



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:06 AM GMT

PDB ID : 3H1I  
Title : Stigmatellin and antimycin bound cytochrome bc1 complex from chicken  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.  
Deposited on : 2009-04-12  
Resolution : 3.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



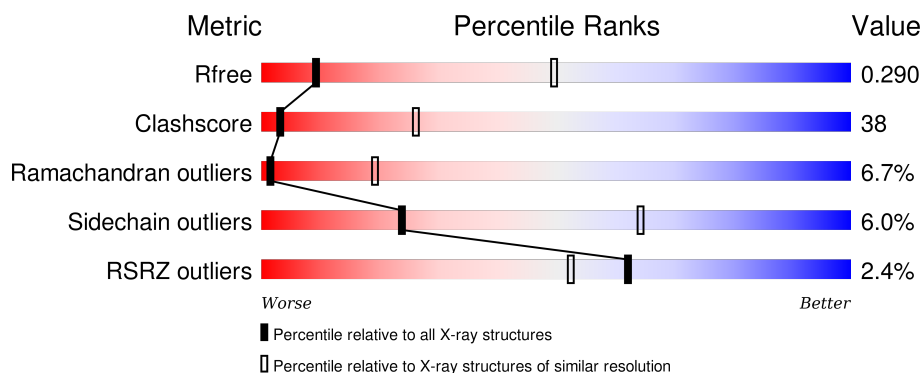
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.53 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)


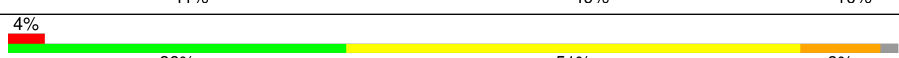

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>0%</div> <div> <div>41%</div> <div>52%</div> <div>7%</div> </div> </div>
1	N	446	<div> <div>2%</div> <div> <div>39%</div> <div>52%</div> <div>7%</div> </div> </div>
2	B	441	<div> <div>0%</div> <div> <div>36%</div> <div>52%</div> <div>7%</div> <div>5%</div> </div> </div>
2	O	441	<div> <div>2%</div> <div> <div>38%</div> <div>50%</div> <div>7%</div> </div> </div>
3	C	380	<div> <div>39%</div> <div>53%</div> <div>7%</div> </div>

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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
13	FES	E	501	-	-	X	-
14	SMA	P	3001	-	-	-	X
15	ANY	C	2002	X	-	-	-
15	ANY	P	3002	X	-	-	-
16	CDL	D	2003	-	-	-	X
16	CDL	P	3004	-	-	-	X
16	CDL	Q	3003	-	-	-	X
17	PEE	A	2008	-	-	-	X
17	PEE	C	2007	-	-	-	X
17	PEE	E	2005	-	-	-	X
17	PEE	P	3005	-	-	-	X
17	PEE	P	3007	-	-	-	X

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	PLC	E	2009	-	-	-	X
18	PLC	R	3009	-	-	-	X
19	UNL	C	2010	-	-	-	X
19	UNL	E	3103	-	-	-	X
19	UNL	R	2103	-	-	-	X
20	GOL	C	2011	-	-	-	X
20	GOL	P	3011	-	-	-	X



## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32701 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

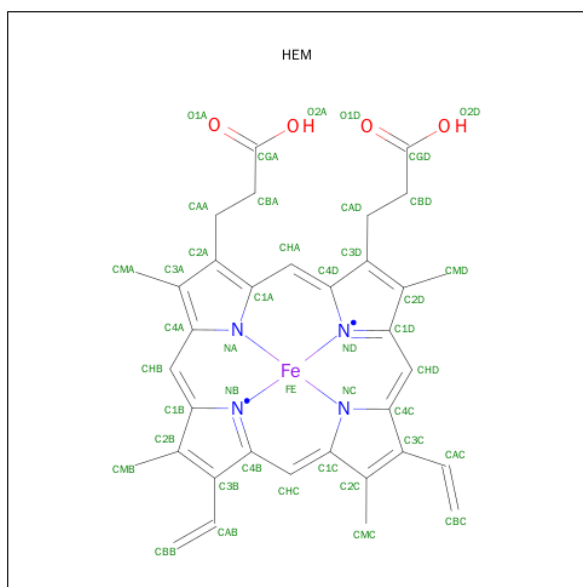
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

- Molecule 10 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total 497	C 321	N 87	O 89	0	0	0
10	W	59	Total 478	C 311	N 85	O 82	0	0	0

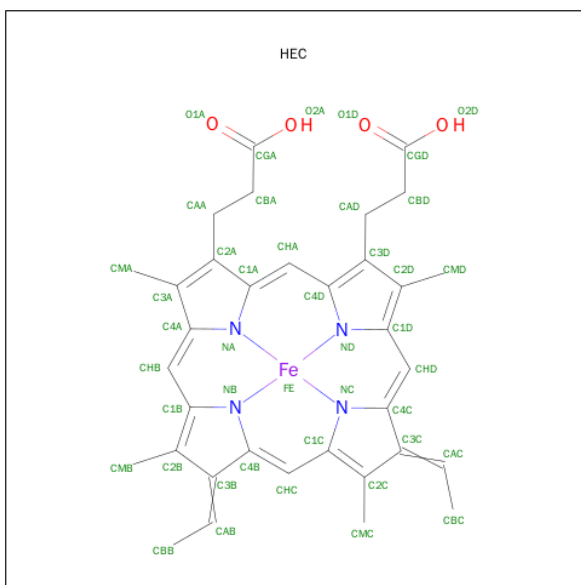
- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

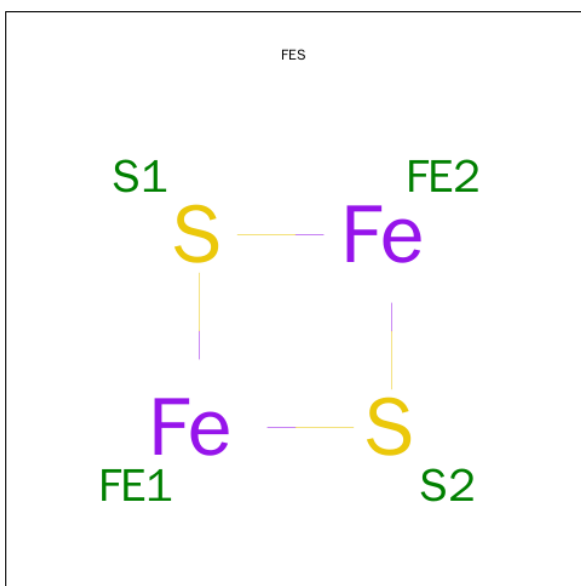
- Molecule 12 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total 4	Fe 2	S 2	0	0
13	R	1	Total 4	Fe 2	S 2	0	0



- 
- The chemical structure of SMA (Silymarin) is shown with atom labels. The structure consists of a flavanone core (chromone) substituted with a methoxy group (O1, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C820, C821, C822, C823, C824, C825, C826, C827, C828, C82

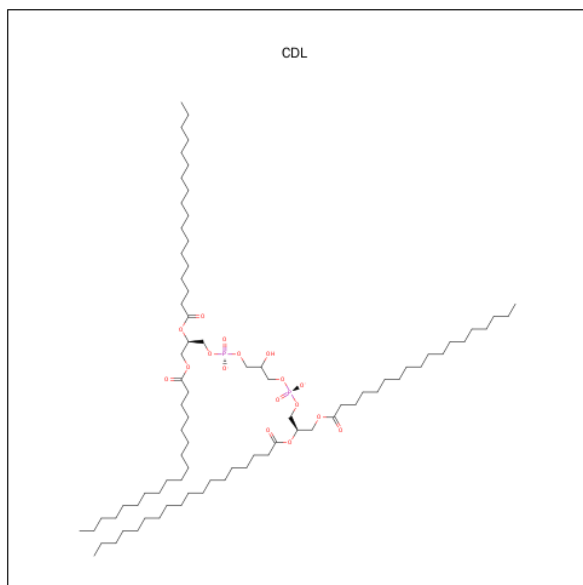
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total 37	C 30	O 7	0	0
14	P	1	Total 37	C 30	O 7	0	0

-



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	N	O	0	0
			37	26	2	9		
15	P	1	Total	C	N	O	0	0
			37	26	2	9		

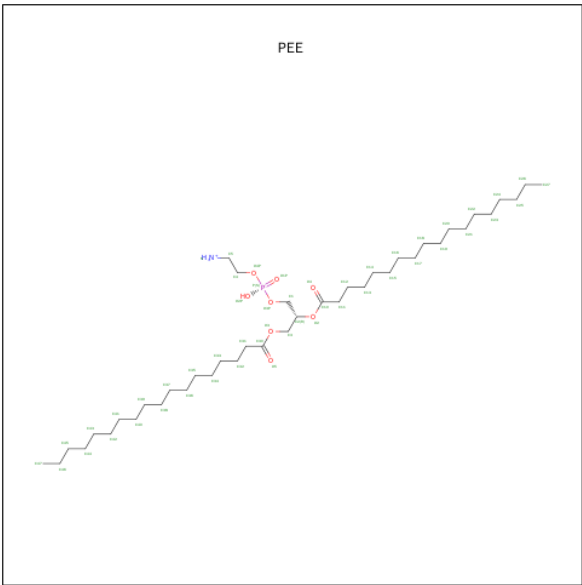
- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	P	0	0
			50	31	17	2		
16	C	1	Total	C	O	P	0	0
			40	21	17	2		
16	Q	1	Total	C	O	P	0	0
			50	31	17	2		
16	P	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 17 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).

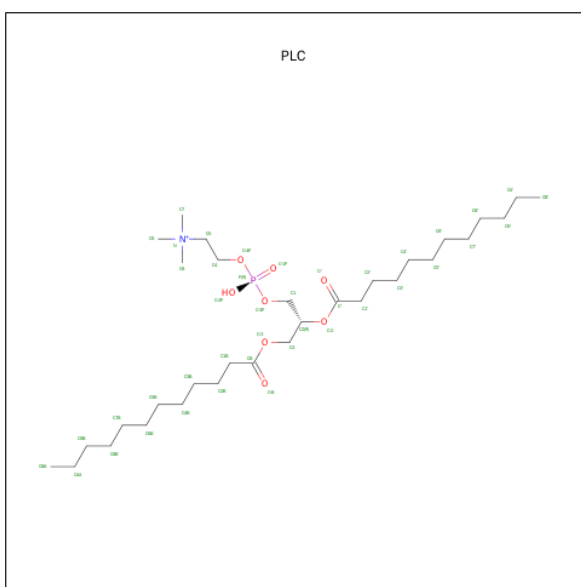




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
17	A	1	Total	C	O	P		0	0
			21	12	8	1			
17	P	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
17	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
17	N	1	Total	O	P			0	0
			5	4	1				

- Molecule 18 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).





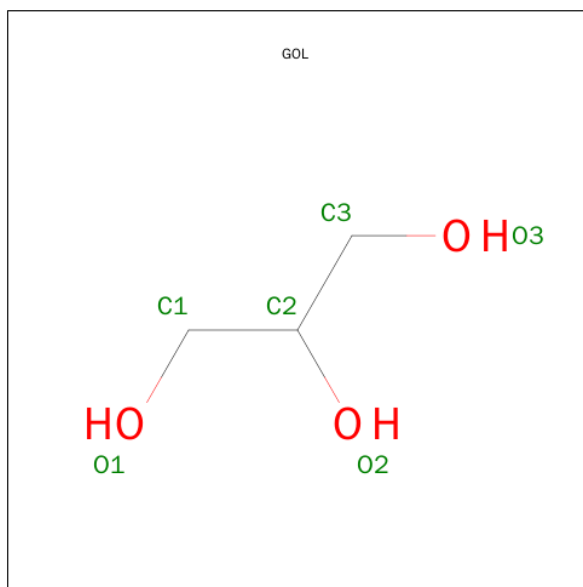
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
18	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

- Molecule 19 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	P	3	Total	O	0	0
			3	3		
19	R	1	Total	O	0	0
			1	1		
19	A	1	Total	O	0	0
			1	1		
19	C	3	Total	O	0	0
			3	3		
19	E	2	Total	O	0	0
			2	2		

- Molecule 20 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





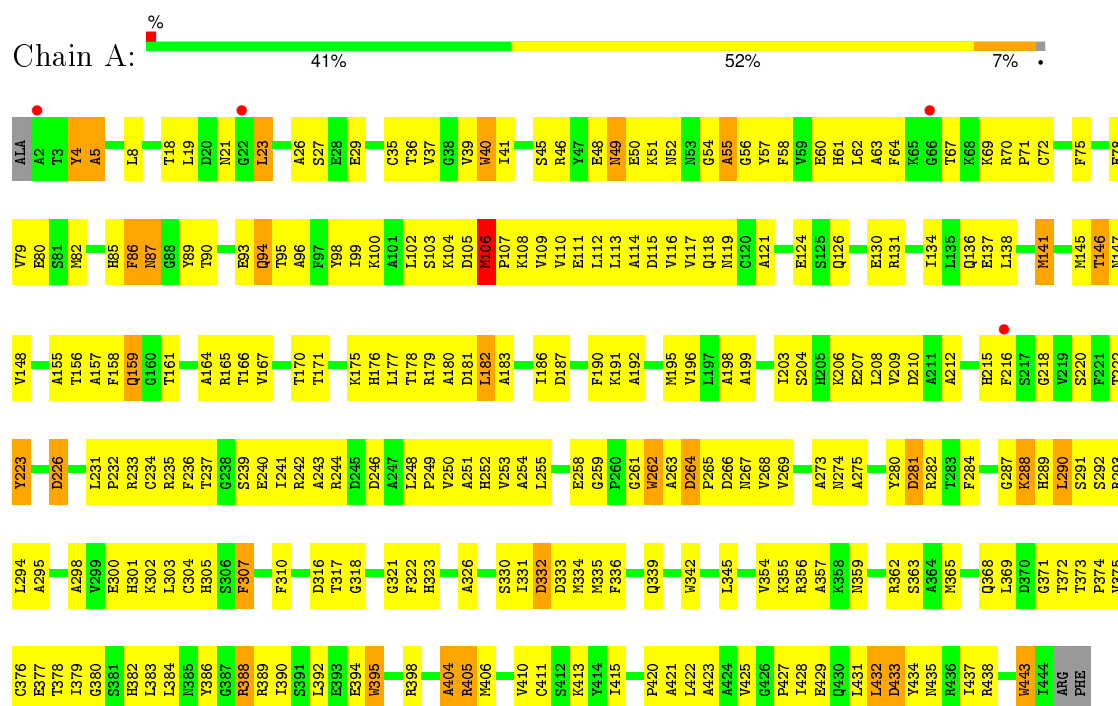
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		



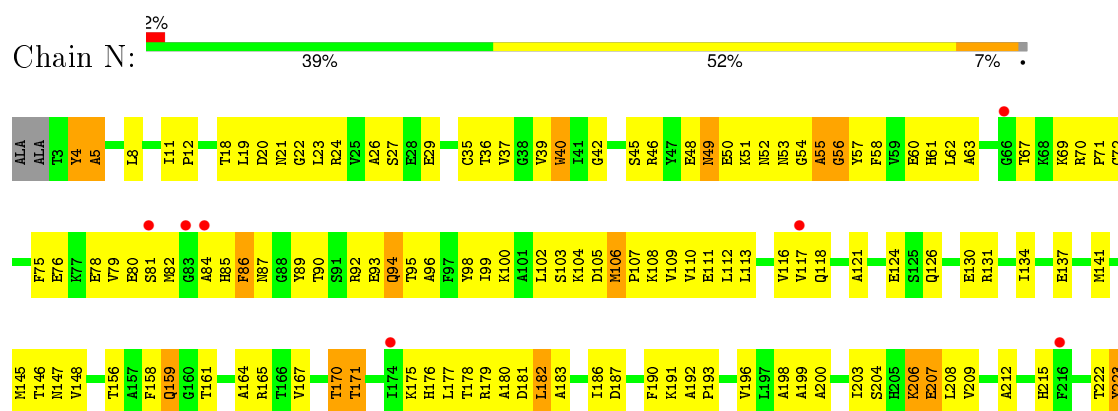
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

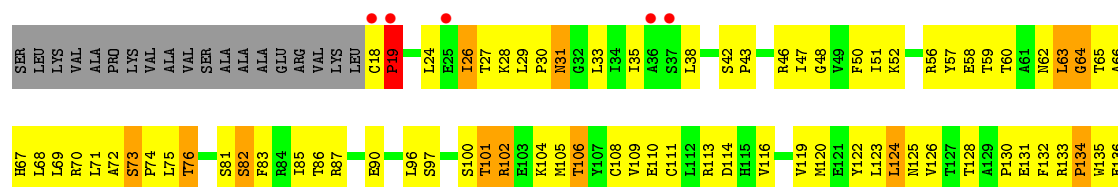
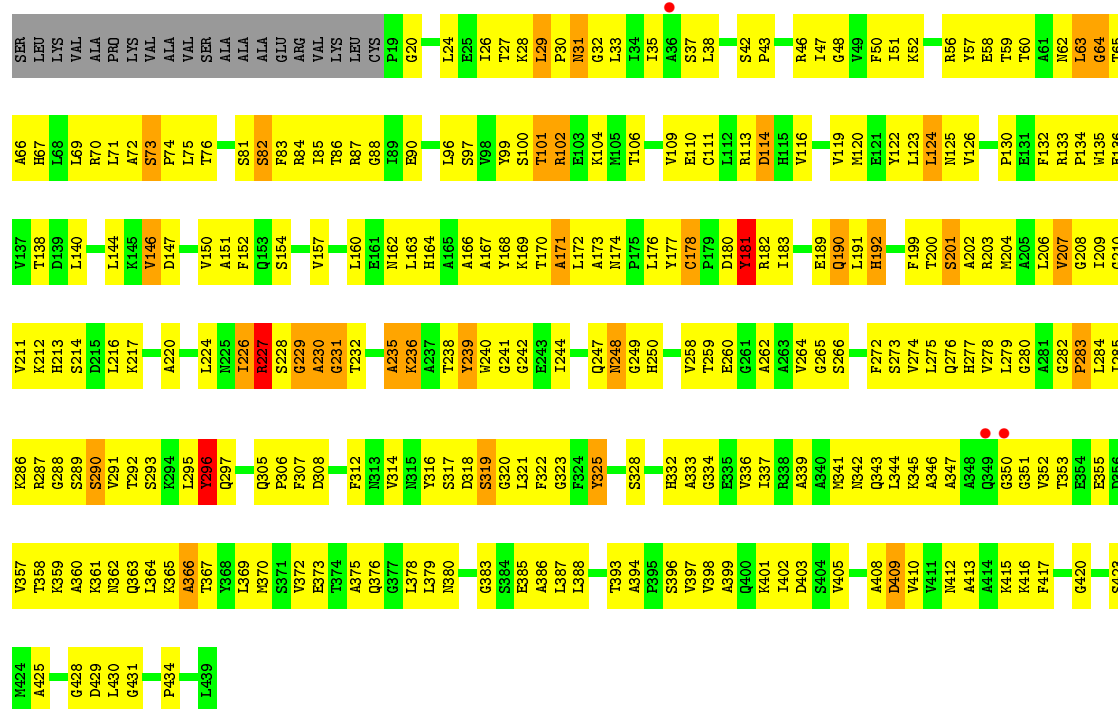
#### • Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL



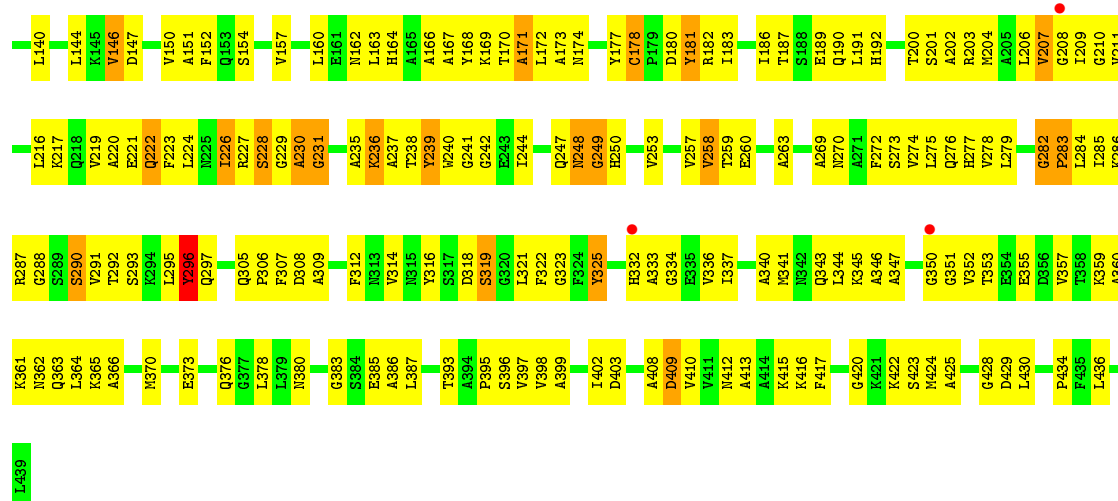
#### • Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL



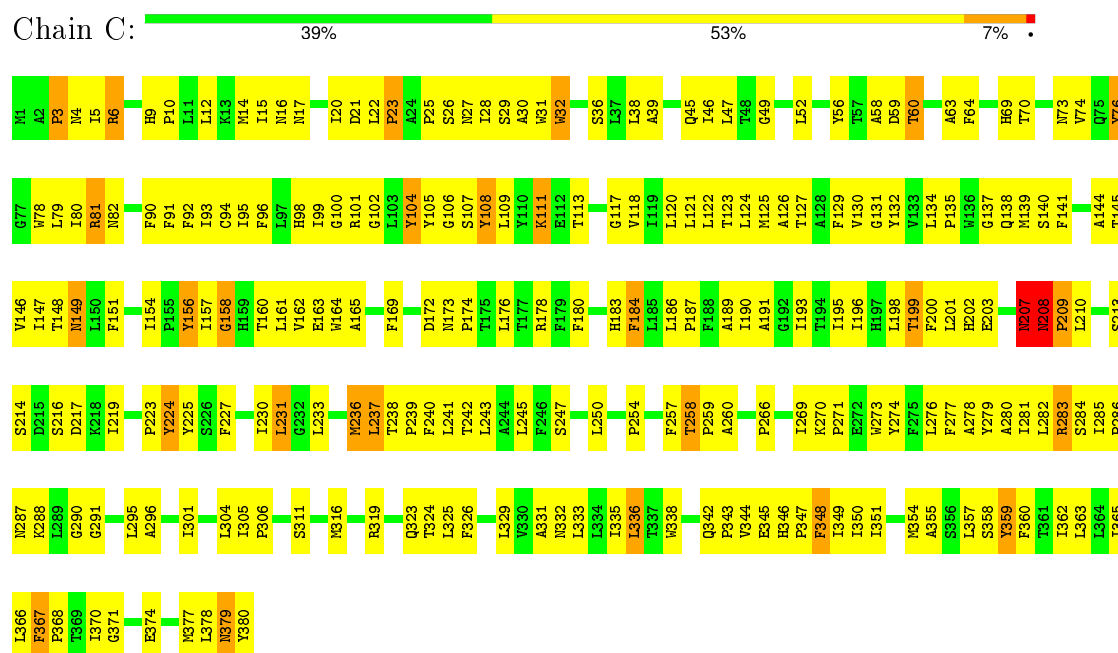




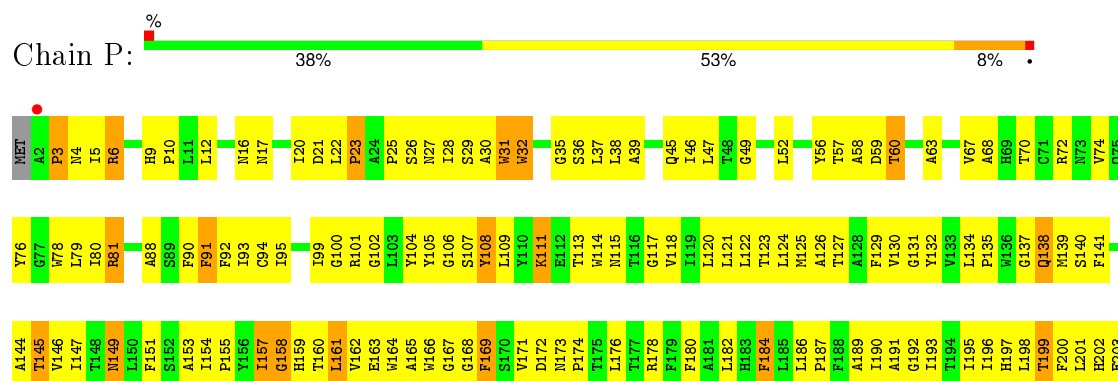




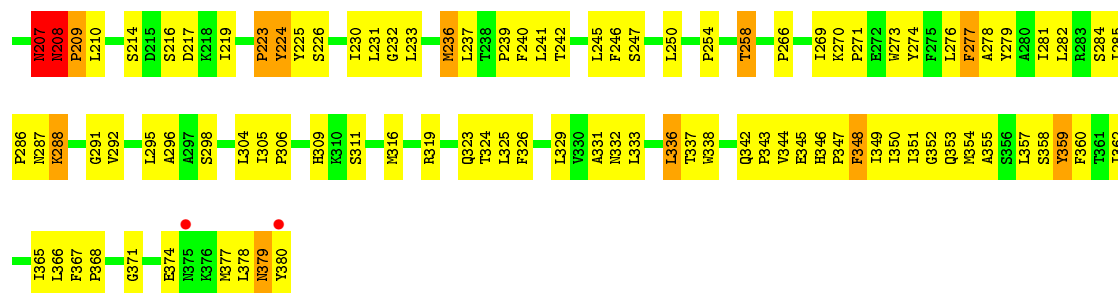
• Molecule 3: Cytochrome b



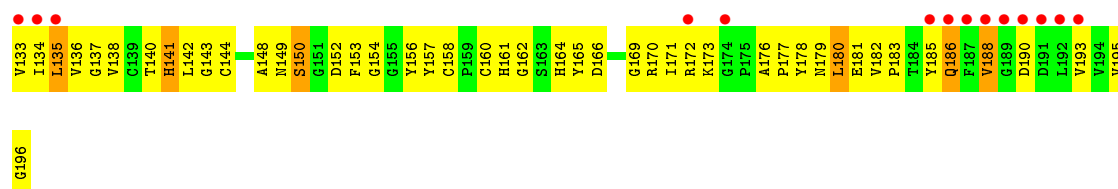
• Molecule 3: Cytochrome b



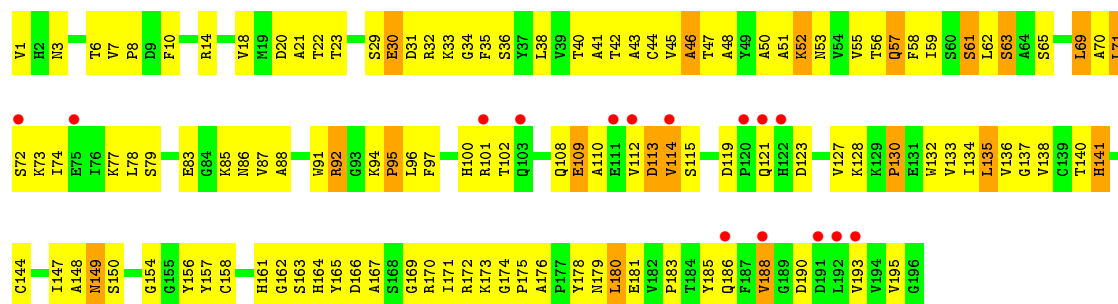




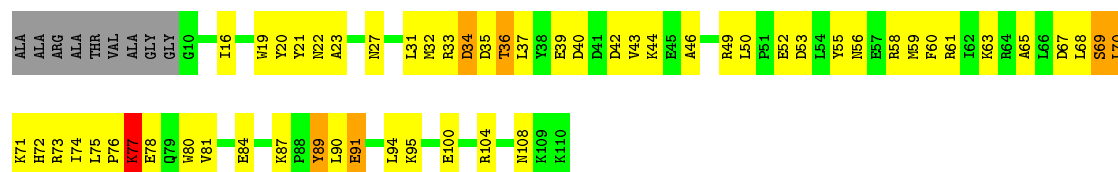




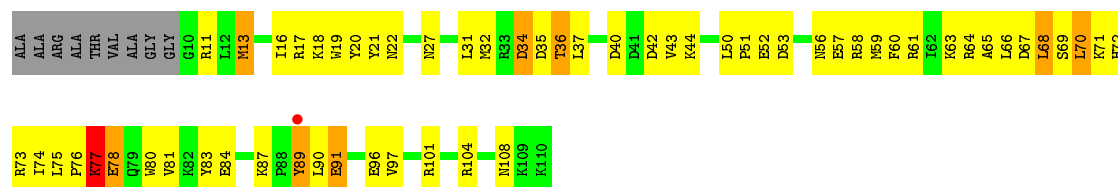
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



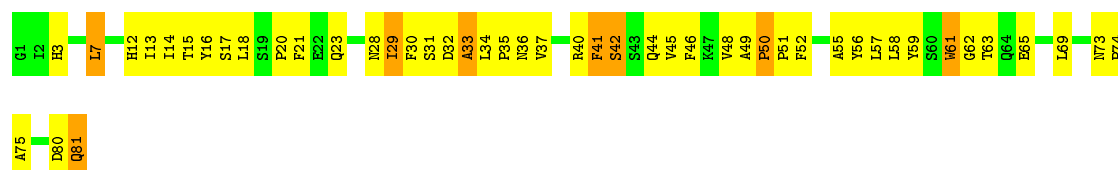
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN



• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN

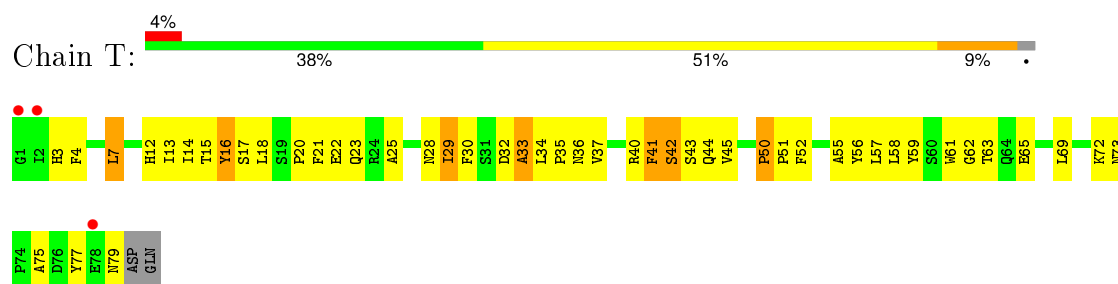


• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

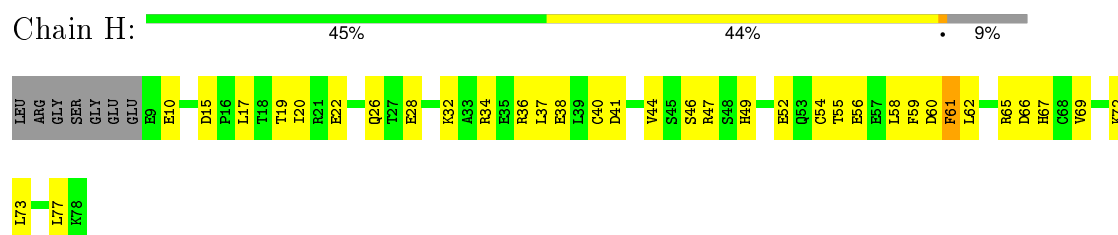




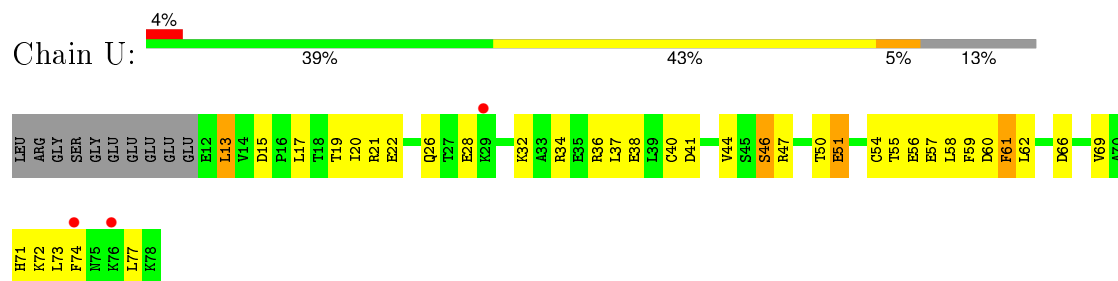
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



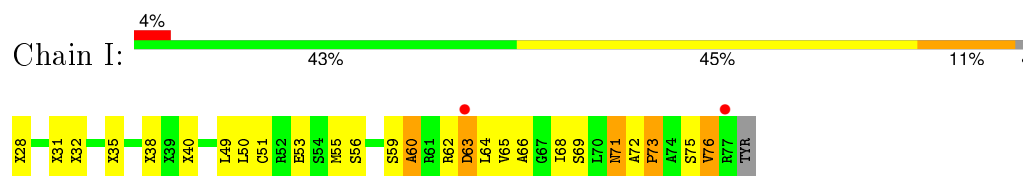
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



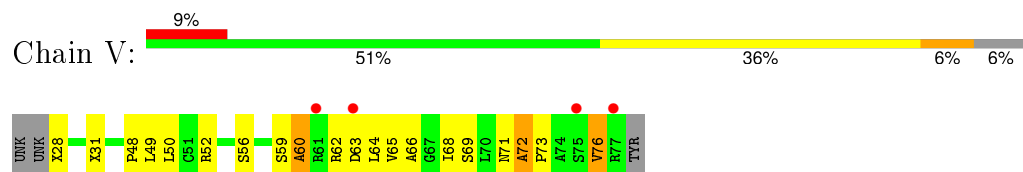
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



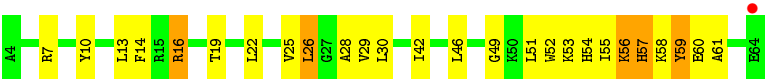
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



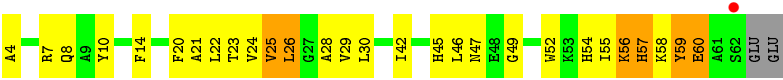
• Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN







● Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.69Å 181.67Å 240.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.53 49.53 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.99-3.53) 90.6 (49.53-3.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.263 , 0.306 0.250 , 0.290	Depositor DCC
$R_{free}$ test set	2551 reflections (3.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.5	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 85476 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	32701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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: GOL, CDL, UNL, PLC, FES, HEC, HEM, PEE, ANY, SMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/3511	0.69	0/4757
1	N	0.49	0/3508	0.69	0/4753
2	B	0.43	0/3196	0.67	0/4334
2	O	0.44	0/3202	0.67	0/4343
3	C	0.59	0/3122	0.76	0/4273
3	P	0.53	0/3114	0.72	0/4263
4	D	0.52	0/1956	0.69	0/2658
4	Q	0.43	0/1956	0.67	0/2658
5	E	0.43	0/1547	0.70	3/2103 (0.1%)
5	R	0.46	0/1547	0.71	1/2103 (0.0%)
6	F	0.55	0/911	0.70	0/1219
6	S	0.49	0/911	0.65	0/1219
7	G	0.56	0/698	0.68	0/946
7	T	0.49	0/680	0.64	0/923
8	H	0.48	0/582	0.61	0/779
8	U	0.39	0/561	0.58	0/751
9	I	0.45	0/218	0.69	0/293
9	V	0.44	0/218	0.66	0/293
10	J	0.48	0/508	0.62	0/682
10	W	0.46	0/489	0.63	0/658
All	All	0.49	0/32435	0.69	4/44008 (0.0%)

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
3	C	0	1

There are no bond length outliers.



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	LEU	N-CA-C	5.94	127.03	111.00
5	E	143	GLY	N-CA-C	5.88	127.80	113.10
5	E	71	LEU	N-CA-C	5.87	126.84	111.00
5	E	70	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	104	TYR	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	3440	0	3353	266	0
1	N	3437	0	3349	273	0
2	B	3141	0	3142	276	0
2	O	3147	0	3146	300	0
3	C	3020	0	3070	259	0
3	P	3012	0	3058	284	0
4	D	1898	0	1846	154	0
4	Q	1898	0	1846	161	0
5	E	1513	0	1478	136	0
5	R	1513	0	1478	120	0
6	F	891	0	893	65	0
6	S	891	0	893	73	0
7	G	676	0	659	58	0
7	T	658	0	647	63	0
8	H	574	0	548	27	0
8	U	553	0	535	38	0
9	I	285	0	239	30	0
9	V	275	0	238	30	0
10	J	497	0	490	25	0
10	W	478	0	478	33	0
11	C	86	0	60	20	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	86	0	60	22	0
12	D	43	0	30	6	0
12	Q	43	0	30	4	0
13	E	4	0	0	2	0
13	R	4	0	0	1	0
14	C	37	0	42	3	0
14	P	37	0	42	4	0
15	C	37	0	28	3	0
15	P	37	0	29	1	0
16	C	40	0	24	2	0
16	D	50	0	44	1	0
16	P	40	0	24	2	0
16	Q	50	0	44	5	0
17	A	21	0	13	0	0
17	C	49	0	72	2	0
17	E	50	0	77	1	0
17	N	5	0	0	0	0
17	P	99	0	149	6	0
18	E	32	0	38	2	0
18	R	32	0	38	3	0
19	A	1	0	0	0	0
19	C	3	0	0	0	0
19	E	2	0	0	0	0
19	P	3	0	0	0	0
19	R	1	0	0	0	0
20	C	6	0	8	1	0
20	P	6	0	8	0	0
All	All	32701	0	32246	2460	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 38.

All (2460) 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)
3:P:157:ILE:HG13	3:P:158:GLY:H	1.04	1.15
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.19	1.12
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.67	1.07
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.36	1.04
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.38	1.03
3:P:46:ILE:HA	11:P:501:HEM:HMC2	1.40	1.02

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:ILE:HD12	7:T:29:ILE:H	1.25	1.01
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.43	1.00
3:P:271:PRO:HA	14:P:3001:SMA:H10	1.42	1.00
4:D:47:ALA:H	4:D:50:ASN:HD22	1.07	0.97
3:C:46:ILE:HA	11:C:501:HEM:HMC2	1.43	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.97
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.31	0.95
2:B:207:VAL:HG12	2:B:208:GLY:H	1.29	0.95
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.33	0.94
7:G:29:ILE:HD12	7:G:29:ILE:H	1.30	0.93
12:D:501:HEC:HBB3	12:D:501:HEC:HMB1	1.50	0.93
5:E:103:GLN:HA	5:E:106:ILE:HB	1.49	0.93
8:U:13:LEU:H	8:U:13:LEU:HD23	1.34	0.93
2:O:207:VAL:HG12	2:O:208:GLY:H	1.34	0.92
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.51	0.92
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.31	0.91
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.52	0.91
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
3:P:157:ILE:HG13	3:P:158:GLY:N	1.81	0.90
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.54	0.90
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.11	0.90
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.50	0.90
1:A:137:GLU:O	1:A:141:MET:HG3	1.73	0.89
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.53	0.89
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.08	0.89
3:C:127:THR:HG21	11:C:501:HEM:HBB2	1.53	0.88
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.53	0.88
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.55	0.88
4:D:32:VAL:HG11	4:D:186:VAL:HB	1.56	0.88
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.56	0.87
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.37	0.87
3:P:127:THR:HG21	11:P:501:HEM:HBB2	1.56	0.87
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.21	0.86
17:P:3007:PEE:H7	7:T:44:GLN:HE21	1.38	0.86
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.40	0.86
17:C:2007:PEE:H7	7:G:44:GLN:HE21	1.38	0.86
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.11	0.85
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.58	0.85
2:B:47:ILE:HG12	2:B:120:MET:HE3	1.58	0.85
1:N:137:GLU:O	1:N:141:MET:HG3	1.77	0.85
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.59	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:61:ARG:HH21	6:S:89:TYR:HE2	1.24	0.84
2:O:361:LYS:O	2:O:365:LYS:HG3	1.77	0.84
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.07	0.84
1:N:388:ARG:HG3	1:N:388:ARG:HH21	1.41	0.84
4:Q:215:LEU:HD22	5:R:46:ALA:HB1	1.60	0.84
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.58	0.84
5:R:128:LYS:O	5:R:130:PRO:HD3	1.78	0.83
4:D:235:MET:HB3	7:G:15:THR:HG22	1.61	0.83
3:C:46:ILE:HA	11:C:501:HEM:CMC	2.07	0.83
2:B:76:THR:HG22	2:B:82:SER:H	1.43	0.83
2:B:274:VAL:O	2:B:278:VAL:HG23	1.78	0.83
1:A:206:LYS:O	1:A:209:VAL:HG12	1.78	0.83
10:J:16:ARG:HB3	10:J:19:THR:HG23	1.60	0.83
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.77	0.83
2:O:398:VAL:O	2:O:402:ILE:HG13	1.79	0.83
2:O:274:VAL:O	2:O:278:VAL:HG23	1.78	0.83
4:D:47:ALA:N	4:D:50:ASN:HD22	1.75	0.82
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.61	0.82
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.13	0.82
1:A:130:GLU:O	1:A:134:ILE:HG13	1.80	0.82
2:B:47:ILE:HG12	2:B:120:MET:CE	2.08	0.82
3:C:101:ARG:HD2	3:C:102:GLY:N	1.94	0.81
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.80	0.81
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.62	0.81
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.44	0.81
3:C:247:SER:OG	3:C:250:LEU:HB2	1.81	0.81
12:Q:501:HEC:HBB3	12:Q:501:HEC:HMB1	1.63	0.81
3:P:101:ARG:HD2	3:P:102:GLY:N	1.96	0.81
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.45	0.80
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.63	0.80
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.11	0.80
3:C:101:ARG:C	3:C:101:ARG:HD2	2.01	0.80
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.64	0.80
2:O:128:THR:HA	2:O:226:ILE:HD11	1.63	0.80
3:P:46:ILE:HA	11:P:501:HEM:CMC	2.11	0.80
2:O:150:VAL:HG23	2:O:151:ALA:H	1.47	0.80
3:C:146:VAL:HG21	14:C:2001:SMA:H6	1.63	0.80
5:E:73:LYS:HB3	5:E:195:VAL:O	1.80	0.80
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79
2:O:150:VAL:HG23	2:O:151:ALA:N	1.97	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:ARG:C	3:P:101:ARG:HD2	2.02	0.79
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.62	0.79
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.17	0.79
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.65	0.79
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.64	0.78
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.65	0.78
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.84	0.78
2:B:325:TYR:HD1	9:I:60:ALA:HB2	1.49	0.78
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.18	0.78
2:B:150:VAL:HG23	2:B:151:ALA:N	1.98	0.78
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.47	0.78
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.17	0.78
4:Q:200:GLN:HE21	18:R:3009:PLC:H51	1.48	0.78
2:B:361:LYS:O	2:B:365:LYS:HG3	1.83	0.78
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.64	0.78
1:A:362:ARG:O	1:A:365:MET:HB3	1.84	0.78
1:N:390:ILE:HG23	1:N:394:GLU:OE1	1.84	0.78
3:C:132:TYR:O	3:C:135:PRO:HD2	1.84	0.78
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.13	0.77
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.48	0.77
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.64	0.77
3:C:113:THR:HG21	3:C:201:LEU:HD13	1.67	0.77
2:B:398:VAL:O	2:B:402:ILE:HG13	1.84	0.77
1:A:4:TYR:HA	2:B:113:ARG:HD3	1.66	0.77
7:T:29:ILE:O	7:T:33:ALA:HB3	1.84	0.77
2:B:43:PRO:O	2:B:113:ARG:HG3	1.85	0.77
2:O:76:THR:CG2	2:O:82:SER:H	1.97	0.77
3:P:118:VAL:N	11:P:502:HEM:HBC2	1.99	0.77
1:N:90:THR:O	1:N:167:VAL:HG11	1.84	0.77
2:B:227:ARG:HE	2:B:227:ARG:HA	1.49	0.77
2:B:46:ARG:NH2	2:B:376:GLN:HG3	1.99	0.77
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.66	0.77
1:A:255:LEU:HD13	1:A:422:LEU:HD13	1.65	0.76
1:N:49:ASN:ND2	1:N:52:ASN:H	1.83	0.76
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.49	0.76
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.15	0.76
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.68	0.76
2:O:56:ARG:HB2	2:O:171:ALA:HB1	1.67	0.76
8:H:34:ARG:O	8:H:38:GLU:HG2	1.84	0.76
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.68	0.75
3:C:355:ALA:O	3:C:358:SER:HB3	1.86	0.75

