:LEU:CD1	2:C:245:ARG:HE	2.13	0.61
1:A:118:PHE:CE2	1:A:162:LEU:HD22	2.35	0.61
1:A:270:PHE:HE2	1:A:275:GLU:HB3	1.63	0.61
2:B:5:ASP:HB3	2:B:116:TYR:CE2	2.36	0.61
2:C:339:ARG:HH22	2:C:464:ASP:HA	1.66	0.61
1:A:128:SER:O	1:A:131:TYR:HB3	2.01	0.61
2:B:38:LYS:HB2	2:B:56:TRP:CZ3	2.35	0.61
2:B:486:ALA:HB3	2:B:489:ALA:CB	2.31	0.61
2:C:71:TYR:HE2	2:C:75:LEU:HD11	1.66	0.61
2:C:149:TYR:O	5:C:530:SAM:CB	2.49	0.61
1:A:74:SER:OG	1:A:78:ILE:HD13	2.01	0.61
1:A:78:ILE:HD12	1:A:111:LEU:CD2	2.30	0.61
1:A:347:MET:CE	1:A:360:ILE:HD12	2.29	0.61
2:B:215:LEU:CD1	2:B:245:ARG:HE	2.13	0.61
1:A:15:VAL:HA	1:A:18:VAL:HG22	1.83	0.61
2:B:55:ARG:NE	2:B:57:ASP:HB2	2.15	0.61
2:B:315:LEU:O	2:B:325:ARG:HD3	2.01	0.61
2:C:249:THR:O	2:C:254:GLY:HA3	2.01	0.61
1:A:39:ASP:O	1:A:60:VAL:HG11	2.00	0.60
2:C:287:ASN:HB3	2:C:290:LEU:HB2	1.84	0.60
2:C:456:ARG:O	2:C:460:SER:HA	2.00	0.60
1:A:294:ASN:HB2	3:D:14:DG:C5'	2.31	0.60
2:B:35:LEU:O	2:B:39:MET:HG2	2.02	0.60
2:C:93:VAL:CG1	2:C:223:ARG:HD3	2.21	0.60
1:A:164:GLU:O	1:A:168:ILE:HG13	2.02	0.60
1:A:209:LEU:HG	1:A:218:PRO:HA	1.83	0.60
1:A:248:VAL:HG12	1:A:249:GLY:H	1.66	0.60
1:A:297:LEU:O	1:A:298:GLU:HG2	2.01	0.60
2:B:90:PHE:O	2:B:93:VAL:HG13	2.01	0.60
1:A:248:VAL:HG11	1:A:269:ARG:C	2.26	0.60
1:A:328:ASP:OD1	1:A:375:VAL:HG22	2.02	0.60
2:B:287:ASN:HB3	2:B:290:LEU:HB2	1.84	0.60
1:A:233:THR:HG22	1:A:322:ARG:HB3	1.81	0.60
2:B:118:GLY:HA2	2:B:123:SER:HB2	1.83	0.60
2:C:106:LEU:HD23	2:C:106:LEU:O	2.01	0.60
2:B:106:LEU:O	2:B:106:LEU:HD23	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:MET:O	2:B:231:LEU:HD13	2.00	0.60
1:A:101:GLU:HG2	1:A:102:CYS:H	1.65	0.60
2:C:163:LEU:O	2:C:163:LEU:HD13	2.01	0.60
1:A:143:ASN:ND2	3:D:5:DA:P	2.74	0.60
1:A:160:PRO:CG	1:A:165:GLN:HG2	2.21	0.60
1:A:253:LEU:HD23	1:A:253:LEU:C	2.27	0.60
2:B:293:MET:HE1	2:B:310:VAL:HG11	1.83	0.60
1:A:25:VAL:HB	1:A:104:PHE:O	2.02	0.60
1:A:83:SER:CA	1:A:147:ILE:HG22	2.24	0.60
1:A:162:LEU:HD13	1:A:162:LEU:O	2.02	0.60
1:A:319:LYS:HE2	3:D:16:DG:N7	2.16	0.60
2:C:244:ILE:N	2:C:244:ILE:HD12	2.17	0.60
2:C:275:THR:HG21	5:C:530:SAM:HN61	1.67	0.60
1:A:319:LYS:HZ1	3:D:15:DT:H4'	1.67	0.59
1:A:209:LEU:HD12	1:A:209:LEU:N	2.16	0.59
1:A:209:LEU:HB3	1:A:216:PHE:CE2	2.33	0.59
1:A:232:LEU:HD12	1:A:365:ILE:CG2	2.32	0.59
2:B:149:TYR:CD1	5:B:530:SAM:O3'	2.46	0.59
2:C:5:ASP:HB3	2:C:116:TYR:CE2	2.35	0.59
1:A:46:ALA:HA	1:A:107:PHE:HZ	1.65	0.59
2:C:90:PHE:O	2:C:93:VAL:HG22	2.03	0.59
1:A:309:LEU:HD22	1:A:310:GLN:H	1.65	0.59
2:B:90:PHE:O	2:B:93:VAL:HG22	2.03	0.59
2:C:35:LEU:O	2:C:39:MET:HG2	2.02	0.59
2:C:90:PHE:O	2:C:93:VAL:HG13	2.01	0.59
2:C:334:LEU:HA	2:C:357:PHE:HB3	1.84	0.59
1:A:263:VAL:HG23	1:A:263:VAL:O	2.03	0.59
1:A:280:ARG:HB3	1:A:315:LEU:HD11	1.85	0.59
2:B:55:ARG:HE	2:B:57:ASP:HB2	1.67	0.59
2:C:489:ALA:O	2:C:493:LEU:HD23	2.02	0.59
2:B:269:PHE:CD1	3:D:6:DA:C6	2.90	0.59
2:B:524:PHE:CE2	2:B:528:LYS:HD2	2.37	0.59
2:C:269:PHE:CD1	4:E:6:DA:C4	2.90	0.59
1:A:70:SER:OG	3:D:1:DG:C3'	2.51	0.59
1:A:143:ASN:CG	3:D:5:DA:OP2	2.46	0.59
1:A:349:ASN:HB2	2:C:430:ALA:CB	2.32	0.59
1:A:353:THR:HG23	2:C:351:LYS:HE2	1.85	0.59
1:A:409:LEU:HD23	1:A:409:LEU:C	2.27	0.59
1:A:157:ILE:HD12	1:A:157:ILE:C	2.28	0.59
4:E:16:DT:H2''	4:E:17:DG:N7	2.18	0.59
1:A:32:ALA:HB3	1:A:35:TYR:HD2	1.62	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:PHE:CB	4:E:6:DA:O4'	2.50	0.59
2:C:524:PHE:CE2	2:C:528:LYS:HD2	2.37	0.59
1:A:20:THR:HG23	1:A:21:LEU:N	2.17	0.59
1:A:131:TYR:HE1	1:A:155:ILE:CD1	2.16	0.59
1:A:215:ASN:HD21	2:C:492:GLU:CG	2.14	0.59
1:A:226:LEU:CD2	1:A:365:ILE:HG12	2.32	0.59
2:B:230:LEU:C	2:B:230:LEU:HD13	2.28	0.59
2:B:290:LEU:HD13	2:B:324:ILE:HD12	1.85	0.59
2:C:269:PHE:CD1	4:E:6:DA:C6	2.91	0.59
1:A:6:LEU:CD2	1:A:10:TRP:HB2	2.17	0.58
1:A:83:SER:OG	1:A:146:ASN:HB3	2.02	0.58
2:B:76:VAL:HG13	2:C:69:GLN:OE1	2.03	0.58
1:A:143:ASN:OD1	3:D:5:DA:OP2	2.20	0.58
1:A:144:ILE:N	2:B:316:PHE:HZ	2.00	0.58
1:A:284:GLN:H	1:A:322:ARG:NH2	2.00	0.58
2:B:269:PHE:CE2	2:B:311:PRO:HB3	2.37	0.58
2:B:334:LEU:HA	2:B:357:PHE:HB3	1.85	0.58
2:B:489:ALA:O	2:B:493:LEU:HD23	2.02	0.58
2:C:72:ARG:HG3	2:C:73:LYS:N	2.18	0.58
1:A:3:ALA:O	2:B:488:GLU:OE1	2.21	0.58
1:A:143:ASN:ND2	3:D:5:DA:OP1	2.36	0.58
1:A:351:VAL:HG12	1:A:352:LYS:O	2.04	0.58
2:C:6:LEU:HG	2:C:10:LEU:HD13	1.85	0.58
1:A:49:ILE:CG1	1:A:107:PHE:HE2	2.13	0.58
1:A:186:PHE:HD1	1:A:395:ILE:CG2	2.15	0.58
1:A:253:LEU:H	1:A:316:TYR:HA	1.68	0.58
2:B:246:LEU:HD13	2:B:246:LEU:C	2.28	0.58
2:C:246:LEU:C	2:C:246:LEU:HD13	2.28	0.58
1:A:312:GLN:HG2	1:A:313:ASN:N	2.19	0.58
2:B:275:THR:HG21	5:B:530:SAM:HN61	1.68	0.58
2:C:6:LEU:O	2:C:10:LEU:HD13	2.02	0.58
2:C:494:VAL:HA	2:C:497:LEU:HD13	1.85	0.58
1:A:36:LEU:HD22	1:A:36:LEU:N	2.18	0.58
1:A:139:SER:CB	2:B:466:SER:HB3	2.22	0.58
1:A:225:LYS:HB2	1:A:228:PHE:HE1	1.66	0.58
2:B:244:ILE:HD12	2:B:244:ILE:N	2.17	0.58
2:B:268:PRO:HD3	5:B:530:SAM:C5'	2.33	0.58
1:A:140:ALA:HB1	2:B:351:LYS:HZ1	1.69	0.58
1:A:209:LEU:HB3	1:A:217:GLU:O	2.03	0.58
1:A:345:ASN:HD22	2:C:469:LYS:HE2	1.67	0.58
2:B:6:LEU:HD23	2:B:130:MET:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ILE:O	2:B:160:ILE:HD13	2.03	0.58
2:B:218:VAL:HG12	2:B:220:GLY:N	2.19	0.58
2:C:118:GLY:HA2	2:C:123:SER:HB2	1.83	0.58
4:E:1:DG:H2'	4:E:2:DT:C7	2.34	0.58
5:B:530:SAM:HE1	3:D:6:DA:H62	1.67	0.58
2:C:55:ARG:HE	2:C:57:ASP:HB2	1.67	0.58
2:C:156:ILE:O	2:C:160:ILE:HD13	2.03	0.58
2:C:268:PRO:HD3	5:C:530:SAM:C5'	2.34	0.58
1:A:231:ILE:HG22	1:A:324:ARG:HB3	1.84	0.58
1:A:265:GLN:CG	1:A:269:ARG:HH21	2.03	0.58
1:A:412:SER:CA	2:B:495:GLN:HG3	2.33	0.58
1:A:11:VAL:HG12	1:A:12:ILE:N	2.19	0.58
1:A:26:THR:HG23	1:A:69:GLU:HG2	1.84	0.58
1:A:215:ASN:CG	2:C:492:GLU:HB2	2.28	0.58
1:A:306:LEU:N	1:A:306:LEU:HD12	2.19	0.58
1:A:349:ASN:HB2	2:C:430:ALA:HB1	1.85	0.58
2:C:17:LEU:HB2	2:C:27:TYR:CD1	2.39	0.58
1:A:46:ALA:HB3	4:E:14:DG:H5'	1.86	0.57
1:A:279:ASN:HB3	4:E:1:DG:OP1	2.04	0.57
1:A:294:ASN:ND2	3:D:14:DG:H5''	2.18	0.57
2:B:2:ASN:H	2:B:129:ASP:CG	2.11	0.57
2:B:114:ASP:C	2:B:116:TYR:H	2.12	0.57
2:C:275:THR:CG2	5:C:530:SAM:N6	2.67	0.57
1:A:372:LEU:HD13	1:A:372:LEU:C	2.29	0.57
2:B:153:ARG:HB3	2:B:154:PRO:HD3	1.86	0.57
2:C:222:ARG:CZ	2:C:226:LEU:HD11	2.34	0.57
1:A:182:THR:HG21	1:A:399:VAL:HG22	1.85	0.57
1:A:305:LEU:HD22	1:A:306:LEU:O	2.04	0.57
2:B:93:VAL:CG1	2:B:223:ARG:HD3	2.20	0.57
2:B:494:VAL:HA	2:B:497:LEU:HD13	1.85	0.57
1:A:241:SER:O	1:A:243:PRO:HD3	2.04	0.57
1:A:293:TYR:HE2	4:E:5:DC:H41	1.52	0.57
2:B:9:LYS:HZ1	2:B:113:LEU:HB2	1.67	0.57
2:B:222:ARG:CZ	2:B:226:LEU:HD11	2.34	0.57
2:B:401:PHE:O	2:B:404:VAL:HG22	2.05	0.57
2:C:230:LEU:C	2:C:230:LEU:HD13	2.29	0.57
1:A:85:GLY:CA	4:E:14:DG:H8	2.15	0.57
1:A:188:GLN:HE22	1:A:192:ILE:CG1	2.16	0.57
2:C:148:GLN:O	5:C:530:SAM:CE	2.52	0.57
2:C:163:LEU:HD13	2:C:163:LEU:C	2.29	0.57
1:A:53:LYS:CE	1:A:97:HIS:HE1	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:HE2	1:A:275:GLU:CA	2.17	0.57
1:A:355:SER:H	2:C:312:ASP:HB3	1.69	0.57
2:C:122:LYS:HZ1	2:C:124:ARG:HG2	1.69	0.57
1:A:274:SER:O	1:A:278:LEU:HB2	2.04	0.57
1:A:345:ASN:HA	2:C:469:LYS:HZ1	1.68	0.57
2:C:38:LYS:HB2	2:C:56:TRP:CH2	2.40	0.57
2:C:218:VAL:HG12	2:C:220:GLY:N	2.19	0.57
1:A:233:THR:HG23	1:A:316:TYR:OH	2.04	0.57
3:D:10:DC:O2	3:D:11:DG:H1'	2.04	0.57
1:A:74:SER:O	1:A:100:PHE:HA	2.05	0.57
1:A:86:SER:OG	1:A:90:VAL:HB	2.05	0.57
2:B:432:SER:O	2:B:436:LYS:HB2	2.05	0.57
2:C:28:VAL:HG23	2:C:29:ASN:N	2.19	0.57
2:C:290:LEU:HD13	2:C:324:ILE:HD12	1.87	0.57
1:A:251:PRO:HG3	1:A:269:ARG:CZ	2.35	0.56
2:C:153:ARG:HB3	2:C:154:PRO:HD3	1.86	0.56
2:B:17:LEU:HB2	2:B:27:TYR:CD1	2.39	0.56
1:A:222:VAL:HG12	1:A:223:PHE:N	2.18	0.56
1:A:305:LEU:HD23	1:A:306:LEU:H	1.68	0.56
1:A:346:ALA:HA	2:C:431:ASP:O	2.04	0.56
2:C:114:ASP:C	2:C:116:TYR:H	2.12	0.56
2:C:350:VAL:CG1	4:E:6:DA:C4'	2.83	0.56
1:A:26:THR:HG22	1:A:70:SER:HB3	1.86	0.56
1:A:45:ARG:CA	1:A:104:PHE:HE1	2.18	0.56
1:A:61:PHE:HE2	1:A:66:LEU:HB2	1.71	0.56
1:A:412:SER:HB2	2:B:495:GLN:NE2	2.18	0.56
2:C:34:LEU:HB3	2:C:110:MET:SD	2.44	0.56
2:C:94:SER:H	2:C:223:ARG:NH1	2.04	0.56
2:C:153:ARG:HB3	2:C:154:PRO:CD	2.36	0.56
4:E:1:DG:H2'	4:E:2:DT:H73	1.88	0.56
1:A:33:ILE:HG23	1:A:34:ASN:N	2.20	0.56
1:A:168:ILE:HD11	1:A:417:ALA:HB1	1.86	0.56
1:A:433:LEU:HD13	1:A:443:LEU:CD1	2.34	0.56
2:B:28:VAL:HG23	2:B:29:ASN:N	2.19	0.56
2:B:34:LEU:HB3	2:B:110:MET:SD	2.44	0.56
2:B:358:THR:HG22	2:B:359:LYS:N	2.21	0.56
2:C:279:ARG:HH21	2:C:281:PHE:HZ	1.54	0.56
1:A:39:ASP:CG	1:A:62:VAL:HA	2.29	0.56
1:A:44:ILE:HG23	1:A:101:GLU:CD	2.31	0.56
1:A:259:ARG:HD3	3:D:14:DG:OP1	2.05	0.56
1:A:274:SER:HA	1:A:278:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG12	1:A:303:CYS:N	2.20	0.56
2:B:248:ASN:O	2:B:253:ASP:HB2	2.06	0.56
1:A:252:ILE:HD11	1:A:316:TYR:C	2.29	0.56
1:A:319:LYS:NZ	3:D:15:DT:H4'	2.20	0.56
1:A:378:GLN:O	1:A:382:VAL:HG23	2.05	0.56
1:A:104:PHE:CE1	1:A:107:PHE:CE1	2.94	0.56
2:C:142:THR:HG23	2:C:143:LYS:N	2.21	0.56
1:A:239:LEU:HD23	1:A:240:SER:N	2.21	0.56
1:A:444:LEU:HD23	1:A:444:LEU:O	2.06	0.56
2:B:71:TYR:HE2	2:B:75:LEU:HD11	1.64	0.56
1:A:26:THR:HG23	1:A:69:GLU:CG	2.35	0.55
1:A:175:LEU:HD13	1:A:175:LEU:C	2.31	0.55
2:C:401:PHE:O	2:C:404:VAL:HG22	2.05	0.55
1:A:365:ILE:HG23	1:A:366:LYS:N	2.21	0.55
2:C:38:LYS:HD3	2:C:56:TRP:CE2	2.41	0.55
2:C:103:ILE:HG23	2:C:104:THR:N	2.21	0.55
2:C:440:GLN:CB	2:C:484:VAL:CG2	2.74	0.55
2:C:450:PHE:CZ	2:C:467:TRP:CZ3	2.94	0.55
2:B:62:ARG:HD2	2:B:70:PHE:CG	2.41	0.55
2:B:384:MET:HE3	2:B:385:PRO:HD2	1.88	0.55
1:A:17:THR:HG23	1:A:18:VAL:N	2.21	0.55
1:A:61:PHE:CE2	1:A:66:LEU:HA	2.41	0.55
1:A:217:GLU:HG3	1:A:218:PRO:HD2	1.89	0.55
2:B:38:LYS:HD3	2:B:56:TRP:CE2	2.41	0.55
2:B:63:ILE:N	2:B:67:GLN:HB2	2.21	0.55
1:A:236:ARG:HG2	1:A:237:ASN:H	1.72	0.55
1:A:255:ILE:HG23	1:A:256:SER:N	2.21	0.55
1:A:291:THR:HG23	1:A:291:THR:O	2.05	0.55
2:B:148:GLN:O	5:B:530:SAM:CE	2.53	0.55
2:B:153:ARG:HB3	2:B:154:PRO:CD	2.36	0.55
1:A:164:GLU:CG	1:A:423:THR:HA	2.36	0.55
2:B:275:THR:CG2	5:B:530:SAM:N6	2.68	0.55
2:B:316:PHE:HB3	2:B:462:SER:OG	2.06	0.55
2:B:338:LEU:HD13	2:B:401:PHE:CD1	2.42	0.55
2:C:94:SER:H	2:C:223:ARG:HH12	1.55	0.55
2:C:384:MET:HE3	2:C:385:PRO:HD2	1.89	0.55
2:B:38:LYS:HB2	2:B:56:TRP:CH2	2.40	0.55
2:B:43:THR:CG2	2:B:45:GLN:HB2	2.37	0.55
2:B:193:THR:O	2:B:194:ASN:HB2	2.06	0.55
2:C:81:ASP:HB2	2:C:83:LYS:NZ	2.22	0.55
1:A:20:THR:HG22	1:A:111:LEU:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:HB1	1:A:82:MET:HE1	1.88	0.55
1:A:144:ILE:HG12	2:B:316:PHE:CE1	2.41	0.55
1:A:162:LEU:HD13	1:A:162:LEU:C	2.32	0.55
2:B:215:LEU:HD13	2:B:245:ARG:NE	2.17	0.55
2:C:353:ASN:HD21	2:C:381:ARG:NH2	2.05	0.55
1:A:25:VAL:HG11	1:A:103:SER:O	2.07	0.55
1:A:78:ILE:HG13	1:A:110:VAL:O	2.06	0.55
1:A:103:SER:HG	1:A:107:PHE:CB	2.19	0.55
1:A:205:VAL:HG23	1:A:205:VAL:O	2.06	0.55
1:A:431:PRO:O	1:A:434:ILE:HG12	2.05	0.55
2:C:248:ASN:O	2:C:253:ASP:HB2	2.06	0.55
1:A:57:THR:HG23	1:A:57:THR:O	2.07	0.55
1:A:144:ILE:HG23	1:A:146:ASN:H	1.72	0.55
1:A:330:LEU:CD2	1:A:332:GLU:H	2.19	0.55
1:A:345:ASN:HD22	2:C:469:LYS:CE	2.20	0.55
1:A:354:THR:OG1	2:C:312:ASP:HB3	2.07	0.55
2:B:259:LYS:HB2	2:B:301:HIS:CE1	2.42	0.55
2:B:442:LEU:HG	2:B:448:ARG:HH12	1.69	0.55
2:C:390:ARG:HG3	2:C:391:THR:N	2.22	0.55
1:A:142:ALA:HB1	2:B:312:ASP:CB	2.36	0.54
1:A:254:ARG:HG2	1:A:255:ILE:H	1.72	0.54
2:B:94:SER:H	2:B:223:ARG:NH1	2.05	0.54
2:C:193:THR:O	2:C:194:ASN:HB2	2.06	0.54
2:C:222:ARG:HD3	2:C:246:LEU:CB	2.37	0.54
2:B:427:THR:HG22	2:B:428:GLU:N	2.21	0.54
2:C:113:LEU:HD23	2:C:113:LEU:C	2.32	0.54
2:C:265:THR:HG23	2:C:267:PRO:HD3	1.89	0.54
2:C:269:PHE:HB3	4:E:6:DA:C5'	2.37	0.54
4:E:17:DG:H2''	4:E:18:DA:N7	2.21	0.54
1:A:15:VAL:CG2	1:A:155:ILE:HG23	2.36	0.54
1:A:144:ILE:HB	2:B:316:PHE:CZ	2.42	0.54
2:B:103:ILE:HG23	2:B:104:THR:N	2.21	0.54
2:C:358:THR:HG22	2:C:359:LYS:N	2.21	0.54
2:C:436:LYS:HG2	2:C:437:ASN:ND2	2.22	0.54
1:A:7:PRO:HG2	1:A:418:PHE:O	2.07	0.54
1:A:289:LEU:CG	1:A:320:LEU:HD11	2.37	0.54
1:A:319:LYS:HE3	3:D:15:DT:O5'	2.07	0.54
1:A:357:GLN:HG2	1:A:358:LYS:H	1.73	0.54
1:A:104:PHE:CE2	1:A:106:ALA:HB3	2.43	0.54
1:A:251:PRO:HA	1:A:269:ARG:CG	2.30	0.54
2:B:17:LEU:HB2	2:B:27:TYR:CE1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:PHE:CZ	2:B:467:TRP:CZ3	2.95	0.54
2:C:6:LEU:HD23	2:C:130:MET:HB2	1.89	0.54
2:C:338:LEU:HD13	2:C:401:PHE:CD1	2.41	0.54
1:A:144:ILE:CG1	2:B:316:PHE:CZ	2.91	0.54
1:A:348:MET:CE	2:C:470:ASP:H	2.19	0.54
2:B:1:MET:HB3	2:B:129:ASP:OD1	2.08	0.54
2:B:71:TYR:CZ	2:B:75:LEU:HD21	2.43	0.54
2:B:390:ARG:HG3	2:B:391:THR:N	2.23	0.54
2:C:43:THR:CG2	2:C:45:GLN:HB2	2.37	0.54
2:C:63:ILE:N	2:C:67:GLN:HB2	2.23	0.54
2:C:269:PHE:CE2	2:C:311:PRO:HD3	2.43	0.54
1:A:168:ILE:HG23	1:A:413:ILE:HD13	1.88	0.54
1:A:290:PHE:CE2	1:A:360:ILE:HG21	2.43	0.54
1:A:355:SER:HB2	2:C:312:ASP:HB2	1.88	0.54
2:C:60:LYS:HE3	2:C:111:ASP:OD2	2.07	0.54
2:C:62:ARG:HD2	2:C:70:PHE:CB	2.37	0.54
2:C:71:TYR:CZ	2:C:75:LEU:HD21	2.43	0.54
2:C:350:VAL:HG11	4:E:6:DA:C4'	2.38	0.54
1:A:270:PHE:HE2	1:A:275:GLU:N	2.06	0.54
1:A:349:ASN:HB2	2:C:430:ALA:C	2.33	0.54
2:B:6:LEU:HB3	2:B:130:MET:CG	2.37	0.54
2:B:113:LEU:HD23	2:B:113:LEU:C	2.32	0.54
2:B:142:THR:HG23	2:B:143:LYS:N	2.21	0.54
2:C:275:THR:HG21	5:C:530:SAM:C6	2.38	0.54
1:A:92:LYS:HG3	1:A:93:SER:N	2.23	0.54
1:A:345:ASN:HD21	2:C:430:ALA:HA	1.73	0.54
2:B:60:LYS:HE3	2:B:111:ASP:OD2	2.07	0.54
2:B:94:SER:H	2:B:223:ARG:HH12	1.56	0.54
1:A:428:ALA:HB2	1:A:443:LEU:CD2	2.35	0.54
2:B:434:GLU:OE1	2:B:465:ILE:HG23	2.08	0.54
2:C:427:THR:HG22	2:C:428:GLU:N	2.21	0.54
1:A:138:LEU:HD22	1:A:138:LEU:N	2.23	0.53
1:A:212:LYS:HD3	1:A:217:GLU:OE1	2.08	0.53
1:A:246:SER:O	1:A:248:VAL:HG23	2.08	0.53
1:A:255:ILE:HD13	3:D:14:DG:C5'	2.35	0.53
2:C:313:ASN:ND2	4:E:5:DC:H5''	2.22	0.53
1:A:232:LEU:HD23	1:A:232:LEU:C	2.32	0.53
1:A:272:GLU:HG3	1:A:275:GLU:OE2	2.08	0.53
1:A:293:TYR:HE2	4:E:5:DC:N4	2.05	0.53
1:A:299:PHE:HE2	1:A:347:MET:HG2	1.69	0.53
2:B:222:ARG:HD3	2:B:246:LEU:CB	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:ARG:HH21	2:B:281:PHE:HZ	1.54	0.53
2:C:17:LEU:HB2	2:C:27:TYR:CE1	2.42	0.53
2:C:322:THR:CA	2:C:325:ARG:HH21	2.21	0.53
1:A:77:ASP:HA	1:A:95:HIS:HE2	1.72	0.53
1:A:252:ILE:CG1	1:A:317:PRO:HD3	2.29	0.53
1:A:254:ARG:HG2	1:A:255:ILE:N	2.22	0.53
1:A:332:GLU:CB	1:A:382:VAL:HG11	2.39	0.53
2:B:336:THR:HG22	2:B:337:ILE:N	2.23	0.53
2:C:2:ASN:ND2	2:C:3:ASN:H	2.07	0.53
2:C:62:ARG:HD2	2:C:70:PHE:CG	2.43	0.53
2:C:70:PHE:HE2	2:C:74:MET:HE3	1.68	0.53
2:C:92:ASN:HB3	2:C:219:PRO:CB	2.38	0.53
2:C:259:LYS:HB2	2:C:301:HIS:CE1	2.43	0.53
