



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:57 PM UTC

PDB ID : 3QZ1 / pdb_00003qz1
Title : Crystal Structure of Bovine Steroid of 21-hydroxylase (P450c21)
Authors : Zhao, B.; Waterman, M.R.
Deposited on : 2011-03-04
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

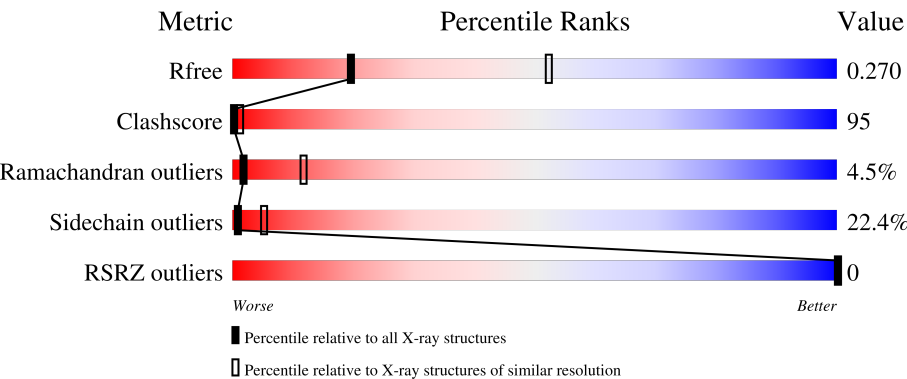
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	22%46%19%•10%
1	B	496	22%47%16%•12%
1	C	496	23%43%18%•12%
1	D	496	20%46%18%•12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3QZ	A	501	-	-	X	-
3	3QZ	B	501	-	-	X	-
3	3QZ	C	501	-	-	X	-
3	3QZ	D	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14525 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.

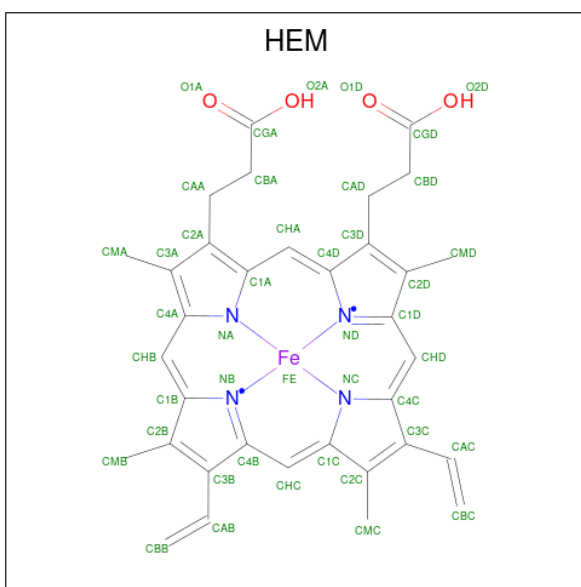
- Molecule 1 is a protein called Steroid 21-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3571	2294	639	618	20			
1	B	436	Total	C	N	O	S	0	0	0
			3506	2259	621	607	19			
1	C	437	Total	C	N	O	S	0	0	0
			3504	2257	619	609	19			
1	D	434	Total	C	N	O	S	0	0	0
			3483	2245	613	606	19			

There are 8 discrepancies between the modelled and reference sequences:

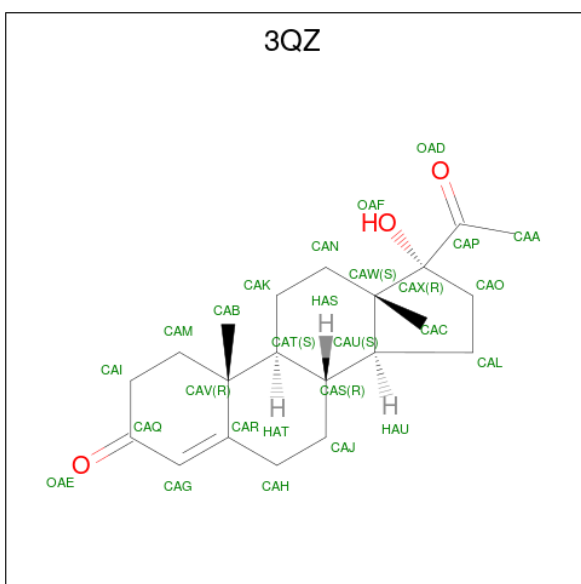
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ARG	THR	engineered mutation	UNP P00191
A	442	ALA	LEU	engineered mutation	UNP P00191
B	241	ARG	THR	engineered mutation	UNP P00191
B	442	ALA	LEU	engineered mutation	UNP P00191
C	241	ARG	THR	engineered mutation	UNP P00191
C	442	ALA	LEU	engineered mutation	UNP P00191
D	241	ARG	THR	engineered mutation	UNP P00191
D	442	ALA	LEU	engineered mutation	UNP P00191

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (9beta)-17-hydroxypregn-4-ene-3,20-dione (CCD ID: 3QZ) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	21	3		
3	A	1	Total	C	O	0	0
			24	21	3		
3	B	1	Total	C	O	0	0
			24	21	3		
3	B	1	Total	C	O	0	0
			24	21	3		
3	C	1	Total	C	O	0	0
			24	21	3		
3	C	1	Total	C	O	0	0
			24	21	3		
3	D	1	Total	C	O	0	0
			24	21	3		
3	D	1	Total	C	O	0	0
			24	21	3		

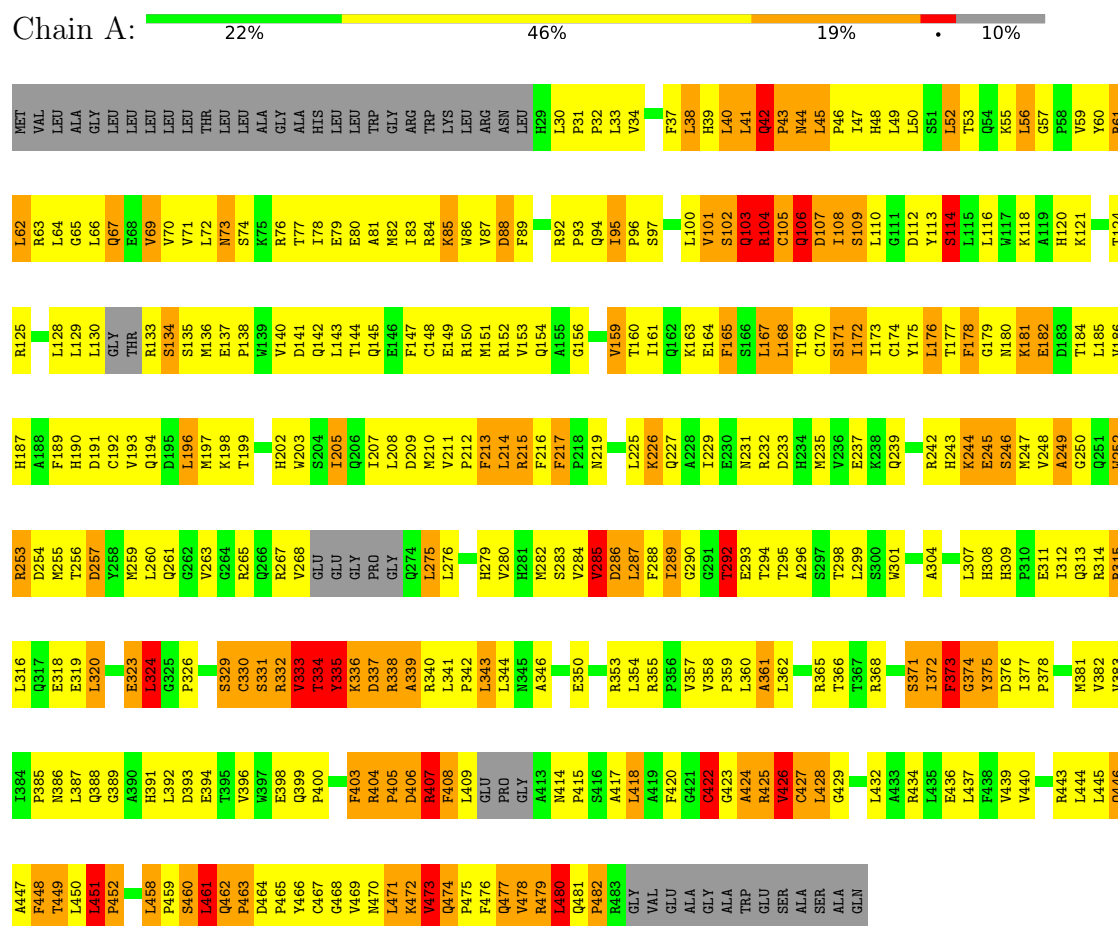
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	28	Total	O	0	0
			28	28		
4	C	22	Total	O	0	0
			22	22		
4	D	25	Total	O	0	0
			25	25		

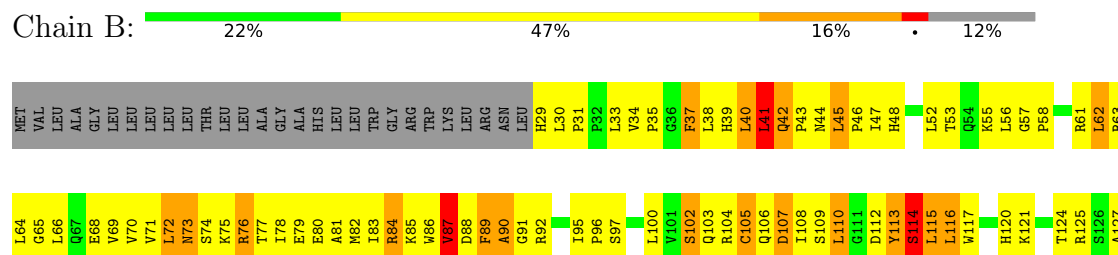
3 Residue-property plots

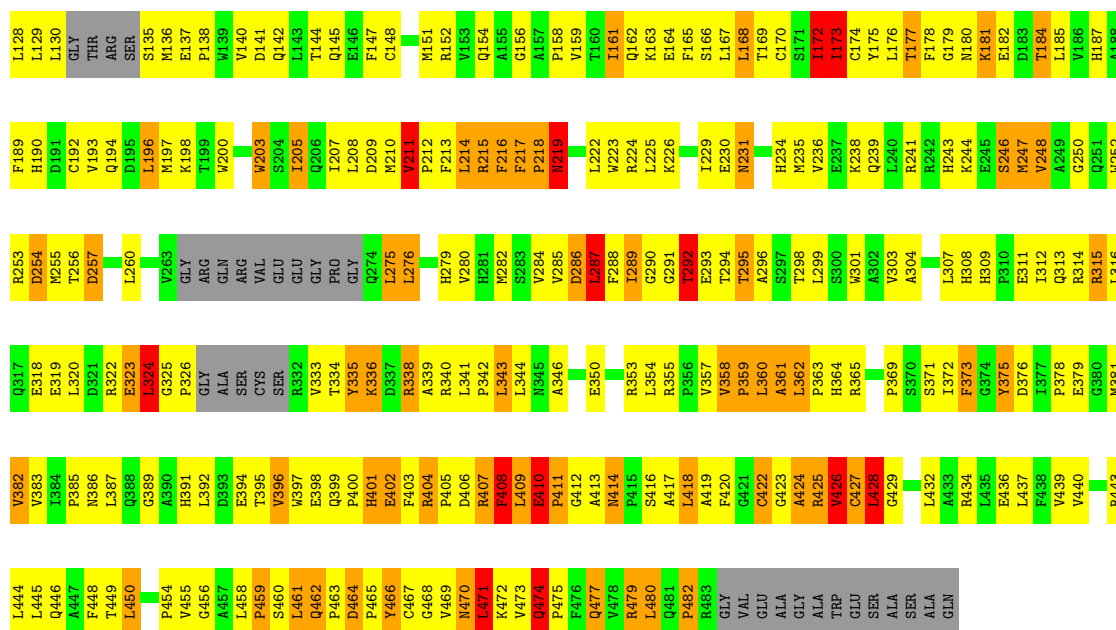
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Steroid 21-hydroxylase