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:MET:CE	6:F:87:LYS:H	1.98	0.75
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.69	0.75
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.01	0.75
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.01	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.66	0.75
4:Q:129:SER:HB3	4:Q:152:TYR:CE2	2.22	0.75
1:N:429:GLU:OE1	7:T:7:LEU:HB2	1.87	0.74
4:Q:120:ARG:HH11	4:Q:120:ARG:HG2	1.51	0.74
6:F:89:TYR:HD1	6:F:90:LEU:N	1.84	0.74
1:N:362:ARG:O	1:N:365:MET:HB3	1.86	0.74
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.70	0.74
3:P:132:TYR:O	3:P:135:PRO:HD2	1.88	0.74
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.23	0.74
3:C:271:PRO:HA	14:C:2001:SMA:H10	1.69	0.74
2:O:325:TYR:HD1	9:V:60:ALA:HB2	1.50	0.74
5:R:58:PHE:O	5:R:61:SER:HB3	1.87	0.73
3:P:319:ARG:HB3	3:P:374:GLU:OE1	1.89	0.73
2:B:199:PHE:O	2:B:226:ILE:HG12	1.88	0.73
2:B:207:VAL:HG12	2:B:208:GLY:N	2.02	0.73
1:N:19:LEU:HB3	1:N:21:ASN:OD1	1.88	0.73
1:A:390:ILE:HG23	1:A:394:GLU:OE1	1.88	0.73
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.54	0.73
1:N:45:SER:HA	1:N:48:GLU:HG3	1.69	0.73
5:E:102:THR:O	5:E:106:ILE:HG13	1.88	0.73
2:O:248:ASN:HD22	2:O:248:ASN:C	1.92	0.73
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.73
2:B:169:LYS:O	2:B:170:THR:HG23	1.88	0.73
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.04	0.73
2:O:345:LYS:C	2:O:347:ALA:H	1.92	0.73
8:U:34:ARG:O	8:U:38:GLU:HG2	1.89	0.73
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.70	0.73
3:C:332:ASN:HD21	3:C:359:TYR:N	1.86	0.73
2:B:76:THR:CG2	2:B:82:SER:H	2.02	0.73
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.04	0.73
2:O:221:GLU:HG3	2:O:222:GLN:H	1.54	0.73
3:P:120:LEU:HD22	11:P:502:HEM:CBB	2.18	0.72
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.71	0.72
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.52	0.72
2:B:357:VAL:O	2:B:361:LYS:HG3	1.89	0.72
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.71	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.23	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.25	0.72
6:S:89:TYR:HD1	6:S:90:LEU:N	1.88	0.72
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.05	0.72
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.89	0.72
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.24	0.72
2:B:162:ASN:O	2:B:244:ILE:HD12	1.90	0.72
1:N:223:TYR:HD2	1:N:223:TYR:H	1.37	0.72
2:O:71:LEU:O	2:O:74:PRO:HD2	1.90	0.72
2:B:248:ASN:HD22	2:B:248:ASN:C	1.92	0.72
1:N:69:LYS:CE	1:N:70:ARG:HH21	2.02	0.72
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.24	0.72
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.20	0.72
5:R:53:ASN:O	5:R:57:GLN:HG3	1.90	0.72
4:Q:8:PRO:HG2	4:Q:10:PHE:HE1	1.53	0.72
1:A:90:THR:O	1:A:167:VAL:HG11	1.89	0.72
2:B:227:ARG:NE	2:B:227:ARG:HA	2.05	0.71
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.53	0.71
3:P:277:PHE:CD1	3:P:278:ALA:N	2.58	0.71
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.71
4:Q:223:LYS:O	4:Q:223:LYS:HD3	1.90	0.71
9:I:71:ASN:HD22	9:I:71:ASN:H	1.36	0.71
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.71	0.71
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.24	0.71
8:H:40:CYS:O	8:H:44:VAL:HG23	1.89	0.71
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.52	0.71
3:P:184:PHE:CD2	11:P:501:HEM:HBC1	2.26	0.71
1:N:130:GLU:O	1:N:134:ILE:HG13	1.90	0.71
2:B:111:CYS:HB3	2:B:119:VAL:HG11	1.72	0.71
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.72	0.71
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.39	0.71
5:E:141:HIS:O	5:E:142:LEU:HD23	1.91	0.71
1:A:294:LEU:HD11	1:A:334:MET:CE	2.20	0.71
4:D:46:VAL:HG12	4:D:47:ALA:N	2.06	0.70
3:C:189:ALA:O	3:C:193:ILE:HG13	1.90	0.70
1:A:45:SER:HA	1:A:48:GLU:HG3	1.71	0.70
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.71	0.70
1:N:373:THR:HB	1:N:374:PRO:HD3	1.71	0.70
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.27	0.70
5:E:53:ASN:O	5:E:57:GLN:HG3	1.91	0.70
1:A:269:VAL:HG11	1:A:410:VAL:HG21	1.73	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.73	0.70
1:A:49:ASN:ND2	1:A:52:ASN:H	1.89	0.70
1:N:294:LEU:HD11	1:N:334:MET:CE	2.21	0.70
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.31	0.70
1:A:373:THR:HB	1:A:374:PRO:HD3	1.73	0.70
4:D:231:LYS:O	6:F:71:LYS:HE3	1.91	0.70
4:D:222:MET:HE3	5:E:40:THR:HG23	1.74	0.70
7:G:29:ILE:O	7:G:33:ALA:HB3	1.92	0.70
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.74	0.70
4:Q:215:LEU:HD22	5:R:46:ALA:CB	2.21	0.70
4:Q:171:TYR:OH	4:Q:182:ILE:HA	1.91	0.70
2:O:219:VAL:O	2:O:223:PHE:HB2	1.92	0.70
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.74	0.70
2:O:24:LEU:HD13	2:O:38:LEU:HB2	1.72	0.70
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.74	0.70
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.25	0.70
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.74	0.70
3:C:134:LEU:HB2	3:C:135:PRO:HD3	1.73	0.70
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.73	0.70
3:C:92:PHE:O	3:C:95:ILE:HG22	1.92	0.70
3:P:189:ALA:O	3:P:193:ILE:HG13	1.91	0.70
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.73	0.70
8:U:73:LEU:HD12	8:U:73:LEU:O	1.92	0.70
2:O:47:ILE:HG12	2:O:120:MET:HE3	1.72	0.70
1:A:223:TYR:HD2	1:A:223:TYR:H	1.38	0.69
3:P:126:ALA:O	3:P:129:PHE:HB3	1.92	0.69
6:F:61:ARG:NH2	6:F:89:TYR:HE2	1.89	0.69
5:E:58:PHE:O	5:E:61:SER:HB3	1.92	0.69
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.27	0.69
3:P:247:SER:OG	3:P:250:LEU:HB2	1.91	0.69
2:B:150:VAL:HG23	2:B:151:ALA:H	1.56	0.69
4:D:215:LEU:HD22	5:E:46:ALA:HB1	1.74	0.69
1:N:206:LYS:O	1:N:209:VAL:HG12	1.92	0.69
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.58	0.69
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.22	0.69
4:D:47:ALA:N	4:D:50:ASN:ND2	2.41	0.69
16:C:2004:CDL:OA4	7:G:40:ARG:HD2	1.92	0.69
2:O:154:SER:O	2:O:157:VAL:HG12	1.92	0.69
2:O:226:ILE:HG22	2:O:227:ARG:N	2.07	0.69
2:O:150:VAL:CG2	2:O:151:ALA:H	2.06	0.69
2:O:357:VAL:O	2:O:361:LYS:HG3	1.93	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:49:ASN:C	1:N:49:ASN:HD22	1.95	0.69
7:G:41:PHE:CD2	7:G:41:PHE:C	2.66	0.69
7:G:41:PHE:HD2	7:G:41:PHE:C	1.96	0.69
1:A:429:GLU:OE1	7:G:7:LEU:HB2	1.92	0.69
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.08	0.69
2:O:43:PRO:O	2:O:113:ARG:HG3	1.93	0.69
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.28	0.69
3:P:92:PHE:O	3:P:95:ILE:HG22	1.93	0.69
1:N:161:THR:HG21	1:N:235:ARG:H	1.57	0.69
3:P:146:VAL:HG21	14:P:3001:SMA:H6	1.74	0.69
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.22	0.69
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.27	0.68
2:O:47:ILE:HG12	2:O:120:MET:CE	2.22	0.68
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.74	0.68
4:D:120:ARG:HH11	4:D:120:ARG:HG2	1.56	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
2:O:207:VAL:HG12	2:O:208:GLY:N	2.07	0.68
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.28	0.68
3:C:282:LEU:HD23	3:C:282:LEU:O	1.94	0.68
2:B:312:PHE:N	2:B:323:GLY:O	2.22	0.68
5:R:109:GLU:HG3	5:R:167:ALA:HB3	1.76	0.68
8:H:73:LEU:HD12	8:H:73:LEU:O	1.93	0.68
4:D:223:LYS:HD3	4:D:223:LYS:O	1.94	0.68
3:P:135:PRO:HG3	11:P:501:HEM:O1D	1.94	0.68
3:P:113:THR:HG21	3:P:201:LEU:HD13	1.74	0.68
1:A:49:ASN:C	1:A:49:ASN:HD22	1.97	0.68
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.08	0.68
2:B:341:MET:O	2:B:344:LEU:N	2.26	0.68
1:A:209:VAL:O	1:A:212:ALA:HB3	1.94	0.68
3:C:319:ARG:HB3	3:C:374:GLU:OE1	1.93	0.68
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.75	0.68
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.75	0.68
1:N:246:ASP:HA	1:N:427:PRO:HB3	1.74	0.68
4:D:46:VAL:HG12	4:D:47:ALA:H	1.59	0.67
3:P:104:TYR:HD2	3:P:105:TYR:CE1	2.11	0.67
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.58	0.67
2:B:353:THR:HG22	2:B:355:GLU:H	1.58	0.67
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.75	0.67
3:C:269:ILE:HG23	3:C:269:ILE:O	1.93	0.67
1:A:136:GLN:HG2	9:I:51:CYS:HB3	1.77	0.67
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	1.77	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:94:PRO:HG2	4:Q:95:TYR:HD1	1.60	0.67
3:C:118:VAL:N	11:C:502:HEM:HBC2	2.10	0.67
8:U:32:LYS:O	8:U:36:ARG:HG3	1.94	0.67
2:B:345:LYS:C	2:B:347:ALA:H	1.95	0.67
2:B:359:LYS:HA	2:B:362:ASN:ND2	2.10	0.67
1:A:69:LYS:CE	1:A:70:ARG:HH21	2.03	0.67
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.60	0.67
2:O:75:LEU:CD2	2:O:136:GLU:HB3	2.24	0.67
5:R:77:LYS:HE2	5:R:79:SER:CB	2.24	0.67
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.75	0.67
2:B:62:ASN:O	2:B:65:THR:HG22	1.95	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.77	0.67
2:O:248:ASN:ND2	2:O:250:HIS:H	1.93	0.67
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.76	0.67
5:E:40:THR:HG21	17:E:2005:PEE:O2P	1.96	0.67
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.60	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.93	0.67
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.30	0.66
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.77	0.66
4:D:94:PRO:HG2	4:D:95:TYR:CD1	2.30	0.66
1:A:136:GLN:NE2	9:I:50:LEU:HB2	2.09	0.66
4:D:47:ALA:H	4:D:50:ASN:ND2	1.86	0.66
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.31	0.66
5:R:113:ASP:C	5:R:115:SER:H	1.99	0.66
7:T:41:PHE:C	7:T:41:PHE:CD2	2.67	0.66
2:B:212:LYS:HD2	2:B:214:SER:OG	1.94	0.66
3:P:254:PRO:HB2	4:Q:118:ASN:O	1.96	0.66
3:P:332:ASN:HD21	3:P:359:TYR:N	1.94	0.66
2:O:293:SER:OG	2:O:296:TYR:HB2	1.96	0.66
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.20	0.66
6:F:33:ARG:O	6:F:36:THR:HG23	1.96	0.66
7:T:41:PHE:C	7:T:41:PHE:HD2	1.99	0.66
9:V:72:ALA:HB1	9:V:73:PRO:HD3	1.77	0.66
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.31	0.66
2:O:29:LEU:HD12	2:O:33:LEU:HD23	1.78	0.66
1:A:182:LEU:HD23	1:A:182:LEU:N	2.11	0.66
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.96	0.66
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.26	0.66
2:O:47:ILE:N	2:O:47:ILE:HD12	2.08	0.66
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.10	0.66
3:P:355:ALA:O	3:P:358:SER:HB3	1.96	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:94:PRO:HG2	4:Q:95:TYR:CD1	2.30	0.65
2:O:111:CYS:HB3	2:O:119:VAL:HG11	1.78	0.65
4:Q:198:HIS:O	4:Q:201:ARG:HB3	1.95	0.65
4:D:198:HIS:O	4:D:201:ARG:HB3	1.96	0.65
3:C:316:MET:HG2	3:C:319:ARG:HH21	1.61	0.65
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.78	0.65
3:C:135:PRO:HG3	11:C:501:HEM:O1D	1.97	0.65
4:Q:47:ALA:N	4:Q:50:ASN:ND2	2.43	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.11	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
4:Q:46:VAL:HG12	4:Q:47:ALA:N	2.12	0.65
2:O:72:ALA:CB	2:O:75:LEU:HD12	2.25	0.65
1:N:295:ALA:O	1:N:298:ALA:HB3	1.96	0.65
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.78	0.65
3:C:254:PRO:HB2	4:D:118:ASN:O	1.95	0.65
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.88	0.65
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.77	0.65
1:A:161:THR:HG21	1:A:234:CYS:HA	1.77	0.65
2:B:47:ILE:HD12	2:B:47:ILE:N	2.11	0.65
6:S:50:LEU:HD21	6:S:90:LEU:HD12	1.79	0.65
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.60	0.65
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.78	0.65
8:U:13:LEU:HD23	8:U:13:LEU:N	2.08	0.65
4:Q:10:PHE:HD1	4:Q:10:PHE:H	1.43	0.65
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.79	0.65
3:P:157:ILE:HD12	3:P:161:LEU:HD12	1.79	0.65
3:C:277:PHE:CD1	3:C:278:ALA:N	2.64	0.65
1:A:5:ALA:O	1:A:8:LEU:HB2	1.97	0.65
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.64	0.65
1:A:388:ARG:NH2	1:A:388:ARG:HG3	2.12	0.64
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.17	0.64
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.27	0.64
12:D:501:HEC:HMC1	12:D:501:HEC:HBC3	1.79	0.64
2:O:29:LEU:CD2	2:O:30:PRO:HD2	2.27	0.64
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.63	0.64
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.79	0.64
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.31	0.64
5:R:91:TRP:CE3	5:R:96:LEU:HD22	2.33	0.64
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.80	0.64
2:B:102:ARG:HH11	2:B:102:ARG:HG2	1.62	0.64
5:R:166:ASP:HB3	5:R:172:ARG:HH11	1.61	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:63:LYS:HD3	7:T:13:ILE:HG21	1.79	0.64
6:S:13:MET:HA	6:S:16:ILE:HB	1.79	0.64
3:P:6:ARG:HD3	3:P:16:ASN:OD1	1.97	0.64
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.13	0.64
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.33	0.64
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.32	0.64
2:O:359:LYS:HA	2:O:362:ASN:ND2	2.12	0.64
1:A:35:CYS:HA	1:A:372:THR:HG21	1.78	0.64
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.32	0.64
2:O:353:THR:HG22	2:O:355:GLU:H	1.62	0.64
4:Q:46:VAL:HG12	4:Q:47:ALA:H	1.63	0.64
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.28	0.64
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.33	0.64
1:N:23:LEU:HA	1:N:192:ALA:O	1.98	0.64
3:P:157:ILE:O	3:P:159:HIS:N	2.31	0.64
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.66	0.64
1:N:379:ILE:HG12	1:N:389:ARG:HE	1.64	0.64
1:N:432:LEU:HD23	1:N:433:ASP:H	1.62	0.63
4:D:218:LEU:HD13	5:E:43:ALA:HA	1.80	0.63
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.25	0.63
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.34	0.63
6:S:13:MET:O	6:S:17:ARG:HG3	1.97	0.63
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.80	0.63
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.34	0.63
7:T:41:PHE:HD2	7:T:41:PHE:O	1.80	0.63
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.38	0.63
4:D:10:PHE:N	4:D:10:PHE:CD1	2.66	0.63
6:F:31:LEU:HD21	6:F:65:ALA:HB2	1.79	0.63
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.63
2:B:71:LEU:O	2:B:74:PRO:HD2	1.98	0.63
2:B:72:ALA:CB	2:B:75:LEU:HD12	2.29	0.63
5:E:166:ASP:HB3	5:E:172:ARG:HH11	1.63	0.63
4:D:171:TYR:OH	4:D:182:ILE:HA	1.99	0.63
2:O:62:ASN:O	2:O:65:THR:HG22	1.98	0.63
4:D:235:MET:HE3	6:F:60:PHE:CE1	2.31	0.63
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.80	0.63
1:N:5:ALA:O	1:N:8:LEU:HB2	1.98	0.63
1:N:35:CYS:HA	1:N:372:THR:HG21	1.81	0.63
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.62	0.63
1:N:49:ASN:ND2	1:N:51:LYS:H	1.96	0.63
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.63	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:165:TYR:CE2	5:R:180:LEU:HG	2.33	0.63
1:N:253:VAL:HG11	1:N:335:MET:HE1	1.81	0.63
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.79	0.63
5:R:73:LYS:HB3	5:R:195:VAL:O	1.98	0.63
5:R:32:ARG:HH12	7:T:22:GLU:CD	2.01	0.63
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.28	0.63
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.81	0.63
2:O:341:MET:O	2:O:344:LEU:N	2.30	0.63
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.79	0.63
7:G:58:LEU:HD12	7:G:58:LEU:O	1.99	0.63
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.12	0.62
2:O:147:ASP:OD1	9:V:68:ILE:HD11	1.98	0.62
3:C:30:ALA:O	3:C:32:TRP:N	2.31	0.62
4:D:164:ILE:HG21	4:D:182:ILE:HG21	1.81	0.62
6:S:68:LEU:O	6:S:71:LYS:N	2.26	0.62
3:C:207:ASN:O	3:C:208:ASN:HB3	1.98	0.62
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.79	0.62
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.14	0.62
1:N:105:ASP:O	1:N:109:VAL:HG23	1.99	0.62
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.34	0.62
3:C:36:SER:O	3:C:39:ALA:HB3	1.99	0.62
3:C:316:MET:HG2	3:C:319:ARG:NH2	2.14	0.62
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.62
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.82	0.62
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
3:P:70:THR:HA	3:P:74:VAL:CG2	2.29	0.62
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.34	0.62
9:I:65:VAL:HG12	9:I:66:ALA:N	2.15	0.62
2:B:220:ALA:O	2:B:224:LEU:HB2	1.98	0.62
6:S:67:ASP:OD1	6:S:71:LYS:HD2	1.99	0.62
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.35	0.62
1:N:49:ASN:HD21	1:N:52:ASN:H	1.46	0.62
1:A:406:MET:O	1:A:410:VAL:HG23	1.99	0.62
6:S:11:ARG:HG2	6:S:11:ARG:O	2.00	0.62
1:N:61:HIS:CE1	1:N:137:GLU:OE1	2.53	0.62
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.64	0.62
6:F:68:LEU:O	6:F:71:LYS:N	2.30	0.62
4:Q:197:GLU:HG2	4:Q:198:HIS:N	2.15	0.62
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.82	0.62
12:D:501:HEC:HMB1	12:D:501:HEC:CBB	2.28	0.62
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.64	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.80	0.62
2:O:226:ILE:HG22	2:O:227:ARG:H	1.63	0.62
5:R:109:GLU:O	5:R:123:ASP:HB2	1.99	0.62
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.34	0.62
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.35	0.62
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.35	0.62
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.15	0.61
3:P:95:ILE:CD1	3:P:121:LEU:HD13	2.29	0.61
5:R:109:GLU:OE1	5:R:166:ASP:HB2	2.00	0.61
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.15	0.61
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.81	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.34	0.61
4:D:116:ILE:HG23	4:D:117:VAL:N	2.14	0.61
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.82	0.61
8:H:58:LEU:HG	8:H:62:LEU:HD12	1.82	0.61
1:A:161:THR:HG21	1:A:235:ARG:H	1.65	0.61
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.61
2:B:58:GLU:OE1	2:B:64:GLY:N	2.33	0.61
3:C:63:ALA:HB2	3:C:176:LEU:HD21	1.80	0.61
1:N:406:MET:O	1:N:410:VAL:HG23	2.00	0.61
4:D:8:PRO:HG2	4:D:10:PHE:HE1	1.63	0.61
2:B:109:VAL:CG1	2:B:123:LEU:HB2	2.30	0.61
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.66	0.61
4:D:43:MET:HE3	4:D:91:PHE:HE2	1.65	0.61
2:B:150:VAL:CG2	2:B:151:ALA:H	2.13	0.61
5:R:109:GLU:CG	5:R:167:ALA:HB3	2.30	0.61
2:B:239:TYR:CE1	2:B:260:GLU:HB2	2.35	0.61
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.16	0.61
3:C:345:GLU:O	3:C:349:ILE:HG13	2.01	0.61
3:P:282:LEU:HD23	3:P:282:LEU:C	2.20	0.61
2:O:150:VAL:CG2	2:O:151:ALA:N	2.62	0.61
2:B:150:VAL:CG2	2:B:151:ALA:N	2.63	0.61
1:N:49:ASN:C	1:N:49:ASN:ND2	2.51	0.61
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.30	0.61
4:D:94:PRO:HG2	4:D:95:TYR:HD1	1.66	0.61
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.66	0.61
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.82	0.61
4:D:223:LYS:HD3	4:D:223:LYS:C	2.20	0.61
2:O:312:PHE:N	2:O:323:GLY:O	2.32	0.61
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.81	0.61
4:D:167:GLU:O	4:D:169:LEU:N	2.34	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:3:LEU:N	4:Q:3:LEU:HD23	2.15	0.61
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.36	0.61
1:A:335:MET:CG	1:A:339:GLN:HE21	2.13	0.61
3:C:70:THR:HA	3:C:74:VAL:HG23	1.82	0.61
1:A:156:THR:HA	5:E:7:VAL:HG21	1.83	0.61
4:D:218:LEU:HD13	5:E:43:ALA:CA	2.31	0.61
1:N:307:PHE:CD1	1:N:307:PHE:C	2.74	0.61
1:N:281:ASP:O	1:N:284:PHE:HD1	1.84	0.61
5:R:34:GLY:HA2	10:W:10:TYR:HB2	1.83	0.61
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.01	0.60
3:C:30:ALA:C	3:C:32:TRP:H	2.04	0.60
3:C:282:LEU:HD23	3:C:282:LEU:C	2.21	0.60
3:P:242:THR:N	4:Q:208:MET:HE1	2.15	0.60
6:S:32:MET:CE	6:S:87:LYS:H	2.13	0.60
4:D:155:GLY:C	4:D:157:ALA:H	2.04	0.60
3:C:184:PHE:CD2	11:C:501:HEM:HBC1	2.35	0.60
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.02	0.60
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.31	0.60
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.83	0.60
3:C:173:ASN:N	3:C:174:PRO:HD2	2.16	0.60
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.83	0.60
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.15	0.60
1:A:27:SER:HB2	1:A:199:ALA:O	2.01	0.60
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.35	0.60
3:P:70:THR:HA	3:P:74:VAL:HG23	1.83	0.60
2:O:312:PHE:HE1	9:V:62:ARG:O	1.84	0.60
1:N:388:ARG:NH2	1:N:388:ARG:HG3	2.15	0.60
1:A:89:TYR:O	1:A:95:THR:HG23	2.01	0.60
3:P:123:THR:HG22	3:P:190:ILE:HD11	1.83	0.60
5:E:128:LYS:O	5:E:130:PRO:HD3	2.02	0.60
1:N:182:LEU:HD23	1:N:182:LEU:N	2.17	0.60
3:P:134:LEU:HB2	3:P:135:PRO:HD3	1.82	0.60
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.37	0.60
1:N:182:LEU:O	1:N:186:ILE:HG13	2.00	0.60
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.67	0.60
2:B:396:SER:O	2:B:399:ALA:HB3	2.01	0.60
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.84	0.60
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.65	0.60
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.37	0.60
1:N:86:PHE:CD2	1:N:99:ILE:HD11	2.36	0.60
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.83	0.60
2:O:219:VAL:HG13	2:O:223:PHE:CD1	2.37	0.60
2:B:109:VAL:HG13	2:B:123:LEU:HB2	1.84	0.60
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.82	0.59
2:B:230:ALA:O	2:B:232:THR:N	2.35	0.59
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.84	0.59
1:N:86:PHE:HB3	2:O:285:ILE:HG22	1.83	0.59
3:P:325:LEU:HD21	3:P:366:LEU:CB	2.32	0.59
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.36	0.59
1:N:255:LEU:HD13	1:N:422:LEU:CD1	2.31	0.59
2:B:140:LEU:HD12	2:B:140:LEU:O	2.02	0.59
2:B:332:HIS:O	2:B:336:VAL:HG23	2.02	0.59
1:N:18:THR:HG23	1:N:24:ARG:HG2	1.84	0.59
2:O:332:HIS:O	2:O:336:VAL:HG23	2.02	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.13	0.59
3:P:27:ASN:ND2	3:P:209:PRO:HD2	2.16	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.00	0.59
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.59
1:N:161:THR:HG21	1:N:234:CYS:HA	1.83	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.59
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.03	0.59
10:J:25:VAL:O	10:J:29:VAL:HG23	2.01	0.59
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.37	0.59
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.37	0.59
2:O:227:ARG:HG3	2:O:228:SER:N	2.17	0.59
2:O:73:SER:N	2:O:74:PRO:HD2	2.17	0.59
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.84	0.59
4:Q:167:GLU:O	4:Q:169:LEU:N	2.36	0.59
3:P:21:ASP:O	3:P:23:PRO:HD3	2.01	0.59
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.32	0.59
3:C:21:ASP:O	3:C:23:PRO:HD3	2.03	0.59
2:B:248:ASN:HD21	2:B:250:HIS:HB3	1.66	0.59
9:V:65:VAL:HG12	9:V:66:ALA:N	2.17	0.59
1:A:310:PHE:HE1	1:A:322:PHE:N	2.00	0.59
5:E:171:ILE:HG12	5:E:176:ALA:O	2.02	0.59
2:O:220:ALA:O	2:O:224:LEU:HB2	2.01	0.59
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.38	0.59
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.84	0.59
4:D:215:LEU:HD22	5:E:46:ALA:CB	2.31	0.59
2:B:295:LEU:HA	2:B:343:GLN:HG2	1.85	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.21	0.59
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.83	0.59
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.59
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.59
16:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.03	0.59
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.36	0.59
3:P:173:ASN:N	3:P:174:PRO:HD2	2.17	0.58
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.38	0.58
3:C:104:TYR:HD2	3:C:105:TYR:CE1	2.21	0.58
3:P:154:ILE:HG23	3:P:155:PRO:HD2	1.84	0.58
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.17	0.58
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.85	0.58
1:N:45:SER:HA	1:N:48:GLU:CG	2.33	0.58
7:G:41:PHE:O	7:G:41:PHE:HD2	1.85	0.58
5:E:38:LEU:HA	10:J:14:PHE:CE1	2.38	0.58
4:D:130:LEU:HD12	4:D:150:ASN:ND2	2.17	0.58
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.03	0.58
1:A:241:ILE:HG23	1:A:241:ILE:O	2.03	0.58
6:S:61:ARG:NH2	6:S:89:TYR:HE2	1.95	0.58
2:B:75:LEU:CD2	2:B:136:GLU:HB3	2.33	0.58
3:C:76:TYR:CE1	5:E:57:GLN:HG2	2.39	0.58
1:N:253:VAL:HG11	1:N:335:MET:CE	2.33	0.58
4:D:120:ARG:NH1	4:D:120:ARG:HG2	2.19	0.58
2:O:162:ASN:O	2:O:244:ILE:HD12	2.03	0.58
2:O:58:GLU:OE1	2:O:64:GLY:N	2.36	0.58
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.85	0.58
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.86	0.58
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.85	0.58
2:O:207:VAL:O	2:O:216:LEU:HD21	2.03	0.58
3:P:26:SER:HA	3:P:219:ILE:CD1	2.33	0.58
1:A:45:SER:HA	1:A:48:GLU:CG	2.34	0.58
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.38	0.58
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.83	0.58
3:P:36:SER:O	3:P:39:ALA:HB3	2.03	0.58
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.38	0.58
3:P:52:LEU:HD13	11:P:501:HEM:HBD1	1.85	0.58
4:D:43:MET:HE3	4:D:91:PHE:CE2	2.38	0.58
3:C:311:SER:HB2	3:C:319:ARG:HH11	1.68	0.58
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.38	0.58
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.85	0.58
5:E:185:TYR:O	5:E:186:GLN:HB2	2.04	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ARG:CZ	2:B:164:HIS:CD2	2.87	0.58
3:P:120:LEU:HD22	11:P:502:HEM:HBB1	1.84	0.58
9:V:65:VAL:O	9:V:76:VAL:HG23	2.04	0.58
1:A:310:PHE:CE1	1:A:322:PHE:N	2.71	0.58
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.38	0.58
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.33	0.58
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.68	0.58
3:P:333:LEU:HD11	17:P:3007:PEE:H38	1.86	0.58
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.31	0.58
1:A:379:ILE:HG12	1:A:389:ARG:HE	1.69	0.58
4:D:167:GLU:C	4:D:169:LEU:H	2.06	0.58
3:P:141:PHE:O	3:P:144:ALA:HB3	2.04	0.58
5:R:69:LEU:HD13	5:R:71:LEU:HD11	1.85	0.58
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.58
3:P:130:VAL:HG23	3:P:131:GLY:N	2.19	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.38	0.58
1:N:410:VAL:O	1:N:413:LYS:HB3	2.03	0.58
2:O:109:VAL:HG13	2:O:123:LEU:HB2	1.86	0.58
2:B:189:GLU:O	2:B:191:LEU:N	2.36	0.58
6:S:71:LYS:O	6:S:72:HIS:HB2	2.04	0.58
3:C:247:SER:HG	3:C:250:LEU:HB2	1.68	0.58
2:B:203:ARG:O	2:B:387:LEU:HD11	2.04	0.58
5:R:57:GLN:OE1	18:R:3009:PLC:H12	2.03	0.58
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.85	0.58
3:C:105:TYR:CE2	3:C:209:PRO:HA	2.38	0.58
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.39	0.57
2:O:248:ASN:C	2:O:248:ASN:ND2	2.54	0.57
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.85	0.57
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.39	0.57
1:A:40:TRP:O	1:A:384:LEU:HD22	2.04	0.57
4:D:116:ILE:HG23	4:D:117:VAL:H	1.69	0.57
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.38	0.57
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.22	0.57
4:Q:224:ARG:HH12	16:Q:3003:CDL:HB21	1.69	0.57
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.24	0.57
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.34	0.57
1:A:49:ASN:ND2	1:A:49:ASN:C	2.56	0.57
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.57
3:P:166:TRP:CD1	3:P:171:VAL:HG22	2.40	0.57
6:F:32:MET:HE3	6:F:87:LYS:H	1.67	0.57
2:B:189:GLU:O	2:B:192:HIS:N	2.37	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.57	0.57
3:P:76:TYR:CE1	5:R:57:GLN:HG2	2.40	0.57
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.39	0.57
8:U:40:CYS:O	8:U:44:VAL:HG23	2.04	0.57
3:P:282:LEU:O	3:P:282:LEU:HD23	2.04	0.57
2:B:67:HIS:O	2:B:70:ARG:HB3	2.04	0.57
2:B:293:SER:OG	2:B:296:TYR:HB2	2.05	0.57
2:O:27:THR:HG22	2:O:28:LYS:N	2.17	0.57
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.40	0.57
7:T:42:SER:O	7:T:45:VAL:HG12	2.05	0.57
1:A:86:PHE:HB3	2:B:285:ILE:HG22	1.86	0.57
1:A:178:THR:HB	1:A:181:ASP:OD1	2.05	0.57
3:P:184:PHE:HA	11:P:501:HEM:CBC	2.34	0.57
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.87	0.57
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.40	0.57
2:B:318:ASP:O	2:B:319:SER:HB2	2.04	0.57
1:N:254:ALA:HB3	1:N:423:ALA:HB3	1.87	0.57
3:P:137:GLY:N	3:P:140:SER:HB2	2.20	0.57
6:S:21:TYR:CD2	6:S:21:TYR:C	2.78	0.57
2:B:258:VAL:HB	2:B:322:PHE:O	2.05	0.57
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.03	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.19	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
3:P:5:ILE:HG22	3:P:12:LEU:HD12	1.86	0.57
1:N:239:SER:HB2	7:T:17:SER:O	2.04	0.57
4:D:42:SER:HB2	4:D:112:ASP:OD2	2.04	0.57
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.25	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.87	0.57
2:O:146:VAL:HG12	2:O:147:ASP:N	2.19	0.57
3:P:207:ASN:O	3:P:208:ASN:HB3	2.03	0.57
3:P:269:ILE:O	3:P:269:ILE:HG23	2.05	0.57
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	1.87	0.57
4:D:227:TRP:O	4:D:228:SER:C	2.41	0.57
2:O:42:SER:OG	2:O:43:PRO:HD2	2.05	0.57
3:P:30:ALA:C	3:P:32:TRP:H	2.09	0.57
4:D:10:PHE:HD1	4:D:10:PHE:H	1.52	0.57
10:W:56:LYS:HE2	10:W:60:GLU:CD	2.25	0.57
6:F:27:ASN:HB2	6:F:81:VAL:HB	1.86	0.57
5:E:108:GLN:O	5:E:112:VAL:HG23	2.04	0.57
2:O:209:ILE:HG22	2:O:210:GLY:N	2.19	0.57
1:A:49:ASN:HD21	1:A:52:ASN:H	1.53	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:135:LEU:CD2	5:R:169:GLY:HA3	2.35	0.57
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.40	0.57
4:D:168:ILE:HG12	4:D:168:ILE:O	2.05	0.57
3:C:120:LEU:HD22	11:C:502:HEM:CBB	2.35	0.56
1:N:394:GLU:O	1:N:395:TRP:C	2.44	0.56
4:D:232:SER:HB3	7:G:23:GLN:NE2	2.19	0.56
10:W:14:PHE:CD2	10:W:14:PHE:N	2.70	0.56
3:C:126:ALA:O	3:C:129:PHE:HB3	2.04	0.56
5:E:35:PHE:O	5:E:38:LEU:N	2.38	0.56
1:N:333:ASP:O	1:N:336:PHE:HB3	2.05	0.56
2:B:86:THR:O	2:B:90:GLU:HG3	2.05	0.56
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.56
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.87	0.56
10:W:22:LEU:N	10:W:22:LEU:HD23	2.20	0.56
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.86	0.56
2:B:272:PHE:O	2:B:275:LEU:N	2.38	0.56
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.40	0.56
6:F:72:HIS:O	6:F:73:ARG:HD3	2.05	0.56
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.34	0.56
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.69	0.56
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.35	0.56
1:A:46:ARG:HD3	1:A:231:LEU:HD13	1.88	0.56
3:P:230:ILE:HG23	17:P:3005:PEE:H25	1.88	0.56
6:S:68:LEU:O	6:S:70:LEU:N	2.38	0.56
6:S:73:ARG:HG3	6:S:73:ARG:HH11	1.70	0.56
7:T:58:LEU:O	7:T:58:LEU:HD12	2.06	0.56
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.40	0.56
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.38	0.56
1:A:180:ALA:O	1:A:183:ALA:HB3	2.05	0.56
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.05	0.56
5:E:103:GLN:HA	5:E:106:ILE:CB	2.30	0.56
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.86	0.56
2:O:308:ASP:OD1	9:V:56:SER:HA	2.06	0.56
3:P:106:GLY:HA2	3:P:108:TYR:CD2	2.39	0.56
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.87	0.56
4:Q:218:LEU:HD13	5:R:43:ALA:HA	1.87	0.56
4:Q:155:GLY:C	4:Q:157:ALA:H	2.08	0.56
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.86	0.56
3:C:22:LEU:HD12	3:C:23:PRO:N	2.20	0.56
1:A:23:LEU:HA	1:A:192:ALA:O	2.06	0.56
5:R:44:CYS:HB3	10:W:24:VAL:HG11	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:MET:HE3	6:F:60:PHE:HE1	1.69	0.56
1:A:332:ASP:O	1:A:333:ASP:C	2.43	0.56
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.39	0.56
5:R:62:LEU:O	5:R:63:SER:O	2.23	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
5:E:148:ALA:HA	5:E:156:TYR:CD2	2.41	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.56
3:C:70:THR:HA	3:C:74:VAL:CG2	2.36	0.56
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.06	0.56
4:Q:47:ALA:HB1	4:Q:89:ASP:O	2.05	0.56
6:F:32:MET:O	6:F:35:ASP:HB2	2.06	0.56
12:Q:501:HEC:HBC3	12:Q:501:HEC:HMC1	1.87	0.56
2:B:333:ALA:O	2:B:337:ILE:HG13	2.05	0.56
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.41	0.56
10:J:22:LEU:N	10:J:22:LEU:HD23	2.20	0.56
3:C:45:GLN:CB	11:C:501:HEM:HAB	2.36	0.56
2:O:396:SER:O	2:O:399:ALA:HB3	2.06	0.56
1:N:335:MET:CG	1:N:339:GLN:HE21	2.18	0.56
7:G:42:SER:O	7:G:45:VAL:HG12	2.06	0.56
3:C:285:ILE:N	3:C:285:ILE:HD12	2.21	0.56
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.86	0.56
2:O:345:LYS:C	2:O:347:ALA:N	2.59	0.56
5:E:29:SER:HA	5:E:32:ARG:HH21	1.71	0.56
2:B:239:TYR:HE1	2:B:260:GLU:N	2.04	0.56
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.71	0.56
2:O:47:ILE:N	2:O:47:ILE:CD1	2.68	0.56
1:N:209:VAL:O	1:N:212:ALA:HB3	2.05	0.56
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.06	0.56
6:S:27:ASN:HB2	6:S:81:VAL:HB	1.87	0.56
2:O:239:TYR:CD1	2:O:260:GLU:HB2	2.42	0.56
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.36	0.55
3:P:45:GLN:CB	11:P:501:HEM:HAB	2.36	0.55
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.32	0.55
3:P:231:LEU:HD11	4:Q:220:TYR:HA	1.88	0.55
2:B:146:VAL:HG12	2:B:147:ASP:N	2.22	0.55
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.70	0.55
1:A:186:ILE:O	1:A:190:PHE:HB2	2.06	0.55
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.55
5:R:1:VAL:HG23	5:R:3:ASN:H	1.70	0.55
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.41	0.55
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.15	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.88	0.55
3:P:27:ASN:ND2	3:P:208:ASN:OD1	2.35	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.04	0.55
3:C:9:HIS:ND1	3:C:10:PRO:HD2	2.21	0.55
1:N:318:GLY:O	1:N:319:LEU:HD23	2.07	0.55
1:A:106:MET:O	1:A:110:VAL:HG23	2.06	0.55
5:E:171:ILE:N	5:E:179:ASN:OD1	2.37	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.55
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.22	0.55
1:A:342:TRP:O	1:A:345:LEU:HB2	2.06	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.88	0.55
3:P:276:LEU:O	3:P:279:TYR:HB3	2.06	0.55
4:Q:167:GLU:C	4:Q:169:LEU:H	2.10	0.55
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.41	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.06	0.55
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.69	0.55
2:O:273:SER:O	2:O:276:GLN:HB3	2.07	0.55
2:B:27:THR:HG22	2:B:28:LYS:H	1.71	0.55
5:E:136:VAL:O	5:E:138:VAL:N	2.37	0.55
3:C:365:ILE:HG22	3:C:366:LEU:HD23	1.86	0.55
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.41	0.55
4:Q:235:MET:HE3	6:S:60:PHE:CE1	2.40	0.55
6:F:71:LYS:O	6:F:72:HIS:HB2	2.04	0.55
6:F:63:LYS:HD3	7:G:13:ILE:HG21	1.88	0.55
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.72	0.55
3:P:117:GLY:C	11:P:502:HEM:HBC2	2.27	0.55
2:O:170:THR:O	2:O:172:LEU:N	2.40	0.55
4:Q:129:SER:HB3	4:Q:152:TYR:CD2	2.41	0.55
2:B:248:ASN:ND2	2:B:248:ASN:C	2.56	0.55
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.41	0.55
2:B:47:ILE:CD1	2:B:47:ILE:N	2.70	0.55
2:B:292:THR:O	2:B:292:THR:HG22	2.06	0.55
3:P:316:MET:HG2	3:P:319:ARG:HH21	1.70	0.55
1:N:19:LEU:O	1:N:21:ASN:N	2.40	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.55
1:N:86:PHE:O	2:O:285:ILE:HA	2.06	0.55
6:S:32:MET:O	6:S:35:ASP:HB2	2.06	0.55
3:P:137:GLY:H	3:P:140:SER:HB2	1.72	0.55
1:A:75:PHE:O	1:A:79:VAL:HG23	2.07	0.55
3:C:79:LEU:HD12	3:C:79:LEU:O	2.06	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:GLY:O	2:B:231:GLY:N	2.39	0.55
4:Q:220:TYR:CE2	16:Q:3003:CDL:H722	2.42	0.55
1:N:4:TYR:HA	2:O:113:ARG:HD3	1.89	0.55
6:S:13:MET:HB2	6:S:17:ARG:NH1	2.21	0.55
10:W:59:TYR:O	10:W:60:GLU:O	2.24	0.55
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.42	0.55
1:N:281:ASP:HB3	1:N:284:PHE:HE1	1.71	0.55
5:R:188:VAL:O	5:R:188:VAL:HG23	2.06	0.55
2:O:122:TYR:O	2:O:126:VAL:HG23	2.07	0.55
2:B:393:THR:CG2	2:B:397:VAL:HB	2.37	0.55
4:Q:120:ARG:NH1	4:Q:120:ARG:HG2	2.18	0.55
2:O:272:PHE:O	2:O:276:GLN:N	2.40	0.55
6:S:32:MET:HE1	6:S:87:LYS:HG2	1.88	0.55
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.55
2:O:81:SER:O	2:O:83:PHE:N	2.40	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.88	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.42	0.54
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.54
5:R:10:PHE:CD1	7:T:18:LEU:HD21	2.42	0.54
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.42	0.54
1:N:124:GLU:HG2	1:N:124:GLU:O	2.08	0.54
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.07	0.54
5:R:83:GLU:CG	5:R:102:THR:HG22	2.28	0.54
3:P:231:LEU:CD1	4:Q:220:TYR:HA	2.37	0.54
3:P:27:ASN:HD21	3:P:208:ASN:CG	2.10	0.54
1:A:410:VAL:O	1:A:413:LYS:HB3	2.08	0.54
2:O:239:TYR:CD2	2:O:240:TRP:N	2.75	0.54
5:E:136:VAL:HB	5:E:181:GLU:HB3	1.88	0.54
3:C:156:TYR:N	3:C:156:TYR:CD2	2.74	0.54
2:B:272:PHE:O	2:B:276:GLN:N	2.37	0.54
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.42	0.54
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.43	0.54
2:O:258:VAL:HB	2:O:322:PHE:O	2.06	0.54
3:C:286:PRO:HA	5:R:175:PRO:HB3	1.90	0.54
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.54
3:P:37:LEU:HD21	3:P:232:GLY:O	2.07	0.54
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.16	0.54
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.54
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.42	0.54
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.88	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
8:U:13:LEU:CD2	8:U:13:LEU:H	2.15	0.54
3:C:380:TYR:OH	6:F:34:ASP:HA	2.08	0.54
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.87	0.54
1:A:339:GLN:HE22	1:A:437:ILE:HG23	1.71	0.54
1:N:206:LYS:O	1:N:208:LEU:N	2.40	0.54
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.69	0.54
3:C:347:PRO:O	3:C:350:ILE:HG22	2.08	0.54
3:C:162:VAL:O	3:C:163:GLU:C	2.45	0.54
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.07	0.54
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.43	0.54
1:A:269:VAL:HG11	1:A:410:VAL:CG2	2.38	0.54
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.88	0.54
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.54
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.88	0.54
3:P:101:ARG:HH22	11:P:502:HEM:CGA	2.21	0.54
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.89	0.54
4:D:191:ARG:O	4:D:192:TRP:C	2.45	0.54
3:P:273:TRP:CE3	3:P:274:TYR:HA	2.43	0.54
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.54
5:R:140:THR:HG21	5:R:178:TYR:HB2	1.89	0.54
2:O:63:LEU:O	2:O:65:THR:N	2.38	0.54
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.54
6:S:72:HIS:O	6:S:73:ARG:HD3	2.07	0.54
3:P:95:ILE:HD13	3:P:121:LEU:HD12	1.90	0.54
1:A:295:ALA:O	1:A:298:ALA:HB3	2.08	0.54
6:F:52:GLU:HG2	6:F:56:ASN:ND2	2.22	0.54
3:P:236:MET:O	3:P:239:PRO:HD2	2.08	0.54
2:O:350:GLY:O	2:O:352:VAL:N	2.32	0.54
2:B:31:ASN:HD22	2:B:32:GLY:H	1.56	0.54
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.90	0.54
5:E:83:GLU:HA	5:E:100:HIS:CG	2.43	0.54
4:Q:191:ARG:O	4:Q:192:TRP:C	2.45	0.54
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.43	0.54
1:A:248:LEU:HB3	1:A:249:PRO:HD2	1.90	0.54
1:N:158:PHE:O	1:N:159:GLN:O	2.26	0.54
1:N:371:GLY:O	1:N:375:VAL:HG23	2.08	0.54
6:F:74:ILE:HG13	6:F:75:LEU:N	2.22	0.54
4:D:142:VAL:HG23	4:D:142:VAL:O	2.08	0.54
3:C:6:ARG:HD3	3:C:16:ASN:OD1	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:433:ASP:O	1:N:437:ILE:HG13	2.08	0.54
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.89	0.54
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.54
3:P:366:LEU:HD23	3:P:366:LEU:N	2.23	0.54
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.39	0.53
3:P:104:TYR:HD2	3:P:105:TYR:CD1	2.27	0.53
2:O:97:SER:HA	9:V:69:SER:HA	1.90	0.53
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.53
5:R:136:VAL:O	5:R:138:VAL:N	2.35	0.53
3:P:316:MET:HG2	3:P:319:ARG:NH2	2.23	0.53
3:C:160:THR:O	3:C:163:GLU:HB3	2.09	0.53
5:E:177:PRO:O	5:E:178:TYR:HD1	1.91	0.53
2:O:318:ASP:O	2:O:319:SER:HB2	2.08	0.53
6:F:50:LEU:HD21	6:F:90:LEU:HD12	1.89	0.53
3:P:113:THR:HG21	3:P:201:LEU:CD1	2.39	0.53
4:Q:164:ILE:HD11	4:Q:183:ALA:HB2	1.89	0.53
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.71	0.53
7:G:81:GLN:O	8:H:47:ARG:HA	2.08	0.53
2:O:428:GLY:O	2:O:430:LEU:HG	2.08	0.53
4:Q:222:MET:HE3	5:R:40:THR:HA	1.90	0.53
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.49	0.53
2:B:239:TYR:HE1	2:B:260:GLU:H	1.56	0.53
6:F:67:ASP:OD1	6:F:71:LYS:HD2	2.08	0.53
3:C:242:THR:N	4:D:208:MET:HE1	2.22	0.53
4:D:167:GLU:C	4:D:169:LEU:N	2.62	0.53
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.53
3:C:325:LEU:HD21	3:C:366:LEU:CB	2.38	0.53
1:N:304:CYS:HA	1:N:326:ALA:HB2	1.91	0.53
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.08	0.53
1:A:307:PHE:CD1	1:A:307:PHE:C	2.82	0.53
1:N:411:CYS:O	1:N:415:ILE:HG13	2.09	0.53
5:E:62:LEU:O	5:E:63:SER:O	2.27	0.53
5:R:51:ALA:O	5:R:52:LYS:C	2.47	0.53
2:O:207:VAL:CG1	2:O:208:GLY:H	2.16	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.74	0.53
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.48	0.53
2:O:109:VAL:CG1	2:O:123:LEU:HB2	2.38	0.53
3:P:273:TRP:CE3	3:P:274:TYR:N	2.77	0.53
2:B:122:TYR:O	2:B:126:VAL:HG23	2.08	0.53
3:C:148:THR:O	3:C:151:PHE:HD1	1.92	0.53
4:D:44:ASP:N	4:D:44:ASP:OD1	2.42	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:LEU:HB3	11:C:502:HEM:HAB	1.90	0.53
3:C:113:THR:HG21	3:C:201:LEU:CD1	2.37	0.53
9:I:71:ASN:HD22	9:I:71:ASN:N	1.97	0.53
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.90	0.53
2:O:67:HIS:O	2:O:70:ARG:HB3	2.09	0.53
4:Q:44:ASP:OD1	4:Q:44:ASP:N	2.40	0.53
3:C:123:THR:HG21	3:C:190:ILE:HG13	1.89	0.53
1:N:330:SER:O	1:N:331:ILE:C	2.46	0.53
8:U:13:LEU:CD2	8:U:13:LEU:N	2.71	0.53
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.53
4:D:197:GLU:HG2	4:D:198:HIS:N	2.24	0.53
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.89	0.53
8:U:58:LEU:HG	8:U:62:LEU:HD12	1.91	0.53
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.44	0.53
1:N:26:ALA:O	1:N:198:ALA:HA	2.09	0.53
2:B:350:GLY:O	2:B:352:VAL:N	2.39	0.53
4:D:158:ILE:HG12	4:D:159:GLY:H	1.74	0.53
2:B:312:PHE:CD1	9:I:60:ALA:HB1	2.44	0.53
2:O:147:ASP:O	2:O:150:VAL:HG22	2.08	0.53
1:A:432:LEU:HD23	1:A:433:ASP:H	1.72	0.53
10:J:59:TYR:CD1	10:J:59:TYR:N	2.77	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
2:O:239:TYR:HD2	2:O:240:TRP:N	2.07	0.53
3:P:78:TRP:CD2	3:P:79:LEU:N	2.77	0.53
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.44	0.53
4:D:76:GLU:H	4:D:76:GLU:CD	2.12	0.53
2:B:207:VAL:CG1	2:B:208:GLY:H	2.12	0.53
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.08	0.53
2:B:200:THR:O	2:B:202:ALA:N	2.42	0.53
1:A:255:LEU:HD12	1:A:421:ALA:O	2.08	0.53
3:C:311:SER:HB2	3:C:319:ARG:NH1	2.24	0.53
3:P:245:LEU:O	4:Q:201:ARG:CG	2.57	0.53
6:S:77:LYS:HA	6:S:80:TRP:NE1	2.23	0.53
1:N:281:ASP:O	1:N:284:PHE:CD1	2.61	0.53
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.24	0.53
2:B:209:ILE:HG22	2:B:210:GLY:N	2.24	0.53
2:B:307:PHE:CD1	2:B:308:ASP:N	2.77	0.53
4:D:68:VAL:HG12	4:D:69:GLU:N	2.23	0.53
5:R:35:PHE:O	5:R:38:LEU:N	2.42	0.52
1:N:22:GLY:O	1:N:193:PRO:HA	2.09	0.52
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.90	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52
6:S:104:ARG:O	6:S:108:ASN:ND2	2.42	0.52
5:E:34:GLY:CA	10:J:10:TYR:HB2	2.39	0.52
10:W:59:TYR:CD1	10:W:59:TYR:N	2.76	0.52
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.75	0.52
3:P:285:ILE:N	3:P:285:ILE:HD12	2.24	0.52
3:C:49:GLY:HA3	11:C:501:HEM:C2C	2.44	0.52
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.35	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.52
5:R:108:GLN:C	5:R:110:ALA:H	2.13	0.52
1:N:170:THR:HG22	1:N:171:THR:H	1.73	0.52
1:N:170:THR:HG22	1:N:171:THR:N	2.25	0.52
1:N:40:TRP:O	1:N:384:LEU:HD22	2.09	0.52
2:O:226:ILE:CG2	2:O:227:ARG:H	2.23	0.52
1:N:356:ARG:O	1:N:357:ALA:C	2.47	0.52
1:N:86:PHE:CG	1:N:99:ILE:HG12	2.44	0.52
1:N:186:ILE:O	1:N:190:PHE:HB2	2.08	0.52
3:C:326:PHE:O	3:C:329:LEU:HB3	2.08	0.52
1:N:180:ALA:O	1:N:183:ALA:HB3	2.09	0.52
3:P:162:VAL:O	3:P:163:GLU:C	2.47	0.52
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.22	0.52
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.69	0.52
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.09	0.52
3:P:138:GLN:HG2	3:P:258:THR:HG22	1.92	0.52
2:B:97:SER:HA	9:I:69:SER:HA	1.92	0.52
3:C:52:LEU:HD11	3:C:81:ARG:HA	1.92	0.52
2:B:182:ARG:NH2	2:B:190:GLN:OE1	2.43	0.52
2:O:307:PHE:CD1	2:O:308:ASP:N	2.78	0.52
3:P:326:PHE:O	3:P:329:LEU:HB3	2.08	0.52
8:H:19:THR:O	8:H:22:GLU:HB2	2.09	0.52
5:R:148:ALA:O	5:R:149:ASN:HB2	2.10	0.52
1:N:342:TRP:O	1:N:345:LEU:HB2	2.10	0.52
9:V:31:UNK:C	9:V:73:PRO:HG2	2.39	0.52
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.44	0.52
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.91	0.52
3:P:347:PRO:HG3	7:T:62:GLY:HA2	1.90	0.52
3:C:279:TYR:CZ	3:C:283:ARG:HD3	2.45	0.52
4:D:186:VAL:O	4:D:190:LEU:HG	2.10	0.52
6:F:58:ARG:HA	6:F:61:ARG:NH2	2.25	0.52
3:P:107:SER:C	3:P:109:LEU:H	2.13	0.52
1:A:239:SER:HB2	7:G:17:SER:O	2.09	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD11	1:A:334:MET:HE3	1.92	0.52
1:A:45:SER:HA	1:A:48:GLU:CD	2.30	0.52
3:C:245:LEU:HD13	4:D:205:GLY:HA2	1.92	0.52
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.74	0.52
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.52
1:A:287:GLY:O	1:A:289:HIS:N	2.43	0.52
4:Q:55:THR:HG1	4:Q:56:HIS:CE1	2.23	0.52
5:R:157:TYR:HE1	5:R:162:GLY:HA2	1.72	0.52
5:E:34:GLY:HA2	10:J:10:TYR:HB2	1.92	0.52
10:W:42:ILE:O	10:W:46:LEU:HG	2.10	0.52
5:E:41:ALA:O	5:E:44:CYS:HB2	2.09	0.52
3:P:186:LEU:O	3:P:187:PRO:C	2.46	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.10	0.52
3:C:183:HIS:O	3:C:187:PRO:HD3	2.10	0.52
6:F:32:MET:HE3	6:F:87:LYS:CG	2.32	0.52
17:P:3005:PEE:O2P	5:R:40:THR:HG21	2.10	0.52
3:C:3:PRO:HG2	3:C:4:ASN:H	1.75	0.52
2:B:345:LYS:C	2:B:347:ALA:N	2.63	0.52
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.52
2:B:28:LYS:HG2	2:B:28:LYS:O	2.10	0.52
2:B:31:ASN:N	2:B:31:ASN:HD22	2.08	0.52
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.33	0.51
3:C:101:ARG:CD	3:C:102:GLY:N	2.71	0.51
2:B:428:GLY:O	2:B:430:LEU:N	2.43	0.51
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.19	0.51
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.92	0.51
8:H:15:ASP:O	8:H:17:LEU:N	2.43	0.51
1:A:404:ALA:O	1:A:405:ARG:C	2.48	0.51
6:F:58:ARG:HA	6:F:61:ARG:CZ	2.41	0.51
3:P:201:LEU:O	3:P:203:GLU:N	2.43	0.51
2:O:135:TRP:O	2:O:136:GLU:C	2.46	0.51
3:C:201:LEU:O	3:C:203:GLU:N	2.44	0.51
2:B:428:GLY:O	2:B:430:LEU:HG	2.10	0.51
2:O:272:PHE:O	2:O:275:LEU:N	2.42	0.51
3:C:208:ASN:OD1	3:C:208:ASN:C	2.48	0.51
1:A:159:GLN:NE2	1:A:237:THR:HG21	2.25	0.51
2:O:29:LEU:CD1	2:O:33:LEU:HD23	2.41	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.32	0.51
3:P:9:HIS:ND1	3:P:10:PRO:HD2	2.25	0.51
3:P:284:SER:O	3:P:286:PRO:HD3	2.11	0.51
2:B:63:LEU:O	2:B:65:THR:N	2.43	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:26:SER:HA	3:P:219:ILE:HD11	1.92	0.51
1:N:89:TYR:O	1:N:95:THR:HG23	2.11	0.51
1:A:239:SER:HB2	7:G:18:LEU:HA	1.91	0.51
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.51
3:C:332:ASN:O	3:C:336:LEU:HD12	2.11	0.51
2:B:239:TYR:CD2	2:B:240:TRP:N	2.78	0.51
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.46	0.51
6:F:68:LEU:O	6:F:70:LEU:N	2.44	0.51
5:R:38:LEU:CA	10:W:14:PHE:CE1	2.94	0.51
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.58	0.51
2:B:229:GLY:C	2:B:231:GLY:H	2.13	0.51
3:C:210:LEU:HD11	6:F:69:SER:HB2	1.91	0.51
6:F:104:ARG:O	6:F:108:ASN:ND2	2.44	0.51
2:B:50:PHE:CD1	2:B:50:PHE:N	2.78	0.51
2:O:101:THR:OG1	2:O:104:LYS:HB3	2.11	0.51
2:B:181:TYR:CE1	2:O:249:GLY:HA3	2.45	0.51
2:O:187:THR:OG1	2:O:189:GLU:HB2	2.10	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
2:B:102:ARG:NH1	2:B:172:LEU:O	2.44	0.51
2:O:385:GLU:C	2:O:387:LEU:H	2.13	0.51
2:O:226:ILE:CG2	2:O:227:ARG:N	2.73	0.51
8:H:37:LEU:O	8:H:38:GLU:C	2.48	0.51
3:P:237:LEU:O	3:P:241:LEU:HG	2.10	0.51
1:A:356:ARG:O	1:A:357:ALA:C	2.47	0.51
3:P:139:MET:O	3:P:140:SER:C	2.49	0.51
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.45	0.51
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.75	0.51
2:B:177:TYR:O	2:B:178:CYS:C	2.49	0.51
1:A:180:ALA:O	1:A:183:ALA:N	2.44	0.51
2:O:86:THR:O	2:O:90:GLU:HG3	2.11	0.51
3:C:5:ILE:HG22	3:C:12:LEU:HD12	1.93	0.51
2:O:81:SER:C	2:O:83:PHE:N	2.64	0.51
1:N:61:HIS:ND1	1:N:134:ILE:HG12	2.25	0.51
4:Q:183:ALA:HA	4:Q:186:VAL:HG12	1.93	0.51
1:A:394:GLU:O	1:A:395:TRP:C	2.49	0.51
6:S:16:ILE:O	6:S:19:TRP:HB3	2.10	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
1:A:86:PHE:O	2:B:285:ILE:HA	2.10	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.92	0.51
1:N:171:THR:O	1:N:175:LYS:HG3	2.11	0.51
4:D:43:MET:HG2	4:D:91:PHE:HD2	1.76	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:ILE:CD1	7:G:29:ILE:H	2.01	0.51
7:G:29:ILE:O	7:G:34:LEU:HG	2.11	0.51
6:F:87:LYS:O	6:F:89:TYR:N	2.44	0.51
5:R:31:ASP:OD2	10:W:7:ARG:HG3	2.11	0.51
1:N:388:ARG:HD3	1:N:388:ARG:H	1.76	0.51
4:Q:227:TRP:O	4:Q:228:SER:C	2.49	0.51
3:P:107:SER:HB2	11:P:502:HEM:HMD3	1.93	0.51
2:O:221:GLU:O	2:O:223:PHE:N	2.43	0.51
3:P:245:LEU:HD13	4:Q:205:GLY:HA2	1.91	0.51
2:O:308:ASP:OD2	9:V:59:SER:HB2	2.11	0.51
5:E:186:GLN:HE21	5:E:188:VAL:HG12	1.75	0.51
1:A:114:ALA:HA	1:A:216:PHE:HE2	1.76	0.51
10:J:42:ILE:O	10:J:46:LEU:HG	2.11	0.51
3:C:231:LEU:CD1	4:D:220:TYR:HA	2.41	0.51
3:P:345:GLU:O	3:P:349:ILE:HG13	2.11	0.51
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.92	0.51
3:C:245:LEU:O	4:D:201:ARG:CG	2.58	0.51
3:C:304:LEU:O	3:C:305:ILE:C	2.50	0.51
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.10	0.51
5:R:41:ALA:O	5:R:44:CYS:HB2	2.11	0.51
5:R:108:GLN:O	5:R:110:ALA:N	2.44	0.51
3:P:230:ILE:O	3:P:233:LEU:HB3	2.11	0.51
1:N:107:PRO:HG2	1:N:108:LYS:H	1.75	0.51
2:B:385:GLU:C	2:B:387:LEU:H	2.14	0.51
4:D:54:VAL:HG11	4:D:192:TRP:CE2	2.45	0.51
7:G:55:ALA:O	7:G:56:TYR:C	2.48	0.51
7:T:55:ALA:O	7:T:58:LEU:N	2.44	0.51
1:N:332:ASP:O	1:N:333:ASP:C	2.50	0.51
6:F:40:ASP:O	6:F:44:LYS:HG3	2.11	0.51
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.41	0.50
3:C:92:PHE:CA	3:C:95:ILE:HG22	2.38	0.50
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.26	0.50
3:C:230:ILE:O	3:C:233:LEU:HB3	2.11	0.50
2:O:272:PHE:HB3	2:O:322:PHE:CE1	2.46	0.50
7:T:56:TYR:O	7:T:59:TYR:HB3	2.11	0.50
4:Q:134:TYR:CD1	4:Q:162:PRO:HG3	2.46	0.50
2:B:370:MET:O	2:B:373:GLU:HG3	2.11	0.50
3:P:134:LEU:HD21	3:P:180:PHE:HA	1.92	0.50
7:G:34:LEU:O	7:G:37:VAL:N	2.45	0.50
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.47	0.50
1:N:27:SER:HB2	1:N:199:ALA:O	2.11	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LEU:O	2:B:279:LEU:HD12	2.12	0.50
5:E:29:SER:CB	5:E:32:ARG:HH21	2.25	0.50
4:D:232:SER:CB	7:G:23:GLN:HE22	2.23	0.50
3:P:332:ASN:ND2	3:P:359:TYR:HA	2.26	0.50
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.26	0.50
2:O:263:ALA:HA	2:O:319:SER:O	2.11	0.50
2:O:393:THR:CG2	2:O:397:VAL:HB	2.42	0.50
2:B:100:SER:HA	2:B:104:LYS:O	2.11	0.50
5:R:74:ILE:HG23	5:R:74:ILE:O	2.11	0.50
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.76	0.50
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.46	0.50
1:N:45:SER:HA	1:N:48:GLU:CD	2.31	0.50
5:R:35:PHE:O	5:R:36:SER:C	2.50	0.50
3:C:273:TRP:CE3	3:C:274:TYR:N	2.79	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.93	0.50
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.92	0.50
3:P:129:PHE:CD1	3:P:147:ILE:HD12	2.46	0.50
2:B:81:SER:O	2:B:83:PHE:N	2.45	0.50
2:O:227:ARG:HG3	2:O:228:SER:H	1.77	0.50
1:A:253:VAL:HG11	1:A:335:MET:CE	2.40	0.50
1:A:55:ALA:O	1:A:57:TYR:N	2.44	0.50
2:O:275:LEU:O	2:O:275:LEU:HD12	2.11	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.92	0.50
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.41	0.50
4:D:102:ARG:NH1	4:D:107:GLY:O	2.44	0.50
3:C:104:TYR:HD2	3:C:105:TYR:CD1	2.29	0.50
1:A:124:GLU:O	1:A:124:GLU:HG2	2.11	0.50
4:D:47:ALA:HB1	4:D:89:ASP:O	2.12	0.50
6:F:32:MET:HE1	6:F:87:LYS:H	1.75	0.50
1:N:335:MET:O	1:N:338:ALA:HB3	2.11	0.50
1:N:269:VAL:HG11	1:N:410:VAL:CG2	2.39	0.50
3:P:354:MET:O	3:P:357:LEU:N	2.45	0.50
4:D:26:VAL:HG13	4:D:189:PHE:HD1	1.76	0.50
2:B:393:THR:HG23	2:B:397:VAL:HB	1.94	0.50
3:C:284:SER:O	3:C:286:PRO:HD3	2.12	0.50
3:P:198:LEU:HD11	15:P:3002:ANY:O4	2.12	0.50
8:U:66:ASP:O	8:U:69:VAL:HB	2.11	0.50
1:N:54:GLY:O	1:N:55:ALA:C	2.49	0.50
1:A:138:LEU:HD22	5:E:3:ASN:ND2	2.26	0.50
1:A:206:LYS:O	1:A:209:VAL:CG1	2.56	0.50
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.77	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:VAL:O	5:E:48:ALA:HB3	2.11	0.50
4:Q:235:MET:HE1	6:S:63:LYS:C	2.32	0.50
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.92	0.50
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.47	0.50
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.93	0.50
10:W:22:LEU:H	10:W:22:LEU:HD23	1.75	0.50
3:C:273:TRP:HA	3:C:276:LEU:HG	1.93	0.50
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.77	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.94	0.50
6:S:89:TYR:CD1	6:S:90:LEU:N	2.75	0.50
5:E:29:SER:OG	5:E:30:GLU:N	2.44	0.50
6:F:73:ARG:HG3	6:F:73:ARG:HH11	1.75	0.50
1:N:180:ALA:O	1:N:183:ALA:N	2.45	0.50
3:C:273:TRP:CE3	3:C:274:TYR:HA	2.47	0.50
1:N:55:ALA:O	1:N:57:TYR:N	2.45	0.50
3:C:139:MET:O	3:C:140:SER:C	2.50	0.50
3:C:354:MET:O	3:C:357:LEU:N	2.45	0.50
6:F:21:TYR:C	6:F:21:TYR:CD2	2.84	0.50
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.39	0.50
4:Q:215:LEU:O	4:Q:215:LEU:HD12	2.12	0.50
1:A:333:ASP:O	1:A:336:PHE:HB3	2.12	0.50
5:R:78:LEU:HD21	5:R:193:VAL:HG11	1.92	0.50
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.50
5:E:171:ILE:HG23	5:E:171:ILE:O	2.12	0.50
4:Q:167:GLU:HG3	8:U:13:LEU:HD11	1.94	0.50
2:B:272:PHE:HB3	2:B:322:PHE:CE1	2.47	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.12	0.50
1:A:161:THR:HB	1:A:234:CYS:SG	2.51	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HB	2.47	0.50
2:O:66:ALA:O	2:O:69:LEU:HB3	2.12	0.50
1:N:310:PHE:HE1	1:N:322:PHE:N	2.10	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.11	0.50
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.94	0.49
1:A:233:ARG:NH1	1:A:233:ARG:HG3	2.27	0.49
2:B:206:LEU:HG	2:B:206:LEU:O	2.11	0.49
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.93	0.49
3:P:242:THR:N	4:Q:208:MET:CE	2.75	0.49
4:Q:232:SER:CB	7:T:23:GLN:HE22	2.25	0.49
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.41	0.49
1:A:411:CYS:O	1:A:415:ILE:HG13	2.11	0.49
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.47	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:HIS:O	1:A:177:LEU:C	2.50	0.49
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.47	0.49
8:H:32:LYS:O	8:H:36:ARG:HG3	2.12	0.49
1:N:40:TRP:CD1	1:N:96:ALA:CB	2.95	0.49
1:A:107:PRO:HG2	1:A:108:LYS:H	1.76	0.49
1:A:4:TYR:O	1:A:5:ALA:C	2.51	0.49
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.94	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.77	0.49
2:O:345:LYS:O	2:O:347:ALA:N	2.46	0.49
8:U:37:LEU:O	8:U:38:GLU:C	2.51	0.49
3:C:241:LEU:CB	4:D:208:MET:HE2	2.42	0.49
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.42	0.49
1:N:356:ARG:O	1:N:359:ASN:N	2.46	0.49
1:N:45:SER:CA	1:N:48:GLU:HG3	2.41	0.49
6:S:63:LYS:O	6:S:63:LYS:HG2	2.12	0.49
8:H:58:LEU:HG	8:H:62:LEU:CD1	2.43	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB2	1.95	0.49
1:A:21:ASN:HD22	1:A:192:ALA:CB	2.25	0.49
3:C:186:LEU:O	3:C:187:PRO:C	2.51	0.49
10:J:60:GLU:O	10:J:61:ALA:HB3	2.12	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
8:H:66:ASP:O	8:H:69:VAL:HB	2.12	0.49
1:N:104:LYS:O	1:N:107:PRO:HD2	2.13	0.49
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.94	0.49
2:B:272:PHE:HZ	2:B:416:LYS:HD3	1.78	0.49
6:F:16:ILE:O	6:F:19:TRP:HB3	2.13	0.49
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.48	0.49
5:E:152:ASP:C	5:E:153:PHE:CD1	2.85	0.49
1:A:220:SER:HB2	1:A:226:ASP:OD1	2.12	0.49
3:P:80:ILE:O	3:P:81:ARG:C	2.51	0.49
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.42	0.49