2:C:336:THR:HG22	2:C:337:ILE:N	2.23	0.53
1:A:35:TYR:O	1:A:62:VAL:HB	2.09	0.53
1:A:196:PHE:CD2	1:A:200:VAL:HG21	2.43	0.53
1:A:395:ILE:HG23	1:A:396:GLU:N	2.23	0.53
1:A:402:ALA:HA	1:A:405:ARG:HD3	1.90	0.53
2:B:70:PHE:CZ	2:B:74:MET:HE3	2.44	0.53
4:E:1:DG:N9	4:E:2:DT:H72	2.23	0.53
1:A:144:ILE:HG22	1:A:146:ASN:H	1.71	0.53
1:A:293:TYR:CD1	1:A:319:LYS:CD	2.91	0.53
2:B:81:ASP:HB2	2:B:83:LYS:NZ	2.22	0.53
2:C:350:VAL:HG11	4:E:6:DA:C1'	2.38	0.53
1:A:35:TYR:OH	1:A:68:LYS:HD3	2.09	0.53
1:A:134:LYS:HA	2:B:431:ASP:O	2.08	0.53
1:A:143:ASN:ND2	3:D:5:DA:OP2	2.41	0.53
1:A:223:PHE:HE1	1:A:369:VAL:CG1	2.20	0.53
1:A:332:GLU:HB3	1:A:382:VAL:HG11	1.91	0.53
2:B:92:ASN:HB3	2:B:219:PRO:CB	2.38	0.53
2:B:440:GLN:HG3	2:B:484:VAL:HB	1.89	0.53
2:B:488:GLU:CD	2:B:488:GLU:H	2.17	0.53
2:C:222:ARG:NE	2:C:246:LEU:HB2	2.23	0.53
2:C:344:ILE:HD11	2:C:345:PHE:CE1	2.44	0.53
2:C:481:GLU:CB	2:C:482:PRO:HD3	2.37	0.53
1:A:243:PRO:O	1:A:246:SER:HB3	2.09	0.53
1:A:370:VAL:HG22	1:A:371:LEU:N	2.24	0.53
1:A:433:LEU:CB	1:A:443:LEU:HD22	2.38	0.53
2:B:1:MET:HE3	2:B:129:ASP:OD1	2.09	0.53
2:B:438:THR:O	2:B:485:LEU:HA	2.08	0.53
2:C:6:LEU:HB3	2:C:130:MET:CG	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:CD	1:A:235:LEU:H	2.17	0.53
2:C:70:PHE:CZ	2:C:74:MET:HE3	2.43	0.53
1:A:35:TYR:CE1	1:A:68:LYS:HD2	2.43	0.53
1:A:196:PHE:HZ	1:A:384:ARG:HD2	1.68	0.53
1:A:316:TYR:HD2	1:A:320:LEU:HB3	1.74	0.53
2:B:222:ARG:NE	2:B:246:LEU:HB2	2.23	0.53
2:B:440:GLN:CB	2:B:484:VAL:CG2	2.75	0.53
1:A:193:LEU:HD12	1:A:388:LEU:HD22	1.90	0.53
2:B:6:LEU:HB3	2:B:130:MET:HG2	1.91	0.53
2:B:431:ASP:OD2	2:B:488:GLU:CB	2.56	0.53
1:A:327:LYS:HG3	1:A:328:ASP:N	2.25	0.52
1:A:410:THR:O	1:A:414:LEU:HG	2.09	0.52
2:B:232:HIS:O	2:B:233:ASP:HB2	2.09	0.52
2:B:305:ARG:NH1	2:B:409:PRO:HG2	2.24	0.52
1:A:159:ILE:HG23	1:A:159:ILE:O	2.08	0.52
1:A:354:THR:HG23	1:A:356:GLY:N	2.24	0.52
1:A:136:SER:HB2	2:B:469:LYS:HE3	1.90	0.52
2:B:85:LEU:HD21	2:B:238:LEU:HD21	1.92	0.52
2:C:438:THR:O	2:C:485:LEU:HA	2.09	0.52
1:A:309:LEU:HD23	1:A:310:GLN:H	1.72	0.52
2:B:4:ASN:O	2:B:7:VAL:HG12	2.10	0.52
2:B:275:THR:HG21	5:B:530:SAM:C6	2.39	0.52
2:C:3:ASN:HA	2:C:130:MET:SD	2.49	0.52
2:C:62:ARG:CD	2:C:70:PHE:HB2	2.39	0.52
1:A:147:ILE:HG23	1:A:147:ILE:O	2.08	0.52
2:B:213:ILE:HG22	2:B:214:GLY:N	2.24	0.52
2:C:304:GLY:H	2:C:359:LYS:HB3	1.75	0.52
1:A:80:ILE:O	1:A:93:SER:HA	2.09	0.52
1:A:98:LEU:CB	1:A:99:PRO:HD2	2.32	0.52
2:C:285:THR:HG22	2:C:286:SER:N	2.23	0.52
1:A:10:TRP:NE1	1:A:418:PHE:CD1	2.77	0.52
1:A:10:TRP:N	1:A:10:TRP:CE3	2.77	0.52
1:A:84:SER:CA	1:A:146:ASN:HD22	2.22	0.52
1:A:158:PRO:HG2	1:A:418:PHE:CE2	2.45	0.52
2:B:344:ILE:HD11	2:B:345:PHE:CE1	2.44	0.52
2:C:293:MET:HE1	2:C:310:VAL:HG11	1.92	0.52
1:A:80:ILE:CG2	1:A:94:ALA:HB3	2.40	0.52
1:A:308:LYS:HB2	1:A:312:GLN:O	2.10	0.52
1:A:394:THR:HG23	1:A:395:ILE:N	2.24	0.52
2:B:285:THR:HG22	2:B:286:SER:N	2.23	0.52
2:C:268:PRO:HD3	5:C:530:SAM:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:488:GLU:CD	2:C:488:GLU:H	2.17	0.52
1:A:55:ASP:O	1:A:98:LEU:HD12	2.10	0.52
1:A:235:LEU:HD11	1:A:315:LEU:CD2	2.40	0.52
1:A:352:LYS:HD3	2:C:382:THR:HG21	1.91	0.52
2:B:6:LEU:HD22	2:B:117:ASN:HB2	1.92	0.52
4:E:15:DT:H3'	4:E:16:DT:C6	2.45	0.52
1:A:101:GLU:HG2	1:A:102:CYS:N	2.25	0.52
1:A:118:PHE:CZ	1:A:162:LEU:HD11	2.42	0.52
1:A:341:PRO:HA	1:A:344:ARG:CG	2.39	0.52
2:B:122:LYS:HZ2	2:B:124:ARG:HG2	1.75	0.52
2:B:376:TRP:CZ3	2:B:447:TRP:NE1	2.78	0.52
4:E:15:DT:H5'	4:E:16:DT:C7	2.40	0.52
1:A:179:VAL:HG23	1:A:180:ASP:N	2.24	0.51
1:A:412:SER:N	2:B:495:GLN:HG3	2.24	0.51
2:B:429:VAL:HG11	2:B:443:ALA:HB1	1.91	0.51
2:C:313:ASN:HB3	4:E:5:DC:OP1	2.11	0.51
2:B:229:CYS:SG	2:B:244:ILE:HD11	2.50	0.51
2:C:229:CYS:SG	2:C:244:ILE:HD11	2.50	0.51
2:C:305:ARG:NH1	2:C:409:PRO:HG2	2.24	0.51
2:C:339:ARG:NH2	2:C:465:ILE:H	2.08	0.51
1:A:78:ILE:CG1	1:A:111:LEU:HD23	2.39	0.51
2:B:62:ARG:HD2	2:B:70:PHE:CB	2.40	0.51
2:B:122:LYS:HZ1	2:B:124:ARG:HG2	1.74	0.51
2:C:213:ILE:HG22	2:C:214:GLY:N	2.24	0.51
1:A:143:ASN:HB3	2:B:316:PHE:CE1	2.45	0.51
1:A:252:ILE:HG21	1:A:268:ILE:HG23	1.89	0.51
2:C:172:GLN:HG2	2:C:173:ASP:N	2.26	0.51
1:A:28:LYS:CB	1:A:65:ASN:HD21	2.22	0.51
1:A:80:ILE:HD11	1:A:107:PHE:HB3	1.92	0.51
1:A:313:ASN:C	1:A:313:ASN:HD22	2.19	0.51
2:B:98:THR:HG23	2:C:94:SER:OG	2.11	0.51
2:C:232:HIS:O	2:C:233:ASP:HB2	2.09	0.51
2:C:313:ASN:HA	2:C:316:PHE:CE1	2.46	0.51
1:A:293:TYR:HB2	3:D:15:DT:OP2	2.10	0.51
2:B:304:GLY:H	2:B:359:LYS:HB3	1.76	0.51
2:B:455:ILE:O	2:B:459:LYS:HB2	2.10	0.51
2:B:486:ALA:HB3	2:B:489:ALA:HB3	1.91	0.51
2:C:138:ASN:OD1	2:C:146:ALA:HB2	2.10	0.51
5:C:530:SAM:HE1	4:E:6:DA:H62	1.69	0.51
1:A:61:PHE:CE2	1:A:66:LEU:CA	2.94	0.51
1:A:170:GLU:O	1:A:174:THR:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:CD2	1:A:320:LEU:HD11	2.40	0.51
1:A:312:GLN:HG2	1:A:313:ASN:H	1.76	0.51
1:A:322:ARG:HG2	1:A:323:ALA:N	2.26	0.51
2:B:456:ARG:O	2:B:460:SER:HA	2.10	0.51
2:C:85:LEU:HD21	2:C:238:LEU:HD21	1.91	0.51
1:A:18:VAL:O	1:A:116:LEU:HD23	2.11	0.51
1:A:96:GLN:HG3	1:A:96:GLN:O	2.09	0.51
1:A:118:PHE:CE2	1:A:166:LYS:HG3	2.45	0.51
1:A:285:ASP:HB3	1:A:308:LYS:CB	2.40	0.51
1:A:444:LEU:HD23	1:A:444:LEU:C	2.36	0.51
1:A:10:TRP:NE1	1:A:160:PRO:HB3	2.26	0.51
1:A:41:LEU:HD21	1:A:101:GLU:HA	1.93	0.51
1:A:167:ILE:HG23	1:A:168:ILE:N	2.24	0.51
1:A:270:PHE:HE2	1:A:275:GLU:CB	2.23	0.51
2:B:138:ASN:OD1	2:B:146:ALA:HB2	2.10	0.51
2:B:268:PRO:HD3	5:B:530:SAM:O4'	2.10	0.51
2:C:217:LEU:O	2:C:219:PRO:HD3	2.11	0.51
2:C:287:ASN:ND2	2:C:290:LEU:H	2.08	0.51
2:C:431:ASP:OD2	2:C:488:GLU:CB	2.57	0.51
1:A:118:PHE:HZ	1:A:162:LEU:CD1	2.24	0.51
1:A:131:TYR:CE2	1:A:135:ILE:CD1	2.94	0.51
1:A:135:ILE:O	1:A:138:LEU:HD23	2.11	0.51
1:A:137:SER:CB	2:B:432:SER:CB	2.88	0.51
1:A:215:ASN:OD1	2:C:489:ALA:CA	2.52	0.51
1:A:248:VAL:HG13	1:A:270:PHE:CA	2.40	0.51
2:B:172:GLN:HG2	2:B:173:ASP:N	2.26	0.51
2:C:283:HIS:H	2:C:294:GLN:NE2	2.02	0.51
1:A:122:ILE:HG23	1:A:123:ALA:N	2.25	0.50
2:B:243:ALA:HB3	2:B:244:ILE:HD12	1.93	0.50
2:B:515:LEU:HD22	2:B:515:LEU:N	2.26	0.50
2:C:6:LEU:HB3	2:C:130:MET:HG2	1.93	0.50
2:C:315:LEU:HD22	2:C:463:LEU:CB	2.41	0.50
2:C:376:TRP:CZ3	2:C:447:TRP:NE1	2.78	0.50
2:B:24:TYR:CD2	2:B:27:TYR:CE2	2.95	0.50
2:B:265:THR:HG23	2:B:267:PRO:HD3	1.92	0.50
2:C:1:MET:CE	2:C:132:GLU:HG3	2.41	0.50
2:C:322:THR:HG23	2:C:323:ASP:N	2.26	0.50
1:A:7:PRO:HG2	1:A:418:PHE:CB	2.41	0.50
1:A:61:PHE:HZ	1:A:66:LEU:HA	1.76	0.50
1:A:336:ILE:HG23	1:A:337:PHE:N	2.26	0.50
2:B:287:ASN:ND2	2:B:290:LEU:H	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:ARG:HD3	2:C:410:HIS:ND1	2.26	0.50
1:A:104:PHE:CE2	1:A:106:ALA:CB	2.95	0.50
2:B:3:ASN:HA	2:B:130:MET:SD	2.52	0.50
2:B:73:LYS:HA	2:C:72:ARG:HH12	1.76	0.50
2:C:63:ILE:HG13	2:C:104:THR:HG21	1.94	0.50
2:C:243:ALA:HB3	2:C:244:ILE:HD12	1.94	0.50
2:C:268:PRO:HD3	5:C:530:SAM:H5'2	1.93	0.50
2:C:515:LEU:HD22	2:C:515:LEU:N	2.26	0.50
1:A:164:GLU:HA	1:A:167:ILE:HG22	1.93	0.50
2:B:28:VAL:HB	2:B:131:TYR:OH	2.12	0.50
2:B:436:LYS:HG2	2:B:437:ASN:ND2	2.27	0.50
2:C:88:ALA:HB2	2:C:241:GLY:CA	2.42	0.50
1:A:49:ILE:CD1	1:A:107:PHE:CE2	2.94	0.50
1:A:118:PHE:CZ	1:A:162:LEU:CD1	2.95	0.50
1:A:118:PHE:CE2	1:A:162:LEU:CD2	2.95	0.50
2:B:3:ASN:HB2	2:B:130:MET:SD	2.52	0.50
2:B:287:ASN:HD22	2:B:289:GLN:N	2.10	0.50
2:C:90:PHE:HA	2:C:93:VAL:CG1	2.41	0.50
1:A:22:ILE:HG23	1:A:108:CYS:SG	2.51	0.50
2:B:217:LEU:O	2:B:219:PRO:HD3	2.11	0.50
2:B:220:GLY:HA2	2:B:223:ARG:CZ	2.41	0.50
2:B:486:ALA:HB3	2:B:489:ALA:HB2	1.93	0.50
2:C:26:ASN:O	2:C:30:GLU:HG2	2.12	0.50
2:C:29:ASN:HB2	2:C:224:LEU:HD11	1.94	0.50
2:C:322:THR:O	2:C:326:ARG:HG3	2.11	0.50
2:C:340:LEU:HD12	2:C:352:THR:OG1	2.12	0.50
1:A:15:VAL:O	1:A:18:VAL:HG22	2.12	0.50
1:A:48:ASN:HB3	1:A:54:PHE:CE1	2.47	0.50
1:A:131:TYR:CE1	1:A:155:ILE:CD1	2.94	0.50
2:C:28:VAL:HB	2:C:131:TYR:OH	2.12	0.50
2:C:177:GLY:O	2:C:225:ALA:HB2	2.12	0.50
3:D:17:DC:H2''	3:D:18:DA:C8	2.46	0.50
1:A:253:LEU:C	1:A:317:PRO:HD2	2.37	0.50
1:A:316:TYR:HE2	1:A:320:LEU:O	1.95	0.50
1:A:348:MET:HE2	2:C:469:LYS:HA	1.94	0.50
2:B:88:ALA:HB2	2:B:241:GLY:CA	2.42	0.50
2:C:6:LEU:HD22	2:C:117:ASN:HB2	1.94	0.50
2:C:55:ARG:HG2	2:C:58:ASP:OD2	2.11	0.50
2:C:474:ILE:HG23	2:C:474:ILE:O	2.10	0.50
1:A:44:ILE:HG22	1:A:54:PHE:CE1	2.46	0.49
1:A:290:PHE:HE2	1:A:360:ILE:HG21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:HB3	2:C:431:ASP:C	2.37	0.49
2:B:106:LEU:HD22	2:B:110:MET:HE3	1.91	0.49
2:B:178:THR:O	2:B:179:ALA:HB3	2.12	0.49
2:B:474:ILE:O	2:B:474:ILE:HG23	2.10	0.49
2:C:280:THR:HG22	2:C:281:PHE:N	2.26	0.49
1:A:44:ILE:HG13	1:A:103:SER:OG	2.12	0.49
1:A:44:ILE:CG2	1:A:54:PHE:CZ	2.95	0.49
2:B:55:ARG:HG2	2:B:58:ASP:OD2	2.12	0.49
1:A:7:PRO:HG2	1:A:418:PHE:HB3	1.93	0.49
1:A:103:SER:HG	1:A:107:PHE:HB2	1.77	0.49
1:A:171:LYS:HE2	1:A:409:LEU:HD11	1.95	0.49
1:A:308:LYS:HE3	1:A:312:GLN:O	2.12	0.49
1:A:334:ILE:HG23	1:A:335:GLU:N	2.26	0.49
1:A:410:THR:HG23	1:A:411:GLN:N	2.27	0.49
1:A:433:LEU:HB2	1:A:443:LEU:HD22	1.94	0.49
2:B:29:ASN:HB2	2:B:224:LEU:HD11	1.94	0.49
2:C:287:ASN:HD22	2:C:289:GLN:N	2.09	0.49
2:C:350:VAL:HG11	4:E:6:DA:H1'	1.92	0.49
1:A:294:ASN:CG	3:D:14:DG:H5''	2.38	0.49
1:A:320:LEU:HD23	1:A:321:ILE:O	2.12	0.49
1:A:330:LEU:HD23	1:A:331:PRO:CD	2.41	0.49
2:B:5:ASP:HB2	2:B:116:TYR:HE2	1.76	0.49
2:B:162:LEU:HD22	2:B:405:TYR:CD2	2.47	0.49
2:B:220:GLY:CA	2:B:223:ARG:HH21	2.25	0.49
2:B:280:THR:HG22	2:B:281:PHE:N	2.26	0.49
2:B:305:ARG:HD3	2:B:410:HIS:ND1	2.26	0.49
2:C:220:GLY:CA	2:C:223:ARG:HH21	2.26	0.49
2:C:376:TRP:CZ2	2:C:415:ARG:HB2	2.47	0.49
1:A:215:ASN:ND2	2:C:492:GLU:CB	2.52	0.49
1:A:354:THR:O	1:A:357:GLN:HB2	2.12	0.49
1:A:371:LEU:HG	1:A:373:PRO:HD3	1.93	0.49
2:B:417:GLU:HA	2:B:447:TRP:HD1	1.77	0.49
2:C:417:GLU:HA	2:C:447:TRP:HD1	1.77	0.49
1:A:126:THR:HG23	1:A:127:LYS:N	2.27	0.49
1:A:161:PRO:O	1:A:165:GLN:HG3	2.12	0.49
2:B:70:PHE:HE2	2:B:74:MET:HE3	1.72	0.49
2:C:28:VAL:O	2:C:131:TYR:HE1	1.96	0.49
1:A:112:ARG:H	1:A:112:ARG:NE	2.11	0.49
1:A:443:LEU:O	1:A:447:ILE:HG12	2.13	0.49
2:C:63:ILE:HG13	2:C:104:THR:CG2	2.43	0.49
2:C:285:THR:HG22	2:C:287:ASN:N	2.07	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:LEU:HD22	2:C:463:LEU:HB3	1.94	0.49
1:A:144:ILE:CB	2:B:316:PHE:HZ	2.25	0.49
1:A:371:LEU:HD23	1:A:371:LEU:N	2.24	0.49
2:B:26:ASN:O	2:B:30:GLU:HG2	2.12	0.49
2:B:268:PRO:CG	5:B:530:SAM:C8	2.83	0.49
1:A:49:ILE:HD12	1:A:82:MET:CG	2.38	0.49
1:A:415:ALA:O	1:A:418:PHE:HB2	2.12	0.49
1:A:71:GLN:HG2	1:A:102:CYS:CB	2.28	0.49
1:A:212:LYS:HG2	1:A:214:ARG:H	1.77	0.49
1:A:225:LYS:HB2	1:A:228:PHE:HD1	1.75	0.49
2:B:155:LEU:O	2:B:159:ILE:HG13	2.13	0.49
2:B:177:GLY:O	2:B:225:ALA:HB2	2.12	0.49
2:B:344:ILE:HG13	2:B:345:PHE:N	2.28	0.49
2:B:376:TRP:CZ2	2:B:415:ARG:HB2	2.48	0.49
2:B:529:GLU:OXT	2:B:529:GLU:HG2	2.12	0.49
2:C:6:LEU:HD23	2:C:130:MET:CG	2.42	0.49
2:C:333:HIS:HD2	2:C:371:CYS:O	1.96	0.49
3:D:15:DT:H5"	3:D:16:DG:P	2.53	0.49
1:A:43:LEU:HB2	1:A:61:PHE:HB2	1.95	0.48
2:B:268:PRO:HD3	5:B:530:SAM:H5'2	1.94	0.48
2:C:178:THR:O	2:C:179:ALA:HB3	2.12	0.48
3:D:1:DG:C5	3:D:2:DT:C7	2.95	0.48
1:A:32:ALA:CB	1:A:35:TYR:CE2	2.94	0.48
1:A:197:ARG:CZ	1:A:341:PRO:HD3	2.43	0.48
1:A:234:GLU:C	4:E:2:DT:OP2	2.56	0.48
1:A:252:ILE:HD11	1:A:316:TYR:O	2.12	0.48
2:B:283:HIS:H	2:B:294:GLN:NE2	2.02	0.48
2:B:448:ARG:HD3	2:B:467:TRP:CZ2	2.44	0.48
2:C:162:LEU:HD22	2:C:405:TYR:CD2	2.48	0.48
1:A:22:ILE:HG12	1:A:110:VAL:HG23	1.95	0.48
1:A:89:VAL:HG21	1:A:135:ILE:HG22	1.95	0.48
1:A:235:LEU:HD23	1:A:236:ARG:O	2.14	0.48
1:A:248:VAL:CG1	1:A:269:ARG:HB3	2.38	0.48
2:B:63:ILE:HG13	2:B:104:THR:CG2	2.43	0.48
2:B:219:PRO:O	2:B:223:ARG:HG3	2.14	0.48
2:C:6:LEU:HD23	2:C:130:MET:HG2	1.96	0.48
2:C:167:PRO:O	2:C:168:ARG:HB2	2.14	0.48
2:C:344:ILE:HG13	2:C:345:PHE:N	2.28	0.48
2:B:167:PRO:O	2:B:168:ARG:HB2	2.13	0.48
2:B:338:LEU:HD12	2:B:378:TYR:HB3	1.95	0.48
2:B:379:ASP:O	2:B:446:ARG:HD3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:GLY:O	2:C:131:TYR:HB3	2.14	0.48
2:C:529:GLU:OXT	2:C:529:GLU:HG2	2.12	0.48
1:A:110:VAL:O	1:A:110:VAL:HG13	2.13	0.48
1:A:235:LEU:HD11	1:A:315:LEU:HD21	1.94	0.48
1:A:248:VAL:CG1	1:A:249:GLY:H	2.25	0.48
1:A:274:SER:CA	1:A:278:LEU:HD23	2.43	0.48
1:A:387:GLN:OE1	1:A:387:GLN:HA	2.13	0.48
2:B:2:ASN:ND2	2:B:3:ASN:H	2.10	0.48
2:B:262:ILE:HG22	2:B:263:VAL:N	2.28	0.48
2:B:269:PHE:CB	3:D:6:DA:O4'	2.61	0.48
2:C:268:PRO:CG	5:C:530:SAM:C8	2.81	0.48
2:B:433:GLU:CA	2:B:436:LYS:HB2	2.42	0.48
2:C:4:ASN:O	2:C:7:VAL:HG12	2.12	0.48
2:C:29:ASN:HD22	2:C:224:LEU:HD11	1.78	0.48
2:C:106:LEU:HD22	2:C:110:MET:HE3	1.91	0.48
1:A:235:LEU:HD22	1:A:316:TYR:O	2.14	0.48
2:B:63:ILE:HG13	2:B:104:THR:HG21	1.94	0.48
2:C:122:LYS:CE	2:C:124:ARG:HG2	2.44	0.48
4:E:15:DT:H5'	4:E:16:DT:H73	1.95	0.48
1:A:142:ALA:HA	2:B:312:ASP:CB	2.35	0.48
1:A:281:HIS:HE1	4:E:1:DG:H3'	1.77	0.48
2:B:217:LEU:HD21	2:B:274:GLY:O	2.14	0.48
2:C:163:LEU:HG	2:C:262:ILE:CG2	2.43	0.48
2:C:217:LEU:HD22	2:C:275:THR:HG23	1.93	0.48
1:A:234:GLU:HB3	4:E:2:DT:O5'	2.14	0.48
1:A:314:LEU:HD23	1:A:315:LEU:C	2.38	0.48
1:A:333:TYR:HB2	1:A:382:VAL:CG2	2.44	0.48
2:B:9:LYS:HZ2	2:B:113:LEU:HB2	1.77	0.48
2:B:153:ARG:N	2:B:154:PRO:HD2	2.29	0.48
2:C:220:GLY:HA2	2:C:223:ARG:CZ	2.41	0.48
2:C:346:TYR:CD1	2:C:347:ALA:N	2.82	0.48
1:A:39:ASP:OD1	1:A:63:PRO:HD3	2.13	0.48
1:A:41:LEU:HD22	1:A:42:PRO:O	2.13	0.48
1:A:270:PHE:HD2	1:A:274:SER:CB	2.22	0.48
1:A:278:LEU:HD22	1:A:278:LEU:N	2.29	0.48
1:A:413:ILE:CG1	1:A:417:ALA:HB2	2.42	0.48
2:B:90:PHE:HA	2:B:93:VAL:CG1	2.41	0.48
2:B:346:TYR:CD1	2:B:347:ALA:N	2.82	0.48
2:C:6:LEU:HG	2:C:10:LEU:HD11	1.96	0.48
2:C:219:PRO:O	2:C:223:ARG:HG3	2.13	0.48
2:C:486:ALA:HB3	2:C:489:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:OE2	1:A:464:SER:HB3	2.14	0.47
1:A:253:LEU:HD11	1:A:263:VAL:CG2	2.38	0.47
1:A:280:ARG:HB3	1:A:315:LEU:HD21	1.96	0.47
1:A:316:TYR:HB2	1:A:317:PRO:HD2	1.95	0.47
1:A:330:LEU:HD23	1:A:330:LEU:C	2.39	0.47
2:B:63:ILE:CA	2:B:67:GLN:HB2	2.44	0.47
2:C:207:GLN:HA	2:C:211:ALA:CB	2.39	0.47
2:C:338:LEU:HD12	2:C:378:TYR:HB3	1.95	0.47
1:A:62:VAL:CG1	1:A:63:PRO:N	2.77	0.47
1:A:148:LYS:HG2	1:A:149:PRO:HD2	1.92	0.47
1:A:270:PHE:CZ	1:A:315:LEU:CD1	2.95	0.47
1:A:358:LYS:HG3	3:D:14:DG:O6	2.14	0.47
2:B:28:VAL:O	2:B:131:TYR:HE1	1.97	0.47
2:B:160:ILE:N	2:B:160:ILE:HD12	2.29	0.47
2:B:195:ASP:O	2:B:196:LEU:HB2	2.14	0.47
2:C:153:ARG:N	2:C:154:PRO:HD2	2.29	0.47
2:C:339:ARG:HH21	2:C:465:ILE:H	1.62	0.47
1:A:250:HIS:CD2	1:A:270:PHE:CE1	2.99	0.47
1:A:270:PHE:HB3	1:A:280:ARG:NH1	2.29	0.47
1:A:409:LEU:HD23	1:A:409:LEU:O	2.13	0.47