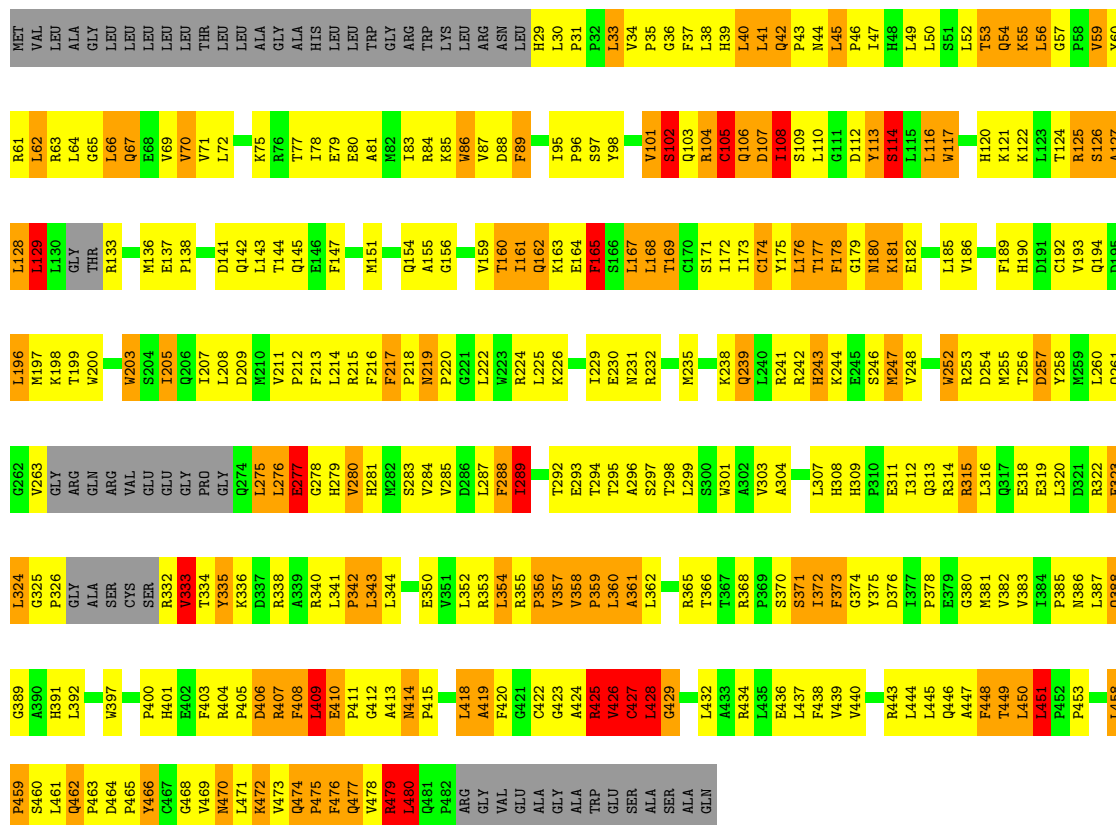
• Molecule 1: Steroid 21-hydroxylase





• Molecule 1: Steroid 21-hydroxylase

Chain C: 23% 43% 18% 12%



• Molecule 1: Steroid 21-hydroxylase

Chain D: 20% 46% 18% 12%

A447	M381	E319	T256	Q194	L130	MET
F448	V382	L320	D257	D195	GLY	VAL
T449		D321	Y258	L196	THR	LEU
L450	P385	R322	M259	M197	ARG	ALA
L451	R386	E323	L260	K198	GLY	GLY
P452	L387	L324	Q261	T199	S135	LEU
P453		G325	G262	W200	M136	LEU
	H391	P326	V263	D201	E137	LEU
L458	L392	GLY	GLY	R202	P138	LEU
P459	D393	ALA	ARG	W203		LEU
S460	E394	SER	GLN	S204	D141	THR
L461	T395	CYS	ARG	I205	Q142	LEU
Q462	V396	SER	VAL	Q206	L143	LEU
P463	V397	ARG	GLU	I207	T144	ALA
D464		V333	T334	L208	Q145	GLY
P465	P400	T334	GLY	D209	E146	ALA
Y466	H401	V335	PRO	M210	F147	HIS
Q467	E402	K336	GLY	V211	C148	LEU
G468	F403	D337	Q274	P212	E149	LEU
V469	R404	R338	L275	F213	R150	TRP
M470	P405	A339	L276	L214	M151	GLY
L471	D406	R340	E277	R215	R152	ARG
K472	R407	L341	Q278	F216	V153	TRP
V473	F408	P342	H279	F217	Q154	LYS
Q474	L409	L343	V280	P218	V87	LEU
P475	E410	L344	H281	N219	D88	ARG
F476	P411	R345	M282	P220		ASN
Q477	G412	A346	S283	G221	V159	LEU
V478	A413	T347	V284	L222	T160	H29
R479	N414		V285	W223	I161	I95
L480	P415	E350	D286	R224	Q162	P96
Q481	S416	V351	L287	K225	K163	L30
PRO	A417	L352	F288	L226	E164	P31
ARG	L418	R353	T289		F165	L33
GLY	A419	L354	T292	I229	S166	L34
VAL	F420	R355	E293	E230	L168	P32
GLU	G421	P356	T294	N231	T169	L35
ALA	G422	V357		R232	C170	G36
GLY	G423	V358	S297	D233	I172	F37
ALA	A424	P359	H294	H234	S171	L38
TRP	R425	L360	T298	M235	I173	H39
GLU	Y426	A361	L299	V236	C174	L40
SER	G427	L362	S300	E237	Y175	L41
ALA	L428	P363	W301	K238	S109	P43
ALA	G429	H364	A302	Q239	L110	N44
SER	E430	R365	V303	L240	T177	L45
ALA	S431	T366	A304	R241	F178	P46
GLN	L432	T367		R242	G179	I47
	A433	R368	L307	H243	N180	
	R434	P369	H308	K244	K181	L50
	L435	S370	H309	E245	E182	S61
	E436	S371	P310	S246	L116	L52
		I372	E311	M247	T184	T63
	V439	P373	I312	V248	L185	Q54
	V440	G374	Q313	A249	V186	K55
		Y375	R314			L56
		D376	R315		F189	G57
	R443	P378	L316	W252	H190	P58
	L444		Q317	R253	D191	
	L445		D254	D254	C192	R61
	Q446		E318	M255	V193	L62

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.87Å 168.00Å 111.84Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 95.1 (30.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.297 0.262 , 0.270	Depositor DCC
R_{free} test set	4871 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 173.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,k,-l	Depositor
Outliers	0 of 48073 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14525	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3QZ, HEM

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	0.70	1/3659 (0.0%)	1.14	40/4971 (0.8%)
1	B	0.68	0/3595	1.13	38/4888 (0.8%)
1	C	0.65	1/3592 (0.0%)	1.15	41/4884 (0.8%)
1	D	0.73	2/3571 (0.1%)	1.15	36/4856 (0.7%)
All	All	0.69	4/14417 (0.0%)	1.14	155/19599 (0.8%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	463	PRO	CA-CB	-9.71	1.40	1.53
1	A	463	PRO	C-O	-5.66	1.17	1.23
1	D	106	GLN	CA-CB	-5.48	1.45	1.53
1	C	289	ILE	CA-CB	5.42	1.61	1.54

