



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:00 PM GMT

PDB ID : 1VYH
Title : PAF-AH HOLOENZYME: LIS1/ALFA2
Authors : Tarricone, C.; Perrina, F.; Monzani, S.; Massimiliano, L.; Knapp, S.; Tsai, L.-H.; Derewenda, Z.S.; Musacchio, A.
Deposited on : 2004-04-30
Resolution : 3.40 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
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

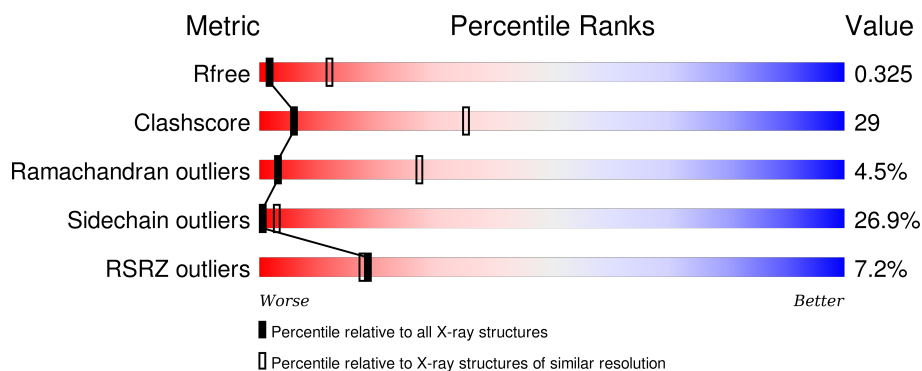
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 ≥ 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	229	<div> <div>2%</div> <div>50% 34% 10% 5%</div> </div>
1	B	229	<div> <div>2%</div> <div>50% 38% 7% 5%</div> </div>
1	E	229	<div> <div></div> <div>54% 37% • 5%</div> </div>
1	F	229	<div> <div>3%</div> <div>55% 31% 9% • 5%</div> </div>
1	I	229	<div> <div>%</div> <div>48% 40% 7% 5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	229	
1	M	229	
1	N	229	
1	Q	229	
1	R	229	
2	C	410	
2	D	410	
2	G	410	
2	H	410	
2	K	410	
2	L	410	
2	O	410	
2	P	410	
2	S	410	
2	T	410	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41590 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 PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	B	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	E	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	F	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	I	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	J	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	M	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	N	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	Q	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	R	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			

- Molecule 2 is a protein called PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	D	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	G	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	K	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	L	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	O	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	P	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	S	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	T	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			

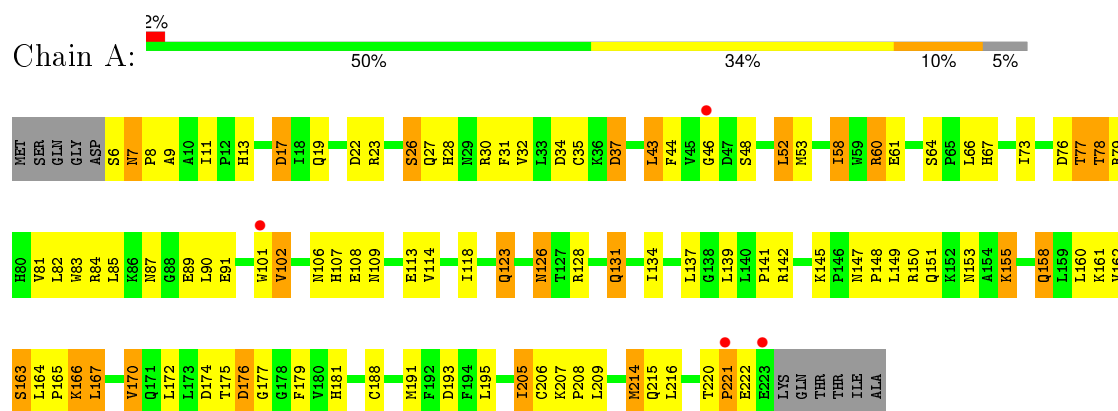
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	SER	ALA	CONFLICT	UNP P43034
C	276	ARG	GLU	CONFLICT	UNP P43034
D	199	SER	ALA	CONFLICT	UNP P43034
D	276	ARG	GLU	CONFLICT	UNP P43034
G	199	SER	ALA	CONFLICT	UNP P43034
G	276	ARG	GLU	CONFLICT	UNP P43034
H	199	SER	ALA	CONFLICT	UNP P43034
H	276	ARG	GLU	CONFLICT	UNP P43034
K	199	SER	ALA	CONFLICT	UNP P43034
K	276	ARG	GLU	CONFLICT	UNP P43034
L	199	SER	ALA	CONFLICT	UNP P43034
L	276	ARG	GLU	CONFLICT	UNP P43034
O	199	SER	ALA	CONFLICT	UNP P43034
O	276	ARG	GLU	CONFLICT	UNP P43034
P	199	SER	ALA	CONFLICT	UNP P43034
P	276	ARG	GLU	CONFLICT	UNP P43034
S	199	SER	ALA	CONFLICT	UNP P43034
S	276	ARG	GLU	CONFLICT	UNP P43034
T	199	SER	ALA	CONFLICT	UNP P43034
T	276	ARG	GLU	CONFLICT	UNP P43034

3 Residue-property plots [i](#)

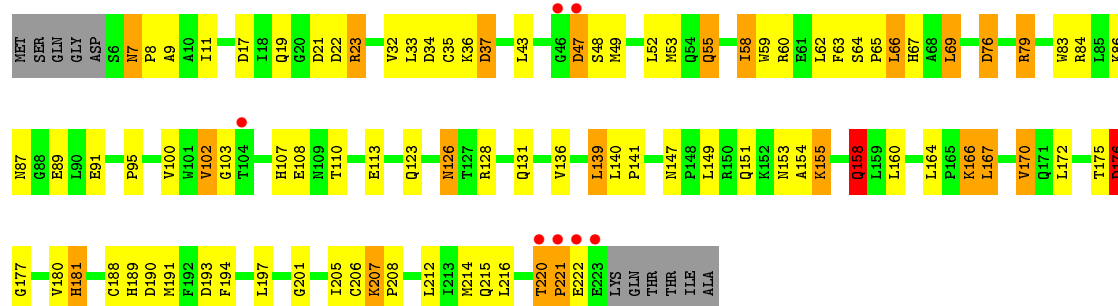
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

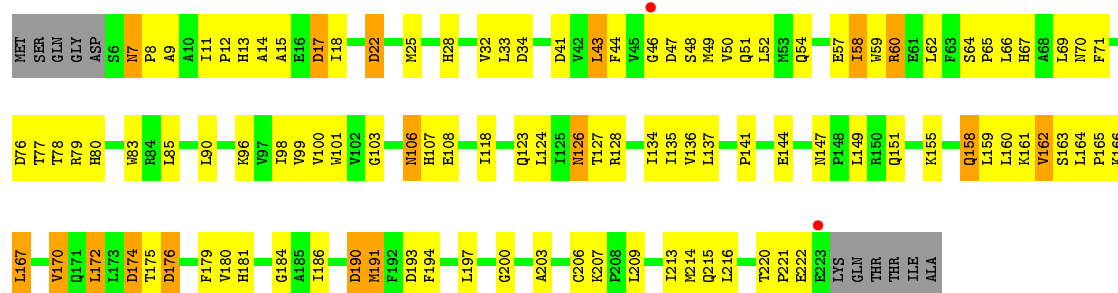




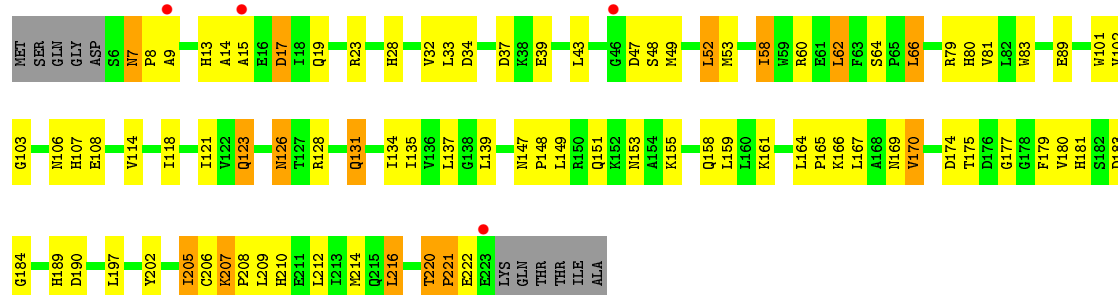
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



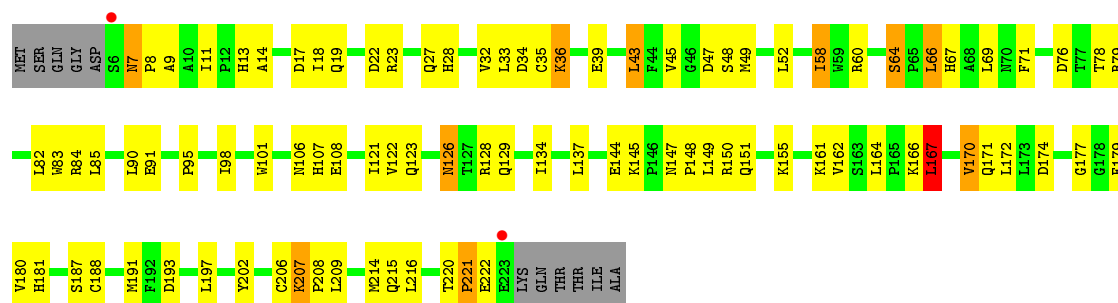
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



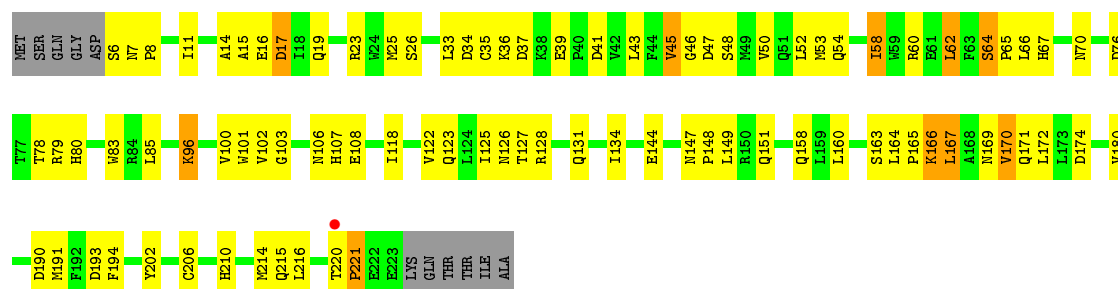
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



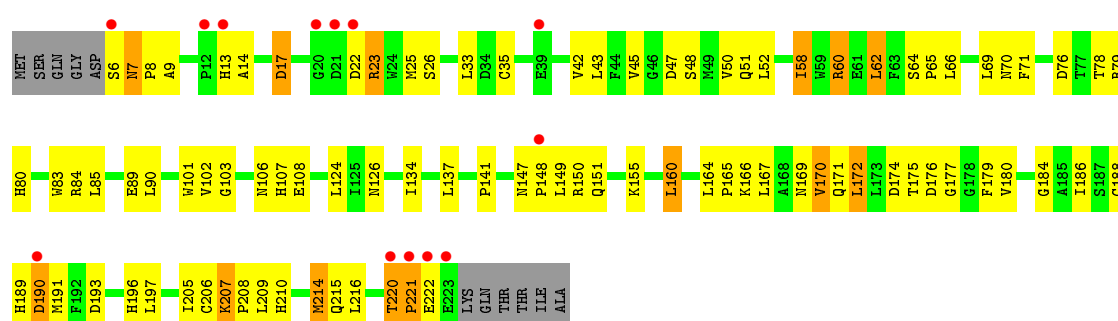
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



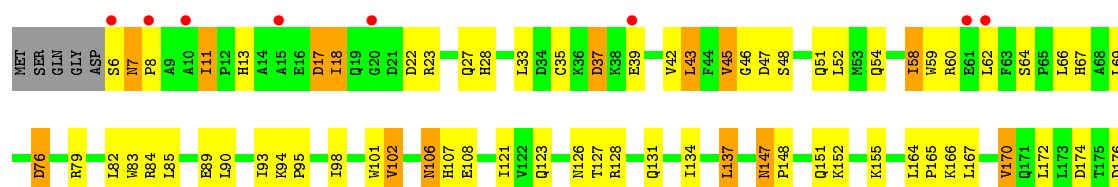
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

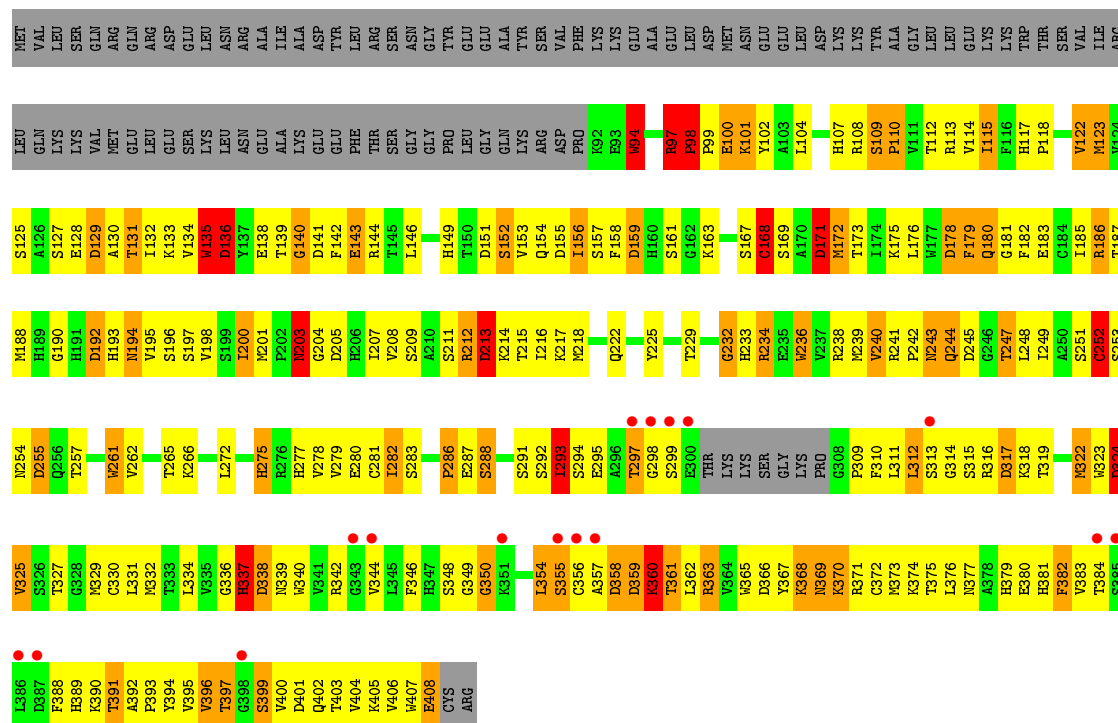
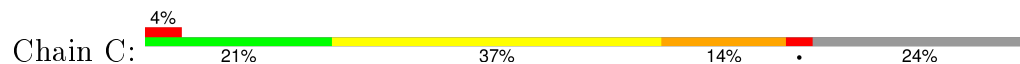


- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

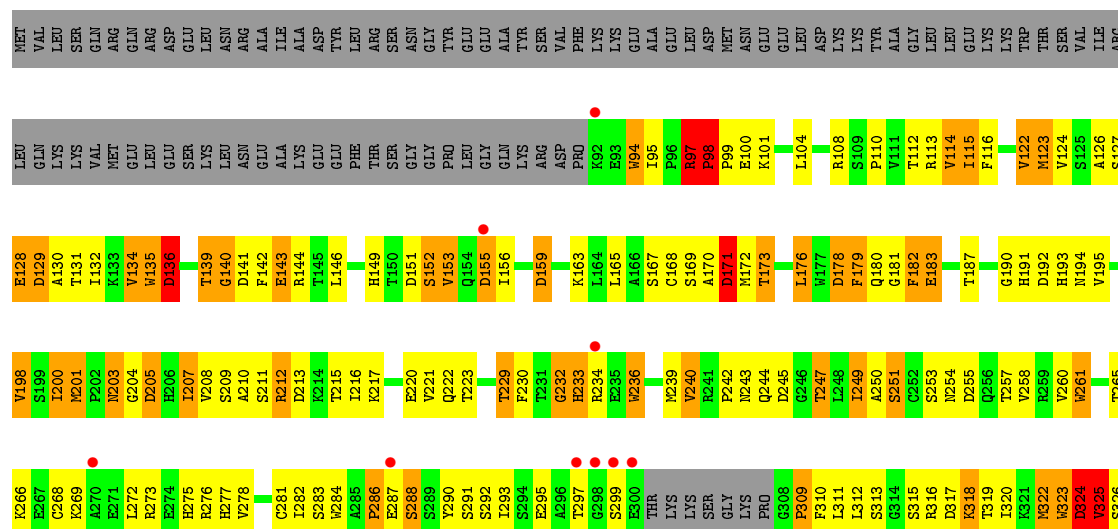
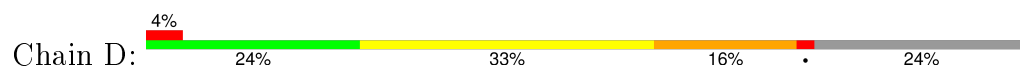


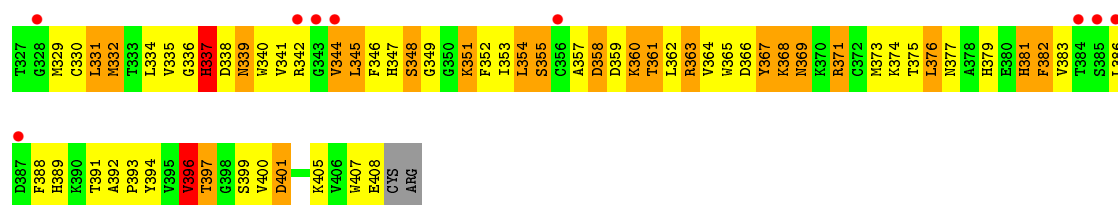


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

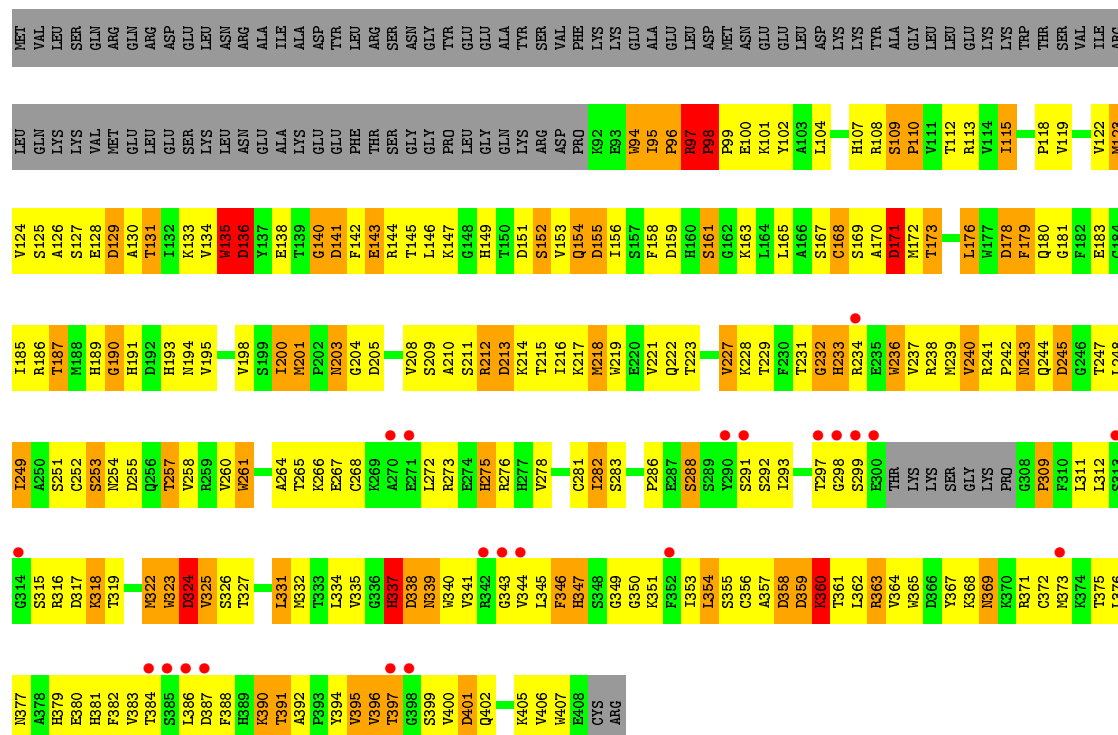
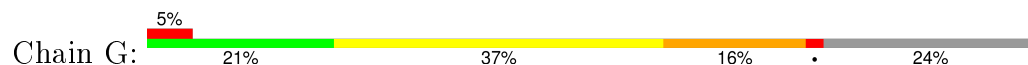


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

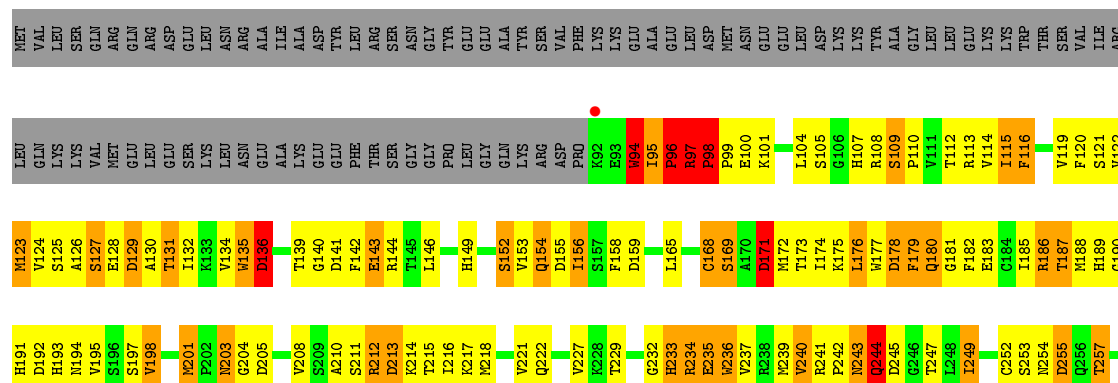
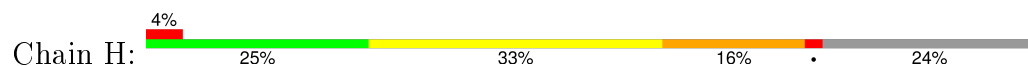


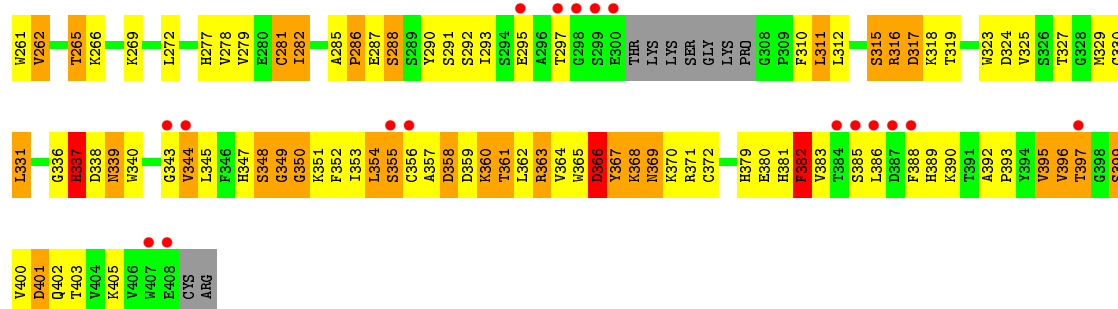


- Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

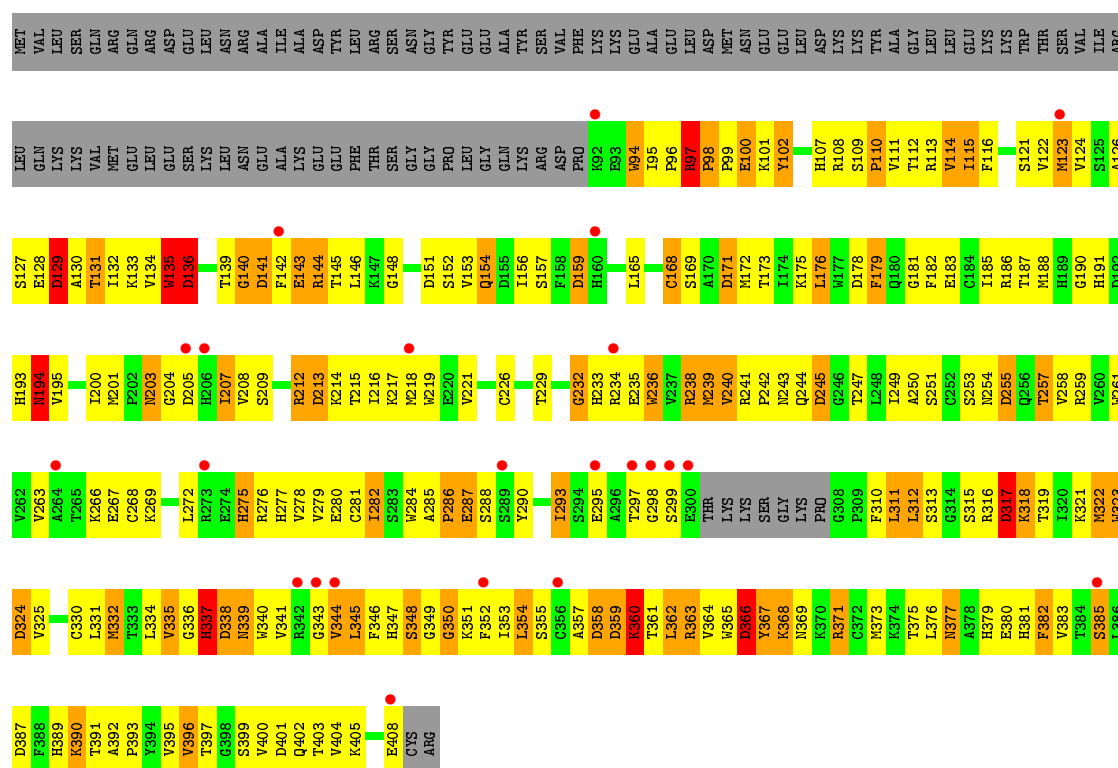
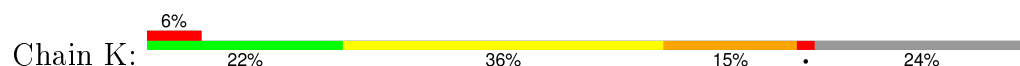


- Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

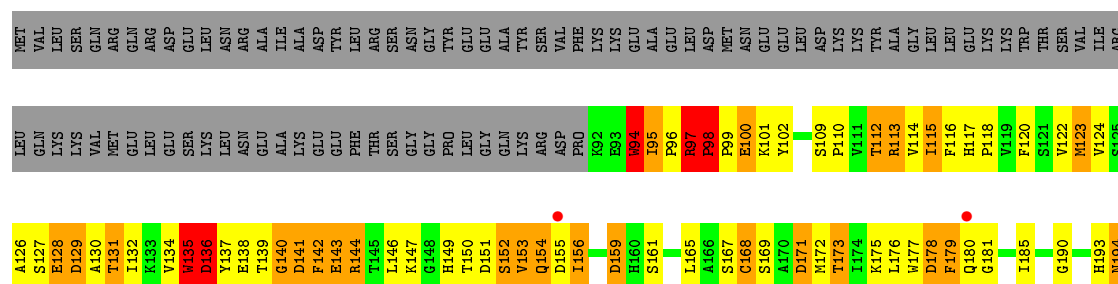
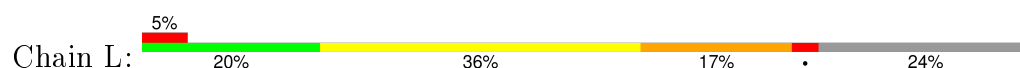


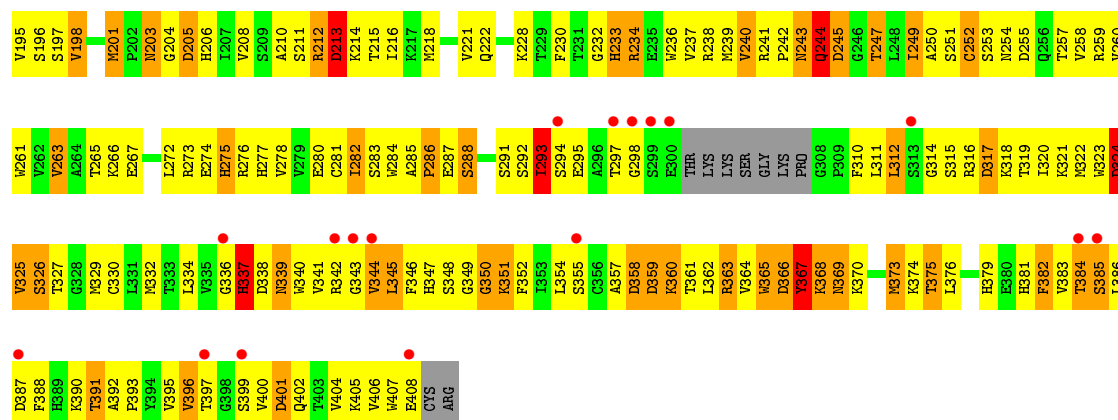


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

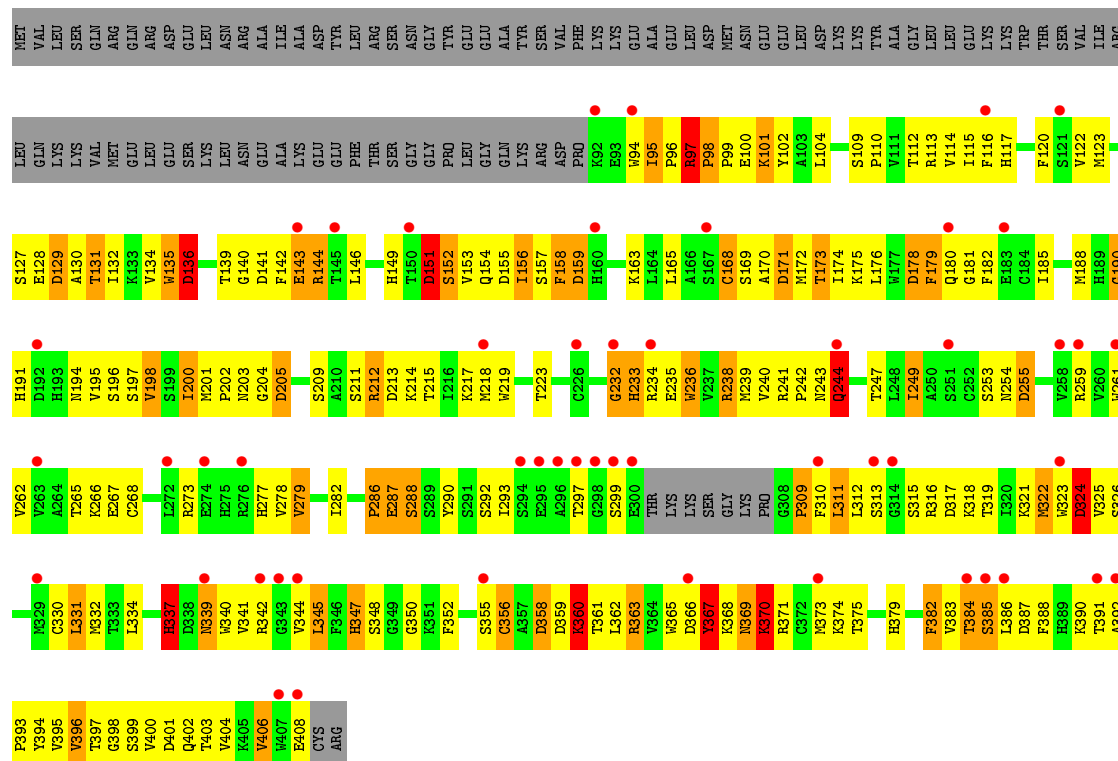
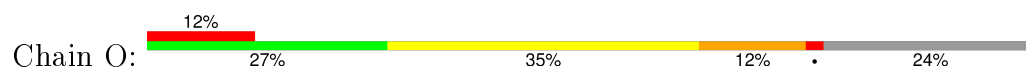


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

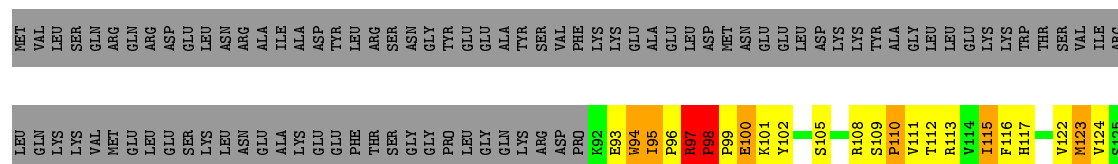
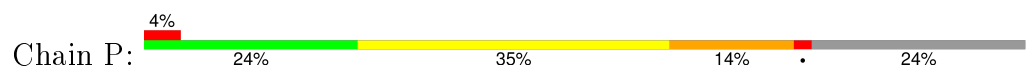


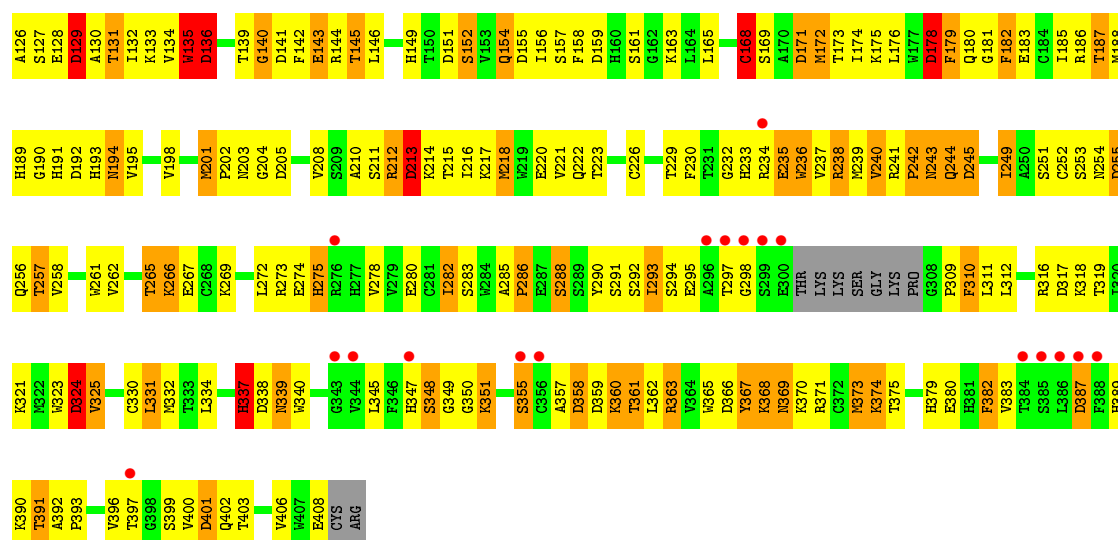


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

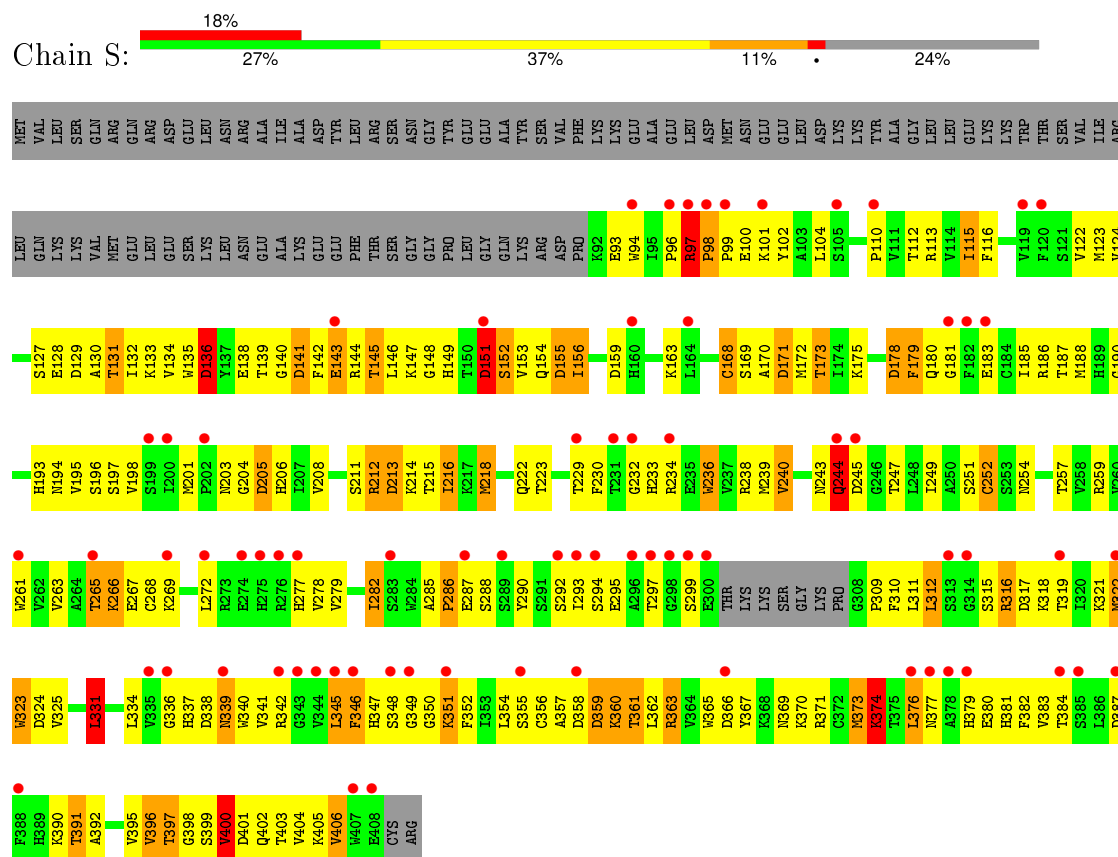


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

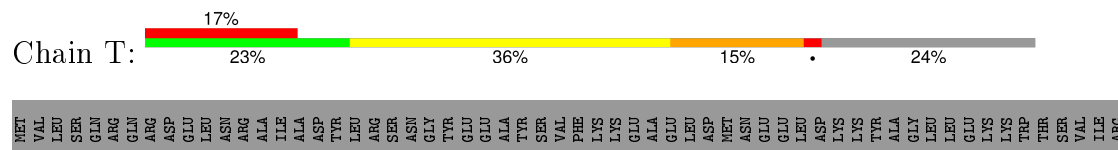


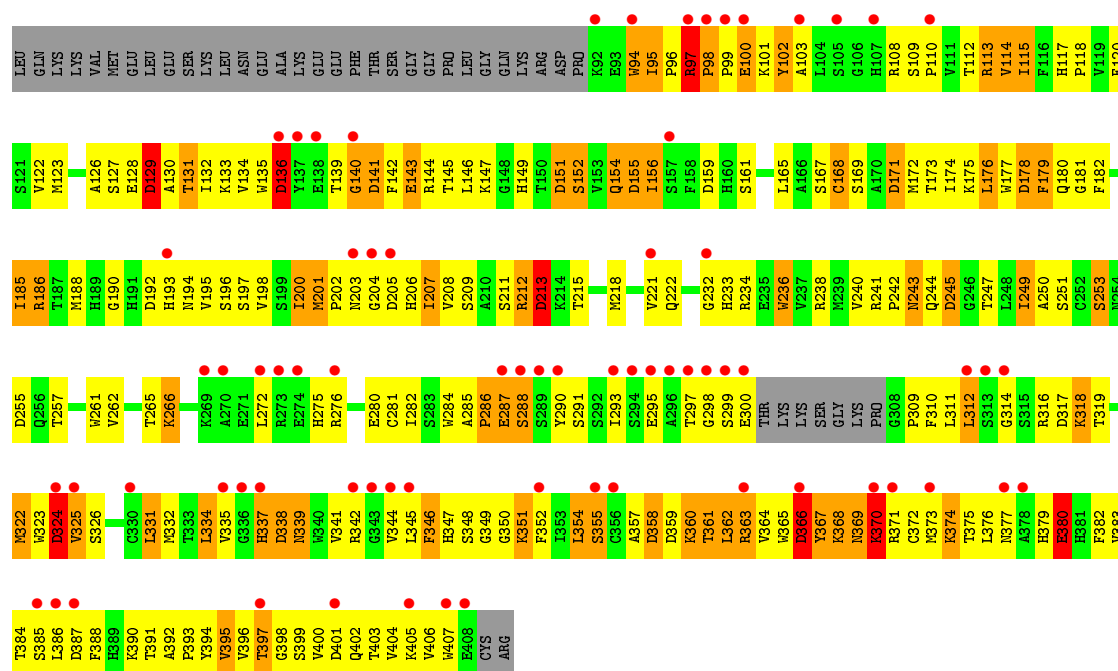


- Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT



- Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	205.77Å 101.22Å 246.13Å 90.00° 98.06° 90.00°	Depositor
Resolution (Å)	200.00 – 3.40 29.93 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (200.00-3.40) 96.4 (29.93-3.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.264 , 0.307 0.301 , 0.325	Depositor DCC
R_{free} test set	5385 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	88.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -0.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 134482 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.82	0/1742	0.94	7/2364 (0.3%)
1	B	0.63	0/1742	0.85	3/2364 (0.1%)
1	E	0.74	0/1742	0.89	6/2364 (0.3%)
1	F	0.84	0/1742	0.97	10/2364 (0.4%)
1	I	0.66	0/1742	0.89	5/2364 (0.2%)
1	J	0.62	0/1742	0.84	6/2364 (0.3%)
1	M	0.53	0/1742	0.80	5/2364 (0.2%)
1	N	0.48	0/1742	0.80	5/2364 (0.2%)
1	Q	0.45	0/1742	0.77	4/2364 (0.2%)
1	R	0.46	0/1742	0.75	6/2364 (0.3%)
2	C	0.90	2/2518 (0.1%)	1.12	17/3414 (0.5%)
2	D	0.72	0/2518	1.02	11/3414 (0.3%)
2	G	0.72	0/2518	1.02	13/3414 (0.4%)
2	H	0.87	1/2518 (0.0%)	1.12	12/3414 (0.4%)
2	K	0.58	0/2518	0.93	13/3414 (0.4%)
2	L	0.80	1/2518 (0.0%)	1.08	17/3414 (0.5%)
2	O	0.56	0/2518	0.88	10/3414 (0.3%)
2	P	0.79	1/2518 (0.0%)	1.09	18/3414 (0.5%)
2	S	0.56	0/2518	0.89	9/3414 (0.3%)
2	T	0.61	0/2518	0.95	14/3414 (0.4%)
All	All	0.69	5/42600 (0.0%)	0.95	191/57780 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	F	0	1
2	C	0	3
2	D	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	5
2	H	0	5
2	K	0	4
2	L	0	4
2	O	0	4
2	P	0	4
2	S	0	2
2	T	0	2
All	All	0	44