2:B:39:MET:SD	2:B:115:TRP:CH2	3.07	0.47
2:B:94:SER:OG	2:C:98:THR:HG23	2.13	0.47
2:B:230:LEU:HD13	2:B:230:LEU:O	2.14	0.47
2:B:333:HIS:HD2	2:B:371:CYS:O	1.96	0.47
1:A:154:LEU:HD23	1:A:154:LEU:C	2.39	0.47
1:A:236:ARG:HB2	4:E:2:DT:C7	2.45	0.47
1:A:330:LEU:HD21	1:A:332:GLU:HB2	1.96	0.47
1:A:388:LEU:HD23	1:A:388:LEU:C	2.39	0.47
2:B:435:ASN:ND2	2:B:467:TRP:HB2	2.25	0.47
1:A:39:ASP:OD2	1:A:60:VAL:HG12	2.14	0.47
2:B:93:VAL:O	2:B:93:VAL:HG23	2.15	0.47
2:B:376:TRP:CD1	2:B:415:ARG:HH11	2.33	0.47
2:C:6:LEU:CG	2:C:130:MET:HG2	2.45	0.47
2:C:24:TYR:CD2	2:C:27:TYR:CE2	2.95	0.47
2:C:376:TRP:CD1	2:C:415:ARG:HH11	2.32	0.47
3:D:18:DA:C6	3:D:19:DA:C6	3.03	0.47
1:A:62:VAL:HG12	1:A:63:PRO:N	2.29	0.47
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.94	0.47
1:A:225:LYS:HB2	1:A:227:ASN:HD21	1.80	0.47
1:A:308:LYS:HG3	1:A:309:LEU:O	2.13	0.47
2:B:118:GLY:HA2	2:B:123:SER:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ARG:HH11	2:B:410:HIS:CD2	2.32	0.47
2:C:230:LEU:HD13	2:C:230:LEU:O	2.14	0.47
2:C:269:PHE:HB2	4:E:6:DA:O4'	2.13	0.47
2:C:440:GLN:HG3	2:C:484:VAL:HB	1.88	0.47
1:A:10:TRP:HE1	1:A:160:PRO:HB3	1.79	0.47
1:A:10:TRP:CD2	1:A:418:PHE:O	2.67	0.47
1:A:103:SER:OG	1:A:107:PHE:HB2	2.13	0.47
1:A:145:ASN:ND2	1:A:145:ASN:H	2.13	0.47
1:A:232:LEU:HD13	1:A:366:LYS:HE3	1.97	0.47
1:A:265:GLN:HG2	1:A:266:ASN:H	1.79	0.47
1:A:353:THR:HG23	1:A:353:THR:O	2.14	0.47
2:B:6:LEU:CG	2:B:130:MET:HG2	2.45	0.47
2:B:43:THR:HG22	2:B:45:GLN:HB2	1.97	0.47
2:B:128:GLY:CA	2:B:231:LEU:HD22	2.33	0.47
2:B:245:ARG:HH22	2:B:253:ASP:C	2.23	0.47
2:B:269:PHE:CD1	2:B:269:PHE:N	2.83	0.47
2:B:484:VAL:HA	2:B:490:MET:HE2	1.97	0.47
2:C:39:MET:SD	2:C:115:TRP:CH2	3.07	0.47
2:C:195:ASP:O	2:C:196:LEU:HB2	2.15	0.47
2:C:209:HIS:O	2:C:236:GLY:HA2	2.14	0.47
2:C:245:ARG:HG2	2:C:246:LEU:N	2.30	0.47
2:C:379:ASP:O	2:C:446:ARG:HD3	2.15	0.47
2:C:438:THR:HG23	2:C:442:LEU:HD23	1.97	0.47
2:C:484:VAL:HA	2:C:490:MET:HE2	1.97	0.47
3:D:15:DT:H5''	3:D:16:DG:OP2	2.14	0.47
1:A:186:PHE:CD1	1:A:395:ILE:CG2	2.95	0.47
1:A:223:PHE:O	1:A:224:LYS:HG3	2.15	0.47
1:A:250:HIS:HD2	1:A:251:PRO:O	1.98	0.47
1:A:215:ASN:HD21	2:C:492:GLU:HG3	1.79	0.47
1:A:235:LEU:HD13	1:A:316:TYR:O	2.14	0.47
1:A:239:LEU:HD23	1:A:240:SER:H	1.79	0.47
2:B:440:GLN:HB2	2:B:484:VAL:CB	2.44	0.47
2:C:155:LEU:O	2:C:159:ILE:HG13	2.14	0.47
2:C:275:THR:CG2	5:C:530:SAM:HN61	2.28	0.47
1:A:144:ILE:CB	2:B:316:PHE:CZ	2.97	0.47
1:A:235:LEU:O	1:A:318:ASP:HA	2.15	0.47
1:A:352:LYS:HE2	2:C:468:LEU:N	2.18	0.47
2:B:6:LEU:CD2	2:B:130:MET:HE3	2.44	0.47
2:B:25:GLN:HA	2:B:138:ASN:OD1	2.15	0.47
2:B:62:ARG:CD	2:B:70:PHE:HB2	2.45	0.47
2:B:209:HIS:O	2:B:236:GLY:HA2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:LEU:CD2	2:C:130:MET:HE3	2.45	0.47
2:C:313:ASN:HA	2:C:316:PHE:CZ	2.49	0.47
2:C:377:VAL:HB	2:C:467:TRP:HH2	1.78	0.47
1:A:39:ASP:CB	1:A:62:VAL:HG22	2.44	0.46
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.37	0.46
1:A:355:SER:H	2:C:312:ASP:HB2	1.80	0.46
2:B:439:ASP:CA	2:B:485:LEU:HD22	2.39	0.46
2:B:450:PHE:HZ	2:B:467:TRP:CZ3	2.31	0.46
2:C:43:THR:HG22	2:C:45:GLN:HB2	1.97	0.46
2:C:93:VAL:O	2:C:93:VAL:HG23	2.14	0.46
2:C:217:LEU:HD21	2:C:274:GLY:O	2.14	0.46
2:C:271:SER:O	2:C:272:ALA:HB3	2.16	0.46
2:C:455:ILE:O	2:C:459:LYS:HB2	2.15	0.46
5:C:530:SAM:CE	4:E:6:DA:H61	2.05	0.46
1:A:61:PHE:HE2	1:A:66:LEU:CB	2.28	0.46
1:A:80:ILE:HD11	1:A:107:PHE:HD2	1.80	0.46
1:A:144:ILE:HG23	1:A:146:ASN:N	2.31	0.46
1:A:145:ASN:H	1:A:145:ASN:HD22	1.62	0.46
2:B:122:LYS:CE	2:B:124:ARG:HG2	2.44	0.46
2:B:201:GLY:HA2	2:B:204:GLN:OE1	2.15	0.46
2:B:245:ARG:HG2	2:B:246:LEU:N	2.30	0.46
2:B:524:PHE:HE2	2:B:528:LYS:HD2	1.81	0.46
2:C:22:VAL:HG12	2:C:23:SER:O	2.15	0.46
2:C:245:ARG:HH22	2:C:253:ASP:C	2.23	0.46
1:A:25:VAL:HB	1:A:104:PHE:C	2.40	0.46
1:A:46:ALA:CA	1:A:107:PHE:CE1	2.95	0.46
1:A:234:GLU:HG3	4:E:2:DT:C2'	2.43	0.46
1:A:293:TYR:C	1:A:295:GLY:H	2.23	0.46
2:C:3:ASN:HB2	2:C:130:MET:SD	2.55	0.46
2:C:172:GLN:CD	2:C:257:LEU:HD23	2.40	0.46
2:C:201:GLY:HA2	2:C:204:GLN:OE1	2.15	0.46
2:C:296:ILE:HD13	2:C:308:VAL:HG21	1.96	0.46
1:A:117:ILE:HD13	1:A:159:ILE:CD1	2.45	0.46
1:A:357:GLN:HG2	1:A:358:LYS:N	2.28	0.46
2:B:172:GLN:CD	2:B:257:LEU:HD23	2.41	0.46
2:B:459:LYS:O	2:B:460:SER:HB2	2.16	0.46
1:A:89:VAL:CG2	1:A:135:ILE:CG2	2.93	0.46
1:A:164:GLU:OE2	1:A:422:LEU:HB2	2.16	0.46
1:A:271:LEU:O	1:A:274:SER:HB3	2.15	0.46
2:C:378:TYR:HE1	2:C:419:GLU:HG2	1.81	0.46
1:A:252:ILE:O	1:A:252:ILE:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:O	1:A:258:VAL:HB	2.16	0.46
1:A:290:PHE:CD2	1:A:291:THR:N	2.83	0.46
1:A:349:ASN:CB	2:C:430:ALA:CB	2.94	0.46
2:B:22:VAL:HG12	2:B:23:SER:O	2.15	0.46
2:B:231:LEU:HD12	2:B:231:LEU:N	2.30	0.46
2:B:408:ASP:OD2	2:B:410:HIS:HB2	2.16	0.46
2:B:459:LYS:HB3	2:B:462:SER:H	1.80	0.46
2:C:305:ARG:HH11	2:C:410:HIS:CD2	2.32	0.46
1:A:6:LEU:HD23	1:A:7:PRO:CD	2.44	0.46
1:A:53:LYS:HE2	1:A:97:HIS:CE1	2.51	0.46
1:A:142:ALA:HB1	2:B:312:ASP:C	2.41	0.46
1:A:193:LEU:HD23	1:A:193:LEU:C	2.40	0.46
1:A:196:PHE:CE1	1:A:200:VAL:CG2	2.95	0.46
1:A:355:SER:HB3	2:C:316:PHE:CZ	2.50	0.46
2:B:29:ASN:HD22	2:B:224:LEU:HD11	1.78	0.46
2:C:25:GLN:HA	2:C:138:ASN:OD1	2.15	0.46
2:C:75:LEU:HB3	2:C:93:VAL:HG23	1.97	0.46
2:C:215:LEU:HD13	2:C:245:ARG:NE	2.17	0.46
2:C:228:ASN:O	2:C:232:HIS:HD2	1.99	0.46
2:C:322:THR:HB	2:C:325:ARG:NH2	2.25	0.46
1:A:182:THR:HG23	1:A:183:LYS:N	2.29	0.46
1:A:197:ARG:HE	1:A:340:SER:HA	1.80	0.46
1:A:242:LYS:HA	1:A:243:PRO:HD2	1.82	0.46
1:A:252:ILE:HG22	1:A:269:ARG:HA	1.96	0.46
2:B:287:ASN:HD21	2:B:289:GLN:HB2	1.81	0.46
2:C:85:LEU:CD2	2:C:238:LEU:CD2	2.94	0.46
2:C:231:LEU:N	2:C:231:LEU:HD12	2.30	0.46
2:C:344:ILE:HD11	2:C:345:PHE:HE1	1.81	0.46
1:A:27:TYR:CE1	1:A:28:LYS:HE2	2.51	0.46
1:A:225:LYS:HD2	1:A:228:PHE:HE1	1.81	0.46
2:B:269:PHE:CD1	3:D:6:DA:C4	3.02	0.46
2:B:431:ASP:O	2:B:432:SER:HB3	2.15	0.46
2:C:118:GLY:HA2	2:C:123:SER:CB	2.45	0.46
2:C:160:ILE:HD12	2:C:160:ILE:N	2.29	0.46
3:D:1:DG:C4	3:D:2:DT:H71	2.51	0.46
4:E:16:DT:C2	4:E:17:DG:C6	3.04	0.46
2:B:296:ILE:HD13	2:B:308:VAL:HG21	1.98	0.46
2:C:222:ARG:O	2:C:226:LEU:HG	2.16	0.46
1:A:61:PHE:CE1	1:A:65:ASN:CG	2.94	0.45
1:A:133:ASN:CG	2:B:431:ASP:HB2	2.41	0.45
1:A:175:LEU:CD1	1:A:406:VAL:HG21	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HD13	1:A:315:LEU:HD22	1.96	0.45
1:A:325:LEU:CD1	1:A:329:ALA:HB3	2.24	0.45
2:B:3:ASN:HD22	2:B:7:VAL:CG1	2.22	0.45
2:B:271:SER:O	2:B:272:ALA:HB3	2.15	0.45
1:A:44:ILE:HD11	1:A:103:SER:CB	2.45	0.45
1:A:227:ASN:H	1:A:227:ASN:HD22	1.63	0.45
1:A:355:SER:N	2:C:312:ASP:HB2	2.31	0.45
2:B:62:ARG:CD	2:B:70:PHE:CB	2.95	0.45
2:B:73:LYS:HA	2:C:72:ARG:NH1	2.30	0.45
2:B:275:THR:CG2	5:B:530:SAM:HN61	2.29	0.45
2:C:29:ASN:HD22	2:C:224:LEU:HD12	1.80	0.45
2:C:63:ILE:CA	2:C:67:GLN:HB2	2.45	0.45
2:C:85:LEU:CD2	2:C:238:LEU:HD22	2.46	0.45
2:C:305:ARG:HH12	2:C:409:PRO:HG2	1.82	0.45
2:C:341:PRO:HA	2:C:381:ARG:HG3	1.99	0.45
2:C:482:PRO:HA	2:C:485:LEU:HG	1.99	0.45
1:A:79:VAL:HG12	1:A:80:ILE:N	2.31	0.45
1:A:131:TYR:HE1	1:A:155:ILE:HD12	1.80	0.45
1:A:215:ASN:ND2	2:C:492:GLU:HG3	2.30	0.45
1:A:427:ARG:CB	1:A:447:ILE:HD12	2.36	0.45
2:B:75:LEU:HB3	2:B:93:VAL:HG23	1.97	0.45
2:B:481:GLU:CB	2:B:482:PRO:HD3	2.37	0.45
2:C:5:ASP:HB2	2:C:116:TYR:HE2	1.76	0.45
2:C:408:ASP:OD2	2:C:410:HIS:HB2	2.16	0.45
1:A:70:SER:O	3:D:1:DG:P	2.75	0.45
1:A:118:PHE:CZ	1:A:166:LYS:HG3	2.51	0.45
1:A:252:ILE:HG22	1:A:268:ILE:C	2.42	0.45
2:B:17:LEU:HB3	2:B:22:VAL:HB	1.99	0.45
2:B:186:ASP:HA	2:B:212:PHE:CZ	2.51	0.45
2:B:228:ASN:O	2:B:232:HIS:HD2	1.99	0.45
2:B:430:ALA:HB3	2:B:467:TRP:O	2.16	0.45
2:C:524:PHE:HE2	2:C:528:LYS:HD2	1.80	0.45
1:A:175:LEU:CD1	1:A:406:VAL:CG2	2.94	0.45
1:A:248:VAL:HG13	1:A:270:PHE:N	2.32	0.45
1:A:434:ILE:HG13	1:A:435:SER:N	2.32	0.45
2:B:32:ALA:HB2	2:B:131:TYR:CE1	2.52	0.45
2:B:39:MET:HA	2:B:39:MET:CE	2.33	0.45
2:B:275:THR:HG21	5:B:530:SAM:C5	2.47	0.45
2:C:186:ASP:HA	2:C:212:PHE:CZ	2.51	0.45
1:A:10:TRP:NE1	1:A:160:PRO:HA	2.31	0.45
1:A:18:VAL:O	1:A:113:PRO:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:O	1:A:19:THR:HG23	2.15	0.45
1:A:26:THR:HG21	1:A:70:SER:HB3	1.95	0.45
1:A:293:TYR:CE2	4:E:5:DC:N4	2.84	0.45
1:A:299:PHE:C	1:A:300:VAL:HG23	2.42	0.45
2:B:85:LEU:CD2	2:B:238:LEU:HD22	2.47	0.45
2:B:85:LEU:CD2	2:B:238:LEU:CD2	2.94	0.45
2:B:222:ARG:O	2:B:226:LEU:HG	2.16	0.45
2:C:122:LYS:HD3	2:C:124:ARG:CG	2.47	0.45
2:C:128:GLY:CA	2:C:231:LEU:HD22	2.33	0.45
1:A:81:ALA:HA	1:A:92:LYS:O	2.17	0.45
1:A:214:ARG:HD2	1:A:369:VAL:HG12	1.97	0.45
2:B:345:PHE:CD2	3:D:6:DA:C2	3.05	0.45
2:B:420:TRP:HB2	2:B:425:GLU:OE1	2.17	0.45
2:C:28:VAL:CG2	2:C:224:LEU:CD2	2.95	0.45
1:A:10:TRP:NE1	1:A:160:PRO:CA	2.80	0.45
1:A:63:PRO:O	1:A:66:LEU:HB3	2.17	0.45
1:A:236:ARG:HB2	4:E:2:DT:H71	1.99	0.45
1:A:314:LEU:HD23	1:A:315:LEU:CA	2.46	0.45
1:A:352:LYS:HD3	2:C:382:THR:CG2	2.46	0.45
2:B:429:VAL:HG12	2:B:430:ALA:N	2.31	0.45
2:C:269:PHE:CD1	2:C:269:PHE:N	2.83	0.45
2:C:275:THR:HG21	5:C:530:SAM:C5	2.47	0.45
2:C:287:ASN:HD21	2:C:289:GLN:HB2	1.81	0.45
2:C:430:ALA:HB1	2:C:469:LYS:HZ3	1.82	0.45
1:A:293:TYR:O	1:A:294:ASN:CB	2.64	0.45
1:A:355:SER:CB	2:C:312:ASP:HB2	2.47	0.45
2:B:68:LEU:HD23	2:B:68:LEU:C	2.42	0.45
2:B:85:LEU:HD23	2:B:238:LEU:HD22	1.98	0.45
2:B:164:LYS:HE3	2:B:407:GLU:O	2.17	0.45
2:C:85:LEU:HD23	2:C:238:LEU:HD22	1.99	0.45
2:C:448:ARG:HD3	2:C:467:TRP:NE1	2.30	0.45
1:A:10:TRP:CH2	1:A:164:GLU:OE1	2.70	0.45
1:A:114:GLU:C	1:A:116:LEU:H	2.25	0.45
1:A:212:LYS:HG2	1:A:213:TRP:N	2.32	0.45
1:A:292:ARG:HD3	1:A:293:TYR:HE1	1.82	0.45
2:B:28:VAL:CG2	2:B:224:LEU:CD2	2.95	0.45
2:B:29:ASN:HD22	2:B:224:LEU:HD12	1.80	0.45
2:B:170:VAL:H	2:B:261:HIS:CD2	2.26	0.45
2:C:115:TRP:CH2	2:C:122:LYS:CE	2.94	0.45
1:A:55:ASP:OD1	1:A:98:LEU:HG	2.17	0.44
1:A:248:VAL:HG12	1:A:250:HIS:N	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:HG2	1:A:332:GLU:OE1	2.17	0.44
2:B:17:LEU:HD21	2:B:106:LEU:CD1	2.48	0.44
2:B:122:LYS:HD3	2:B:124:ARG:CG	2.47	0.44
2:B:250:LEU:HA	2:B:279:ARG:NH2	2.33	0.44
2:C:17:LEU:HD21	2:C:106:LEU:CD1	2.47	0.44
2:C:32:ALA:HB2	2:C:131:TYR:CE1	2.51	0.44
2:C:130:MET:HB2	2:C:130:MET:HE2	1.81	0.44
2:C:334:LEU:HA	2:C:357:PHE:CB	2.46	0.44
2:C:338:LEU:HD13	2:C:401:PHE:CE1	2.52	0.44
2:C:430:ALA:HB1	2:C:469:LYS:NZ	2.32	0.44
2:C:459:LYS:O	2:C:460:SER:HB2	2.17	0.44
1:A:15:VAL:CA	1:A:18:VAL:HG22	2.46	0.44
1:A:215:ASN:ND2	2:C:492:GLU:CG	2.79	0.44
1:A:254:ARG:HG2	1:A:255:ILE:HG22	1.98	0.44
1:A:290:PHE:HB3	1:A:321:ILE:HG22	1.92	0.44
1:A:330:LEU:CD2	1:A:332:GLU:HB2	2.47	0.44
1:A:360:ILE:O	1:A:360:ILE:HG23	2.17	0.44
2:B:3:ASN:CB	2:B:130:MET:SD	3.06	0.44
2:B:43:THR:HG21	2:B:45:GLN:HB2	2.00	0.44
2:B:344:ILE:HD11	2:B:345:PHE:HE1	1.82	0.44
2:C:420:TRP:HB2	2:C:425:GLU:OE1	2.17	0.44
1:A:7:PRO:HG2	1:A:418:PHE:C	2.42	0.44
1:A:416:LYS:O	1:A:422:LEU:HG	2.16	0.44
2:C:149:TYR:CD1	5:C:530:SAM:C3'	2.99	0.44
2:C:451:SER:O	2:C:455:ILE:HG13	2.17	0.44
3:D:1:DG:C5	3:D:2:DT:H73	2.52	0.44
4:E:18:DA:C6	4:E:19:DA:C6	3.06	0.44
1:A:35:TYR:CD1	1:A:65:ASN:CG	2.95	0.44
1:A:42:PRO:HB3	1:A:57:THR:CG2	2.42	0.44
1:A:352:LYS:HB2	2:C:466:SER:CB	2.47	0.44
2:B:277:ILE:HD13	2:B:291:CYS:SG	2.57	0.44
2:B:384:MET:CB	2:B:385:PRO:HD2	2.37	0.44
2:C:3:ASN:CB	2:C:130:MET:SD	3.05	0.44
2:C:17:LEU:HD22	2:C:22:VAL:HG21	2.00	0.44
2:C:62:ARG:CD	2:C:70:PHE:CB	2.95	0.44
1:A:78:ILE:CD1	1:A:111:LEU:CD2	2.95	0.44
1:A:257:SER:HB2	1:A:266:ASN:HD21	1.81	0.44
1:A:294:ASN:HD22	3:D:14:DG:H8	1.64	0.44
2:B:438:THR:HG23	2:B:442:LEU:HD23	1.98	0.44
2:C:164:LYS:HE3	2:C:407:GLU:O	2.17	0.44
2:C:279:ARG:NE	2:C:281:PHE:CZ	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HE2	1:A:97:HIS:HE1	1.82	0.44
1:A:325:LEU:HD13	1:A:329:ALA:HB1	1.95	0.44
1:A:385:VAL:HG12	1:A:389:PHE:HE1	1.82	0.44
2:B:135:LEU:HD23	2:B:135:LEU:C	2.41	0.44
2:B:252:SER:O	2:B:255:GLU:HG2	2.18	0.44
2:C:287:ASN:HD22	2:C:290:LEU:H	1.66	0.44
1:A:15:VAL:CG2	1:A:155:ILE:CG2	2.95	0.44
1:A:73:ILE:HG22	1:A:100:PHE:HB3	1.94	0.44
1:A:253:LEU:CD1	1:A:263:VAL:CG2	2.93	0.44
2:B:39:MET:CA	2:B:39:MET:CE	2.95	0.44
2:B:115:TRP:CH2	2:B:122:LYS:CE	2.94	0.44
2:B:128:GLY:O	2:B:131:TYR:HB3	2.18	0.44
2:B:149:TYR:O	5:B:530:SAM:HB1	2.18	0.44
2:B:287:ASN:HD22	2:B:290:LEU:H	1.66	0.44
2:B:482:PRO:HA	2:B:485:LEU:HG	1.99	0.44
2:B:488:GLU:HG2	2:B:489:ALA:N	2.33	0.44
2:C:135:LEU:HD23	2:C:135:LEU:C	2.42	0.44
2:C:158:THR:OG1	2:C:398:LEU:HD13	2.18	0.44
2:C:277:ILE:HD13	2:C:291:CYS:SG	2.57	0.44
1:A:271:LEU:HD22	1:A:273:CYS:N	2.13	0.44
1:A:410:THR:HA	1:A:413:ILE:HG22	1.99	0.44
2:B:158:THR:OG1	2:B:398:LEU:HD13	2.18	0.44
2:C:39:MET:HA	2:C:39:MET:CE	2.33	0.44
2:C:250:LEU:HA	2:C:279:ARG:NH2	2.33	0.44
1:A:118:PHE:CZ	1:A:166:LYS:CE	2.95	0.44
1:A:223:PHE:CG	1:A:224:LYS:N	2.85	0.44
1:A:254:ARG:HH21	1:A:256:SER:HB2	1.74	0.44
2:B:17:LEU:HD22	2:B:22:VAL:HG21	2.00	0.44
2:B:215:LEU:HD22	2:B:245:ARG:HH21	1.83	0.44
2:C:252:SER:O	2:C:255:GLU:HG2	2.18	0.44
1:A:187:GLU:O	1:A:190:PRO:HD2	2.18	0.43
1:A:262:HIS:HD2	1:A:263:VAL:H	1.66	0.43
1:A:288:LEU:HG	1:A:289:LEU:N	2.32	0.43
2:C:68:LEU:HD23	2:C:68:LEU:C	2.42	0.43
2:C:459:LYS:HD3	2:C:459:LYS:HA	1.80	0.43
2:C:488:GLU:HG2	2:C:489:ALA:N	2.32	0.43
1:A:10:TRP:CZ2	1:A:417:ALA:O	2.71	0.43
1:A:143:ASN:HD22	2:B:313:ASN:CG	2.26	0.43
1:A:203:GLY:O	1:A:204:ALA:HB3	2.18	0.43
1:A:225:LYS:HB2	1:A:227:ASN:ND2	2.33	0.43
1:A:286:GLY:CA	1:A:305:LEU:HD21	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:HD23	1:A:320:LEU:C	2.43	0.43
2:B:6:LEU:HD23	2:B:130:MET:CG	2.48	0.43
2:C:17:LEU:HB3	2:C:22:VAL:HB	1.99	0.43
1:A:25:VAL:HG11	1:A:103:SER:C	2.43	0.43
1:A:196:PHE:CD1	1:A:200:VAL:HG21	2.54	0.43
1:A:426:TRP:HE3	1:A:447:ILE:CB	2.31	0.43
2:B:6:LEU:CB	2:B:130:MET:HG2	2.47	0.43
2:B:459:LYS:HD3	2:B:459:LYS:HA	1.81	0.43
1:A:16:SER:HA	1:A:19:THR:HG22	2.01	0.43
1:A:45:ARG:HA	1:A:104:PHE:CD1	2.51	0.43
1:A:232:LEU:HD21	1:A:321:ILE:CD1	2.45	0.43
1:A:320:LEU:HD23	1:A:321:ILE:C	2.43	0.43
2:B:207:GLN:HA	2:B:211:ALA:CB	2.39	0.43
2:C:17:LEU:CB	2:C:27:TYR:CD1	3.01	0.43
2:C:275:THR:CB	5:C:530:SAM:HN61	2.31	0.43
2:C:439:ASP:CA	2:C:485:LEU:HD22	2.38	0.43
1:A:291:THR:CG2	1:A:302:VAL:HB	2.48	0.43
1:A:291:THR:HG22	1:A:302:VAL:HB	1.99	0.43
2:B:220:GLY:HA2	2:B:223:ARG:NH2	2.34	0.43
2:B:283:HIS:HB3	2:B:320:LYS:HE3	2.00	0.43
2:B:312:ASP:CG	2:B:351:LYS:HB3	2.43	0.43
2:B:315:LEU:HD22	2:B:463:LEU:HB3	2.00	0.43
2:B:338:LEU:HD13	2:B:401:PHE:CE1	2.53	0.43
2:C:106:LEU:HD23	2:C:106:LEU:C	2.43	0.43
2:C:169:GLU:OE1	2:C:262:ILE:HD11	2.18	0.43
1:A:44:ILE:CG1	1:A:103:SER:CB	2.96	0.43