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	ARG	N-CA-C	21.79	139.81	113.23
1	A	88	ASP	N-CA-C	14.80	127.12	111.14
1	C	480	LEU	N-CA-C	12.34	126.92	109.15
1	B	409	LEU	N-CA-C	-11.88	98.20	113.17
1	B	217	PHE	N-CA-C	-11.69	93.59	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	VAL	N-CA-C	10.69	121.52	110.72
1	B	424	ALA	N-CA-C	-10.27	99.90	111.71
1	D	419	ALA	N-CA-C	-10.17	99.42	112.23
1	D	479	ARG	N-CA-C	9.95	132.00	110.80
1	B	479	ARG	N-CA-C	9.62	131.30	110.80
1	A	292	THR	N-CA-C	9.45	121.58	111.28
1	D	214	LEU	N-CA-C	9.37	123.81	112.38
1	B	113	TYR	N-CA-C	-9.20	98.78	110.19
1	A	422	CYS	N-CA-C	-9.18	91.91	107.23
1	B	287	LEU	N-CA-C	-8.82	101.75	111.36
1	B	335	TYR	N-CA-C	8.70	129.33	110.80
1	D	73	ASN	N-CA-C	8.67	122.60	112.72
1	A	479	ARG	N-CA-C	8.66	123.95	111.56
1	C	426	VAL	N-CA-C	8.56	118.64	110.42
1	D	480	LEU	N-CA-C	8.54	123.03	107.99
1	A	452	PRO	N-CA-C	8.53	118.66	110.47
1	B	428	LEU	N-CA-C	-8.50	97.91	110.06
1	A	424	ALA	N-CA-C	-8.29	102.26	112.38
1	B	360	LEU	N-CA-C	-8.23	101.01	112.45
1	C	277	GLU	N-CA-C	8.21	120.22	111.28
1	C	174	CYS	N-CA-C	8.20	120.00	111.14
1	C	114	SER	N-CA-C	-8.19	93.35	110.80
1	D	293	GLU	N-CA-C	8.15	119.79	111.07
1	C	108	ILE	N-CA-CB	-8.02	102.92	112.07
1	D	374	GLY	N-CA-C	-8.01	102.52	112.77
1	D	114	SER	N-CA-C	-7.86	94.06	110.80
1	A	334	THR	N-CA-C	7.51	120.58	109.24
1	C	424	ALA	N-CA-C	-7.45	103.16	111.28
1	C	419	ALA	N-CA-C	-7.39	104.51	113.97
1	C	411	PRO	N-CA-C	-7.30	104.34	113.84
1	A	171	SER	N-CA-C	7.29	122.24	113.12
1	C	288	PHE	N-CA-C	7.29	126.33	110.80
1	D	429	GLY	N-CA-C	7.24	122.64	114.67
1	A	249	ALA	N-CA-C	7.19	120.95	111.75
1	A	360	LEU	N-CA-C	-7.18	104.09	112.92
1	C	129	LEU	N-CA-C	7.16	122.45	113.43
1	D	106	GLN	N-CA-C	7.15	120.94	111.28
1	C	108	ILE	N-CA-C	7.15	119.33	109.46
1	D	202	HIS	N-CA-C	7.10	121.41	110.20
1	C	411	PRO	N-CA-CB	7.06	110.54	103.48
1	B	425	ARG	N-CA-C	-6.97	94.79	107.75
1	D	174	CYS	N-CA-C	6.93	118.52	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	410	GLU	N-CA-C	6.89	125.03	109.81
1	A	451	LEU	CA-C-N	6.83	124.65	119.66
1	A	451	LEU	C-N-CA	6.83	124.65	119.66
1	D	288	PHE	N-CA-C	6.79	125.26	110.80
1	D	414	ASN	N-CA-C	6.79	118.26	109.64
1	C	425	ARG	N-CA-C	-6.73	99.52	109.62
1	B	480	LEU	N-CA-C	6.72	120.42	109.59
1	C	426	VAL	CB-CA-C	-6.71	103.38	111.97
1	A	480	LEU	N-CA-C	6.71	119.62	109.23
1	B	336	LYS	N-CA-C	-6.56	105.31	113.38
1	D	360	LEU	N-CA-C	-6.55	105.03	113.16
1	D	424	ALA	N-CA-C	-6.51	104.43	112.38
1	A	42	GLN	CA-C-N	6.49	126.40	119.85
1	A	42	GLN	C-N-CA	6.49	126.40	119.85
1	A	94	GLN	N-CA-C	-6.45	97.17	108.20
1	B	246	SER	N-CA-C	-6.44	105.29	112.57
1	A	43	PRO	N-CA-C	6.41	121.57	111.38
1	C	333	VAL	N-CA-C	6.37	122.58	109.34
1	B	426	VAL	CB-CA-C	-6.36	104.29	111.80
1	D	292	THR	N-CA-C	6.35	118.21	111.28
1	C	478	VAL	CB-CA-C	-6.31	104.35	111.80
1	D	277	GLU	N-CA-C	6.31	118.16	111.28
1	A	403	PHE	N-CA-C	-6.29	100.59	109.96
1	B	408	PHE	N-CA-C	6.28	118.76	108.52
1	B	106	GLN	CB-CA-C	-6.25	109.38	116.63
1	B	471	LEU	N-CA-C	6.22	118.74	110.53
1	A	104	ARG	N-CA-C	-6.13	104.60	111.28
1	C	217	PHE	N-CA-C	-6.09	101.37	109.84
1	B	358	VAL	N-CA-C	-6.06	100.82	107.73
1	D	358	VAL	CA-C-N	6.04	127.40	119.84
1	D	358	VAL	C-N-CA	6.04	127.40	119.84
1	B	419	ALA	N-CA-C	-6.02	104.79	111.71
1	D	480	LEU	N-CA-CB	-6.02	101.38	110.35
1	D	477	GLN	N-CA-C	5.99	119.03	110.10
1	B	173	ILE	N-CA-C	5.99	116.17	110.42
1	C	117	TRP	N-CA-C	-5.98	104.76	111.28
1	D	113	TYR	N-CA-C	-5.93	102.84	110.19
1	A	88	ASP	CB-CA-C	-5.90	101.58	110.90
1	B	276	LEU	N-CA-C	5.90	117.94	110.33
1	D	108	ILE	N-CA-C	5.87	117.61	109.45
1	B	41	LEU	N-CA-C	-5.87	102.92	110.19
1	B	292	THR	N-CA-C	5.86	118.62	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	ASP	N-CA-C	5.85	121.47	113.16
1	C	164	GLU	N-CA-C	-5.85	104.98	111.71
1	A	448	PHE	N-CA-C	5.82	118.69	109.50
1	C	113	TYR	N-CA-C	-5.80	100.73	109.60
1	C	361	ALA	CB-CA-C	-5.79	109.92	116.63
1	C	428	LEU	N-CA-C	-5.76	98.99	108.49
1	D	112	ASP	N-CA-C	-5.72	103.37	110.41
1	B	87	VAL	N-CA-C	5.71	116.49	110.72
1	B	338	ARG	N-CA-C	-5.69	106.26	113.43
1	C	102	SER	N-CA-C	5.65	117.52	111.36
1	A	329	SER	N-CA-C	5.65	117.44	108.79
1	D	361	ALA	CB-CA-C	-5.65	110.08	116.63
1	B	480	LEU	N-CA-CB	-5.65	101.60	110.69
1	B	114	SER	N-CA-C	-5.63	98.81	110.80
1	A	361	ALA	CB-CA-C	-5.61	110.09	116.54
1	A	427	CYS	N-CA-C	-5.60	100.01	108.52
1	A	213	PHE	N-CA-C	-5.59	106.53	113.19
1	D	315	ARG	N-CA-C	-5.59	105.34	111.82
1	C	289	ILE	N-CA-C	-5.56	104.87	113.16
1	C	480	LEU	N-CA-CB	-5.51	100.56	109.60
1	C	127	ALA	N-CA-C	-5.51	105.38	111.71
1	B	90	ALA	N-CA-C	-5.47	106.60	113.72
1	C	427	CYS	N-CA-C	-5.46	99.17	110.80
1	B	414	ASN	CA-C-N	5.46	126.66	119.84
1	B	414	ASN	C-N-CA	5.46	126.66	119.84
1	D	477	GLN	CB-CA-C	-5.46	101.39	109.90
1	C	243	HIS	N-CA-C	-5.45	106.99	113.97
1	B	412	GLY	N-CA-C	-5.45	100.27	113.18
1	D	338	ARG	N-CA-C	5.45	116.90	111.07
1	D	425	ARG	N-CA-C	-5.40	106.54	113.02
1	A	320	LEU	N-CA-C	5.38	117.96	111.40
1	A	103	GLN	CB-CA-C	-5.37	109.93	117.23
1	C	414	ASN	CA-C-N	5.35	125.61	119.83
1	C	414	ASN	C-N-CA	5.35	125.61	119.83
1	A	393	ASP	N-CA-C	-5.33	102.02	109.96
1	C	358	VAL	CA-C-N	5.30	126.47	119.84
1	C	358	VAL	C-N-CA	5.30	126.47	119.84
1	C	451	LEU	CA-C-N	5.30	125.84	120.38
1	C	451	LEU	C-N-CA	5.30	125.84	120.38
1	C	315	ARG	N-CA-C	-5.29	105.68	111.82
1	A	315	ARG	N-CA-C	-5.27	105.71	111.82
1	C	105	CYS	N-CA-C	5.27	122.02	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ILE	N-CA-C	-5.26	104.39	111.44
1	D	412	GLY	N-CA-C	-5.25	100.75	113.18
1	A	57	GLY	CA-C-N	5.24	124.87	119.05
1	A	57	GLY	C-N-CA	5.24	124.87	119.05
1	B	315	ARG	N-CA-C	-5.23	105.76	111.82
1	A	285	VAL	CB-CA-C	-5.22	105.29	111.97
1	A	339	ALA	N-CA-C	-5.21	106.78	113.23
1	B	172	ILE	N-CA-C	-5.19	105.48	110.72
1	A	114	SER	N-CA-C	-5.17	99.78	110.80
1	B	219	ASN	N-CA-C	-5.16	101.60	109.64
1	B	211	VAL	CA-C-N	5.13	124.75	119.05
1	B	211	VAL	C-N-CA	5.13	124.75	119.05
1	D	83	ILE	N-CA-C	5.12	116.54	111.67
1	C	165	PHE	N-CA-C	-5.08	105.74	111.28
1	C	356	PRO	N-CA-C	-5.07	103.22	111.03
1	D	83	ILE	CB-CA-C	-5.06	105.83	111.80
1	A	95	ILE	N-CA-C	-5.05	97.97	108.88
1	A	473	VAL	CB-CA-C	-5.04	103.03	111.29
1	C	360	LEU	N-CA-C	-5.04	106.92	113.16
1	D	193	VAL	CB-CA-C	-5.03	105.44	112.02
1	A	425	ARG	N-CA-C	-5.01	107.33	113.50
1	A	73	ASN	N-CA-C	5.01	116.41	109.54
1	B	254	ASP	N-CA-C	5.01	117.48	109.81
1	B	401	HIS	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	425	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3571	0	3632	723	1
1	B	3506	0	3567	673	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3504	0	3555	646	1
1	D	3483	0	3539	741	2
2	A	43	0	30	6	0
2	B	43	0	30	5	0
2	C	43	0	30	13	0
2	D	43	0	30	11	0
3	A	48	0	60	19	0
3	B	48	0	60	20	0
3	C	48	0	60	13	0
3	D	48	0	60	10	0
4	A	22	0	0	17	2
4	B	28	0	0	8	0
4	C	22	0	0	11	1
4	D	25	0	0	14	0
All	All	14525	0	14653	2772	5

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 95.