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	168	CYS	CB-SG	-5.86	1.72	1.81
2	C	168	CYS	CB-SG	-5.44	1.73	1.81
2	C	252	CYS	CB-SG	-5.15	1.73	1.81
2	L	365	TRP	CB-CG	-5.15	1.41	1.50
2	P	168	CYS	CB-SG	-5.13	1.73	1.81

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	171	ASP	CB-CG-OD2	9.44	126.80	118.30
2	D	358	ASP	CB-CG-OD2	8.41	125.87	118.30
1	J	174	ASP	CB-CG-OD2	8.41	125.87	118.30
2	H	136	ASP	N-CA-C	8.22	133.18	111.00
2	H	358	ASP	CB-CG-OD2	7.98	125.48	118.30
2	H	255	ASP	CB-CG-OD2	7.76	125.28	118.30
2	P	255	ASP	CB-CG-OD2	7.70	125.23	118.30
1	R	174	ASP	CB-CG-OD2	7.65	125.19	118.30
2	P	358	ASP	CB-CG-OD2	7.58	125.13	118.30
2	C	317	ASP	CB-CG-OD2	7.53	125.08	118.30
1	N	174	ASP	CB-CG-OD2	7.51	125.06	118.30
2	H	178	ASP	CB-CG-OD2	7.48	125.03	118.30
2	P	242	PRO	N-CD-CG	-7.48	91.98	103.20
2	G	324	ASP	CB-CG-OD2	7.43	124.98	118.30
2	C	136	ASP	N-CA-C	7.37	130.89	111.00
2	L	324	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	17	ASP	CB-CG-OD2	7.19	124.77	118.30
2	P	136	ASP	N-CA-C	7.10	130.17	111.00
2	G	136	ASP	N-CA-C	7.07	130.08	111.00
1	M	174	ASP	CB-CG-OD2	7.05	124.64	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	136	ASP	N-CA-C	6.94	129.75	111.00
2	C	338	ASP	CB-CG-OD2	6.92	124.53	118.30
2	D	401	ASP	CB-CG-OD2	6.86	124.47	118.30
2	D	171	ASP	CB-CG-OD2	6.85	124.47	118.30
2	H	192	ASP	CB-CG-OD2	6.79	124.41	118.30
2	L	136	ASP	N-CA-C	6.77	129.29	111.00
2	C	255	ASP	CB-CG-OD2	6.74	124.37	118.30
1	F	190	ASP	CB-CG-OD2	6.73	124.36	118.30
2	G	338	ASP	CB-CG-OD2	6.69	124.32	118.30
1	N	76	ASP	CB-CG-OD2	6.69	124.32	118.30
2	L	171	ASP	CB-CG-OD2	6.67	124.31	118.30
2	H	171	ASP	CB-CG-OD2	6.66	124.30	118.30
2	D	151	ASP	CB-CG-OD2	6.63	124.27	118.30
2	H	366	ASP	CB-CG-OD2	6.62	124.26	118.30
1	F	62	LEU	CB-CG-CD2	-6.62	99.75	111.00
2	G	171	ASP	CB-CG-OD2	6.61	124.25	118.30
1	Q	174	ASP	CB-CG-OD2	6.57	124.21	118.30
2	K	129	ASP	CB-CG-OD2	6.51	124.16	118.30
2	P	324	ASP	CB-CG-OD2	6.51	124.16	118.30
2	P	178	ASP	CB-CG-OD2	6.49	124.14	118.30
2	K	359	ASP	CB-CG-OD2	6.49	124.14	118.30
2	P	171	ASP	CB-CA-C	-6.38	97.63	110.40
2	T	324	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	34	ASP	CB-CG-OD2	6.32	123.99	118.30
2	C	358	ASP	CB-CG-OD2	6.30	123.97	118.30
2	D	205	ASP	CB-CG-OD2	6.29	123.96	118.30
2	S	136	ASP	N-CA-C	6.29	127.98	111.00
1	F	47	ASP	CB-CG-OD2	6.28	123.95	118.30
1	E	21	ASP	CB-CG-OD2	6.24	123.92	118.30
2	T	358	ASP	CB-CG-OD2	6.23	123.91	118.30
1	I	176	ASP	CB-CG-OD2	6.23	123.91	118.30
2	C	324	ASP	CB-CG-OD2	6.21	123.89	118.30
2	P	136	ASP	CB-CG-OD2	6.19	123.87	118.30
1	J	190	ASP	CB-CG-OD2	6.18	123.86	118.30
2	S	338	ASP	CB-CG-OD2	6.17	123.86	118.30
2	D	155	ASP	CB-CG-OD2	6.17	123.85	118.30
1	N	17	ASP	CB-CG-OD2	6.16	123.84	118.30
2	O	358	ASP	CB-CG-OD2	6.15	123.83	118.30
1	J	17	ASP	CB-CG-OD2	6.13	123.82	118.30
1	R	47	ASP	CB-CG-OD2	6.11	123.80	118.30
2	T	151	ASP	CB-CG-OD2	6.11	123.80	118.30
2	G	358	ASP	CB-CG-OD2	6.08	123.77	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	76	ASP	CB-CG-OD2	6.07	123.76	118.30
2	O	178	ASP	CB-CG-OD2	6.07	123.76	118.30
2	G	155	ASP	CB-CG-OD2	6.06	123.76	118.30
2	T	136	ASP	N-CA-C	6.00	127.20	111.00
2	L	213	ASP	CB-CG-OD2	6.00	123.70	118.30
2	T	387	ASP	CB-CG-OD2	6.00	123.70	118.30
2	K	338	ASP	CB-CG-OD2	5.99	123.69	118.30
2	L	401	ASP	CB-CG-OD2	5.99	123.69	118.30
2	P	338	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	192	ASP	CB-CG-OD2	5.98	123.68	118.30
1	I	22	ASP	CB-CG-OD2	5.96	123.66	118.30
2	S	387	ASP	CB-CG-OD2	5.95	123.66	118.30
2	T	338	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	176	ASP	CB-CG-OD2	5.91	123.62	118.30
1	F	76	ASP	CB-CG-OD2	5.91	123.62	118.30
1	I	17	ASP	CB-CG-OD2	5.90	123.61	118.30
2	K	136	ASP	N-CA-C	5.89	126.89	111.00
2	G	387	ASP	CB-CG-OD2	5.88	123.59	118.30
2	D	338	ASP	CB-CG-OD2	5.88	123.59	118.30
2	O	255	ASP	CB-CG-OD2	5.86	123.57	118.30
2	O	136	ASP	CB-CG-OD2	5.81	123.53	118.30
1	N	47	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	174	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	22	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	37	ASP	CB-CG-OD2	5.77	123.49	118.30
1	F	22	ASP	CB-CG-OD2	5.76	123.48	118.30
2	L	205	ASP	CB-CG-OD2	5.75	123.48	118.30
2	P	192	ASP	CB-CG-OD2	5.74	123.46	118.30
1	Q	17	ASP	CB-CG-OD2	5.72	123.45	118.30
1	J	183	ASP	CB-CG-OD2	5.72	123.45	118.30
1	M	22	ASP	CB-CG-OD2	5.72	123.44	118.30
2	L	338	ASP	CB-CG-OD2	5.71	123.44	118.30
2	O	205	ASP	CB-CG-OD2	5.71	123.44	118.30
2	C	159	ASP	CB-CG-OD2	5.71	123.43	118.30
2	H	382	PHE	N-CA-CB	5.70	120.86	110.60
2	T	401	ASP	CB-CG-OD2	5.70	123.43	118.30
2	C	178	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	17	ASP	CB-CG-OD2	5.64	123.38	118.30
2	C	401	ASP	CB-CG-OD2	5.64	123.37	118.30
2	L	358	ASP	CB-CG-OD2	5.64	123.37	118.30
2	H	338	ASP	CB-CG-OD2	5.60	123.34	118.30
2	T	141	ASP	CB-CG-OD2	5.58	123.32	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	401	ASP	CB-CG-OD2	5.58	123.32	118.30
2	T	245	ASP	CB-CG-OD2	5.58	123.32	118.30
2	P	151	ASP	CB-CG-OD2	5.57	123.32	118.30
2	L	171	ASP	CB-CA-C	-5.57	99.26	110.40
1	I	190	ASP	CB-CG-OD2	5.57	123.31	118.30
1	M	193	ASP	CB-CG-OD2	5.56	123.30	118.30
2	S	151	ASP	CB-CG-OD2	5.56	123.30	118.30
2	T	129	ASP	CB-CG-OD2	5.56	123.30	118.30
1	R	76	ASP	CB-CG-OD2	5.55	123.30	118.30
1	Q	47	ASP	CB-CG-OD2	5.53	123.28	118.30
2	G	245	ASP	CB-CG-OD2	5.53	123.27	118.30
2	P	155	ASP	CB-CG-OD2	5.52	123.27	118.30
2	L	94	TRP	N-CA-C	5.52	125.89	111.00
1	E	216	LEU	CA-CB-CG	5.51	127.97	115.30
2	L	136	ASP	CB-CG-OD2	5.48	123.24	118.30
2	L	151	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	17	ASP	CB-CG-OD2	5.48	123.23	118.30
2	K	141	ASP	CB-CG-OD2	5.46	123.22	118.30
2	G	401	ASP	CB-CG-OD2	5.45	123.21	118.30
2	P	245	ASP	CB-CG-OD2	5.44	123.20	118.30
2	S	155	ASP	CB-CG-OD2	5.44	123.20	118.30
2	G	146	LEU	CA-CB-CG	5.44	127.81	115.30
2	S	136	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	174	ASP	CB-CG-OD2	5.39	123.15	118.30
2	K	255	ASP	CB-CG-OD2	5.38	123.15	118.30
2	K	366	ASP	CB-CG-OD2	5.38	123.14	118.30
2	O	324	ASP	CB-CG-OD2	5.37	123.14	118.30
2	T	155	ASP	CB-CG-OD2	5.33	123.10	118.30
2	H	98	PRO	N-CA-C	5.33	125.95	112.10
2	C	98	PRO	N-CA-C	5.32	125.94	112.10
2	S	141	ASP	CB-CG-OD2	5.32	123.08	118.30
2	C	94	TRP	N-CA-C	5.31	125.34	111.00
2	D	324	ASP	CB-CG-OD2	5.31	123.08	118.30
2	S	245	ASP	CB-CG-OD2	5.30	123.07	118.30
2	L	141	ASP	CB-CG-OD2	5.30	123.07	118.30
2	K	387	ASP	CB-CG-OD2	5.29	123.06	118.30
2	L	98	PRO	N-CA-C	5.29	125.84	112.10
2	L	387	ASP	CB-CG-OD2	5.26	123.04	118.30
2	C	192	ASP	CB-CG-OD2	5.26	123.03	118.30
1	I	174	ASP	CB-CG-OD2	5.25	123.03	118.30
2	O	136	ASP	N-CA-C	5.25	125.18	111.00
1	E	174	ASP	CB-CG-OD2	5.25	123.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	214	MET	CG-SD-CE	5.25	108.60	100.20
1	Q	190	ASP	CB-CG-OD2	5.25	123.02	118.30
2	H	401	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	102	VAL	CB-CA-C	-5.24	101.44	111.40
2	C	151	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	176	ASP	CB-CG-OD2	5.22	123.00	118.30
2	K	151	ASP	CB-CG-OD2	5.22	123.00	118.30
2	H	94	TRP	N-CA-C	5.22	125.09	111.00
1	N	190	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	359	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	176	ASP	N-CA-C	5.21	125.07	111.00
2	G	141	ASP	CB-CG-OD2	5.21	122.99	118.30
1	R	37	ASP	CB-CG-OD2	5.21	122.99	118.30
1	J	34	ASP	CB-CG-OD2	5.21	122.98	118.30
2	G	359	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	22	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	98	PRO	N-CA-C	5.18	125.58	112.10
1	M	34	ASP	CB-CG-OD2	5.17	122.95	118.30
1	F	158	GLN	CB-CA-C	-5.17	100.07	110.40
2	G	98	PRO	N-CA-C	5.17	125.53	112.10
2	P	366	ASP	CB-CG-OD2	5.16	122.95	118.30
2	K	213	ASP	CB-CG-OD2	5.15	122.94	118.30
2	K	317	ASP	CB-CG-OD2	5.15	122.93	118.30
1	F	170	VAL	CB-CA-C	-5.13	101.66	111.40
2	C	213	ASP	CB-CA-C	-5.12	100.17	110.40
1	E	47	ASP	CB-CG-OD2	5.12	122.90	118.30
2	T	366	ASP	CB-CG-OD2	5.11	122.90	118.30
2	P	98	PRO	N-CA-C	5.11	125.38	112.10
1	A	76	ASP	CB-CG-OD2	5.11	122.89	118.30
2	P	387	ASP	CB-CG-OD2	5.10	122.89	118.30
2	K	358	ASP	CB-CG-OD2	5.09	122.88	118.30
2	T	213	ASP	CB-CG-OD2	5.09	122.88	118.30
2	C	376	LEU	CA-CB-CG	5.08	126.97	115.30
2	O	159	ASP	CB-CG-OD2	5.07	122.87	118.30
2	L	366	ASP	CB-CG-OD2	5.07	122.86	118.30
2	T	192	ASP	CB-CG-OD2	5.07	122.86	118.30
2	P	129	ASP	CB-CG-OD2	5.06	122.86	118.30
2	O	151	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	172	LEU	CB-CG-CD2	-5.04	102.43	111.00
2	S	205	ASP	CB-CG-OD2	5.04	122.84	118.30
2	O	387	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	47	ASP	CB-CG-OD2	5.03	122.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	142	PHE	CB-CA-C	-5.03	100.34	110.40
2	K	324	ASP	CB-CG-OD2	5.01	122.81	118.30
1	R	22	ASP	CB-CG-OD2	5.00	122.81	118.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	THR	Peptide
2	C	135	TRP	Peptide
2	C	337	HIS	Peptide
2	C	97	ARG	Peptide
2	D	135	TRP	Peptide
2	D	323	TRP	Peptide
2	D	335	VAL	Peptide
2	D	337	HIS	Peptide
2	D	367	TYR	Peptide
2	D	396	VAL	Peptide
2	D	97	ARG	Peptide
1	E	175	THR	Peptide
1	E	6	SER	Mainchain
1	F	175	THR	Peptide
2	G	135	TRP	Peptide
2	G	335	VAL	Peptide
2	G	337	HIS	Peptide
2	G	96	PRO	Peptide
2	G	97	ARG	Peptide
2	H	135	TRP	Peptide
2	H	316	ARG	Peptide
2	H	337	HIS	Peptide
2	H	96	PRO	Peptide
2	H	97	ARG	Peptide
2	K	135	TRP	Peptide
2	K	337	HIS	Peptide
2	K	367	TYR	Peptide
2	K	97	ARG	Peptide
2	L	135	TRP	Peptide
2	L	337	HIS	Peptide
2	L	367	TYR	Peptide
2	L	97	ARG	Peptide
2	O	135	TRP	Peptide
2	O	337	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	O	367	TYR	Peptide
2	O	97	ARG	Peptide
2	P	135	TRP	Peptide
2	P	182	PHE	Peptide
2	P	337	HIS	Peptide
2	P	97	ARG	Peptide
2	S	135	TRP	Peptide
2	S	97	ARG	Peptide
2	T	135	TRP	Peptide
2	T	97	ARG	Peptide

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	1705	0	1701	69	0
1	B	1705	0	1701	64	0
1	E	1705	0	1701	59	0
1	F	1705	0	1701	67	0
1	I	1705	0	1701	63	1
1	J	1705	0	1701	56	0
1	M	1705	0	1701	49	0
1	N	1705	0	1701	40	0
1	Q	1705	0	1701	53	0
1	R	1705	0	1701	31	0
2	C	2454	0	2371	212	0
2	D	2454	0	2371	184	0
2	G	2454	0	2371	204	0
2	H	2454	0	2371	207	0
2	K	2454	0	2371	182	0
2	L	2454	0	2371	227	0
2	O	2454	0	2371	149	0
2	P	2454	0	2371	204	0
2	S	2454	0	2371	138	0
2	T	2454	0	2371	162	1
All	All	41590	0	40720	2361	1

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 29.