1:A:89:VAL:CG2	1:A:135:ILE:HG22	2.47	0.43
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.82	0.43
1:A:130:LEU:HD23	1:A:130:LEU:C	2.42	0.43
1:A:248:VAL:CG1	1:A:270:PHE:N	2.82	0.43
1:A:300:VAL:CG1	1:A:301:GLY:N	2.80	0.43
2:B:279:ARG:NE	2:B:281:PHE:CZ	2.86	0.43
2:B:322:THR:O	2:B:326:ARG:HG3	2.18	0.43
2:B:376:TRP:CE3	2:B:447:TRP:NE1	2.87	0.43
2:C:20:GLY:HA2	2:C:102:GLN:CG	2.37	0.43
2:C:43:THR:HG21	2:C:45:GLN:HB2	2.00	0.43
2:C:269:PHE:CZ	2:C:311:PRO:HD3	2.53	0.43
4:E:1:DG:H2"	4:E:2:DT:H6	1.84	0.43
1:A:48:ASN:HB3	1:A:54:PHE:CD1	2.54	0.43
1:A:80:ILE:HD11	1:A:107:PHE:CD2	2.53	0.43
1:A:131:TYR:CE1	1:A:155:ILE:HD12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HG23	1:A:268:ILE:HG23	1.92	0.43
1:A:411:GLN:HB3	2:B:491:GLY:O	2.19	0.43
2:B:166:GLN:HB3	2:B:167:PRO:HD2	2.01	0.43
1:A:133:ASN:HA	2:B:469:LYS:NZ	2.34	0.43
1:A:175:LEU:C	1:A:175:LEU:CD1	2.92	0.43
1:A:254:ARG:CG	1:A:255:ILE:H	2.30	0.43
1:A:409:LEU:C	1:A:409:LEU:CD2	2.91	0.43
2:B:14:CYS:SG	2:B:31:LEU:HD11	2.59	0.43
2:B:17:LEU:CB	2:B:27:TYR:CD1	3.01	0.43
2:B:497:LEU:HD12	2:B:497:LEU:N	2.34	0.43
2:C:1:MET:SD	2:C:129:ASP:HA	2.58	0.43
2:C:497:LEU:N	2:C:497:LEU:HD12	2.34	0.43
1:A:17:THR:CG2	1:A:18:VAL:N	2.82	0.43
1:A:20:THR:CG2	1:A:21:LEU:N	2.82	0.43
1:A:26:THR:HG21	1:A:70:SER:H	1.84	0.43
1:A:78:ILE:HG22	1:A:96:GLN:CG	2.44	0.43
2:B:380:LEU:O	2:B:380:LEU:HD23	2.19	0.43
2:C:322:THR:CG2	2:C:323:ASP:N	2.82	0.43
1:A:112:ARG:H	1:A:112:ARG:CD	2.32	0.43
1:A:155:ILE:HG23	1:A:155:ILE:O	2.19	0.43
1:A:197:ARG:CZ	1:A:340:SER:HA	2.48	0.43
1:A:222:VAL:CG1	1:A:223:PHE:N	2.82	0.43
1:A:254:ARG:HA	1:A:317:PRO:HG2	2.01	0.43
1:A:299:PHE:CZ	1:A:347:MET:CE	2.95	0.43
1:A:426:TRP:CE3	1:A:447:ILE:CB	3.00	0.43
2:B:62:ARG:HH11	2:B:66:GLU:HG2	1.84	0.43
2:B:275:THR:CB	5:B:530:SAM:HN61	2.32	0.43
2:B:378:TYR:HE1	2:B:419:GLU:HG2	1.84	0.43
2:C:115:TRP:CE3	2:C:127:PHE:CE1	3.07	0.43
1:A:89:VAL:O	1:A:89:VAL:HG22	2.19	0.42
1:A:142:ALA:O	2:B:316:PHE:CZ	2.72	0.42
1:A:365:ILE:CG2	1:A:366:LYS:N	2.82	0.42
2:B:224:LEU:HD12	2:B:224:LEU:N	2.34	0.42
2:B:269:PHE:CZ	2:B:311:PRO:HD3	2.54	0.42
2:B:305:ARG:HH12	2:B:409:PRO:HG2	1.82	0.42
2:B:334:LEU:HA	2:B:357:PHE:CB	2.46	0.42
2:C:6:LEU:CB	2:C:117:ASN:HB2	2.47	0.42
2:C:122:LYS:HZ2	2:C:124:ARG:HG2	1.81	0.42
1:A:10:TRP:CE2	1:A:418:PHE:CA	2.94	0.42
1:A:35:TYR:CD1	1:A:65:ASN:ND2	2.87	0.42
1:A:72:LYS:HB3	3:D:1:DG:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.47	0.42
1:A:287:ASP:HB2	1:A:322:ARG:HH21	1.84	0.42
1:A:385:VAL:CG1	1:A:389:PHE:HE1	2.32	0.42
2:B:161:HIS:O	2:B:164:LYS:HG3	2.19	0.42
2:B:251:GLY:HA2	2:B:278:THR:OG1	2.19	0.42
2:C:34:LEU:CB	2:C:110:MET:SD	3.07	0.42
2:C:103:ILE:CG2	2:C:104:THR:N	2.82	0.42
2:C:213:ILE:CG2	2:C:214:GLY:N	2.82	0.42
2:C:450:PHE:CE1	2:C:467:TRP:CZ3	3.07	0.42
2:C:493:LEU:HD22	2:C:493:LEU:N	2.34	0.42
1:A:10:TRP:CE3	1:A:418:PHE:O	2.72	0.42
1:A:104:PHE:CZ	1:A:106:ALA:HB3	2.54	0.42
1:A:117:ILE:HD12	1:A:165:GLN:OE1	2.19	0.42
1:A:118:PHE:CZ	1:A:162:LEU:HD21	2.53	0.42
1:A:212:LYS:CG	1:A:213:TRP:N	2.83	0.42
1:A:224:LYS:O	1:A:370:VAL:HG12	2.20	0.42
1:A:233:THR:O	1:A:321:ILE:HG13	2.19	0.42
1:A:255:ILE:CG2	1:A:256:SER:N	2.83	0.42
1:A:265:GLN:CG	1:A:266:ASN:N	2.82	0.42
1:A:347:MET:CE	1:A:360:ILE:CD1	2.96	0.42
2:C:62:ARG:HH11	2:C:66:GLU:HG2	1.84	0.42
2:C:215:LEU:HD22	2:C:245:ARG:HH21	1.83	0.42
2:C:269:PHE:CG	4:E:6:DA:C4	3.07	0.42
1:A:41:LEU:HD23	1:A:42:PRO:HD2	1.98	0.42
1:A:121:PHE:CZ	1:A:160:PRO:HG3	2.55	0.42
1:A:142:ALA:O	2:B:316:PHE:CE2	2.72	0.42
1:A:198:GLN:NE2	2:C:491:GLY:HA3	2.34	0.42
1:A:254:ARG:CG	1:A:255:ILE:N	2.83	0.42
1:A:315:LEU:HD23	1:A:316:TYR:O	2.19	0.42
2:B:277:ILE:O	2:B:277:ILE:HG22	2.20	0.42
2:B:377:VAL:HG12	2:B:378:TYR:N	2.34	0.42
2:C:358:THR:CG2	2:C:359:LYS:N	2.83	0.42
3:D:1:DG:C4	3:D:2:DT:C7	3.03	0.42
4:E:1:DG:C4	4:E:2:DT:H72	2.55	0.42
1:A:22:ILE:CG2	1:A:108:CYS:SG	3.07	0.42
1:A:126:THR:CG2	1:A:127:LYS:N	2.83	0.42
1:A:239:LEU:CD2	1:A:240:SER:N	2.82	0.42
1:A:333:TYR:CA	1:A:382:VAL:HG22	2.46	0.42
1:A:395:ILE:CG2	1:A:396:GLU:N	2.83	0.42
1:A:410:THR:CG2	1:A:411:GLN:N	2.83	0.42
1:A:417:ALA:HA	1:A:422:LEU:HG	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:SER:N	2:B:479:LEU:HD12	2.35	0.42
2:C:14:CYS:SG	2:C:31:LEU:HD11	2.59	0.42
2:C:170:VAL:H	2:C:261:HIS:CD2	2.27	0.42
2:C:220:GLY:HA3	2:C:223:ARG:HH21	1.85	0.42
1:A:15:VAL:HA	1:A:18:VAL:CG2	2.49	0.42
1:A:61:PHE:CE2	1:A:66:LEU:HB2	2.54	0.42
1:A:144:ILE:HG12	2:B:316:PHE:HZ	1.81	0.42
1:A:167:ILE:CG2	1:A:168:ILE:N	2.83	0.42
1:A:334:ILE:CG2	1:A:335:GLU:N	2.83	0.42
2:B:115:TRP:CE3	2:B:127:PHE:CE1	3.07	0.42
2:B:269:PHE:HB2	3:D:6:DA:N9	2.28	0.42
2:C:142:THR:CG2	2:C:143:LYS:N	2.83	0.42
2:C:220:GLY:HA2	2:C:223:ARG:NH2	2.34	0.42
2:C:262:ILE:HG22	2:C:263:VAL:N	2.34	0.42
2:C:336:THR:CG2	2:C:337:ILE:N	2.83	0.42
1:A:144:ILE:N	2:B:316:PHE:CZ	2.83	0.42
1:A:182:THR:CG2	1:A:183:LYS:N	2.83	0.42
1:A:223:PHE:CZ	1:A:369:VAL:HG13	2.49	0.42
1:A:229:GLU:OE2	1:A:329:ALA:HB2	2.20	0.42
1:A:232:LEU:HG	1:A:321:ILE:CD1	2.46	0.42
1:A:444:LEU:C	1:A:444:LEU:CD2	2.93	0.42
2:B:106:LEU:HD23	2:B:106:LEU:C	2.43	0.42
2:B:136:GLN:HG2	2:B:140:ASN:HD21	1.85	0.42
2:B:213:ILE:CG2	2:B:214:GLY:N	2.83	0.42
2:B:285:THR:HG22	2:B:287:ASN:N	2.07	0.42
2:C:85:LEU:HD21	2:C:238:LEU:CD2	2.50	0.42
2:C:151:THR:HG22	2:C:152:PRO:N	2.34	0.42
2:C:166:GLN:HB3	2:C:167:PRO:HD2	2.00	0.42
2:C:222:ARG:HH12	2:C:226:LEU:HD11	1.81	0.42
2:C:224:LEU:HD12	2:C:224:LEU:N	2.34	0.42
2:C:354:VAL:CG1	2:C:356:PHE:CZ	3.03	0.42
2:C:478:SER:N	2:C:479:LEU:HD12	2.35	0.42
1:A:54:PHE:CD2	1:A:54:PHE:O	2.73	0.42
1:A:104:PHE:CE1	1:A:107:PHE:CD1	3.08	0.42
1:A:164:GLU:CG	1:A:423:THR:CA	2.95	0.42
1:A:255:ILE:CG2	3:D:14:DG:H5'	2.47	0.42
1:A:330:LEU:HD22	1:A:333:TYR:N	2.30	0.42
1:A:332:GLU:HB3	1:A:382:VAL:CG1	2.50	0.42
2:B:22:VAL:HG13	2:B:96:THR:OG1	2.20	0.42
2:B:123:SER:O	2:B:127:PHE:HD1	2.03	0.42
2:B:479:LEU:HD12	2:B:479:LEU:N	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:PHE:CD1	4:E:6:DA:N7	2.86	0.42
2:C:435:ASN:HD21	2:C:467:TRP:HB2	1.84	0.42
1:A:6:LEU:CD1	1:A:12:ILE:CD1	2.95	0.42
1:A:142:ALA:HB1	2:B:312:ASP:CA	2.50	0.42
1:A:414:LEU:O	1:A:418:PHE:CD2	2.73	0.42
2:B:216:GLU:HG2	2:B:221:THR:HB	2.01	0.42
2:B:305:ARG:HD3	2:B:410:HIS:CG	2.55	0.42
2:B:493:LEU:HD22	2:B:493:LEU:N	2.34	0.42
2:C:3:ASN:HB2	2:C:7:VAL:CB	2.44	0.42
2:C:20:GLY:N	2:C:102:GLN:HG3	2.34	0.42
1:A:122:ILE:CG2	1:A:123:ALA:N	2.83	0.42
1:A:193:LEU:C	1:A:193:LEU:CD2	2.93	0.42
1:A:230:SER:HA	1:A:324:ARG:O	2.19	0.42
1:A:253:LEU:O	1:A:316:TYR:HB2	2.19	0.42
1:A:289:LEU:HD11	1:A:320:LEU:HD21	1.97	0.42
1:A:302:VAL:CG1	1:A:303:CYS:N	2.83	0.42
1:A:312:GLN:CG	1:A:313:ASN:N	2.82	0.42
1:A:388:LEU:C	1:A:388:LEU:CD2	2.93	0.42
2:B:151:THR:HG22	2:B:152:PRO:N	2.34	0.42
2:B:481:GLU:HB2	2:B:482:PRO:CD	2.41	0.42
2:C:72:ARG:CG	2:C:73:LYS:N	2.82	0.42
2:C:123:SER:O	2:C:127:PHE:HD1	2.03	0.42
2:C:161:HIS:O	2:C:164:LYS:HG3	2.19	0.42
2:C:376:TRP:CE3	2:C:447:TRP:NE1	2.87	0.42
2:C:427:THR:CG2	2:C:428:GLU:N	2.83	0.42
2:C:459:LYS:HB3	2:C:462:SER:H	1.85	0.42
1:A:61:PHE:CE1	1:A:69:GLU:OE1	2.74	0.41
1:A:270:PHE:CD2	1:A:271:LEU:O	2.73	0.41
1:A:415:ALA:CB	2:B:492:GLU:HG2	2.34	0.41
2:B:451:SER:O	2:B:455:ILE:HG13	2.19	0.41
2:C:149:TYR:CD1	5:C:530:SAM:H3'	2.55	0.41
2:C:305:ARG:HD3	2:C:410:HIS:CG	2.55	0.41
1:A:7:PRO:HG3	1:A:415:ALA:O	2.20	0.41
1:A:20:THR:HG23	1:A:111:LEU:HB2	1.99	0.41
1:A:80:ILE:HD13	1:A:107:PHE:HD2	1.81	0.41
2:B:20:GLY:N	2:B:102:GLN:HG3	2.34	0.41
2:B:103:ILE:CG2	2:B:104:THR:N	2.83	0.41
2:B:122:LYS:CD	2:B:124:ARG:HG2	2.50	0.41
2:C:22:VAL:HG13	2:C:96:THR:OG1	2.20	0.41
2:C:263:VAL:CG2	2:C:300:LEU:CD2	2.95	0.41
2:C:479:LEU:HD12	2:C:479:LEU:N	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:484:VAL:CG2	2:C:485:LEU:N	2.83	0.41
4:E:1:DG:C4	4:E:2:DT:C5	3.07	0.41
4:E:16:DT:C2'	4:E:17:DG:C8	2.99	0.41
1:A:10:TRP:CE2	1:A:160:PRO:CA	3.00	0.41
1:A:33:ILE:CG2	1:A:34:ASN:N	2.82	0.41
1:A:70:SER:HA	3:D:1:DG:H5'	2.03	0.41
1:A:130:LEU:C	1:A:130:LEU:CD2	2.94	0.41
1:A:159:ILE:HA	1:A:160:PRO:HD2	1.83	0.41
1:A:328:ASP:O	1:A:329:ALA:HB2	2.20	0.41
1:A:336:ILE:CG2	1:A:337:PHE:N	2.83	0.41
2:B:85:LEU:HD21	2:B:238:LEU:CD2	2.50	0.41
2:B:142:THR:CG2	2:B:143:LYS:N	2.83	0.41
2:B:217:LEU:HD22	2:B:275:THR:HG23	1.94	0.41
2:B:269:PHE:CE2	2:B:311:PRO:CB	3.02	0.41
2:C:6:LEU:CB	2:C:130:MET:HG2	2.50	0.41
2:C:122:LYS:CD	2:C:124:ARG:HG2	2.49	0.41
1:A:10:TRP:CD1	1:A:159:ILE:C	2.99	0.41
1:A:44:ILE:HG12	1:A:103:SER:HA	2.02	0.41
2:B:68:LEU:C	2:B:68:LEU:CD2	2.94	0.41
2:B:344:ILE:CD1	2:B:345:PHE:CE1	3.03	0.41
2:B:345:PHE:CD2	3:D:6:DA:H2	2.38	0.41
2:C:39:MET:CA	2:C:39:MET:CE	2.95	0.41
2:C:167:PRO:C	2:C:169:GLU:H	2.28	0.41
2:C:277:ILE:O	2:C:277:ILE:HG22	2.20	0.41
1:A:71:GLN:HG3	1:A:103:SER:O	2.19	0.41
1:A:158:PRO:CG	1:A:418:PHE:CE2	3.03	0.41
1:A:416:LYS:O	1:A:422:LEU:HD23	2.20	0.41
2:B:106:LEU:CD2	2:B:106:LEU:C	2.94	0.41
1:A:26:THR:HG21	3:D:2:DT:H72	2.03	0.41
1:A:41:LEU:HD11	1:A:73:ILE:HG12	2.02	0.41
1:A:61:PHE:CZ	1:A:66:LEU:CA	3.00	0.41
2:B:62:ARG:HB3	2:B:67:GLN:HA	2.03	0.41
2:B:167:PRO:C	2:B:169:GLU:H	2.28	0.41
2:B:220:GLY:HA2	2:B:223:ARG:HH21	1.85	0.41
2:B:358:THR:CG2	2:B:359:LYS:N	2.83	0.41
2:C:251:GLY:HA2	2:C:278:THR:OG1	2.19	0.41
2:C:420:TRP:O	2:C:420:TRP:CD1	2.73	0.41
1:A:6:LEU:HA	1:A:7:PRO:HD2	1.79	0.41
1:A:42:PRO:HG2	1:A:101:GLU:HG3	2.03	0.41
1:A:209:LEU:N	1:A:209:LEU:CD1	2.83	0.41
1:A:316:TYR:CE2	1:A:320:LEU:O	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:N	1:A:422:LEU:CD2	2.83	0.41
2:B:38:LYS:HA	2:B:56:TRP:CE3	2.56	0.41
2:B:63:ILE:HG12	2:B:64:GLY:N	2.36	0.41
2:B:283:HIS:N	2:B:294:GLN:HE22	2.05	0.41
2:B:484:VAL:CG2	2:B:485:LEU:N	2.83	0.41
2:C:88:ALA:HB2	2:C:241:GLY:HA2	2.02	0.41
1:A:12:ILE:CD1	1:A:12:ILE:N	2.83	0.41
1:A:126:THR:O	1:A:131:TYR:CD2	2.74	0.41
1:A:136:SER:HB2	2:B:469:LYS:CE	2.51	0.41
1:A:232:LEU:CD2	1:A:232:LEU:C	2.94	0.41
1:A:247:GLY:C	1:A:248:VAL:CG2	2.94	0.41
1:A:353:THR:CG2	2:C:351:LYS:CE	2.95	0.41
1:A:394:THR:CG2	1:A:395:ILE:N	2.82	0.41
1:A:426:TRP:HE3	1:A:447:ILE:HG21	1.84	0.41
2:B:190:LYS:HA	2:B:193:THR:OG1	2.21	0.41
2:B:440:GLN:CB	2:B:484:VAL:HB	2.50	0.41
2:C:216:GLU:HG2	2:C:221:THR:HB	2.01	0.41
2:C:269:PHE:HD1	4:E:6:DA:C5	2.25	0.41
2:C:334:LEU:HD12	2:C:357:PHE:HB3	2.03	0.41
1:A:8:GLU:CD	1:A:464:SER:HB3	2.46	0.41
1:A:27:TYR:CE2	1:A:28:LYS:O	2.74	0.41
1:A:41:LEU:CD2	1:A:42:PRO:N	2.78	0.41
1:A:45:ARG:O	1:A:107:PHE:CZ	2.74	0.41
1:A:138:LEU:HD22	1:A:138:LEU:H	1.83	0.41
1:A:316:TYR:CD2	1:A:317:PRO:O	2.74	0.41
2:B:103:ILE:O	2:B:107:VAL:HG23	2.21	0.41
2:B:220:GLY:HA3	2:B:223:ARG:HH21	1.84	0.41
2:B:427:THR:CG2	2:B:428:GLU:N	2.83	0.41
2:C:68:LEU:C	2:C:68:LEU:CD2	2.94	0.41
2:C:70:PHE:HE2	2:C:74:MET:CE	2.32	0.41
2:C:135:LEU:C	2:C:135:LEU:CD2	2.94	0.41
2:C:148:GLN:OE1	4:E:6:DA:C8	2.74	0.41
2:C:163:LEU:CG	2:C:262:ILE:HG21	2.48	0.41
2:C:216:GLU:HG3	2:C:218:VAL:O	2.21	0.41
2:C:244:ILE:N	2:C:244:ILE:CD1	2.84	0.41
2:C:246:LEU:HD13	2:C:247:GLY:N	2.36	0.41
2:C:344:ILE:CD1	2:C:345:PHE:CE1	3.04	0.41
2:C:377:VAL:HG12	2:C:378:TYR:N	2.35	0.41
2:C:408:ASP:OD1	2:C:409:PRO:HD2	2.21	0.41
1:A:11:VAL:CG1	1:A:12:ILE:N	2.83	0.41
1:A:36:LEU:N	1:A:36:LEU:CD2	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:CG2	1:A:101:GLU:CD	2.94	0.41
1:A:86:SER:C	1:A:88:SER:H	2.29	0.41
1:A:299:PHE:CD2	1:A:347:MET:HG2	2.54	0.41
1:A:356:GLY:N	2:C:316:PHE:CZ	2.89	0.41
1:A:372:LEU:C	1:A:372:LEU:CD1	2.94	0.41
1:A:411:GLN:OE1	2:B:491:GLY:HA3	2.20	0.41
1:A:414:LEU:O	1:A:418:PHE:CG	2.74	0.41
2:B:88:ALA:HB2	2:B:241:GLY:HA2	2.02	0.41
2:B:336:THR:CG2	2:B:337:ILE:N	2.83	0.41
2:C:450:PHE:HZ	2:C:467:TRP:CZ3	2.38	0.41
2:C:515:LEU:HD22	2:C:515:LEU:H	1.86	0.41
1:A:27:TYR:CD2	1:A:28:LYS:O	2.74	0.40
1:A:74:SER:O	1:A:100:PHE:CD2	2.74	0.40
1:A:154:LEU:C	1:A:154:LEU:CD2	2.94	0.40
1:A:253:LEU:C	1:A:253:LEU:CD2	2.93	0.40
1:A:268:ILE:HG12	1:A:269:ARG:N	2.36	0.40
1:A:294:ASN:ND2	3:D:13:DC:C2'	2.60	0.40
2:B:28:VAL:CG2	2:B:29:ASN:N	2.85	0.40
2:B:113:LEU:C	2:B:113:LEU:CD2	2.94	0.40
2:B:135:LEU:C	2:B:135:LEU:CD2	2.94	0.40
2:B:279:ARG:NH2	2:B:281:PHE:HZ	2.19	0.40
2:B:390:ARG:CG	2:B:391:THR:N	2.85	0.40
2:B:420:TRP:O	2:B:420:TRP:CD1	2.73	0.40
2:C:136:GLN:HG2	2:C:140:ASN:HD21	1.86	0.40
2:C:283:HIS:HB3	2:C:320:LYS:HE3	2.03	0.40
1:A:89:VAL:HG22	1:A:135:ILE:HG21	2.03	0.40
1:A:236:ARG:CG	1:A:237:ASN:N	2.82	0.40
2:B:216:GLU:HG3	2:B:218:VAL:O	2.21	0.40
2:B:237:ASN:HD22	2:B:238:LEU:N	2.19	0.40
2:B:432:SER:HB2	2:B:433:GLU:H	1.62	0.40
2:C:38:LYS:HA	2:C:56:TRP:CE3	2.56	0.40
2:C:62:ARG:HD3	2:C:70:PHE:HB2	2.02	0.40
2:C:115:TRP:CZ3	2:C:127:PHE:CE1	3.09	0.40
2:C:390:ARG:CG	2:C:391:THR:N	2.84	0.40
1:A:49:ILE:CG1	1:A:107:PHE:CE2	2.98	0.40
1:A:232:LEU:HD11	1:A:321:ILE:CD1	2.48	0.40
1:A:290:PHE:CD1	1:A:302:VAL:O	2.74	0.40
1:A:303:CYS:SG	1:A:304:GLY:N	2.95	0.40
2:B:246:LEU:C	2:B:246:LEU:CD1	2.94	0.40
2:C:106:LEU:CD2	2:C:106:LEU:C	2.94	0.40
2:C:190:LYS:HA	2:C:193:THR:OG1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:440:GLN:HB2	2:C:484:VAL:CB	2.45	0.40
3:D:10:DC:H2''	3:D:11:DG:O5'	2.21	0.40
3:D:18:DA:C2	4:E:4:DG:N2	2.89	0.40
1:A:54:PHE:CE1	1:A:56:THR:O	2.75	0.40
1:A:54:PHE:CE2	1:A:101:GLU:OE1	2.74	0.40
1:A:125:PHE:CE1	1:A:418:PHE:HZ	2.32	0.40
1:A:137:SER:OG	1:A:138:LEU:HD22	2.21	0.40
1:A:252:ILE:HD12	1:A:315:LEU:C	2.46	0.40
1:A:292:ARG:O	1:A:359:GLY:HA2	2.22	0.40
1:A:305:LEU:CD2	1:A:306:LEU:N	2.82	0.40
1:A:350:CYS:N	2:C:432:SER:HB3	2.37	0.40
2:B:34:LEU:CB	2:B:110:MET:SD	3.07	0.40
2:B:148:GLN:OE1	3:D:6:DA:C8	2.74	0.40
2:B:246:LEU:HD13	2:B:247:GLY:N	2.36	0.40
2:B:334:LEU:HD12	2:B:357:PHE:HB3	2.03	0.40
2:C:103:ILE:O	2:C:107:VAL:HG23	2.21	0.40
2:C:230:LEU:C	2:C:230:LEU:CD1	2.94	0.40
2:C:345:PHE:CD2	4:E:6:DA:C2	3.10	0.40
2:C:429:VAL:HG12	2:C:430:ALA:N	2.37	0.40
3:D:1:DG:C8	3:D:2:DT:H71	2.56	0.40
1:A:54:PHE:CZ	1:A:56:THR:O	2.74	0.40
1:A:75:PRO:HG3	1:A:111:LEU:CD1	2.41	0.40
1:A:98:LEU:CB	1:A:99:PRO:CD	2.99	0.40
1:A:223:PHE:CD1	1:A:370:VAL:O	2.74	0.40
1:A:232:LEU:HD23	1:A:233:THR:C	2.46	0.40
2:B:6:LEU:CB	2:B:117:ASN:HB2	2.45	0.40
2:B:269:PHE:N	2:B:269:PHE:HD1	2.18	0.40
2:B:316:PHE:C	2:B:316:PHE:CD1	2.98	0.40
2:B:350:VAL:O	2:B:350:VAL:HG23	2.20	0.40
2:C:38:LYS:CD	2:C:56:TRP:CE2	3.04	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	462/464 (100%)	433 (94%)	22 (5%)	7 (2%)	8	40
2	B	527/529 (100%)	503 (95%)	18 (3%)	6 (1%)	11	46
2	C	527/529 (100%)	503 (95%)	20 (4%)	4 (1%)	16	54
All	All	1516/1522 (100%)	1439 (95%)	60 (4%)	17 (1%)	14	46