All (2772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PRO:CG	1:D:471:LEU:HB3	1.12	1.59
1:D:463:PRO:HG3	1:D:471:LEU:CB	1.17	1.57
1:D:463:PRO:HB3	1:D:471:LEU:CG	1.32	1.54
1:D:106:GLN:HB2	1:D:279:HIS:CE1	1.40	1.53
1:D:463:PRO:CB	1:D:471:LEU:HG	1.31	1.52
1:A:294:THR:CG2	3:A:501:3QZ:HAAA	1.40	1.48
1:A:294:THR:CG2	3:A:501:3QZ:CAA	1.96	1.43
1:A:252:TRP:CE3	1:A:253:ARG:HG3	1.53	1.42
1:A:475:PRO:CB	1:A:477:GLN:HE22	1.34	1.40
1:A:472:LYS:CE	1:A:473:VAL:H	1.35	1.38
1:C:55:LYS:HG2	1:C:56:LEU:CD2	1.54	1.37
1:D:46:PRO:HG3	1:D:466:TYR:CE2	1.56	1.37
1:B:62:LEU:HD23	1:B:63:ARG:N	1.41	1.35
1:A:472:LYS:CE	1:A:473:VAL:N	1.90	1.34
1:C:62:LEU:HD23	1:C:63:ARG:N	1.41	1.34
1:B:288:PHE:CD2	1:B:289:ILE:HD11	1.62	1.33
1:D:106:GLN:CB	1:D:279:HIS:CE1	2.11	1.33
1:B:189:PHE:CE2	1:B:288:PHE:CZ	2.16	1.32
1:A:62:LEU:HD23	1:A:63:ARG:N	1.41	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HE2	1:B:252:TRP:CZ3	1.47	1.31
1:C:159:VAL:HG12	1:C:476:PHE:CE2	1.65	1.31
1:D:62:LEU:HD23	1:D:63:ARG:N	1.42	1.31
1:D:473:VAL:CG1	1:D:474:GLN:H	1.43	1.31
1:B:178:PHE:CE2	1:B:252:TRP:CZ3	2.18	1.30
1:B:284:VAL:C	1:B:288:PHE:HB2	1.55	1.30
1:B:284:VAL:O	1:B:288:PHE:CB	1.79	1.30
1:B:288:PHE:CD2	1:B:289:ILE:CD1	2.15	1.29
1:A:42:GLN:HG2	4:A:613:HOH:O	1.22	1.29
1:A:475:PRO:HB2	1:A:477:GLN:NE2	1.46	1.29
1:D:463:PRO:HB3	1:D:471:LEU:CD1	1.62	1.29
1:D:94:GLN:OE1	1:D:99:LYS:HE2	1.30	1.28
1:B:294:THR:CG2	3:B:501:3QZ:HAAA	1.62	1.28
1:A:463:PRO:O	1:A:466:TYR:CE1	1.86	1.28
1:B:214:LEU:HD23	1:B:216:PHE:CD2	1.69	1.27
1:D:105:CYS:HB2	4:D:613:HOH:O	1.35	1.26
1:B:288:PHE:C	1:B:289:ILE:HD12	1.60	1.26
1:B:116:LEU:HD23	1:B:116:LEU:C	1.61	1.25
1:B:189:PHE:CE2	1:B:288:PHE:HZ	1.52	1.25
1:A:472:LYS:HE2	1:A:473:VAL:N	1.46	1.25
1:D:418:LEU:HD23	1:D:422:CYS:SG	1.77	1.25
1:C:276:LEU:HD23	1:C:277:GLU:N	1.52	1.24
1:A:177:THR:HB	1:A:288:PHE:CE1	1.70	1.24
1:B:178:PHE:HE2	1:B:252:TRP:CH2	1.53	1.24
1:A:37:PHE:O	1:A:38:LEU:HD23	1.31	1.24
1:D:96:PRO:HG2	1:D:209:ASP:OD1	1.37	1.23
1:D:165:PHE:HE1	1:D:293:GLU:OE2	1.16	1.23
1:B:294:THR:CG2	3:B:501:3QZ:CAA	2.17	1.23
1:D:214:LEU:HD23	1:D:216:PHE:CD1	1.70	1.23
1:A:332:ARG:NE	1:A:332:ARG:HA	1.48	1.22
1:A:449:THR:HB	1:A:480:LEU:O	1.33	1.22
1:D:168:LEU:O	1:D:172:ILE:HD13	1.39	1.22
1:D:116:LEU:C	1:D:116:LEU:HD23	1.62	1.22
1:A:294:THR:HG21	3:A:501:3QZ:CAA	1.60	1.21
1:C:116:LEU:HD23	1:C:116:LEU:C	1.62	1.21
1:A:461:LEU:O	1:A:462:GLN:CG	1.88	1.21
1:B:284:VAL:HG12	1:B:288:PHE:CD1	1.75	1.21
1:D:106:GLN:HG2	1:D:279:HIS:NE2	1.56	1.21
1:D:275:LEU:HD12	1:D:275:LEU:O	1.40	1.20
1:C:179:GLY:N	1:C:254:ASP:OD1	1.73	1.20
1:D:202:HIS:O	1:D:205:ILE:HG22	1.41	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:HG	1:A:452:PRO:HD2	1.24	1.19
1:B:214:LEU:CD2	1:B:216:PHE:HD2	1.55	1.19
1:B:72:LEU:C	1:B:73:ASN:HD22	1.50	1.19
1:D:40:LEU:HD12	1:D:40:LEU:O	1.42	1.18
1:D:55:LYS:HD2	1:D:56:LEU:CD2	1.74	1.18
1:D:168:LEU:HD23	1:D:292:THR:O	1.39	1.18
1:D:461:LEU:HD22	1:D:462:GLN:O	1.41	1.18
1:B:284:VAL:O	1:B:288:PHE:HB2	1.05	1.17
1:A:324:LEU:HD12	1:A:332:ARG:HG2	1.26	1.17
1:A:108:ILE:HG13	1:A:286:ASP:OD2	1.43	1.16
1:B:471:LEU:H	1:B:471:LEU:CD1	1.51	1.16
1:D:461:LEU:O	1:D:461:LEU:HD23	1.43	1.16
1:A:461:LEU:C	1:A:461:LEU:HD23	1.69	1.16
1:D:463:PRO:CB	1:D:471:LEU:CG	1.99	1.16
1:A:472:LYS:HE3	1:A:473:VAL:HG23	1.28	1.16
1:D:461:LEU:HD23	1:D:461:LEU:C	1.69	1.15
1:D:111:GLY:O	1:D:425:ARG:NH2	1.78	1.15
1:C:40:LEU:HD12	1:C:40:LEU:O	1.46	1.15
1:C:62:LEU:HD23	1:C:62:LEU:C	1.67	1.15
1:B:471:LEU:N	1:B:471:LEU:HD12	1.58	1.14
1:C:358:VAL:CG1	2:C:500:HEM:HMA3	1.77	1.14
1:A:89:PHE:CZ	1:A:372:ILE:CG1	2.30	1.14
1:B:62:LEU:HD23	1:B:62:LEU:C	1.73	1.14
1:C:412:GLY:O	4:C:604:HOH:O	1.63	1.14
1:D:165:PHE:CE1	1:D:293:GLU:OE2	1.99	1.14
1:C:219:ASN:OD1	1:C:220:PRO:HD2	1.44	1.13
1:D:116:LEU:HD23	1:D:117:TRP:N	1.62	1.13
1:D:52:LEU:O	1:D:56:LEU:HD23	1.46	1.13
1:D:62:LEU:HD23	1:D:62:LEU:C	1.72	1.13
1:A:283:SER:O	1:A:287:LEU:CD1	1.96	1.13
1:A:461:LEU:O	1:A:462:GLN:HG2	0.97	1.13
1:B:41:LEU:HD23	1:B:41:LEU:N	1.56	1.13
1:B:288:PHE:O	1:B:289:ILE:HD12	1.49	1.13
1:B:116:LEU:HD23	1:B:117:TRP:N	1.62	1.13
1:C:297:SER:HB2	1:C:357:VAL:HG21	1.30	1.13
1:C:178:PHE:HA	1:C:254:ASP:OD2	1.49	1.13
1:A:252:TRP:CZ3	1:A:253:ARG:HD2	1.84	1.12
1:B:174:CYS:O	1:B:179:GLY:HA2	1.49	1.12
1:C:55:LYS:CE	1:C:56:LEU:HD21	1.77	1.12
1:C:448:PHE:HB3	1:C:479:ARG:O	1.49	1.12
1:D:46:PRO:CG	1:D:466:TYR:CE2	2.33	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:O	1:A:461:LEU:HD23	1.48	1.12
1:B:210:MET:CG	3:B:502:3QZ:HAG	1.78	1.12
1:D:196:LEU:HD23	3:D:501:3QZ:CAI	1.79	1.12
1:A:40:LEU:HD12	1:A:40:LEU:O	1.49	1.12
1:A:252:TRP:HZ3	1:A:253:ARG:HD2	0.95	1.11
1:D:168:LEU:H	1:D:168:LEU:CD1	1.61	1.11
1:D:65:GLY:O	1:D:66:LEU:HD12	1.49	1.11
1:B:193:VAL:HG13	1:B:289:ILE:CG2	1.79	1.11
1:B:288:PHE:HD2	1:B:289:ILE:CD1	1.55	1.11
1:B:402:GLU:OE1	1:B:402:GLU:HA	1.49	1.11
1:D:404:ARG:HD2	1:D:404:ARG:O	1.50	1.11
1:D:418:LEU:CD2	1:D:422:CYS:SG	2.38	1.11
1:C:162:GLN:HA	1:C:162:GLN:HE21	1.03	1.10
1:D:38:LEU:HB3	1:D:41:LEU:HD12	1.18	1.10
1:A:62:LEU:HD23	1:A:62:LEU:C	1.69	1.10
1:D:473:VAL:HG12	1:D:474:GLN:N	1.52	1.10
1:C:181:LYS:O	1:C:181:LYS:HG2	1.50	1.10
1:C:212:PRO:O	1:C:216:PHE:CE2	2.04	1.10
1:A:178:PHE:CA	1:A:243:HIS:HE1	1.62	1.10
1:A:214:LEU:HD21	1:A:216:PHE:CA	1.81	1.10
1:C:276:LEU:CD2	1:C:278:GLY:H	1.64	1.10
1:D:420:PHE:CZ	2:D:500:HEM:HBB2	1.86	1.10
1:A:252:TRP:HB2	1:A:257:ASP:CG	1.77	1.10
1:A:196:LEU:HD23	3:A:501:3QZ:HAI	1.31	1.09
1:B:128:LEU:CG	1:B:287:LEU:HD21	1.80	1.09
1:C:463:PRO:HG3	1:C:471:LEU:HB3	1.27	1.09
1:D:407:ARG:HH11	1:D:407:ARG:CG	1.65	1.09
1:A:459:PRO:HG3	1:A:475:PRO:HB3	1.34	1.09
1:C:212:PRO:O	1:C:216:PHE:HE2	1.33	1.09