All (2361) 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)
2:L:312:LEU:HD21	2:L:346:PHE:CE1	1.64	1.32
2:K:315:SER:OG	2:K:317:ASP:HB2	1.21	1.27
2:L:312:LEU:CD2	2:L:346:PHE:HE1	1.51	1.24
2:L:239:MET:HE3	2:L:241:ARG:HH21	1.05	1.19
2:D:168:CYS:SG	2:D:198:VAL:HB	1.85	1.16
2:T:332:MET:SD	2:T:367:TYR:HB2	1.87	1.15
2:T:159:ASP:HA	2:T:200:ILE:HG21	1.28	1.14
2:P:297:THR:HG22	2:P:298:GLY:H	1.04	1.13
2:S:310:PHE:CE2	2:S:324:ASP:HB3	1.83	1.13
2:P:310:PHE:CD2	2:P:324:ASP:HB2	1.85	1.12
2:P:129:ASP:HB3	2:P:131:THR:OG1	1.50	1.11
2:C:97:ARG:HG3	2:C:98:PRO:HD3	1.20	1.10
2:C:129:ASP:HB3	2:C:131:THR:OG1	1.51	1.10
2:H:115:ILE:HD12	2:H:156:ILE:HG22	1.34	1.09
2:D:339:ASN:ND2	2:D:340:TRP:H	1.49	1.09
2:D:260:VAL:HG21	2:D:325:VAL:HG12	1.34	1.09
2:K:336:GLY:HA2	2:K:365:TRP:HH2	1.12	1.09
2:C:379:HIS:NE2	2:C:397:THR:HG22	1.66	1.09
2:K:336:GLY:HA2	2:K:365:TRP:CH2	1.88	1.08
2:L:239:MET:CE	2:L:241:ARG:HH21	1.63	1.08
2:C:379:HIS:NE2	2:C:397:THR:CG2	2.17	1.07
2:T:311:LEU:HD23	2:T:323:TRP:HB2	1.32	1.07
2:H:366:ASP:OD1	2:H:368:LYS:HB3	1.53	1.07
2:H:211:SER:HB3	2:H:213:ASP:HB2	1.36	1.07
2:T:310:PHE:CE2	2:T:324:ASP:HB2	1.88	1.07
2:P:310:PHE:HD2	2:P:324:ASP:HB2	1.13	1.06
2:P:211:SER:HB3	2:P:213:ASP:HB2	1.32	1.06
2:G:129:ASP:HB3	2:G:131:THR:OG1	1.57	1.05
2:C:115:ILE:HD12	2:C:156:ILE:HG22	1.38	1.04
2:C:193:HIS:CD2	2:C:194:ASN:H	1.75	1.04
2:H:186:ARG:HH11	2:H:186:ARG:HG2	1.18	1.04
2:C:144:ARG:NH1	2:C:181:GLY:O	1.90	1.03
2:T:288:SER:HB2	2:T:350:GLY:HA3	1.38	1.03
2:L:366:ASP:OD1	2:L:368:LYS:HB3	1.58	1.03
2:H:178:ASP:HB2	2:H:185:ILE:HD11	1.41	1.02
1:A:8:PRO:O	1:A:79:ARG:HD3	1.60	1.01
2:S:366:ASP:HB2	2:S:373:MET:HG2	1.42	1.01
1:B:107:HIS:O	1:B:108:GLU:HB2	1.56	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:ASN:HD22	2:D:340:TRP:N	1.56	1.00
2:P:191:HIS:CE1	2:P:217:LYS:HG3	1.97	1.00
2:H:339:ASN:HD22	2:H:340:TRP:N	1.59	1.00
2:C:359:ASP:O	2:C:361:THR:HB	1.60	1.00
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.24	1.00
2:C:127:SER:OG	2:C:129:ASP:HB2	1.62	0.99
2:D:260:VAL:HG21	2:D:325:VAL:CG1	1.92	0.99
1:F:36:LYS:HE2	1:F:37:ASP:OD2	1.63	0.98
2:G:360:LYS:HD3	2:G:379:HIS:O	1.63	0.98
2:T:94:TRP:HH2	2:T:391:THR:O	1.48	0.97
1:F:107:HIS:O	1:F:108:GLU:HB2	1.62	0.97
2:S:359:ASP:O	2:S:361:THR:N	1.98	0.97
2:C:171:ASP:O	2:C:172:MET:HG3	1.63	0.97
2:H:339:ASN:ND2	2:H:340:TRP:H	1.60	0.97
1:F:67:HIS:HE1	2:H:339:ASN:HD21	1.12	0.96
1:A:11:ILE:O	1:A:79:ARG:HD2	1.63	0.96
1:I:107:HIS:O	1:I:108:GLU:HB2	1.61	0.96
2:H:379:HIS:NE2	2:H:397:THR:CG2	2.28	0.96
2:C:98:PRO:HB3	2:C:99:PRO:HD2	1.48	0.95
2:L:144:ARG:NH2	2:L:181:GLY:HA2	1.81	0.95
2:H:168:CYS:SG	2:H:198:VAL:HB	2.06	0.95
2:K:310:PHE:CE2	2:K:324:ASP:HB3	2.00	0.95
2:L:317:ASP:HB3	2:L:319:THR:OG1	1.65	0.95
2:D:115:ILE:HD12	2:D:156:ILE:HG22	1.49	0.95
2:D:129:ASP:HB3	2:D:131:THR:OG1	1.66	0.95
2:P:297:THR:CG2	2:P:298:GLY:H	1.81	0.94
2:P:112:THR:HG21	2:P:154:GLN:HA	1.49	0.94
2:L:312:LEU:HD21	2:L:346:PHE:HE1	0.79	0.94
2:H:126:ALA:HB2	2:H:156:ILE:HD12	1.50	0.94
2:C:275:HIS:ND1	2:C:317:ASP:OD2	2.01	0.94
1:M:181:HIS:CE1	2:P:108:ARG:HE	1.86	0.94
1:M:85:LEU:HD22	1:M:90:LEU:HD11	1.49	0.93
2:L:359:ASP:O	2:L:361:THR:N	2.00	0.93
2:K:315:SER:HG	2:K:317:ASP:HB2	1.34	0.93
2:P:201:MET:HE1	2:P:242:PRO:HB3	1.51	0.92
2:P:98:PRO:HB3	2:P:99:PRO:HD2	1.51	0.92
2:T:312:LEU:HB2	2:T:344:VAL:HG11	1.52	0.92
2:O:310:PHE:CE2	2:O:324:ASP:HB3	2.05	0.91
2:P:297:THR:HG22	2:P:298:GLY:N	1.86	0.91
2:G:359:ASP:OD1	2:G:361:THR:HB	1.69	0.91
2:T:392:ALA:HB1	2:T:393:PRO:CD	2.00	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:107:HIS:O	1:J:108:GLU:HB2	1.70	0.91
2:C:193:HIS:HD2	2:C:194:ASN:H	1.00	0.91
2:L:358:ASP:HA	2:L:382:PHE:HB3	1.52	0.91
2:C:97:ARG:HG3	2:C:98:PRO:CD	2.02	0.90
2:H:97:ARG:HG3	2:H:98:PRO:HD3	1.51	0.90
2:O:337:HIS:HE1	2:O:375:THR:HG23	1.34	0.90
2:L:351:LYS:HB2	2:L:352:PHE:CD1	2.06	0.90
2:G:159:ASP:HA	2:G:200:ILE:HG21	1.51	0.90
2:S:249:ILE:HG22	2:S:261:TRP:HB2	1.53	0.90
2:L:355:SER:O	2:L:362:LEU:HD12	1.71	0.90
1:R:107:HIS:O	1:R:108:GLU:HB2	1.72	0.90
1:Q:101:TRP:CE3	1:Q:137:LEU:HD12	2.08	0.89
2:K:126:ALA:HB2	2:K:156:ILE:HD12	1.55	0.89
2:H:358:ASP:HA	2:H:382:PHE:HB3	1.54	0.89
2:C:252:CYS:HB2	2:C:282:ILE:HD11	1.55	0.89
2:L:340:TRP:O	2:L:357:ALA:HB1	1.71	0.88
2:L:129:ASP:HB3	2:L:131:THR:OG1	1.72	0.88
2:L:312:LEU:HD23	2:L:312:LEU:H	1.36	0.88
1:J:39:GLU:OE2	2:L:238:ARG:NH2	2.05	0.88
2:T:310:PHE:CE2	2:T:324:ASP:CB	2.56	0.88
2:L:312:LEU:HD23	2:L:312:LEU:N	1.86	0.88
2:P:201:MET:CE	2:P:242:PRO:HB3	2.04	0.88
2:D:317:ASP:HB2	2:D:319:THR:OG1	1.74	0.88
2:H:347:HIS:HD2	2:H:349:GLY:H	1.17	0.87
2:K:323:TRP:HA	2:K:331:LEU:HG	1.57	0.87
2:L:239:MET:HE3	2:L:241:ARG:NH2	1.87	0.87
2:D:159:ASP:HA	2:D:200:ILE:HG21	1.56	0.87
1:Q:107:HIS:O	1:Q:108:GLU:HB2	1.73	0.87
2:D:254:ASN:HA	2:D:278:VAL:HG13	1.55	0.87
2:C:374:LYS:HG3	2:C:375:THR:H	1.37	0.86
2:H:399:SER:HB2	2:H:401:ASP:OD1	1.75	0.86
2:O:337:HIS:CE1	2:O:361:THR:HG21	2.10	0.86
2:L:379:HIS:NE2	2:L:397:THR:HG23	1.89	0.86
2:H:278:VAL:HB	2:H:316:ARG:HD2	1.57	0.86
2:T:309:PRO:HG2	2:T:325:VAL:HG23	1.56	0.86
2:C:254:ASN:HA	2:C:278:VAL:HG13	1.58	0.86
2:H:186:ARG:HH11	2:H:186:ARG:CG	1.87	0.85
2:S:382:PHE:O	2:S:399:SER:HB2	1.76	0.85
2:C:379:HIS:HE1	2:C:405:LYS:HG3	1.40	0.85
2:H:129:ASP:HB3	2:H:131:THR:OG1	1.76	0.85
2:C:159:ASP:HA	2:C:200:ILE:HG21	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:THR:HG23	1:E:80:HIS:CE1	2.12	0.85
2:T:168:CYS:SG	2:T:198:VAL:HB	2.16	0.84
2:G:350:GLY:O	2:G:367:TYR:OH	1.93	0.84
2:D:339:ASN:HD22	2:D:340:TRP:H	0.86	0.84
1:M:78:THR:H	1:M:106:ASN:HD21	1.24	0.84
2:C:144:ARG:NH2	2:C:181:GLY:HA2	1.92	0.84
2:C:112:THR:HG21	2:C:154:GLN:HA	1.59	0.84
2:T:392:ALA:HB1	2:T:393:PRO:HD3	1.59	0.84
2:D:98:PRO:HB3	2:D:99:PRO:HD2	1.59	0.84
2:C:374:LYS:HG3	2:C:375:THR:N	1.92	0.84
1:E:84:ARG:HD2	1:E:89:GLU:OE2	1.78	0.84
2:O:337:HIS:H	2:O:337:HIS:CD2	1.94	0.83
2:H:112:THR:HG21	2:H:154:GLN:HA	1.60	0.83
2:L:193:HIS:HD2	2:L:194:ASN:H	1.24	0.83
2:H:350:GLY:O	2:H:367:TYR:OH	1.95	0.83
2:K:173:THR:HG23	2:K:187:THR:HG23	1.60	0.83
1:I:118:ILE:HD13	1:I:160:LEU:HD11	1.60	0.83
2:P:133:LYS:HG2	2:P:145:THR:HG23	1.61	0.83
2:O:392:ALA:HB1	2:O:393:PRO:CD	2.09	0.83
2:T:178:ASP:HB2	2:T:185:ILE:HD11	1.61	0.82
2:C:379:HIS:CE1	2:C:405:LYS:HG3	2.14	0.82
2:G:388:PHE:HD1	2:G:395:VAL:HG13	1.43	0.82
2:T:369:ASN:HB2	2:T:371:ARG:NH2	1.93	0.82
2:T:383:VAL:HA	2:T:399:SER:HB3	1.61	0.82
2:C:178:ASP:HB2	2:C:185:ILE:HD11	1.60	0.82
2:G:399:SER:OG	2:G:401:ASP:OD1	1.95	0.82
2:L:193:HIS:CD2	2:L:194:ASN:H	1.97	0.82
2:L:239:MET:HE2	2:L:241:ARG:HE	1.42	0.82
2:D:340:TRP:O	2:D:357:ALA:HB1	1.80	0.82
2:C:152:SER:O	2:C:169:SER:HB2	1.80	0.82
2:D:236:TRP:O	2:D:253:SER:HB2	1.80	0.82
2:L:94:TRP:HH2	2:L:391:THR:O	1.61	0.82
2:L:359:ASP:OD1	2:L:361:THR:HB	1.78	0.82
2:H:114:VAL:HG11	2:H:396:VAL:HB	1.60	0.81
2:T:288:SER:HB2	2:T:350:GLY:CA	2.10	0.81
2:G:332:MET:SD	2:G:367:TYR:HB2	2.20	0.81
2:P:156:ILE:CG2	2:P:165:LEU:HD11	2.10	0.81
2:H:255:ASP:OD2	2:H:257:THR:HB	1.80	0.81
2:C:359:ASP:O	2:C:361:THR:N	2.14	0.81
2:G:379:HIS:NE2	2:G:397:THR:HG23	1.96	0.81
2:P:334:LEU:HB3	2:P:365:TRP:CZ3	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:ILE:HG22	2:L:124:VAL:HB	1.63	0.81
2:D:359:ASP:O	2:D:361:THR:N	2.13	0.81
2:P:149:HIS:CE1	2:P:175:LYS:HG3	2.16	0.81
2:S:366:ASP:HB2	2:S:373:MET:CG	2.09	0.81
2:O:112:THR:HG21	2:O:154:GLN:HA	1.63	0.81
2:S:337:HIS:HB2	2:S:363:ARG:NE	1.96	0.81
1:I:15:ALA:HB2	1:I:80:HIS:CD2	2.15	0.81
2:C:203:ASN:O	2:C:205:ASP:N	2.13	0.80
2:S:383:VAL:HA	2:S:399:SER:HB3	1.63	0.80
2:C:334:LEU:HB3	2:C:365:TRP:CZ3	2.16	0.80
2:P:211:SER:CB	2:P:213:ASP:HB2	2.11	0.80
2:H:96:PRO:HD2	2:H:97:ARG:HG2	1.62	0.80
2:S:278:VAL:HB	2:S:316:ARG:HG3	1.61	0.80
2:L:310:PHE:CE2	2:L:324:ASP:HB2	2.17	0.80
2:H:254:ASN:HA	2:H:278:VAL:HG13	1.63	0.80
2:G:340:TRP:O	2:G:357:ALA:HB1	1.82	0.80
2:L:343:GLY:O	2:L:344:VAL:HG23	1.83	0.80
1:F:207:LYS:HB3	1:F:208:PRO:CD	2.11	0.79
2:H:149:HIS:CE1	2:H:175:LYS:HG3	2.17	0.79
2:H:379:HIS:HD2	2:H:383:VAL:HG22	1.47	0.79
2:H:347:HIS:CD2	2:H:349:GLY:H	2.00	0.79
2:K:312:LEU:HD21	2:K:322:MET:HG2	1.65	0.79
2:T:361:THR:HG22	2:T:363:ARG:HG2	1.64	0.79
2:C:312:LEU:HD21	2:C:346:PHE:CE1	2.17	0.79
2:C:115:ILE:CD1	2:C:156:ILE:HG22	2.13	0.78
1:B:181:HIS:CE1	2:C:108:ARG:HE	2.01	0.78
2:O:213:ASP:HB3	2:O:215:THR:HB	1.66	0.78
1:A:137:LEU:HD21	1:A:209:LEU:HD13	1.66	0.78
2:P:337:HIS:H	2:P:337:HIS:CD2	2.01	0.78
2:H:94:TRP:CH2	2:H:392:ALA:C	2.56	0.78
2:H:115:ILE:HD12	2:H:156:ILE:CG2	2.12	0.78
1:E:84:ARG:HB3	1:E:89:GLU:OE2	1.84	0.78
2:H:337:HIS:H	2:H:337:HIS:CD2	1.99	0.77
2:O:337:HIS:H	2:O:337:HIS:HD2	1.28	0.77
2:C:383:VAL:HA	2:C:399:SER:HB2	1.66	0.77
2:G:282:ILE:CG2	2:G:311:LEU:HD12	2.14	0.77
2:O:382:PHE:O	2:O:399:SER:HB2	1.84	0.77
2:G:98:PRO:HB3	2:G:99:PRO:HD2	1.65	0.77
2:P:144:ARG:NH2	2:P:181:GLY:HA2	1.99	0.77
2:K:249:ILE:HG22	2:K:261:TRP:HB2	1.65	0.77
2:H:178:ASP:OD1	2:H:180:GLN:HB2	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:ASP:HB3	2:C:319:THR:OG1	1.85	0.77
2:C:171:ASP:O	2:C:172:MET:CG	2.32	0.77
1:F:189:HIS:HD2	2:G:402:GLN:HE22	1.32	0.77
2:S:149:HIS:CE1	2:S:175:LYS:HG3	2.20	0.77
2:L:332:MET:SD	2:L:367:TYR:HB2	2.25	0.77
1:Q:137:LEU:HD21	1:Q:209:LEU:HD13	1.67	0.77
1:F:140:LEU:HB3	1:F:141:PRO:HD2	1.67	0.77
2:D:203:ASN:O	2:D:205:ASP:N	2.18	0.77
2:P:178:ASP:OD1	2:P:180:GLN:HB2	1.84	0.77
1:A:107:HIS:O	1:A:108:GLU:HB2	1.84	0.77
2:H:97:ARG:CG	2:H:98:PRO:HD3	2.14	0.76
2:O:132:ILE:HG12	2:O:156:ILE:HD11	1.66	0.76
2:O:249:ILE:HG22	2:O:261:TRP:HB2	1.66	0.76
2:O:392:ALA:HB1	2:O:393:PRO:HD3	1.67	0.76
1:Q:60:ARG:HA	1:Q:64:SER:OG	1.86	0.76
2:D:250:ALA:HB2	2:D:284:TRP:CZ2	2.21	0.76
2:L:382:PHE:O	2:L:399:SER:HB2	1.85	0.76
2:G:210:ALA:HB2	2:G:240:VAL:HG22	1.67	0.76
2:D:324:ASP:OD1	2:D:331:LEU:HD11	1.84	0.76
2:T:94:TRP:CH2	2:T:391:THR:O	2.36	0.76
2:K:126:ALA:HB2	2:K:156:ILE:CD1	2.14	0.76
2:L:272:LEU:HB3	2:L:323:TRP:CZ3	2.20	0.76
2:S:112:THR:HG21	2:S:154:GLN:HA	1.65	0.76
2:G:337:HIS:HE1	2:G:375:THR:OG1	1.67	0.76
2:H:379:HIS:CD2	2:H:383:VAL:HG22	2.20	0.76
2:P:379:HIS:NE2	2:P:397:THR:HG22	2.01	0.76
2:L:98:PRO:HB3	2:L:99:PRO:HD2	1.65	0.76
2:P:359:ASP:O	2:P:361:THR:N	2.19	0.75
2:P:144:ARG:NH1	2:P:181:GLY:O	2.19	0.75
2:O:127:SER:OG	2:O:129:ASP:HB2	1.86	0.75
2:O:383:VAL:HA	2:O:399:SER:HB3	1.69	0.75
2:S:396:VAL:HG13	2:S:406:VAL:HG13	1.66	0.75
1:A:118:ILE:HD12	1:A:160:LEU:HD11	1.67	0.75
1:E:78:THR:HG23	1:E:106:ASN:HD21	1.50	0.75
2:H:272:LEU:HB3	2:H:323:TRP:CZ3	2.22	0.75
2:P:233:HIS:CD2	2:P:253:SER:OG	2.40	0.75
2:L:392:ALA:HB1	2:L:393:PRO:HD2	1.69	0.75
1:A:81:VAL:HG21	1:A:102:VAL:HG11	1.66	0.75
2:D:311:LEU:O	2:D:323:TRP:HD1	1.69	0.75
2:T:354:LEU:HD22	2:T:364:VAL:HG22	1.69	0.75
1:M:107:HIS:O	1:M:108:GLU:HB2	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:379:HIS:NE2	2:H:397:THR:HG23	2.02	0.74
2:T:127:SER:OG	2:T:129:ASP:HB2	1.87	0.74
2:S:337:HIS:HB2	2:S:363:ARG:HE	1.49	0.74
2:C:337:HIS:CD2	2:C:337:HIS:H	2.05	0.74
2:T:395:VAL:HG23	2:T:407:TRP:HB2	1.68	0.74
2:L:127:SER:OG	2:L:129:ASP:HB2	1.87	0.74
1:I:14:ALA:HB2	1:I:83:TRP:CE2	2.23	0.74
2:L:239:MET:CE	2:L:241:ARG:NH2	2.46	0.74
2:H:98:PRO:HB3	2:H:99:PRO:CD	2.16	0.74
2:D:134:VAL:O	2:D:143:GLU:HB2	1.86	0.74
1:B:189:HIS:HD2	2:C:402:GLN:HE22	1.35	0.74
2:L:312:LEU:CD2	2:L:346:PHE:CE1	2.44	0.74
2:T:249:ILE:HG22	2:T:261:TRP:HB2	1.67	0.74
2:T:112:THR:HG21	2:T:154:GLN:HA	1.69	0.74
2:K:112:THR:HG21	2:K:154:GLN:HA	1.68	0.74
2:L:213:ASP:HB3	2:L:215:THR:OG1	1.86	0.74
2:P:156:ILE:HG23	2:P:165:LEU:HD11	1.69	0.74
1:F:158:GLN:HE21	1:F:158:GLN:CA	2.00	0.74
2:G:203:ASN:O	2:G:205:ASP:N	2.20	0.74
2:C:127:SER:HG	2:C:129:ASP:HB2	1.51	0.74
2:K:282:ILE:HA	2:K:312:LEU:O	1.87	0.74
2:L:254:ASN:HA	2:L:278:VAL:HG13	1.69	0.74
2:P:236:TRP:CH2	2:P:238:ARG:NH2	2.56	0.74
2:G:312:LEU:HD22	2:G:322:MET:HG2	1.69	0.74
1:E:181:HIS:CE1	2:H:108:ARG:HE	2.05	0.74
2:G:191:HIS:CE1	2:G:217:LYS:HG3	2.23	0.74
2:L:152:SER:O	2:L:169:SER:CB	2.36	0.74
1:N:19:GLN:HE22	1:N:23:ARG:HH11	1.34	0.74
2:K:193:HIS:CD2	2:K:194:ASN:H	2.05	0.74
2:H:366:ASP:CG	2:H:368:LYS:HB3	2.07	0.74
1:E:73:ILE:HD12	1:E:84:ARG:NE	2.03	0.74
2:C:193:HIS:CD2	2:C:194:ASN:N	2.54	0.73
2:L:115:ILE:HD12	2:L:156:ILE:HG23	1.69	0.73
2:G:156:ILE:CG2	2:G:165:LEU:HD11	2.18	0.73
2:C:193:HIS:HD2	2:C:194:ASN:N	1.81	0.73
2:K:98:PRO:HB3	2:K:99:PRO:HD2	1.68	0.73
2:T:129:ASP:HB3	2:T:131:THR:OG1	1.88	0.73
2:L:94:TRP:CH2	2:L:391:THR:O	2.40	0.73
2:H:354:LEU:HD21	2:H:364:VAL:HG22	1.70	0.73
1:F:158:GLN:HA	1:F:158:GLN:HE21	1.53	0.73
2:D:379:HIS:NE2	2:D:397:THR:HG23	2.04	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:322:MET:HB2	2:K:332:MET:HG3	1.71	0.73
2:S:383:VAL:HA	2:S:399:SER:CB	2.19	0.73
2:H:203:ASN:O	2:H:205:ASP:N	2.21	0.73
2:L:337:HIS:CD2	2:L:337:HIS:H	2.06	0.72
2:S:203:ASN:O	2:S:205:ASP:N	2.21	0.72
2:K:254:ASN:HA	2:K:278:VAL:HG13	1.71	0.72
2:L:203:ASN:O	2:L:205:ASP:N	2.21	0.72
2:L:171:ASP:HB2	2:L:173:THR:OG1	1.88	0.72
2:S:132:ILE:HG12	2:S:156:ILE:HD11	1.70	0.72
2:S:193:HIS:CD2	2:S:194:ASN:H	2.05	0.72
2:O:312:LEU:HD22	2:O:322:MET:HG2	1.71	0.72
2:L:399:SER:OG	2:L:401:ASP:OD1	2.07	0.72
2:D:201:MET:CE	2:D:242:PRO:HB3	2.20	0.72
1:R:82:LEU:HG	1:R:121:ILE:HG13	1.72	0.72
2:K:310:PHE:CD2	2:K:324:ASP:HB3	2.25	0.72
2:H:94:TRP:CH2	2:H:392:ALA:O	2.42	0.72
1:F:8:PRO:HA	1:F:11:ILE:HD12	1.71	0.72
2:T:334:LEU:HB2	2:T:365:TRP:CZ3	2.25	0.72
2:D:317:ASP:CB	2:D:319:THR:OG1	2.36	0.72
2:P:358:ASP:HA	2:P:382:PHE:HB2	1.70	0.72
2:P:235:GLU:HA	2:P:235:GLU:OE1	1.88	0.72
1:B:58:ILE:HD11	1:B:206:CYS:HB2	1.71	0.72
2:H:347:HIS:HD2	2:H:349:GLY:N	1.88	0.72
2:C:340:TRP:O	2:C:357:ALA:HB1	1.89	0.72
2:T:213:ASP:HB3	2:T:215:THR:HB	1.70	0.72
2:T:347:HIS:CG	2:T:348:SER:H	2.08	0.72
2:T:265:THR:O	2:T:266:LYS:HG2	1.89	0.71
2:C:178:ASP:OD1	2:C:180:GLN:HB2	1.90	0.71
2:D:277:HIS:ND1	2:D:316:ARG:HB2	2.05	0.71
2:K:339:ASN:HD22	2:K:340:TRP:H	1.35	0.71
2:O:114:VAL:HG11	2:O:396:VAL:HB	1.71	0.71
2:L:117:HIS:CD2	2:L:118:PRO:HD2	2.25	0.71
2:D:362:LEU:HD11	2:D:386:LEU:HD13	1.72	0.71
2:L:171:ASP:CB	2:L:173:THR:OG1	2.38	0.71
2:G:315:SER:HB3	2:G:317:ASP:HB2	1.73	0.71
2:K:156:ILE:HG23	2:K:165:LEU:HD11	1.72	0.71
2:H:144:ARG:NH1	2:H:181:GLY:O	2.23	0.71
2:O:337:HIS:CE1	2:O:375:THR:HG23	2.24	0.71
2:L:168:CYS:SG	2:L:198:VAL:HB	2.30	0.71
2:L:278:VAL:HB	2:L:316:ARG:HD2	1.73	0.71
1:J:107:HIS:O	1:J:108:GLU:CB	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:354:LEU:HD13	2:K:362:LEU:HD11	1.73	0.71
1:I:78:THR:H	1:I:106:ASN:HD21	1.39	0.71
2:D:339:ASN:ND2	2:D:340:TRP:CD1	2.59	0.71
2:L:132:ILE:HB	2:L:146:LEU:HB2	1.73	0.71
2:C:315:SER:OG	2:C:316:ARG:N	2.22	0.71
2:K:207:ILE:HD12	2:K:221:VAL:HG22	1.73	0.71
2:H:317:ASP:HB3	2:H:319:THR:OG1	1.91	0.71
2:K:203:ASN:O	2:K:205:ASP:N	2.23	0.71
1:I:126:ASN:HD22	1:I:126:ASN:C	1.95	0.71
2:G:379:HIS:HD2	2:G:383:VAL:HG22	1.56	0.70
2:T:103:ALA:HA	2:T:405:LYS:HG2	1.73	0.70
2:P:236:TRP:O	2:P:253:SER:HB2	1.89	0.70
1:N:78:THR:H	1:N:106:ASN:HD21	1.36	0.70
2:D:366:ASP:OD1	2:D:368:LYS:HB3	1.91	0.70
2:S:366:ASP:CB	2:S:373:MET:HG2	2.18	0.70
2:D:126:ALA:HB2	2:D:156:ILE:HD11	1.74	0.70
2:K:354:LEU:CD2	2:K:364:VAL:HG22	2.21	0.70
1:J:8:PRO:O	1:J:79:ARG:HD3	1.91	0.70
2:G:360:LYS:CD	2:G:379:HIS:O	2.39	0.70
2:H:340:TRP:O	2:H:357:ALA:HB1	1.92	0.70
2:C:149:HIS:CE1	2:C:175:LYS:HG3	2.26	0.70
1:E:77:THR:HG23	1:E:80:HIS:ND1	2.06	0.70
1:F:207:LYS:HB3	1:F:208:PRO:HD3	1.72	0.70
2:D:272:LEU:HD13	2:D:323:TRP:CD2	2.25	0.70
1:I:191:MET:HB3	1:I:194:PHE:HA	1.72	0.70
1:I:8:PRO:O	1:I:79:ARG:CD	2.39	0.70
2:S:317:ASP:HB3	2:S:319:THR:OG1	1.91	0.70
1:E:103:GLY:HA2	1:E:106:ASN:HD22	1.56	0.70
1:B:189:HIS:HD2	2:C:402:GLN:NE2	1.89	0.70
1:I:8:PRO:O	1:I:79:ARG:HD2	1.91	0.70
2:S:359:ASP:OD1	2:S:361:THR:HG22	1.92	0.70
1:B:58:ILE:HD11	1:B:206:CYS:CB	2.21	0.70
2:D:193:HIS:CD2	2:D:194:ASN:H	2.10	0.70
2:T:351:LYS:HB2	2:T:352:PHE:CD1	2.26	0.70
2:T:366:ASP:OD1	2:T:368:LYS:HB3	1.92	0.70
2:L:347:HIS:CD2	2:L:349:GLY:H	2.10	0.70
2:O:178:ASP:HB2	2:O:185:ILE:HD11	1.73	0.70
2:K:363:ARG:HB2	2:K:365:TRP:HE1	1.54	0.69
2:C:337:HIS:CE1	2:C:363:ARG:HG2	2.27	0.69
2:O:203:ASN:O	2:O:205:ASP:N	2.23	0.69
2:L:345:LEU:HD11	2:L:388:PHE:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:58:ILE:HD11	1:M:206:CYS:CB	2.21	0.69
2:T:203:ASN:O	2:T:205:ASP:N	2.25	0.69
2:K:275:HIS:CE1	2:K:321:LYS:HG3	2.27	0.69
2:T:272:LEU:HB3	2:T:323:TRP:CZ3	2.26	0.69
2:L:317:ASP:CB	2:L:319:THR:OG1	2.40	0.69
1:J:175:THR:HG21	1:J:205:ILE:HD13	1.73	0.69
1:N:60:ARG:HA	1:N:64:SER:HB2	1.72	0.69
2:P:379:HIS:HD2	2:P:383:VAL:HG22	1.56	0.69
2:P:262:VAL:HG12	2:P:262:VAL:O	1.90	0.69
2:D:337:HIS:HB2	2:D:363:ARG:HH21	1.56	0.69
2:C:291:SER:HB2	2:C:367:TYR:HE1	1.57	0.69
2:D:397:THR:O	2:D:397:THR:HG22	1.90	0.69
2:L:347:HIS:HD2	2:L:349:GLY:H	1.39	0.69
2:L:178:ASP:OD1	2:L:180:GLN:HB2	1.92	0.69
1:N:58:ILE:HD11	1:N:206:CYS:HB2	1.75	0.69
2:L:124:VAL:HG22	2:L:134:VAL:HG22	1.75	0.69
2:T:173:THR:O	2:T:174:ILE:HG13	1.93	0.69
2:H:193:HIS:CD2	2:H:212:ARG:HD2	2.27	0.69
2:P:358:ASP:HA	2:P:382:PHE:CB	2.23	0.69
1:F:176:ASP:OD1	1:F:177:GLY:O	2.11	0.69
1:I:77:THR:HB	1:I:106:ASN:ND2	2.07	0.69
2:O:360:LYS:HB2	2:O:379:HIS:O	1.92	0.69
2:D:101:LYS:HD3	2:D:408:GLU:HG3	1.73	0.69
2:P:203:ASN:O	2:P:205:ASP:N	2.25	0.69
1:E:164:LEU:HD12	1:E:172:LEU:HB2	1.74	0.69
2:H:98:PRO:CB	2:H:99:PRO:CD	2.70	0.68
1:M:8:PRO:O	1:M:79:ARG:HD3	1.92	0.68
2:T:287:GLU:HG2	2:T:287:GLU:O	1.93	0.68
2:H:97:ARG:HG3	2:H:98:PRO:CD	2.22	0.68
2:H:337:HIS:N	2:H:337:HIS:CD2	2.61	0.68
2:T:253:SER:OG	2:T:255:ASP:OD1	2.10	0.68
2:K:316:ARG:C	2:K:318:LYS:H	1.97	0.68
2:S:366:ASP:HB2	2:S:373:MET:HB3	1.74	0.68
2:T:97:ARG:O	2:T:407:TRP:HE3	1.77	0.68
2:K:316:ARG:O	2:K:318:LYS:N	2.26	0.68
2:T:311:LEU:CD2	2:T:323:TRP:HB2	2.18	0.68
1:F:139:LEU:HB2	1:F:153:ASN:HB3	1.76	0.68
2:P:129:ASP:CB	2:P:131:THR:OG1	2.38	0.68
2:G:360:LYS:O	2:G:360:LYS:HD2	1.94	0.68
2:G:381:HIS:ND1	2:G:382:PHE:N	2.40	0.68
2:P:220:GLU:HB3	2:P:223:THR:OG1	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:334:LEU:HB3	2:C:365:TRP:CE3	2.29	0.68
2:P:310:PHE:HD2	2:P:324:ASP:CB	1.99	0.67
2:H:213:ASP:O	2:H:214:LYS:HB2	1.95	0.67
1:M:137:LEU:HD21	1:M:209:LEU:HD13	1.76	0.67
2:T:312:LEU:HD21	2:T:346:PHE:CE1	2.29	0.67
2:S:98:PRO:HB3	2:S:99:PRO:HD2	1.76	0.67
2:T:98:PRO:HB3	2:T:99:PRO:CD	2.23	0.67
2:P:98:PRO:HB3	2:P:99:PRO:CD	2.23	0.67
2:C:337:HIS:N	2:C:337:HIS:CD2	2.62	0.67
1:A:107:HIS:O	1:A:108:GLU:CB	2.43	0.67
2:D:354:LEU:HD22	2:D:364:VAL:HG22	1.75	0.67
2:K:350:GLY:O	2:K:367:TYR:OH	2.06	0.67
2:T:98:PRO:HB3	2:T:99:PRO:HD2	1.77	0.67
2:C:127:SER:OG	2:C:129:ASP:CB	2.42	0.67
2:S:358:ASP:HA	2:S:382:PHE:HB2	1.77	0.67
2:D:233:HIS:HB3	2:D:255:ASP:OD2	1.93	0.67
1:E:137:LEU:HD11	1:E:209:LEU:HD22	1.75	0.67
2:L:123:MET:HG2	2:L:124:VAL:N	2.09	0.67
2:C:213:ASP:HB3	2:C:215:THR:OG1	1.95	0.67
2:O:149:HIS:CE1	2:O:175:LYS:HG3	2.30	0.67
2:C:251:SER:HB3	2:C:261:TRP:HE1	1.58	0.67
2:T:129:ASP:N	2:T:130:ALA:HA	2.10	0.67
2:G:337:HIS:HB2	2:G:363:ARG:HH21	1.60	0.67
2:L:233:HIS:CD2	2:L:253:SER:OG	2.47	0.67
2:L:358:ASP:HA	2:L:382:PHE:CB	2.24	0.67
2:T:156:ILE:HG12	2:T:165:LEU:HD11	1.74	0.67
2:T:310:PHE:HE2	2:T:324:ASP:CB	2.08	0.67
2:L:134:VAL:O	2:L:143:GLU:HB2	1.95	0.67
1:B:118:ILE:HD12	1:B:160:LEU:HD11	1.76	0.67
2:C:134:VAL:O	2:C:143:GLU:HB2	1.95	0.67
2:O:215:THR:HG21	2:O:217:LYS:HE2	1.75	0.67
2:O:398:GLY:CA	2:O:404:VAL:HG22	2.25	0.67
2:S:347:HIS:HB2	2:S:352:PHE:O	1.94	0.67
1:Q:78:THR:H	1:Q:106:ASN:HD21	1.41	0.67
2:K:173:THR:CG2	2:K:187:THR:HG23	2.25	0.66
2:P:392:ALA:HB1	2:P:393:PRO:HD3	1.75	0.66
2:K:315:SER:OG	2:K:317:ASP:CB	2.18	0.66
2:L:337:HIS:N	2:L:337:HIS:CD2	2.60	0.66
2:H:128:GLU:HA	2:H:152:SER:OG	1.95	0.66
2:D:251:SER:HB3	2:D:261:TRP:HE1	1.61	0.66
2:L:149:HIS:HE2	2:L:167:SER:HG	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:374:LYS:HE2	2:P:375:THR:H	1.58	0.66
2:T:132:ILE:HB	2:T:146:LEU:HB2	1.76	0.66
1:M:126:ASN:H	1:M:126:ASN:HD22	1.44	0.66
2:L:260:VAL:HG21	2:L:325:VAL:HG11	1.76	0.66
2:G:354:LEU:N	2:G:354:LEU:HD23	2.09	0.66
1:A:43:LEU:HD22	1:A:44:PHE:N	2.09	0.66
2:S:311:LEU:HD22	2:S:325:VAL:HG22	1.77	0.66
2:H:186:ARG:CG	2:H:186:ARG:NH1	2.53	0.66
2:T:334:LEU:CB	2:T:365:TRP:CZ3	2.79	0.66
2:C:217:LYS:HG3	2:C:229:THR:HG23	1.77	0.66
2:T:324:ASP:HB3	2:T:331:LEU:HD21	1.78	0.66
2:H:178:ASP:CB	2:H:185:ILE:HD11	2.23	0.66
2:C:171:ASP:C	2:C:172:MET:CG	2.63	0.66
2:O:168:CYS:SG	2:O:198:VAL:HB	2.36	0.66
2:H:94:TRP:HH2	2:H:392:ALA:C	1.98	0.66
2:O:254:ASN:HA	2:O:278:VAL:HG22	1.77	0.66
1:A:67:HIS:CE1	2:C:340:TRP:CE2	2.83	0.66
2:K:360:LYS:HB3	2:K:381:HIS:O	1.96	0.66
2:H:243:ASN:HD21	2:H:245:ASP:HB3	1.61	0.66
2:G:173:THR:HG22	2:G:187:THR:HG23	1.78	0.66
2:G:252:CYS:HB2	2:G:282:ILE:HD11	1.77	0.66
2:P:94:TRP:CH2	2:P:392:ALA:C	2.68	0.66
2:L:336:GLY:HA2	2:L:365:TRP:CH2	2.31	0.66
2:C:98:PRO:HB3	2:C:99:PRO:CD	2.24	0.66
2:L:126:ALA:HB2	2:L:156:ILE:HD12	1.78	0.66
2:P:144:ARG:CZ	2:P:181:GLY:HA2	2.26	0.66
2:P:310:PHE:CE2	2:P:324:ASP:HB2	2.31	0.66
2:H:210:ALA:HB2	2:H:240:VAL:HG22	1.78	0.66
1:F:53:MET:HG2	1:F:59:TRP:HE3	1.61	0.66
2:K:253:SER:OG	2:K:255:ASP:OD1	2.12	0.66
1:J:126:ASN:C	1:J:126:ASN:HD22	2.00	0.66
2:P:337:HIS:HD2	2:P:337:HIS:H	1.42	0.66
1:B:189:HIS:CD2	2:C:402:GLN:HE22	2.14	0.66
2:K:144:ARG:NH2	2:K:181:GLY:CA	2.59	0.66
2:G:109:SER:HA	2:G:402:GLN:HE21	1.61	0.65
2:D:369:ASN:HD22	2:D:371:ARG:HH12	1.42	0.65
2:P:212:ARG:HG2	2:P:236:TRP:CE2	2.31	0.65
2:C:309:PRO:HG2	2:C:325:VAL:HG23	1.78	0.65
1:I:209:LEU:O	1:I:213:ILE:HG13	1.97	0.65
1:A:77:THR:HB	1:A:106:ASN:ND2	2.11	0.65
2:H:272:LEU:HD13	2:H:323:TRP:CD2	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:347:HIS:CG	2:T:348:SER:N	2.65	0.65
2:D:345:LEU:CD1	2:D:388:PHE:HB2	2.26	0.65
2:L:112:THR:HG21	2:L:154:GLN:HA	1.77	0.65
2:P:134:VAL:O	2:P:143:GLU:HB2	1.97	0.65
1:F:67:HIS:CE1	2:H:339:ASN:HD21	2.03	0.65
2:O:213:ASP:HB3	2:O:215:THR:CB	2.27	0.65
1:J:8:PRO:O	1:J:79:ARG:CD	2.44	0.65
1:Q:58:ILE:HD11	1:Q:206:CYS:HB2	1.79	0.65
2:T:332:MET:SD	2:T:367:TYR:CB	2.77	0.65
2:P:212:ARG:HG2	2:P:236:TRP:CD2	2.32	0.65
2:T:236:TRP:O	2:T:253:SER:HB2	1.96	0.65
2:S:98:PRO:HB3	2:S:99:PRO:CD	2.26	0.65
2:K:233:HIS:HD2	2:K:257:THR:HG22	1.62	0.65
2:K:148:GLY:O	2:K:175:LYS:HE3	1.96	0.65
2:O:98:PRO:HB3	2:O:99:PRO:HD2	1.79	0.65
2:G:334:LEU:HD13	2:G:365:TRP:CE3	2.31	0.65
2:S:211:SER:HB3	2:S:213:ASP:HB2	1.79	0.65
2:L:310:PHE:HE2	2:L:324:ASP:HB2	1.60	0.65
2:O:278:VAL:HB	2:O:316:ARG:HD2	1.79	0.65
1:B:189:HIS:CD2	2:C:402:GLN:NE2	2.64	0.65
2:K:144:ARG:HH22	2:K:181:GLY:HA2	1.62	0.65
1:B:8:PRO:O	1:B:79:ARG:CD	2.45	0.65
2:H:366:ASP:OD1	2:H:368:LYS:CB	2.39	0.65
1:B:181:HIS:CE1	2:C:108:ARG:NE	2.65	0.65
2:S:366:ASP:HB2	2:S:373:MET:CB	2.27	0.64
2:G:358:ASP:HA	2:G:382:PHE:CB	2.27	0.64
2:D:253:SER:OG	2:D:255:ASP:OD1	2.15	0.64
2:D:272:LEU:HD13	2:D:323:TRP:CE3	2.32	0.64
2:K:97:ARG:HE	2:K:98:PRO:HD3	1.62	0.64
2:T:211:SER:OG	2:T:213:ASP:HB2	1.97	0.64
2:C:102:TYR:HE2	2:C:139:THR:O	1.79	0.64
2:O:144:ARG:NH2	2:O:181:GLY:HA2	2.12	0.64
2:G:144:ARG:NH1	2:G:181:GLY:O	2.30	0.64
2:H:201:MET:CE	2:H:242:PRO:HB3	2.27	0.64
1:J:28:HIS:ND1	1:J:89:GLU:OE2	2.25	0.64
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.02	0.64
2:H:367:TYR:HD2	2:H:367:TYR:N	1.95	0.64
2:L:98:PRO:HB3	2:L:99:PRO:CD	2.27	0.64
2:H:144:ARG:NH2	2:H:181:GLY:HA2	2.12	0.64
2:O:337:HIS:N	2:O:337:HIS:CD2	2.65	0.64
2:G:168:CYS:SG	2:G:198:VAL:HB	2.38	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:166:LYS:O	2.15	0.64
2:H:249:ILE:HG22	2:H:261:TRP:HB2	1.78	0.64
1:J:135:ILE:HD13	1:J:212:LEU:HD23	1.77	0.64
2:C:368:LYS:HG2	2:C:369:ASN:OD1	1.97	0.64
2:L:152:SER:O	2:L:169:SER:HB2	1.97	0.64
2:P:252:CYS:HB2	2:P:282:ILE:HD11	1.79	0.64
2:K:312:LEU:CD2	2:K:322:MET:HG2	2.26	0.64
2:K:358:ASP:HA	2:K:382:PHE:HB2	1.79	0.64
2:D:173:THR:CG2	2:D:187:THR:HG23	2.27	0.64
2:T:362:LEU:HB3	2:T:376:LEU:HD12	1.79	0.64
2:T:322:MET:HB3	2:T:331:LEU:HB2	1.80	0.64
2:K:144:ARG:NH1	2:K:181:GLY:O	2.30	0.64
2:D:179:PHE:C	2:D:181:GLY:N	2.49	0.64
2:D:210:ALA:HB2	2:D:240:VAL:HG22	1.80	0.64
2:G:341:VAL:HA	2:G:357:ALA:HB2	1.79	0.64
2:L:156:ILE:HG12	2:L:165:LEU:HD11	1.80	0.64
1:E:55:GLN:HA	1:E:55:GLN:NE2	2.12	0.64
2:O:110:PRO:HG2	2:O:128:GLU:OE1	1.98	0.64
2:C:101:LYS:HZ3	2:C:408:GLU:HG3	1.62	0.64
2:L:297:THR:HG22	2:L:298:GLY:H	1.62	0.64
2:L:281:CYS:HB2	2:L:314:GLY:H	1.63	0.64
2:K:337:HIS:HE1	2:K:375:THR:OG1	1.80	0.64
2:L:392:ALA:HB1	2:L:393:PRO:CD	2.27	0.64
2:K:382:PHE:O	2:K:399:SER:HB2	1.97	0.64
1:A:164:LEU:N	1:A:165:PRO:HD2	2.12	0.64
2:K:316:ARG:HG2	2:K:340:TRP:CG	2.33	0.63
2:O:213:ASP:CB	2:O:215:THR:HB	2.28	0.63
2:P:251:SER:O	2:P:258:VAL:HG22	1.98	0.63
1:Q:84:ARG:HB3	1:Q:89:GLU:OE2	1.98	0.63
2:D:362:LEU:HB3	2:D:376:LEU:HD12	1.81	0.63
2:D:98:PRO:HB3	2:D:99:PRO:CD	2.28	0.63
2:H:252:CYS:HB2	2:H:282:ILE:HD11	1.79	0.63
2:G:127:SER:OG	2:G:129:ASP:HB2	1.99	0.63
2:P:124:VAL:HG22	2:P:134:VAL:HG22	1.81	0.63
2:P:193:HIS:CD2	2:P:194:ASN:H	2.17	0.63
2:G:379:HIS:CD2	2:G:383:VAL:HG22	2.33	0.63
2:L:379:HIS:CD2	2:L:383:VAL:HG13	2.34	0.63
2:H:399:SER:CB	2:H:401:ASP:OD1	2.46	0.63
2:K:360:LYS:HZ1	2:K:377:ASN:HB3	1.64	0.63
2:T:169:SER:OG	2:T:171:ASP:CG	2.37	0.63
2:H:351:LYS:O	2:H:367:TYR:HE2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:VAL:HA	2:D:357:ALA:HB2	1.80	0.63
2:C:144:ARG:HH22	2:C:181:GLY:HA2	1.61	0.63
1:F:189:HIS:HD2	2:G:402:GLN:NE2	1.97	0.63
2:O:310:PHE:CE2	2:O:324:ASP:CB	2.81	0.63
2:C:337:HIS:HD2	2:C:337:HIS:H	1.44	0.63
2:H:316:ARG:HG2	2:H:340:TRP:CD2	2.34	0.62
2:H:169:SER:OG	2:H:171:ASP:N	2.23	0.62
2:D:310:PHE:HD2	2:D:324:ASP:HB3	1.64	0.62
1:A:141:PRO:HB3	1:A:150:ARG:HD3	1.81	0.62
1:F:181:HIS:CE1	2:G:108:ARG:NE	2.67	0.62
2:O:172:MET:HA	2:O:195:VAL:HG23	1.81	0.62
2:H:126:ALA:HB2	2:H:156:ILE:CD1	2.28	0.62
2:O:129:ASP:HB3	2:O:131:THR:N	2.13	0.62
2:C:369:ASN:O	2:C:371:ARG:N	2.32	0.62
2:H:312:LEU:HD11	2:H:353:ILE:HG12	1.80	0.62
2:P:309:PRO:O	2:P:325:VAL:HG23	1.98	0.62
1:A:58:ILE:HD11	1:A:206:CYS:HB2	1.80	0.62
2:P:210:ALA:HB2	2:P:240:VAL:HG22	1.82	0.62
2:G:291:SER:HB2	2:G:367:TYR:HE1	1.62	0.62
2:H:173:THR:HG23	2:H:187:THR:HG23	1.82	0.62
2:L:98:PRO:CB	2:L:99:PRO:HD2	2.29	0.62
2:D:362:LEU:HB3	2:D:376:LEU:CD1	2.29	0.62
2:K:354:LEU:HD22	2:K:364:VAL:HG22	1.82	0.62
1:F:181:HIS:CE1	2:G:108:ARG:HE	2.18	0.62
2:D:213:ASP:HB3	2:D:215:THR:CB	2.30	0.62
2:G:281:CYS:SG	2:G:344:VAL:HG23	2.40	0.62
2:D:172:MET:HA	2:D:195:VAL:HG23	1.81	0.62
1:I:134:ILE:HB	1:I:170:VAL:HG13	1.82	0.62
1:N:45:VAL:HG11	1:N:85:LEU:HD21	1.81	0.62
2:P:152:SER:O	2:P:169:SER:HB2	1.99	0.62
1:I:107:HIS:O	1:I:108:GLU:CB	2.39	0.62
2:L:144:ARG:NH2	2:L:181:GLY:CA	2.60	0.62
2:D:207:ILE:HD12	2:D:221:VAL:HG22	1.82	0.62
1:M:101:TRP:CD1	1:M:137:LEU:HB2	2.35	0.62
2:O:98:PRO:HB3	2:O:99:PRO:CD	2.30	0.62
1:N:58:ILE:HD11	1:N:206:CYS:CB	2.30	0.62
1:I:41:ASP:OD1	1:I:96:LYS:NZ	2.32	0.62
2:G:388:PHE:CD1	2:G:395:VAL:HG13	2.31	0.62
2:D:115:ILE:HD12	2:D:156:ILE:CG2	2.27	0.62
1:E:73:ILE:HD12	1:E:84:ARG:HE	1.65	0.62
2:P:253:SER:OG	2:P:255:ASP:OD1	2.05	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:334:LEU:HD13	2:T:365:TRP:CE3	2.35	0.62
2:K:129:ASP:HB3	2:K:131:THR:OG1	2.00	0.62
2:O:334:LEU:HD13	2:O:365:TRP:CD2	2.35	0.62
2:K:337:HIS:N	2:K:337:HIS:CD2	2.68	0.62
2:L:359:ASP:OD1	2:L:361:THR:CB	2.48	0.62
2:H:388:PHE:HD1	2:H:395:VAL:HG13	1.64	0.62
2:L:239:MET:HE2	2:L:241:ARG:NE	2.15	0.61
2:T:392:ALA:HB1	2:T:393:PRO:HD2	1.82	0.61
1:F:164:LEU:O	1:F:166:LYS:O	2.18	0.61
1:F:139:LEU:HD23	1:F:139:LEU:N	2.14	0.61
2:P:382:PHE:O	2:P:399:SER:HB2	2.00	0.61
2:O:312:LEU:HA	2:O:321:LYS:O	2.00	0.61
1:I:144:GLU:HG3	1:I:194:PHE:CE2	2.35	0.61
2:H:98:PRO:CB	2:H:99:PRO:HD2	2.30	0.61
2:H:203:ASN:CG	2:H:203:ASN:O	2.38	0.61
2:G:278:VAL:HB	2:G:316:ARG:HD2	1.82	0.61
1:M:58:ILE:HD11	1:M:206:CYS:HB2	1.83	0.61
2:H:367:TYR:N	2:H:367:TYR:CD2	2.67	0.61
2:L:211:SER:HB3	2:L:213:ASP:HB2	1.82	0.61
2:D:322:MET:HB2	2:D:332:MET:HB2	1.81	0.61
2:S:272:LEU:HD22	2:S:323:TRP:CE3	2.35	0.61
2:D:132:ILE:HB	2:D:146:LEU:HB2	1.82	0.61
2:K:285:ALA:HB3	2:K:310:PHE:HB2	1.80	0.61
2:G:124:VAL:HG22	2:G:134:VAL:HG22	1.83	0.61
2:T:233:HIS:CE1	2:T:251:SER:OG	2.54	0.61
2:P:368:LYS:HE3	2:P:369:ASN:OD1	2.01	0.61
2:S:312:LEU:HA	2:S:321:LYS:O	1.99	0.61
2:T:272:LEU:HD13	2:T:323:TRP:CD2	2.36	0.61
2:T:288:SER:CB	2:T:350:GLY:CA	2.79	0.61
2:H:316:ARG:HG2	2:H:340:TRP:CG	2.36	0.61
1:M:85:LEU:HD22	1:M:90:LEU:CD1	2.26	0.61
2:G:317:ASP:HB3	2:G:319:THR:OG1	2.00	0.61
2:S:342:ARG:HD2	2:S:384:THR:HA	1.83	0.61
2:G:282:ILE:HG22	2:G:311:LEU:HD12	1.82	0.61
2:P:96:PRO:HD2	2:P:97:ARG:HG2	1.83	0.61
2:L:136:ASP:OD1	2:L:139:THR:HB	2.01	0.61
1:E:133:LYS:HD3	1:E:216:LEU:HD12	1.83	0.61
1:Q:85:LEU:HD22	1:Q:90:LEU:HG	1.82	0.61
2:G:334:LEU:HB3	2:G:365:TRP:CZ3	2.36	0.60
2:T:185:ILE:HG22	2:T:186:ARG:HE	1.66	0.60
2:D:310:PHE:CD2	2:D:324:ASP:HB3	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:293:ILE:HG23	2:P:294:SER:N	2.16	0.60
1:A:147:ASN:HD22	1:A:149:LEU:H	1.49	0.60
2:H:281:CYS:SG	2:H:343:GLY:HA2	2.41	0.60
2:D:213:ASP:HB3	2:D:215:THR:OG1	2.01	0.60
2:S:312:LEU:HD21	2:S:346:PHE:CE1	2.36	0.60
1:R:58:ILE:HD11	1:R:206:CYS:HB2	1.83	0.60
2:G:112:THR:HG21	2:G:154:GLN:HA	1.83	0.60
1:F:67:HIS:HE1	2:H:339:ASN:ND2	1.93	0.60
2:D:355:SER:O	2:D:362:LEU:HD12	2.01	0.60
2:P:337:HIS:N	2:P:337:HIS:CD2	2.68	0.60
2:H:361:THR:HG23	2:H:363:ARG:HG3	1.82	0.60
1:J:137:LEU:HD11	1:J:209:LEU:HD22	1.83	0.60
2:D:339:ASN:ND2	2:D:340:TRP:N	2.30	0.60
2:G:191:HIS:NE2	2:G:209:SER:OG	2.34	0.60
2:C:233:HIS:CD2	2:C:253:SER:OG	2.54	0.60
1:J:197:LEU:HB2	1:J:202:TYR:CE1	2.37	0.60
2:P:316:ARG:HG2	2:P:340:TRP:CD2	2.36	0.60
2:O:355:SER:OG	2:O:363:ARG:HB2	2.02	0.60
2:D:347:HIS:CD2	2:D:351:LYS:HD2	2.37	0.60
1:A:84:ARG:HD2	1:A:89:GLU:OE2	2.02	0.60
2:C:98:PRO:CB	2:C:99:PRO:HD2	2.29	0.60
2:C:379:HIS:NE2	2:C:397:THR:HG21	2.16	0.60
2:O:356:CYS:SG	2:O:383:VAL:HG12	2.42	0.60
2:P:123:MET:HG2	2:P:124:VAL:N	2.15	0.60
2:C:388:PHE:HA	2:C:395:VAL:HG12	1.82	0.60
2:K:239:MET:HE3	2:K:241:ARG:HH21	1.66	0.60
2:H:120:PHE:CZ	2:L:294:SER:HA	2.37	0.60
2:L:379:HIS:HD2	2:L:383:VAL:HG13	1.66	0.60
2:L:141:ASP:C	2:L:143:GLU:H	2.04	0.60
2:C:123:MET:HE1	2:C:404:VAL:HG11	1.82	0.60
1:N:164:LEU:N	1:N:165:PRO:HD2	2.16	0.60
2:O:322:MET:HE2	2:O:331:LEU:HD12	1.84	0.60
2:O:322:MET:HB2	2:O:332:MET:HB2	1.83	0.60
2:P:359:ASP:O	2:P:361:THR:HB	2.00	0.60
1:A:155:LYS:O	1:A:158:GLN:HB3	2.02	0.60
2:D:379:HIS:NE2	2:D:397:THR:CG2	2.65	0.60
2:L:117:HIS:CD2	2:L:118:PRO:CD	2.84	0.60
2:T:288:SER:CB	2:T:350:GLY:HA3	2.24	0.60
2:C:249:ILE:HG22	2:C:261:TRP:HB2	1.84	0.60
2:L:368:LYS:O	2:L:369:ASN:ND2	2.35	0.59
2:P:337:HIS:HE1	2:P:375:THR:OG1	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:PRO:HB3	2:G:99:PRO:CD	2.31	0.59
2:P:141:ASP:O	2:P:143:GLU:N	2.35	0.59
1:B:60:ARG:HA	1:B:64:SER:HB2	1.84	0.59
2:P:367:TYR:H	2:P:367:TYR:HD2	1.50	0.59
2:S:96:PRO:HD2	2:S:97:ARG:HG2	1.84	0.59
2:H:98:PRO:HB3	2:H:99:PRO:HD2	1.83	0.59
2:H:110:PRO:HG3	2:H:400:VAL:HG13	1.84	0.59
2:H:272:LEU:HB3	2:H:323:TRP:CH2	2.36	0.59
1:I:58:ILE:HD11	1:I:206:CYS:HB2	1.84	0.59
2:G:126:ALA:HB2	2:G:156:ILE:HD11	1.84	0.59
2:C:393:PRO:O	2:C:394:TYR:CG	2.55	0.59
2:K:312:LEU:HD11	2:K:353:ILE:HD13	1.83	0.59
2:G:341:VAL:HA	2:G:357:ALA:CB	2.33	0.59
2:S:341:VAL:HA	2:S:357:ALA:CB	2.31	0.59
1:R:8:PRO:O	1:R:79:ARG:HD3	2.03	0.59
2:P:98:PRO:CB	2:P:99:PRO:HD2	2.28	0.59
1:F:8:PRO:O	1:F:79:ARG:CD	2.50	0.59
2:C:149:HIS:NE2	2:C:175:LYS:HG3	2.17	0.59
2:D:337:HIS:CD2	2:D:337:HIS:N	2.69	0.59
2:L:141:ASP:O	2:L:143:GLU:N	2.34	0.59
2:D:345:LEU:HD11	2:D:388:PHE:HB2	1.85	0.59
2:O:312:LEU:HB2	2:O:344:VAL:HG11	1.85	0.59
2:P:111:VAL:HG13	2:P:126:ALA:O	2.02	0.59
2:L:150:THR:HB	2:L:171:ASP:OD1	2.02	0.59
2:D:173:THR:HG22	2:D:187:THR:HG23	1.85	0.59
2:G:115:ILE:HG22	2:G:124:VAL:HB	1.84	0.59
2:K:353:ILE:HG13	2:K:367:TYR:CD2	2.38	0.59
2:C:213:ASP:HB3	2:C:215:THR:CB	2.33	0.59
2:P:278:VAL:HB	2:P:316:ARG:HD2	1.84	0.59
1:N:62:LEU:HG	1:N:210:HIS:CD2	2.38	0.59
1:A:83:TRP:CE2	1:A:87:ASN:ND2	2.71	0.59
2:H:215:THR:HG22	2:H:216:ILE:N	2.18	0.59
2:P:337:HIS:CD2	2:P:363:ARG:HG2	2.37	0.59
2:P:317:ASP:HB3	2:P:319:THR:OG1	2.02	0.59
2:C:239:MET:HE3	2:C:241:ARG:HH21	1.68	0.59
2:S:310:PHE:CD2	2:S:324:ASP:HB3	2.35	0.59
2:P:383:VAL:HA	2:P:399:SER:HB3	1.84	0.59
1:J:207:LYS:HB3	1:J:208:PRO:HD3	1.85	0.59
2:K:397:THR:O	2:K:404:VAL:HA	2.03	0.59
2:H:193:HIS:HD2	2:H:212:ARG:HD2	1.67	0.58
2:O:211:SER:HB3	2:O:213:ASP:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:110:PRO:O	2:O:127:SER:HB2	2.03	0.58
2:D:193:HIS:HD2	2:D:194:ASN:H	1.51	0.58
1:R:58:ILE:HD11	1:R:206:CYS:CB	2.33	0.58
2:P:288:SER:HB2	2:P:350:GLY:HA3	1.84	0.58
2:D:341:VAL:HA	2:D:357:ALA:CB	2.33	0.58
1:E:78:THR:HG23	1:E:106:ASN:ND2	2.18	0.58
2:S:213:ASP:HB3	2:S:215:THR:CB	2.32	0.58
2:K:379:HIS:NE2	2:K:397:THR:HG22	2.18	0.58
2:G:201:MET:CE	2:G:242:PRO:HB3	2.32	0.58
2:C:310:PHE:CE2	2:C:324:ASP:HB2	2.36	0.58
2:S:172:MET:HA	2:S:195:VAL:HG23	1.85	0.58
2:K:124:VAL:HG22	2:K:134:VAL:HG22	1.84	0.58
2:K:354:LEU:HD21	2:K:364:VAL:HG22	1.85	0.58
1:I:103:GLY:O	1:I:106:ASN:HB2	2.04	0.58
1:A:78:THR:H	1:A:106:ASN:HD21	1.50	0.58
1:A:147:ASN:ND2	1:A:149:LEU:HB2	2.18	0.58
1:I:100:VAL:HB	1:I:136:VAL:HG22	1.85	0.58
2:S:249:ILE:CG2	2:S:261:TRP:HB2	2.31	0.58
2:H:233:HIS:CD2	2:H:253:SER:OG	2.56	0.58
2:L:213:ASP:O	2:L:214:LYS:HB2	2.03	0.58
2:T:98:PRO:CB	2:T:99:PRO:CD	2.82	0.58
2:P:116:PHE:CZ	2:P:396:VAL:HG23	2.38	0.58
2:S:178:ASP:HB2	2:S:185:ILE:HD11	1.86	0.58
2:O:359:ASP:O	2:O:361:THR:N	2.32	0.58
2:T:168:CYS:SG	2:T:195:VAL:HG12	2.42	0.58
2:K:313:SER:O	2:K:321:LYS:N	2.33	0.58
2:D:374:LYS:HG3	2:D:375:THR:N	2.19	0.58
1:N:147:ASN:HD22	1:N:149:LEU:H	1.51	0.58
2:C:136:ASP:O	2:C:140:GLY:N	2.34	0.58
2:T:117:HIS:CE1	2:T:120:PHE:H	2.21	0.58
2:G:169:SER:OG	2:G:170:ALA:N	2.33	0.58
2:C:172:MET:HA	2:C:195:VAL:HG23	1.86	0.58
1:F:207:LYS:CB	1:F:208:PRO:CD	2.78	0.58
2:G:212:ARG:HG2	2:G:236:TRP:CD2	2.38	0.58
1:J:62:LEU:HD23	1:J:210:HIS:HB2	1.85	0.58
1:F:47:ASP:OD2	1:F:49:MET:HG2	2.04	0.58
1:J:7:ASN:HD22	1:J:7:ASN:C	2.07	0.58
1:B:79:ARG:HH11	1:B:79:ARG:HG3	1.69	0.58
2:O:96:PRO:HD2	2:O:97:ARG:HG2	1.85	0.58
2:G:218:MET:CE	2:G:228:LYS:HD2	2.34	0.58
2:L:337:HIS:CE1	2:L:375:THR:OG1	2.57	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:341:VAL:HA	2:L:357:ALA:HB2	1.86	0.58
2:H:355:SER:OG	2:H:363:ARG:HD3	2.03	0.58
2:G:358:ASP:HA	2:G:382:PHE:HB2	1.84	0.58
2:H:152:SER:O	2:H:169:SER:HB2	2.04	0.58
2:L:146:LEU:HD13	2:L:177:TRP:CE3	2.39	0.58
2:S:134:VAL:O	2:S:143:GLU:HB2	2.04	0.58
1:R:164:LEU:N	1:R:165:PRO:HD2	2.19	0.58
1:A:83:TRP:CD2	1:A:87:ASN:ND2	2.72	0.58
2:G:193:HIS:CD2	2:G:194:ASN:H	2.22	0.58
2:K:339:ASN:ND2	2:K:340:TRP:H	2.01	0.57
2:H:217:LYS:HG3	2:H:229:THR:HG23	1.86	0.57
2:S:317:ASP:O	2:S:318:LYS:HB2	2.04	0.57
1:E:103:GLY:O	1:E:106:ASN:HB2	2.03	0.57
2:T:207:ILE:HD12	2:T:221:VAL:HG22	1.85	0.57
2:P:272:LEU:HD13	2:P:323:TRP:CD2	2.39	0.57
2:L:337:HIS:HE1	2:L:375:THR:OG1	1.86	0.57
1:Q:64:SER:HB2	1:Q:65:PRO:HD3	1.85	0.57
2:C:101:LYS:O	2:C:102:TYR:CD1	2.57	0.57
1:N:134:ILE:HB	1:N:170:VAL:HG13	1.86	0.57
2:L:354:LEU:HD22	2:L:364:VAL:HG22	1.86	0.57
1:J:189:HIS:CD2	2:K:402:GLN:HE22	2.22	0.57
2:L:129:ASP:N	2:L:130:ALA:HA	2.18	0.57
2:D:315:SER:OG	2:D:316:ARG:N	2.37	0.57
1:I:147:ASN:ND2	1:I:149:LEU:HB2	2.19	0.57
2:S:309:PRO:O	2:S:324:ASP:HA	2.04	0.57
1:Q:107:HIS:O	1:Q:108:GLU:CB	2.47	0.57
2:T:178:ASP:OD1	2:T:180:GLN:HB2	2.04	0.57
2:D:216:ILE:HD11	2:D:251:SER:HB2	1.86	0.57
2:L:260:VAL:HG21	2:L:325:VAL:CG1	2.34	0.57
2:G:232:GLY:HA3	2:G:261:TRP:HH2	1.69	0.57
2:T:141:ASP:C	2:T:143:GLU:H	2.07	0.57
2:K:278:VAL:O	2:K:315:SER:HB2	2.05	0.57
2:K:339:ASN:HD22	2:K:340:TRP:N	2.01	0.57
2:C:97:ARG:CG	2:C:98:PRO:HD3	2.15	0.57
2:K:259:ARG:HB2	2:K:261:TRP:HE1	1.69	0.57
2:C:360:LYS:HB3	2:C:379:HIS:O	2.03	0.57
2:H:255:ASP:OD2	2:H:257:THR:CB	2.53	0.57
2:L:272:LEU:HB3	2:L:323:TRP:CE3	2.39	0.57
2:C:233:HIS:CE1	2:C:251:SER:HG	2.23	0.57
2:H:243:ASN:ND2	2:H:245:ASP:HB3	2.19	0.57
2:G:187:THR:HG22	2:G:189:HIS:CD2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ALA:HB2	1:E:83:TRP:CE2	2.40	0.57
2:L:293:ILE:HG22	2:L:294:SER:N	2.20	0.57
2:T:312:LEU:HD12	2:T:344:VAL:HG12	1.85	0.57
2:H:98:PRO:HB3	2:H:99:PRO:HD3	1.86	0.57
2:S:98:PRO:CB	2:S:99:PRO:CD	2.82	0.57
2:H:201:MET:HE3	2:H:242:PRO:HB3	1.86	0.57
2:C:366:ASP:HB2	2:C:373:MET:HG2	1.86	0.57
2:K:141:ASP:C	2:K:143:GLU:H	2.08	0.57
1:B:22:ASP:OD2	1:B:25:MET:HB2	2.05	0.57
2:K:217:LYS:HD3	2:K:226:CYS:SG	2.44	0.57
2:H:367:TYR:HD2	2:H:367:TYR:H	1.52	0.57
1:I:8:PRO:HA	1:I:11:ILE:HD12	1.84	0.57
1:B:8:PRO:O	1:B:79:ARG:HD2	2.05	0.57
1:M:164:LEU:O	1:M:166:LYS:O	2.23	0.57
2:P:243:ASN:HD21	2:P:245:ASP:HB3	1.70	0.57
2:G:107:HIS:NE2	2:G:125:SER:OG	2.36	0.57
1:I:58:ILE:O	1:I:58:ILE:HG13	2.03	0.57
2:C:94:TRP:HH2	2:C:391:THR:O	1.86	0.57
1:M:14:ALA:HB2	1:M:83:TRP:CE2	2.40	0.57
2:O:136:ASP:OD1	2:O:139:THR:HB	2.04	0.57
2:L:135:TRP:N	2:L:135:TRP:CD1	2.72	0.57
2:K:335:VAL:O	2:K:335:VAL:HG12	2.03	0.57
2:O:396:VAL:HG13	2:O:406:VAL:HG13	1.87	0.57
2:P:392:ALA:HB1	2:P:393:PRO:CD	2.34	0.57
2:D:347:HIS:CD2	2:D:349:GLY:H	2.22	0.57
1:B:164:LEU:O	1:B:166:LYS:O	2.22	0.57
2:H:186:ARG:HG2	2:H:186:ARG:NH1	2.00	0.57
2:T:361:THR:CG2	2:T:363:ARG:HG2	2.34	0.57
2:L:98:PRO:CB	2:L:99:PRO:CD	2.83	0.57
2:K:144:ARG:NH2	2:K:181:GLY:HA3	2.20	0.57
2:C:310:PHE:HE2	2:C:324:ASP:HB2	1.70	0.57
1:B:78:THR:H	1:B:106:ASN:HD21	1.53	0.57
2:G:172:MET:HA	2:G:195:VAL:HG23	1.86	0.57
2:P:127:SER:OG	2:P:128:GLU:N	2.37	0.56
2:G:397:THR:CG2	2:G:407:TRP:HE1	2.18	0.56
2:D:98:PRO:CB	2:D:99:PRO:HD2	2.34	0.56
1:M:147:ASN:HD22	1:M:149:LEU:H	1.52	0.56
2:C:334:LEU:HD13	2:C:365:TRP:CE3	2.38	0.56
2:P:172:MET:HA	2:P:195:VAL:CG2	2.34	0.56
1:N:164:LEU:O	1:N:166:LYS:O	2.23	0.56
2:K:171:ASP:C	2:K:172:MET:HG3	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:397:THR:HG22	2:L:407:TRP:HE1	1.70	0.56
2:D:397:THR:HG21	2:D:407:TRP:HE1	1.70	0.56
1:F:8:PRO:O	1:F:79:ARG:HD3	2.05	0.56
2:T:115:ILE:HD13	2:T:156:ILE:HG22	1.87	0.56
1:B:7:ASN:HD22	1:B:8:PRO:HD2	1.70	0.56
2:D:169:SER:OG	2:D:170:ALA:N	2.38	0.56
2:D:336:GLY:CA	2:D:365:TRP:HH2	2.17	0.56
2:K:233:HIS:CD2	2:K:257:THR:HG22	2.40	0.56
2:C:309:PRO:O	2:C:325:VAL:HG23	2.04	0.56
2:H:281:CYS:SG	2:H:344:VAL:HG23	2.46	0.56
1:E:107:HIS:O	1:E:108:GLU:HB2	2.05	0.56
1:R:84:ARG:NH1	1:R:89:GLU:OE1	2.37	0.56
2:P:215:THR:CG2	2:P:229:THR:CG2	2.84	0.56
2:P:173:THR:HG21	2:P:175:LYS:HE2	1.86	0.56
2:L:320:ILE:HB	2:L:334:LEU:HB2	1.87	0.56
2:H:355:SER:OG	2:H:363:ARG:CD	2.54	0.56
2:D:397:THR:O	2:D:397:THR:CG2	2.53	0.56
2:P:288:SER:CB	2:P:350:GLY:HA3	2.36	0.56
2:K:281:CYS:SG	2:K:343:GLY:HA2	2.46	0.56
2:G:211:SER:HB3	2:G:213:ASP:HB2	1.86	0.56
2:K:316:ARG:C	2:K:318:LYS:N	2.55	0.56
2:L:337:HIS:CE1	2:L:363:ARG:HG2	2.41	0.56
2:T:351:LYS:HB2	2:T:352:PHE:CE1	2.40	0.56
2:S:141:ASP:C	2:S:143:GLU:H	2.08	0.56
2:H:140:GLY:O	2:H:141:ASP:OD1	2.24	0.56
2:T:317:ASP:O	2:T:319:THR:HG23	2.06	0.56
2:H:277:HIS:ND1	2:H:278:VAL:N	2.53	0.56
2:H:172:MET:HA	2:H:195:VAL:HG23	1.87	0.56
2:T:212:ARG:HG2	2:T:236:TRP:CG	2.40	0.56
2:G:187:THR:CG2	2:G:189:HIS:NE2	2.69	0.56
2:P:141:ASP:C	2:P:143:GLU:H	2.09	0.56
2:S:141:ASP:O	2:S:143:GLU:N	2.39	0.56
2:L:252:CYS:SG	2:L:282:ILE:HG12	2.46	0.56
1:F:191:MET:HB3	1:F:194:PHE:HA	1.86	0.56
2:P:117:HIS:HD2	2:P:158:PHE:CZ	2.24	0.56
2:G:379:HIS:NE2	2:G:397:THR:CG2	2.68	0.56
2:O:158:PHE:CE2	2:O:165:LEU:HB2	2.41	0.56
2:G:254:ASN:HA	2:G:278:VAL:HG13	1.88	0.56
2:K:213:ASP:HB3	2:K:215:THR:HB	1.88	0.56
2:L:176:LEU:HD11	2:L:221:VAL:HG13	1.86	0.56
2:L:239:MET:HE2	2:L:241:ARG:HH21	1.63	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:129:ASP:N	2:P:130:ALA:HA	2.20	0.56
2:C:337:HIS:NE2	2:C:363:ARG:HG2	2.20	0.56
2:O:129:ASP:N	2:O:130:ALA:HA	2.21	0.56
2:L:336:GLY:HA2	2:L:365:TRP:HH2	1.69	0.56
2:P:171:ASP:O	2:P:172:MET:HB2	2.06	0.56
2:C:240:VAL:O	2:C:241:ARG:HD3	2.06	0.56
1:J:164:LEU:N	1:J:165:PRO:HD2	2.21	0.56
1:Q:141:PRO:HB3	1:Q:150:ARG:HD3	1.86	0.56
2:G:337:HIS:CE1	2:G:375:THR:OG1	2.53	0.55
2:G:140:GLY:O	2:G:141:ASP:OD1	2.24	0.55
2:T:141:ASP:O	2:T:143:GLU:N	2.38	0.55
2:L:249:ILE:HG22	2:L:261:TRP:HB2	1.87	0.55
2:T:341:VAL:HA	2:T:357:ALA:CB	2.36	0.55
1:E:110:THR:O	1:E:114:VAL:HG23	2.05	0.55
2:K:337:HIS:CE1	2:K:363:ARG:HG2	2.41	0.55
2:L:213:ASP:HB3	2:L:215:THR:CB	2.36	0.55
2:T:287:GLU:O	2:T:287:GLU:CG	2.55	0.55
2:C:168:CYS:SG	2:C:198:VAL:HB	2.46	0.55
1:R:67:HIS:NE2	2:T:358:ASP:OD2	2.29	0.55
2:C:317:ASP:CB	2:C:319:THR:OG1	2.55	0.55
2:C:141:ASP:O	2:C:143:GLU:N	2.39	0.55
2:G:187:THR:HG22	2:G:189:HIS:NE2	2.21	0.55
1:Q:58:ILE:O	1:Q:58:ILE:HG13	2.05	0.55
2:S:213:ASP:HB3	2:S:215:THR:HB	1.87	0.55
1:B:46:GLY:HA2	1:B:102:VAL:HG22	1.89	0.55
2:O:345:LEU:HD11	2:O:388:PHE:H	1.69	0.55
2:G:397:THR:HG22	2:G:405:LYS:HB2	1.88	0.55
2:O:322:MET:HG3	2:O:332:MET:HB2	1.88	0.55
2:H:337:HIS:NE2	2:H:363:ARG:HG2	2.22	0.55
2:G:317:ASP:O	2:G:318:LYS:HB2	2.05	0.55
1:Q:164:LEU:N	1:Q:165:PRO:HD2	2.21	0.55
1:Q:13:HIS:H	1:Q:83:TRP:HB2	1.72	0.55
1:E:7:ASN:C	1:E:7:ASN:ND2	2.59	0.55
2:P:135:TRP:CD1	2:P:135:TRP:N	2.74	0.55
2:L:144:ARG:HH22	2:L:181:GLY:HA2	1.66	0.55
2:L:379:HIS:CE1	2:L:405:LYS:HG3	2.41	0.55
2:C:213:ASP:O	2:C:214:LYS:HB2	2.06	0.55
2:K:212:ARG:HG2	2:K:236:TRP:CD2	2.41	0.55
2:K:236:TRP:O	2:K:253:SER:HB2	2.07	0.55
1:I:85:LEU:HD22	1:I:90:LEU:HD11	1.89	0.55
2:C:312:LEU:HD21	2:C:346:PHE:CZ	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:312:LEU:CD2	2:G:322:MET:HG2	2.35	0.55
2:O:398:GLY:HA3	2:O:404:VAL:HG22	1.89	0.55
2:G:141:ASP:C	2:G:143:GLU:H	2.10	0.55
2:G:201:MET:HE3	2:G:242:PRO:HB3	1.88	0.55
1:Q:164:LEU:O	1:Q:166:LYS:O	2.25	0.55
2:C:212:ARG:HG2	2:C:236:TRP:CD2	2.41	0.55
2:P:211:SER:HB3	2:P:213:ASP:CB	2.23	0.55
2:P:132:ILE:HB	2:P:146:LEU:HB2	1.89	0.55
2:D:232:GLY:HA3	2:D:261:TRP:HH2	1.71	0.55
2:P:126:ALA:HB2	2:P:156:ILE:HD11	1.89	0.55
2:K:193:HIS:HD2	2:K:194:ASN:HB2	1.72	0.55
1:A:31:PHE:HD1	1:A:89:GLU:OE2	1.89	0.55
2:O:141:ASP:C	2:O:143:GLU:H	2.10	0.55
1:F:110:THR:HG23	1:F:113:GLU:OE1	2.06	0.55
2:K:277:HIS:ND1	2:K:316:ARG:HB2	2.22	0.55
2:P:334:LEU:HB3	2:P:365:TRP:CE3	2.42	0.55
2:L:117:HIS:ND1	2:L:120:PHE:HB2	2.22	0.55
2:D:358:ASP:HA	2:D:382:PHE:HB3	1.88	0.55
2:L:110:PRO:HG2	2:L:128:GLU:HG3	1.89	0.55
2:G:129:ASP:N	2:G:130:ALA:HA	2.22	0.55
2:S:315:SER:HB3	2:S:317:ASP:HB2	1.89	0.55
2:P:236:TRP:CZ2	2:P:238:ARG:NH2	2.74	0.55
1:F:155:LYS:O	1:F:158:GLN:HB2	2.06	0.55
2:O:345:LEU:HD12	2:O:388:PHE:HB2	1.88	0.55
2:H:109:SER:HA	2:H:402:GLN:HE21	1.72	0.55
1:E:28:HIS:O	1:E:32:VAL:HG23	2.06	0.55
1:I:164:LEU:N	1:I:165:PRO:HD2	2.22	0.55
2:P:310:PHE:CD2	2:P:324:ASP:CB	2.75	0.54
2:D:337:HIS:CD2	2:D:337:HIS:H	2.23	0.54
1:E:164:LEU:O	1:E:166:LYS:O	2.26	0.54
2:C:368:LYS:O	2:C:369:ASN:CG	2.46	0.54
1:E:39:GLU:OE2	2:G:238:ARG:NH2	2.39	0.54
1:N:107:HIS:O	1:N:108:GLU:HB3	2.07	0.54
2:S:129:ASP:HB3	2:S:131:THR:OG1	2.07	0.54
2:C:110:PRO:HB2	2:C:128:GLU:HG3	1.89	0.54
2:L:343:GLY:HA3	2:L:386:LEU:CD2	2.37	0.54
2:K:357:ALA:HB3	2:K:359:ASP:OD2	2.08	0.54
1:I:172:LEU:HD21	1:I:174:ASP:HB2	1.88	0.54
2:S:309:PRO:HG2	2:S:325:VAL:HB	1.88	0.54
2:H:214:LYS:NZ	2:H:234:ARG:HH21	2.06	0.54
2:L:351:LYS:HB2	2:L:352:PHE:CE1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:14:ALA:HB2	1:N:83:TRP:CE2	2.42	0.54
2:C:280:GLU:OE1	2:C:342:ARG:HD2	2.08	0.54
2:L:401:ASP:O	2:L:402:GLN:HB2	2.07	0.54
2:H:171:ASP:O	2:H:172:MET:HG3	2.08	0.54
2:L:324:ASP:OD2	2:L:326:SER:OG	2.14	0.54
2:P:235:GLU:HB3	2:P:254:ASN:HB2	1.88	0.54
2:P:102:TYR:HB2	2:P:406:VAL:HB	1.90	0.54
2:T:159:ASP:CA	2:T:200:ILE:HG21	2.19	0.54
2:G:357:ALA:HB3	2:G:359:ASP:OD2	2.08	0.54
2:H:336:GLY:O	2:H:337:HIS:O	2.26	0.54
2:P:236:TRP:CZ3	2:P:238:ARG:NH2	2.76	0.54
2:K:381:HIS:ND1	2:K:382:PHE:N	2.54	0.54
2:H:282:ILE:HA	2:H:312:LEU:O	2.07	0.54
2:G:141:ASP:O	2:G:143:GLU:N	2.41	0.54
2:T:134:VAL:O	2:T:143:GLU:HB2	2.07	0.54
2:C:245:ASP:HB3	2:C:247:THR:OG1	2.07	0.54
2:L:407:TRP:N	2:L:407:TRP:CD1	2.75	0.54
2:D:355:SER:OG	2:D:363:ARG:HD3	2.08	0.54
2:K:107:HIS:CE1	2:K:133:LYS:HG3	2.43	0.54
2:K:232:GLY:HA3	2:K:261:TRP:HH2	1.72	0.54
2:H:119:VAL:HG11	2:L:293:ILE:HG23	1.90	0.54
2:G:339:ASN:HB3	2:G:358:ASP:HB2	1.90	0.54
2:S:254:ASN:HA	2:S:278:VAL:HG13	1.89	0.54
2:G:179:PHE:C	2:G:181:GLY:N	2.61	0.54
2:C:94:TRP:CH2	2:C:391:THR:O	2.61	0.54
1:R:164:LEU:O	1:R:166:LYS:O	2.26	0.54
2:K:172:MET:HA	2:K:195:VAL:HG23	1.90	0.54
2:S:129:ASP:N	2:S:130:ALA:HA	2.23	0.54
1:I:47:ASP:OD2	1:I:49:MET:HG2	2.07	0.54
2:K:132:ILE:HB	2:K:146:LEU:HB2	1.90	0.54
2:O:98:PRO:CB	2:O:99:PRO:CD	2.86	0.54
1:Q:207:LYS:HB3	1:Q:208:PRO:CD	2.38	0.54
1:B:137:LEU:HD21	1:B:209:LEU:HD13	1.90	0.54
2:G:109:SER:HA	2:G:402:GLN:NE2	2.23	0.54
2:L:293:ILE:CG2	2:L:294:SER:N	2.71	0.54
1:A:60:ARG:HA	1:A:64:SER:HB2	1.89	0.54
2:L:144:ARG:NH1	2:L:181:GLY:O	2.41	0.54
2:H:155:ASP:H	2:H:168:CYS:HB2	1.73	0.54
2:T:337:HIS:HB2	2:T:363:ARG:NH2	2.23	0.54
2:T:388:PHE:HD1	2:T:395:VAL:HG13	1.73	0.54
2:L:334:LEU:HD13	2:L:365:TRP:CD2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:213:ASP:O	2:S:214:LYS:HB2	2.07	0.54
2:L:280:GLU:OE1	2:L:342:ARG:HD3	2.08	0.54
2:P:295:GLU:OE1	2:P:331:LEU:HD13	2.08	0.54
2:D:127:SER:OG	2:D:128:GLU:N	2.37	0.54
2:G:400:VAL:C	2:G:402:GLN:H	2.10	0.53
2:P:179:PHE:C	2:P:181:GLY:N	2.60	0.53
1:I:8:PRO:O	1:I:79:ARG:HD3	2.07	0.53
1:Q:58:ILE:HD11	1:Q:206:CYS:CB	2.37	0.53
2:G:123:MET:HE1	2:G:135:TRP:CD1	2.42	0.53
2:D:287:GLU:O	2:D:287:GLU:HG3	2.07	0.53
2:T:297:THR:HG22	2:T:298:GLY:H	1.74	0.53
2:S:216:ILE:HG23	2:S:240:VAL:HG11	1.91	0.53
2:H:311:LEU:O	2:H:311:LEU:HD23	2.08	0.53
2:O:313:SER:OG	2:O:323:TRP:NE1	2.39	0.53
2:O:340:TRP:O	2:O:358:ASP:N	2.40	0.53
2:G:343:GLY:O	2:G:355:SER:HB2	2.09	0.53
2:H:310:PHE:HA	2:H:323:TRP:O	2.08	0.53
2:H:134:VAL:O	2:H:143:GLU:HB2	2.08	0.53
1:E:7:ASN:ND2	1:E:9:ALA:H	2.06	0.53
2:T:201:MET:SD	2:T:208:VAL:CG2	2.96	0.53
2:P:217:LYS:HG2	2:P:229:THR:HG23	1.90	0.53
1:M:126:ASN:HD22	1:M:126:ASN:N	2.04	0.53
2:C:114:VAL:HG13	2:C:123:MET:HE3	1.89	0.53
2:D:178:ASP:OD1	2:D:180:GLN:HB2	2.09	0.53
2:C:169:SER:OG	2:C:171:ASP:CG	2.46	0.53
2:L:139:THR:HG21	2:L:141:ASP:OD2	2.08	0.53
1:B:8:PRO:O	1:B:79:ARG:HD3	2.07	0.53
1:A:58:ILE:HD11	1:A:206:CYS:CB	2.39	0.53
1:A:58:ILE:O	1:A:58:ILE:HG13	2.08	0.53
1:M:197:LEU:HB2	1:M:202:TYR:CE1	2.43	0.53
1:A:26:SER:HB3	1:B:194:PHE:CE1	2.43	0.53
2:C:379:HIS:CD2	2:C:397:THR:CG2	2.90	0.53
2:T:310:PHE:HE2	2:T:324:ASP:HB3	1.72	0.53
2:P:239:MET:HE2	2:P:241:ARG:HE	1.73	0.53
2:T:169:SER:HB2	2:T:171:ASP:OD1	2.08	0.53
1:F:158:GLN:NE2	1:F:158:GLN:CA	2.71	0.53
2:P:203:ASN:OD1	2:P:203:ASN:O	2.27	0.53
1:J:207:LYS:HB3	1:J:208:PRO:CD	2.39	0.53
1:F:189:HIS:CD2	2:G:402:GLN:NE2	2.77	0.53
2:G:379:HIS:CD2	2:G:399:SER:HB3	2.44	0.53
2:L:211:SER:CB	2:L:213:ASP:HB2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:VAL:HB	2:K:399:SER:H	1.74	0.53
2:C:122:VAL:HG22	2:C:136:ASP:H	1.74	0.53
2:O:136:ASP:O	2:O:140:GLY:N	2.36	0.53
2:P:216:ILE:HB	2:P:230:PHE:HB2	1.90	0.53
2:H:176:LEU:HD11	2:H:221:VAL:HG13	1.90	0.53
2:K:259:ARG:HB2	2:K:261:TRP:NE1	2.24	0.53
2:O:171:ASP:HB2	2:O:173:THR:OG1	2.08	0.53
1:I:164:LEU:O	1:I:166:LYS:O	2.25	0.53
2:D:281:CYS:HB3	2:D:344:VAL:CG2	2.38	0.53
1:A:109:ASN:HA	1:A:113:GLU:OE1	2.09	0.53
2:C:336:GLY:HA3	2:C:365:TRP:HH2	1.73	0.53
2:D:114:VAL:CG1	2:D:123:MET:HE3	2.39	0.53
2:G:126:ALA:CB	2:G:156:ILE:HD11	2.39	0.53
2:P:272:LEU:HB3	2:P:323:TRP:CZ3	2.44	0.53
1:I:147:ASN:HD21	1:I:149:LEU:HB2	1.74	0.53
2:K:215:THR:HG23	2:K:229:THR:HG23	1.90	0.53
1:I:193:ASP:O	1:J:23:ARG:HD2	2.09	0.53
2:S:363:ARG:HB2	2:S:365:TRP:HE1	1.73	0.53
1:Q:45:VAL:HG12	1:Q:71:PHE:HB2	1.91	0.53
2:T:179:PHE:C	2:T:181:GLY:N	2.62	0.53
2:G:339:ASN:ND2	2:G:340:TRP:H	2.07	0.53
2:D:233:HIS:NE2	2:D:251:SER:OG	2.41	0.53
2:T:355:SER:OG	2:T:363:ARG:HD2	2.09	0.53
2:C:393:PRO:O	2:C:394:TYR:CD2	2.62	0.53
2:S:265:THR:O	2:S:266:LYS:HG2	2.09	0.53
1:E:147:ASN:ND2	1:F:21:ASP:HB3	2.25	0.53
2:D:176:LEU:HD11	2:D:221:VAL:HG13	1.91	0.52
2:S:132:ILE:HB	2:S:146:LEU:HB2	1.91	0.52
2:T:213:ASP:HB3	2:T:215:THR:CB	2.39	0.52
2:L:345:LEU:HD11	2:L:388:PHE:CB	2.39	0.52
1:J:212:LEU:HG	1:J:216:LEU:HD22	1.90	0.52
2:C:262:VAL:HG12	2:C:265:THR:H	1.74	0.52
2:L:171:ASP:C	2:L:172:MET:HG3	2.30	0.52
2:L:233:HIS:HB3	2:L:255:ASP:OD2	2.09	0.52
2:G:248:LEU:O	2:G:249:ILE:HD12	2.10	0.52
2:K:141:ASP:O	2:K:143:GLU:N	2.43	0.52
2:C:243:ASN:HD22	2:C:248:LEU:H	1.57	0.52
1:M:60:ARG:HA	1:M:64:SER:HB2	1.89	0.52
1:B:44:PHE:HB3	1:B:50:VAL:CG1	2.39	0.52
2:P:201:MET:HE3	2:P:242:PRO:HB3	1.89	0.52
2:G:282:ILE:HG21	2:G:311:LEU:HD12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:PRO:CB	2:G:99:PRO:HD2	2.37	0.52
2:S:98:PRO:CB	2:S:99:PRO:HD2	2.38	0.52
2:O:398:GLY:HA2	2:O:404:VAL:HG22	1.92	0.52
2:C:217:LYS:CG	2:C:229:THR:HG23	2.40	0.52
2:P:282:ILE:HG21	2:P:311:LEU:HD12	1.91	0.52
2:S:216:ILE:HB	2:S:230:PHE:HD1	1.74	0.52
1:E:193:ASP:O	1:F:23:ARG:HD2	2.09	0.52
2:O:369:ASN:O	2:O:370:LYS:HB2	2.09	0.52
1:F:107:HIS:O	1:F:108:GLU:CB	2.45	0.52
2:P:233:HIS:HD2	2:P:257:THR:HG22	1.73	0.52
2:D:136:ASP:O	2:D:140:GLY:N	2.40	0.52
2:C:277:HIS:ND1	2:C:316:ARG:HB2	2.24	0.52
2:D:179:PHE:C	2:D:181:GLY:H	2.11	0.52
1:I:64:SER:N	1:I:65:PRO:CD	2.72	0.52
2:S:93:GLU:HA	2:S:351:LYS:NZ	2.25	0.52
2:C:358:ASP:HA	2:C:382:PHE:HB3	1.92	0.52
2:G:210:ALA:HB2	2:G:240:VAL:CG2	2.37	0.52
2:T:212:ARG:HG2	2:T:236:TRP:CD2	2.44	0.52
2:O:173:THR:O	2:O:174:ILE:HG13	2.09	0.52
2:K:129:ASP:N	2:K:130:ALA:HA	2.24	0.52
2:C:388:PHE:CD1	2:C:395:VAL:CG1	2.92	0.52
2:C:392:ALA:HB1	2:C:393:PRO:CD	2.39	0.52
2:D:127:SER:O	2:D:153:VAL:HG23	2.09	0.52
2:L:116:PHE:CE1	2:L:396:VAL:HG22	2.45	0.52
2:K:251:SER:OG	2:K:259:ARG:HB2	2.10	0.52
2:H:401:ASP:N	2:H:401:ASP:OD1	2.33	0.52
1:A:101:TRP:CE3	1:A:137:LEU:HD12	2.44	0.52
2:P:282:ILE:HA	2:P:312:LEU:O	2.10	0.52
2:D:144:ARG:NH1	2:D:181:GLY:O	2.43	0.52
2:K:383:VAL:HG13	2:K:397:THR:HG23	1.91	0.52
2:C:155:ASP:HB3	2:C:198:VAL:HG12	1.90	0.52
1:Q:207:LYS:HB3	1:Q:208:PRO:HD3	1.92	0.52
2:S:252:CYS:SG	2:S:282:ILE:HG12	2.49	0.52
2:O:367:TYR:CD2	2:O:367:TYR:N	2.75	0.52
2:P:213:ASP:HB3	2:P:215:THR:CB	2.40	0.52
2:L:193:HIS:CD2	2:L:194:ASN:N	2.73	0.52
2:H:187:THR:HG22	2:H:189:HIS:NE2	2.25	0.52
2:K:401:ASP:OD1	2:K:403:THR:OG1	2.27	0.52
2:D:191:HIS:HA	2:D:213:ASP:OD2	2.10	0.52
2:P:293:ILE:CG2	2:P:294:SER:N	2.73	0.52
1:R:11:ILE:O	1:R:79:ARG:HD2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:389:HIS:ND1	2:K:392:ALA:HB3	2.23	0.52
2:K:136:ASP:O	2:K:140:GLY:N	2.40	0.52
1:B:84:ARG:HB3	1:B:84:ARG:HH11	1.74	0.52
2:C:135:TRP:CD1	2:C:135:TRP:N	2.75	0.52
2:C:129:ASP:N	2:C:130:ALA:HA	2.25	0.52
2:H:379:HIS:CE1	2:H:405:LYS:HG3	2.45	0.52
2:C:252:CYS:CB	2:C:282:ILE:HD11	2.34	0.52
2:H:236:TRP:O	2:H:253:SER:HB2	2.09	0.52
2:C:382:PHE:O	2:C:399:SER:HB2	2.10	0.52
2:O:132:ILE:HB	2:O:146:LEU:HB2	1.90	0.52
2:T:334:LEU:HB3	2:T:365:TRP:CZ3	2.45	0.52
2:K:144:ARG:HH22	2:K:181:GLY:CA	2.20	0.52
2:G:155:ASP:H	2:G:168:CYS:HB2	1.75	0.52
2:H:141:ASP:C	2:H:143:GLU:H	2.12	0.52
2:T:136:ASP:O	2:T:140:GLY:N	2.38	0.52
2:S:251:SER:OG	2:S:259:ARG:HB2	2.08	0.52
2:S:345:LEU:HB3	2:S:354:LEU:HB2	1.92	0.52
2:K:114:VAL:HG23	2:K:385:SER:HB2	1.92	0.52
1:A:142:ARG:NH2	1:A:195:LEU:HD13	2.24	0.52
2:C:173:THR:CG2	2:C:187:THR:HG23	2.40	0.52
2:S:336:GLY:HA3	2:S:365:TRP:CH2	2.45	0.52
2:C:336:GLY:HA3	2:C:365:TRP:CH2	2.45	0.52
2:D:193:HIS:HD2	2:D:194:ASN:HB2	1.74	0.52
2:L:149:HIS:NE2	2:L:175:LYS:HG3	2.25	0.52
2:D:312:LEU:HD11	2:D:353:ILE:HD13	1.92	0.52
2:C:171:ASP:OD2	2:C:173:THR:OG1	2.22	0.52
2:D:156:ILE:HG23	2:D:165:LEU:HD11	1.92	0.52
2:H:236:TRP:O	2:H:253:SER:CB	2.58	0.52
2:P:399:SER:OG	2:P:401:ASP:OD1	2.27	0.52
1:A:67:HIS:CE1	2:C:340:TRP:CD2	2.97	0.52
2:S:211:SER:CB	2:S:213:ASP:HB2	2.40	0.52