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	296	SER
1	A	326	THR
1	A	248	VAL
2	B	472	ASP
2	C	472	ASP
1	A	2	SER
2	B	4	ASN
2	B	272	ALA
2	B	432	SER
2	C	4	ASN
2	C	272	ALA
1	A	206	ASN
1	A	215	ASN
2	B	464	ASP
2	B	274	GLY
2	C	274	GLY

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	398/398 (100%)	388 (98%)	10 (2%)	42	63
2	B	452/452 (100%)	443 (98%)	9 (2%)	48	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	452/452 (100%)	442 (98%)	10 (2%)	45 64
All	All	1302/1302 (100%)	1273 (98%)	29 (2%)	45 64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	TRP
1	A	28	LYS
1	A	112	ARG
1	A	145	ASN
1	A	234	GLU
1	A	239	LEU
1	A	284	GLN
1	A	313	ASN
1	A	444	LEU
2	B	87	GLN
2	B	113	LEU
2	B	259	LYS
2	B	287	ASN
2	B	346	TYR
2	B	453	GLU
2	B	484	VAL
2	B	488	GLU
2	B	492	GLU
2	C	87	GLN
2	C	113	LEU
2	C	259	LYS
2	C	287	ASN
2	C	346	TYR
2	C	434	GLU
2	C	453	GLU
2	C	484	VAL
2	C	488	GLU
2	C	492	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	ASN
1	A	65	ASN
1	A	96	GLN
1	A	97	HIS
1	A	124	HIS
1	A	133	ASN
1	A	143	ASN
1	A	146	ASN
1	A	191	GLN
1	A	215	ASN
1	A	220	HIS
1	A	227	ASN
1	A	237	ASN
1	A	244	ASN
1	A	250	HIS
1	A	262	HIS
1	A	265	GLN
1	A	279	ASN
1	A	281	HIS
1	A	294	ASN
1	A	312	GLN
1	A	313	ASN
1	A	345	ASN
1	A	349	ASN
1	A	357	GLN
1	A	368	GLN
1	A	398	GLN
1	A	407	ASN
2	B	2	ASN
2	B	3	ASN
2	B	4	ASN
2	B	25	GLN
2	B	29	ASN
2	B	87	GLN
2	B	91	HIS
2	B	194	ASN
2	B	232	HIS
2	B	237	ASN
2	B	240	HIS
2	B	256	ASN
2	B	261	HIS
2	B	276	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	287	ASN
2	B	294	GLN
2	B	301	HIS
2	B	348	GLN
2	B	397	HIS
2	B	399	GLN
2	B	410	HIS
2	B	435	ASN
2	B	437	ASN
2	C	2	ASN
2	C	3	ASN
2	C	4	ASN
2	C	25	GLN
2	C	29	ASN
2	C	69	GLN
2	C	87	GLN
2	C	91	HIS
2	C	92	ASN
2	C	194	ASN
2	C	232	HIS
2	C	237	ASN
2	C	240	HIS
2	C	256	ASN
2	C	261	HIS
2	C	276	ASN
2	C	287	ASN
2	C	294	GLN
2	C	301	HIS
2	C	348	GLN
2	C	353	ASN
2	C	397	HIS
2	C	399	GLN
2	C	410	HIS
2	C	435	ASN
2	C	437	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	SAM	B	530	-	27,29,29	1.26	5 (18%)	34,42,42	1.91	10 (29%)
5	SAM	C	530	-	27,29,29	1.25	5 (18%)	34,42,42	1.91	10 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAM	B	530	-	-	2/17/33/33	0/3/3/3
5	SAM	C	530	-	-	2/17/33/33	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	530	SAM	C2-N1	2.90	1.39	1.33
5	C	530	SAM	C2-N1	2.88	1.39	1.33
5	C	530	SAM	C2-N3	2.72	1.38	1.33
5	B	530	SAM	C2-N3	2.71	1.38	1.33
5	B	530	SAM	C5-N7	-2.57	1.34	1.39
5	C	530	SAM	C5-N7	-2.56	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	530	SAM	OXT-C	-2.44	1.22	1.30
5	B	530	SAM	OXT-C	-2.42	1.22	1.30
5	B	530	SAM	C8-N7	2.13	1.35	1.31
5	C	530	SAM	C8-N7	2.08	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	530	SAM	N3-C2-N1	-5.24	120.65	128.58
5	B	530	SAM	N3-C2-N1	-5.22	120.69	128.58
5	B	530	SAM	C5-C4-N3	-3.87	121.38	126.72
5	C	530	SAM	C5-C4-N3	-3.84	121.43	126.72
5	C	530	SAM	OXT-C-O	-3.65	115.81	124.08
5	B	530	SAM	OXT-C-O	-3.62	115.87	124.08
5	B	530	SAM	C5-N7-C8	3.37	108.74	103.45
5	C	530	SAM	C5-N7-C8	3.35	108.72	103.45
5	C	530	SAM	N9-C8-N7	-3.14	109.48	113.94
5	B	530	SAM	N9-C8-N7	-3.14	109.48	113.94
5	B	530	SAM	C4-C5-N7	-3.02	107.13	110.58
5	C	530	SAM	C4-C5-N7	-2.98	107.17	110.58
5	B	530	SAM	C2-N3-C4	2.74	118.53	111.83
5	C	530	SAM	C2-N3-C4	2.73	118.50	111.83
5	B	530	SAM	C6-C5-C4	2.36	120.40	117.18
5	C	530	SAM	C6-C5-C4	2.32	120.34	117.18
5	B	530	SAM	C5-C4-N9	2.21	108.22	105.81
5	C	530	SAM	O2'-C2'-C3'	2.16	118.75	111.82
5	C	530	SAM	C5-C4-N9	2.15	108.15	105.81
5	B	530	SAM	O2'-C2'-C3'	2.14	118.67	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