1:C:447:ALA:HB3	1:C:448:PHE:CE2	1.87	1.09
1:C:159:VAL:CG1	1:C:476:PHE:CE2	2.35	1.08
1:A:252:TRP:HZ3	1:A:253:ARG:CD	1.66	1.08
1:C:407:ARG:HH11	1:C:407:ARG:HG3	0.93	1.08
1:B:169:THR:HG22	1:B:173:ILE:HD11	1.34	1.08
1:D:106:GLN:CB	1:D:279:HIS:NE2	2.15	1.08
1:D:168:LEU:H	1:D:168:LEU:HD12	0.95	1.08
1:D:242:ARG:HG2	1:D:242:ARG:NH1	1.56	1.08
1:D:242:ARG:HH11	1:D:242:ARG:CG	1.65	1.08
1:A:193:VAL:HG22	1:A:289:ILE:HG22	1.31	1.08
1:A:171:SER:O	1:A:175:TYR:CE1	2.07	1.08
1:B:409:LEU:O	1:B:409:LEU:HD23	1.49	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HB3	1:A:41:LEU:HD21	1.36	1.07
1:A:89:PHE:CZ	1:A:372:ILE:HG12	1.85	1.07
1:B:176:LEU:O	1:B:176:LEU:HD23	1.53	1.07
1:C:102:SER:OG	1:C:105:CYS:HA	1.55	1.07
1:C:358:VAL:HG11	2:C:500:HEM:CMA	1.85	1.07
1:C:407:ARG:HH11	1:C:407:ARG:CG	1.66	1.07
1:D:214:LEU:HD21	1:D:216:PHE:HA	1.35	1.07
1:B:128:LEU:HD21	1:B:287:LEU:HD23	1.30	1.07
1:C:40:LEU:HD12	1:C:40:LEU:C	1.75	1.07
1:C:167:LEU:O	1:C:167:LEU:HD23	1.54	1.07
1:A:283:SER:O	1:A:287:LEU:HD11	1.54	1.07
1:D:106:GLN:CG	1:D:279:HIS:NE2	2.16	1.07
1:D:372:ILE:O	1:D:373:PHE:HB3	1.53	1.06
1:B:294:THR:HG21	3:B:501:3QZ:HAAA	1.12	1.06
1:A:472:LYS:HE2	1:A:473:VAL:H	0.96	1.06
1:B:418:LEU:HD12	1:B:418:LEU:N	1.58	1.06
1:D:430:GLU:OE2	4:D:617:HOH:O	1.72	1.06
1:A:214:LEU:HD21	1:A:216:PHE:HA	1.34	1.06
1:B:92:ARG:NH1	1:B:363:PRO:O	1.89	1.06
1:D:65:GLY:C	1:D:66:LEU:HD12	1.79	1.06
1:D:168:LEU:CD2	1:D:292:THR:O	2.04	1.06
1:D:373:PHE:CD1	1:D:373:PHE:C	2.30	1.06
1:A:404:ARG:HH11	1:A:404:ARG:CG	1.69	1.05
1:B:89:PHE:HE2	1:B:372:ILE:HD11	1.19	1.05
1:A:219:ASN:ND2	4:A:621:HOH:O	1.71	1.05
1:C:276:LEU:HD23	1:C:276:LEU:C	1.80	1.05
1:D:214:LEU:CD2	1:D:216:PHE:HD1	1.67	1.05
1:D:85:LYS:HG3	1:D:88:ASP:OD2	1.54	1.05
1:B:410:GLU:OE2	1:B:411:PRO:HG3	1.53	1.05
1:C:423:GLY:O	1:C:426:VAL:HG13	1.55	1.05
1:D:252:TRP:CZ3	1:D:253:ARG:CZ	2.40	1.05
1:A:214:LEU:HG	1:A:216:PHE:H	1.21	1.04
1:A:287:LEU:H	1:A:287:LEU:HD12	1.12	1.04
1:B:409:LEU:O	1:B:411:PRO:HD3	1.54	1.04
1:A:161:ILE:O	1:A:165:PHE:HB2	1.56	1.04
1:C:55:LYS:HE2	1:C:56:LEU:HD21	1.04	1.04
1:C:89:PHE:CE2	1:C:372:ILE:CD1	2.41	1.04
1:C:418:LEU:H	1:C:418:LEU:HD12	0.89	1.04
1:A:294:THR:HG23	3:A:501:3QZ:CAA	1.81	1.04
1:A:332:ARG:C	1:A:333:VAL:HG23	1.82	1.04
1:B:214:LEU:HD21	1:B:216:PHE:HA	1.40	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:HD12	1:C:418:LEU:N	1.62	1.04
1:C:472:LYS:C	1:C:472:LYS:HZ3	1.66	1.04
1:D:55:LYS:HG3	1:D:56:LEU:CD2	1.88	1.04
1:B:396:VAL:CG1	1:B:397:TRP:CE3	2.42	1.03
1:A:214:LEU:CD2	1:A:216:PHE:CD2	2.41	1.03
1:C:465:PRO:HG2	1:C:471:LEU:HD22	1.40	1.03
1:D:463:PRO:HB2	1:D:471:LEU:HG	1.32	1.03
1:A:460:SER:O	1:A:461:LEU:HB3	1.59	1.03
1:B:460:SER:HA	1:B:472:LYS:HE2	1.39	1.03
1:A:177:THR:HB	1:A:288:PHE:CZ	1.94	1.02
1:B:210:MET:HG2	3:B:502:3QZ:HAG	1.07	1.02
1:D:55:LYS:CD	1:D:56:LEU:HD21	1.88	1.02
1:A:214:LEU:CG	1:A:216:PHE:H	1.71	1.02
1:D:407:ARG:HH11	1:D:407:ARG:HG3	1.25	1.02
1:A:252:TRP:CE3	1:A:253:ARG:CG	2.43	1.02
1:A:252:TRP:CZ3	1:A:253:ARG:CD	2.41	1.02
1:A:373:PHE:CD1	1:A:373:PHE:C	2.36	1.02
1:A:52:LEU:O	1:A:56:LEU:HD23	1.58	1.01
1:C:55:LYS:HE2	1:C:56:LEU:CD2	1.89	1.01
1:C:232:ARG:NH1	3:C:501:3QZ:HAG	1.75	1.01
1:B:285:VAL:HA	1:B:288:PHE:HB3	1.39	1.01
1:D:252:TRP:CE3	1:D:253:ARG:HD2	1.94	1.01
1:A:67:GLN:HA	1:A:67:GLN:OE1	1.60	1.01
1:A:244:LYS:HG2	1:A:260:LEU:HD21	1.41	1.01
1:B:294:THR:HG21	3:B:501:3QZ:CAA	1.87	1.01
1:A:472:LYS:HE2	1:A:472:LYS:CA	1.90	1.01
1:C:408:PHE:O	1:C:408:PHE:HD1	1.43	1.01
1:A:332:ARG:O	1:A:333:VAL:HG23	1.61	1.01
1:A:404:ARG:O	1:A:404:ARG:HG2	1.56	1.01
1:C:294:THR:HG21	3:C:501:3QZ:HAAA	1.41	1.01
1:C:407:ARG:O	1:C:413:ALA:HB1	1.59	1.01
1:A:463:PRO:O	1:A:466:TYR:HE1	1.27	1.00
1:B:128:LEU:HD21	1:B:287:LEU:CD2	1.90	1.00
1:B:448:PHE:HD1	1:B:479:ARG:O	1.43	1.00
1:C:67:GLN:OE1	1:C:67:GLN:HA	1.59	1.00
1:D:196:LEU:CD2	3:D:501:3QZ:HAI	1.90	1.00
1:A:332:ARG:HA	1:A:332:ARG:HE	0.94	1.00
1:A:178:PHE:CA	1:A:243:HIS:CE1	2.44	1.00
1:C:276:LEU:HD21	1:C:278:GLY:H	1.24	1.00
1:A:446:GLN:O	1:A:481:GLN:NE2	1.94	1.00
1:D:346:ALA:HB1	1:D:405:PRO:O	1.62	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD12	1:B:418:LEU:H	0.85	1.00
1:D:97:SER:HB2	1:D:209:ASP:OD2	1.60	1.00
1:A:404:ARG:HH11	1:A:404:ARG:HG3	1.23	1.00
1:D:55:LYS:HD2	1:D:56:LEU:HD21	1.00	0.99
1:D:275:LEU:HD12	1:D:275:LEU:C	1.87	0.99
1:A:335:TYR:CD2	1:A:336:LYS:N	2.30	0.99
1:B:189:PHE:CZ	1:B:288:PHE:HZ	1.79	0.99
1:D:432:LEU:HD23	1:D:432:LEU:O	1.61	0.99
1:B:176:LEU:HD23	1:B:176:LEU:C	1.86	0.99
1:B:288:PHE:HD2	1:B:289:ILE:HD13	1.22	0.99
1:B:396:VAL:HG12	1:B:397:TRP:CE3	1.98	0.99
1:A:472:LYS:C	1:A:472:LYS:HZ3	1.70	0.99
1:A:214:LEU:CD2	1:A:216:PHE:H	1.75	0.99
1:A:472:LYS:NZ	1:A:472:LYS:HB3	1.75	0.99
1:D:38:LEU:HB3	1:D:41:LEU:CD1	1.91	0.99
1:A:463:PRO:O	1:A:466:TYR:CD1	2.16	0.99
1:A:472:LYS:HE2	1:A:472:LYS:C	1.87	0.99
1:B:41:LEU:HD23	1:B:41:LEU:H	1.22	0.99
1:A:178:PHE:HA	1:A:243:HIS:CE1	1.98	0.99
1:C:358:VAL:HG11	2:C:500:HEM:C3A	1.98	0.99
1:C:472:LYS:HA	1:C:472:LYS:HE2	1.44	0.98
1:D:407:ARG:NH1	1:D:407:ARG:HB2	1.77	0.98
1:D:214:LEU:CD2	1:D:216:PHE:H	1.76	0.98
1:B:169:THR:O	1:B:173:ILE:HG12	1.62	0.98
1:B:214:LEU:O	1:B:215:ARG:HG3	1.63	0.98
1:D:211:VAL:O	1:D:211:VAL:HG12	1.61	0.98
1:A:357:VAL:HG12	1:A:469:VAL:CG1	1.93	0.98
1:B:396:VAL:HG11	1:B:397:TRP:CZ3	1.98	0.98
1:C:104:ARG:C	1:C:105:CYS:SG	2.46	0.98
1:A:50:LEU:O	1:A:53:THR:HG23	1.64	0.98
1:B:169:THR:O	1:B:173:ILE:CG1	2.11	0.98
1:A:106:GLN:OE1	1:A:116:LEU:HD13	1.62	0.98
1:B:178:PHE:CE2	1:B:252:TRP:CH2	2.46	0.98
1:D:215:ARG:HB3	1:D:217:PHE:CE1	1.98	0.98
1:D:407:ARG:HH11	1:D:407:ARG:CB	1.76	0.98
1:A:38:LEU:CB	1:A:41:LEU:HD21	1.93	0.97
1:A:472:LYS:NZ	1:A:473:VAL:N	2.11	0.97