2:L:110:PRO:HG2	2:L:128:GLU:OE1	2.10	0.52
2:C:117:HIS:CD2	2:C:118:PRO:HD2	2.45	0.52
2:C:107:HIS:CE1	2:C:133:LYS:HG3	2.44	0.52
2:H:158:PHE:CE2	2:H:165:LEU:HD13	2.44	0.52
2:T:193:HIS:CD2	2:T:194:ASN:H	2.27	0.52
1:J:14:ALA:HB2	1:J:83:TRP:CE2	2.44	0.52
2:H:379:HIS:NE2	2:H:397:THR:HG22	2.18	0.51
2:L:179:PHE:C	2:L:181:GLY:N	2.64	0.51
2:O:191:HIS:CE1	2:O:217:LYS:HD2	2.45	0.51
2:C:215:THR:HG22	2:C:216:ILE:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:218:MET:HE2	2:G:228:LYS:HD2	1.91	0.51
1:B:44:PHE:HB3	1:B:50:VAL:HG11	1.92	0.51
1:Q:193:ASP:OD2	1:Q:196:HIS:ND1	2.43	0.51
2:D:245:ASP:HB3	2:D:247:THR:OG1	2.10	0.51
2:L:315:SER:OG	2:L:316:ARG:N	2.44	0.51
2:D:129:ASP:N	2:D:130:ALA:HA	2.24	0.51
2:K:345:LEU:O	2:K:353:ILE:HG23	2.11	0.51
2:C:359:ASP:O	2:C:361:THR:CB	2.48	0.51
2:L:337:HIS:N	2:L:337:HIS:HD2	2.08	0.51
2:T:98:PRO:CB	2:T:99:PRO:HD2	2.39	0.51
2:C:141:ASP:C	2:C:143:GLU:H	2.11	0.51
2:H:171:ASP:C	2:H:172:MET:HG3	2.31	0.51
2:H:237:VAL:HA	2:H:253:SER:HB3	1.93	0.51
2:H:173:THR:HG21	2:H:175:LYS:HE2	1.91	0.51
2:O:358:ASP:HA	2:O:382:PHE:HB2	1.92	0.51
1:M:58:ILE:HD11	1:M:206:CYS:SG	2.51	0.51
2:L:149:HIS:CE1	2:L:175:LYS:HG3	2.45	0.51
2:G:213:ASP:HB3	2:G:215:THR:CB	2.41	0.51
2:D:149:HIS:CD2	2:D:153:VAL:HG13	2.45	0.51
2:K:243:ASN:ND2	2:K:245:ASP:HB2	2.26	0.51
2:S:206:HIS:HB3	2:S:218:MET:SD	2.50	0.51
1:A:101:TRP:CD2	1:A:137:LEU:HD12	2.46	0.51
1:E:181:HIS:CE1	2:H:108:ARG:NE	2.75	0.51
2:L:345:LEU:CD1	2:L:388:PHE:HB2	2.39	0.51
2:G:144:ARG:NH2	2:G:181:GLY:HA2	2.25	0.51
2:P:275:HIS:CE1	2:P:321:LYS:HE2	2.45	0.51
2:P:213:ASP:O	2:P:214:LYS:HB2	2.10	0.51
2:O:213:ASP:O	2:O:214:LYS:HB2	2.11	0.51
2:D:123:MET:HE1	2:D:135:TRP:CD1	2.46	0.51
2:S:133:LYS:HG2	2:S:145:THR:HG23	1.93	0.51
2:P:187:THR:HG22	2:P:189:HIS:NE2	2.26	0.51
2:L:201:MET:CE	2:L:242:PRO:HB3	2.41	0.51
2:K:361:THR:HG21	2:K:375:THR:HG23	1.92	0.51
2:P:156:ILE:HG22	2:P:157:SER:N	2.25	0.51
2:H:361:THR:CG2	2:H:363:ARG:HG3	2.41	0.51
1:A:163:SER:O	1:A:166:LYS:HG3	2.11	0.51
2:L:201:MET:HE3	2:L:242:PRO:HB3	1.92	0.51
2:L:275:HIS:CE1	2:L:321:LYS:HG3	2.46	0.51
2:G:272:LEU:HD13	2:G:323:TRP:CD2	2.45	0.51
2:S:136:ASP:O	2:S:140:GLY:N	2.40	0.51
2:C:109:SER:OG	2:C:110:PRO:HD2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:322:MET:HB2	2:O:332:MET:H	1.75	0.51
2:L:136:ASP:O	2:L:140:GLY:N	2.37	0.51
2:D:311:LEU:O	2:D:323:TRP:CD1	2.57	0.51
2:D:136:ASP:OD1	2:D:139:THR:HB	2.11	0.51
2:P:94:TRP:HH2	2:P:392:ALA:CA	2.24	0.51
2:K:179:PHE:C	2:K:181:GLY:N	2.64	0.51
2:D:211:SER:HB3	2:D:213:ASP:HB2	1.92	0.51
2:S:360:LYS:CE	2:S:377:ASN:HB3	2.41	0.51
2:G:131:THR:HG22	2:G:145:THR:HG22	1.93	0.51
2:C:282:ILE:HG23	2:C:312:LEU:O	2.10	0.51
2:D:216:ILE:HB	2:D:230:PHE:HB2	1.92	0.51
2:L:94:TRP:CH2	2:L:392:ALA:C	2.84	0.51
2:L:334:LEU:HD13	2:L:365:TRP:CE3	2.45	0.51
1:N:122:VAL:HG11	1:N:170:VAL:HG11	1.93	0.51
1:J:118:ILE:HA	1:J:121:ILE:HD12	1.91	0.51
1:N:144:GLU:HG3	1:N:194:PHE:CE2	2.45	0.51
2:G:360:LYS:HE3	2:G:377:ASN:HB3	1.93	0.51
1:M:11:ILE:O	1:M:79:ARG:HD2	2.11	0.51
2:C:232:GLY:HA3	2:C:261:TRP:HH2	1.75	0.51
2:D:173:THR:HG21	2:D:187:THR:HG23	1.93	0.51
2:G:218:MET:O	2:G:227:VAL:HG23	2.10	0.51
2:T:339:ASN:O	2:T:357:ALA:HB1	2.11	0.51
1:M:39:GLU:OE2	2:O:238:ARG:NH2	2.44	0.51
2:O:159:ASP:HA	2:O:200:ILE:HG21	1.92	0.51
1:M:45:VAL:HG12	1:M:71:PHE:HB2	1.93	0.51
2:L:277:HIS:ND1	2:L:316:ARG:HB2	2.26	0.50
2:L:139:THR:CG2	2:L:141:ASP:OD2	2.59	0.50
2:S:336:GLY:HA3	2:S:365:TRP:HH2	1.76	0.50
2:D:140:GLY:O	2:D:141:ASP:OD1	2.28	0.50
2:L:178:ASP:HB2	2:L:185:ILE:HD11	1.93	0.50
2:O:360:LYS:CB	2:O:379:HIS:O	2.59	0.50
2:G:136:ASP:O	2:G:140:GLY:N	2.41	0.50
2:T:397:THR:O	2:T:404:VAL:HA	2.10	0.50
2:C:144:ARG:CZ	2:C:181:GLY:HA2	2.41	0.50
2:K:96:PRO:HD2	2:K:97:ARG:HG2	1.93	0.50
1:M:122:VAL:O	1:M:126:ASN:ND2	2.44	0.50
2:O:309:PRO:HG2	2:O:325:VAL:HB	1.94	0.50
2:K:297:THR:HG22	2:K:298:GLY:H	1.76	0.50
1:B:15:ALA:HB2	1:B:80:HIS:CD2	2.46	0.50
1:I:162:VAL:HG12	1:I:163:SER:N	2.26	0.50
2:H:214:LYS:HZ1	2:H:234:ARG:HH21	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:373:MET:O	2:S:374:LYS:HB3	2.11	0.50
2:L:129:ASP:HB3	2:L:131:THR:N	2.27	0.50
2:L:123:MET:CE	2:L:404:VAL:HG11	2.42	0.50
2:D:272:LEU:HB3	2:D:323:TRP:CZ3	2.46	0.50
2:T:112:THR:HG21	2:T:154:GLN:HG3	1.93	0.50
2:S:132:ILE:HG12	2:S:156:ILE:CD1	2.38	0.50
2:L:168:CYS:SG	2:L:195:VAL:HG12	2.50	0.50
2:O:178:ASP:OD1	2:O:180:GLN:HB2	2.11	0.50
2:S:350:GLY:O	2:S:367:TYR:OH	2.27	0.50
2:P:122:VAL:HG22	2:P:136:ASP:H	1.76	0.50
2:O:288:SER:HB2	2:O:350:GLY:HA3	1.92	0.50
2:G:400:VAL:O	2:G:400:VAL:HG12	2.11	0.50
2:O:383:VAL:HA	2:O:399:SER:CB	2.40	0.50
2:S:193:HIS:CG	2:S:194:ASN:H	2.30	0.50
1:F:8:PRO:O	1:F:79:ARG:HD2	2.10	0.50
2:C:233:HIS:CE1	2:C:251:SER:OG	2.63	0.50
2:K:399:SER:OG	2:K:401:ASP:OD1	2.29	0.50
2:T:114:VAL:HG11	2:T:404:VAL:HG11	1.93	0.50
1:I:107:HIS:CE1	1:J:19:GLN:HG2	2.46	0.50
2:D:129:ASP:HB3	2:D:131:THR:CB	2.40	0.50
2:P:178:ASP:HB2	2:P:185:ILE:HD11	1.92	0.50
2:P:317:ASP:CB	2:P:319:THR:OG1	2.60	0.50
1:J:164:LEU:O	1:J:166:LYS:O	2.28	0.50
2:G:309:PRO:HG2	2:G:325:VAL:HG23	1.93	0.50
1:F:7:ASN:ND2	1:F:9:ALA:H	2.10	0.50
1:A:126:ASN:HD22	1:A:126:ASN:C	2.14	0.50
2:D:182:PHE:HB3	2:D:183:GLU:HG2	1.92	0.50
2:K:350:GLY:O	2:K:367:TYR:CZ	2.64	0.50
2:C:179:PHE:C	2:C:181:GLY:N	2.65	0.50
2:L:379:HIS:HE1	2:L:405:LYS:HG3	1.76	0.50
1:E:15:ALA:HB2	1:E:80:HIS:CD2	2.46	0.50
2:H:212:ARG:HG2	2:H:236:TRP:CD2	2.47	0.50
2:K:360:LYS:HZ3	2:K:377:ASN:HD22	1.58	0.50
1:F:53:MET:HG2	1:F:59:TRP:CE3	2.46	0.50
2:G:144:ARG:CZ	2:G:181:GLY:HA2	2.42	0.50
2:P:171:ASP:O	2:P:172:MET:CB	2.60	0.50
2:O:141:ASP:O	2:O:143:GLU:N	2.44	0.50
2:P:400:VAL:C	2:P:402:GLN:H	2.13	0.50
2:P:174:ILE:HB	2:P:188:MET:HE2	1.93	0.50
2:O:347:HIS:HB2	2:O:352:PHE:HB2	1.94	0.50
2:T:396:VAL:HG12	2:T:406:VAL:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:ILE:HG22	2:H:124:VAL:HB	1.93	0.50
2:G:128:GLU:HA	2:G:152:SER:OG	2.12	0.50
2:L:395:VAL:O	2:L:407:TRP:HD1	1.93	0.50
2:O:337:HIS:HE1	2:O:375:THR:CG2	2.16	0.50
2:D:336:GLY:HA2	2:D:365:TRP:HH2	1.75	0.50
2:C:392:ALA:HB1	2:C:393:PRO:HD2	1.94	0.50
2:G:369:ASN:ND2	2:G:371:ARG:HD2	2.26	0.50
2:T:342:ARG:HG3	2:T:384:THR:HA	1.93	0.50
2:C:234:ARG:HD3	2:C:234:ARG:O	2.11	0.50
2:S:311:LEU:O	2:S:323:TRP:HD1	1.94	0.50
2:O:310:PHE:HA	2:O:323:TRP:O	2.11	0.50
2:S:148:GLY:O	2:S:175:LYS:HE3	2.12	0.50
2:D:369:ASN:HD22	2:D:371:ARG:NH1	2.10	0.50
1:N:107:HIS:O	1:N:108:GLU:CB	2.60	0.50
2:D:281:CYS:HB3	2:D:344:VAL:HG23	1.94	0.50
2:S:179:PHE:C	2:S:181:GLY:N	2.64	0.50
2:O:190:GLY:HA3	2:O:219:TRP:HH2	1.75	0.50
2:K:316:ARG:HG2	2:K:340:TRP:CD2	2.47	0.50
2:G:360:LYS:CE	2:G:377:ASN:HD22	2.24	0.50
1:M:90:LEU:HD22	1:M:129:GLN:HG3	1.93	0.50
2:G:156:ILE:HG22	2:G:165:LEU:HD11	1.90	0.50
2:P:169:SER:OG	2:P:171:ASP:CB	2.60	0.50
2:S:312:LEU:HD21	2:S:346:PHE:HE1	1.73	0.50
2:D:392:ALA:HB1	2:D:393:PRO:HD2	1.94	0.50
2:C:114:VAL:HG11	2:C:396:VAL:HB	1.94	0.50
1:M:134:ILE:HB	1:M:170:VAL:HG13	1.94	0.50
1:J:134:ILE:HB	1:J:170:VAL:HG13	1.92	0.50
2:P:93:GLU:HA	2:P:351:LYS:NZ	2.27	0.50
1:I:44:PHE:HB3	1:I:50:VAL:CG1	2.41	0.50
2:C:152:SER:O	2:C:169:SER:CB	2.54	0.49
2:H:379:HIS:HD2	2:H:383:VAL:CG2	2.22	0.49
2:D:318:LYS:HB3	2:D:337:HIS:O	2.11	0.49
2:S:316:ARG:HD3	2:S:340:TRP:CE2	2.47	0.49
2:T:383:VAL:HA	2:T:399:SER:CB	2.37	0.49
2:L:367:TYR:H	2:L:367:TYR:HD2	1.59	0.49
2:K:98:PRO:HB3	2:K:99:PRO:CD	2.39	0.49
2:S:171:ASP:HB2	2:S:173:THR:OG1	2.11	0.49
1:J:58:ILE:HD11	1:J:206:CYS:CB	2.42	0.49
2:C:288:SER:HB2	2:C:350:GLY:HA3	1.93	0.49
2:P:217:LYS:HD3	2:P:226:CYS:SG	2.51	0.49
2:D:123:MET:HG2	2:D:124:VAL:N	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:233:HIS:CD2	2:K:253:SER:OG	2.65	0.49
2:O:144:ARG:NH2	2:O:181:GLY:CA	2.75	0.49
2:O:179:PHE:C	2:O:181:GLY:N	2.64	0.49
2:H:201:MET:HE1	2:H:242:PRO:HB3	1.94	0.49
2:C:366:ASP:OD1	2:C:368:LYS:HB3	2.11	0.49
2:H:109:SER:HA	2:H:402:GLN:NE2	2.27	0.49
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.94	0.49
2:C:243:ASN:O	2:C:244:GLN:C	2.49	0.49
1:M:7:ASN:ND2	1:M:9:ALA:H	2.11	0.49
2:D:397:THR:HG22	2:D:405:LYS:HB2	1.94	0.49
2:C:123:MET:CE	2:C:404:VAL:HG11	2.43	0.49
2:S:216:ILE:CG2	2:S:240:VAL:HG11	2.42	0.49
1:E:23:ARG:NH2	1:F:193:ASP:OD2	2.42	0.49
1:F:212:LEU:O	1:F:215:GLN:HB3	2.12	0.49
2:G:159:ASP:CA	2:G:200:ILE:HG21	2.35	0.49
1:I:13:HIS:H	1:I:83:TRP:HB2	1.77	0.49
2:L:203:ASN:H	2:L:203:ASN:HD22	1.60	0.49
2:G:317:ASP:CB	2:G:319:THR:OG1	2.61	0.49
1:E:166:LYS:O	1:E:167:LEU:HB2	2.13	0.49
2:P:94:TRP:HH2	2:P:391:THR:O	1.95	0.49
2:G:354:LEU:HD22	2:G:364:VAL:HG22	1.93	0.49
2:G:123:MET:CE	2:G:135:TRP:CD1	2.95	0.49
2:H:120:PHE:HD2	2:L:369:ASN:HB3	1.76	0.49
2:H:127:SER:OG	2:H:128:GLU:N	2.46	0.49
2:C:389:HIS:O	2:C:391:THR:N	2.46	0.49
2:G:213:ASP:HB3	2:G:215:THR:HB	1.95	0.49
2:O:345:LEU:CD1	2:O:388:PHE:HB2	2.42	0.49
2:G:272:LEU:HB3	2:G:323:TRP:CZ3	2.48	0.49
2:D:383:VAL:HA	2:D:399:SER:HB3	1.94	0.49
1:I:159:LEU:HD23	1:I:159:LEU:N	2.27	0.49
2:K:353:ILE:HG13	2:K:367:TYR:HD2	1.78	0.49
2:C:312:LEU:HD22	2:C:322:MET:HG2	1.93	0.49
2:D:98:PRO:CB	2:D:99:PRO:CD	2.90	0.49
2:D:208:VAL:HG21	2:D:249:ILE:HD11	1.95	0.49
2:D:216:ILE:CD1	2:D:251:SER:HB2	2.42	0.49
2:T:361:THR:HG22	2:T:363:ARG:CG	2.39	0.49
2:O:358:ASP:OD1	2:O:382:PHE:CD2	2.64	0.49
2:O:334:LEU:HD13	2:O:365:TRP:CE2	2.47	0.49
1:F:19:GLN:HE22	1:F:23:ARG:HH11	1.59	0.49
2:H:132:ILE:HB	2:H:146:LEU:HB2	1.93	0.49
1:R:106:ASN:HD22	1:R:106:ASN:N	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:HIS:CE1	2:K:340:TRP:CE2	3.00	0.49
2:G:339:ASN:HD22	2:G:340:TRP:H	1.60	0.49
2:H:129:ASP:N	2:H:130:ALA:HA	2.28	0.49
2:L:249:ILE:HD12	2:L:263:VAL:HG23	1.95	0.49
2:C:281:CYS:SG	2:C:342:ARG:C	2.91	0.49
1:M:36:LYS:O	2:O:212:ARG:NH2	2.46	0.49
2:G:129:ASP:CB	2:G:131:THR:OG1	2.46	0.49
2:G:98:PRO:CB	2:G:99:PRO:CD	2.90	0.49
2:O:129:ASP:HB3	2:O:131:THR:OG1	2.13	0.49
2:P:316:ARG:HG2	2:P:340:TRP:CG	2.48	0.49
2:G:213:ASP:O	2:G:214:LYS:HB2	2.12	0.49
2:L:116:PHE:CZ	2:L:396:VAL:HG22	2.47	0.49
2:S:360:LYS:HE2	2:S:377:ASN:HB3	1.93	0.49
1:E:177:GLY:O	1:E:179:PHE:N	2.43	0.49
1:E:109:ASN:O	1:E:152:LYS:HE3	2.13	0.49
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.70	0.49
2:K:272:LEU:HD13	2:K:323:TRP:CE2	2.48	0.49
2:C:233:HIS:HB3	2:C:255:ASP:CG	2.33	0.49
2:C:368:LYS:O	2:C:369:ASN:ND2	2.46	0.49
2:K:115:ILE:HG22	2:K:124:VAL:HB	1.94	0.49
1:I:60:ARG:HA	1:I:64:SER:OG	2.12	0.49
1:J:180:VAL:HG12	1:J:184:GLY:HA2	1.95	0.49
2:G:401:ASP:C	2:G:402:GLN:HG3	2.32	0.49
2:C:382:PHE:O	2:C:399:SER:CB	2.61	0.49
2:O:277:HIS:ND1	2:O:316:ARG:HB2	2.28	0.49
2:D:122:VAL:HG22	2:D:136:ASP:N	2.28	0.49
2:C:153:VAL:HA	2:C:168:CYS:O	2.13	0.49
1:N:46:GLY:HA2	1:N:102:VAL:HG22	1.94	0.49
2:L:210:ALA:HB2	2:L:240:VAL:HG22	1.95	0.48
2:T:132:ILE:HG12	2:T:156:ILE:HD11	1.94	0.48
2:P:347:HIS:HD2	2:P:349:GLY:H	1.60	0.48
2:C:397:THR:HB	2:C:407:TRP:HE1	1.78	0.48
2:H:379:HIS:HE1	2:H:405:LYS:HG3	1.77	0.48
2:O:392:ALA:CB	2:O:393:PRO:CD	2.87	0.48
2:O:98:PRO:CB	2:O:99:PRO:HD2	2.42	0.48
2:H:141:ASP:O	2:H:143:GLU:N	2.44	0.48
2:C:243:ASN:HD22	2:C:248:LEU:N	2.11	0.48
2:L:315:SER:HB3	2:L:317:ASP:HB2	1.95	0.48
2:S:316:ARG:HA	2:S:340:TRP:CD1	2.49	0.48
2:D:97:ARG:HG3	2:D:98:PRO:HD3	1.94	0.48
1:N:58:ILE:HG13	1:N:58:ILE:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:236:TRP:HD1	2:L:237:VAL:N	2.11	0.48
2:C:155:ASP:HB2	2:C:197:SER:HA	1.94	0.48
2:S:349:GLY:HA3	2:S:351:LYS:HD2	1.95	0.48
2:S:93:GLU:HA	2:S:351:LYS:HZ2	1.77	0.48
2:K:243:ASN:O	2:K:244:GLN:C	2.51	0.48
2:P:101:LYS:HG2	2:P:408:GLU:OE2	2.13	0.48
1:M:78:THR:N	1:M:106:ASN:HD21	2.04	0.48
2:O:382:PHE:O	2:O:400:VAL:HG23	2.14	0.48
2:K:360:LYS:NZ	2:K:377:ASN:HB3	2.27	0.48
2:P:169:SER:OG	2:P:171:ASP:HB2	2.13	0.48
2:T:201:MET:HG3	2:T:206:HIS:HB2	1.95	0.48
2:G:233:HIS:HB3	2:G:255:ASP:OD2	2.13	0.48
2:C:182:PHE:CD2	2:C:182:PHE:C	2.85	0.48
2:L:381:HIS:ND1	2:L:382:PHE:N	2.61	0.48
2:S:278:VAL:HB	2:S:316:ARG:CG	2.39	0.48
2:C:203:ASN:O	2:C:203:ASN:CG	2.52	0.48
2:P:255:ASP:O	2:P:256:GLN:HB2	2.13	0.48
2:P:262:VAL:CG1	2:P:265:THR:H	2.26	0.48
2:P:389:HIS:HE1	2:P:391:THR:HG22	1.77	0.48
2:C:293:ILE:CG2	2:C:294:SER:N	2.77	0.48
1:R:147:ASN:HB2	1:R:148:PRO:HD2	1.96	0.48
2:G:190:GLY:HA3	2:G:219:TRP:HH2	1.79	0.48
1:B:154:ALA:HA	1:B:157:ASN:HD22	1.78	0.48
2:G:152:SER:O	2:G:169:SER:CB	2.61	0.48
2:G:243:ASN:HD21	2:G:245:ASP:HB3	1.78	0.48
2:C:286:PRO:HB2	2:C:287:GLU:H	1.46	0.48
1:F:84:ARG:HD2	1:F:89:GLU:OE2	2.14	0.48
1:R:43:LEU:HB3	1:R:98:ILE:HG12	1.94	0.48
2:K:278:VAL:HB	2:K:316:ARG:HD2	1.95	0.48
2:K:250:ALA:HB2	2:K:284:TRP:CZ2	2.48	0.48
2:D:337:HIS:NE2	2:D:363:ARG:HG2	2.29	0.48
2:H:347:HIS:CD2	2:H:348:SER:N	2.81	0.48
2:L:171:ASP:O	2:L:172:MET:HG3	2.13	0.48
2:C:104:LEU:HD12	2:C:404:VAL:HB	1.96	0.48
1:Q:160:LEU:HB3	1:Q:172:LEU:HD13	1.96	0.48
1:M:47:ASP:OD2	1:M:49:MET:HG2	2.13	0.48
2:K:337:HIS:HD2	2:K:337:HIS:N	2.12	0.48
2:P:337:HIS:CE1	2:P:363:ARG:HG2	2.48	0.48
1:J:7:ASN:ND2	1:J:7:ASN:C	2.67	0.48
2:P:293:ILE:CG2	2:P:294:SER:H	2.26	0.48
2:P:168:CYS:SG	2:P:198:VAL:HB	2.54	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:LEU:HD21	1:I:71:PHE:CD1	2.49	0.48
1:I:28:HIS:O	1:I:32:VAL:HG23	2.14	0.48
2:K:152:SER:O	2:K:169:SER:HA	2.14	0.48
2:P:127:SER:C	2:P:129:ASP:H	2.17	0.48
2:C:98:PRO:CB	2:C:99:PRO:CD	2.88	0.48
2:K:353:ILE:HB	2:K:365:TRP:HB2	1.95	0.48
2:G:395:VAL:HG23	2:G:407:TRP:HB2	1.96	0.48
2:K:176:LEU:HD11	2:K:221:VAL:HG13	1.94	0.48
2:L:233:HIS:HD1	2:L:233:HIS:H	1.62	0.48
2:G:178:ASP:OD2	2:G:180:GLN:HB2	2.13	0.48
2:L:101:LYS:NZ	2:L:408:GLU:OE1	2.47	0.48
1:I:141:PRO:HB2	1:I:186:ILE:HD11	1.96	0.48
2:G:133:LYS:HG2	2:G:145:THR:HG23	1.95	0.48
2:P:236:TRP:HD1	2:P:237:VAL:N	2.12	0.48
2:D:397:THR:CG2	2:D:407:TRP:HE1	2.26	0.48
2:L:354:LEU:CD2	2:L:364:VAL:HG13	2.44	0.48
1:I:46:GLY:HA3	1:I:50:VAL:HG21	1.95	0.48
1:B:88:GLY:HA2	1:B:91:GLU:HG3	1.96	0.48
2:C:225:TYR:CD2	1:F:154:ALA:HB1	2.49	0.48
2:T:337:HIS:HB2	2:T:363:ARG:HH21	1.79	0.47
2:D:258:VAL:HB	2:D:272:LEU:HB2	1.96	0.47
1:J:7:ASN:HD22	1:J:8:PRO:N	2.12	0.47
2:K:131:THR:HG21	2:K:145:THR:CG2	2.44	0.47
1:Q:22:ASP:OD2	1:Q:25:MET:HB2	2.14	0.47
1:J:131:GLN:OE1	1:J:131:GLN:N	2.38	0.47
1:M:95:PRO:HD2	1:M:129:GLN:OE1	2.14	0.47
2:P:337:HIS:CG	2:P:363:ARG:HG2	2.49	0.47
2:G:315:SER:OG	2:G:316:ARG:N	2.47	0.47
1:F:166:LYS:HA	2:P:203:ASN:HD22	1.80	0.47
2:P:94:TRP:CH2	2:P:391:THR:O	2.68	0.47
1:N:191:MET:HB3	1:N:194:PHE:HA	1.96	0.47
2:O:288:SER:CB	2:O:350:GLY:HA3	2.44	0.47
2:H:123:MET:HE2	2:H:135:TRP:HD1	1.78	0.47
1:E:43:LEU:HD13	1:E:45:VAL:HG13	1.96	0.47
2:T:238:ARG:HD3	2:T:280:GLU:HG3	1.96	0.47
2:S:400:VAL:C	2:S:402:GLN:H	2.17	0.47
2:D:320:ILE:HB	2:D:334:LEU:HB2	1.95	0.47
2:S:309:PRO:O	2:S:325:VAL:HG23	2.14	0.47
2:K:261:TRP:N	2:K:261:TRP:CD1	2.82	0.47
2:H:366:ASP:C	2:H:368:LYS:N	2.68	0.47
2:S:277:HIS:HB3	2:S:316:ARG:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:381:HIS:ND1	2:S:382:PHE:N	2.60	0.47
2:H:345:LEU:HD13	2:H:388:PHE:HB2	1.96	0.47
2:G:134:VAL:O	2:G:143:GLU:HB2	2.14	0.47
1:J:58:ILE:HD11	1:J:206:CYS:HB3	1.95	0.47
2:G:96:PRO:HD2	2:G:97:ARG:HG2	1.94	0.47
2:K:348:SER:OG	2:K:390:LYS:HA	2.15	0.47
2:K:219:TRP:CD1	2:K:219:TRP:N	2.83	0.47
2:H:279:VAL:HA	2:H:315:SER:HB2	1.97	0.47
2:H:153:VAL:HA	2:H:168:CYS:O	2.13	0.47
2:G:358:ASP:HA	2:G:382:PHE:HB3	1.94	0.47
2:C:252:CYS:HB2	2:C:282:ILE:CD1	2.36	0.47
2:L:214:LYS:HZ2	2:L:234:ARG:HH22	1.62	0.47
2:P:389:HIS:ND1	2:P:392:ALA:N	2.45	0.47
2:D:173:THR:CG2	2:D:187:THR:CG2	2.93	0.47
1:Q:160:LEU:HD22	1:Q:164:LEU:HG	1.95	0.47
2:S:216:ILE:HB	2:S:230:PHE:CD1	2.49	0.47
1:I:179:PHE:O	1:I:186:ILE:HG12	2.15	0.47
2:T:133:LYS:HG2	2:T:145:THR:HG23	1.97	0.47
2:O:232:GLY:HA3	2:O:261:TRP:HH2	1.80	0.47
2:K:212:ARG:HG2	2:K:236:TRP:CG	2.49	0.47
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.95	0.47
2:P:330:CYS:SG	2:P:332:MET:O	2.72	0.47
2:K:400:VAL:C	2:K:402:GLN:H	2.18	0.47
2:K:396:VAL:HA	2:K:405:LYS:O	2.14	0.47
2:H:235:GLU:HA	2:H:235:GLU:OE1	2.09	0.47
2:S:373:MET:O	2:S:374:LYS:CB	2.61	0.47
2:C:149:HIS:NE2	2:C:167:SER:OG	2.47	0.47
1:E:181:HIS:CD2	2:H:108:ARG:HD2	2.50	0.47
2:T:102:TYR:O	2:T:405:LYS:HA	2.14	0.47
1:J:126:ASN:C	1:J:126:ASN:ND2	2.66	0.47
2:K:131:THR:CG2	2:K:145:THR:CG2	2.93	0.47
2:H:281:CYS:SG	2:H:343:GLY:CA	3.02	0.47
2:K:114:VAL:HG12	2:K:123:MET:HE3	1.97	0.47
2:G:233:HIS:HD2	2:G:257:THR:HG22	1.78	0.47
1:M:19:GLN:HE22	1:M:23:ARG:HH11	1.60	0.47
1:R:45:VAL:HG11	1:R:85:LEU:HD21	1.96	0.47
2:T:250:ALA:HB2	2:T:284:TRP:CZ2	2.50	0.47
1:M:67:HIS:HE1	2:O:339:ASN:HD21	1.63	0.47
1:M:85:LEU:HB3	1:M:90:LEU:HD12	1.96	0.47
2:L:379:HIS:CD2	2:L:399:SER:HB3	2.49	0.47
2:T:171:ASP:OD1	2:T:171:ASP:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ASN:HD22	2:C:203:ASN:H	1.62	0.47
2:L:344:VAL:HG12	2:L:344:VAL:O	2.14	0.47
2:G:312:LEU:HD22	2:G:322:MET:CG	2.43	0.47
1:F:103:GLY:HA3	1:F:139:LEU:HD11	1.96	0.47
2:G:354:LEU:CD2	2:G:354:LEU:N	2.77	0.47
1:I:47:ASP:OD2	1:I:49:MET:N	2.40	0.47
2:K:389:HIS:HB3	2:K:392:ALA:O	2.15	0.47
2:G:369:ASN:HD22	2:G:371:ARG:HD2	1.80	0.47
1:I:50:VAL:HG12	1:I:70:ASN:HD21	1.79	0.47
2:L:216:ILE:HB	2:L:230:PHE:HB2	1.96	0.47
1:Q:76:ASP:HA	1:Q:80:HIS:ND1	2.30	0.47
1:N:54:GLN:NE2	1:N:70:ASN:HB3	2.29	0.47
2:S:243:ASN:O	2:S:244:GLN:C	2.53	0.47
1:E:197:LEU:HB2	1:E:202:TYR:CE1	2.50	0.47
1:Q:7:ASN:ND2	1:Q:9:ALA:H	2.13	0.47
1:J:15:ALA:HB2	1:J:80:HIS:CD2	2.50	0.47
1:R:46:GLY:HA2	1:R:102:VAL:HG22	1.95	0.47
2:H:286:PRO:HB2	2:H:287:GLU:H	1.52	0.47
1:E:38:LYS:HA	1:E:38:LYS:HD3	1.66	0.47
2:L:144:ARG:CZ	2:L:181:GLY:HA2	2.42	0.47
2:S:334:LEU:HB3	2:S:365:TRP:CZ3	2.50	0.47
2:L:258:VAL:HB	2:L:272:LEU:HB2	1.96	0.47
2:L:281:CYS:HB2	2:L:314:GLY:N	2.28	0.47
2:O:288:SER:CB	2:O:350:GLY:CA	2.93	0.47
2:T:149:HIS:NE2	2:T:167:SER:OG	2.40	0.47
1:A:188:CYS:HA	1:A:191:MET:O	2.14	0.47
2:G:297:THR:HG22	2:G:298:GLY:H	1.79	0.47
2:T:281:CYS:HB2	2:T:314:GLY:H	1.80	0.47
2:K:242:PRO:O	2:K:284:TRP:CD1	2.68	0.47
2:D:126:ALA:HB2	2:D:156:ILE:CD1	2.43	0.47
2:K:258:VAL:HB	2:K:272:LEU:HB2	1.97	0.47
2:P:172:MET:HA	2:P:195:VAL:HG23	1.96	0.47
2:C:122:VAL:HG22	2:C:136:ASP:N	2.30	0.47
2:C:117:HIS:HD2	2:C:158:PHE:CE2	2.32	0.47
1:A:23:ARG:O	1:A:27:GLN:HG3	2.14	0.47
1:F:147:ASN:HD22	1:F:149:LEU:H	1.61	0.47
2:L:243:ASN:O	2:L:244:GLN:C	2.52	0.47
2:O:324:ASP:H	2:O:331:LEU:HD21	1.80	0.47
2:P:374:LYS:HE2	2:P:375:THR:N	2.28	0.47
1:J:175:THR:CG2	1:J:205:ILE:HD13	2.44	0.47
2:K:191:HIS:CE1	2:K:217:LYS:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:149:HIS:NE2	2:G:167:SER:OG	2.38	0.47
2:T:110:PRO:HG2	2:T:128:GLU:OE1	2.15	0.46
2:G:312:LEU:HD21	2:G:346:PHE:CE1	2.49	0.46
2:L:336:GLY:HA2	2:L:365:TRP:CZ2	2.50	0.46
1:B:7:ASN:HD22	1:B:8:PRO:CD	2.27	0.46
2:P:169:SER:OG	2:P:171:ASP:CG	2.54	0.46
1:Q:180:VAL:HG12	1:Q:184:GLY:HA2	1.97	0.46
2:O:104:LEU:HD13	2:O:135:TRP:CG	2.51	0.46
1:J:181:HIS:CD2	2:K:108:ARG:HD2	2.50	0.46
1:N:67:HIS:HE1	2:P:339:ASN:HD21	1.64	0.46
2:H:348:SER:OG	2:H:390:LYS:HA	2.15	0.46
2:T:110:PRO:HG3	2:T:400:VAL:HG13	1.97	0.46
2:T:100:GLU:CD	2:T:405:LYS:HD3	2.35	0.46
2:O:171:ASP:C	2:O:172:MET:HG3	2.36	0.46
2:O:334:LEU:HD22	2:O:365:TRP:CE3	2.50	0.46
2:T:341:VAL:HA	2:T:357:ALA:HB2	1.96	0.46
2:H:135:TRP:N	2:H:135:TRP:CD1	2.83	0.46
2:K:366:ASP:CG	2:K:368:LYS:HB3	2.35	0.46
2:S:398:GLY:HA3	2:S:404:VAL:HG22	1.96	0.46
2:L:113:ARG:HD3	2:L:385:SER:HB3	1.97	0.46
1:B:180:VAL:HG12	1:B:184:GLY:HA2	1.97	0.46
1:I:22:ASP:OD2	1:I:25:MET:HB2	2.15	0.46
1:E:140:LEU:HB3	1:E:141:PRO:HD2	1.97	0.46
2:H:357:ALA:HB3	2:H:359:ASP:OD2	2.14	0.46
2:C:169:SER:OG	2:C:171:ASP:OD1	2.33	0.46
2:H:179:PHE:C	2:H:181:GLY:N	2.69	0.46
1:J:197:LEU:HB2	1:J:202:TYR:CD1	2.51	0.46
2:L:101:LYS:NZ	2:L:408:GLU:CD	2.69	0.46
2:O:152:SER:O	2:O:169:SER:HA	2.15	0.46
1:R:134:ILE:HB	1:R:170:VAL:HG13	1.97	0.46
2:C:127:SER:C	2:C:129:ASP:H	2.19	0.46
2:H:191:HIS:CE1	2:H:217:LYS:HD2	2.50	0.46
2:C:144:ARG:NH2	2:C:181:GLY:CA	2.73	0.46
1:A:19:GLN:HG2	1:B:107:HIS:CE1	2.51	0.46
2:S:363:ARG:HB2	2:S:365:TRP:NE1	2.30	0.46
2:G:337:HIS:HB2	2:G:363:ARG:HE	1.80	0.46
2:K:95:ILE:HA	2:K:96:PRO:HD3	1.73	0.46
2:K:207:ILE:CD1	2:K:221:VAL:HG22	2.42	0.46
2:L:110:PRO:HB3	2:L:400:VAL:HG22	1.97	0.46
2:D:312:LEU:HG	2:D:346:PHE:CE1	2.50	0.46
2:P:347:HIS:CG	2:P:348:SER:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:311:LEU:HD23	2:T:323:TRP:CB	2.24	0.46
2:G:127:SER:C	2:G:129:ASP:H	2.18	0.46
2:O:312:LEU:CD2	2:O:322:MET:HG2	2.44	0.46
2:H:95:ILE:HA	2:H:96:PRO:HD3	1.67	0.46
2:P:383:VAL:HA	2:P:399:SER:CB	2.44	0.46
2:D:141:ASP:C	2:D:143:GLU:H	2.19	0.46
2:K:193:HIS:CD2	2:K:194:ASN:N	2.80	0.46
1:B:39:GLU:OE2	2:D:316:ARG:NH2	2.31	0.46
2:P:262:VAL:HG12	2:P:265:THR:H	1.79	0.46
2:L:251:SER:OG	2:L:259:ARG:HB2	2.15	0.46
1:I:200:GLY:O	1:I:203:ALA:HB3	2.15	0.46
1:E:188:CYS:HA	1:E:191:MET:O	2.16	0.46
2:C:110:PRO:O	2:C:127:SER:HB2	2.15	0.46
2:L:310:PHE:CD2	2:L:324:ASP:HB2	2.50	0.46
2:H:337:HIS:N	2:H:337:HIS:HD2	2.09	0.46
2:D:213:ASP:HB3	2:D:215:THR:HB	1.96	0.46
1:N:166:LYS:O	1:N:167:LEU:HB2	2.16	0.46
2:H:123:MET:CE	2:H:135:TRP:CD1	2.98	0.46
2:S:110:PRO:HB3	2:S:400:VAL:HG13	1.97	0.46
2:S:285:ALA:HA	2:S:286:PRO:HD3	1.78	0.46
2:G:102:TYR:HB2	2:G:406:VAL:HB	1.97	0.46
2:T:113:ARG:HA	2:T:113:ARG:HD3	1.75	0.46
2:T:392:ALA:CB	2:T:393:PRO:CD	2.77	0.46
2:H:288:SER:HB2	2:H:350:GLY:HA3	1.98	0.46
1:Q:103:GLY:O	1:Q:106:ASN:HB2	2.15	0.46
1:J:13:HIS:H	1:J:83:TRP:HB2	1.79	0.46
1:B:100:VAL:HB	1:B:136:VAL:HG22	1.98	0.46
1:J:220:THR:HA	1:J:221:PRO:HD3	1.74	0.46
2:L:366:ASP:HB2	2:L:373:MET:HG2	1.98	0.46
2:G:135:TRP:N	2:G:135:TRP:CD1	2.83	0.46
1:M:166:LYS:O	1:M:167:LEU:HB2	2.15	0.46
2:O:159:ASP:HB3	2:O:200:ILE:HD13	1.97	0.46
1:M:43:LEU:HB3	1:M:98:ILE:HG23	1.97	0.46
2:O:101:LYS:HB2	2:O:408:GLU:HG3	1.96	0.46
2:S:362:LEU:HD23	2:S:376:LEU:CD1	2.46	0.46
1:I:180:VAL:HG12	1:I:184:GLY:HA2	1.98	0.46
2:G:110:PRO:O	2:G:127:SER:HB2	2.16	0.46
2:L:362:LEU:HD23	2:L:376:LEU:CD1	2.46	0.46
2:O:117:HIS:HD2	2:O:158:PHE:CE1	2.33	0.46
2:P:205:ASP:C	2:P:221:VAL:HG23	2.36	0.46
2:C:369:ASN:C	2:C:371:ARG:H	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ALA:HB2	1:E:83:TRP:CD2	2.50	0.46
2:H:136:ASP:O	2:H:140:GLY:N	2.39	0.46
1:M:177:GLY:O	1:M:179:PHE:N	2.48	0.46
2:H:215:THR:CG2	2:H:229:THR:CG2	2.94	0.46
1:Q:101:TRP:CD2	1:Q:137:LEU:HD12	2.51	0.46
2:S:342:ARG:HB3	2:S:384:THR:O	2.16	0.46
2:H:187:THR:HG22	2:H:189:HIS:CD2	2.50	0.46
2:P:95:ILE:HA	2:P:96:PRO:HD3	1.68	0.46
2:G:216:ILE:HD11	2:G:251:SER:HB2	1.97	0.46
2:P:285:ALA:HA	2:P:286:PRO:HD3	1.82	0.46
1:E:207:LYS:HB3	1:E:208:PRO:CD	2.46	0.46
1:A:131:GLN:N	1:A:131:GLN:OE1	2.43	0.46
2:H:217:LYS:CG	2:H:229:THR:HG23	2.45	0.45
2:G:152:SER:O	2:G:169:SER:HA	2.16	0.45
2:L:339:ASN:HB3	2:L:358:ASP:HB2	1.98	0.45
1:F:139:LEU:CB	1:F:153:ASN:HB3	2.45	0.45
1:A:53:MET:CE	1:A:206:CYS:SG	3.04	0.45
2:K:110:PRO:HG2	2:K:128:GLU:OE1	2.16	0.45
2:P:340:TRP:N	2:P:340:TRP:CD1	2.83	0.45
1:I:158:GLN:HB3	1:I:159:LEU:HD23	1.96	0.45
1:M:28:HIS:O	1:M:32:VAL:HG23	2.17	0.45
1:E:173:LEU:C	1:E:173:LEU:HD12	2.37	0.45
2:S:379:HIS:CE1	2:S:405:LYS:HG3	2.51	0.45
2:T:130:ALA:HB2	2:T:152:SER:HA	1.97	0.45
2:T:128:GLU:HA	2:T:152:SER:OG	2.15	0.45
2:K:381:HIS:CG	2:K:382:PHE:H	2.35	0.45
2:P:350:GLY:O	2:P:367:TYR:OH	2.23	0.45
2:C:211:SER:OG	2:C:212:ARG:N	2.49	0.45
2:P:109:SER:C	2:P:402:GLN:HG2	2.36	0.45
1:Q:7:ASN:HA	1:Q:8:PRO:HD2	1.86	0.45
1:Q:191:MET:HG3	1:Q:197:LEU:HD23	1.98	0.45
2:C:132:ILE:HB	2:C:146:LEU:HB2	1.97	0.45
2:H:116:PHE:CE1	2:H:389:HIS:HB2	2.50	0.45
2:T:393:PRO:HG2	2:T:394:TYR:CE2	2.50	0.45
2:O:359:ASP:OD1	2:O:361:THR:HB	2.16	0.45
2:S:340:TRP:O	2:S:357:ALA:HB1	2.17	0.45
2:C:337:HIS:HB2	2:C:363:ARG:HH21	1.80	0.45
2:L:350:GLY:O	2:L:367:TYR:OH	2.32	0.45
2:S:102:TYR:HB2	2:S:406:VAL:HG23	1.99	0.45
1:F:139:LEU:CD2	1:F:139:LEU:N	2.78	0.45
2:L:212:ARG:HG2	2:L:236:TRP:CD2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:127:SER:OG	2:K:128:GLU:N	2.50	0.45
2:P:136:ASP:O	2:P:140:GLY:N	2.41	0.45
2:G:178:ASP:HB2	2:G:185:ILE:HD11	1.98	0.45
1:J:66:LEU:HA	1:J:66:LEU:HD12	1.81	0.45
1:I:54:GLN:HG2	1:I:59:TRP:CE2	2.52	0.45
2:C:110:PRO:HG2	2:C:128:GLU:OE1	2.15	0.45
2:K:241:ARG:HA	2:K:242:PRO:HD3	1.78	0.45
2:H:213:ASP:O	2:H:214:LYS:CB	2.64	0.45
2:G:355:SER:OG	2:G:363:ARG:HD2	2.15	0.45
1:N:45:VAL:HG23	1:N:100:VAL:HG22	1.99	0.45
2:G:201:MET:HE1	2:G:242:PRO:HB3	1.98	0.45
1:J:147:ASN:HD22	1:J:149:LEU:H	1.64	0.45
2:S:341:VAL:HA	2:S:357:ALA:HB2	1.96	0.45
2:H:94:TRP:CZ2	2:H:393:PRO:HA	2.51	0.45
2:O:379:HIS:ND1	2:O:401:ASP:OD2	2.48	0.45
2:T:126:ALA:HB2	2:T:156:ILE:HD12	1.99	0.45
1:B:64:SER:N	1:B:65:PRO:CD	2.78	0.45
2:P:332:MET:CE	2:P:367:TYR:HB2	2.46	0.45
2:G:171:ASP:C	2:G:172:MET:HG3	2.37	0.45
2:H:107:HIS:NE2	2:H:125:SER:OG	2.30	0.45
2:O:243:ASN:O	2:O:244:GLN:C	2.54	0.45
2:K:135:TRP:CD1	2:K:135:TRP:N	2.81	0.45
2:P:98:PRO:CB	2:P:99:PRO:CD	2.85	0.45
2:O:374:LYS:HG3	2:O:375:THR:N	2.31	0.45
2:L:205:ASP:O	2:L:206:HIS:ND1	2.49	0.45
2:S:215:THR:CG2	2:S:229:THR:HG23	2.47	0.45
1:N:62:LEU:HA	1:N:62:LEU:HD12	1.79	0.45
2:D:149:HIS:NE2	2:D:167:SER:OG	2.45	0.45
2:H:285:ALA:HA	2:H:286:PRO:HD3	1.82	0.45
2:O:152:SER:O	2:O:169:SER:CB	2.65	0.45
1:J:147:ASN:HB2	1:J:148:PRO:HD2	1.98	0.45
1:E:47:ASP:OD2	1:E:49:MET:HG2	2.17	0.45
1:F:83:TRP:O	1:F:87:ASN:ND2	2.49	0.45
1:F:189:HIS:CD2	2:G:402:GLN:HE22	2.21	0.45
2:S:342:ARG:H	2:S:357:ALA:HA	1.82	0.45
2:T:152:SER:O	2:T:169:SER:HA	2.17	0.45
2:D:193:HIS:CD2	2:D:194:ASN:N	2.82	0.45
2:C:94:TRP:CH2	2:C:392:ALA:C	2.90	0.45
2:P:243:ASN:O	2:P:244:GLN:C	2.53	0.45
1:E:7:ASN:HD22	1:E:7:ASN:C	2.20	0.45
2:O:94:TRP:HB2	2:O:347:HIS:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ARG:O	1:E:26:SER:HB2	2.17	0.45
2:O:201:MET:HE3	2:O:202:PRO:HD2	1.99	0.45
2:S:152:SER:O	2:S:169:SER:HA	2.17	0.45
2:S:212:ARG:HG2	2:S:236:TRP:CD2	2.51	0.45
2:C:173:THR:HG22	2:C:187:THR:HG23	1.98	0.45
2:L:397:THR:CG2	2:L:407:TRP:HE1	2.30	0.45
2:D:337:HIS:HD2	2:D:337:HIS:H	1.63	0.45
1:A:43:LEU:C	1:A:43:LEU:HD22	2.37	0.45
2:D:149:HIS:HD2	2:D:153:VAL:HG13	1.81	0.45
2:L:274:GLU:O	2:L:321:LYS:HE3	2.17	0.45
1:R:85:LEU:HD22	1:R:90:LEU:HG	1.98	0.45
1:A:181:HIS:ND1	2:D:108:ARG:NH2	2.64	0.45
2:O:342:ARG:HB3	2:O:384:THR:O	2.17	0.45
2:L:95:ILE:HA	2:L:96:PRO:HD3	1.67	0.45
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.52	0.45
2:C:173:THR:HG21	2:C:175:LYS:HE2	1.98	0.45
2:O:393:PRO:O	2:O:394:TYR:CD2	2.70	0.45
2:H:94:TRP:CH2	2:H:393:PRO:HA	2.52	0.45
2:G:173:THR:CG2	2:G:187:THR:HG23	2.46	0.45
1:B:79:ARG:HH11	1:B:79:ARG:CG	2.30	0.45
2:K:127:SER:C	2:K:129:ASP:H	2.20	0.45
2:T:243:ASN:O	2:T:244:GLN:C	2.54	0.45
2:D:116:PHE:CE1	2:D:396:VAL:HG22	2.52	0.45
1:N:53:MET:HG3	1:N:202:TYR:CD2	2.51	0.45
2:S:272:LEU:HD13	2:S:323:TRP:CD2	2.51	0.45
2:T:310:PHE:CE2	2:T:324:ASP:HB3	2.44	0.45
2:P:233:HIS:HB3	2:P:255:ASP:CG	2.37	0.45
2:L:203:ASN:H	2:L:203:ASN:ND2	2.15	0.45
2:O:144:ARG:HH22	2:O:181:GLY:HA2	1.79	0.45
2:K:379:HIS:CD2	2:K:383:VAL:HG22	2.51	0.45
2:G:258:VAL:HB	2:G:272:LEU:HB2	1.99	0.45
2:K:152:SER:O	2:K:169:SER:HB2	2.16	0.45
2:K:216:ILE:CG2	2:K:240:VAL:HG11	2.47	0.45
1:Q:220:THR:HA	1:Q:221:PRO:HD3	1.74	0.45
2:H:379:HIS:CD2	2:H:397:THR:HG23	2.52	0.44
2:D:124:VAL:HG22	2:D:134:VAL:HG13	1.97	0.44
2:K:281:CYS:SG	2:K:343:GLY:CA	3.06	0.44
2:L:285:ALA:HA	2:L:286:PRO:HD3	1.68	0.44
2:D:243:ASN:O	2:D:244:GLN:C	2.55	0.44
1:N:11:ILE:O	1:N:79:ARG:HD2	2.17	0.44
2:P:249:ILE:HG22	2:P:261:TRP:CD1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:HB2	1:A:123:GLN:HE21	1.49	0.44
1:B:207:LYS:HB3	1:B:208:PRO:HD3	1.99	0.44
2:D:212:ARG:HG2	2:D:236:TRP:CE2	2.51	0.44
2:D:201:MET:HE2	2:D:242:PRO:HB3	1.97	0.44
2:O:233:HIS:HB3	2:O:255:ASP:OD1	2.17	0.44
2:G:337:HIS:HB2	2:G:363:ARG:NH2	2.30	0.44
1:E:103:GLY:HA2	1:E:106:ASN:ND2	2.29	0.44
2:T:103:ALA:CA	2:T:405:LYS:HG2	2.44	0.44
1:J:7:ASN:HA	1:J:8:PRO:HD2	1.81	0.44
2:D:381:HIS:O	2:D:382:PHE:C	2.55	0.44
1:I:50:VAL:HG12	1:I:70:ASN:ND2	2.32	0.44
2:K:152:SER:O	2:K:169:SER:CB	2.66	0.44
1:R:39:GLU:OE2	2:T:238:ARG:NH2	2.50	0.44
1:B:43:LEU:HD21	1:B:71:PHE:CD1	2.52	0.44
1:B:13:HIS:H	1:B:83:TRP:HB2	1.81	0.44
1:M:188:CYS:HA	1:M:191:MET:O	2.17	0.44
2:D:309:PRO:O	2:D:325:VAL:CG2	2.65	0.44
2:K:241:ARG:HG2	2:K:282:ILE:HD12	1.99	0.44
2:S:339:ASN:HB3	2:S:358:ASP:CB	2.47	0.44
2:P:379:HIS:NE2	2:P:397:THR:CG2	2.76	0.44
1:A:46:GLY:HA2	1:A:102:VAL:HG13	1.98	0.44
1:I:7:ASN:HA	1:I:8:PRO:HD2	1.85	0.44
2:H:208:VAL:HG21	2:H:249:ILE:HD11	1.99	0.44
2:C:155:ASP:H	2:C:168:CYS:HB2	1.82	0.44
2:K:94:TRP:NE1	2:K:393:PRO:HB3	2.32	0.44
1:Q:147:ASN:HB2	1:Q:148:PRO:HD2	1.99	0.44
1:M:66:LEU:HA	1:M:66:LEU:HD12	1.74	0.44
2:H:213:ASP:HB3	2:H:215:THR:CB	2.48	0.44
2:O:311:LEU:HD23	2:O:323:TRP:HB2	2.00	0.44
2:G:288:SER:HB2	2:G:350:GLY:HA3	1.98	0.44
2:O:127:SER:C	2:O:129:ASP:H	2.21	0.44
2:K:233:HIS:HD2	2:K:257:THR:CG2	2.28	0.44
1:J:28:HIS:O	1:J:32:VAL:HG23	2.17	0.44
1:J:53:MET:HG3	1:J:202:TYR:CD2	2.53	0.44
2:O:95:ILE:HA	2:O:96:PRO:HD3	1.75	0.44
2:T:276:ARG:HB2	2:T:317:ASP:OD1	2.17	0.44
1:Q:14:ALA:HB2	1:Q:83:TRP:CE2	2.52	0.44
2:G:95:ILE:HD11	2:G:97:ARG:NH2	2.32	0.44
2:T:149:HIS:CE1	2:T:175:LYS:HG3	2.53	0.44
2:T:95:ILE:HA	2:T:96:PRO:HD3	1.81	0.44
2:O:236:TRP:O	2:O:253:SER:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:210:HIS:NE2	1:Q:214:MET:SD	2.90	0.44
2:T:380:GLU:HG2	2:T:380:GLU:H	1.43	0.44
2:C:359:ASP:O	2:C:360:LYS:C	2.56	0.44
2:G:350:GLY:O	2:G:367:TYR:CZ	2.71	0.44
2:G:253:SER:OG	2:G:254:ASN:N	2.49	0.44
2:D:354:LEU:CD2	2:D:364:VAL:HG22	2.46	0.44
1:J:189:HIS:CD2	2:K:402:GLN:NE2	2.85	0.44
2:T:122:VAL:HG22	2:T:136:ASP:H	1.82	0.44
1:B:15:ALA:HB2	1:B:80:HIS:NE2	2.32	0.44
2:H:146:LEU:HD13	2:H:177:TRP:CE3	2.53	0.44
1:N:8:PRO:O	1:N:79:ARG:HD3	2.18	0.44
2:H:239:MET:HE2	2:H:241:ARG:HE	1.81	0.44
1:A:193:ASP:O	1:B:23:ARG:HD2	2.18	0.44
2:H:365:TRP:CZ3	2:H:372:CYS:HB2	2.53	0.44
2:K:363:ARG:HB2	2:K:365:TRP:NE1	2.28	0.44
2:H:120:PHE:HZ	2:L:294:SER:HA	1.80	0.44
2:O:310:PHE:HE2	2:O:324:ASP:HB3	1.71	0.44
2:T:171:ASP:C	2:T:172:MET:HG3	2.38	0.44
2:D:97:ARG:HG3	2:D:98:PRO:CD	2.47	0.44
2:L:193:HIS:HD2	2:L:194:ASN:HB2	1.81	0.44
2:P:355:SER:OG	2:P:363:ARG:HD2	2.18	0.44
2:H:356:CYS:HA	2:H:361:THR:O	2.18	0.44
2:L:291:SER:HB2	2:L:367:TYR:HE1	1.82	0.44
2:G:158:PHE:CE2	2:G:165:LEU:HD13	2.53	0.44
1:N:64:SER:N	1:N:65:PRO:CD	2.80	0.44
1:M:101:TRP:CG	1:M:137:LEU:HB2	2.53	0.44
2:C:233:HIS:HB3	2:C:255:ASP:OD1	2.17	0.44
2:C:242:PRO:HA	2:C:249:ILE:HD12	2.00	0.44
2:L:237:VAL:HA	2:L:253:SER:HB3	2.00	0.44
2:O:198:VAL:HG23	2:O:209:SER:HB3	1.99	0.44
1:E:8:PRO:HA	1:E:11:ILE:HD12	1.98	0.44
1:E:7:ASN:HD22	1:E:8:PRO:N	2.16	0.44
1:A:139:LEU:HB2	1:A:153:ASN:HB3	1.98	0.44
1:F:64:SER:N	1:F:65:PRO:CD	2.81	0.44
2:L:245:ASP:HB3	2:L:247:THR:OG1	2.17	0.44
2:K:242:PRO:HA	2:K:249:ILE:HD12	1.99	0.44
2:K:338:ASP:H	2:K:363:ARG:HH21	1.66	0.44
2:P:217:LYS:HE2	2:P:229:THR:CG2	2.47	0.44
2:G:401:ASP:N	2:G:401:ASP:OD1	2.37	0.44
2:T:288:SER:CB	2:T:350:GLY:HA2	2.47	0.44
2:L:373:MET:HE2	2:L:373:MET:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:361:THR:HG23	2:L:375:THR:HG23	2.00	0.44
2:C:374:LYS:CG	2:C:375:THR:N	2.70	0.44
2:L:324:ASP:OD1	2:L:327:THR:OG1	2.23	0.44
1:F:8:PRO:HA	1:F:11:ILE:CD1	2.44	0.44
2:L:155:ASP:HB2	2:L:197:SER:HA	1.99	0.44
1:N:118:ILE:O	1:N:122:VAL:HG23	2.18	0.44
2:L:250:ALA:HB2	2:L:284:TRP:CZ2	2.52	0.44
2:P:215:THR:HG23	2:P:229:THR:HG22	2.00	0.44
2:H:127:SER:C	2:H:129:ASP:H	2.21	0.44
2:H:169:SER:OG	2:H:171:ASP:CG	2.56	0.44
2:T:155:ASP:H	2:T:168:CYS:HB2	1.82	0.44
2:P:144:ARG:CZ	2:P:181:GLY:O	2.66	0.44
2:L:212:ARG:HG2	2:L:236:TRP:CG	2.53	0.44
2:H:136:ASP:OD1	2:H:139:THR:N	2.50	0.44
2:S:127:SER:OG	2:S:128:GLU:N	2.51	0.44
2:L:116:PHE:HE2	2:L:137:TYR:CD2	2.36	0.44
2:D:110:PRO:HG3	2:D:400:VAL:HG13	2.00	0.44
2:P:347:HIS:CG	2:P:348:SER:H	2.36	0.44
1:R:13:HIS:H	1:R:83:TRP:HB2	1.83	0.44
1:F:205:ILE:O	1:F:208:PRO:HG2	2.17	0.44
2:T:349:GLY:HA3	2:T:351:LYS:HG3	1.99	0.44
2:C:213:ASP:O	2:C:214:LYS:CB	2.65	0.44
1:B:78:THR:O	1:B:82:LEU:HD12	2.18	0.44
2:K:94:TRP:HE3	2:K:347:HIS:HE1	1.66	0.44
2:S:151:ASP:HB3	2:S:170:ALA:HB3	1.98	0.44
1:J:49:MET:HB3	1:J:101:TRP:CZ3	2.53	0.44
2:D:217:LYS:HE2	2:D:229:THR:OG1	2.18	0.44
2:H:262:VAL:HG12	2:H:265:THR:H	1.81	0.44
2:D:129:ASP:HB3	2:D:131:THR:HG1	1.76	0.43
2:H:112:THR:HG21	2:H:154:GLN:HG3	2.00	0.43
2:D:249:ILE:HG22	2:D:261:TRP:CD1	2.52	0.43
2:P:233:HIS:HB3	2:P:255:ASP:OD2	2.18	0.43
2:P:233:HIS:CE1	2:P:251:SER:OG	2.71	0.43
2:K:193:HIS:HD2	2:K:194:ASN:H	1.61	0.43
2:L:334:LEU:HB3	2:L:365:TRP:CZ3	2.53	0.43
2:D:210:ALA:HB2	2:D:240:VAL:CG2	2.46	0.43
2:G:97:ARG:HA	2:G:376:LEU:HD11	2.00	0.43
2:K:317:ASP:HB3	2:K:319:THR:OG1	2.18	0.43
2:C:129:ASP:CB	2:C:131:THR:OG1	2.43	0.43
2:H:214:LYS:NZ	2:H:234:ARG:NH2	2.65	0.43
2:O:156:ILE:HG12	2:O:165:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:58:ILE:HG13	1:R:58:ILE:O	2.17	0.43
1:E:83:TRP:CD2	1:E:87:ASN:ND2	2.86	0.43
1:E:83:TRP:CE2	1:E:87:ASN:ND2	2.86	0.43
1:E:13:HIS:H	1:E:83:TRP:HB2	1.83	0.43
2:L:242:PRO:O	2:L:284:TRP:CD1	2.71	0.43
2:T:396:VAL:CG1	2:T:406:VAL:HG13	2.48	0.43
2:G:95:ILE:HA	2:G:96:PRO:HD3	1.74	0.43
2:O:152:SER:O	2:O:169:SER:HB2	2.17	0.43
2:H:110:PRO:HB2	2:H:128:GLU:HG3	2.00	0.43
2:H:288:SER:C	2:H:290:TYR:H	2.20	0.43
2:O:114:VAL:HG23	2:O:385:SER:HB2	2.00	0.43
1:J:7:ASN:ND2	1:J:9:ALA:H	2.16	0.43
2:K:134:VAL:O	2:K:143:GLU:HB2	2.18	0.43
2:C:281:CYS:HB2	2:C:314:GLY:HA3	1.99	0.43
1:A:220:THR:HA	1:A:221:PRO:HD3	1.72	0.43
2:D:155:ASP:H	2:D:168:CYS:HB2	1.82	0.43
2:K:312:LEU:HB3	2:K:344:VAL:HG11	1.99	0.43
1:I:15:ALA:HB2	1:I:80:HIS:HD2	1.77	0.43
1:F:59:TRP:C	1:F:59:TRP:CD1	2.91	0.43
2:C:309:PRO:HG2	2:C:325:VAL:CG2	2.48	0.43
1:A:77:THR:HB	1:A:106:ASN:HD21	1.82	0.43
1:A:166:LYS:O	1:A:167:LEU:HB2	2.17	0.43
2:O:367:TYR:HD2	2:O:367:TYR:H	1.62	0.43
2:C:107:HIS:NE2	2:C:125:SER:OG	2.42	0.43
1:M:207:LYS:HB3	1:M:208:PRO:CD	2.49	0.43
2:C:186:ARG:HB2	2:C:186:ARG:HE	1.58	0.43
2:T:272:LEU:HD11	2:T:311:LEU:HD21	1.99	0.43
2:G:152:SER:O	2:G:169:SER:OG	2.37	0.43
2:G:347:HIS:CE1	2:G:388:PHE:HE2	2.36	0.43
2:L:132:ILE:HG23	2:L:156:ILE:HD11	1.99	0.43
2:P:373:MET:O	2:P:374:LYS:HB2	2.18	0.43
1:E:164:LEU:N	1:E:165:PRO:CD	2.81	0.43
2:P:94:TRP:CH2	2:P:392:ALA:CA	3.02	0.43
2:C:102:TYR:HB2	2:C:406:VAL:HB	2.00	0.43
2:G:104:LEU:HB3	2:G:135:TRP:CZ3	2.53	0.43
1:Q:160:LEU:HD23	1:Q:160:LEU:HA	1.81	0.43
1:I:164:LEU:H	1:I:165:PRO:HD2	1.81	0.43
2:G:376:LEU:HD23	2:G:376:LEU:HA	1.92	0.43
2:T:398:GLY:HA2	2:T:403:THR:O	2.18	0.43
2:T:374:LYS:HG3	2:T:375:THR:N	2.33	0.43
1:M:220:THR:HA	1:M:221:PRO:HD3	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:400:VAL:O	2:G:400:VAL:CG1	2.67	0.43
2:G:339:ASN:HD22	2:G:340:TRP:N	2.15	0.43
2:G:340:TRP:CD1	2:G:340:TRP:N	2.86	0.43
2:T:172:MET:HA	2:T:195:VAL:HG23	2.00	0.43
2:T:155:ASP:OD2	2:T:198:VAL:O	2.36	0.43
2:D:101:LYS:HD3	2:D:408:GLU:CG	2.47	0.43
2:G:242:PRO:HA	2:G:249:ILE:HD12	2.00	0.43
1:I:50:VAL:HG22	1:I:101:TRP:HB3	2.01	0.43
1:B:216:LEU:HA	1:B:216:LEU:HD12	1.84	0.43
2:G:94:TRP:CH2	2:G:392:ALA:C	2.92	0.43
2:O:279:VAL:HA	2:O:315:SER:HA	2.00	0.43
2:G:397:THR:HB	2:G:407:TRP:HE1	1.83	0.43
2:K:286:PRO:HB2	2:K:287:GLU:H	1.50	0.43
2:L:318:LYS:HB3	2:L:337:HIS:O	2.18	0.43
2:C:391:THR:HG22	2:C:392:ALA:N	2.33	0.43
2:P:116:PHE:CZ	2:P:396:VAL:CG2	3.01	0.43
2:G:261:TRP:CD1	2:G:261:TRP:N	2.86	0.43
1:E:107:HIS:O	1:E:108:GLU:CB	2.67	0.43
2:K:102:TYR:CZ	2:K:139:THR:O	2.72	0.43
2:S:136:ASP:OD1	2:S:139:THR:HB	2.19	0.43
2:H:123:MET:HE2	2:H:135:TRP:CD1	2.53	0.43
1:B:47:ASP:HA	1:B:73:ILE:O	2.19	0.43
1:F:63:PHE:HA	1:F:66:LEU:HD22	2.00	0.43
2:P:345:LEU:HA	2:P:345:LEU:HD23	1.87	0.43
1:N:103:GLY:O	1:N:106:ASN:HB2	2.18	0.43
1:Q:85:LEU:HD23	1:Q:85:LEU:HA	1.83	0.43
2:G:241:ARG:HA	2:G:242:PRO:HD3	1.78	0.43
2:C:324:ASP:OD1	2:C:327:THR:HG23	2.19	0.43
1:B:49:MET:HB3	1:B:101:TRP:CZ3	2.54	0.43
2:H:360:LYS:HD2	2:H:380:GLU:O	2.19	0.43
2:G:397:THR:HG21	2:G:407:TRP:HE1	1.84	0.43
1:B:7:ASN:HD21	1:B:113:GLU:HB3	1.82	0.43
1:A:164:LEU:N	1:A:165:PRO:CD	2.80	0.43
2:G:216:ILE:HD11	2:G:251:SER:CB	2.48	0.43
2:K:336:GLY:HA2	2:K:365:TRP:CZ2	2.45	0.43
2:C:312:LEU:HD12	2:C:344:VAL:CG1	2.49	0.43
2:H:288:SER:CB	2:H:350:GLY:HA3	2.48	0.43
2:O:316:ARG:HG2	2:O:340:TRP:CG	2.54	0.43
2:T:97:ARG:O	2:T:407:TRP:CE3	2.65	0.43
1:M:8:PRO:O	1:M:79:ARG:CD	2.64	0.43
2:L:336:GLY:CA	2:L:365:TRP:HH2	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:SER:O	2:D:169:SER:HA	2.19	0.43
2:S:252:CYS:HB2	2:S:282:ILE:HD11	2.01	0.43
2:H:287:GLU:HG2	2:H:287:GLU:H	1.50	0.43
1:B:47:ASP:OD2	1:B:47:ASP:C	2.57	0.43
1:I:99:VAL:HG22	1:I:135:ILE:HB	2.01	0.43
2:C:330:CYS:SG	2:C:332:MET:O	2.77	0.43
2:O:265:THR:HB	2:O:267:GLU:HG2	2.00	0.43
2:T:285:ALA:HA	2:T:286:PRO:HD3	1.81	0.43
1:F:220:THR:HA	1:F:221:PRO:HD3	1.81	0.43
1:A:205:ILE:HD13	1:A:205:ILE:HA	1.80	0.43
2:G:109:SER:HB3	2:G:128:GLU:HB2	2.00	0.42
2:S:359:ASP:OD1	2:S:361:THR:CG2	2.65	0.42
2:O:392:ALA:HB1	2:O:393:PRO:HD2	1.95	0.42
2:H:355:SER:OG	2:H:363:ARG:HD2	2.19	0.42
2:O:233:HIS:CE1	2:O:261:TRP:HZ2	2.37	0.42
2:P:237:VAL:HA	2:P:253:SER:HB3	2.01	0.42
2:G:334:LEU:HD13	2:G:365:TRP:CD2	2.54	0.42
1:A:53:MET:HE2	1:A:206:CYS:SG	2.59	0.42
2:G:236:TRP:HD1	2:G:237:VAL:N	2.17	0.42
1:R:164:LEU:N	1:R:165:PRO:CD	2.82	0.42
1:N:125:ILE:HG22	1:N:134:ILE:HD11	2.01	0.42
1:B:82:LEU:HG	1:B:121:ILE:HG13	2.01	0.42
1:A:142:ARG:NH2	1:A:195:LEU:CD1	2.81	0.42
2:P:275:HIS:ND1	2:P:321:LYS:HE2	2.34	0.42
1:Q:147:ASN:HD22	1:Q:149:LEU:H	1.67	0.42
1:A:214:MET:HA	1:A:214:MET:CE	2.49	0.42
2:G:391:THR:O	2:G:391:THR:CG2	2.66	0.42
2:G:356:CYS:HB2	2:G:383:VAL:CG1	2.49	0.42
1:M:187:SER:HB2	2:P:108:ARG:NH2	2.34	0.42
2:L:288:SER:HB2	2:L:350:GLY:HA3	2.00	0.42
2:G:118:PRO:HD3	2:G:158:PHE:CD1	2.54	0.42
2:H:354:LEU:HD13	2:H:362:LEU:HD11	2.00	0.42
2:H:203:ASN:OD1	2:H:203:ASN:O	2.37	0.42
2:D:277:HIS:ND1	2:D:316:ARG:CB	2.79	0.42
1:J:135:ILE:HD11	1:J:216:LEU:HD23	2.01	0.42
2:D:399:SER:HB2	2:D:400:VAL:H	1.55	0.42
1:B:133:LYS:HD3	1:B:216:LEU:HG	2.01	0.42
1:A:134:ILE:HB	1:A:170:VAL:HG13	2.01	0.42
1:Q:189:HIS:HD2	2:T:402:GLN:NE2	2.17	0.42
2:O:317:ASP:HB2	2:O:319:THR:OG1	2.19	0.42
2:K:159:ASP:HA	2:K:200:ILE:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:241:ARG:HA	2:O:242:PRO:HD3	1.80	0.42
2:T:332:MET:CE	2:T:370:LYS:HG3	2.50	0.42
1:A:19:GLN:HG2	1:B:107:HIS:NE2	2.34	0.42
2:O:340:TRP:HB2	2:O:358:ASP:HB2	2.00	0.42
2:O:397:THR:O	2:O:404:VAL:HA	2.19	0.42
2:H:243:ASN:O	2:H:244:GLN:C	2.58	0.42
2:D:347:HIS:CG	2:D:348:SER:N	2.87	0.42
1:F:188:CYS:HA	1:F:191:MET:O	2.19	0.42
1:N:15:ALA:HB2	1:N:80:HIS:NE2	2.34	0.42
1:J:139:LEU:HD12	1:J:153:ASN:HA	2.00	0.42
2:K:337:HIS:NE2	2:K:363:ARG:HG2	2.34	0.42
2:H:315:SER:OG	2:H:316:ARG:N	2.52	0.42
2:S:317:ASP:O	2:S:318:LYS:CB	2.68	0.42
2:L:193:HIS:HD2	2:L:194:ASN:N	2.03	0.42
2:D:359:ASP:O	2:D:359:ASP:CG	2.58	0.42
2:O:400:VAL:C	2:O:402:GLN:H	2.23	0.42
2:L:112:THR:HG21	2:L:154:GLN:HG3	2.00	0.42
2:D:171:ASP:O	2:D:172:MET:HG3	2.20	0.42
1:N:118:ILE:HD13	1:N:160:LEU:HD11	2.02	0.42
2:D:286:PRO:HB2	2:D:287:GLU:H	1.48	0.42
2:P:400:VAL:C	2:P:402:GLN:N	2.73	0.42
1:A:23:ARG:HD2	1:B:193:ASP:O	2.19	0.42
1:F:197:LEU:HD22	1:F:201:GLY:HA3	2.00	0.42
2:H:397:THR:O	2:H:397:THR:HG22	2.19	0.42
2:K:285:ALA:HA	2:K:286:PRO:HD3	1.75	0.42
2:S:340:TRP:O	2:S:358:ASP:N	2.51	0.42
2:T:169:SER:CB	2:T:171:ASP:OD1	2.67	0.42
1:A:114:VAL:O	1:A:118:ILE:HG13	2.20	0.42
1:B:146:PRO:HG3	2:G:189:HIS:CE1	2.54	0.42
2:S:213:ASP:O	2:S:214:LYS:CB	2.68	0.42
2:C:102:TYR:CE2	2:C:139:THR:O	2.66	0.42
1:B:166:LYS:O	1:B:167:LEU:O	2.38	0.42
1:R:28:HIS:ND1	1:R:89:GLU:OE2	2.44	0.42
2:L:252:CYS:SG	2:L:282:ILE:CG1	3.08	0.42
2:K:317:ASP:O	2:K:318:LYS:HB2	2.20	0.42
2:G:151:ASP:HB3	2:G:170:ALA:HB3	2.00	0.42
2:D:126:ALA:CB	2:D:156:ILE:HD11	2.47	0.42
2:S:379:HIS:HD2	2:S:383:VAL:HG22	1.84	0.42
2:C:159:ASP:CA	2:C:200:ILE:HG21	2.40	0.42
2:T:169:SER:HG	2:T:171:ASP:CG	2.23	0.42
2:H:367:TYR:O	2:H:369:ASN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:379:HIS:CD2	2:T:383:VAL:HG22	2.55	0.42
2:D:208:VAL:HG12	2:D:209:SER:N	2.35	0.42
2:C:363:ARG:HB2	2:C:365:TRP:HE1	1.85	0.42
1:I:11:ILE:HA	1:I:12:PRO:HD2	1.90	0.42
2:L:286:PRO:HB2	2:L:287:GLU:H	1.53	0.42
2:P:110:PRO:HB2	2:P:128:GLU:HG3	2.01	0.42
1:Q:50:VAL:HG12	1:Q:70:ASN:OD1	2.20	0.42
2:H:233:HIS:HB3	2:H:255:ASP:CG	2.40	0.42
2:C:316:ARG:HD3	2:C:340:TRP:CE2	2.55	0.42
2:P:265:THR:O	2:P:266:LYS:HG2	2.20	0.42
2:G:153:VAL:HA	2:G:168:CYS:O	2.20	0.42
2:S:355:SER:O	2:S:362:LEU:HD12	2.19	0.42
1:M:207:LYS:HB3	1:M:208:PRO:HD3	2.01	0.42
2:K:238:ARG:HD2	2:K:280:GLU:HG2	2.00	0.42
1:E:64:SER:N	1:E:65:PRO:CD	2.82	0.42
2:D:220:GLU:HB3	2:D:223:THR:OG1	2.20	0.42
1:F:100:VAL:HB	1:F:136:VAL:HG22	2.02	0.42
2:L:102:TYR:HB2	2:L:406:VAL:HB	2.01	0.42
2:P:100:GLU:H	2:P:100:GLU:HG3	1.72	0.42
2:L:240:VAL:O	2:L:241:ARG:HD3	2.20	0.42
2:C:171:ASP:O	2:C:172:MET:CB	2.68	0.42
2:L:129:ASP:CB	2:L:131:THR:H	2.32	0.42
2:K:213:ASP:O	2:K:214:LYS:HB2	2.19	0.42
2:S:127:SER:C	2:S:129:ASP:H	2.23	0.42
2:P:187:THR:CG2	2:P:189:HIS:NE2	2.82	0.42
2:C:272:LEU:HB3	2:C:323:TRP:CZ3	2.55	0.42
1:J:47:ASP:OD2	1:J:47:ASP:C	2.58	0.42
2:P:241:ARG:HA	2:P:242:PRO:HD3	1.81	0.42
2:L:391:THR:HG22	2:L:392:ALA:N	2.35	0.42
2:L:123:MET:HE3	2:L:404:VAL:HG11	2.00	0.42
2:T:337:HIS:H	2:T:337:HIS:CD2	2.37	0.42
2:P:293:ILE:HG23	2:P:294:SER:H	1.85	0.42
1:R:7:ASN:HA	1:R:8:PRO:HD2	1.88	0.42
2:P:274:GLU:O	2:P:321:LYS:HE3	2.20	0.42
2:P:122:VAL:HG22	2:P:136:ASP:N	2.34	0.42
1:E:24:TRP:HE3	1:E:25:MET:HG2	1.84	0.42
1:R:93:ILE:HD12	1:R:95:PRO:HD3	2.02	0.42
2:O:286:PRO:HB2	2:O:287:GLU:H	1.53	0.42
1:A:85:LEU:HD22	1:A:90:LEU:HG	2.02	0.42
2:L:293:ILE:HG22	2:L:294:SER:H	1.85	0.42
2:H:277:HIS:CE1	2:H:278:VAL:HG23	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:240:VAL:O	2:P:241:ARG:HD3	2.20	0.42
2:S:397:THR:O	2:S:405:LYS:N	2.32	0.42
2:P:212:ARG:HG2	2:P:236:TRP:CG	2.55	0.42
2:T:262:VAL:HG12	2:T:265:THR:H	1.84	0.42
2:G:275:HIS:CE1	2:G:315:SER:HB2	2.55	0.42
2:T:117:HIS:HA	2:T:118:PRO:HD3	1.90	0.42
2:L:400:VAL:O	2:L:400:VAL:HG12	2.20	0.42
1:I:166:LYS:O	1:I:167:LEU:HB2	2.18	0.42
1:R:90:LEU:HD23	1:R:90:LEU:HA	1.88	0.42
1:A:177:GLY:O	1:A:179:PHE:N	2.49	0.42
1:A:207:LYS:N	1:A:208:PRO:HD2	2.35	0.42
2:L:351:LYS:CB	2:L:352:PHE:CE1	3.03	0.41
2:G:159:ASP:OD2	2:G:161:SER:OG	2.28	0.41
2:D:394:TYR:HA	2:D:407:TRP:O	2.20	0.41
2:O:153:VAL:HA	2:O:168:CYS:O	2.20	0.41
1:J:135:ILE:CD1	1:J:212:LEU:HD23	2.48	0.41
1:R:11:ILE:O	1:R:11:ILE:HG22	2.20	0.41
2:K:366:ASP:OD1	2:K:368:LYS:HB3	2.20	0.41
2:K:209:SER:O	2:K:216:ILE:HG23	2.20	0.41
1:Q:189:HIS:CD2	2:T:402:GLN:NE2	2.88	0.41
2:D:288:SER:C	2:D:290:TYR:H	2.22	0.41
2:O:151:ASP:HB3	2:O:170:ALA:HB3	2.01	0.41
1:F:95:PRO:O	1:F:131:GLN:NE2	2.53	0.41
2:S:323:TRP:HA	2:S:331:LEU:HD23	2.02	0.41
2:C:110:PRO:HG3	2:C:400:VAL:HG13	2.03	0.41
2:H:233:HIS:HB3	2:H:255:ASP:OD1	2.20	0.41
2:P:337:HIS:NE2	2:P:363:ARG:HG2	2.35	0.41
2:P:373:MET:HG3	2:P:373:MET:O	2.20	0.41
2:D:104:LEU:HD13	2:D:135:TRP:CG	2.55	0.41
1:F:166:LYS:O	1:F:167:LEU:HB2	2.20	0.41
2:H:312:LEU:HD23	2:H:312:LEU:HA	1.86	0.41
2:P:291:SER:O	2:P:293:ILE:HG22	2.20	0.41
1:M:13:HIS:H	1:M:83:TRP:HB2	1.85	0.41
2:G:272:LEU:HD22	2:G:323:TRP:CE3	2.55	0.41
2:G:243:ASN:O	2:G:244:GLN:C	2.57	0.41
1:F:84:ARG:O	1:F:89:GLU:HG3	2.20	0.41
2:G:178:ASP:C	2:G:178:ASP:OD1	2.58	0.41
2:K:347:HIS:CG	2:K:348:SER:N	2.88	0.41
1:Q:8:PRO:O	1:Q:79:ARG:CD	2.68	0.41
1:F:32:VAL:O	1:F:35:CYS:HB2	2.21	0.41
1:B:111:ALA:HB1	1:B:155:LYS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ILE:O	1:E:121:ILE:HB	2.21	0.41
1:A:30:ARG:HD2	1:B:188:CYS:SG	2.60	0.41
1:Q:69:LEU:HA	1:Q:69:LEU:HD23	1.73	0.41
2:S:322:MET:HB3	2:S:331:LEU:HB2	2.02	0.41
2:G:397:THR:CB	2:G:407:TRP:HE1	2.33	0.41
2:C:312:LEU:N	2:C:312:LEU:HD23	2.35	0.41
2:L:141:ASP:C	2:L:143:GLU:N	2.72	0.41
2:C:381:HIS:O	2:C:382:PHE:C	2.58	0.41
2:P:144:ARG:CZ	2:P:181:GLY:CA	2.96	0.41
2:P:368:LYS:O	2:P:369:ASN:CG	2.59	0.41
2:P:116:PHE:CE1	2:P:396:VAL:HG23	2.55	0.41
2:C:281:CYS:SG	2:C:342:ARG:O	2.79	0.41
2:P:102:TYR:OH	2:P:139:THR:HA	2.19	0.41
2:O:288:SER:HB3	2:O:350:GLY:CA	2.50	0.41
2:G:324:ASP:OD2	2:G:327:THR:HG23	2.20	0.41
1:J:103:GLY:HA2	1:J:106:ASN:ND2	2.35	0.41
1:R:101:TRP:CZ2	1:R:137:LEU:HD12	2.56	0.41
1:R:18:ILE:HG13	1:R:18:ILE:H	1.61	0.41
1:F:126:ASN:HD22	1:F:126:ASN:C	2.23	0.41
2:T:369:ASN:HB2	2:T:371:ARG:HH21	1.78	0.41
2:D:171:ASP:C	2:D:172:MET:HG3	2.41	0.41
2:D:389:HIS:ND1	2:D:392:ALA:HB3	2.35	0.41
2:G:218:MET:HE3	2:G:228:LYS:HD2	2.00	0.41
2:K:171:ASP:O	2:K:172:MET:CB	2.67	0.41
2:G:260:VAL:HG21	2:G:325:VAL:HG11	2.02	0.41
1:Q:147:ASN:ND2	1:Q:149:LEU:HB2	2.35	0.41
1:Q:177:GLY:O	1:Q:179:PHE:N	2.49	0.41
2:D:352:PHE:CE2	2:D:373:MET:SD	3.14	0.41
1:B:179:PHE:O	1:B:186:ILE:HG12	2.21	0.41
2:G:127:SER:OG	2:G:129:ASP:CB	2.66	0.41
2:G:131:THR:CG2	2:G:145:THR:HG22	2.51	0.41
2:D:250:ALA:HB2	2:D:284:TRP:HZ2	1.80	0.41
2:P:358:ASP:HA	2:P:382:PHE:HB3	2.00	0.41
2:L:155:ASP:H	2:L:168:CYS:HB2	1.85	0.41
2:G:353:ILE:C	2:G:354:LEU:HD23	2.40	0.41
2:O:134:VAL:O	2:O:143:GLU:HB2	2.20	0.41
1:Q:7:ASN:C	1:Q:7:ASN:ND2	2.73	0.41
2:T:316:ARG:C	2:T:318:LYS:H	2.22	0.41
2:H:330:CYS:SG	2:H:331:LEU:N	2.93	0.41
1:R:54:GLN:HG3	1:R:59:TRP:CE2	2.55	0.41
1:N:50:VAL:HG23	1:N:101:TRP:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:287:GLU:H	2:S:287:GLU:HG2	1.72	0.41
2:G:394:TYR:HA	2:G:407:TRP:O	2.21	0.41
2:H:381:HIS:ND1	2:H:382:PHE:N	2.66	0.41
2:D:205:ASP:C	2:D:221:VAL:HG23	2.41	0.41
2:H:171:ASP:O	2:H:172:MET:CB	2.68	0.41
2:D:201:MET:SD	2:D:208:VAL:HG23	2.61	0.41
2:S:337:HIS:HB2	2:S:363:ARG:CZ	2.50	0.41
2:L:203:ASN:CG	2:L:203:ASN:O	2.59	0.41
2:D:172:MET:HA	2:D:195:VAL:CG2	2.50	0.41
2:T:176:LEU:HD11	2:T:221:VAL:HG13	2.02	0.41
2:T:358:ASP:OD1	2:T:382:PHE:CD2	2.73	0.41
1:B:209:LEU:O	1:B:213:ILE:HG13	2.20	0.41
2:L:101:LYS:HZ3	2:L:408:GLU:CD	2.23	0.41
1:Q:188:CYS:HA	1:Q:191:MET:O	2.21	0.41
1:Q:62:LEU:HG	1:Q:210:HIS:CG	2.55	0.41
1:A:90:LEU:HA	1:A:90:LEU:HD23	1.73	0.41
1:I:124:LEU:O	1:I:127:THR:HB	2.21	0.41
1:E:70:ASN:C	1:E:70:ASN:OD1	2.58	0.41
2:T:291:SER:HB2	2:T:367:TYR:CE1	2.55	0.41
2:G:110:PRO:HB2	2:G:128:GLU:HG3	2.03	0.41
2:D:141:ASP:O	2:D:143:GLU:N	2.54	0.41
1:I:126:ASN:C	1:I:126:ASN:ND2	2.68	0.41
2:D:171:ASP:O	2:D:172:MET:CB	2.69	0.41
1:N:164:LEU:N	1:N:165:PRO:CD	2.82	0.41
2:H:197:SER:OG	2:H:239:MET:HA	2.21	0.41
1:N:15:ALA:HB2	1:N:80:HIS:CD2	2.56	0.41
1:F:160:LEU:HA	1:F:160:LEU:HD23	1.93	0.41
2:K:100:GLU:HG3	2:K:100:GLU:H	1.69	0.41
2:D:355:SER:N	2:D:363:ARG:O	2.54	0.41
2:S:339:ASN:HB3	2:S:358:ASP:HB3	2.03	0.41
2:P:115:ILE:HD12	2:P:156:ILE:HB	2.02	0.41
1:E:137:LEU:HD23	1:E:137:LEU:HA	1.92	0.41
2:L:159:ASP:OD2	2:L:161:SER:OG	2.39	0.41
2:S:153:VAL:HA	2:S:168:CYS:O	2.20	0.41
1:M:82:LEU:CD2	1:M:121:ILE:HG13	2.50	0.41
2:S:391:THR:HG22	2:S:392:ALA:N	2.36	0.41
1:A:7:ASN:HD21	1:A:9:ALA:HB3	1.86	0.41
1:A:7:ASN:ND2	1:A:9:ALA:H	2.19	0.41
1:M:27:GLN:NE2	1:N:193:ASP:HB2	2.35	0.41
2:D:401:ASP:N	2:D:401:ASP:OD1	2.54	0.41
2:C:97:ARG:CG	2:C:98:PRO:CD	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:213:ASP:HB3	2:P:215:THR:HB	2.03	0.41
2:S:97:ARG:HB3	2:S:374:LYS:HE2	2.03	0.41
1:Q:50:VAL:CG2	1:Q:101:TRP:HB3	2.51	0.41
2:D:317:ASP:O	2:D:318:LYS:HB2	2.21	0.41
2:D:355:SER:HB3	2:D:365:TRP:HE1	1.85	0.41
2:S:358:ASP:OD1	2:S:382:PHE:CD2	2.74	0.41
2:P:361:THR:HG23	2:P:362:LEU:N	2.35	0.41
1:F:155:LYS:O	1:F:158:GLN:CB	2.69	0.41
2:H:144:ARG:CZ	2:H:181:GLY:HA2	2.51	0.41
1:F:53:MET:CE	1:F:206:CYS:SG	3.09	0.41
2:S:178:ASP:OD2	2:S:180:GLN:HB2	2.21	0.41
1:Q:164:LEU:N	1:Q:165:PRO:CD	2.84	0.41
2:D:313:SER:O	2:D:320:ILE:HA	2.20	0.41
1:A:207:LYS:HB3	1:A:208:PRO:HD3	2.01	0.41
1:B:177:GLY:O	1:B:179:PHE:N	2.49	0.41
2:P:208:VAL:HG22	2:P:218:MET:HG2	2.03	0.41
2:G:176:LEU:HD11	2:G:221:VAL:HG13	2.02	0.41
2:S:115:ILE:HG22	2:S:124:VAL:HB	2.01	0.41
2:K:311:LEU:C	2:K:311:LEU:HD23	2.40	0.41
1:M:69:LEU:HD23	1:M:69:LEU:HA	1.57	0.41
1:M:144:GLU:HG2	1:M:145:LYS:HG3	2.03	0.41
2:S:197:SER:CB	2:S:239:MET:HA	2.51	0.41
2:K:153:VAL:HA	2:K:168:CYS:O	2.20	0.41
2:C:100:GLU:H	2:C:100:GLU:HG3	1.70	0.41
1:F:69:LEU:HA	1:F:69:LEU:HD23	1.65	0.41
2:L:100:GLU:CD	2:L:405:LYS:HE2	2.41	0.41
2:O:337:HIS:CE1	2:O:375:THR:CG2	2.98	0.41
2:H:351:LYS:HB2	2:H:352:PHE:CD1	2.55	0.41
1:J:8:PRO:O	1:J:79:ARG:HD2	2.19	0.41
1:I:7:ASN:ND2	1:I:9:ALA:H	2.18	0.41
2:T:146:LEU:HB3	2:T:177:TRP:CZ3	2.56	0.41
2:K:212:ARG:HG2	2:K:236:TRP:CE2	2.56	0.41
2:D:210:ALA:CB	2:D:240:VAL:HG22	2.49	0.41
2:P:116:PHE:HE1	2:P:387:ASP:O	2.04	0.41
2:O:309:PRO:O	2:O:325:VAL:HG23	2.21	0.41
2:C:293:ILE:HG22	2:C:294:SER:N	2.36	0.41
1:R:137:LEU:HD21	1:R:209:LEU:HD13	2.03	0.41
1:Q:23:ARG:HD2	1:R:193:ASP:O	2.20	0.41
1:J:177:GLY:O	1:J:179:PHE:N	2.49	0.41
1:B:90:LEU:O	1:B:129:GLN:NE2	2.54	0.41
1:B:81:VAL:O	1:B:85:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:ASP:O	1:N:96:LYS:N	2.49	0.41
1:B:197:LEU:HB2	1:B:202:TYR:CE1	2.55	0.41
2:C:329:MET:HA	2:C:329:MET:CE	2.51	0.41
1:F:58:ILE:HG13	1:F:58:ILE:O	2.20	0.41
2:C:354:LEU:N	2:C:354:LEU:HD23	2.36	0.41
2:K:361:THR:HG22	2:K:363:ARG:HG3	2.03	0.40
2:P:191:HIS:HE1	2:P:217:LYS:HG3	1.74	0.40
2:D:336:GLY:HA2	2:D:365:TRP:CH2	2.55	0.40
2:D:230:PHE:CD1	2:D:230:PHE:N	2.89	0.40
1:I:77:THR:HB	1:I:106:ASN:HD21	1.85	0.40
2:K:233:HIS:HB3	2:K:255:ASP:OD2	2.21	0.40
2:D:94:TRP:H	2:D:351:LYS:NZ	2.18	0.40
2:G:228:LYS:NZ	2:G:264:ALA:O	2.54	0.40
2:L:342:ARG:NH2	2:L:384:THR:HG23	2.35	0.40
2:K:136:ASP:OD1	2:K:139:THR:HB	2.21	0.40
1:I:101:TRP:CD1	1:I:137:LEU:HB2	2.56	0.40
2:C:297:THR:HG22	2:C:298:GLY:H	1.86	0.40
2:T:241:ARG:HA	2:T:242:PRO:HD3	1.79	0.40
1:J:52:LEU:HA	1:J:52:LEU:HD23	1.78	0.40
2:O:362:LEU:HD12	2:O:362:LEU:HA	1.88	0.40
2:H:359:ASP:OD2	2:H:359:ASP:N	2.54	0.40
2:S:379:HIS:CD2	2:S:383:VAL:HG22	2.55	0.40
2:T:131:THR:CG2	2:T:145:THR:HG22	2.51	0.40
2:H:94:TRP:HH2	2:H:392:ALA:O	1.94	0.40
1:J:175:THR:CB	1:J:205:ILE:HD13	2.51	0.40
2:G:104:LEU:HD21	2:G:140:GLY:HA3	2.04	0.40
2:S:173:THR:HG22	2:S:187:THR:CG2	2.51	0.40
2:T:117:HIS:ND1	2:T:120:PHE:N	2.65	0.40
1:B:103:GLY:O	1:B:106:ASN:HB2	2.20	0.40
1:Q:160:LEU:O	1:Q:164:LEU:HB2	2.22	0.40
2:S:345:LEU:HA	2:S:345:LEU:HD22	1.91	0.40
1:Q:8:PRO:O	1:Q:79:ARG:HD3	2.21	0.40
2:D:116:PHE:CZ	2:D:396:VAL:HG22	2.57	0.40
2:O:262:VAL:HG12	2:O:265:THR:H	1.86	0.40
1:E:180:VAL:HG12	1:E:184:GLY:HA2	2.03	0.40
2:O:155:ASP:HB2	2:O:197:SER:HA	2.02	0.40
2:L:312:LEU:CD2	2:L:312:LEU:N	2.64	0.40
2:C:359:ASP:OD1	2:C:361:THR:HB	2.22	0.40
2:D:200:ILE:HG13	2:D:207:ILE:HG13	2.03	0.40
2:S:278:VAL:O	2:S:315:SER:OG	2.34	0.40
2:C:355:SER:OG	2:C:363:ARG:CD	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:132:ILE:HG12	2:O:156:ILE:CD1	2.45	0.40
2:O:259:ARG:HD2	2:O:261:TRP:CZ2	2.56	0.40
2:L:153:VAL:HA	2:L:168:CYS:O	2.22	0.40
2:K:354:LEU:HA	2:K:354:LEU:HD22	1.90	0.40
2:C:233:HIS:NE2	2:C:251:SER:OG	2.53	0.40
2:P:340:TRP:O	2:P:357:ALA:HB1	2.22	0.40
1:I:64:SER:N	1:I:65:PRO:HD3	2.36	0.40
1:B:207:LYS:HB3	1:B:208:PRO:CD	2.50	0.40
1:E:56:TYR:OH	1:F:55:GLN:HG3	2.20	0.40
1:J:123:GLN:HE21	1:J:123:GLN:HB2	1.64	0.40
2:C:317:ASP:O	2:C:318:LYS:HB2	2.21	0.40
2:K:272:LEU:HD13	2:K:323:TRP:CD2	2.56	0.40
2:L:146:LEU:HD13	2:L:177:TRP:CD2	2.57	0.40
2:D:94:TRP:CH2	2:D:392:ALA:C	2.95	0.40
1:N:147:ASN:HB2	1:N:148:PRO:HD2	2.03	0.40
1:N:220:THR:HA	1:N:221:PRO:HD3	1.72	0.40
2:G:386:LEU:HA	2:G:396:VAL:O	2.22	0.40
2:P:297:THR:CG2	2:P:298:GLY:N	2.55	0.40
2:K:334:LEU:O	2:K:336:GLY:N	2.55	0.40
2:H:288:SER:C	2:H:290:TYR:N	2.75	0.40
2:H:173:THR:HG22	2:H:174:ILE:N	2.37	0.40
2:P:193:HIS:CD2	2:P:194:ASN:N	2.87	0.40
2:S:171:ASP:O	2:S:172:MET:CB	2.69	0.40
2:G:233:HIS:CE1	2:G:251:SER:OG	2.74	0.40
1:A:28:HIS:O	1:A:32:VAL:HG23	2.21	0.40
1:B:42:VAL:HG13	1:B:97:VAL:HB	2.04	0.40
1:Q:134:ILE:HB	1:Q:170:VAL:HG13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:LYS:CB	2:T:300:GLU:O[2_556]	1.91	0.29