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.47	0.49
2:B:75:LEU:HD11	2:B:140:LEU:HD23	1.95	0.49
5:E:113:ASP:C	5:E:115:SER:H	2.16	0.49
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.12	0.49
3:P:192:GLY:O	3:P:195:ILE:HB	2.12	0.49
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.13	0.49
3:C:92:PHE:C	3:C:95:ILE:HG22	2.32	0.49
5:R:127:VAL:HG11	5:R:133:VAL:HA	1.95	0.49
4:Q:116:ILE:HG23	4:Q:117:VAL:H	1.76	0.49
3:C:26:SER:HA	3:C:219:ILE:CD1	2.43	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:MET:HE1	6:F:20:TYR:HD1	1.77	0.49
2:O:239:TYR:HE1	2:O:260:GLU:N	2.11	0.49
3:C:366:LEU:HD23	3:C:366:LEU:N	2.28	0.49
3:P:79:LEU:O	3:P:79:LEU:HD12	2.12	0.49
2:B:408:ALA:O	2:B:410:VAL:N	2.46	0.49
5:E:51:ALA:O	5:E:52:LYS:C	2.50	0.49
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.49
4:D:55:THR:HG1	4:D:56:HIS:CE1	2.30	0.49
3:C:78:TRP:CD2	3:C:79:LEU:N	2.80	0.49
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.94	0.49
5:R:29:SER:OG	5:R:30:GLU:N	2.46	0.49
2:O:292:THR:HG22	2:O:292:THR:O	2.12	0.49
7:G:45:VAL:HG13	7:G:46:PHE:N	2.28	0.49
3:P:30:ALA:O	3:P:32:TRP:N	2.45	0.49
2:B:31:ASN:ND2	2:B:32:GLY:H	2.11	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.13	0.49
5:R:114:VAL:HG12	5:R:114:VAL:O	2.12	0.49
1:N:420:PRO:HD2	1:N:434:TYR:OH	2.13	0.49
2:B:72:ALA:O	2:B:75:LEU:HB2	2.12	0.49
5:E:29:SER:HA	5:E:32:ARG:HE	1.78	0.49
3:P:172:ASP:C	3:P:174:PRO:HD2	2.33	0.49
2:B:209:ILE:HD11	2:B:378:LEU:HG	1.94	0.49
4:D:24:SER:OG	10:J:55:ILE:HD11	2.13	0.49
1:N:241:ILE:O	1:N:241:ILE:HG23	2.11	0.49
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.14	0.49
4:Q:47:ALA:O	4:Q:49:ARG:N	2.46	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.12	0.49
1:N:255:LEU:O	1:N:321:GLY:HA3	2.13	0.49
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.48	0.49
3:C:172:ASP:C	3:C:174:PRO:HD2	2.33	0.49
4:D:109:LEU:O	4:D:111:PRO:HD3	2.12	0.49
2:O:81:SER:O	2:O:82:SER:C	2.52	0.48
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.28	0.48
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.48	0.48
5:R:165:TYR:HA	5:R:170:ARG:O	2.13	0.48
4:D:215:LEU:O	4:D:215:LEU:HD12	2.13	0.48
2:B:27:THR:HG22	2:B:28:LYS:N	2.28	0.48
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.26	0.48
8:U:61:PHE:O	8:U:62:LEU:C	2.50	0.48
1:N:310:PHE:CE1	1:N:322:PHE:N	2.81	0.48
5:E:113:ASP:HB3	5:E:116:LYS:HB2	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:25:VAL:O	10:W:29:VAL:HG23	2.13	0.48
3:P:287:ASN:O	3:P:288:LYS:C	2.50	0.48
7:G:29:ILE:HD12	7:G:29:ILE:N	2.13	0.48
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.48
1:A:334:MET:O	1:A:335:MET:C	2.51	0.48
2:B:239:TYR:HD2	2:B:240:TRP:N	2.12	0.48
3:C:365:ILE:C	3:C:368:PRO:HD2	2.33	0.48
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.95	0.48
8:U:59:PHE:O	8:U:60:ASP:C	2.52	0.48
2:B:325:TYR:CD2	2:B:325:TYR:C	2.87	0.48
12:Q:501:HEC:CBB	12:Q:501:HEC:HMB1	2.40	0.48
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.13	0.48
1:N:334:MET:O	1:N:335:MET:C	2.52	0.48
1:N:404:ALA:O	1:N:405:ARG:C	2.52	0.48
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.94	0.48
3:C:287:ASN:O	3:C:288:LYS:C	2.52	0.48
1:A:36:THR:OG1	1:A:100:LYS:HG2	2.13	0.48
1:N:63:ALA:O	1:N:116:VAL:HG11	2.13	0.48
3:P:157:ILE:O	3:P:158:GLY:C	2.52	0.48
1:A:239:SER:CB	7:G:18:LEU:HA	2.43	0.48
2:B:135:TRP:O	2:B:136:GLU:C	2.51	0.48
2:O:307:PHE:H	9:V:52:ARG:HG2	1.78	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CD2	2.49	0.48
1:A:170:THR:HG22	1:A:171:THR:N	2.29	0.48
3:P:184:PHE:CG	11:P:501:HEM:HBC1	2.49	0.48
4:Q:167:GLU:C	4:Q:169:LEU:N	2.65	0.48
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.13	0.48
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.95	0.48
3:P:311:SER:HB2	3:P:319:ARG:HH11	1.79	0.48
1:N:4:TYR:O	1:N:5:ALA:C	2.52	0.48
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.96	0.48
2:B:31:ASN:N	2:B:31:ASN:ND2	2.61	0.48
5:R:163:SER:HA	5:R:174:GLY:HA3	1.94	0.48
5:E:69:LEU:HD13	5:E:71:LEU:HD11	1.96	0.48
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.48
5:E:142:LEU:HD22	3:P:149:ASN:HB3	1.96	0.48
4:D:131:LEU:HD11	12:D:501:HEC:HMB2	1.96	0.48
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.44	0.48
2:O:75:LEU:HD21	2:O:136:GLU:HB3	1.95	0.48
1:A:21:ASN:HB3	1:A:218:GLY:O	2.12	0.48
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.44	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.94	0.48
3:P:158:GLY:O	3:P:161:LEU:N	2.47	0.48
3:P:127:THR:O	3:P:130:VAL:HG22	2.14	0.48
2:B:167:ALA:C	2:B:168:TYR:CD1	2.87	0.48
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.96	0.48
2:O:272:PHE:HZ	2:O:416:LYS:HD3	1.79	0.48
3:C:245:LEU:O	4:D:201:ARG:HG2	2.14	0.48
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.14	0.48
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.95	0.48
2:O:253:VAL:HG13	2:O:430:LEU:CD2	2.44	0.48
5:R:134:ILE:C	5:R:135:LEU:HG	2.33	0.48
1:N:85:HIS:CD2	2:O:284:LEU:HB3	2.48	0.48
4:D:28:ARG:O	4:D:29:GLY:C	2.52	0.48
3:P:273:TRP:CE3	3:P:274:TYR:CA	2.97	0.48
3:C:164:TRP:O	3:C:165:ALA:C	2.50	0.48
2:O:177:TYR:O	2:O:178:CYS:C	2.51	0.48
5:E:55:VAL:O	5:E:56:THR:C	2.52	0.48
2:B:66:ALA:O	2:B:69:LEU:HB3	2.14	0.48
2:O:29:LEU:HD23	2:O:30:PRO:HD2	1.95	0.48
3:P:191:ALA:O	3:P:195:ILE:HG12	2.13	0.48
1:N:93:GLU:O	1:N:93:GLU:HG3	2.14	0.48
1:N:93:GLU:O	1:N:94:GLN:HB2	2.14	0.48
1:A:191:LYS:O	1:A:195:MET:HG3	2.13	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.14	0.48
4:D:218:LEU:HD13	5:E:43:ALA:N	2.28	0.48
4:D:26:VAL:CG1	4:D:189:PHE:HD1	2.27	0.48
2:O:163:LEU:HD13	2:O:425:ALA:CB	2.44	0.48
1:N:178:THR:HG22	1:N:180:ALA:H	1.79	0.48
1:A:63:ALA:O	1:A:116:VAL:HG11	2.14	0.48
1:A:244:ARG:HH22	1:A:429:GLU:CD	2.17	0.47
3:P:304:LEU:O	3:P:305:ILE:C	2.52	0.47
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.49	0.47
3:P:246:PHE:CZ	4:Q:205:GLY:C	2.87	0.47
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.29	0.47
3:P:3:PRO:HG2	3:P:4:ASN:H	1.78	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.28	0.47
3:C:196:ILE:O	3:C:199:THR:N	2.46	0.47
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.79	0.47
7:G:61:TRP:CE3	7:G:62:GLY:N	2.82	0.47
4:D:161:ALA:O	4:D:162:PRO:C	2.53	0.47
2:O:206:LEU:O	2:O:206:LEU:HG	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:182:ARG:NH2	2:O:190:GLN:OE1	2.47	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.49	0.47
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.47
1:N:35:CYS:HB2	1:N:200:ALA:O	2.14	0.47
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.80	0.47
2:B:163:LEU:HD13	2:B:425:ALA:CB	2.43	0.47
3:P:107:SER:O	3:P:109:LEU:N	2.47	0.47
3:P:120:LEU:HB3	11:P:502:HEM:HAB	1.96	0.47
3:P:201:LEU:HD11	11:P:502:HEM:HAD2	1.95	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.14	0.47
7:T:4:PHE:CD2	7:T:7:LEU:HD11	2.49	0.47
2:B:166:ALA:O	2:B:242:GLY:N	2.37	0.47
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.44	0.47
3:P:154:ILE:CG2	3:P:155:PRO:HD2	2.43	0.47
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.96	0.47
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.28	0.47
1:N:145:MET:O	1:N:146:THR:C	2.52	0.47
5:E:52:LYS:HD3	5:E:56:THR:OG1	2.13	0.47
1:A:171:THR:O	1:A:175:LYS:HG3	2.14	0.47
9:V:49:LEU:O	9:V:50:LEU:HG	2.14	0.47
1:N:287:GLY:O	1:N:289:HIS:N	2.47	0.47
6:S:58:ARG:HA	6:S:61:ARG:CZ	2.44	0.47
4:Q:26:VAL:HG13	4:Q:189:PHE:HD1	1.79	0.47
4:Q:26:VAL:CG1	4:Q:189:PHE:HD1	2.27	0.47
1:N:45:SER:OG	1:N:92:ARG:HA	2.13	0.47
4:D:200:GLN:HE21	18:E:2009:PLC:H51	1.79	0.47
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.50	0.47
3:C:165:ALA:O	3:C:178:ARG:HD2	2.14	0.47
5:E:152:ASP:O	5:E:153:PHE:CD1	2.67	0.47
3:P:31:TRP:O	3:P:101:ARG:HG3	2.13	0.47
8:H:37:LEU:O	8:H:40:CYS:N	2.47	0.47
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.49	0.47
1:A:106:MET:HE3	1:A:208:LEU:CD1	2.45	0.47
3:C:123:THR:HG22	3:C:190:ILE:HD11	1.95	0.47
6:F:19:TRP:O	6:F:22:ASN:N	2.47	0.47
7:T:16:TYR:N	7:T:16:TYR:CD1	2.82	0.47
5:E:85:LYS:HG2	5:E:86:ASN:N	2.29	0.47
1:A:69:LYS:HE3	1:A:70:ARG:NH2	2.14	0.47
2:B:81:SER:C	2:B:83:PHE:N	2.65	0.47
3:P:117:GLY:HA3	11:P:502:HEM:HBC2	1.97	0.47
3:C:371:GLY:O	3:C:374:GLU:HB2	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:GLN:O	2:B:347:ALA:HB2	2.15	0.47
7:G:49:ALA:O	7:G:50:PRO:C	2.53	0.47
7:G:56:TYR:O	7:G:59:TYR:HB3	2.15	0.47
2:O:259:THR:O	2:O:260:GLU:C	2.51	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.28	0.47
6:F:52:GLU:HG2	6:F:56:ASN:HD21	1.78	0.47
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.47	0.47
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.47
4:Q:130:LEU:HD12	4:Q:150:ASN:ND2	2.30	0.47
10:W:26:LEU:O	10:W:30:LEU:HG	2.14	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.13	0.47
7:T:34:LEU:O	7:T:37:VAL:N	2.47	0.47
1:N:422:LEU:HD22	1:N:437:ILE:HD12	1.96	0.47
6:S:90:LEU:O	6:S:91:GLU:C	2.53	0.47
3:C:95:ILE:HD13	3:C:121:LEU:HD12	1.96	0.47
2:B:239:TYR:HD1	2:B:260:GLU:HB2	1.76	0.47
1:A:29:GLU:HG3	1:A:203:ILE:O	2.15	0.47
3:C:78:TRP:CG	3:C:79:LEU:N	2.83	0.47
2:O:67:HIS:ND1	2:O:177:TYR:HA	2.30	0.47
3:P:347:PRO:O	3:P:350:ILE:HG22	2.14	0.47
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.29	0.47
1:N:176:HIS:O	1:N:177:LEU:C	2.53	0.47
8:U:15:ASP:O	8:U:17:LEU:N	2.48	0.47
4:D:47:ALA:O	4:D:50:ASN:N	2.38	0.47
4:D:182:ILE:O	4:D:184:LYS:N	2.48	0.47
3:P:277:PHE:CD1	3:P:277:PHE:C	2.88	0.47
1:N:103:SER:O	1:N:106:MET:HB2	2.15	0.47
3:C:92:PHE:HA	3:C:95:ILE:CG2	2.41	0.47
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.95	0.47
8:H:44:VAL:HG22	8:H:52:GLU:HG2	1.97	0.47
1:A:45:SER:CA	1:A:48:GLU:HG3	2.42	0.47
1:N:253:VAL:CG1	1:N:335:MET:HE1	2.45	0.47
1:A:27:SER:CB	1:A:199:ALA:O	2.62	0.47
3:C:241:LEU:HB3	4:D:208:MET:HE2	1.97	0.47
9:I:65:VAL:HG12	9:I:66:ALA:H	1.79	0.47
6:F:77:LYS:HA	6:F:80:TRP:NE1	2.30	0.47
3:C:213:SER:HB2	6:F:39:GLU:OE2	2.15	0.47
3:P:122:LEU:O	3:P:125:MET:HB2	2.13	0.47
3:P:210:LEU:HD12	6:S:66:LEU:HD23	1.96	0.47
4:Q:158:ILE:HG12	4:Q:159:GLY:H	1.80	0.47
5:E:126:ARG:O	5:E:182:VAL:HG11	2.15	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:29:LEU:HD22	2:O:30:PRO:HD2	1.96	0.47
2:O:200:THR:O	2:O:202:ALA:N	2.47	0.47
2:O:275:LEU:O	2:O:279:LEU:HD12	2.15	0.47
6:S:76:PRO:O	6:S:78:GLU:N	2.48	0.47
2:O:209:ILE:HD11	2:O:378:LEU:HG	1.97	0.47
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.50	0.47
1:N:67:THR:HA	1:N:121:ALA:H	1.78	0.47
3:P:130:VAL:HG23	3:P:131:GLY:H	1.80	0.47
1:N:42:GLY:HA2	1:N:384:LEU:HD21	1.97	0.47
2:O:309:ALA:HA	2:O:325:TYR:O	2.15	0.47
1:N:388:ARG:NH2	1:N:388:ARG:CG	2.78	0.47
4:Q:220:TYR:HE2	16:Q:3003:CDL:H722	1.79	0.47
4:Q:230:LEU:O	6:S:70:LEU:HD11	2.15	0.47
4:Q:191:ARG:O	4:Q:194:ALA:N	2.46	0.47
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.62	0.47
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.47
1:A:281:ASP:HB3	1:A:284:PHE:CE1	2.50	0.47
3:P:380:TYR:OH	6:S:34:ASP:HA	2.15	0.47
2:B:412:ASN:O	2:B:415:LYS:N	2.47	0.47
4:D:46:VAL:CG1	4:D:47:ALA:N	2.76	0.47
1:N:105:ASP:O	1:N:106:MET:C	2.54	0.47
1:N:106:MET:O	1:N:110:VAL:HG23	2.14	0.47
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.96	0.47
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.55	0.47
1:A:54:GLY:O	1:A:55:ALA:C	2.54	0.47
3:P:29:SER:O	3:P:32:TRP:HB2	2.15	0.47
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.50	0.47
8:H:61:PHE:O	8:H:62:LEU:C	2.53	0.47
1:N:280:TYR:CG	1:N:281:ASP:N	2.83	0.47
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.47
2:O:100:SER:HB3	2:O:105:MET:HA	1.97	0.47
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.50	0.47
3:C:199:THR:HG22	3:C:200:PHE:N	2.30	0.47
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.45	0.47
2:B:176:LEU:O	2:B:176:LEU:HD12	2.15	0.47
2:O:428:GLY:O	2:O:430:LEU:N	2.47	0.46
3:C:101:ARG:HD2	3:C:102:GLY:CA	2.45	0.46
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.29	0.46
1:A:235:ARG:NH2	5:E:14:ARG:NH2	2.63	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
2:O:393:THR:HG23	2:O:397:VAL:HB	1.96	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LYS:O	4:D:66:GLU:HG3	2.15	0.46
1:A:305:HIS:ND1	9:I:35:UNK:CB	2.79	0.46
5:E:148:ALA:O	5:E:149:ASN:HB2	2.15	0.46
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.30	0.46
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.80	0.46
5:R:47:THR:O	5:R:48:ALA:C	2.52	0.46
1:N:435:ASN:O	1:N:438:ARG:HB3	2.15	0.46
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.30	0.46
3:P:63:ALA:CB	3:P:176:LEU:HD21	2.44	0.46
3:C:30:ALA:C	3:C:32:TRP:N	2.67	0.46
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.46
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.81	0.46
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.30	0.46
3:C:4:ASN:O	3:C:4:ASN:OD1	2.33	0.46
2:O:314:VAL:HG11	2:O:316:TYR:CZ	2.50	0.46
1:N:19:LEU:C	1:N:21:ASN:H	2.18	0.46
1:N:307:PHE:HA	1:N:324:PHE:HA	1.97	0.46
1:A:86:PHE:CD2	1:A:99:ILE:HD11	2.50	0.46
1:A:21:ASN:HD22	1:A:192:ALA:HB1	1.79	0.46
5:R:136:VAL:HB	5:R:181:GLU:HB3	1.97	0.46
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.78	0.46
1:A:330:SER:O	1:A:331:ILE:C	2.53	0.46
3:P:104:TYR:CD2	3:P:105:TYR:CE1	2.97	0.46
1:A:372:THR:O	1:A:373:THR:C	2.54	0.46
3:P:59:ASP:O	3:P:60:THR:C	2.54	0.46
5:R:38:LEU:CA	10:W:14:PHE:HE1	2.28	0.46
3:C:172:ASP:OD1	3:C:173:ASN:N	2.43	0.46
3:P:365:ILE:C	3:P:368:PRO:HD2	2.36	0.46
1:A:438:ARG:NH1	1:A:438:ARG:HG3	2.30	0.46
2:B:280:GLY:HA3	2:B:293:SER:OG	2.16	0.46
3:C:285:ILE:HG21	3:C:290:GLY:HA3	1.98	0.46
3:P:281:ILE:O	3:P:285:ILE:HD13	2.16	0.46
2:B:101:THR:OG1	2:B:104:LYS:HB3	2.16	0.46
3:C:122:LEU:O	3:C:125:MET:HB2	2.15	0.46
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.81	0.46
7:G:33:ALA:O	7:G:34:LEU:C	2.54	0.46
6:F:36:THR:O	6:F:37:LEU:C	2.54	0.46
6:F:89:TYR:CD1	6:F:90:LEU:N	2.73	0.46
2:B:189:GLU:C	2:B:191:LEU:N	2.67	0.46
4:Q:182:ILE:O	4:Q:184:LYS:N	2.49	0.46
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.41	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.98	0.46
2:B:239:TYR:C	2:B:239:TYR:CD2	2.89	0.46
3:C:338:TRP:CE2	7:G:59:TYR:HD1	2.32	0.46
2:O:239:TYR:CE1	2:O:260:GLU:HB2	2.50	0.46
3:P:350:ILE:HG23	3:P:351:ILE:N	2.30	0.46
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.50	0.46
1:A:104:LYS:O	1:A:107:PRO:HD2	2.16	0.46
3:P:277:PHE:HD2	17:P:3007:PEE:H77	1.79	0.46
1:A:388:ARG:NH2	1:A:388:ARG:CG	2.77	0.46
3:C:277:PHE:CD1	3:C:277:PHE:C	2.88	0.46
3:C:270:LYS:HA	3:C:271:PRO:HD3	1.77	0.46
5:R:171:ILE:O	5:R:171:ILE:HG23	2.16	0.46
2:O:113:ARG:O	2:O:116:VAL:HG23	2.16	0.46
3:P:332:ASN:HD21	3:P:359:TYR:CA	2.29	0.46
4:D:10:PHE:N	4:D:10:PHE:HD1	2.07	0.46
1:N:284:PHE:CE2	9:V:71:ASN:O	2.69	0.46
2:O:166:ALA:HB2	2:O:244:ILE:CD1	2.46	0.46
3:P:295:LEU:O	3:P:296:ALA:C	2.54	0.46
1:N:112:LEU:HG	1:N:112:LEU:H	1.48	0.46
3:C:219:ILE:HD11	3:C:225:TYR:CE1	2.51	0.46
2:O:168:TYR:CD2	2:O:237:ALA:HB1	2.51	0.46
3:C:335:ILE:O	3:C:336:LEU:C	2.53	0.46
10:W:14:PHE:HD2	10:W:14:PHE:N	2.13	0.46
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.64	0.46
3:C:258:THR:HG22	3:C:258:THR:O	2.15	0.46
3:C:357:LEU:HD12	3:C:357:LEU:HA	1.68	0.46
10:J:52:TRP:O	10:J:56:LYS:HB2	2.15	0.46
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.98	0.46
6:S:18:LYS:HA	6:S:83:TYR:CD1	2.50	0.46
4:Q:121:HIS:C	4:Q:123:GLY:H	2.18	0.46
3:P:199:THR:HG22	3:P:200:PHE:N	2.31	0.46
4:Q:29:GLY:HA3	4:Q:185:ASP:O	2.16	0.46
2:O:128:THR:CA	2:O:226:ILE:HD11	2.41	0.46
8:H:40:CYS:O	8:H:41:ASP:C	2.54	0.46
3:P:25:PRO:HG2	3:P:207:ASN:O	2.16	0.46
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.29	0.46
3:P:56:TYR:OH	3:P:176:LEU:HD11	2.16	0.46
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.34	0.46
3:C:344:VAL:CG1	3:C:349:ILE:HD11	2.46	0.46
2:B:67:HIS:ND1	2:B:177:TYR:HA	2.31	0.46
2:O:241:GLY:HA2	2:O:423:SER:OG	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:ARG:O	8:H:69:VAL:HG23	2.15	0.46
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.97	0.46
5:R:29:SER:HA	5:R:32:ARG:HE	1.81	0.46
2:B:113:ARG:O	2:B:116:VAL:HG23	2.15	0.46
2:B:72:ALA:CA	2:B:75:LEU:HD12	2.46	0.46
5:E:29:SER:CA	5:E:32:ARG:HH21	2.29	0.46
3:P:355:ALA:HA	3:P:358:SER:HB3	1.97	0.46
3:C:70:THR:O	3:C:70:THR:HG22	2.15	0.46
3:P:166:TRP:NE1	3:P:171:VAL:HG22	2.31	0.46
3:P:198:LEU:HA	3:P:198:LEU:HD23	1.64	0.46
4:D:109:LEU:HG	4:D:109:LEU:O	2.15	0.46
8:U:17:LEU:HD11	8:U:21:ARG:HE	1.81	0.46
1:A:93:GLU:O	1:A:94:GLN:HB2	2.16	0.46
1:A:243:ALA:O	1:A:425:VAL:HA	2.16	0.46
5:E:122:HIS:O	5:E:124:LEU:N	2.49	0.46
8:U:46:SER:OG	8:U:47:ARG:N	2.48	0.46
2:O:63:LEU:C	2:O:65:THR:H	2.20	0.46
6:S:58:ARG:HA	6:S:61:ARG:NH2	2.30	0.46
3:C:117:GLY:HA3	11:C:502:HEM:HBC2	1.97	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.46	0.46
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.96	0.46
4:Q:5:LEU:HG	4:Q:152:TYR:HE1	1.81	0.46
6:S:74:ILE:HG13	6:S:75:LEU:N	2.30	0.46
3:C:104:TYR:CD2	3:C:105:TYR:CE1	3.04	0.46
2:O:378:LEU:C	2:O:380:ASN:N	2.70	0.46
1:A:103:SER:O	1:A:106:MET:HB2	2.15	0.46
5:E:140:THR:HG21	5:E:178:TYR:HB2	1.97	0.46
7:G:81:GLN:OXT	8:H:49:HIS:HB3	2.16	0.46
3:C:183:HIS:O	3:C:187:PRO:CD	2.64	0.46
3:C:378:LEU:O	3:C:379:ASN:CB	2.63	0.46
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.51	0.45
2:B:76:THR:HG22	2:B:82:SER:N	2.21	0.45
3:C:269:ILE:CG2	3:C:269:ILE:O	2.63	0.45
4:Q:5:LEU:HG	4:Q:152:TYR:CE1	2.51	0.45
3:P:332:ASN:O	3:P:336:LEU:HD12	2.16	0.45
5:R:150:SER:OG	5:R:157:TYR:HB3	2.16	0.45
3:P:338:TRP:CE2	7:T:59:TYR:CD1	3.02	0.45
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.31	0.45
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.98	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
5:R:18:VAL:O	5:R:18:VAL:HG23	2.15	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:242:ARG:O	7:T:14:ILE:HA	2.15	0.45
3:C:295:LEU:O	3:C:296:ALA:C	2.51	0.45
3:P:100:GLY:O	3:P:101:ARG:C	2.54	0.45
3:P:208:ASN:C	3:P:208:ASN:OD1	2.54	0.45
1:N:301:HIS:HB2	1:N:303:LEU:HD21	1.97	0.45
1:N:235:ARG:NH2	5:R:14:ARG:NH2	2.65	0.45
7:T:41:PHE:HE2	7:T:45:VAL:HB	1.81	0.45
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.46	0.45
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.46	0.45
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.50	0.45
1:A:147:ASN:O	1:A:148:VAL:C	2.55	0.45
4:Q:42:SER:HB2	4:Q:112:ASP:OD2	2.16	0.45
3:C:141:PHE:O	3:C:144:ALA:HB3	2.16	0.45
8:H:59:PHE:O	8:H:60:ASP:C	2.54	0.45
2:B:57:TYR:CD1	2:B:57:TYR:N	2.84	0.45
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.97	0.45
3:C:38:LEU:HB3	11:C:502:HEM:CMB	2.46	0.45
3:P:117:GLY:CA	11:P:502:HEM:HBC2	2.46	0.45
2:B:42:SER:OG	2:B:43:PRO:HD2	2.16	0.45
1:N:49:ASN:HD21	1:N:52:ASN:N	2.13	0.45
3:P:27:ASN:HD22	3:P:209:PRO:HD2	1.82	0.45
1:N:22:GLY:C	1:N:193:PRO:HA	2.35	0.45
5:E:35:PHE:O	5:E:38:LEU:HB3	2.17	0.45
1:A:21:ASN:ND2	1:A:192:ALA:HB1	2.30	0.45
1:N:178:THR:HB	1:N:181:ASP:OD1	2.16	0.45
3:C:273:TRP:CE3	3:C:274:TYR:CA	3.00	0.45
1:N:354:VAL:HG23	1:N:355:LYS:N	2.31	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45
2:O:422:LYS:O	2:O:436:LEU:HD21	2.16	0.45
7:T:29:ILE:CD1	7:T:29:ILE:H	2.00	0.45
4:D:46:VAL:HB	4:D:91:PHE:CD2	2.51	0.45
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.77	0.45
3:C:52:LEU:HD13	11:C:501:HEM:HBD1	1.97	0.45
2:B:247:GLN:NE2	2:B:429:ASP:HA	2.16	0.45
4:Q:28:ARG:O	4:Q:29:GLY:C	2.53	0.45
1:A:433:ASP:O	1:A:437:ILE:HG13	2.16	0.45
1:N:206:LYS:O	1:N:207:GLU:C	2.55	0.45
3:C:316:MET:HA	3:C:319:ARG:HE	1.81	0.45
2:B:99:TYR:HA	9:I:66:ALA:O	2.16	0.45
2:O:209:ILE:CG2	2:O:210:GLY:N	2.80	0.45
4:D:48:PHE:CE2	4:D:65:ALA:HA	2.51	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:408:ALA:O	2:O:410:VAL:N	2.48	0.45
3:P:164:TRP:O	3:P:165:ALA:C	2.54	0.45
3:P:157:ILE:CG1	3:P:158:GLY:H	1.96	0.45
5:E:119:ASP:CB	5:E:179:ASN:ND2	2.59	0.45
6:F:32:MET:O	6:F:33:ARG:C	2.53	0.45
2:B:275:LEU:O	2:B:275:LEU:HD12	2.16	0.45
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.52	0.45
3:P:377:MET:HE1	6:S:20:TYR:HD1	1.82	0.45
5:R:135:LEU:HA	5:R:183:PRO:HD3	1.98	0.45
5:R:113:ASP:C	5:R:115:SER:N	2.65	0.45
2:O:209:ILE:O	2:O:211:VAL:HG22	2.16	0.45
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.34	0.45
2:O:235:ALA:O	2:O:236:LYS:C	2.54	0.45
5:R:55:VAL:O	5:R:56:THR:C	2.54	0.45
6:S:52:GLU:HG2	6:S:56:ASN:ND2	2.31	0.45
8:U:19:THR:O	8:U:22:GLU:HB2	2.16	0.45
3:P:182:LEU:HD23	14:P:3001:SMA:H26	1.98	0.45
3:C:45:GLN:HB3	11:C:501:HEM:HAB	1.99	0.45
3:P:92:PHE:C	3:P:95:ILE:HG22	2.37	0.45
3:P:95:ILE:O	3:P:99:ILE:HG13	2.16	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.51	0.45
1:N:187:ASP:O	1:N:191:LYS:HE3	2.16	0.45
1:A:87:ASN:ND2	1:A:98:TYR:OH	2.50	0.45
3:C:285:ILE:N	3:C:285:ILE:CD1	2.79	0.45
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.97	0.45
1:A:289:HIS:O	1:A:290:LEU:C	2.55	0.45
3:C:231:LEU:HD11	4:D:220:TYR:HA	1.98	0.45
10:W:20:PHE:O	10:W:23:THR:HB	2.17	0.45
1:A:261:GLY:O	1:A:262:TRP:C	2.55	0.45
5:E:161:HIS:HB2	13:E:501:FES:S1	2.56	0.45
3:P:295:LEU:O	3:P:298:SER:OG	2.29	0.45
2:B:73:SER:N	2:B:74:PRO:HD2	2.31	0.45
1:N:84:ALA:HB1	1:N:99:ILE:CG2	2.47	0.45
2:O:259:THR:HG22	2:O:260:GLU:N	2.31	0.45
6:S:40:ASP:O	6:S:44:LYS:HG3	2.15	0.45
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.97	0.45
3:P:271:PRO:CA	14:P:3001:SMA:H10	2.31	0.45
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.95	0.45
6:S:77:LYS:HA	6:S:80:TRP:CD1	2.51	0.45
10:W:21:ALA:O	10:W:24:VAL:N	2.50	0.45
2:B:412:ASN:O	2:B:413:ALA:C	2.56	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:36:THR:O	6:S:37:LEU:C	2.54	0.45
4:Q:221:TYR:CE1	7:T:25:ALA:HB2	2.51	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
3:C:331:ALA:HB2	7:G:52:PHE:CD2	2.52	0.45
3:P:129:PHE:CD1	3:P:129:PHE:C	2.89	0.45
6:S:65:ALA:O	6:S:68:LEU:HB2	2.17	0.45
3:P:35:GLY:O	3:P:38:LEU:HB2	2.16	0.45
6:S:19:TRP:O	6:S:22:ASN:N	2.50	0.45
3:C:173:ASN:O	3:C:174:PRO:C	2.53	0.45
2:B:67:HIS:ND1	2:B:178:CYS:N	2.65	0.45
1:N:261:GLY:HA2	1:N:317:THR:O	2.17	0.45
3:C:365:ILE:O	3:C:368:PRO:HD2	2.17	0.45
1:A:249:PRO:HG2	1:A:250:VAL:H	1.81	0.45
1:N:288:LYS:HE3	1:N:289:HIS:NE2	2.31	0.45
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.32	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.67	0.45
1:A:266:ASP:O	1:A:267:ASN:C	2.54	0.45
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.99	0.45
6:S:96:GLU:O	6:S:97:VAL:C	2.55	0.45
5:E:165:TYR:HA	5:E:170:ARG:O	2.17	0.45
1:A:61:HIS:ND1	1:A:134:ILE:HG12	2.32	0.45
2:O:203:ARG:O	2:O:387:LEU:HD11	2.17	0.45
2:O:279:LEU:O	2:O:295:LEU:HB3	2.17	0.45
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.30	0.45
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.71	0.45
2:B:84:ARG:O	2:B:88:GLY:N	2.47	0.45
3:P:130:VAL:O	3:P:131:GLY:C	2.56	0.44
3:C:49:GLY:HA3	11:C:501:HEM:C3C	2.52	0.44
3:C:63:ALA:CB	3:C:176:LEU:HD21	2.46	0.44
2:B:325:TYR:HD2	2:B:325:TYR:C	2.19	0.44
2:O:171:ALA:O	2:O:174:ASN:HB2	2.16	0.44
2:O:47:ILE:HG22	2:O:48:GLY:N	2.31	0.44
5:R:87:VAL:HG12	5:R:88:ALA:N	2.32	0.44
2:B:379:LEU:HG	2:B:379:LEU:O	2.15	0.44
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.44
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.82	0.44
1:N:368:GLN:O	1:N:374:PRO:HB3	2.18	0.44
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.99	0.44
3:P:38:LEU:HD21	3:P:95:ILE:N	2.32	0.44
9:I:49:LEU:O	9:I:50:LEU:HG	2.17	0.44
9:I:49:LEU:HB3	9:I:55:MET:CG	2.48	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:ND2	1:A:51:LYS:N	2.65	0.44
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.30	0.44
3:C:316:MET:CG	3:C:319:ARG:HH21	2.29	0.44
1:A:300:GLU:HG2	1:A:301:HIS:CE1	2.52	0.44
3:P:323:GLN:O	3:P:326:PHE:HB3	2.17	0.44
1:A:289:HIS:O	1:A:290:LEU:O	2.34	0.44
8:H:56:GLU:O	8:H:59:PHE:HB2	2.16	0.44
10:W:4:ALA:N	10:W:8:GLN:HE21	2.16	0.44
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.52	0.44
1:A:62:LEU:HD21	1:A:126:GLN:HG3	1.99	0.44
5:E:87:VAL:HG12	5:E:88:ALA:N	2.31	0.44
3:P:151:PHE:C	3:P:153:ALA:N	2.70	0.44
2:B:59:THR:HG22	2:B:60:THR:N	2.31	0.44
5:E:135:LEU:HA	5:E:183:PRO:HD3	1.99	0.44
5:E:141:HIS:HB3	13:E:501:FES:S2	2.57	0.44
7:G:30:PHE:O	7:G:35:PRO:CD	2.65	0.44
4:Q:224:ARG:O	4:Q:225:HIS:C	2.55	0.44
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.44
3:C:98:HIS:CD2	11:C:502:HEM:NC	2.85	0.44
6:S:73:ARG:NH1	7:T:32:ASP:OD1	2.49	0.44
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.48	0.44
2:B:259:THR:O	2:B:260:GLU:C	2.56	0.44
2:O:279:LEU:O	2:O:295:LEU:CB	2.66	0.44
4:Q:208:MET:C	4:Q:208:MET:SD	2.96	0.44
3:C:156:TYR:HD2	3:C:156:TYR:N	2.16	0.44
4:D:183:ALA:HA	4:D:186:VAL:HG12	2.00	0.44
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.53	0.44
3:C:100:GLY:O	3:C:101:ARG:C	2.54	0.44
3:P:22:LEU:HD12	3:P:23:PRO:HD2	1.98	0.44
3:C:332:ASN:ND2	3:C:359:TYR:CA	2.81	0.44
1:N:294:LEU:O	1:N:298:ALA:HB2	2.17	0.44
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.44
2:O:277:HIS:HB2	2:O:360:ALA:HB1	1.98	0.44
4:D:22:ASP:O	4:D:25:SER:N	2.51	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.82	0.44
2:B:235:ALA:O	2:B:236:LYS:C	2.54	0.44
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.50	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.32	0.44
1:A:67:THR:HB	1:A:119:ASN:O	2.17	0.44
5:E:160:CYS:HB3	5:E:161:HIS:CE1	2.53	0.44
4:Q:43:MET:HE3	4:Q:91:PHE:HE2	1.82	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:26:VAL:HG13	4:Q:189:PHE:HA	2.00	0.44
5:E:57:GLN:OE1	18:E:2009:PLC:H12	2.18	0.44
1:N:253:VAL:O	1:N:323:HIS:HA	2.17	0.44
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.97	0.44
3:C:29:SER:HB2	16:C:2004:CDL:HB21	2.00	0.44
1:N:191:LYS:C	1:N:193:PRO:HD2	2.38	0.44
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.85	0.44
5:E:122:HIS:C	5:E:124:LEU:N	2.71	0.44
1:N:36:THR:OG1	1:N:100:LYS:HG2	2.18	0.44
3:P:145:THR:O	3:P:149:ASN:HB2	2.17	0.44
3:C:184:PHE:HA	11:C:501:HEM:CBC	2.48	0.44
1:N:419:CYS:SG	7:T:21:PHE:HB2	2.58	0.44
4:Q:55:THR:OG1	4:Q:56:HIS:CE1	2.69	0.44
8:U:40:CYS:O	8:U:41:ASP:C	2.55	0.44
5:E:29:SER:O	5:E:30:GLU:C	2.56	0.44
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.98	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
3:P:108:TYR:HE1	3:P:309:HIS:HB2	1.81	0.44
1:N:86:PHE:CE2	1:N:99:ILE:HD11	2.53	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.18	0.44
6:F:77:LYS:HA	6:F:80:TRP:CD1	2.53	0.44
1:A:105:ASP:O	1:A:106:MET:C	2.55	0.44
1:N:248:LEU:HB3	1:N:249:PRO:HD2	1.99	0.44
7:G:73:ASN:O	7:G:75:ALA:N	2.50	0.44
2:O:50:PHE:CD2	2:O:106:THR:HG23	2.53	0.44
2:B:189:GLU:O	2:B:190:GLN:C	2.55	0.44
2:O:253:VAL:HG13	2:O:430:LEU:HD22	1.99	0.44
1:N:372:THR:O	1:N:373:THR:C	2.56	0.44
1:N:277:ILE:HG22	1:N:277:ILE:O	2.17	0.44
2:O:306:PRO:HB3	9:V:52:ARG:N	2.32	0.44
6:S:75:LEU:O	6:S:80:TRP:NE1	2.39	0.44
9:I:65:VAL:CG1	9:I:66:ALA:N	2.81	0.44
2:B:96:LEU:HD13	2:B:109:VAL:HG12	2.00	0.44
4:Q:102:ARG:HG2	4:Q:102:ARG:NH1	2.33	0.44
6:F:16:ILE:O	6:F:19:TRP:N	2.48	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.72	0.44
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.82	0.44
3:P:146:VAL:O	3:P:147:ILE:C	2.56	0.44
5:R:29:SER:HA	5:R:32:ARG:HH21	1.82	0.44
11:C:502:HEM:HBB2	11:C:502:HEM:CMB	2.48	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:NH1	2:B:172:LEU:HD21	2.33	0.44
4:Q:29:GLY:O	4:Q:32:VAL:HB	2.18	0.44
3:C:198:LEU:HD11	15:C:2002:ANY:O4	2.17	0.44
2:B:264:VAL:HG11	2:B:388:LEU:CD1	2.41	0.44
1:A:57:TYR:O	1:A:60:GLU:N	2.51	0.44
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.53	0.44
5:R:112:VAL:HG12	5:R:113:ASP:N	2.32	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.44
3:P:151:PHE:N	3:P:151:PHE:CD1	2.85	0.44
1:A:304:CYS:HA	1:A:326:ALA:HB2	2.00	0.44
2:O:229:GLY:O	2:O:231:GLY:N	2.49	0.44
2:O:269:ALA:O	2:O:270:ASN:C	2.56	0.44
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.51	0.44
1:N:81:SER:HB2	2:O:359:LYS:HE2	1.99	0.44
1:A:206:LYS:C	1:A:209:VAL:HG12	2.37	0.44
1:A:207:GLU:O	1:A:210:ASP:HB2	2.17	0.44
3:C:107:SER:HB2	11:C:502:HEM:HMD3	2.00	0.44
2:B:163:LEU:HD13	2:B:425:ALA:HB2	1.99	0.44
3:P:95:ILE:CD1	3:P:121:LEU:CD1	2.89	0.44
1:N:19:LEU:C	1:N:21:ASN:N	2.72	0.44
4:Q:235:MET:CE	6:S:64:ARG:HA	2.48	0.44
3:P:354:MET:O	3:P:358:SER:N	2.41	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.44
3:C:129:PHE:C	3:C:129:PHE:CD1	2.88	0.44
2:O:163:LEU:CD1	2:O:425:ALA:HB2	2.47	0.44
3:C:123:THR:O	3:C:124:LEU:C	2.56	0.44
1:N:55:ALA:C	1:N:57:TYR:N	2.71	0.44
5:E:1:VAL:HG23	5:E:3:ASN:H	1.83	0.44
1:A:254:ALA:HB3	1:A:423:ALA:HB3	2.00	0.44
1:N:266:ASP:O	1:N:267:ASN:C	2.56	0.44
2:O:370:MET:O	2:O:373:GLU:HG3	2.18	0.44
1:N:388:ARG:HD3	1:N:388:ARG:N	2.33	0.43
2:B:169:LYS:HD2	2:B:238:THR:HG21	2.00	0.43
4:D:227:TRP:O	4:D:230:LEU:N	2.50	0.43
2:O:100:SER:HA	2:O:104:LYS:O	2.18	0.43
8:H:66:ASP:O	8:H:67:HIS:C	2.55	0.43
1:A:291:SER:OG	2:B:87:ARG:HD3	2.18	0.43
7:G:34:LEU:O	7:G:35:PRO:C	2.56	0.43
4:Q:225:HIS:CE1	7:T:20:PRO:HB2	2.53	0.43
2:B:81:SER:O	2:B:82:SER:C	2.57	0.43
2:B:171:ALA:O	2:B:174:ASN:HB2	2.17	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.99	0.43
3:P:60:THR:HG23	3:P:173:ASN:HA	2.00	0.43
2:B:344:LEU:HA	2:B:344:LEU:HD12	1.89	0.43
2:O:296:TYR:O	2:O:297:GLN:C	2.57	0.43
3:P:245:LEU:HD12	4:Q:208:MET:HE2	2.00	0.43
4:Q:197:GLU:O	4:Q:199:ASP:N	2.51	0.43
4:D:204:MET:O	4:D:205:GLY:C	2.56	0.43
7:G:48:VAL:O	7:G:51:PRO:HD2	2.18	0.43
4:D:189:PHE:O	4:D:191:ARG:N	2.50	0.43
2:O:166:ALA:O	2:O:242:GLY:N	2.35	0.43
2:O:408:ALA:O	2:O:409:ASP:C	2.56	0.43
3:P:111:LYS:O	3:P:114:TRP:HB3	2.18	0.43
2:O:160:LEU:HD12	9:V:64:LEU:HB2	1.99	0.43
5:E:135:LEU:HD22	5:E:180:LEU:HD12	1.99	0.43
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.43
3:C:92:PHE:O	3:C:96:PHE:CD2	2.71	0.43
6:S:67:ASP:HA	6:S:70:LEU:CD2	2.46	0.43
4:Q:235:MET:HE1	6:S:64:ARG:N	2.34	0.43
3:C:242:THR:N	4:D:208:MET:CE	2.80	0.43
6:F:31:LEU:HD21	6:F:65:ALA:CB	2.48	0.43
7:G:57:LEU:C	7:G:59:TYR:N	2.70	0.43
1:A:301:HIS:HB2	1:A:303:LEU:HD21	1.99	0.43
3:P:78:TRP:CG	3:P:79:LEU:N	2.86	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.84	0.43
1:N:94:GLN:NE2	1:N:381:SER:OG	2.44	0.43
2:O:235:ALA:O	2:O:236:LYS:O	2.36	0.43
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.82	0.43
2:O:124:LEU:HG	2:O:125:ASN:N	2.34	0.43
3:P:184:PHE:CD2	3:P:184:PHE:C	2.92	0.43
7:T:33:ALA:O	7:T:34:LEU:C	2.57	0.43
2:O:207:VAL:CG1	2:O:208:GLY:N	2.79	0.43
5:R:32:ARG:HD2	7:T:21:PHE:O	2.18	0.43
4:Q:227:TRP:O	4:Q:230:LEU:N	2.50	0.43
2:O:167:ALA:C	2:O:168:TYR:CD1	2.92	0.43
3:P:371:GLY:O	3:P:374:GLU:HB2	2.18	0.43
3:P:29:SER:HB2	16:P:3004:CDL:HB21	2.00	0.43
1:A:155:ALA:O	5:E:7:VAL:HG23	2.19	0.43
4:D:155:GLY:C	4:D:157:ALA:N	2.71	0.43
10:J:22:LEU:H	10:J:22:LEU:HD23	1.82	0.43
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.54	0.43
2:O:50:PHE:CD1	2:O:50:PHE:N	2.86	0.43
1:A:354:VAL:HG23	1:A:355:LYS:N	2.33	0.43
3:C:93:ILE:O	3:C:94:CYS:C	2.56	0.43
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.32	0.43
5:E:74:ILE:HG23	5:E:74:ILE:O	2.17	0.43
2:O:31:ASN:H	2:O:31:ASN:ND2	2.17	0.43
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.53	0.43
2:O:72:ALA:O	2:O:75:LEU:HB2	2.18	0.43
2:B:135:TRP:O	2:B:138:THR:N	2.51	0.43
8:U:37:LEU:O	8:U:40:CYS:N	2.50	0.43
3:P:22:LEU:HD12	3:P:23:PRO:CD	2.49	0.43
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.31	0.43
1:N:294:LEU:HD23	1:N:307:PHE:CE1	2.53	0.43
2:O:306:PRO:HA	9:V:52:ARG:HG3	2.00	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HB3	2.54	0.43
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.53	0.43
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.54	0.43
3:P:123:THR:O	3:P:124:LEU:C	2.57	0.43
2:O:239:TYR:C	2:O:239:TYR:CD2	2.91	0.43
4:Q:109:LEU:HA	4:Q:110:PRO:HD2	1.91	0.43
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.18	0.43
4:D:206:LEU:O	4:D:207:LYS:C	2.57	0.43
6:F:42:ASP:O	6:F:43:VAL:C	2.55	0.43
10:J:26:LEU:O	10:J:30:LEU:HG	2.18	0.43
1:A:292:SER:O	1:A:293:ARG:C	2.55	0.43
5:R:94:LYS:O	5:R:95:PRO:O	2.37	0.43
4:Q:43:MET:HE3	4:Q:91:PHE:CE2	2.52	0.43
5:R:29:SER:O	5:R:30:GLU:C	2.56	0.43
3:P:232:GLY:HA2	16:Q:3003:CDL:H121	2.00	0.43
3:C:101:ARG:C	3:C:101:ARG:CD	2.77	0.43
3:C:117:GLY:C	11:C:502:HEM:HBC2	2.39	0.43
3:P:101:ARG:HD2	3:P:102:GLY:CA	2.48	0.43
3:C:28:ILE:HD12	15:C:2002:ANY:H3	2.00	0.43
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.25	0.43
1:N:429:GLU:CD	7:T:7:LEU:HB2	2.37	0.43
1:A:86:PHE:CG	1:A:99:ILE:HG12	2.54	0.43
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.00	0.43
1:N:317:THR:HG23	1:N:318:GLY:N	2.33	0.43
5:R:52:LYS:HD3	5:R:52:LYS:C	2.39	0.43
1:N:351:GLU:OE2	1:N:404:ALA:HB3	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.83	0.43
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.49	0.43
5:R:141:HIS:HB3	13:R:501:FES:S2	2.58	0.43
3:C:95:ILE:CD1	3:C:121:LEU:HD13	2.49	0.43
2:B:163:LEU:O	2:B:167:ALA:N	2.52	0.43
1:N:382:HIS:HE1	1:N:390:ILE:O	2.02	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.81	0.43
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.49	0.43
4:D:116:ILE:CG2	4:D:117:VAL:N	2.82	0.43
3:P:88:ALA:O	3:P:91:PHE:HB3	2.19	0.43
3:C:104:TYR:HB2	3:C:326:PHE:CE1	2.53	0.43
3:P:138:GLN:NE2	3:P:266:PRO:HD3	2.34	0.43
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.48	0.43
1:A:287:GLY:C	1:A:289:HIS:H	2.22	0.43
1:A:259:GLY:HA3	1:A:318:GLY:HA3	1.99	0.43
3:C:149:ASN:HD22	3:C:149:ASN:HA	1.54	0.43
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.54	0.43
8:H:20:ILE:HG22	8:H:20:ILE:O	2.18	0.43
4:D:46:VAL:CG1	4:D:47:ALA:H	2.30	0.43
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.83	0.43
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.43
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.54	0.43
4:Q:10:PHE:HB3	8:U:74:PHE:CE1	2.54	0.43
2:B:241:GLY:HA2	2:B:423:SER:OG	2.19	0.43
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.47	0.43
1:A:368:GLN:O	1:A:374:PRO:HB3	2.18	0.43
6:F:67:ASP:HA	6:F:70:LEU:CD2	2.47	0.43
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.75	0.43
2:O:344:LEU:HD12	2:O:344:LEU:HA	1.92	0.43
9:V:65:VAL:HG12	9:V:66:ALA:H	1.82	0.43
4:D:130:LEU:HD12	4:D:150:ASN:CG	2.39	0.43
5:R:78:LEU:HG	5:R:193:VAL:HG12	2.00	0.43
1:N:261:GLY:HA2	1:N:314:TYR:O	2.19	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
2:O:350:GLY:C	2:O:352:VAL:H	2.17	0.43
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.54	0.43
3:C:130:VAL:HG23	3:C:131:GLY:N	2.33	0.43
5:E:114:VAL:HG12	5:E:114:VAL:O	2.19	0.43
3:P:169:PHE:HD2	3:P:169:PHE:HA	1.77	0.43
3:C:81:ARG:HH22	20:C:2011:GOL:H2	1.83	0.43
4:Q:47:ALA:O	4:Q:50:ASN:N	2.39	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:182:ARG:HG2	2:O:182:ARG:HH11	1.84	0.43
4:Q:189:PHE:O	4:Q:191:ARG:N	2.52	0.43
3:C:241:LEU:O	3:C:245:LEU:N	2.51	0.43
10:J:14:PHE:HD2	10:J:14:PHE:N	2.15	0.43
1:N:63:ALA:O	1:N:116:VAL:CG1	2.67	0.43
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.43
4:D:209:LEU:HA	4:D:209:LEU:HD23	1.82	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB1	1.84	0.43
3:C:56:TYR:OH	3:C:134:LEU:O	2.30	0.43
2:B:47:ILE:HG22	2:B:48:GLY:N	2.32	0.43
1:A:255:LEU:HA	1:A:421:ALA:O	2.19	0.43
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.18	0.43
1:A:55:ALA:C	1:A:57:TYR:N	2.72	0.43
2:O:102:ARG:CZ	2:O:164:HIS:CD2	3.02	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.01	0.43
7:G:57:LEU:O	7:G:59:TYR:N	2.52	0.43
2:O:337:ILE:O	2:O:340:ALA:HB3	2.18	0.43
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.01	0.43
7:T:55:ALA:O	7:T:56:TYR:C	2.57	0.43
8:U:58:LEU:HG	8:U:62:LEU:CD1	2.49	0.43
3:C:137:GLY:N	3:C:140:SER:HB2	2.33	0.43
5:E:113:ASP:C	5:E:115:SER:N	2.72	0.43
7:G:28:ASN:HB3	7:G:31:SER:OG	2.18	0.43
4:Q:47:ALA:O	4:Q:48:PHE:C	2.56	0.42
2:O:248:ASN:HD22	2:O:250:HIS:H	1.65	0.42
1:N:277:ILE:CD1	1:N:345:LEU:HD11	2.49	0.42
2:O:399:ALA:HA	2:O:402:ILE:HD12	2.00	0.42
1:N:273:ALA:O	1:N:275:ALA:N	2.52	0.42
1:A:422:LEU:HD22	1:A:437:ILE:HD12	2.00	0.42
5:R:97:PHE:O	5:R:134:ILE:HA	2.19	0.42
2:O:47:ILE:CG2	2:O:48:GLY:N	2.81	0.42
3:C:29:SER:O	3:C:32:TRP:HB2	2.18	0.42
3:C:237:LEU:O	3:C:241:LEU:HG	2.19	0.42
2:O:144:LEU:CB	2:O:183:ILE:CD1	2.97	0.42
7:G:55:ALA:O	7:G:58:LEU:N	2.52	0.42
3:C:25:PRO:HG2	3:C:207:ASN:O	2.18	0.42
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.42
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.49	0.42
1:N:261:GLY:O	1:N:262:TRP:C	2.57	0.42
1:N:319:LEU:HA	1:N:319:LEU:HD23	1.73	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.02	0.42
8:U:66:ASP:HA	8:U:69:VAL:CG2	2.49	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.54	0.42
4:D:143:VAL:O	4:D:144:ARG:C	2.57	0.42
3:C:82:ASN:N	3:C:82:ASN:HD22	2.16	0.42
3:C:28:ILE:HG13	3:C:225:TYR:HE2	1.82	0.42
6:F:20:TYR:O	6:F:23:ALA:HB3	2.19	0.42
1:N:284:PHE:HD1	1:N:284:PHE:H	1.66	0.42
5:E:35:PHE:O	5:E:36:SER:C	2.56	0.42
1:N:54:GLY:O	1:N:56:GLY:N	2.52	0.42
2:O:230:ALA:O	2:O:231:GLY:C	2.57	0.42
2:O:412:ASN:O	2:O:413:ALA:C	2.56	0.42
4:D:237:TYR:CD2	4:D:239:PRO:HD3	2.54	0.42
2:B:169:LYS:HB2	2:B:238:THR:HB	2.00	0.42
3:P:107:SER:C	3:P:109:LEU:N	2.72	0.42
3:P:99:ILE:HD11	3:P:121:LEU:HD22	2.01	0.42
1:N:90:THR:HB	1:N:95:THR:HG23	2.02	0.42
2:B:358:THR:HA	2:B:361:LYS:HD2	2.02	0.42
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.46	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
5:E:177:PRO:C	5:E:178:TYR:HD1	2.22	0.42
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.49	0.42
5:E:113:ASP:CB	5:E:116:LYS:HB2	2.49	0.42
4:D:22:ASP:O	4:D:24:SER:N	2.52	0.42
3:C:378:LEU:O	3:C:379:ASN:HB3	2.19	0.42
3:C:141:PHE:HB2	3:C:260:ALA:HB1	2.02	0.42
3:C:154:ILE:HG21	3:C:157:ILE:HD11	2.01	0.42
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.42
1:A:78:GLU:OE1	1:A:108:LYS:CE	2.67	0.42
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.80	0.42
5:R:186:GLN:HE21	5:R:188:VAL:HG12	1.84	0.42
2:O:239:TYR:HE1	2:O:260:GLU:H	1.65	0.42
3:P:196:ILE:O	3:P:197:HIS:C	2.57	0.42
3:C:14:MET:O	3:C:15:ILE:C	2.57	0.42
4:Q:46:VAL:CG1	4:Q:47:ALA:N	2.81	0.42
2:O:247:GLN:HE21	2:O:249:GLY:H	1.68	0.42
5:R:29:SER:O	5:R:31:ASP:N	2.52	0.42
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.42
10:J:13:LEU:O	10:J:19:THR:OG1	2.36	0.42
2:O:168:TYR:HD2	2:O:237:ALA:HB1	1.83	0.42
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.27	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:16:ILE:O	6:S:19:TRP:N	2.52	0.42
3:P:70:THR:HA	3:P:74:VAL:HG21	2.01	0.42
2:B:317:SER:OG	2:B:318:ASP:N	2.52	0.42
1:A:301:HIS:HB2	1:A:303:LEU:CD2	2.50	0.42
8:H:49:HIS:O	8:H:49:HIS:CG	2.71	0.42
1:A:261:GLY:HA2	1:A:317:THR:O	2.20	0.42
7:T:30:PHE:O	7:T:35:PRO:CD	2.67	0.42
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.50	0.42
3:C:380:TYR:HH	6:F:33:ARG:HE	1.68	0.42
6:S:50:LEU:HA	6:S:51:PRO:HD3	1.83	0.42
3:C:193:ILE:H	3:C:193:ILE:HG13	1.67	0.42
5:E:185:TYR:HB2	5:E:186:GLN:H	1.63	0.42
3:C:285:ILE:HB	3:C:291:GLY:HA2	2.01	0.42
2:B:209:ILE:O	2:B:211:VAL:HG22	2.19	0.42
8:H:15:ASP:C	8:H:17:LEU:N	2.72	0.42
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.54	0.42
1:N:439:SER:C	1:N:441:MET:H	2.23	0.42
4:D:121:HIS:C	4:D:123:GLY:H	2.22	0.42
2:O:57:TYR:N	2:O:57:TYR:CD1	2.87	0.42
3:C:243:LEU:HD12	3:C:243:LEU:HA	1.76	0.42
3:P:49:GLY:HA3	11:P:501:HEM:C2C	2.55	0.42
5:R:83:GLU:HA	5:R:100:HIS:CG	2.54	0.42
2:O:76:THR:HG23	2:O:82:SER:HB2	2.02	0.42
2:B:258:VAL:HB	2:B:322:PHE:C	2.40	0.42
3:C:36:SER:HA	15:C:2002:ANY:O7	2.20	0.42
1:N:378:THR:O	1:N:382:HIS:N	2.50	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.19	0.42
3:C:301:ILE:HD13	3:C:363:LEU:HD13	2.02	0.42
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.19	0.42
1:A:284:PHE:HD1	1:A:284:PHE:H	1.66	0.42
3:C:273:TRP:CD2	3:C:274:TYR:N	2.88	0.42
7:T:73:ASN:O	7:T:75:ALA:N	2.53	0.42
10:W:45:HIS:C	10:W:47:ASN:H	2.23	0.42
1:N:257:VAL:HG23	1:N:320:PHE:HB3	2.01	0.42
3:C:191:ALA:O	3:C:195:ILE:HG12	2.20	0.42
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.01	0.42
8:U:50:THR:OG1	8:U:51:GLU:N	2.52	0.42
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.60	0.42
1:N:29:GLU:OE1	1:N:204:SER:HA	2.19	0.42
2:B:163:LEU:CD1	2:B:425:ALA:HB2	2.50	0.42
7:T:12:HIS:O	7:T:13:ILE:HG13	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:301:HIS:HB2	1:N:303:LEU:CD2	2.50	0.42
1:A:178:THR:O	1:A:179:ARG:C	2.57	0.42
3:P:273:TRP:CD2	3:P:274:TYR:N	2.88	0.42
3:C:162:VAL:O	3:C:165:ALA:N	2.52	0.42
1:A:187:ASP:O	1:A:191:LYS:HE3	2.20	0.42
1:A:236:PHE:HB2	1:A:258:GLU:OE1	2.19	0.42
6:F:49:ARG:HH22	6:F:100:GLU:CD	2.23	0.42
5:E:94:LYS:O	5:E:95:PRO:O	2.37	0.42
5:E:149:ASN:O	5:E:150:SER:HB3	2.19	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.53	0.42
1:N:78:GLU:OE1	1:N:108:LYS:CE	2.67	0.42
3:C:38:LEU:HD21	3:C:95:ILE:N	2.35	0.42
6:S:73:ARG:HG3	6:S:73:ARG:NH1	2.33	0.42
5:E:29:SER:O	5:E:31:ASP:N	2.53	0.42
2:O:47:ILE:O	2:O:108:CYS:HB2	2.20	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HB	2.55	0.42
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.33	0.42
4:Q:44:ASP:O	4:Q:90:TYR:HD2	2.03	0.42
5:R:108:GLN:C	5:R:110:ALA:N	2.73	0.42
2:B:50:PHE:HD1	2:B:50:PHE:H	1.68	0.42
5:E:127:VAL:HG11	5:E:133:VAL:HG23	2.02	0.42
4:Q:18:LEU:HD22	4:Q:206:LEU:HD13	2.02	0.42
3:P:223:PRO:HA	3:P:226:SER:OG	2.20	0.42
5:E:141:HIS:HB3	5:E:142:LEU:H	1.66	0.42
4:D:186:VAL:HG21	12:D:501:HEC:HBB3	2.02	0.42
2:B:62:ASN:HD22	2:B:65:THR:HG21	1.85	0.42
1:N:112:LEU:O	1:N:113:LEU:C	2.57	0.42
1:N:433:ASP:OD2	1:N:435:ASN:N	2.53	0.42
3:C:107:SER:C	3:C:109:LEU:H	2.23	0.42
1:A:89:TYR:O	1:A:95:THR:CG2	2.65	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
1:A:40:TRP:CD1	1:A:96:ALA:CB	3.03	0.42
1:A:182:LEU:HD23	1:A:182:LEU:H	1.85	0.42
5:R:91:TRP:O	5:R:92:ARG:C	2.59	0.42
2:O:166:ALA:HB2	2:O:244:ILE:CG1	2.50	0.42
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.20	0.42
1:A:138:LEU:HD22	5:E:3:ASN:HD21	1.84	0.42
5:E:78:LEU:HD21	5:E:193:VAL:HG11	2.02	0.42
1:A:251:ALA:HB1	1:A:428:ILE:HG22	2.02	0.42
3:P:93:ILE:O	3:P:94:CYS:C	2.57	0.42
3:C:80:ILE:O	3:C:81:ARG:C	2.56	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:ILE:O	4:D:185:ASP:N	2.53	0.41
12:D:501:HEC:HBC3	12:D:501:HEC:CMC	2.44	0.41
4:Q:215:LEU:HD12	4:Q:219:LEU:HG	2.02	0.41
4:Q:160:MET:HB2	12:Q:501:HEC:C1D	2.50	0.41
14:C:2001:SMA:H4	5:R:161:HIS:CE1	2.55	0.41
1:A:239:SER:O	1:A:421:ALA:HA	2.20	0.41
9:I:49:LEU:HB3	9:I:55:MET:HG2	2.02	0.41
1:A:356:ARG:O	1:A:359:ASN:N	2.53	0.41
2:O:163:LEU:O	2:O:166:ALA:N	2.52	0.41
2:B:35:ILE:O	2:B:213:HIS:HE1	2.03	0.41
1:N:317:THR:OG1	1:N:318:GLY:N	2.51	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.82	0.41
5:E:78:LEU:HD22	5:E:132:TRP:CD2	2.54	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.55	0.41
3:C:59:ASP:O	3:C:60:THR:C	2.58	0.41
2:O:189:GLU:O	2:O:191:LEU:N	2.53	0.41
3:C:269:ILE:O	3:C:270:LYS:HD3	2.20	0.41
2:O:169:LYS:HB2	2:O:238:THR:HB	2.01	0.41
3:P:6:ARG:CD	3:P:16:ASN:OD1	2.65	0.41
2:O:183:ILE:HD13	2:O:183:ILE:HA	1.88	0.41
4:Q:3:LEU:HD23	4:Q:3:LEU:H	1.85	0.41
7:T:57:LEU:C	7:T:59:TYR:N	2.73	0.41
4:Q:218:LEU:HD13	5:R:43:ALA:CA	2.50	0.41
1:A:158:PHE:O	1:A:159:GLN:O	2.37	0.41
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.55	0.41
2:B:408:ALA:O	2:B:409:ASP:C	2.58	0.41
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.41
3:C:145:THR:O	3:C:149:ASN:HB2	2.20	0.41
3:P:352:GLY:O	3:P:353:GLN:C	2.58	0.41
1:A:233:ARG:NH2	1:A:316:ASP:HB2	2.35	0.41
5:R:45:VAL:O	5:R:48:ALA:HB3	2.21	0.41
2:B:201:SER:N	2:B:227:ARG:O	2.53	0.41
3:C:236:MET:O	3:C:238:THR:N	2.53	0.41
3:P:30:ALA:C	3:P:32:TRP:N	2.72	0.41
1:N:76:GLU:HG2	2:O:285:ILE:HD12	2.03	0.41
1:A:178:THR:HG22	1:A:179:ARG:N	2.36	0.41
2:B:378:LEU:C	2:B:380:ASN:N	2.72	0.41
2:B:431:GLY:HA3	2:O:60:THR:HG21	2.01	0.41
1:N:288:LYS:N	1:N:299:VAL:HG11	2.34	0.41
1:N:249:PRO:HG2	1:N:250:VAL:H	1.85	0.41
5:R:20:ASP:C	5:R:22:THR:H	2.23	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
1:A:80:GLU:CD	2:B:290:SER:HA	2.41	0.41
7:T:77:TYR:C	7:T:79:ASN:H	2.23	0.41
5:E:18:VAL:O	5:E:18:VAL:HG23	2.20	0.41
2:O:26:ILE:HG23	2:O:26:ILE:O	2.20	0.41
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.41
5:R:45:VAL:CG1	10:W:28:ALA:HA	2.37	0.41
6:S:89:TYR:CD1	6:S:89:TYR:C	2.93	0.41
3:C:95:ILE:O	3:C:99:ILE:HG13	2.21	0.41
4:D:197:GLU:HG2	4:D:198:HIS:H	1.83	0.41
2:O:417:PHE:C	2:O:417:PHE:CD2	2.94	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.38	0.41
10:W:55:ILE:O	10:W:56:LYS:C	2.58	0.41
5:E:38:LEU:CA	10:J:14:PHE:CE1	3.01	0.41
3:P:160:THR:O	3:P:163:GLU:HB3	2.21	0.41
5:E:24:SER:OG	5:E:26:GLN:HB2	2.21	0.41
3:P:331:ALA:HB2	7:T:52:PHE:CD2	2.55	0.41
2:B:366:ALA:O	2:B:369:LEU:N	2.53	0.41
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.01	0.41
3:P:57:THR:O	3:P:57:THR:HG22	2.20	0.41
1:N:69:LYS:HE3	1:N:70:ARG:NH2	2.15	0.41
3:P:109:LEU:HA	3:P:109:LEU:HD23	1.85	0.41
1:A:40:TRP:CD2	1:A:380:GLY:HA3	2.56	0.41
2:B:259:THR:HG22	2:B:260:GLU:N	2.34	0.41
2:B:111:CYS:SG	2:B:119:VAL:HG21	2.60	0.41
2:O:144:LEU:HB3	2:O:183:ILE:CD1	2.51	0.41
1:A:86:PHE:HD1	1:A:87:ASN:N	2.18	0.41
8:H:55:THR:O	8:H:58:LEU:N	2.54	0.41
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.56	0.41
1:A:166:THR:HG21	5:E:3:ASN:OD1	2.20	0.41
10:J:55:ILE:O	10:J:56:LYS:C	2.59	0.41
5:E:20:ASP:C	5:E:22:THR:H	2.24	0.41
1:N:291:SER:OG	2:O:87:ARG:HD3	2.20	0.41
4:D:195:GLU:O	4:D:195:GLU:HG3	2.20	0.41
8:U:20:ILE:O	8:U:20:ILE:HG22	2.20	0.41
5:E:134:ILE:C	5:E:135:LEU:HG	2.40	0.41
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.56	0.41
4:Q:48:PHE:CE2	4:Q:65:ALA:HA	2.56	0.41
2:O:362:ASN:HA	2:O:365:LYS:HD2	2.01	0.41
3:P:38:LEU:HB3	11:P:502:HEM:CMB	2.51	0.41
4:D:241:LYS:HA	4:D:241:LYS:CE	2.42	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:60:THR:N	3:P:176:LEU:HD23	2.36	0.41
2:O:283:PRO:CG	9:V:56:SER:HB2	2.47	0.41
9:V:65:VAL:CG1	9:V:66:ALA:N	2.83	0.41
1:A:281:ASP:O	1:A:284:PHE:HD1	2.03	0.41
4:D:42:SER:C	4:D:112:ASP:OD2	2.59	0.41
6:S:18:LYS:HA	6:S:83:TYR:CE1	2.55	0.41
9:I:75:SER:O	9:I:76:VAL:HB	2.20	0.41
4:Q:195:GLU:N	4:Q:196:PRO:HD3	2.36	0.41
1:N:147:ASN:O	1:N:148:VAL:C	2.59	0.41
5:E:33:LYS:HG2	7:G:21:PHE:CD1	2.56	0.41
6:S:53:ASP:O	6:S:57:GLU:HG3	2.21	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.02	0.41
6:F:90:LEU:O	6:F:91:GLU:C	2.59	0.41
2:O:248:ASN:HD21	2:O:250:HIS:CB	2.29	0.41
1:N:434:TYR:O	1:N:435:ASN:C	2.58	0.41
1:A:206:LYS:CA	1:A:209:VAL:HG12	2.50	0.41
3:C:99:ILE:O	3:C:100:GLY:C	2.58	0.41
4:Q:171:TYR:HH	4:Q:182:ILE:HA	1.83	0.41
2:O:227:ARG:NH1	2:O:228:SER:H	2.17	0.41
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.21	0.41
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.36	0.41
3:P:22:LEU:HD12	3:P:23:PRO:N	2.35	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.55	0.41
3:P:332:ASN:ND2	3:P:359:TYR:CA	2.82	0.41
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.83	0.41
3:P:246:PHE:CZ	4:Q:205:GLY:HA3	2.56	0.41
2:O:144:LEU:HB3	2:O:183:ILE:HD11	2.02	0.41
6:S:76:PRO:O	6:S:77:LYS:C	2.59	0.41
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.41
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.55	0.41
1:A:29:GLU:OE1	1:A:204:SER:HA	2.21	0.41
6:F:63:LYS:HD3	7:G:13:ILE:HD13	2.01	0.41
3:P:285:ILE:HB	3:P:291:GLY:HA2	2.03	0.41
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.41
2:O:31:ASN:N	2:O:31:ASN:HD22	2.18	0.41
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.56	0.41
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.41
1:N:80:GLU:CD	2:O:290:SER:HA	2.41	0.41
6:F:87:LYS:CG	6:F:87:LYS:O	2.69	0.41
4:Q:220:TYR:CE1	4:Q:224:ARG:HG3	2.56	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:92:PHE:HA	3:P:95:ILE:CG2	2.45	0.41
2:O:75:LEU:HD11	2:O:140:LEU:HD23	2.03	0.41
1:N:272:VAL:O	1:N:275:ALA:HB3	2.21	0.41
1:A:95:THR:HG22	1:A:96:ALA:N	2.36	0.41
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.46	0.41
3:P:241:LEU:O	3:P:245:LEU:N	2.54	0.41
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.55	0.41
1:A:114:ALA:HA	1:A:216:PHE:CE2	2.55	0.41
3:C:186:LEU:HA	3:C:186:LEU:HD23	1.71	0.41
6:S:52:GLU:HG2	6:S:56:ASN:HD21	1.86	0.41
2:B:235:ALA:O	2:B:236:LYS:O	2.38	0.41
1:A:67:THR:HA	1:A:121:ALA:H	1.85	0.41
4:Q:34:LYS:O	4:Q:38:SER:OG	2.34	0.41
6:F:53:ASP:O	6:F:55:TYR:N	2.53	0.41
3:P:378:LEU:O	3:P:379:ASN:CB	2.68	0.41
4:Q:43:MET:HG2	4:Q:91:PHE:HD2	1.85	0.41
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.41
6:F:89:TYR:HD1	6:F:89:TYR:C	2.24	0.41
1:N:40:TRP:HZ3	1:N:376:CYS:SG	2.27	0.41
2:O:325:TYR:C	2:O:325:TYR:CD2	2.94	0.41
3:P:230:ILE:CG2	17:P:3005:PEE:H25	2.50	0.41
2:O:130:PRO:CB	2:O:132:PHE:CE2	2.95	0.41
1:N:29:GLU:HG3	1:N:203:ILE:O	2.21	0.41
2:B:47:ILE:CG2	2:B:48:GLY:N	2.83	0.41
1:A:210:ASP:C	1:A:212:ALA:N	2.73	0.41
3:P:201:LEU:C	3:P:203:GLU:H	2.24	0.41
3:P:99:ILE:O	3:P:100:GLY:C	2.58	0.41
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.41
2:O:72:ALA:CA	2:O:75:LEU:HD12	2.50	0.41
5:R:50:ALA:HA	18:R:3009:PLC:OB	2.21	0.41
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.56	0.41
1:A:235:ARG:CZ	5:E:14:ARG:NH2	2.84	0.41
3:C:358:SER:O	3:C:362:ILE:HG13	2.21	0.41
3:P:104:TYR:CD1	3:P:316:MET:SD	3.14	0.41
1:N:223:TYR:CD2	1:N:223:TYR:N	2.81	0.41
4:Q:237:TYR:CD2	4:Q:239:PRO:HD3	2.56	0.41
4:D:215:LEU:HD12	4:D:219:LEU:HG	2.03	0.41
7:T:40:ARG:O	7:T:41:PHE:C	2.59	0.41
4:D:208:MET:SD	4:D:208:MET:C	2.99	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.41
6:S:32:MET:HE1	6:S:87:LYS:H	1.85	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.89	0.41
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.02	0.41
3:P:28:ILE:HG13	3:P:225:TYR:HE2	1.84	0.41
1:A:287:GLY:C	1:A:289:HIS:N	2.74	0.41
1:A:288:LYS:HE3	1:A:289:HIS:NE2	2.36	0.41
3:P:165:ALA:O	3:P:178:ARG:HD2	2.20	0.41
6:S:42:ASP:O	6:S:43:VAL:C	2.59	0.41
6:F:43:VAL:O	6:F:46:ALA:N	2.54	0.41
2:O:412:ASN:O	2:O:415:LYS:N	2.53	0.41
2:B:289:SER:O	2:B:290:SER:C	2.58	0.41
2:B:366:ALA:O	2:B:367:THR:C	2.59	0.41
2:B:124:LEU:HG	2:B:125:ASN:N	2.36	0.41
4:D:224:ARG:HH12	16:D:2003:CDL:HB21	1.86	0.41
3:C:367:PHE:HA	3:C:367:PHE:HD2	1.73	0.41
1:N:62:LEU:HD21	1:N:126:GLN:HG3	2.01	0.41
10:J:51:LEU:C	10:J:53:LYS:N	2.74	0.41
3:C:227:PHE:CD2	4:D:226:LYS:HG3	2.56	0.41
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	2.03	0.41
4:D:43:MET:O	4:D:45:TYR:N	2.54	0.41
4:D:47:ALA:O	4:D:49:ARG:N	2.54	0.41
1:A:46:ARG:NH1	1:A:316:ASP:OD1	2.36	0.41
5:R:46:ALA:O	5:R:47:THR:C	2.58	0.41
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.97	0.41
1:A:373:THR:HB	1:A:374:PRO:CD	2.46	0.41
3:P:245:LEU:O	4:Q:201:ARG:HG2	2.20	0.41
2:O:312:PHE:CE1	9:V:62:ARG:O	2.69	0.41
3:P:365:ILE:O	3:P:368:PRO:HD2	2.21	0.41
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.41
1:N:177:LEU:HD23	1:N:177:LEU:HA	1.86	0.41
1:A:157:ALA:HB1	1:A:236:PHE:HE1	1.86	0.41
2:O:62:ASN:O	2:O:65:THR:CG2	2.67	0.40
5:R:29:SER:CB	5:R:32:ARG:HH21	2.34	0.40
2:O:221:GLU:C	2:O:223:PHE:H	2.25	0.40
2:O:295:LEU:O	2:O:296:TYR:C	2.60	0.40
2:B:328:SER:OG	2:B:333:ALA:HA	2.21	0.40
4:D:158:ILE:HG12	4:D:159:GLY:N	2.34	0.40
3:P:78:TRP:CE3	3:P:79:LEU:N	2.89	0.40
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.36	0.40
5:E:122:HIS:C	5:E:124:LEU:H	2.24	0.40
3:P:164:TRP:O	3:P:167:GLY:N	2.54	0.40
2:B:369:LEU:O	2:B:372:VAL:HG22	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ALA:HA	2:B:342:ASN:ND2	2.36	0.40
3:C:64:PHE:HD2	4:D:45:TYR:HH	1.67	0.40
2:B:130:PRO:HB2	2:B:132:PHE:CD2	2.56	0.40
2:O:131:GLU:O	2:O:132:PHE:C	2.59	0.40
1:N:106:MET:HB3	1:N:107:PRO:CD	2.51	0.40
3:P:200:PHE:O	3:P:203:GLU:HB2	2.21	0.40
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.85	0.40
3:C:29:SER:O	3:C:30:ALA:C	2.59	0.40
5:R:113:ASP:O	5:R:115:SER:N	2.53	0.40
3:P:357:LEU:HA	3:P:357:LEU:HD12	1.69	0.40
4:Q:204:MET:O	4:Q:205:GLY:C	2.59	0.40
3:P:273:TRP:HA	3:P:276:LEU:HG	2.02	0.40
1:N:296:ALA:O	1:N:299:VAL:HB	2.22	0.40
3:P:378:LEU:HD23	3:P:378:LEU:HA	1.94	0.40
3:P:378:LEU:O	3:P:379:ASN:HB3	2.22	0.40
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.40
1:N:11:ILE:HA	1:N:12:PRO:HD2	1.86	0.40
4:Q:143:VAL:O	4:Q:144:ARG:C	2.59	0.40
3:P:146:VAL:O	3:P:149:ASN:N	2.54	0.40
3:C:184:PHE:C	3:C:184:PHE:CD2	2.95	0.40
4:D:164:ILE:HD11	4:D:183:ALA:HB2	2.02	0.40
1:N:61:HIS:NE2	1:N:137:GLU:OE1	2.53	0.40
16:Q:3003:CDL:H732	16:Q:3003:CDL:HA61	2.04	0.40
3:P:115:ASN:O	3:P:118:VAL:HG23	2.21	0.40
5:E:10:PHE:O	5:E:14:ARG:HG3	2.22	0.40
2:O:73:SER:N	2:O:74:PRO:CD	2.84	0.40
1:N:86:PHE:HD1	1:N:87:ASN:N	2.19	0.40
3:C:27:ASN:ND2	3:C:209:PRO:HD2	2.36	0.40
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.03	0.40
3:C:346:HIS:CG	3:C:347:PRO:HA	2.56	0.40
3:C:276:LEU:HA	3:C:276:LEU:HD23	1.87	0.40
3:P:67:VAL:O	3:P:68:ALA:C	2.59	0.40
2:O:68:LEU:HD22	2:O:186:ILE:HD12	2.02	0.40
4:Q:175:THR:HA	4:Q:176:PRO:HD3	1.85	0.40
1:A:112:LEU:H	1:A:112:LEU:HG	1.49	0.40
1:A:339:GLN:NE2	1:A:437:ILE:HG23	2.37	0.40
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.21	0.40
2:O:24:LEU:CD1	2:O:38:LEU:HB2	2.46	0.40
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.21	0.40
1:N:246:ASP:HA	1:N:427:PRO:CB	2.48	0.40
6:S:32:MET:HE3	6:S:87:LYS:CB	2.50	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:338:TRP:CZ2	7:T:59:TYR:HD1	2.39	0.40
1:A:241:ILE:O	1:A:241:ILE:CG2	2.70	0.40
2:O:163:LEU:HD12	2:O:163:LEU:HA	1.83	0.40
5:R:186:GLN:O	5:R:193:VAL:HG23	2.21	0.40
3:P:285:ILE:N	3:P:285:ILE:CD1	2.85	0.40
3:P:346:HIS:CG	3:P:347:PRO:HA	2.57	0.40
7:T:61:TRP:CE3	7:T:62:GLY:N	2.89	0.40
5:E:52:LYS:C	5:E:52:LYS:HD3	2.41	0.40
8:U:56:GLU:O	8:U:59:PHE:HB2	2.22	0.40
3:C:280:ALA:O	3:C:281:ILE:C	2.59	0.40
5:E:170:ARG:HA	5:E:179:ASN:CB	2.51	0.40
3:P:184:PHE:CE2	11:P:501:HEM:HBC1	2.57	0.40
3:P:270:LYS:HA	3:P:271:PRO:HD3	1.94	0.40
3:C:56:TYR:OH	3:C:176:LEU:HD11	2.21	0.40
4:Q:46:VAL:HB	4:Q:91:PHE:CD2	2.57	0.40
6:F:89:TYR:C	6:F:89:TYR:CD1	2.94	0.40
3:C:333:LEU:HD11	17:C:2007:PEE:H38	2.04	0.40
1:N:110:VAL:HA	1:N:113:LEU:HD12	2.03	0.40
6:S:89:TYR:C	6:S:89:TYR:HD1	2.23	0.40
1:N:51:LYS:HB2	1:N:51:LYS:HE3	1.94	0.40
1:A:378:THR:O	1:A:382:HIS:N	2.52	0.40
7:G:40:ARG:O	7:G:41:PHE:C	2.59	0.40
7:G:41:PHE:HE2	7:G:45:VAL:HB	1.87	0.40
3:C:311:SER:OG	3:C:319:ARG:HD3	2.21	0.40
2:B:345:LYS:O	2:B:347:ALA:N	2.54	0.40
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.57	0.40
5:E:91:TRP:O	5:E:92:ARG:C	2.59	0.40
1:A:273:ALA:O	1:A:275:ALA:N	2.55	0.40
1:N:283:THR:O	1:N:284:PHE:C	2.59	0.40
3:P:166:TRP:C	3:P:168:GLY:H	2.24	0.40
1:N:158:PHE:O	1:N:159:GLN:C	2.59	0.40
1:A:262:TRP:HE3	1:A:386:TYR:CZ	2.39	0.40
6:F:94:LEU:O	6:F:95:LYS:C	2.60	0.40
6:F:76:PRO:O	6:F:78:GLU:N	2.54	0.40
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	441/446 (99%)	323 (73%)	94 (21%)	24 (5%)	2	25
1	N	440/446 (99%)	320 (73%)	95 (22%)	25 (6%)	2	24
2	B	419/441 (95%)	302 (72%)	77 (18%)	40 (10%)	1	11
2	O	420/441 (95%)	302 (72%)	85 (20%)	33 (8%)	1	14
3	C	378/380 (100%)	284 (75%)	72 (19%)	22 (6%)	2	23
3	P	377/380 (99%)	284 (75%)	73 (19%)	20 (5%)	2	25
4	D	239/241 (99%)	188 (79%)	37 (16%)	14 (6%)	2	23
4	Q	239/241 (99%)	186 (78%)	40 (17%)	13 (5%)	2	25
5	E	194/196 (99%)	136 (70%)	42 (22%)	16 (8%)	1	13
5	R	194/196 (99%)	136 (70%)	36 (19%)	22 (11%)	0	7
6	F	99/110 (90%)	73 (74%)	24 (24%)	2 (2%)	9	50
6	S	99/110 (90%)	73 (74%)	23 (23%)	3 (3%)	5	41
7	G	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	15
7	T	77/81 (95%)	52 (68%)	20 (26%)	5 (6%)	1	20
8	H	68/77 (88%)	46 (68%)	18 (26%)	4 (6%)	2	23
8	U	65/77 (84%)	41 (63%)	20 (31%)	4 (6%)	2	21
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	5
9	V	29/47 (62%)	21 (72%)	4 (14%)	4 (14%)	0	5
10	J	59/61 (97%)	41 (70%)	16 (27%)	2 (3%)	5	39
10	W	57/61 (93%)	36 (63%)	17 (30%)	4 (7%)	1	17
All	All	4002/4160 (96%)	2919 (73%)	816 (20%)	267 (7%)	1	19