1:C:55:LYS:HG2	1:C:56:LEU:HD22	0.99	0.97
1:D:55:LYS:HG3	1:D:56:LEU:HD22	1.45	0.97
1:D:94:GLN:OE1	1:D:99:LYS:CE	2.12	0.97
1:D:168:LEU:HD12	1:D:168:LEU:N	1.80	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:VAL:HG12	1:A:286:ASP:OD1	1.62	0.97
1:D:275:LEU:C	1:D:275:LEU:CD1	2.38	0.97
1:B:128:LEU:CD1	1:B:287:LEU:HD21	1.93	0.97
1:A:43:PRO:HB2	1:A:44:ASN:OD1	1.63	0.97
1:D:473:VAL:HG13	1:D:474:GLN:H	1.29	0.97
1:B:189:PHE:CE2	1:B:288:PHE:CE2	2.52	0.96
1:B:219:ASN:OD1	4:B:626:HOH:O	1.83	0.96
1:D:448:PHE:N	1:D:448:PHE:HD2	1.63	0.96
1:B:350:GLU:HG3	1:B:404:ARG:O	1.65	0.96
1:C:162:GLN:HA	1:C:162:GLN:NE2	1.70	0.96
1:D:375:TYR:O	1:D:377:ILE:HD13	1.63	0.96
1:B:193:VAL:HG22	1:B:289:ILE:HG23	1.48	0.96
1:A:472:LYS:NZ	1:A:473:VAL:O	1.99	0.96
1:C:41:LEU:O	1:C:42:GLN:HB3	1.63	0.96
1:B:33:LEU:HD13	1:B:34:VAL:O	1.64	0.96
1:B:112:ASP:OD2	1:B:365:ARG:NH2	1.97	0.96
1:B:418:LEU:H	1:B:418:LEU:CD1	1.78	0.96
1:C:448:PHE:HD2	1:C:448:PHE:N	1.64	0.96
1:D:350:GLU:HG3	1:D:404:ARG:O	1.64	0.96
1:B:73:ASN:HD22	1:B:73:ASN:N	1.61	0.96
1:B:178:PHE:HB2	1:B:243:HIS:CE1	2.01	0.96
1:B:210:MET:HG2	3:B:502:3QZ:CAG	1.95	0.96
1:C:62:LEU:C	1:C:62:LEU:CD2	2.37	0.96
1:B:214:LEU:HD23	1:B:216:PHE:HD2	0.82	0.95
1:D:196:LEU:HD23	3:D:501:3QZ:HAI	0.96	0.95
1:A:275:LEU:HD12	1:A:275:LEU:O	1.66	0.95
1:C:55:LYS:CG	1:C:56:LEU:CD2	2.43	0.95
1:C:167:LEU:C	1:C:167:LEU:CD2	2.39	0.95
1:B:284:VAL:CG1	1:B:288:PHE:CD1	2.48	0.95
1:D:214:LEU:HD23	1:D:216:PHE:HD1	0.79	0.95
1:C:232:ARG:HH12	3:C:501:3QZ:HAG	1.27	0.95
1:C:358:VAL:CG1	2:C:500:HEM:CMA	2.41	0.95
1:A:246:SER:O	1:A:252:TRP:NE1	1.99	0.95
1:A:335:TYR:HD2	1:A:335:TYR:C	1.74	0.95
1:D:196:LEU:HD21	3:D:501:3QZ:OAE	1.64	0.95
1:D:449:THR:O	1:D:450:LEU:HB2	1.67	0.95
1:B:62:LEU:C	1:B:62:LEU:CD2	2.38	0.95
1:D:164:GLU:O	1:D:168:LEU:CD1	2.14	0.95
1:D:463:PRO:CG	1:D:471:LEU:CB	1.96	0.95
1:C:472:LYS:CA	1:C:472:LYS:CE	2.43	0.95
1:D:55:LYS:CD	1:D:56:LEU:CD2	2.43	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:O	1:B:211:VAL:HG12	1.64	0.94
1:C:358:VAL:HG11	2:C:500:HEM:HMA3	1.44	0.94
1:A:475:PRO:CB	1:A:477:GLN:NE2	2.14	0.94
1:B:178:PHE:CE2	1:B:252:TRP:HZ3	1.76	0.94
1:D:178:PHE:CE1	1:D:242:ARG:NH1	2.35	0.94
1:D:215:ARG:HB3	1:D:217:PHE:HE1	1.31	0.94
1:C:116:LEU:C	1:C:116:LEU:CD2	2.39	0.94
1:C:407:ARG:HG3	1:C:407:ARG:NH1	1.58	0.94
1:D:173:ILE:HA	1:D:288:PHE:CE1	2.02	0.94
1:D:463:PRO:CB	1:D:471:LEU:CB	2.40	0.94
1:B:91:GLY:O	1:B:365:ARG:N	1.98	0.94
1:B:288:PHE:C	1:B:289:ILE:CD1	2.40	0.94
1:A:372:ILE:O	1:A:372:ILE:HG22	1.66	0.94
1:B:89:PHE:N	1:B:89:PHE:HD1	1.66	0.94
1:A:56:LEU:HD22	1:A:56:LEU:H	1.32	0.94
1:A:301:TRP:CE2	1:A:472:LYS:HG2	2.02	0.94
1:A:319:GLU:O	1:A:323:GLU:HB2	1.68	0.94
1:B:34:VAL:HG11	1:B:52:LEU:HD13	1.50	0.94
1:B:214:LEU:HD23	1:B:216:PHE:H	1.32	0.94
1:C:89:PHE:CE2	1:C:372:ILE:HD11	2.02	0.94
1:C:358:VAL:HG13	2:C:500:HEM:HMA3	1.47	0.94
1:A:350:GLU:HG3	1:A:404:ARG:O	1.67	0.94
1:B:177:THR:HG22	1:B:177:THR:O	1.64	0.94
1:B:176:LEU:HD11	1:B:287:LEU:HB3	1.49	0.94
1:C:173:ILE:HA	1:C:288:PHE:CE1	2.03	0.94
1:C:358:VAL:HG13	1:C:358:VAL:O	1.65	0.94
1:D:473:VAL:CG1	1:D:474:GLN:N	2.09	0.94
1:B:214:LEU:CD2	1:B:216:PHE:H	1.80	0.93
1:B:284:VAL:O	1:B:288:PHE:N	2.01	0.93
1:C:276:LEU:CD2	1:C:276:LEU:C	2.41	0.93
1:D:117:TRP:CZ2	1:D:425:ARG:HD3	2.03	0.93
1:D:214:LEU:HD23	1:D:216:PHE:H	1.30	0.93
1:D:447:ALA:C	1:D:448:PHE:CD2	2.46	0.93
1:A:177:THR:CB	1:A:288:PHE:CE1	2.51	0.93
1:C:37:PHE:O	1:C:38:LEU:HD23	1.67	0.93
1:C:169:THR:HG21	1:C:190:HIS:HB2	1.50	0.93
1:C:447:ALA:HB3	1:C:448:PHE:HE2	1.24	0.93
1:D:109:SER:OG	1:D:110:LEU:HD23	1.68	0.93
1:D:46:PRO:HG3	1:D:466:TYR:HE2	0.89	0.93
1:B:284:VAL:CG1	1:B:288:PHE:HD1	1.82	0.93
1:B:357:VAL:HG12	1:B:469:VAL:HG13	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG22	1:A:165:PHE:CD2	2.04	0.93
1:A:161:ILE:HG22	1:A:165:PHE:HD2	1.33	0.93
1:A:332:ARG:HG3	1:A:337:ASP:OD1	1.67	0.93
1:B:248:VAL:HG23	1:B:250:GLY:H	1.33	0.93
1:C:463:PRO:HG3	1:C:471:LEU:CB	1.97	0.93
1:D:461:LEU:C	1:D:461:LEU:CD2	2.37	0.93
1:B:214:LEU:CD2	1:B:216:PHE:CD2	2.40	0.93
1:D:62:LEU:C	1:D:62:LEU:CD2	2.40	0.93
1:A:103:GLN:N	4:A:610:HOH:O	2.00	0.92
1:B:471:LEU:H	1:B:471:LEU:HD12	0.77	0.92
1:B:113:TYR:O	1:B:114:SER:HB3	1.67	0.92
1:D:106:GLN:CG	1:D:279:HIS:CE1	2.52	0.92
1:A:62:LEU:C	1:A:62:LEU:CD2	2.40	0.92
1:C:472:LYS:HE2	1:C:473:VAL:H	1.33	0.92
1:C:472:LYS:HE2	1:C:473:VAL:N	1.84	0.92
1:A:42:GLN:CG	4:A:613:HOH:O	1.89	0.92
1:A:178:PHE:N	1:A:243:HIS:CE1	2.38	0.92
1:A:372:ILE:O	1:A:373:PHE:HB3	1.67	0.92
1:D:373:PHE:C	1:D:373:PHE:HD1	1.69	0.92
1:A:106:GLN:O	1:A:107:ASP:HB3	1.69	0.91
1:B:176:LEU:CD1	1:B:287:LEU:HB3	2.00	0.91
1:D:448:PHE:HB3	1:D:479:ARG:O	1.71	0.91
1:A:475:PRO:CG	1:A:477:GLN:NE2	2.33	0.91
1:C:448:PHE:N	1:C:448:PHE:CD2	2.34	0.91
1:D:471:LEU:HD13	1:D:472:LYS:N	1.85	0.91
1:C:465:PRO:HG2	1:C:471:LEU:CD2	2.00	0.91
1:A:462:GLN:HB2	1:A:466:TYR:OH	1.71	0.91
1:C:55:LYS:CG	1:C:56:LEU:HD22	1.96	0.91
1:C:178:PHE:CA	1:C:254:ASP:OD2	2.19	0.91
1:A:40:LEU:HD12	1:A:40:LEU:C	1.92	0.91
1:C:307:LEU:HD13	1:C:458:LEU:HD22	1.52	0.91
1:C:30:LEU:HG	1:C:31:PRO:HD2	1.51	0.91
1:A:313:GLN:HE22	1:A:450:LEU:CD1	1.83	0.90
1:C:167:LEU:HD23	1:C:167:LEU:C	1.93	0.90
1:D:448:PHE:N	1:D:448:PHE:CD2	2.28	0.90
1:C:116:LEU:HD23	1:C:117:TRP:N	1.85	0.90
1:C:472:LYS:HA	1:C:472:LYS:CE	1.92	0.90
1:A:105:CYS:O	1:A:106:GLN:HB2	1.71	0.90
1:B:71:VAL:HG12	1:B:73:ASN:HD21	1.37	0.90
1:D:69:VAL:HG13	1:D:382:VAL:HB	1.52	0.90
1:A:108:ILE:HD13	1:A:124:THR:HG21	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:VAL:HG12	1:B:397:TRP:CD2	2.06	0.90
1:C:113:TYR:O	1:C:114:SER:HB3	1.72	0.90
1:D:55:LYS:CG	1:D:56:LEU:HD22	2.02	0.90
1:D:214:LEU:O	1:D:214:LEU:HG	1.71	0.90