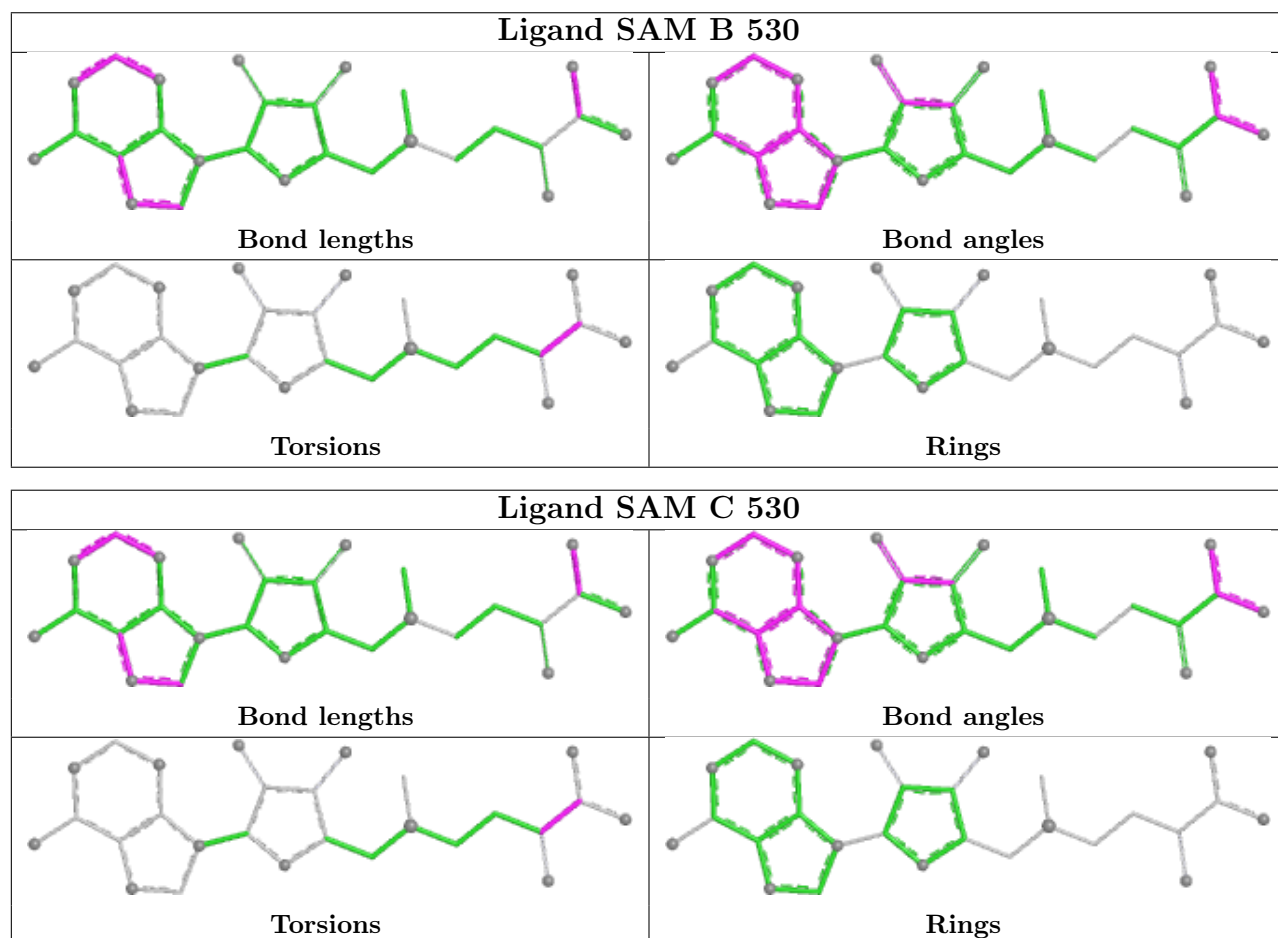
Mol	Chain	Res	Type	Atoms
5	B	530	SAM	OXT-C-CA-CB
5	C	530	SAM	OXT-C-CA-CB
5	B	530	SAM	O-C-CA-CB
5	C	530	SAM	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	530	SAM	28	0
5	C	530	SAM	30	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	292:ARG	C	293:TYR	N	1.68
1	A	295:GLY	C	296:SER	N	1.18