All (267) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	72	CYS
1	A	94	GLN
1	A	159	GLN
1	A	282	ARG
1	A	290	LEU
2	B	29	LEU
2	B	171	ALA
2	B	201	SER
2	B	226	ILE
2	B	230	ALA
2	B	236	LYS
2	B	283	PRO
3	C	31	TRP
3	C	58	ALA
3	C	111	LYS
3	C	224	TYR
3	C	348	PHE
4	D	44	ASP
4	D	198	HIS
5	E	63	SER
5	E	95	PRO
5	E	113	ASP
5	E	141	HIS
6	F	69	SER
7	G	7	LEU
7	G	33	ALA
9	I	63	ASP
10	J	56	LYS
1	N	4	TYR
1	N	55	ALA
1	N	72	CYS
1	N	159	GLN
1	N	206	LYS
1	N	282	ARG
1	N	433	ASP
2	O	171	ALA
2	O	201	SER
2	O	226	ILE
2	O	230	ALA
2	O	236	LYS
2	O	283	PRO
3	P	58	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	P	111	LYS
3	P	224	TYR
4	Q	198	HIS
5	R	63	SER
5	R	95	PRO
5	R	141	HIS
6	S	69	SER
7	T	7	LEU
7	T	33	ALA
10	W	56	LYS
10	W	60	GLU
1	A	288	LYS
1	A	404	ALA
1	A	433	ASP
2	B	20	GLY
2	B	26	ILE
2	B	64	GLY
2	B	110	GLU
2	B	190	GLN
2	B	231	GLY
2	B	249	GLY
2	B	290	SER
2	B	319	SER
2	B	366	ALA
2	B	386	ALA
2	B	420	GLY
3	C	6	ARG
3	C	17	ASN
3	C	202	HIS
4	D	133	GLY
4	D	168	ILE
4	D	177	ALA
4	D	183	ALA
5	E	92	ARG
5	E	137	GLY
5	E	154	GLY
5	E	180	LEU
5	E	188	VAL
6	F	77	LYS
9	I	60	ALA
9	I	73	PRO
9	I	76	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
10	J	57	HIS
1	N	20	ASP
1	N	94	GLN
1	N	207	GLU
1	N	288	LYS
1	N	290	LEU
1	N	404	ALA
2	O	19	PRO
2	O	26	ILE
2	O	64	GLY
2	O	222	GLN
2	O	231	GLY
2	O	290	SER
2	O	351	GLY
2	O	420	GLY
3	P	6	ARG
3	P	17	ASN
3	P	31	TRP
3	P	108	TYR
3	P	158	GLY
3	P	202	HIS
3	P	217	ASP
3	P	348	PHE
4	Q	44	ASP
4	Q	48	PHE
4	Q	133	GLY
4	Q	168	ILE
4	Q	177	ALA
4	Q	183	ALA
5	R	8	PRO
5	R	92	ARG
5	R	109	GLU
5	R	113	ASP
5	R	137	GLY
5	R	180	LEU
6	S	77	LYS
7	T	42	SER
8	U	46	SER
10	W	57	HIS
1	A	4	TYR
1	A	5	ALA
1	A	164	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	222	THR
1	A	274	ASN
2	B	114	ASP
2	B	180	ASP
2	B	265	GLY
2	B	334	GLY
2	B	409	ASP
3	C	3	PRO
3	C	158	GLY
3	C	207	ASN
3	C	217	ASP
3	C	359	TYR
4	D	48	PHE
4	D	166	ASN
4	D	190	LEU
5	E	69	LEU
5	E	70	ALA
5	E	72	SER
5	E	123	ASP
5	E	150	SER
7	G	42	SER
8	H	28	GLU
1	N	222	THR
1	N	262	TRP
1	N	274	ASN
1	N	405	ARG
2	O	110	GLU
2	O	249	GLY
2	O	319	SER
2	O	334	GLY
2	O	346	ALA
2	O	366	ALA
2	O	386	ALA
2	O	409	ASP
3	P	207	ASN
4	Q	162	PRO
4	Q	190	LEU
5	R	21	ALA
5	R	70	ALA
5	R	72	SER
8	U	28	GLU
9	V	48	PRO