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	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	21	65
1	B	216/229 (94%)	196 (91%)	17 (8%)	3 (1%)	14	55
1	E	216/229 (94%)	192 (89%)	22 (10%)	2 (1%)	21	65
1	F	216/229 (94%)	199 (92%)	15 (7%)	2 (1%)	21	65
1	I	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	21	65
1	J	216/229 (94%)	197 (91%)	17 (8%)	2 (1%)	21	65
1	M	216/229 (94%)	197 (91%)	16 (7%)	3 (1%)	14	55
1	N	216/229 (94%)	198 (92%)	16 (7%)	2 (1%)	21	65
1	Q	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	21	65
1	R	216/229 (94%)	199 (92%)	15 (7%)	2 (1%)	21	65
2	C	306/410 (75%)	247 (81%)	35 (11%)	24 (8%)	1	12
2	D	306/410 (75%)	242 (79%)	46 (15%)	18 (6%)	2	19
2	G	306/410 (75%)	238 (78%)	45 (15%)	23 (8%)	1	13
2	H	306/410 (75%)	243 (79%)	38 (12%)	25 (8%)	1	11
2	K	306/410 (75%)	237 (78%)	44 (14%)	25 (8%)	1	11
2	L	306/410 (75%)	243 (79%)	42 (14%)	21 (7%)	1	15
2	O	306/410 (75%)	245 (80%)	43 (14%)	18 (6%)	2	19
2	P	306/410 (75%)	251 (82%)	34 (11%)	21 (7%)	1	15
2	S	306/410 (75%)	242 (79%)	47 (15%)	17 (6%)	2	21
2	T	306/410 (75%)	244 (80%)	43 (14%)	19 (6%)	2	18
All	All	5220/6390 (82%)	4410 (84%)	577 (11%)	233 (4%)	3	27