1:C:297:SER:HB2	1:C:357:VAL:CG2	2.01	0.90
1:A:189:PHE:CZ	1:A:288:PHE:CE2	2.59	0.90
1:D:116:LEU:C	1:D:116:LEU:CD2	2.39	0.90
1:D:473:VAL:HG12	1:D:474:GLN:H	1.10	0.90
1:A:214:LEU:HD21	1:A:216:PHE:CD2	2.07	0.90
1:A:214:LEU:HG	1:A:216:PHE:N	1.86	0.89
1:B:128:LEU:HD11	1:B:287:LEU:HD21	1.50	0.89
1:D:231:ASN:HB3	1:D:235:MET:HE3	1.53	0.89
1:D:472:LYS:HD2	1:D:473:VAL:N	1.87	0.89
1:A:101:VAL:HG23	1:A:101:VAL:O	1.72	0.89
1:D:55:LYS:CG	1:D:56:LEU:CD2	2.50	0.89
1:D:117:TRP:NE1	1:D:425:ARG:NH1	2.21	0.89
1:A:102:SER:OG	4:A:610:HOH:O	1.89	0.89
1:D:377:ILE:HG23	1:D:378:PRO:HD2	1.54	0.89
1:B:41:LEU:N	1:B:41:LEU:CD2	2.35	0.89
1:B:248:VAL:HG23	1:B:250:GLY:N	1.86	0.89
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.86	0.89
1:A:38:LEU:O	1:A:41:LEU:HG	1.72	0.89
1:A:159:VAL:O	1:A:159:VAL:HG22	1.72	0.89
1:A:38:LEU:HB3	1:A:41:LEU:CD2	2.03	0.89
1:A:56:LEU:HD22	1:A:56:LEU:N	1.87	0.89
1:D:178:PHE:HE1	1:D:242:ARG:HH12	1.21	0.89
1:C:162:GLN:NE2	1:C:162:GLN:CA	2.35	0.88
1:A:89:PHE:CZ	1:A:372:ILE:HG13	2.09	0.88
1:A:472:LYS:NZ	1:A:472:LYS:CB	2.35	0.88
1:A:294:THR:HG23	3:A:501:3QZ:HAA	1.51	0.88
1:B:284:VAL:O	1:B:288:PHE:CA	2.21	0.88
1:C:56:LEU:CD2	1:C:56:LEU:N	2.36	0.88
1:A:404:ARG:NH2	1:A:414:ASN:ND2	2.22	0.88
1:B:116:LEU:CD2	1:B:117:TRP:N	2.36	0.88
1:B:288:PHE:CE2	1:B:289:ILE:HD11	2.08	0.88
1:A:103:GLN:NE2	1:A:104:ARG:HD3	1.89	0.88
1:B:407:ARG:HH11	1:B:407:ARG:HG3	1.39	0.88
1:C:425:ARG:O	4:C:606:HOH:O	1.92	0.88
1:A:461:LEU:C	1:A:461:LEU:CD2	2.42	0.88
1:C:62:LEU:CD2	1:C:64:LEU:N	2.36	0.88
1:C:472:LYS:HE2	1:C:472:LYS:CA	2.02	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD22	1:D:56:LEU:N	1.88	0.88
1:B:189:PHE:HE2	1:B:288:PHE:CZ	1.82	0.87
1:D:185:LEU:HD11	1:D:239:GLN:HE22	1.38	0.87
1:D:307:LEU:HD13	1:D:458:LEU:HD22	1.56	0.87
1:D:463:PRO:CB	1:D:471:LEU:HB3	2.03	0.87
1:A:263:VAL:HG13	1:A:275:LEU:HD12	1.57	0.87
1:B:128:LEU:HG	1:B:287:LEU:HD21	1.53	0.87
1:C:276:LEU:CD2	1:C:278:GLY:N	2.35	0.87
1:A:124:THR:HG23	1:A:428:LEU:HD11	1.54	0.87
1:D:423:GLY:O	1:D:426:VAL:HG13	1.73	0.87
1:A:189:PHE:CZ	1:A:288:PHE:HE2	1.92	0.87
1:A:373:PHE:C	1:A:373:PHE:HD1	1.81	0.87
1:B:61:ARG:NH1	1:B:68:GLU:CD	2.33	0.87
1:D:463:PRO:HB3	1:D:471:LEU:HD12	1.55	0.87
1:A:313:GLN:NE2	1:A:450:LEU:HD12	1.89	0.87
1:D:232:ARG:NH1	3:D:501:3QZ:OAE	2.06	0.87
1:A:246:SER:O	1:A:252:TRP:CD1	2.28	0.87
1:D:203:TRP:HA	1:D:206:GLN:HB2	1.57	0.87
1:B:294:THR:CG2	3:B:501:3QZ:HAA	2.04	0.87
1:C:125:ARG:O	1:C:128:LEU:HB2	1.74	0.87
1:C:472:LYS:CE	1:C:473:VAL:N	2.37	0.87
1:D:116:LEU:CD2	1:D:117:TRP:N	2.37	0.87
1:C:87:VAL:HG12	1:C:368:ARG:HH12	1.38	0.87
1:C:231:ASN:HB3	1:C:235:MET:HE3	1.57	0.87
1:D:211:VAL:HG12	1:D:214:LEU:HB2	1.57	0.87
1:D:405:PRO:HD2	1:D:406:ASP:OD1	1.75	0.87
1:A:337:ASP:O	1:A:340:ARG:N	2.08	0.86
1:B:89:PHE:HE2	1:B:372:ILE:CD1	1.88	0.86
1:C:418:LEU:H	1:C:418:LEU:CD1	1.81	0.86
1:D:108:ILE:HD11	1:D:124:THR:HG21	1.56	0.86
1:A:423:GLY:O	1:A:426:VAL:HG13	1.75	0.86
1:D:38:LEU:HD13	1:D:41:LEU:HD11	1.55	0.86
1:D:65:GLY:C	1:D:66:LEU:CD1	2.46	0.86
1:A:341:LEU:HD13	1:A:344:LEU:HD12	1.57	0.86
1:A:472:LYS:HE2	1:A:472:LYS:HA	1.58	0.86
1:B:89:PHE:CE2	1:B:372:ILE:HD11	2.09	0.86
1:B:178:PHE:CD2	1:B:252:TRP:CZ3	2.63	0.86
1:C:341:LEU:HD13	1:C:344:LEU:HD12	1.56	0.86
1:D:373:PHE:HD1	1:D:374:GLY:N	1.74	0.86
1:A:89:PHE:CE1	1:A:372:ILE:HG12	2.08	0.86
1:B:473:VAL:O	1:B:475:PRO:HD3	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:CD2	1:A:216:PHE:N	2.38	0.86
1:B:193:VAL:HG13	1:B:289:ILE:HG22	1.57	0.86
1:B:459:PRO:CG	1:B:472:LYS:HZ1	1.87	0.86
1:D:54:GLN:NE2	1:D:54:GLN:C	2.34	0.86
1:A:337:ASP:O	1:A:339:ALA:N	2.08	0.86
1:D:242:ARG:HG2	1:D:242:ARG:HH11	0.75	0.86
1:A:177:THR:CB	1:A:288:PHE:CZ	2.57	0.86
1:A:472:LYS:CE	1:A:472:LYS:CA	2.50	0.86
1:B:116:LEU:C	1:B:116:LEU:CD2	2.39	0.86
1:B:193:VAL:CG2	1:B:289:ILE:HG23	2.05	0.86
1:C:38:LEU:HB3	1:C:41:LEU:CD1	2.06	0.86
1:B:89:PHE:N	1:B:89:PHE:CD1	2.41	0.85
1:B:285:VAL:CA	1:B:288:PHE:HB3	2.06	0.85
1:B:396:VAL:HG11	1:B:397:TRP:CE3	2.09	0.85
1:D:46:PRO:CG	1:D:466:TYR:HE2	1.77	0.85
1:D:472:LYS:HD2	1:D:473:VAL:H	1.38	0.85
1:A:89:PHE:CE2	1:A:372:ILE:HD11	2.11	0.85
1:A:472:LYS:CE	1:A:472:LYS:C	2.47	0.85
1:B:408:PHE:C	1:B:408:PHE:CD2	2.53	0.85
1:D:407:ARG:NH1	1:D:407:ARG:CB	2.38	0.85
1:A:42:GLN:OE1	4:A:613:HOH:O	1.94	0.85
1:A:449:THR:CB	1:A:480:LEU:O	2.22	0.85
1:C:472:LYS:C	1:C:472:LYS:NZ	2.35	0.85
1:A:168:LEU:HD21	1:A:296:ALA:HB2	1.59	0.85
1:C:333:VAL:O	1:C:333:VAL:HG12	1.75	0.85
1:D:105:CYS:CB	4:D:613:HOH:O	2.03	0.85
1:A:252:TRP:CZ3	1:A:253:ARG:CG	2.59	0.85
1:B:62:LEU:HD23	1:B:63:ARG:CA	2.07	0.85
1:B:407:ARG:HG3	1:B:407:ARG:NH1	1.89	0.85
1:C:101:VAL:HG23	1:C:232:ARG:HH22	1.40	0.85
1:A:45:LEU:CD2	1:A:49:LEU:HG	2.07	0.85
1:A:252:TRP:HE3	1:A:253:ARG:HG3	1.09	0.85
1:D:378:PRO:HG2	1:D:381:MET:HB2	1.57	0.85
1:A:42:GLN:OE1	1:A:48:HIS:CG	2.30	0.85
1:A:177:THR:HG21	1:A:288:PHE:CE2	2.12	0.85
1:A:324:LEU:CD1	1:A:332:ARG:HG2	2.05	0.85
1:B:459:PRO:HG2	1:B:472:LYS:HZ1	1.40	0.85
1:A:252:TRP:CZ3	1:A:253:ARG:HG3	2.10	0.85
1:C:88:ASP:HB2	1:C:89:PHE:CD1	2.11	0.85
1:A:56:LEU:H	1:A:56:LEU:CD2	1.90	0.84
1:A:335:TYR:CD2	1:A:335:TYR:C	2.48	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:CD	4:A:613:HOH:O	2.14	0.84
1:A:332:ARG:HE	1:A:332:ARG:CA	1.86	0.84
1:D:471:LEU:HD13	1:D:472:LYS:C	2.00	0.84
1:B:460:SER:CA	1:B:472:LYS:HE2	2.06	0.84
1:C:31:PRO:HG2	1:C:61:ARG:HG3	1.59	0.84
1:C:62:LEU:HD23	1:C:63:ARG:CA	2.08	0.84
1:A:243:HIS:CD2	1:A:256:THR:HB	2.12	0.84
1:C:104:ARG:O	1:C:105:CYS:SG	2.36	0.84
1:D:110:LEU:CD2	1:D:110:LEU:N	2.40	0.84
1:A:160:THR:OG1	1:A:477:GLN:HG2	1.77	0.84
1:A:357:VAL:HG12	1:A:469:VAL:HG13	1.58	0.84
1:B:168:LEU:HD21	1:B:296:ALA:HB2	1.59	0.84