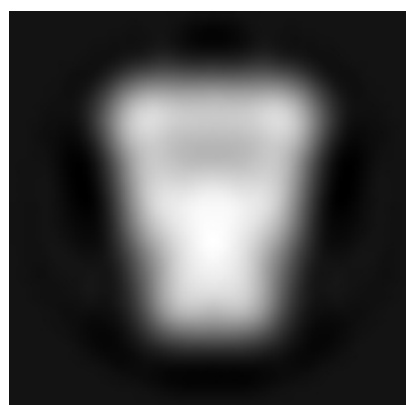
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1534. These allow visual inspection of the internal detail of the map and identification of artifacts.

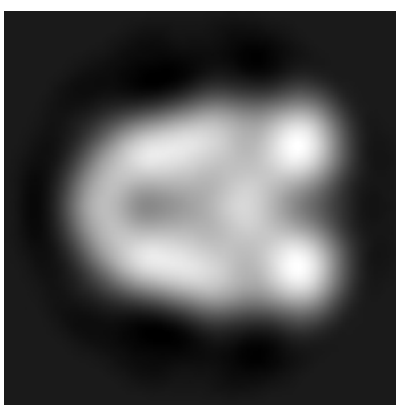
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

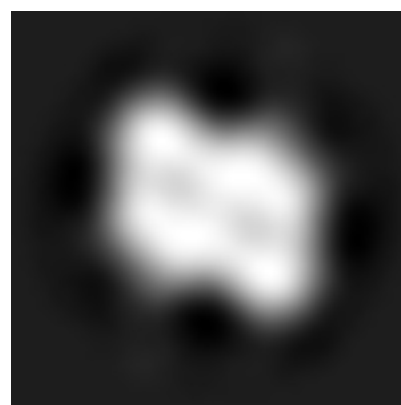
6.1.1 Primary map



X



Y

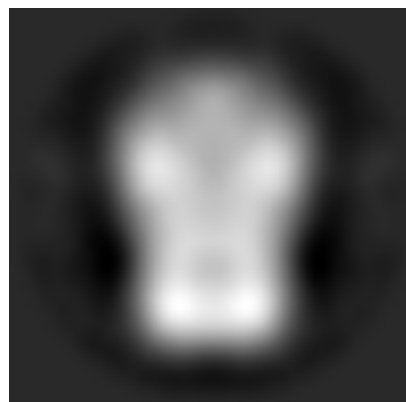


Z

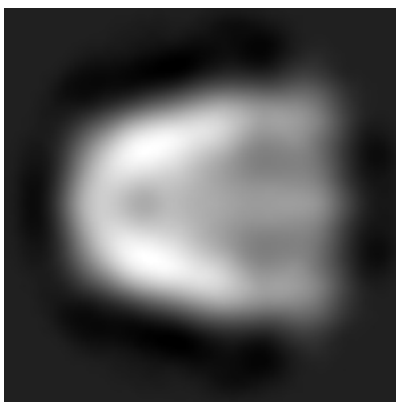
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

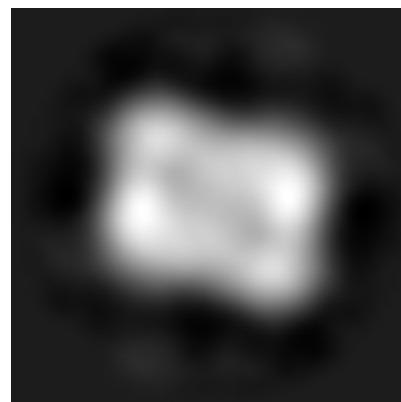
6.2.1 Primary map



X Index: 24



Y Index: 24

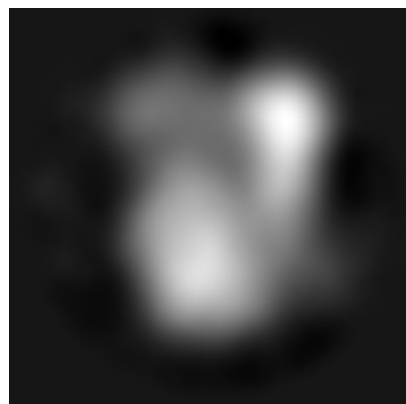


Z Index: 24

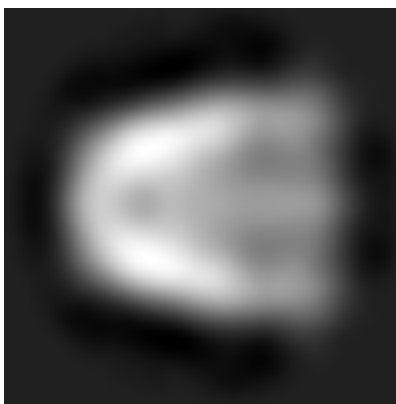
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

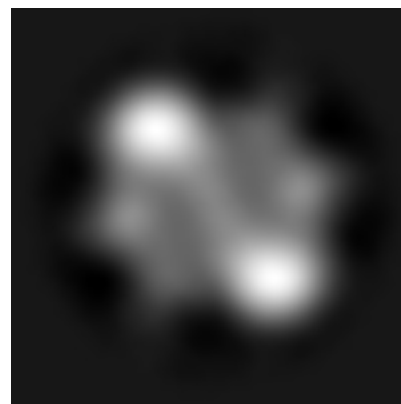
6.3.1 Primary map



X Index: 18



Y Index: 24

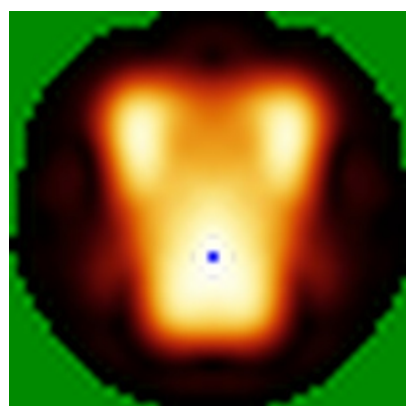


Z Index: 33

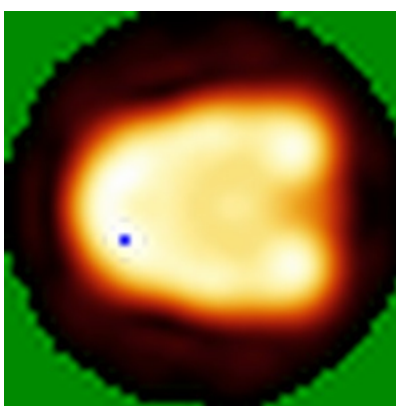
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

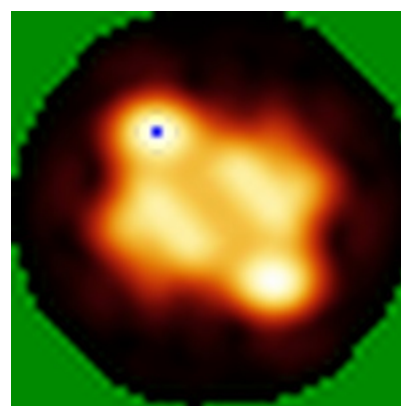
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

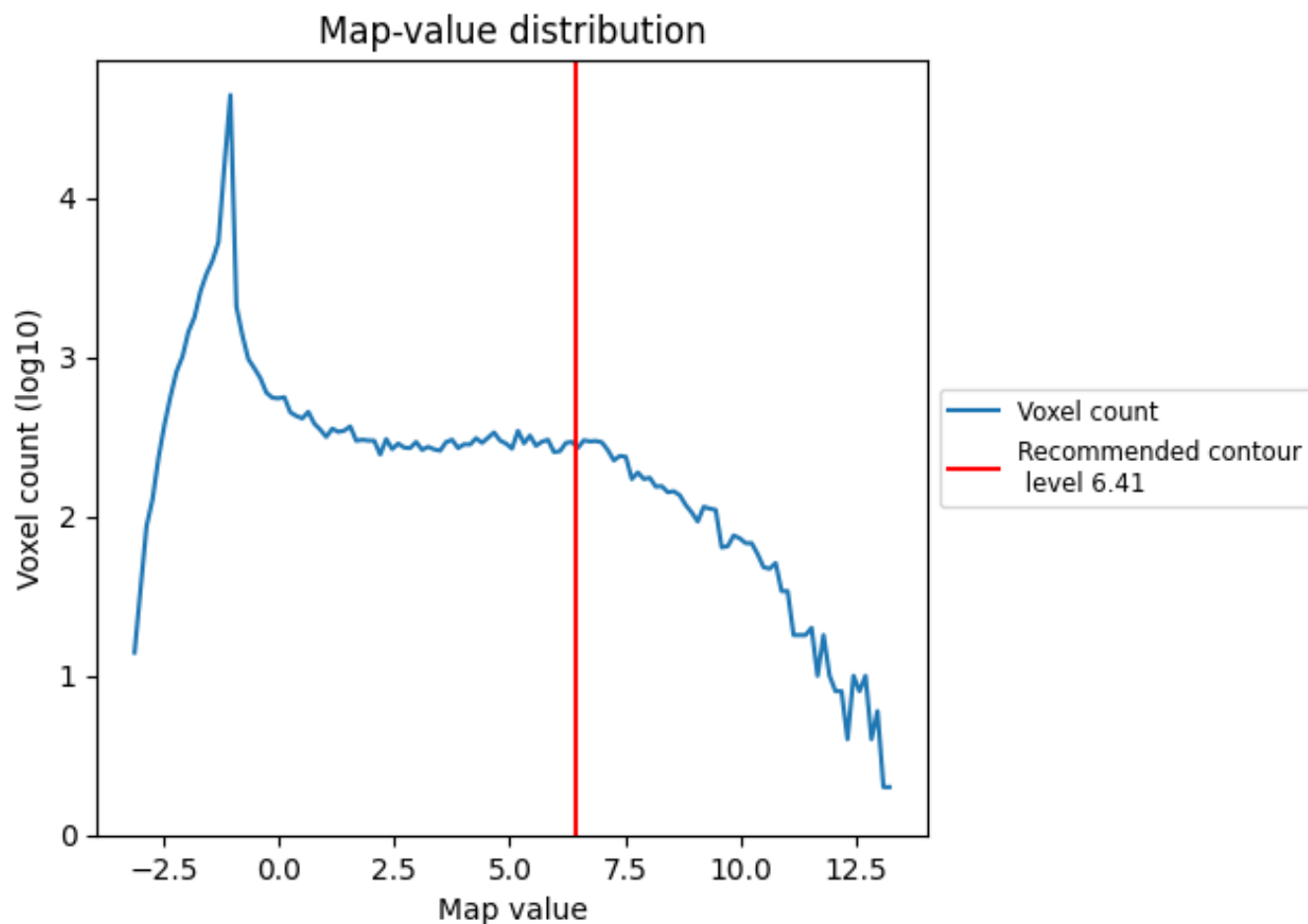
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