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	97	ARG
2	C	98	PRO
2	C	143	GLU
2	C	293	ILE
2	C	360	LYS
2	C	370	LYS
2	D	97	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	98	PRO
2	D	136	ASP
2	D	143	GLU
2	D	286	PRO
2	D	360	LYS
2	D	368	LYS
2	G	97	ARG
2	G	98	PRO
2	G	143	GLU
2	G	286	PRO
2	G	293	ILE
2	G	347	HIS
2	H	97	ARG
2	H	98	PRO
2	H	136	ASP
2	H	142	PHE
2	H	143	GLU
2	H	286	PRO
2	H	293	ILE
2	H	317	ASP
2	H	337	HIS
2	H	368	LYS
2	K	97	ARG
2	K	98	PRO
2	K	143	GLU
2	K	293	ILE
2	K	317	ASP
2	L	97	ARG
2	L	98	PRO
2	L	142	PHE
2	L	143	GLU
2	L	293	ILE
2	L	360	LYS
2	O	97	ARG
2	O	98	PRO
2	O	143	GLU
2	P	97	ARG
2	P	98	PRO
2	P	142	PHE
2	P	143	GLU
2	P	286	PRO
2	P	293	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	360	LYS
2	P	370	LYS
2	S	97	ARG
2	S	98	PRO
2	S	142	PHE
2	S	143	GLU
2	S	360	LYS
2	S	370	LYS
2	S	400	VAL
2	T	97	ARG
2	T	98	PRO
2	T	142	PHE
2	T	143	GLU
2	T	337	HIS
1	B	167	LEU
2	C	136	ASP
2	C	142	PHE
2	C	204	GLY
2	C	286	PRO
2	C	288	SER
2	C	390	LYS
2	D	142	PHE
2	D	204	GLY
2	D	236	TRP
2	D	288	SER
2	D	293	ILE
1	F	167	LEU
2	G	136	ASP
2	G	142	PHE
2	G	204	GLY
2	H	204	GLY
2	H	288	SER
1	J	167	LEU
2	K	142	PHE
2	K	204	GLY
2	K	286	PRO
2	K	288	SER
2	K	335	VAL
2	L	136	ASP
2	L	204	GLY
2	L	286	PRO
2	L	337	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	344	VAL
2	L	390	LYS
2	O	142	PHE
2	O	204	GLY
2	O	286	PRO
2	O	288	SER
2	O	293	ILE
2	O	360	LYS
2	O	368	LYS
2	P	136	ASP
2	P	204	GLY
2	P	213	ASP
2	P	288	SER
1	Q	167	LEU
1	R	167	LEU
2	S	204	GLY
2	S	286	PRO
2	S	288	SER
2	S	293	ILE
2	T	204	GLY
2	T	286	PRO
2	T	293	ILE
2	T	380	GLU
2	C	194	ASN
2	C	213	ASP
2	C	236	TRP
2	C	244	GLN
1	E	167	LEU
2	G	236	TRP
2	G	288	SER
2	G	331	LEU
2	G	337	HIS
2	G	360	LYS
2	H	203	ASN
2	H	236	TRP
2	H	349	GLY
1	I	167	LEU
2	K	136	ASP
2	K	203	ASN
2	K	236	TRP
2	K	360	LYS
2	K	366	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	288	SER
1	M	167	LEU
1	N	167	LEU
2	O	236	TRP
2	O	347	HIS
2	S	236	TRP
2	S	331	LEU
2	S	374	LYS
2	T	288	SER
1	A	167	LEU
2	C	190	GLY
2	C	203	ASN
2	C	350	GLY
2	C	382	PHE
2	D	190	GLY
2	D	203	ASN
2	D	309	PRO
2	G	190	GLY
2	G	213	ASP
2	G	390	LYS
2	H	190	GLY
2	H	213	ASP
2	H	244	GLN
2	H	370	LYS
2	K	190	GLY
2	K	371	ARG
2	K	377	ASN
2	L	190	GLY
2	L	203	ASN
2	L	368	LYS
2	O	190	GLY
2	P	110	PRO
2	P	190	GLY
2	S	190	GLY
2	T	190	GLY
2	T	360	LYS
1	A	221	PRO
2	C	349	GLY
2	H	194	ASN
2	H	292	SER
2	H	350	GLY
2	H	385	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	221	PRO
2	K	368	LYS
2	L	194	ASN
2	L	244	GLN
2	O	370	LYS
2	P	172	MET
2	P	236	TRP
2	T	136	ASP
2	T	236	TRP
2	T	368	LYS
2	T	370	LYS
1	B	221	PRO
2	G	203	ASN
2	G	309	PRO
2	H	366	ASP
2	K	194	ASN
1	M	221	PRO
1	N	221	PRO
2	O	194	ASN
2	O	244	GLN
2	P	194	ASN
2	P	380	GLU
2	S	244	GLN
1	B	148	PRO
2	C	110	PRO
2	D	325	VAL
1	F	221	PRO
2	G	110	PRO
2	K	349	GLY
2	K	350	GLY
1	M	148	PRO
2	C	140	GLY
1	J	221	PRO
2	K	110	PRO
1	Q	221	PRO
1	R	221	PRO
2	C	232	GLY
2	D	232	GLY
1	E	221	PRO
2	G	349	GLY
2	L	232	GLY
2	L	350	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	202	PRO
2	P	232	GLY
2	G	232	GLY
2	H	232	GLY
2	K	232	GLY
2	O	232	GLY
2	O	309	PRO
2	P	140	GLY
2	S	232	GLY
2	T	140	GLY
2	T	202	PRO
2	T	232	GLY
2	D	140	GLY
2	G	140	GLY
2	K	140	GLY
2	L	140	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	185/197 (94%)	145 (78%)	40 (22%)	1	6
1	B	185/197 (94%)	145 (78%)	40 (22%)	1	6
1	E	185/197 (94%)	158 (85%)	27 (15%)	4	21
1	F	185/197 (94%)	149 (80%)	36 (20%)	2	8
1	I	185/197 (94%)	145 (78%)	40 (22%)	1	6
1	J	185/197 (94%)	154 (83%)	31 (17%)	2	14
1	M	185/197 (94%)	153 (83%)	32 (17%)	2	13
1	N	185/197 (94%)	147 (80%)	38 (20%)	1	7
1	Q	185/197 (94%)	148 (80%)	37 (20%)	1	8
1	R	185/197 (94%)	141 (76%)	44 (24%)	1	4
2	C	274/365 (75%)	187 (68%)	87 (32%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	274/365 (75%)	186 (68%)	88 (32%)	0	2
2	G	274/365 (75%)	186 (68%)	88 (32%)	0	2
2	H	274/365 (75%)	189 (69%)	85 (31%)	0	2
2	K	274/365 (75%)	180 (66%)	94 (34%)	0	2
2	L	274/365 (75%)	187 (68%)	87 (32%)	0	2
2	O	274/365 (75%)	189 (69%)	85 (31%)	0	2
2	P	274/365 (75%)	201 (73%)	73 (27%)	0	3
2	S	274/365 (75%)	183 (67%)	91 (33%)	0	2
2	T	274/365 (75%)	182 (66%)	92 (34%)	0	2
All	All	4590/5620 (82%)	3355 (73%)	1235 (27%)	0	3