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	23	LEU
1	A	56	GLY
1	A	71	PRO
1	A	262	TRP
1	A	332	ASP
1	A	405	ARG
2	B	82	SER
2	B	227	ARG
2	B	346	ALA
2	B	351	GLY
3	C	60	THR
3	C	108	TYR
3	C	156	TYR
3	C	379	ASN
4	D	23	HIS
5	E	186	GLN
8	H	72	LYS
1	N	56	GLY
1	N	164	ALA
1	N	332	ASP
2	O	76	THR
2	O	82	SER
2	O	180	ASP
2	O	296	TYR
3	P	3	PRO
3	P	60	THR
3	P	288	LYS
3	P	359	TYR
3	P	379	ASN
4	Q	144	ARG
4	Q	166	ASN
5	R	114	VAL
5	R	121	GLN
8	U	61	PHE
8	U	72	LYS
9	V	72	ALA
9	V	76	VAL
1	A	141	MET
2	B	63	LEU
2	B	235	ALA
2	B	296	TYR
2	B	375	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	401	LYS
3	C	208	ASN
3	C	209	PRO
3	C	237	LEU
4	D	162	PRO
4	D	176	PRO
5	E	21	ALA
7	G	50	PRO
7	G	61	TRP
8	H	46	SER
8	H	61	PHE
1	N	71	PRO
1	N	170	THR
2	O	114	ASP
3	P	157	ILE
3	P	209	PRO
5	R	30	GLU
5	R	46	ALA
5	R	57	GLN
5	R	69	LEU
5	R	130	PRO
5	R	154	GLY
5	R	188	VAL
6	S	68	LEU
7	T	43	SER
9	V	60	ALA
1	A	106	MET
1	A	263	ALA
1	A	268	VAL
2	B	181	TYR
2	B	207	VAL
2	B	229	GLY
2	B	266	SER
3	C	76	TYR
4	D	110	PRO
1	N	5	ALA
2	O	63	LEU
2	O	178	CYS
3	P	208	ASN
4	Q	176	PRO
5	R	149	ASN
7	T	50	PRO