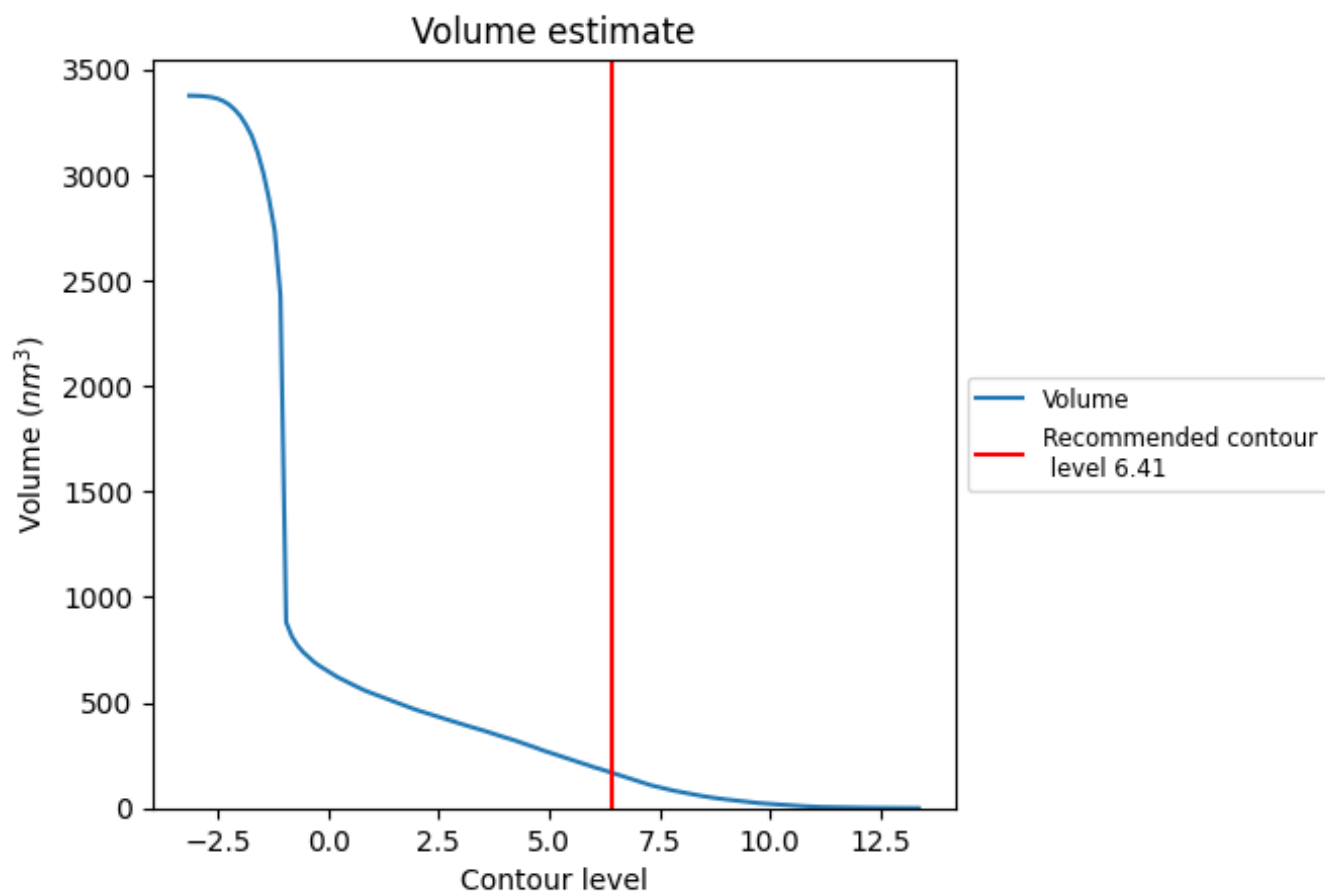
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

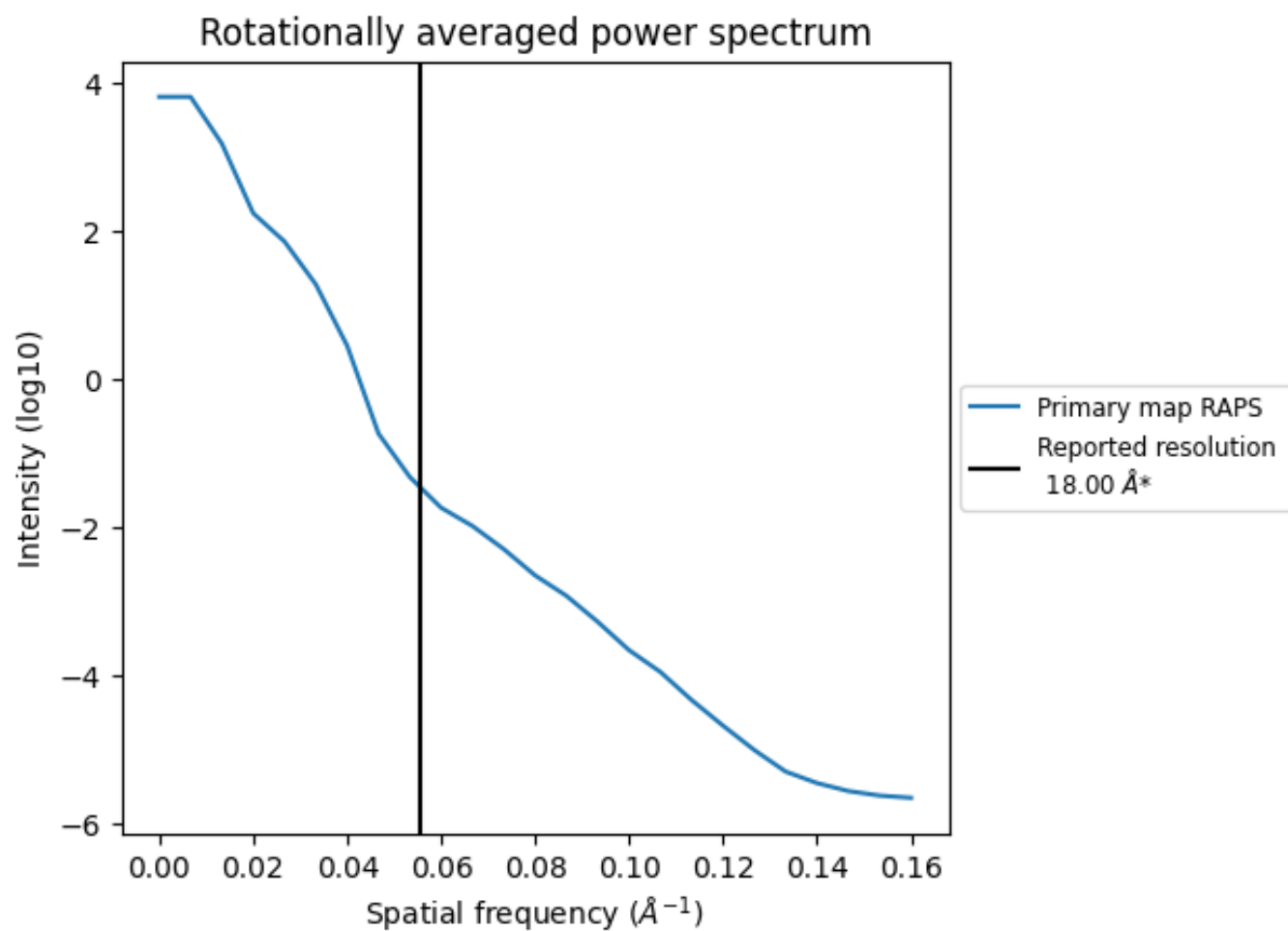
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm^3 ; this corresponds to an approximate mass of 152 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.056 Å⁻¹

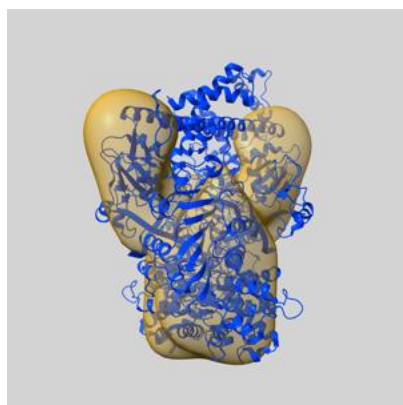
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

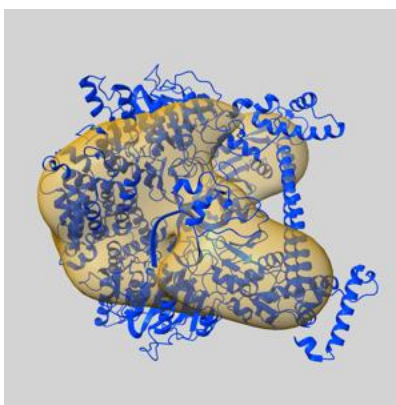
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1534 and PDB model 2Y7H. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

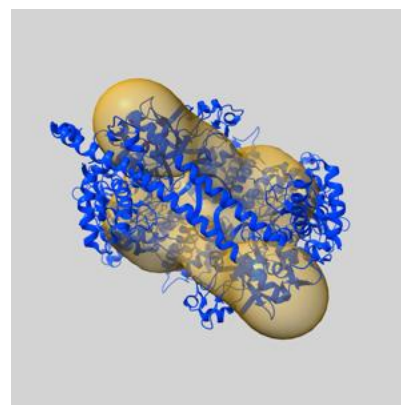
9.1 Map-model overlay [i](#)



X



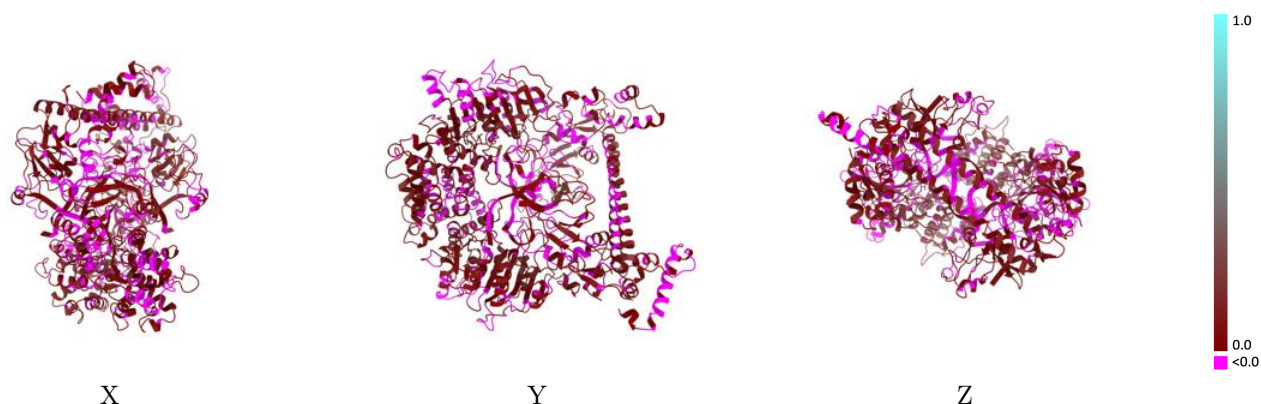
Y



Z

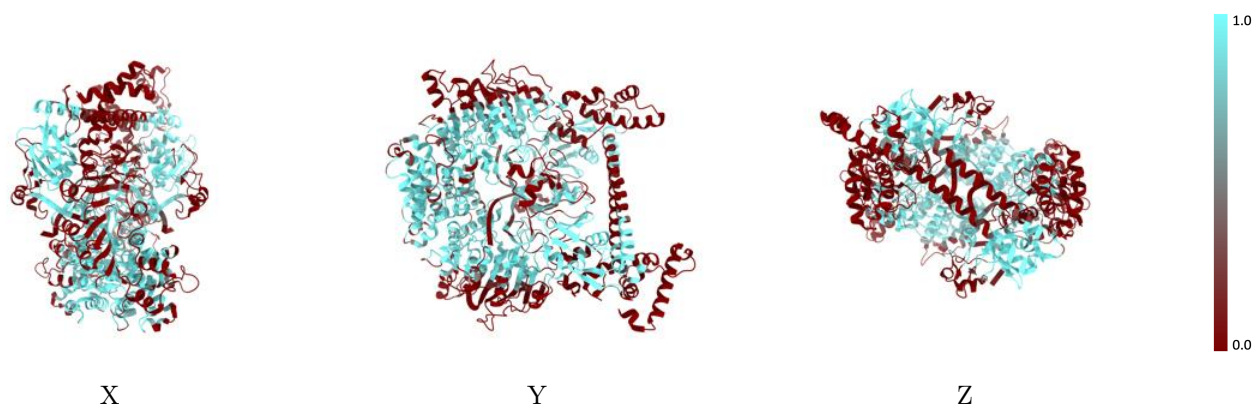
The images above show the 3D surface view of the map at the recommended contour level 6.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



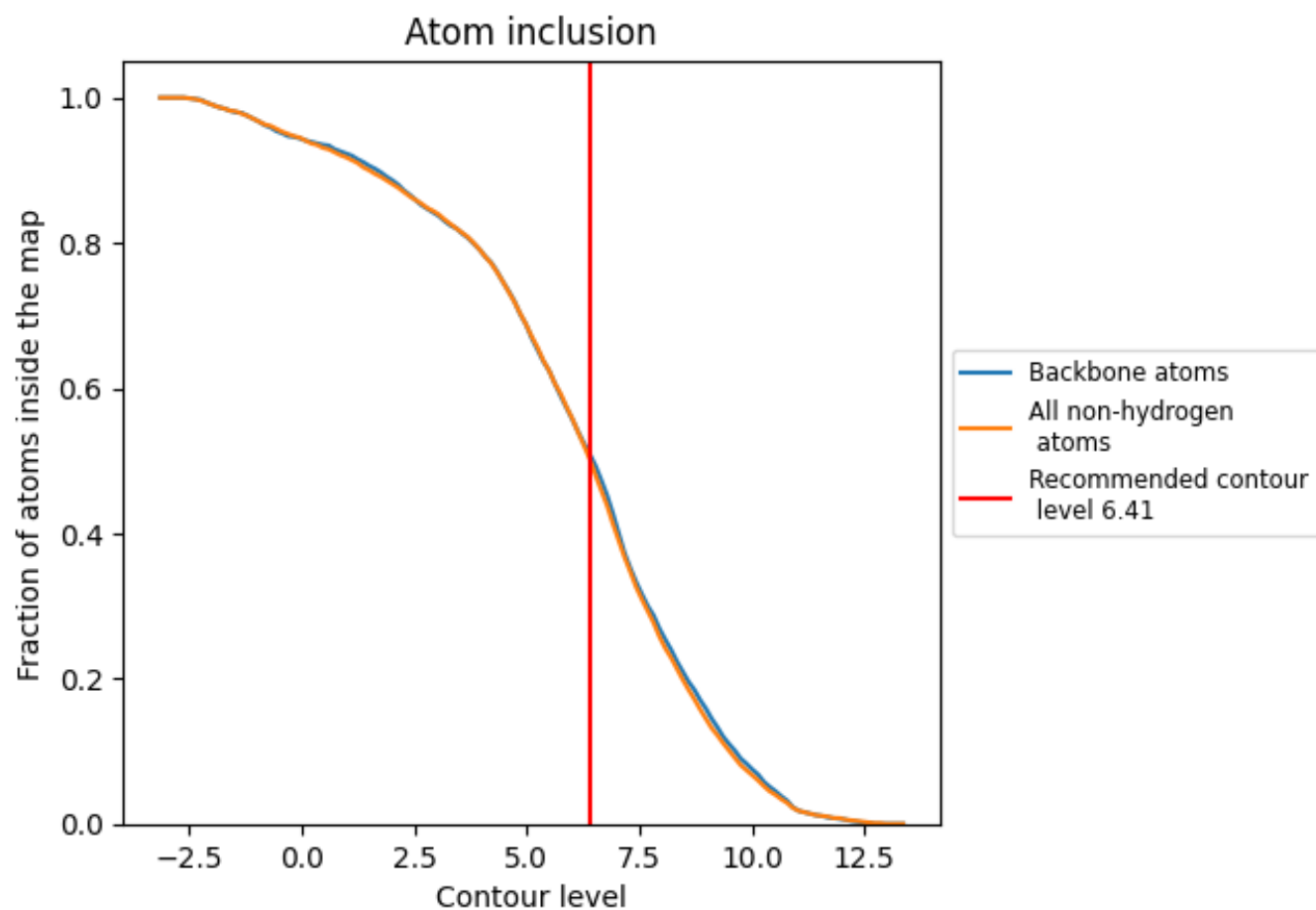
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.41).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5010	0.0340
A	0.4710	0.0330
B	0.5180	0.0400
C	0.5200	0.0350
D	0.4300	-0.0030
E	0.4570	-0.0010