All (1235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	ASN
1	A	13	HIS
1	A	17	ASP
1	A	26	SER
1	A	35	CYS
1	A	37	ASP
1	A	43	LEU
1	A	48	SER
1	A	52	LEU
1	A	58	ILE
1	A	60	ARG
1	A	61	GLU
1	A	66	LEU
1	A	73	ILE
1	A	77	THR
1	A	78	THR
1	A	82	LEU
1	A	91	GLU
1	A	102	VAL
1	A	123	GLN
1	A	126	ASN
1	A	128	ARG
1	A	131	GLN
1	A	145	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	GLN
1	A	155	LYS
1	A	158	GLN
1	A	161	LYS
1	A	162	VAL
1	A	163	SER
1	A	166	LYS
1	A	170	VAL
1	A	172	LEU
1	A	176	ASP
1	A	205	ILE
1	A	214	MET
1	A	215	GLN
1	A	216	LEU
1	A	222	GLU
1	B	17	ASP
1	B	33	LEU
1	B	36	LYS
1	B	37	ASP
1	B	39	GLU
1	B	43	LEU
1	B	52	LEU
1	B	58	ILE
1	B	62	LEU
1	B	64	SER
1	B	66	LEU
1	B	76	ASP
1	B	79	ARG
1	B	82	LEU
1	B	84	ARG
1	B	86	LYS
1	B	91	GLU
1	B	96	LYS
1	B	104	THR
1	B	123	GLN
1	B	126	ASN
1	B	127	THR
1	B	128	ARG
1	B	150	ARG
1	B	151	GLN
1	B	155	LYS
1	B	159	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	162	VAL
1	B	170	VAL
1	B	175	THR
1	B	176	ASP
1	B	181	HIS
1	B	182	SER
1	B	189	HIS
1	B	205	ILE
1	B	207	LYS
1	B	214	MET
1	B	216	LEU
1	B	220	THR
1	B	222	GLU
2	C	94	TRP
2	C	100	GLU
2	C	101	LYS
2	C	109	SER
2	C	113	ARG
2	C	115	ILE
2	C	122	VAL
2	C	123	MET
2	C	129	ASP
2	C	131	THR
2	C	135	TRP
2	C	136	ASP
2	C	138	GLU
2	C	152	SER
2	C	156	ILE
2	C	157	SER
2	C	161	SER
2	C	163	LYS
2	C	168	CYS
2	C	171	ASP
2	C	172	MET
2	C	176	LEU
2	C	179	PHE
2	C	180	GLN
2	C	183	GLU
2	C	186	ARG
2	C	188	MET
2	C	192	ASP
2	C	196	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	200	ILE
2	C	201	MET
2	C	203	ASN
2	C	207	ILE
2	C	208	VAL
2	C	209	SER
2	C	212	ARG
2	C	218	MET
2	C	222	GLN
2	C	234	ARG
2	C	238	ARG
2	C	240	VAL
2	C	243	ASN
2	C	247	THR
2	C	252	CYS
2	C	257	THR
2	C	261	TRP
2	C	266	LYS
2	C	275	HIS
2	C	279	VAL
2	C	282	ILE
2	C	283	SER
2	C	292	SER
2	C	293	ILE
2	C	295	GLU
2	C	297	THR
2	C	299	SER
2	C	311	LEU
2	C	312	LEU
2	C	313	SER
2	C	322	MET
2	C	324	ASP
2	C	325	VAL
2	C	331	LEU
2	C	337	HIS
2	C	338	ASP
2	C	339	ASN
2	C	348	SER
2	C	354	LEU
2	C	355	SER
2	C	356	CYS
2	C	360	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	361	THR
2	C	362	LEU
2	C	363	ARG
2	C	368	LYS
2	C	369	ASN
2	C	370	LYS
2	C	372	CYS
2	C	377	ASN
2	C	380	GLU
2	C	384	THR
2	C	391	THR
2	C	396	VAL
2	C	397	THR
2	C	399	SER
2	C	403	THR
2	C	408	GLU
2	D	94	TRP
2	D	95	ILE
2	D	97	ARG
2	D	98	PRO
2	D	100	GLU
2	D	112	THR
2	D	113	ARG
2	D	114	VAL
2	D	115	ILE
2	D	122	VAL
2	D	123	MET
2	D	128	GLU
2	D	129	ASP
2	D	134	VAL
2	D	136	ASP
2	D	139	THR
2	D	152	SER
2	D	153	VAL
2	D	159	ASP
2	D	163	LYS
2	D	171	ASP
2	D	173	THR
2	D	176	LEU
2	D	178	ASP
2	D	179	PHE
2	D	182	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	183	GLU
2	D	198	VAL
2	D	200	ILE
2	D	201	MET
2	D	207	ILE
2	D	212	ARG
2	D	222	GLN
2	D	229	THR
2	D	233	HIS
2	D	234	ARG
2	D	239	MET
2	D	240	VAL
2	D	247	THR
2	D	249	ILE
2	D	251	SER
2	D	257	THR
2	D	261	TRP
2	D	265	THR
2	D	266	LYS
2	D	268	CYS
2	D	269	LYS
2	D	273	ARG
2	D	275	HIS
2	D	276	ARG
2	D	282	ILE
2	D	283	SER
2	D	291	SER
2	D	292	SER
2	D	295	GLU
2	D	297	THR
2	D	299	SER
2	D	318	LYS
2	D	322	MET
2	D	324	ASP
2	D	325	VAL
2	D	326	SER
2	D	329	MET
2	D	330	CYS
2	D	331	LEU
2	D	332	MET
2	D	337	HIS
2	D	339	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	342	ARG
2	D	344	VAL
2	D	345	LEU
2	D	348	SER
2	D	351	LYS
2	D	354	LEU
2	D	355	SER
2	D	360	LYS
2	D	361	THR
2	D	363	ARG
2	D	367	TYR
2	D	369	ASN
2	D	371	ARG
2	D	376	LEU
2	D	377	ASN
2	D	381	HIS
2	D	382	PHE
2	D	391	THR
2	D	396	VAL
2	D	397	THR
1	E	17	ASP
1	E	18	ILE
1	E	34	ASP
1	E	37	ASP
1	E	43	LEU
1	E	48	SER
1	E	52	LEU
1	E	57	GLU
1	E	66	LEU
1	E	69	LEU
1	E	76	ASP
1	E	77	THR
1	E	92	ASN
1	E	104	THR
1	E	118	ILE
1	E	123	GLN
1	E	126	ASN
1	E	150	ARG
1	E	158	GLN
1	E	170	VAL
1	E	173	LEU
1	E	176	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	189	HIS
1	E	207	LYS
1	E	214	MET
1	E	215	GLN
1	E	216	LEU
1	F	7	ASN
1	F	17	ASP
1	F	23	ARG
1	F	33	LEU
1	F	34	ASP
1	F	37	ASP
1	F	43	LEU
1	F	48	SER
1	F	52	LEU
1	F	55	GLN
1	F	58	ILE
1	F	60	ARG
1	F	66	LEU
1	F	69	LEU
1	F	76	ASP
1	F	79	ARG
1	F	86	LYS
1	F	91	GLU
1	F	102	VAL
1	F	123	GLN
1	F	126	ASN
1	F	128	ARG
1	F	139	LEU
1	F	151	GLN
1	F	155	LYS
1	F	158	GLN
1	F	166	LYS
1	F	170	VAL
1	F	176	ASP
1	F	180	VAL
1	F	181	HIS
1	F	207	LYS
1	F	214	MET
1	F	216	LEU
1	F	220	THR
1	F	222	GLU
2	G	94	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	95	ILE
2	G	97	ARG
2	G	100	GLU
2	G	101	LYS
2	G	109	SER
2	G	113	ARG
2	G	115	ILE
2	G	119	VAL
2	G	122	VAL
2	G	123	MET
2	G	129	ASP
2	G	131	THR
2	G	135	TRP
2	G	136	ASP
2	G	138	GLU
2	G	147	LYS
2	G	152	SER
2	G	154	GLN
2	G	161	SER
2	G	163	LYS
2	G	168	CYS
2	G	171	ASP
2	G	173	THR
2	G	176	LEU
2	G	178	ASP
2	G	179	PHE
2	G	183	GLU
2	G	186	ARG
2	G	187	THR
2	G	200	ILE
2	G	201	MET
2	G	208	VAL
2	G	212	ARG
2	G	218	MET
2	G	222	GLN
2	G	223	THR
2	G	227	VAL
2	G	229	THR
2	G	231	THR
2	G	233	HIS
2	G	234	ARG
2	G	239	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	240	VAL
2	G	243	ASN
2	G	247	THR
2	G	249	ILE
2	G	253	SER
2	G	257	THR
2	G	261	TRP
2	G	265	THR
2	G	266	LYS
2	G	267	GLU
2	G	268	CYS
2	G	273	ARG
2	G	275	HIS
2	G	276	ARG
2	G	282	ILE
2	G	283	SER
2	G	292	SER
2	G	299	SER
2	G	318	LYS
2	G	322	MET
2	G	323	TRP
2	G	324	ASP
2	G	325	VAL
2	G	326	SER
2	G	331	LEU
2	G	338	ASP
2	G	339	ASN
2	G	345	LEU
2	G	346	PHE
2	G	351	LYS
2	G	354	LEU
2	G	360	LYS
2	G	362	LEU
2	G	363	ARG
2	G	368	LYS
2	G	369	ASN
2	G	372	CYS
2	G	373	MET
2	G	380	GLU
2	G	384	THR
2	G	390	LYS
2	G	391	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	395	VAL
2	G	396	VAL
2	G	397	THR
2	H	94	TRP
2	H	95	ILE
2	H	96	PRO
2	H	97	ARG
2	H	98	PRO
2	H	100	GLU
2	H	101	LYS
2	H	104	LEU
2	H	105	SER
2	H	109	SER
2	H	113	ARG
2	H	115	ILE
2	H	116	PHE
2	H	121	SER
2	H	122	VAL
2	H	123	MET
2	H	127	SER
2	H	129	ASP
2	H	131	THR
2	H	136	ASP
2	H	152	SER
2	H	154	GLN
2	H	156	ILE
2	H	159	ASP
2	H	169	SER
2	H	171	ASP
2	H	176	LEU
2	H	179	PHE
2	H	180	GLN
2	H	182	PHE
2	H	183	GLU
2	H	186	ARG
2	H	187	THR
2	H	188	MET
2	H	198	VAL
2	H	201	MET
2	H	212	ARG
2	H	218	MET
2	H	222	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	227	VAL
2	H	233	HIS
2	H	234	ARG
2	H	235	GLU
2	H	240	VAL
2	H	243	ASN
2	H	244	GLN
2	H	247	THR
2	H	249	ILE
2	H	257	THR
2	H	262	VAL
2	H	265	THR
2	H	266	LYS
2	H	269	LYS
2	H	281	CYS
2	H	282	ILE
2	H	291	SER
2	H	295	GLU
2	H	297	THR
2	H	311	LEU
2	H	315	SER
2	H	318	LYS
2	H	324	ASP
2	H	325	VAL
2	H	327	THR
2	H	329	MET
2	H	331	LEU
2	H	337	HIS
2	H	339	ASN
2	H	344	VAL
2	H	348	SER
2	H	354	LEU
2	H	355	SER
2	H	360	LYS
2	H	361	THR
2	H	363	ARG
2	H	367	TYR
2	H	369	ASN
2	H	371	ARG
2	H	382	PHE
2	H	386	LEU
2	H	395	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	396	VAL
2	H	397	THR
2	H	399	SER
2	H	403	THR
1	I	7	ASN
1	I	17	ASP
1	I	18	ILE
1	I	33	LEU
1	I	34	ASP
1	I	43	LEU
1	I	48	SER
1	I	51	GLN
1	I	52	LEU
1	I	57	GLU
1	I	58	ILE
1	I	60	ARG
1	I	62	LEU
1	I	66	LEU
1	I	69	LEU
1	I	76	ASP
1	I	98	ILE
1	I	106	ASN
1	I	123	GLN
1	I	126	ASN
1	I	128	ARG
1	I	151	GLN
1	I	155	LYS
1	I	158	GLN
1	I	161	LYS
1	I	162	VAL
1	I	170	VAL
1	I	172	LEU
1	I	175	THR
1	I	176	ASP
1	I	181	HIS
1	I	190	ASP
1	I	191	MET
1	I	197	LEU
1	I	207	LYS
1	I	214	MET
1	I	215	GLN
1	I	216	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	220	THR
1	I	222	GLU
1	J	7	ASN
1	J	17	ASP
1	J	33	LEU
1	J	37	ASP
1	J	43	LEU
1	J	48	SER
1	J	52	LEU
1	J	58	ILE
1	J	60	ARG
1	J	62	LEU
1	J	64	SER
1	J	66	LEU
1	J	81	VAL
1	J	102	VAL
1	J	114	VAL
1	J	123	GLN
1	J	126	ASN
1	J	128	ARG
1	J	131	GLN
1	J	151	GLN
1	J	155	LYS
1	J	158	GLN
1	J	159	LEU
1	J	161	LYS
1	J	169	ASN
1	J	170	VAL
1	J	205	ILE
1	J	207	LYS
1	J	216	LEU
1	J	220	THR
1	J	222	GLU
2	K	94	TRP
2	K	97	ARG
2	K	100	GLU
2	K	101	LYS
2	K	102	TYR
2	K	109	SER
2	K	113	ARG
2	K	114	VAL
2	K	115	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	116	PHE
2	K	121	SER
2	K	122	VAL
2	K	123	MET
2	K	129	ASP
2	K	131	THR
2	K	135	TRP
2	K	136	ASP
2	K	144	ARG
2	K	154	GLN
2	K	157	SER
2	K	159	ASP
2	K	168	CYS
2	K	171	ASP
2	K	176	LEU
2	K	178	ASP
2	K	179	PHE
2	K	182	PHE
2	K	183	GLU
2	K	185	ILE
2	K	186	ARG
2	K	188	MET
2	K	194	ASN
2	K	201	MET
2	K	207	ILE
2	K	208	VAL
2	K	212	ARG
2	K	218	MET
2	K	234	ARG
2	K	235	GLU
2	K	238	ARG
2	K	239	MET
2	K	240	VAL
2	K	245	ASP
2	K	247	THR
2	K	257	THR
2	K	263	VAL
2	K	266	LYS
2	K	267	GLU
2	K	268	CYS
2	K	269	LYS
2	K	275	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	276	ARG
2	K	279	VAL
2	K	282	ILE
2	K	287	GLU
2	K	290	TYR
2	K	293	ILE
2	K	295	GLU
2	K	299	SER
2	K	311	LEU
2	K	312	LEU
2	K	317	ASP
2	K	318	LYS
2	K	322	MET
2	K	323	TRP
2	K	325	VAL
2	K	330	CYS
2	K	332	MET
2	K	337	HIS
2	K	339	ASN
2	K	341	VAL
2	K	344	VAL
2	K	345	LEU
2	K	346	PHE
2	K	348	SER
2	K	351	LYS
2	K	352	PHE
2	K	354	LEU
2	K	355	SER
2	K	360	LYS
2	K	362	LEU
2	K	363	ARG
2	K	369	ASN
2	K	371	ARG
2	K	373	MET
2	K	376	LEU
2	K	380	GLU
2	K	382	PHE
2	K	385	SER
2	K	390	LYS
2	K	391	THR
2	K	395	VAL
2	K	396	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	408	GLU
2	L	94	TRP
2	L	95	ILE
2	L	97	ARG
2	L	100	GLU
2	L	109	SER
2	L	112	THR
2	L	113	ARG
2	L	114	VAL
2	L	115	ILE
2	L	122	VAL
2	L	123	MET
2	L	128	GLU
2	L	129	ASP
2	L	131	THR
2	L	135	TRP
2	L	136	ASP
2	L	138	GLU
2	L	144	ARG
2	L	147	LYS
2	L	152	SER
2	L	153	VAL
2	L	154	GLN
2	L	156	ILE
2	L	159	ASP
2	L	168	CYS
2	L	173	THR
2	L	178	ASP
2	L	179	PHE
2	L	196	SER
2	L	198	VAL
2	L	201	MET
2	L	208	VAL
2	L	212	ARG
2	L	213	ASP
2	L	218	MET
2	L	222	GLN
2	L	228	LYS
2	L	233	HIS
2	L	234	ARG
2	L	240	VAL
2	L	243	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	244	GLN
2	L	245	ASP
2	L	247	THR
2	L	249	ILE
2	L	252	CYS
2	L	257	THR
2	L	263	VAL
2	L	265	THR
2	L	266	LYS
2	L	267	GLU
2	L	273	ARG
2	L	275	HIS
2	L	276	ARG
2	L	282	ILE
2	L	283	SER
2	L	292	SER
2	L	293	ILE
2	L	295	GLU
2	L	311	LEU
2	L	312	LEU
2	L	317	ASP
2	L	322	MET
2	L	324	ASP
2	L	325	VAL
2	L	326	SER
2	L	329	MET
2	L	330	CYS
2	L	337	HIS
2	L	339	ASN
2	L	345	LEU
2	L	348	SER
2	L	351	LYS
2	L	359	ASP
2	L	360	LYS
2	L	363	ARG
2	L	367	TYR
2	L	369	ASN
2	L	370	LYS
2	L	373	MET
2	L	374	LYS
2	L	375	THR
2	L	382	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	384	THR
2	L	385	SER
2	L	391	THR
2	L	396	VAL
1	M	7	ASN
1	M	17	ASP
1	M	18	ILE
1	M	33	LEU
1	M	35	CYS
1	M	36	LYS
1	M	43	LEU
1	M	48	SER
1	M	52	LEU
1	M	58	ILE
1	M	64	SER
1	M	66	LEU
1	M	84	ARG
1	M	91	GLU
1	M	123	GLN
1	M	126	ASN
1	M	128	ARG
1	M	150	ARG
1	M	151	GLN
1	M	155	LYS
1	M	161	LYS
1	M	162	VAL
1	M	167	LEU
1	M	170	VAL
1	M	171	GLN
1	M	172	LEU
1	M	180	VAL
1	M	207	LYS
1	M	214	MET
1	M	215	GLN
1	M	216	LEU
1	M	222	GLU
1	N	6	SER
1	N	7	ASN
1	N	16	GLU
1	N	17	ASP
1	N	25	MET
1	N	26	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	33	LEU
1	N	34	ASP
1	N	35	CYS
1	N	36	LYS
1	N	37	ASP
1	N	39	GLU
1	N	43	LEU
1	N	45	VAL
1	N	48	SER
1	N	52	LEU
1	N	58	ILE
1	N	62	LEU
1	N	64	SER
1	N	66	LEU
1	N	96	LYS
1	N	123	GLN
1	N	126	ASN
1	N	127	THR
1	N	128	ARG
1	N	131	GLN
1	N	151	GLN
1	N	158	GLN
1	N	163	SER
1	N	166	LYS
1	N	169	ASN
1	N	170	VAL
1	N	171	GLN
1	N	172	LEU
1	N	180	VAL
1	N	214	MET
1	N	215	GLN
1	N	216	LEU
2	O	95	ILE
2	O	97	ARG
2	O	100	GLU
2	O	101	LYS
2	O	102	TYR
2	O	109	SER
2	O	113	ARG
2	O	115	ILE
2	O	116	PHE
2	O	120	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	122	VAL
2	O	123	MET
2	O	129	ASP
2	O	131	THR
2	O	136	ASP
2	O	144	ARG
2	O	151	ASP
2	O	152	SER
2	O	156	ILE
2	O	157	SER
2	O	158	PHE
2	O	163	LYS
2	O	168	CYS
2	O	171	ASP
2	O	173	THR
2	O	176	LEU
2	O	179	PHE
2	O	182	PHE
2	O	188	MET
2	O	196	SER
2	O	198	VAL
2	O	200	ILE
2	O	212	ARG
2	O	218	MET
2	O	223	THR
2	O	233	HIS
2	O	234	ARG
2	O	235	GLU
2	O	238	ARG
2	O	239	MET
2	O	240	VAL
2	O	244	GLN
2	O	247	THR
2	O	249	ILE
2	O	266	LYS
2	O	268	CYS
2	O	273	ARG
2	O	279	VAL
2	O	282	ILE
2	O	287	GLU
2	O	290	TYR
2	O	292	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	297	THR
2	O	299	SER
2	O	311	LEU
2	O	318	LYS
2	O	322	MET
2	O	324	ASP
2	O	326	SER
2	O	330	CYS
2	O	331	LEU
2	O	337	HIS
2	O	339	ASN
2	O	341	VAL
2	O	345	LEU
2	O	348	SER
2	O	356	CYS
2	O	360	LYS
2	O	363	ARG
2	O	366	ASP
2	O	367	TYR
2	O	369	ASN
2	O	370	LYS
2	O	371	ARG
2	O	373	MET
2	O	382	PHE
2	O	384	THR
2	O	385	SER
2	O	386	LEU
2	O	390	LYS
2	O	391	THR
2	O	395	VAL
2	O	396	VAL
2	O	403	THR
2	O	406	VAL
2	P	94	TRP
2	P	95	ILE
2	P	97	ARG
2	P	100	GLU
2	P	105	SER
2	P	113	ARG
2	P	115	ILE
2	P	123	MET
2	P	129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	131	THR
2	P	135	TRP
2	P	136	ASP
2	P	145	THR
2	P	152	SER
2	P	154	GLN
2	P	159	ASP
2	P	161	SER
2	P	163	LYS
2	P	168	CYS
2	P	176	LEU
2	P	178	ASP
2	P	179	PHE
2	P	182	PHE
2	P	183	GLU
2	P	186	ARG
2	P	187	THR
2	P	201	MET
2	P	212	ARG
2	P	213	ASP
2	P	218	MET
2	P	222	GLN
2	P	234	ARG
2	P	235	GLU
2	P	238	ARG
2	P	240	VAL
2	P	243	ASN
2	P	244	GLN
2	P	249	ILE
2	P	257	THR
2	P	265	THR
2	P	266	LYS
2	P	267	GLU
2	P	269	LYS
2	P	273	ARG
2	P	275	HIS
2	P	280	GLU
2	P	282	ILE
2	P	283	SER
2	P	290	TYR
2	P	292	SER
2	P	310	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	318	LYS
2	P	324	ASP
2	P	325	VAL
2	P	331	LEU
2	P	337	HIS
2	P	339	ASN
2	P	348	SER
2	P	351	LYS
2	P	355	SER
2	P	360	LYS
2	P	361	THR
2	P	363	ARG
2	P	367	TYR
2	P	368	LYS
2	P	369	ASN
2	P	371	ARG
2	P	373	MET
2	P	374	LYS
2	P	382	PHE
2	P	390	LYS
2	P	391	THR
2	P	403	THR
1	Q	6	SER
1	Q	7	ASN
1	Q	17	ASP
1	Q	23	ARG
1	Q	26	SER
1	Q	33	LEU
1	Q	35	CYS
1	Q	42	VAL
1	Q	43	LEU
1	Q	48	SER
1	Q	51	GLN
1	Q	52	LEU
1	Q	58	ILE
1	Q	60	ARG
1	Q	62	LEU
1	Q	66	LEU
1	Q	102	VAL
1	Q	124	LEU
1	Q	126	ASN
1	Q	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	155	LYS
1	Q	160	LEU
1	Q	169	ASN
1	Q	170	VAL
1	Q	171	GLN
1	Q	172	LEU
1	Q	175	THR
1	Q	176	ASP
1	Q	186	ILE
1	Q	190	ASP
1	Q	205	ILE
1	Q	207	LYS
1	Q	214	MET
1	Q	215	GLN
1	Q	216	LEU
1	Q	220	THR
1	Q	222	GLU
1	R	6	SER
1	R	7	ASN
1	R	11	ILE
1	R	17	ASP
1	R	18	ILE
1	R	23	ARG
1	R	27	GLN
1	R	33	LEU
1	R	35	CYS
1	R	37	ASP
1	R	42	VAL
1	R	43	LEU
1	R	45	VAL
1	R	48	SER
1	R	51	GLN
1	R	52	LEU
1	R	58	ILE
1	R	60	ARG
1	R	62	LEU
1	R	64	SER
1	R	66	LEU
1	R	69	LEU
1	R	76	ASP
1	R	94	LYS
1	R	102	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	106	ASN
1	R	123	GLN
1	R	126	ASN
1	R	127	THR
1	R	128	ARG
1	R	131	GLN
1	R	137	LEU
1	R	147	ASN
1	R	151	GLN
1	R	152	LYS
1	R	155	LYS
1	R	170	VAL
1	R	172	LEU
1	R	176	ASP
1	R	180	VAL
1	R	187	SER
1	R	214	MET
1	R	216	LEU
1	R	220	THR
2	S	94	TRP
2	S	97	ARG
2	S	100	GLU
2	S	101	LYS
2	S	104	LEU
2	S	113	ARG
2	S	115	ILE
2	S	116	PHE
2	S	122	VAL
2	S	123	MET
2	S	131	THR
2	S	136	ASP
2	S	138	GLU
2	S	144	ARG
2	S	145	THR
2	S	147	LYS
2	S	151	ASP
2	S	152	SER
2	S	155	ASP
2	S	156	ILE
2	S	159	ASP
2	S	163	LYS
2	S	168	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	171	ASP
2	S	173	THR
2	S	178	ASP
2	S	179	PHE
2	S	183	GLU
2	S	186	ARG
2	S	188	MET
2	S	196	SER
2	S	198	VAL
2	S	201	MET
2	S	208	VAL
2	S	212	ARG
2	S	213	ASP
2	S	216	ILE
2	S	218	MET
2	S	222	GLN
2	S	223	THR
2	S	233	HIS
2	S	234	ARG
2	S	238	ARG
2	S	240	VAL
2	S	244	GLN
2	S	247	THR
2	S	252	CYS
2	S	257	THR
2	S	263	VAL
2	S	265	THR
2	S	266	LYS
2	S	267	GLU
2	S	268	CYS
2	S	269	LYS
2	S	279	VAL
2	S	282	ILE
2	S	290	TYR
2	S	292	SER
2	S	294	SER
2	S	295	GLU
2	S	297	THR
2	S	299	SER
2	S	312	LEU
2	S	316	ARG
2	S	322	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	323	TRP
2	S	331	LEU
2	S	339	ASN
2	S	345	LEU
2	S	346	PHE
2	S	348	SER
2	S	351	LYS
2	S	356	CYS
2	S	359	ASP
2	S	361	THR
2	S	363	ARG
2	S	369	ASN
2	S	371	ARG
2	S	373	MET
2	S	374	LYS
2	S	376	LEU
2	S	380	GLU
2	S	390	LYS
2	S	391	THR
2	S	395	VAL
2	S	396	VAL
2	S	397	THR
2	S	400	VAL
2	S	401	ASP
2	S	403	THR
2	S	406	VAL
2	T	94	TRP
2	T	95	ILE
2	T	97	ARG
2	T	100	GLU
2	T	101	LYS
2	T	102	TYR
2	T	108	ARG
2	T	109	SER
2	T	113	ARG
2	T	114	VAL
2	T	115	ILE
2	T	123	MET
2	T	129	ASP
2	T	131	THR
2	T	136	ASP
2	T	139	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	144	ARG
2	T	147	LYS
2	T	151	ASP
2	T	152	SER
2	T	154	GLN
2	T	156	ILE
2	T	161	SER
2	T	168	CYS
2	T	171	ASP
2	T	176	LEU
2	T	178	ASP
2	T	179	PHE
2	T	182	PHE
2	T	185	ILE
2	T	186	ARG
2	T	188	MET
2	T	196	SER
2	T	197	SER
2	T	200	ILE
2	T	201	MET
2	T	207	ILE
2	T	209	SER
2	T	212	ARG
2	T	213	ASP
2	T	218	MET
2	T	222	GLN
2	T	234	ARG
2	T	240	VAL
2	T	243	ASN
2	T	245	ASP
2	T	247	THR
2	T	249	ILE
2	T	253	SER
2	T	257	THR
2	T	266	LYS
2	T	275	HIS
2	T	282	ILE
2	T	287	GLU
2	T	290	TYR
2	T	295	GLU
2	T	299	SER
2	T	312	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	318	LYS
2	T	322	MET
2	T	324	ASP
2	T	325	VAL
2	T	326	SER
2	T	331	LEU
2	T	334	LEU
2	T	335	VAL
2	T	338	ASP
2	T	339	ASN
2	T	345	LEU
2	T	346	PHE
2	T	351	LYS
2	T	354	LEU
2	T	355	SER
2	T	359	ASP
2	T	360	LYS
2	T	361	THR
2	T	362	LEU
2	T	363	ARG
2	T	366	ASP
2	T	367	TYR
2	T	369	ASN
2	T	370	LYS
2	T	372	CYS
2	T	373	MET
2	T	374	LYS
2	T	377	ASN
2	T	380	GLU
2	T	385	SER
2	T	386	LEU
2	T	390	LYS
2	T	395	VAL
2	T	397	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	13	HIS
1	A	19	GLN
1	A	80	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	ASN
1	A	106	ASN
1	A	123	GLN
1	A	126	ASN
1	A	147	ASN
1	A	189	HIS
1	B	7	ASN
1	B	19	GLN
1	B	106	ASN
1	B	107	HIS
1	B	126	ASN
1	B	147	ASN
1	B	157	ASN
1	B	181	HIS
1	B	189	HIS
2	C	193	HIS
2	C	203	ASN
2	C	243	ASN
2	C	256	GLN
2	C	337	HIS
2	C	339	ASN
2	C	402	GLN
2	D	193	HIS
2	D	243	ASN
2	D	339	ASN
2	D	347	HIS
2	D	369	ASN
1	E	7	ASN
1	E	55	GLN
1	E	87	ASN
1	E	106	ASN
1	E	109	ASN
1	E	123	GLN
1	E	147	ASN
1	E	181	HIS
1	F	7	ASN
1	F	19	GLN
1	F	67	HIS
1	F	87	ASN
1	F	106	ASN
1	F	107	HIS
1	F	109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	126	ASN
1	F	147	ASN
1	F	181	HIS
1	F	189	HIS
2	G	160	HIS
2	G	193	HIS
2	G	243	ASN
2	G	337	HIS
2	G	339	ASN
2	G	377	ASN
2	G	402	GLN
2	H	193	HIS
2	H	243	ASN
2	H	337	HIS
2	H	339	ASN
2	H	347	HIS
2	H	402	GLN
1	I	7	ASN
1	I	19	GLN
1	I	87	ASN
1	I	106	ASN
1	I	107	HIS
1	I	109	ASN
1	I	123	GLN
1	I	126	ASN
1	I	147	ASN
1	I	158	GLN
1	I	210	HIS
1	J	7	ASN
1	J	67	HIS
1	J	105	ASN
1	J	123	GLN
1	J	126	ASN
1	J	147	ASN
1	J	189	HIS
2	K	193	HIS
2	K	233	HIS
2	K	243	ASN
2	K	337	HIS
2	K	339	ASN
2	K	369	ASN
2	K	377	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	193	HIS
2	L	203	ASN
2	L	233	HIS
2	L	243	ASN
2	L	337	HIS
2	L	339	ASN
2	L	347	HIS
2	L	379	HIS
2	L	389	HIS
1	M	7	ASN
1	M	19	GLN
1	M	55	GLN
1	M	106	ASN
1	M	109	ASN
1	M	123	GLN
1	M	126	ASN
1	M	147	ASN
1	M	171	GLN
1	M	181	HIS
1	M	210	HIS
1	N	7	ASN
1	N	19	GLN
1	N	54	GLN
1	N	105	ASN
1	N	106	ASN
1	N	109	ASN
1	N	123	GLN
1	N	131	GLN
1	N	147	ASN
1	N	151	GLN
1	N	210	HIS
2	O	337	HIS
2	O	339	ASN
2	O	402	GLN
2	P	154	GLN
2	P	160	HIS
2	P	193	HIS
2	P	203	ASN
2	P	233	HIS
2	P	243	ASN
2	P	337	HIS
2	P	339	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	347	HIS
1	Q	7	ASN
1	Q	19	GLN
1	Q	106	ASN
1	Q	109	ASN
1	Q	147	ASN
1	Q	189	HIS
1	R	7	ASN
1	R	55	GLN
1	R	109	ASN
1	R	131	GLN
1	R	147	ASN
1	R	171	GLN
1	R	210	HIS
2	S	193	HIS
2	S	339	ASN
2	S	402	GLN
2	T	193	HIS
2	T	233	HIS
2	T	243	ASN
2	T	339	ASN
2	T	402	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	A	218/229 (95%)	0.14	4 (1%) 71 65	3, 4, 8, 10	0
1	B	218/229 (95%)	-0.01	4 (1%) 71 65	3, 4, 7, 10	0
1	E	218/229 (95%)	-0.02	1 (0%) 91 89	3, 4, 8, 10	0
1	F	218/229 (95%)	0.24	7 (3%) 51 47	3, 4, 8, 11	0
1	I	218/229 (95%)	0.01	2 (0%) 85 81	3, 5, 8, 10	0
1	J	218/229 (95%)	-0.04	4 (1%) 71 65	3, 5, 7, 10	0
1	M	218/229 (95%)	-0.01	2 (0%) 85 81	3, 5, 7, 10	0
1	N	218/229 (95%)	0.11	1 (0%) 91 89	3, 5, 7, 9	0
1	Q	218/229 (95%)	0.26	13 (5%) 25 23	3, 5, 7, 9	0
1	R	218/229 (95%)	0.46	14 (6%) 23 21	3, 5, 7, 9	0
2	C	310/410 (75%)	0.53	16 (5%) 31 28	3, 5, 63, 78	0
2	D	310/410 (75%)	0.53	18 (5%) 26 24	3, 5, 74, 85	0
2	G	310/410 (75%)	0.58	22 (7%) 19 18	3, 5, 73, 80	0
2	H	310/410 (75%)	0.51	18 (5%) 26 24	3, 5, 65, 82	0
2	K	310/410 (75%)	0.58	23 (7%) 17 17	3, 5, 84, 89	0
2	L	310/410 (75%)	0.48	19 (6%) 25 23	3, 5, 67, 77	0
2	O	310/410 (75%)	1.02	51 (16%) 2 2	3, 5, 90, 94	0
2	P	310/410 (75%)	0.49	18 (5%) 26 24	3, 5, 73, 82	0
2	S	310/410 (75%)	1.30	73 (23%) 1 1	3, 5, 91, 94	0
2	T	310/410 (75%)	1.28	70 (22%) 1 1	3, 5, 91, 95	0
All	All	5280/6390 (82%)	0.48	380 (7%) 18 17	3, 5, 83, 95	0