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	134	PRO
2	O	207	VAL
4	Q	110	PRO
3	C	259	PRO
7	G	74	PRO
1	N	268	VAL
1	N	331	ILE
10	W	25	VAL
2	O	85	ILE
2	B	85	ILE
2	B	178	CYS
2	B	282	GLY
2	O	282	GLY
4	D	122	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 X-ray entries followed by that with respect to entries of similar resolution.

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	365/368 (99%)	342 (94%)	23 (6%)	22	63
1	N	365/368 (99%)	343 (94%)	22 (6%)	24	64
2	B	332/347 (96%)	316 (95%)	16 (5%)	31	71
2	O	333/347 (96%)	315 (95%)	18 (5%)	27	67
3	C	329/329 (100%)	306 (93%)	23 (7%)	19	59
3	P	328/329 (100%)	304 (93%)	24 (7%)	17	57
4	D	200/200 (100%)	192 (96%)	8 (4%)	38	75
4	Q	200/200 (100%)	190 (95%)	10 (5%)	30	69
5	E	166/166 (100%)	156 (94%)	10 (6%)	24	64
5	R	166/166 (100%)	157 (95%)	9 (5%)	27	67
6	F	93/96 (97%)	85 (91%)	8 (9%)	13	49
6	S	93/96 (97%)	83 (89%)	10 (11%)	8	38
7	G	71/71 (100%)	65 (92%)	6 (8%)	13	50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	69/71 (97%)	65 (94%)	4 (6%)	25	65
8	H	65/71 (92%)	63 (97%)	2 (3%)	47	81
8	U	63/71 (89%)	59 (94%)	4 (6%)	22	63
9	I	23/26 (88%)	21 (91%)	2 (9%)	13	49
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	46 (94%)	3 (6%)	23	64
10	W	47/49 (96%)	45 (96%)	2 (4%)	35	74
All	All	3380/3446 (98%)	3176 (94%)	204 (6%)	24	64

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	40	TRP
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	87	ASN
1	A	102	LEU
1	A	106	MET
1	A	146	THR
1	A	182	LEU
1	A	223	TYR
1	A	226	ASP
1	A	264	ASP
1	A	281	ASP
1	A	302	LYS
1	A	307	PHE
1	A	363	SER
1	A	388	ARG
1	A	395	TRP
1	A	420	PRO
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	73	SER
2	B	101	THR
2	B	102	ARG
2	B	106	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	124	LEU
2	B	146	VAL
2	B	152	PHE
2	B	181	TYR
2	B	192	HIS
2	B	227	ARG
2	B	239	TYR
2	B	248	ASN
2	B	296	TYR
2	B	325	TYR
2	B	403	ASP
3	C	23	PRO
3	C	32	TRP
3	C	47	LEU
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	161	LEU
3	C	169	PHE
3	C	184	PHE
3	C	199	THR
3	C	207	ASN
3	C	208	ASN
3	C	214	SER
3	C	216	SER
3	C	223	PRO
3	C	231	LEU
3	C	236	MET
3	C	258	THR
3	C	266	PRO
3	C	283	ARG
3	C	324	THR
3	C	336	LEU
3	C	367	PHE
4	D	10	PHE
4	D	37	CYS
4	D	42	SER
4	D	43	MET
4	D	44	ASP
4	D	179	MET
4	D	215	LEU
4	D	241	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	E	6	THR
5	E	23	THR
5	E	52	LYS
5	E	59	ILE
5	E	61	SER
5	E	65	SER
5	E	123	ASP
5	E	125	ASP
5	E	135	LEU
5	E	190	ASP
6	F	34	ASP
6	F	36	THR
6	F	59	MET
6	F	70	LEU
6	F	77	LYS
6	F	84	GLU
6	F	89	TYR
6	F	91	GLU
7	G	16	TYR
7	G	29	ILE
7	G	41	PHE
7	G	63	THR
7	G	80	ASP
7	G	81	GLN
8	H	10	GLU
8	H	26	GLN
9	I	63	ASP
9	I	71	ASN
10	J	16	ARG
10	J	26	LEU
10	J	59	TYR
1	N	40	TRP
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	171	THR
1	N	182	LEU
1	N	223	TYR
1	N	264	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	N	274	ASN
1	N	281	ASP
1	N	302	LYS
1	N	307	PHE
1	N	363	SER
1	N	388	ARG
1	N	395	TRP
1	N	420	PRO
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	73	SER
2	O	101	THR
2	O	102	ARG
2	O	106	THR
2	O	124	LEU
2	O	146	VAL
2	O	152	PHE
2	O	181	TYR
2	O	192	HIS
2	O	228	SER
2	O	239	TYR
2	O	248	ASN
2	O	258	VAL
2	O	296	TYR
2	O	325	TYR
2	O	403	ASP
3	P	23	PRO
3	P	32	TRP
3	P	47	LEU
3	P	81	ARG
3	P	91	PHE
3	P	138	GLN
3	P	145	THR
3	P	149	ASN
3	P	161	LEU
3	P	169	PHE
3	P	184	PHE
3	P	199	THR
3	P	207	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	P	208	ASN
3	P	214	SER
3	P	216	SER
3	P	223	PRO
3	P	236	MET
3	P	258	THR
3	P	277	PHE
3	P	324	THR
3	P	336	LEU
3	P	337	THR
3	P	367	PHE
4	Q	3	LEU
4	Q	10	PHE
4	Q	13	SER
4	Q	37	CYS
4	Q	42	SER
4	Q	43	MET
4	Q	44	ASP
4	Q	199	ASP
4	Q	215	LEU
4	Q	241	LYS
5	R	6	THR
5	R	23	THR
5	R	52	LYS
5	R	59	ILE
5	R	61	SER
5	R	65	SER
5	R	135	LEU
5	R	147	ILE
5	R	190	ASP
6	S	13	MET
6	S	34	ASP
6	S	36	THR
6	S	59	MET
6	S	70	LEU
6	S	77	LYS
6	S	78	GLU
6	S	84	GLU
6	S	89	TYR
6	S	91	GLU
7	T	16	TYR
7	T	29	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	T	41	PHE
7	T	63	THR
8	U	13	LEU
8	U	26	GLN
8	U	51	GLU
8	U	71	HIS
10	W	26	LEU
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	87	ASN
1	A	118	GLN
1	A	136	GLN
1	A	159	GLN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	332	HIS
2	B	362	ASN
2	B	363	GLN
2	B	376	GLN
2	B	400	GLN
3	C	33	ASN
3	C	73	ASN
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	105	ASN
4	D	200	GLN
4	D	225	HIS
5	E	86	ASN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	56	ASN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
7	G	81	GLN
8	H	26	GLN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	87	ASN
1	N	118	GLN
1	N	136	GLN
1	N	159	GLN
1	N	173	ASN
1	N	274	ASN
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	222	GLN
2	O	247	GLN
2	O	248	ASN
2	O	297	GLN
2	O	329	GLN
2	O	332	HIS
2	O	362	ASN
2	O	363	GLN
2	O	376	GLN
2	O	400	GLN
3	P	33	ASN
3	P	69	HIS
3	P	82	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	P	149	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	105	ASN
4	Q	200	GLN
4	Q	225	HIS
5	R	164	HIS
5	R	186	GLN
6	S	56	ASN
6	S	79	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
17	PEE	A	2008	-	20,20,50	1.79	5 (25%)	21,25,55	0.74	1 (4%)
14	SMA	C	2001	-	35,38,38	1.64	4 (11%)	40,52,52	1.58	5 (12%)
15	ANY	C	2002	-	38,38,41	1.53	5 (13%)	32,52,55	2.13	9 (28%)
16	CDL	C	2004	-	39,39,99	1.25	5 (12%)	41,51,111	1.18	4 (9%)
17	PEE	C	2007	-	48,48,50	1.34	7 (14%)	49,53,55	0.93	5 (10%)
20	GOL	C	2011	-	5,5,5	1.21	0	5,5,5	0.64	0
11	HEM	C	501	3	30,50,50	3.17	8 (26%)	24,82,82	2.38	9 (37%)
11	HEM	C	502	3	30,50,50	3.12	9 (30%)	24,82,82	2.49	8 (33%)
16	CDL	D	2003	-	49,49,99	1.17	4 (8%)	51,61,111	0.93	1 (1%)
12	HEC	D	501	4	24,50,50	2.41	2 (8%)	19,82,82	3.87	6 (31%)
17	PEE	E	2005	-	49,49,50	1.33	9 (18%)	50,54,55	0.94	5 (10%)
18	PLC	E	2009	-	31,31,41	1.68	6 (19%)	35,39,49	0.71	1 (2%)
13	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	PEE	N	3008	-	4,4,50	3.65	3 (75%)	6,6,55	0.59	0
14	SMA	P	3001	-	35,38,38	1.82	5 (14%)	40,52,52	1.54	4 (10%)
15	ANY	P	3002	-	38,38,41	1.78	9 (23%)	32,52,55	2.12	7 (21%)
16	CDL	P	3004	-	39,39,99	1.24	4 (10%)	41,51,111	1.18	3 (7%)
17	PEE	P	3005	-	49,49,50	1.44	9 (18%)	50,54,55	0.94	5 (10%)
17	PEE	P	3007	-	48,48,50	1.32	7 (14%)	49,53,55	0.93	5 (10%)
20	GOL	P	3011	-	5,5,5	1.17	0	5,5,5	0.63	0
11	HEM	P	501	3	30,50,50	3.11	10 (33%)	24,82,82	2.25	8 (33%)
11	HEM	P	502	3	30,50,50	3.21	8 (26%)	24,82,82	2.38	10 (41%)
16	CDL	Q	3003	-	49,49,99	1.14	3 (6%)	51,61,111	0.96	2 (3%)
12	HEC	Q	501	4	24,50,50	2.53	4 (16%)	19,82,82	3.72	7 (36%)
18	PLC	R	3009	-	31,31,41	1.60	8 (25%)	35,39,49	0.58	0
13	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-