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	299	SER	10.1
2	G	299	SER	8.3
2	G	298	GLY	8.1
2	S	336	GLY	7.5
2	P	297	THR	7.0
2	T	300	GLU	6.8
2	O	300	GLU	6.7
2	S	300	GLU	6.7
2	L	299	SER	6.7
1	Q	223	GLU	6.6
2	D	299	SER	6.5
2	T	355	SER	6.3
1	M	223	GLU	6.3
2	O	299	SER	6.2
2	S	299	SER	6.1
2	P	298	GLY	5.7
2	S	297	THR	5.7
1	B	223	GLU	5.7
2	D	298	GLY	5.5
2	T	335	VAL	5.4
2	T	289	SER	5.3
2	S	387	ASP	5.3
2	S	407	TRP	5.2
2	P	299	SER	5.2
1	A	223	GLU	5.2
2	G	300	GLU	5.1
2	T	297	THR	5.1
2	H	298	GLY	5.0
2	T	386	LEU	5.0
2	T	385	SER	4.9
2	S	343	GLY	4.9
2	O	298	GLY	4.9
2	L	298	GLY	4.9
2	H	387	ASP	4.9
2	K	299	SER	4.8
2	T	407	TRP	4.8
2	S	377	ASN	4.7
1	F	221	PRO	4.7
2	D	300	GLU	4.6
2	T	343	GLY	4.6
2	T	98	PRO	4.5
2	T	336	GLY	4.4
2	O	408	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	344	VAL	4.4
2	H	299	SER	4.4
2	O	232	GLY	4.4
2	G	387	ASP	4.4
1	R	185	ALA	4.4
2	S	289	SER	4.4
2	T	298	GLY	4.3
2	O	294	SER	4.3
2	O	180	GLN	4.3
2	S	314	GLY	4.1
2	T	356	CYS	4.1
2	O	385	SER	4.1
2	O	344	VAL	4.1
2	O	386	LEU	4.0
2	C	299	SER	4.0
2	O	251	SER	3.9
2	T	377	ASN	3.9
1	R	61	GLU	3.9
2	T	97	ARG	3.9
2	O	167	SER	3.9
1	F	220	THR	3.9
2	K	300	GLU	3.9
2	S	376	LEU	3.9
2	O	407	TRP	3.8
2	O	366	ASP	3.8
2	P	300	GLU	3.8
2	S	97	ARG	3.8
2	C	298	GLY	3.8
2	O	295	GLU	3.8
2	S	298	GLY	3.8
2	G	297	THR	3.8
2	S	339	ASN	3.8
2	S	294	SER	3.8
2	S	183	GLU	3.8
2	G	384	THR	3.7
2	T	345	LEU	3.7
2	O	384	THR	3.7
2	S	384	THR	3.7
2	T	94	TRP	3.7
1	J	223	GLU	3.6
2	O	92	LYS	3.6
2	T	344	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	297	THR	3.6
1	R	223	GLU	3.6
2	D	343	GLY	3.6
2	G	385	SER	3.6
2	C	385	SER	3.5
2	O	339	ASN	3.5
2	T	387	ASP	3.5
2	O	343	GLY	3.5
2	C	387	ASP	3.5
1	R	20	GLY	3.5
2	O	297	THR	3.5
2	D	234	ARG	3.5
2	L	387	ASP	3.5
2	S	296	ALA	3.5
1	I	223	GLU	3.5
2	T	270	ALA	3.4
2	S	385	SER	3.4
2	G	343	GLY	3.4
2	S	335	VAL	3.4
1	F	223	GLU	3.4
2	T	324	ASP	3.4
2	T	276	ARG	3.4
2	C	384	THR	3.4
2	G	386	LEU	3.4
2	D	385	SER	3.3
2	S	277	HIS	3.3
2	T	408	GLU	3.3
2	S	245	ASP	3.3
2	C	297	THR	3.3
1	R	220	THR	3.2
2	O	391	THR	3.2
2	K	342	ARG	3.2
2	T	157	SER	3.2
2	D	344	VAL	3.2
2	T	366	ASP	3.1
2	O	263	VAL	3.1
2	P	276	ARG	3.1
2	S	345	LEU	3.1
2	P	385	SER	3.1
2	G	344	VAL	3.1
2	T	288	SER	3.1
2	T	274	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	352	PHE	3.1
2	L	343	GLY	3.1
2	P	347	HIS	3.1
2	S	199	SER	3.1
2	D	387	ASP	3.1
2	D	356	CYS	3.0
2	K	264	ALA	3.0
2	C	351	LYS	3.0
2	K	142	PHE	3.0
2	T	107	HIS	3.0
2	O	183	GLU	3.0
1	I	46	GLY	3.0
2	T	342	ARG	3.0
2	T	313	SER	3.0
2	S	351	LYS	3.0
2	O	145	THR	3.0
1	Q	6	SER	3.0
1	R	221	PRO	3.0
2	H	344	VAL	3.0
2	K	234	ARG	3.0
2	L	300	GLU	3.0
2	K	218	MET	2.9
2	K	408	GLU	2.9
2	S	274	GLU	2.9
2	T	330	CYS	2.9
2	D	386	LEU	2.9
2	G	234	ARG	2.9
2	T	103	ALA	2.9
2	C	343	GLY	2.9
2	C	355	SER	2.9
2	C	386	LEU	2.9
2	S	275	HIS	2.9
2	S	232	GLY	2.9
2	S	342	ARG	2.9
2	P	234	ARG	2.9
2	S	94	TRP	2.9
2	S	96	PRO	2.9
2	K	297	THR	2.9
2	S	348	SER	2.9
1	Q	39	GLU	2.8
2	O	226	CYS	2.8
1	J	9	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	343	GLY	2.8
2	P	387	ASP	2.8
1	Q	221	PRO	2.8
2	D	297	THR	2.8
2	K	343	GLY	2.8
2	S	293	ILE	2.8
2	T	269	LYS	2.8
2	S	120	PHE	2.8
2	S	143	GLU	2.8
2	T	136	ASP	2.8
2	S	283	SER	2.8
2	L	336	GLY	2.8
2	S	408	GLU	2.8
2	P	388	PHE	2.8
2	T	204	GLY	2.8
2	S	319	THR	2.7
2	D	270	ALA	2.7
2	T	100	GLU	2.7
2	S	119	VAL	2.7
1	N	220	THR	2.7
2	D	384	THR	2.7
2	H	385	SER	2.7
2	L	384	THR	2.7
2	O	244	GLN	2.7
2	S	164	LEU	2.7
2	T	138	GLU	2.7
2	T	221	VAL	2.7
2	K	160	HIS	2.7
2	K	206	HIS	2.7
1	Q	21	ASP	2.7
2	S	99	PRO	2.7
2	G	342	ARG	2.7
2	O	160	HIS	2.7
2	S	182	PHE	2.7
2	S	269	LYS	2.7
1	Q	22	ASP	2.7
2	G	314	GLY	2.6
2	P	356	CYS	2.6
2	T	205	ASP	2.6
2	O	276	ARG	2.6
2	S	231	THR	2.6
2	L	297	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	373	MET	2.6
2	T	232	GLY	2.6
2	T	378	ALA	2.6
1	R	181	HIS	2.6
2	H	386	LEU	2.6
2	K	205	ASP	2.6
2	S	322	MET	2.6
2	L	385	SER	2.6
2	O	274	GLU	2.6
1	M	6	SER	2.6
2	C	344	VAL	2.6
2	S	244	GLN	2.6
2	L	397	THR	2.6
2	S	313	SER	2.6
2	T	371	ARG	2.5
2	T	290	TYR	2.5
2	S	388	PHE	2.5
2	S	261	TRP	2.5
2	T	293	ILE	2.5
1	R	187	SER	2.5
2	P	343	GLY	2.5
2	T	405	LYS	2.5
2	K	344	VAL	2.5
2	S	379	HIS	2.5
2	O	261	TRP	2.5
2	T	287	GLU	2.5
2	G	373	MET	2.5
2	S	202	PRO	2.5
2	P	384	THR	2.5
2	T	105	SER	2.5
2	S	276	ARG	2.5
2	S	151	ASP	2.5
1	Q	222	GLU	2.5
2	C	300	GLU	2.5
2	O	392	ALA	2.5
1	B	181	HIS	2.5
2	H	295	GLU	2.5
1	Q	20	GLY	2.5
2	G	313	SER	2.5
2	O	355	SER	2.5
2	C	398	GLY	2.4
2	S	287	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	300	GLU	2.4
2	L	294	SER	2.4
2	S	160	HIS	2.4
2	S	110	PRO	2.4
2	K	123	MET	2.4
1	Q	190	ASP	2.4
2	L	344	VAL	2.4
2	K	92	LYS	2.4
2	T	99	PRO	2.4
2	L	408	GLU	2.4
2	T	337	HIS	2.4
2	T	92	LYS	2.4
1	F	104	THR	2.3
2	O	150	THR	2.3
2	G	398	GLY	2.3
2	T	272	LEU	2.3
2	O	192	ASP	2.3
2	P	296	ALA	2.3
2	T	312	LEU	2.3
2	L	342	ARG	2.3
2	D	155	ASP	2.3
2	O	143	GLU	2.3
2	D	92	LYS	2.3
2	K	289	SER	2.3
2	S	378	ALA	2.3
2	G	397	THR	2.3
2	T	373	MET	2.3
2	S	265	THR	2.3
2	S	292	SER	2.3
2	O	218	MET	2.3
2	O	314	GLY	2.3
2	H	408	GLU	2.3
2	T	137	TYR	2.3
2	T	140	GLY	2.3
2	C	313	SER	2.3
2	D	342	ARG	2.2
2	L	155	ASP	2.2
2	S	234	ARG	2.2
1	E	223	GLU	2.2
1	A	46	GLY	2.2
1	Q	12	PRO	2.2
2	G	290	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	342	ARG	2.2
2	P	344	VAL	2.2
1	R	15	ALA	2.2
2	G	270	ALA	2.2
2	K	356	CYS	2.2
2	G	352	PHE	2.2
2	T	314	GLY	2.2
1	R	39	GLU	2.2
2	P	355	SER	2.2
2	H	356	CYS	2.2
2	S	200	ILE	2.2
1	B	46	GLY	2.2
2	S	346	PHE	2.2
2	T	203	ASN	2.2
2	S	349	GLY	2.2
2	H	384	THR	2.2
2	S	98	PRO	2.2
2	T	193	HIS	2.2
2	S	366	ASP	2.2
2	T	273	ARG	2.2
2	H	355	SER	2.2
2	L	180	GLN	2.2
2	S	105	SER	2.2
1	A	221	PRO	2.2
1	A	101	TRP	2.2
1	J	46	GLY	2.2
2	T	370	LYS	2.1
2	O	272	LEU	2.1
2	T	294	SER	2.1
1	R	8	PRO	2.1
2	O	258	VAL	2.1
1	F	47	ASP	2.1
1	F	46	GLY	2.1
2	L	313	SER	2.1
1	F	222	GLU	2.1
2	T	295	GLU	2.1
1	R	10	ALA	2.1
2	G	291	SER	2.1
2	K	352	PHE	2.1
2	L	399	SER	2.1
2	S	355	SER	2.1
2	O	329	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	328	GLY	2.1
2	K	273	ARG	2.1
2	O	259	ARG	2.1
2	O	234	ARG	2.1
1	R	6	SER	2.1
2	H	388	PHE	2.1
2	S	272	LEU	2.1
1	Q	148	PRO	2.1
2	O	310	PHE	2.1
2	K	385	SER	2.1
1	B	60	ARG	2.1
2	K	295	GLU	2.1
2	T	401	ASP	2.1
1	J	15	ALA	2.1
2	K	298	GLY	2.1
2	L	355	SER	2.1
2	P	397	THR	2.1
2	H	407	TRP	2.1
1	Q	13	HIS	2.1
2	C	357	ALA	2.1
2	T	325	VAL	2.1
1	Q	220	THR	2.1
1	R	62	LEU	2.1
2	T	110	PRO	2.1
2	S	101	LYS	2.0
2	T	296	ALA	2.0
2	O	313	SER	2.0
2	O	94	TRP	2.0
2	O	323	TRP	2.0
2	G	271	GLU	2.0
2	T	397	THR	2.0
2	H	92	LYS	2.0
2	D	287	GLU	2.0
2	O	121	SER	2.0
2	S	358	ASP	2.0
2	C	356	CYS	2.0
2	S	181	GLY	2.0
2	O	116	PHE	2.0
2	T	363	ARG	2.0
2	P	386	LEU	2.0
2	H	397	THR	2.0
2	O	296	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	229	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.