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
17	PEE	A	2008	-	-	0/24/24/54	0/0/0/0
14	SMA	C	2001	-	-	0/33/34/34	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ANY	C	2002	-	1/1/10/13	0/35/52/56	0/1/2/2
16	CDL	C	2004	-	-	0/49/49/110	0/0/0/0
17	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
20	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
11	HEM	C	501	3	-	0/10/54/54	0/0/8/8
11	HEM	C	502	3	-	0/10/54/54	0/0/8/8
16	CDL	D	2003	-	-	0/59/59/110	0/0/0/0
12	HEC	D	501	4	-	0/6/54/54	0/0/8/8
17	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
18	PLC	E	2009	-	-	0/35/35/45	0/0/0/0
13	FES	E	501	5	-	0/0/4/4	0/1/1/1
17	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
14	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
15	ANY	P	3002	-	1/1/10/13	0/35/52/56	0/1/2/2
16	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
17	PEE	P	3005	-	-	0/53/53/54	0/0/0/0
17	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
20	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
11	HEM	P	501	3	-	0/10/54/54	0/0/8/8
11	HEM	P	502	3	-	0/10/54/54	0/0/8/8
16	CDL	Q	3003	-	-	0/59/59/110	0/0/0/0
12	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
18	PLC	R	3009	-	-	0/35/35/45	0/0/0/0
13	FES	R	501	5	-	0/0/4/4	0/1/1/1

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	502	HEM	C3B-C4B	-8.91	1.43	1.51
12	Q	501	HEC	C3B-C2B	-8.62	1.31	1.40
11	C	502	HEM	C3C-CAC	-8.32	1.35	1.51
11	C	501	HEM	C3B-C4B	-8.25	1.44	1.51
12	D	501	HEC	C3B-C2B	-8.00	1.32	1.40
11	P	501	HEM	C2D-C3D	-7.90	1.30	1.54
11	C	502	HEM	C2D-C3D	-7.77	1.31	1.54
11	C	501	HEM	C3B-CAB	-7.75	1.36	1.51
11	P	501	HEM	C3B-C4B	-7.57	1.45	1.51
11	P	502	HEM	C3B-CAB	-7.45	1.37	1.51
12	Q	501	HEC	C3C-C2C	-7.38	1.33	1.40
12	D	501	HEC	C3C-C2C	-7.32	1.33	1.40
11	P	502	HEM	C3C-CAC	-6.96	1.38	1.51
11	P	501	HEM	C3C-CAC	-6.79	1.38	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	501	HEM	C3B-CAB	-6.69	1.38	1.51
11	C	501	HEM	C3C-CAC	-6.50	1.39	1.51
11	C	501	HEM	C2D-C3D	-6.48	1.35	1.54
11	P	502	HEM	C2D-C3D	-6.45	1.35	1.54
11	C	502	HEM	C2C-C1C	-6.23	1.40	1.52
11	P	502	HEM	C2C-C1C	-5.91	1.41	1.52
11	C	502	HEM	C3B-CAB	-5.65	1.40	1.51
11	C	502	HEM	C3D-C4D	-5.26	1.44	1.51
11	C	501	HEM	C3D-C4D	-4.08	1.46	1.51
11	C	501	HEM	C2C-C1C	-3.65	1.45	1.52
11	P	501	HEM	C3D-C4D	-3.18	1.47	1.51
11	C	502	HEM	C3B-C4B	-3.03	1.49	1.51
17	P	3007	PEE	C22-C21	-2.89	1.34	1.51
17	C	2007	PEE	C22-C21	-2.83	1.35	1.51
17	P	3005	PEE	C19-C18	-2.83	1.35	1.51
17	E	2005	PEE	C22-C21	-2.82	1.35	1.51
17	C	2007	PEE	C19-C18	-2.76	1.35	1.51
17	P	3007	PEE	C19-C18	-2.71	1.35	1.51
17	E	2005	PEE	C19-C18	-2.69	1.36	1.51
17	P	3005	PEE	C22-C21	-2.69	1.36	1.51
11	C	502	HEM	C2D-C1D	-2.58	1.43	1.51
11	P	501	HEM	FE-NC	-2.54	1.85	1.95
11	P	501	HEM	C2C-C1C	-2.48	1.47	1.52
12	Q	501	HEC	C1C-CHC	-2.30	1.33	1.39
11	P	501	HEM	C1A-CHA	-2.03	1.34	1.39
16	P	3004	CDL	OA8-CA6	-2.00	1.40	1.45
16	P	3004	CDL	OB8-CB7	2.00	1.39	1.33
16	C	2004	CDL	O1-C1	2.04	1.49	1.43
15	P	3002	ANY	C7-N2	2.05	1.38	1.34
11	P	502	HEM	CAA-C2A	2.07	1.55	1.52
18	R	3009	PLC	C1'-C'	2.08	1.56	1.50
17	E	2005	PEE	C1-C2	2.10	1.56	1.50
17	P	3007	PEE	C1-C2	2.11	1.56	1.50
16	D	2003	CDL	OB8-CB7	2.13	1.39	1.33
14	P	3001	SMA	O1-C8A	2.13	1.40	1.36
15	P	3002	ANY	O5-C14	2.14	1.39	1.34
16	C	2004	CDL	OB8-CB7	2.15	1.39	1.33
18	R	3009	PLC	C1B-CB	2.19	1.57	1.50
16	Q	3003	CDL	O1-C1	2.19	1.50	1.43
17	E	2005	PEE	C3-C2	2.20	1.56	1.50
17	E	2005	PEE	C11-C10	2.21	1.57	1.50
16	P	3004	CDL	O1-C1	2.23	1.50	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	2004	CDL	OA6-CA5	2.25	1.41	1.34
18	R	3009	PLC	C3-C2	2.25	1.57	1.50
17	P	3005	PEE	C1-C2	2.27	1.57	1.50
15	P	3002	ANY	C3-C2	2.27	1.43	1.39
17	C	2007	PEE	C1-C2	2.29	1.57	1.50
18	R	3009	PLC	O2-C2	2.30	1.52	1.46
17	A	2008	PEE	C3-C2	2.31	1.57	1.50
15	C	2002	ANY	C10-C9	2.33	1.58	1.53
16	Q	3003	CDL	CA6-CA4	2.34	1.57	1.50
17	C	2007	PEE	C3-C2	2.34	1.57	1.50
17	E	2005	PEE	C31-C30	2.37	1.57	1.50
17	P	3005	PEE	C3-C2	2.38	1.57	1.50
12	Q	501	HEC	CAD-C3D	2.45	1.56	1.52
15	P	3002	ANY	C6-C1	2.45	1.45	1.41
17	P	3007	PEE	C3-C2	2.46	1.57	1.50
15	P	3002	ANY	C13-C12	2.47	1.58	1.53
16	Q	3003	CDL	CA3-CA4	2.50	1.57	1.50
18	E	2009	PLC	C3-C2	2.51	1.57	1.50
17	C	2007	PEE	O3-C30	2.52	1.40	1.33
15	C	2002	ANY	O8-C21	2.53	1.40	1.34
16	D	2003	CDL	O1-C1	2.53	1.51	1.43
17	P	3005	PEE	C11-C10	2.55	1.58	1.50
16	C	2004	CDL	CB3-CB4	2.55	1.57	1.50
16	D	2003	CDL	CA3-CA4	2.57	1.58	1.50
16	C	2004	CDL	CA3-CA4	2.57	1.58	1.50
17	P	3007	PEE	P-O1P	2.68	1.61	1.51
15	C	2002	ANY	C2-C1	2.69	1.44	1.40
16	P	3004	CDL	CA3-CA4	2.70	1.58	1.50
14	C	2001	SMA	C4-C3	2.72	1.49	1.41
17	P	3007	PEE	O3-C30	2.77	1.41	1.33
18	R	3009	PLC	C1-C2	2.83	1.58	1.50
17	E	2005	PEE	O2-C10	2.84	1.42	1.34
18	R	3009	PLC	O3-CB	2.87	1.41	1.33
17	E	2005	PEE	P-O1P	2.87	1.61	1.51
17	P	3005	PEE	C31-C30	2.89	1.59	1.50
17	A	2008	PEE	P-O1P	2.90	1.61	1.51
18	R	3009	PLC	P-O1P	2.91	1.61	1.51
16	D	2003	CDL	CA6-CA4	2.91	1.58	1.50
17	A	2008	PEE	O3-C30	2.92	1.42	1.33
17	A	2008	PEE	C1-C2	2.92	1.59	1.50
17	C	2007	PEE	P-O1P	2.94	1.61	1.51
18	E	2009	PLC	O3-CB	2.95	1.42	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	3008	PEE	P-O4P	2.96	1.65	1.54
17	E	2005	PEE	O3-C30	3.00	1.42	1.33
17	N	3008	PEE	P-O3P	3.06	1.65	1.54
15	P	3002	ANY	O8-C21	3.10	1.41	1.34
17	A	2008	PEE	O2-C10	3.11	1.43	1.34
18	E	2009	PLC	P-O1P	3.14	1.62	1.51
17	P	3005	PEE	O2-C10	3.16	1.43	1.34
17	P	3005	PEE	O3-C30	3.17	1.42	1.33
18	E	2009	PLC	C1-C2	3.18	1.59	1.50
14	P	3001	SMA	C7-C8	3.21	1.44	1.40
18	E	2009	PLC	O2-C2	3.22	1.54	1.46
17	P	3005	PEE	P-O1P	3.24	1.63	1.51
11	C	501	HEM	CBB-CAB	3.24	1.48	1.29
11	C	502	HEM	CBC-CAC	3.28	1.48	1.29
15	C	2002	ANY	C12-C11	3.29	1.59	1.52
17	P	3007	PEE	O2-C10	3.32	1.44	1.34
15	P	3002	ANY	C12-C11	3.33	1.59	1.52
14	P	3001	SMA	C4-C3	3.35	1.51	1.41
14	C	2001	SMA	O1-C2	3.41	1.39	1.35
17	C	2007	PEE	O2-C10	3.42	1.44	1.34
15	P	3002	ANY	C2-C1	3.43	1.46	1.40
11	P	502	HEM	CBB-CAB	3.51	1.49	1.29
18	R	3009	PLC	O2-C'	3.59	1.45	1.34
11	P	502	HEM	CBC-CAC	3.88	1.51	1.29
18	E	2009	PLC	O2-C'	4.16	1.46	1.34
11	P	501	HEM	CBB-CAB	4.17	1.53	1.29
11	P	501	HEM	CBC-CAC	4.18	1.53	1.29
11	C	502	HEM	CBB-CAB	4.50	1.55	1.29
11	C	501	HEM	CBC-CAC	4.59	1.55	1.29
14	C	2001	SMA	C4-C4A	4.99	1.48	1.41
14	C	2001	SMA	C7-C8	5.02	1.47	1.40
14	P	3001	SMA	O1-C2	5.14	1.41	1.35
15	C	2002	ANY	C8-N1	5.40	1.41	1.34
17	N	3008	PEE	P-O1P	5.58	1.61	1.50
15	P	3002	ANY	C8-N1	5.64	1.42	1.34
14	P	3001	SMA	C4-C4A	6.38	1.50	1.41

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	501	HEC	CBC-CAC-C3C	-12.17	100.31	127.35
12	Q	501	HEC	CBC-CAC-C3C	-11.45	101.91	127.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	501	HEC	CBB-CAB-C3B	-6.21	113.56	127.35
12	Q	501	HEC	CBB-CAB-C3B	-6.02	113.97	127.35
15	C	2002	ANY	O5-C14-O6	-5.17	117.22	124.19
15	P	3002	ANY	C25-C22-C23	-5.02	89.40	111.90
11	C	501	HEM	CBA-CAA-C2A	-4.97	103.62	112.53
11	C	502	HEM	C3C-CAC-CBC	-4.78	117.12	124.46
11	P	501	HEM	C3C-CAC-CBC	-4.55	117.47	124.46
14	P	3001	SMA	C3-C4-C4A	-4.45	115.18	121.35
15	C	2002	ANY	C25-C22-C23	-4.32	92.54	111.90
14	C	2001	SMA	C3-C4-C4A	-4.28	115.41	121.35
15	P	3002	ANY	O5-C14-O6	-4.23	118.50	124.19
16	P	3004	CDL	CB4-OB6-CB5	-3.89	108.55	117.89
11	P	502	HEM	CBD-CAD-C3D	-3.85	102.36	113.55
14	C	2001	SMA	C9-C10-C11	-3.75	110.33	114.75
11	C	501	HEM	C3C-CAC-CBC	-3.71	118.77	124.46
16	C	2004	CDL	CB4-OB6-CB5	-3.70	109.00	117.89
11	P	501	HEM	CBA-CAA-C2A	-3.65	105.98	112.53
15	P	3002	ANY	O4-C20-O7	-3.15	119.95	124.19
12	D	501	HEC	CAA-C2A-C3A	-3.11	120.12	129.00
12	Q	501	HEC	CAA-C2A-C3A	-3.06	120.27	129.00
15	C	2002	ANY	O4-C20-O7	-3.05	120.08	124.19
11	C	501	HEM	C3B-CAB-CBB	-3.01	119.83	124.46
14	P	3001	SMA	C9-C10-C11	-2.89	111.34	114.75
11	P	502	HEM	C3C-CAC-CBC	-2.72	120.28	124.46
16	D	2003	CDL	CB4-OB6-CB5	-2.67	111.47	117.89
11	C	502	HEM	CBD-CAD-C3D	-2.65	105.85	113.55
16	Q	3003	CDL	CB4-OB6-CB5	-2.44	112.03	117.89
11	P	502	HEM	CMA-C3A-C4A	-2.38	124.42	128.36
16	P	3004	CDL	CA6-CA4-CA3	-2.21	106.89	112.07
16	Q	3003	CDL	CA6-CA4-CA3	-2.12	107.10	112.07
16	C	2004	CDL	CA6-CA4-CA3	-2.07	107.23	112.07
16	C	2004	CDL	CA4-OA6-CA5	-2.06	112.95	117.89
15	C	2002	ANY	O8-C21-O9	-2.06	119.65	123.89
16	P	3004	CDL	CA4-OA6-CA5	-2.01	113.07	117.89
14	P	3001	SMA	C4-C3-C2	2.01	120.65	117.73
11	P	501	HEM	CMD-C2D-C3D	2.01	123.24	114.35
18	E	2009	PLC	O3-C3-C2	2.04	114.19	108.69
11	C	502	HEM	CMD-C2D-C3D	2.06	123.46	114.35
11	P	502	HEM	C2D-C3D-C4D	2.08	105.02	101.50
14	C	2001	SMA	C4-C3-C2	2.12	120.82	117.73
15	P	3002	ANY	O1-C1-C6	2.17	124.92	121.00
15	C	2002	ANY	C12-O8-C21	2.19	121.83	118.01

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	2004	CDL	OB6-CB4-CB3	2.20	116.12	108.36
17	P	3005	PEE	O3-C3-C2	2.20	114.62	108.69
17	P	3007	PEE	O3-C3-C2	2.21	114.65	108.69
17	A	2008	PEE	O3-C3-C2	2.22	114.65	108.69
17	C	2007	PEE	O3-C3-C2	2.24	114.72	108.69
11	P	502	HEM	CMD-C2D-C3D	2.26	124.35	114.35
15	C	2002	ANY	C23-C22-C21	2.26	118.85	111.03
15	C	2002	ANY	O1-C1-C6	2.27	125.11	121.00
11	P	501	HEM	C2D-C3D-C4D	2.30	105.40	101.50
17	C	2007	PEE	C22-C21-C20	2.35	126.69	114.53
17	P	3007	PEE	C23-C22-C21	2.36	126.74	114.53
17	E	2005	PEE	O3-C3-C2	2.37	115.08	108.69
17	P	3005	PEE	C19-C18-C17	2.39	126.88	114.53
11	C	501	HEM	CAA-C2A-C1A	2.39	129.60	127.01
11	C	501	HEM	CMD-C2D-C3D	2.40	124.98	114.35
17	P	3007	PEE	C22-C21-C20	2.41	126.98	114.53
17	E	2005	PEE	C23-C22-C21	2.44	127.15	114.53
17	C	2007	PEE	C23-C22-C21	2.48	127.33	114.53
17	P	3005	PEE	C23-C22-C21	2.50	127.43	114.53
17	E	2005	PEE	C22-C21-C20	2.50	127.45	114.53
17	P	3005	PEE	C22-C21-C20	2.54	127.64	114.53
15	P	3002	ANY	C12-O8-C21	2.54	122.45	118.01
17	E	2005	PEE	C19-C18-C17	2.55	127.69	114.53
11	P	502	HEM	CAA-C2A-C1A	2.62	129.85	127.01
17	C	2007	PEE	C20-C19-C18	2.62	128.08	114.53
11	C	501	HEM	CMB-C2B-C3B	2.66	123.17	116.53
17	P	3007	PEE	C19-C18-C17	2.68	128.37	114.53
12	Q	501	HEC	CBD-CAD-C3D	2.69	117.34	112.53
15	P	3002	ANY	O7-C20-C9	2.71	129.83	125.20
17	E	2005	PEE	C20-C19-C18	2.76	128.80	114.53
17	C	2007	PEE	C19-C18-C17	2.78	128.86	114.53
12	Q	501	HEC	CAD-C3D-C4D	2.79	130.04	127.01
17	P	3005	PEE	C20-C19-C18	2.81	129.02	114.53
17	P	3007	PEE	C20-C19-C18	2.81	129.04	114.53
14	C	2001	SMA	O7-C7-C8	2.83	117.31	114.47
15	C	2002	ANY	O7-C20-C9	3.09	130.49	125.20
11	C	501	HEM	CAD-C3D-C2D	3.18	122.37	113.22
11	C	502	HEM	CMB-C2B-C3B	3.18	124.48	116.53
11	C	502	HEM	CAD-C3D-C2D	3.21	122.44	113.22
11	P	501	HEM	CAD-C3D-C2D	3.35	122.83	113.22
11	P	502	HEM	CAD-C3D-C2D	3.42	123.04	113.22
11	C	501	HEM	CMC-C2C-C3C	3.43	125.10	116.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	501	HEM	CMB-C2B-C3B	3.65	125.65	116.53
11	P	501	HEM	CMC-C2C-C3C	3.91	126.29	116.53
12	D	501	HEC	CAD-C3D-C4D	4.02	131.38	127.01
11	P	502	HEM	CMB-C2B-C3B	4.45	127.65	116.53
11	C	502	HEM	CAA-C2A-C1A	4.63	132.04	127.01
11	C	502	HEM	CMC-C2C-C3C	4.81	128.53	116.53
12	D	501	HEC	CBA-CAA-C2A	4.93	121.37	112.53
11	P	502	HEM	CMC-C2C-C3C	4.94	128.85	116.53
12	Q	501	HEC	CBA-CAA-C2A	5.10	121.67	112.53
11	P	502	HEM	CAD-C3D-C4D	5.27	131.05	112.47
11	C	502	HEM	CAD-C3D-C4D	5.40	131.53	112.47
11	P	501	HEM	CAD-C3D-C4D	5.46	131.73	112.47
12	Q	501	HEC	CAA-C2A-C1A	6.05	133.58	127.01
12	D	501	HEC	CAA-C2A-C1A	6.11	133.64	127.01
11	C	501	HEM	CAD-C3D-C4D	6.17	134.24	112.47
14	C	2001	SMA	C9-C2-C3	6.34	128.92	120.56
14	P	3001	SMA	C9-C2-C3	6.35	128.94	120.56
15	C	2002	ANY	C25-C22-C21	6.87	134.77	111.03
15	P	3002	ANY	C25-C22-C21	7.04	135.38	111.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	2002	ANY	C22
15	P	3002	ANY	C22

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2001	SMA	3	0
15	C	2002	ANY	3	0
16	C	2004	CDL	2	0
17	C	2007	PEE	2	0
20	C	2011	GOL	1	0
11	C	501	HEM	11	0
11	C	502	HEM	9	0
16	D	2003	CDL	1	0
12	D	501	HEC	6	0
17	E	2005	PEE	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	E	2009	PLC	2	0
13	E	501	FES	2	0
14	P	3001	SMA	4	0
15	P	3002	ANY	1	0
16	P	3004	CDL	2	0
17	P	3005	PEE	3	0
17	P	3007	PEE	3	0
11	P	501	HEM	11	0
11	P	502	HEM	11	0
16	Q	3003	CDL	5	0
12	Q	501	HEC	4	0
18	R	3009	PLC	3	0
13	R	501	FES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/446 (99%)	-0.20	4 (0%) 85 78	40, 85, 131, 143	0
1	N	442/446 (99%)	-0.14	8 (1%) 71 62	42, 91, 131, 143	0
2	B	421/441 (95%)	-0.09	3 (0%) 89 83	63, 107, 145, 173	0
2	O	422/441 (95%)	-0.17	8 (1%) 70 61	50, 97, 140, 150	0
3	C	380/380 (100%)	-0.72	0 100 100	17, 40, 73, 122	0
3	P	379/380 (99%)	-0.50	3 (0%) 87 80	20, 71, 106, 136	0
4	D	241/241 (100%)	-0.47	0 100 100	28, 55, 105, 118	0
4	Q	241/241 (100%)	-0.26	2 (0%) 87 80	51, 93, 136, 148	0
5	E	196/196 (100%)	0.52	40 (20%) 1 1	36, 123, 176, 180	0
5	R	196/196 (100%)	0.16	15 (7%) 16 13	50, 97, 152, 159	0
6	F	101/110 (91%)	-0.64	0 100 100	32, 57, 80, 112	0
6	S	101/110 (91%)	-0.21	1 (0%) 84 76	67, 103, 138, 161	0
7	G	81/81 (100%)	-0.40	0 100 100	38, 66, 112, 123	0
7	T	79/81 (97%)	-0.22	3 (3%) 44 36	62, 112, 176, 184	0
8	H	70/77 (90%)	-0.19	0 100 100	50, 90, 109, 132	0
8	U	67/77 (87%)	0.29	3 (4%) 37 29	129, 151, 171, 173	0
9	I	31/47 (65%)	0.65	2 (6%) 22 16	100, 143, 177, 178	0
9	V	31/47 (65%)	0.66	4 (12%) 5 5	107, 152, 194, 197	0
10	J	61/61 (100%)	-0.24	1 (1%) 74 66	57, 72, 124, 165	0
10	W	59/61 (96%)	0.07	1 (1%) 73 64	62, 89, 125, 148	0
All	All	4042/4160 (97%)	-0.22	98 (2%) 62 52	17, 87, 148, 197	0

All (98) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
5	E	132	TRP	5.4
5	E	134	ILE	4.5
9	I	77	ARG	4.2
5	E	121	GLN	4.0
5	E	111	GLU	3.9
5	E	133	VAL	3.9
10	J	64	GLU	3.9
5	R	188	VAL	3.9
5	E	77	LYS	3.9
5	E	117	LEU	3.8
5	E	127	VAL	3.7
5	E	78	LEU	3.7
5	E	122	HIS	3.7
5	E	128	LYS	3.6
9	V	77	ARG	3.5
5	E	192	LEU	3.5
5	R	122	HIS	3.5
5	E	114	VAL	3.3
5	E	110	ALA	3.3
5	E	112	VAL	3.3
8	U	76	LYS	3.2
5	E	76	ILE	3.1
2	O	36	ALA	3.1
5	E	187	PHE	3.1
1	A	216	PHE	3.1
2	B	350	GLY	3.1
5	E	98	VAL	3.0
5	R	114	VAL	2.9
10	W	62	SER	2.9
5	E	109	GLU	2.9
1	N	83	GLY	2.9
5	E	115	SER	2.9
5	R	111	GLU	2.9
2	O	208	GLY	2.8
7	T	2	ILE	2.8
5	E	174	GLY	2.8
2	O	18	CYS	2.8
3	P	380	TYR	2.8
5	R	75	GLU	2.8
5	E	188	VAL	2.8
5	R	192	LEU	2.8
5	E	96	LEU	2.8
5	R	121	GLN	2.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	E	120	PRO	2.7
1	N	66	GLY	2.7
5	E	185	TYR	2.7
5	E	135	LEU	2.7
5	R	103	GLN	2.7
5	E	172	ARG	2.7
1	A	2	ALA	2.7
8	U	74	PHE	2.7
1	N	370	ASP	2.6
3	P	375	ASN	2.5
3	P	2	ALA	2.5
1	N	81	SER	2.5
5	R	112	VAL	2.5
5	E	191	ASP	2.4
5	E	193	VAL	2.4
5	E	189	GLY	2.4
5	R	120	PRO	2.4
9	I	63	ASP	2.4
5	E	118	ARG	2.3
2	O	332	HIS	2.3
1	A	22	GLY	2.3
1	N	216	PHE	2.3
6	S	89	TYR	2.3
5	E	101	ARG	2.3
4	Q	180	SER	2.2
1	N	84	ALA	2.2
5	R	193	VAL	2.2
5	E	79	SER	2.2
5	R	186	GLN	2.2
5	E	81	ILE	2.2
2	O	19	PRO	2.2
4	Q	67	GLU	2.2
5	R	101	ARG	2.2
5	R	72	SER	2.2
2	B	36	ALA	2.2
5	E	190	ASP	2.2
1	A	66	GLY	2.1
5	E	97	PHE	2.1
1	N	174	ILE	2.1
5	E	113	ASP	2.1
9	V	75	SER	2.1
7	T	78	GLU	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	O	350	GLY	2.1
2	B	349	GLN	2.1
9	V	61	ARG	2.1
5	R	191	ASP	2.1
8	U	29	LYS	2.1
2	O	37	SER	2.1
1	N	117	VAL	2.1
2	O	25	GLU	2.0
7	T	1	GLY	2.0
5	E	129	LYS	2.0
5	E	116	LYS	2.0
9	V	63	ASP	2.0
5	E	186	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	UNL	C	2010	1/-	0.92	0.58	21.00	24,24,24,24	0
19	UNL	R	2103	1/-	0.93	0.57	15.20	12,12,12,12	0
19	UNL	E	3103	1/-	0.90	0.52	10.57	32,32,32,32	0
20	GOL	P	3011	6/6	0.94	0.43	5.83	46,48,50,50	0
17	PEE	P	3007	49/51	0.88	0.43	5.68	63,96,134,135	0
17	PEE	E	2005	50/51	0.85	0.46	5.43	66,86,100,101	0
16	CDL	Q	3003	50/100	0.75	0.40	5.20	116,149,158,158	0
18	PLC	R	3009	32/42	0.83	0.48	4.11	74,93,118,118	0

*Continued on next page...*



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	PEE	A	2008	21/51	0.79	0.35	4.10	121,125,130,130	0
20	GOL	C	2011	6/6	0.91	0.29	3.95	67,70,71,73	0
17	PEE	C	2007	49/51	0.91	0.30	3.75	44,56,90,91	0
17	PEE	P	3005	50/51	0.78	0.46	3.66	75,97,113,115	0
16	CDL	D	2003	50/100	0.83	0.34	2.93	63,103,110,111	0
18	PLC	E	2009	32/42	0.86	0.38	2.90	37,60,94,95	0
16	CDL	P	3004	40/100	0.87	0.27	2.63	101,108,110,110	0
14	SMA	P	3001	37/37	0.94	0.34	2.14	64,69,74,75	0
15	ANY	C	2002	37/40	0.96	0.21	1.46	27,36,48,50	0
15	ANY	P	3002	37/40	0.95	0.24	1.26	65,69,82,82	0
14	SMA	C	2001	37/37	0.97	0.22	1.04	20,30,37,39	0
16	CDL	C	2004	40/100	0.92	0.23	0.95	50,72,90,92	0
11	HEM	C	502	43/43	0.98	0.20	0.90	21,28,43,49	0
11	HEM	P	502	43/43	0.96	0.22	0.80	49,52,70,77	0
11	HEM	P	501	43/43	0.98	0.21	0.64	44,49,55,56	0
11	HEM	C	501	43/43	0.98	0.20	0.27	24,32,36,39	0
12	HEC	D	501	43/43	0.98	0.16	-0.53	34,39,48,55	0
12	HEC	Q	501	43/43	0.97	0.20	-0.70	64,68,72,76	0
13	FES	R	501	4/4	0.99	0.12	-0.95	55,56,58,58	0
13	FES	E	501	4/4	0.99	0.11	-1.70	87,88,89,90	0
19	UNL	C	2104	1/-	0.81	0.43	-	36,36,36,36	0
19	UNL	A	3016	1/-	0.86	0.36	-	10,10,10,10	0
19	UNL	P	2015	1/-	0.92	0.54	-	25,25,25,25	0
19	UNL	P	3010	1/-	0.93	0.35	-	24,24,24,24	0
19	UNL	E	2105	1/-	0.60	0.34	-	35,35,35,35	0
19	UNL	C	3015	1/-	0.63	0.60	-	32,32,32,32	0
17	PEE	N	3008	5/51	0.91	0.36	-	105,105,106,106	0
19	UNL	P	3104	1/-	0.69	0.63	-	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.