1:B:408:PHE:HD2	1:B:410:GLU:N	1.76	0.84
1:B:409:LEU:C	1:B:411:PRO:HD3	2.03	0.84
1:D:106:GLN:HG2	1:D:116:LEU:HD11	1.58	0.84
1:A:169:THR:HG21	1:A:190:HIS:HB2	1.59	0.84
1:B:136:MET:HB3	1:B:175:TYR:CE2	2.13	0.84
1:D:177:THR:HG23	1:D:239:GLN:HG2	1.59	0.84
1:A:375:TYR:N	1:A:375:TYR:CD2	2.42	0.84
1:D:214:LEU:HD21	1:D:216:PHE:CA	2.07	0.83
1:A:103:GLN:HE22	1:A:104:ARG:HD3	1.43	0.83
1:B:62:LEU:CD2	1:B:63:ARG:C	2.51	0.83
1:B:30:LEU:HG	1:B:31:PRO:HD2	1.59	0.83
1:B:448:PHE:CD1	1:B:479:ARG:O	2.32	0.83
1:D:196:LEU:HD11	1:D:229:ILE:HA	1.60	0.83
1:B:176:LEU:HD12	1:B:287:LEU:HD22	1.59	0.83
1:B:214:LEU:O	1:B:217:PHE:CE1	2.31	0.83
1:C:103:GLN:O	1:C:105:CYS:SG	2.36	0.83
1:C:129:LEU:N	1:C:129:LEU:CD1	2.41	0.83
1:C:161:ILE:CD1	1:C:474:GLN:HA	2.08	0.83
1:C:161:ILE:CG1	1:C:475:PRO:HD2	2.09	0.83
1:D:297:SER:HB2	1:D:357:VAL:HG22	1.58	0.83
1:A:106:GLN:OE1	1:A:116:LEU:CD1	2.27	0.83
1:A:407:ARG:HH11	1:A:407:ARG:HG3	1.42	0.83
1:B:113:TYR:HD2	1:B:114:SER:H	1.27	0.83
1:B:172:ILE:HD13	1:B:172:ILE:N	1.93	0.83
1:C:358:VAL:CG1	1:C:358:VAL:O	2.26	0.83
1:B:88:ASP:C	1:B:89:PHE:HD1	1.86	0.83
1:A:161:ILE:CG2	1:A:165:PHE:HD2	1.92	0.82
1:B:193:VAL:HG22	1:B:289:ILE:CG2	2.08	0.82
1:D:215:ARG:CB	1:D:217:PHE:HE1	1.91	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:O	1:A:105:CYS:SG	2.37	0.82
1:C:472:LYS:HZ3	1:C:472:LYS:CB	1.93	0.82
1:D:252:TRP:HE3	1:D:253:ARG:HD2	1.44	0.82
1:A:113:TYR:HD2	1:A:114:SER:H	1.27	0.82
1:A:472:LYS:HB3	1:A:472:LYS:HZ2	1.40	0.82
1:C:59:VAL:HG21	1:C:372:ILE:HG21	1.62	0.82
1:C:232:ARG:NH1	3:C:501:3QZ:CAG	2.43	0.82
1:D:174:CYS:O	1:D:179:GLY:HA2	1.77	0.82
1:A:472:LYS:C	1:A:472:LYS:NZ	2.36	0.82
1:D:358:VAL:HG12	1:D:361:ALA:HA	1.61	0.82
1:D:461:LEU:O	1:D:462:GLN:HB2	1.77	0.82
1:A:358:VAL:CG1	1:A:361:ALA:HA	2.08	0.82
1:D:168:LEU:CD1	1:D:168:LEU:N	2.31	0.82
1:A:472:LYS:HE3	1:A:473:VAL:H	1.39	0.82
1:C:447:ALA:CB	1:C:448:PHE:CE2	2.62	0.82
1:D:451:LEU:HG	1:D:452:PRO:HD2	1.62	0.82
1:D:463:PRO:HG3	1:D:471:LEU:CA	2.09	0.82
1:C:101:VAL:HG23	1:C:101:VAL:O	1.79	0.82
1:A:44:ASN:HB2	1:A:47:ILE:HG12	1.59	0.82
1:C:294:THR:CG2	3:C:501:3QZ:HAAA	2.09	0.82
1:D:105:CYS:O	4:D:604:HOH:O	1.96	0.82
1:D:113:TYR:O	1:D:114:SER:HB3	1.79	0.82
1:A:89:PHE:CD2	1:A:372:ILE:HD11	2.14	0.81
1:D:40:LEU:HD12	1:D:40:LEU:C	1.99	0.81
1:D:420:PHE:HZ	2:D:500:HEM:HBB2	1.43	0.81
1:A:161:ILE:CG2	1:A:165:PHE:CD2	2.63	0.81
1:B:341:LEU:HD13	1:B:344:LEU:HD12	1.60	0.81
1:C:174:CYS:O	1:C:179:GLY:HA2	1.81	0.81
1:D:164:GLU:O	1:D:168:LEU:HD12	1.79	0.81
1:A:178:PHE:H	1:A:243:HIS:CE1	1.96	0.81
1:C:128:LEU:C	1:C:129:LEU:HD12	2.06	0.81
1:C:178:PHE:N	1:C:254:ASP:CG	2.38	0.81
1:C:472:LYS:CE	1:C:473:VAL:H	1.94	0.81
1:D:46:PRO:CD	1:D:466:TYR:CD2	2.63	0.81
1:D:212:PRO:C	1:D:214:LEU:H	1.89	0.81
1:A:32:PRO:O	1:A:61:ARG:HB2	1.81	0.81
1:A:335:TYR:HD2	1:A:336:LYS:N	1.73	0.81
1:D:373:PHE:CD1	1:D:373:PHE:O	2.33	0.81
1:B:360:LEU:O	1:B:361:ALA:HB3	1.78	0.81
1:C:56:LEU:HD22	1:C:56:LEU:N	1.93	0.81
1:B:172:ILE:N	1:B:172:ILE:CD1	2.43	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:PHE:HD1	1:C:408:PHE:C	1.88	0.81
1:D:473:VAL:CG1	1:D:474:GLN:OE1	2.29	0.81
1:A:404:ARG:HG3	1:A:404:ARG:NH1	1.84	0.81
1:B:151:MET:HB3	1:B:479:ARG:HH12	1.44	0.81
1:B:193:VAL:CG1	1:B:289:ILE:CG2	2.59	0.81
1:D:58:PRO:HG3	1:D:76:ARG:HH21	1.43	0.81
1:D:177:THR:HB	1:D:288:PHE:CE1	2.16	0.81
1:A:108:ILE:CG1	1:A:286:ASP:OD2	2.29	0.80
1:A:420:PHE:CZ	2:A:500:HEM:HBB2	2.17	0.80
1:C:62:LEU:CD2	1:C:63:ARG:C	2.54	0.80
1:D:375:TYR:O	1:D:377:ILE:CD1	2.28	0.80
1:C:159:VAL:CG1	1:C:476:PHE:HE2	1.95	0.80
1:C:89:PHE:CZ	1:C:372:ILE:CD1	2.65	0.80
1:D:143:LEU:HD21	1:D:181:LYS:HD2	1.63	0.80
1:A:243:HIS:NE2	1:A:254:ASP:CG	2.40	0.80
1:B:72:LEU:C	1:B:73:ASN:ND2	2.35	0.80
1:A:313:GLN:HE22	1:A:450:LEU:CB	1.95	0.80
1:A:475:PRO:HB2	1:A:477:GLN:HE22	0.64	0.80
1:B:423:GLY:O	1:B:426:VAL:HG13	1.81	0.80
1:C:447:ALA:C	1:C:448:PHE:CD2	2.60	0.80
1:B:128:LEU:CD2	1:B:287:LEU:CD2	2.60	0.80
1:B:294:THR:HG23	3:B:501:3QZ:HAA	1.62	0.80
1:C:81:ALA:HB2	1:C:372:ILE:HG13	1.63	0.80
1:D:404:ARG:HH12	1:D:407:ARG:HB3	1.46	0.80
1:C:128:LEU:C	1:C:129:LEU:CD1	2.55	0.79
1:C:129:LEU:N	1:C:129:LEU:HD13	1.97	0.79
1:D:350:GLU:CG	1:D:404:ARG:O	2.29	0.79
1:D:372:ILE:O	1:D:372:ILE:CG2	2.31	0.79
1:D:463:PRO:CD	1:D:471:LEU:HB3	2.08	0.79
1:B:90:ALA:HB3	1:B:113:TYR:CD1	2.16	0.79
1:B:338:ARG:HB2	4:B:601:HOH:O	1.82	0.79
1:A:286:ASP:O	1:A:290:GLY:HA3	1.81	0.79
1:B:386:ASN:ND2	1:B:389:GLY:H	1.81	0.79
1:C:319:GLU:O	1:C:323:GLU:HB2	1.81	0.79
1:C:160:THR:CG2	1:C:477:GLN:HB2	2.12	0.79
1:C:463:PRO:CG	1:C:471:LEU:HB3	2.10	0.79
1:D:214:LEU:CD2	1:D:216:PHE:N	2.45	0.79
1:A:80:GLU:HG3	1:A:84:ARG:HD3	1.63	0.79
1:B:30:LEU:HD11	1:B:378:PRO:HD3	1.65	0.79
1:C:408:PHE:C	1:C:408:PHE:CD1	2.57	0.79
1:C:464:ASP:N	1:C:465:PRO:HD2	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLN:HB3	1:D:279:HIS:CD2	2.17	0.79
1:D:106:GLN:HB2	1:D:279:HIS:ND1	1.94	0.79
1:D:374:GLY:O	1:D:375:TYR:CD2	2.36	0.79
1:A:287:LEU:HD12	1:A:287:LEU:N	1.96	0.79
1:D:432:LEU:C	1:D:432:LEU:CD2	2.56	0.79
1:B:288:PHE:CD2	1:B:289:ILE:HD13	2.01	0.79
1:D:447:ALA:HB3	1:D:448:PHE:CE2	2.18	0.79
1:A:285:VAL:CG1	1:A:286:ASP:N	2.45	0.78
1:B:62:LEU:HD23	1:B:63:ARG:C	2.08	0.78
1:B:350:GLU:CG	1:B:404:ARG:O	2.31	0.78
1:D:252:TRP:CZ3	1:D:253:ARG:NH1	2.50	0.78
1:A:214:LEU:O	1:A:215:ARG:HB2	1.83	0.78
1:B:62:LEU:CD2	1:B:64:LEU:N	2.47	0.78
1:C:313:GLN:HE21	1:C:445:LEU:HD11	1.46	0.78
1:A:461:LEU:C	1:A:462:GLN:HG2	2.04	0.78
1:B:244:LYS:HE2	1:B:260:LEU:HD11	1.65	0.78
1:D:324:LEU:HG	1:D:340:ARG:HG3	1.66	0.78
1:D:463:PRO:HB3	1:D:471:LEU:HG	0.84	0.78
1:C:372:ILE:HG22	1:C:373:PHE:N	1.95	0.78
1:D:214:LEU:HD23	1:D:216:PHE:N	1.99	0.78
1:A:62:LEU:CD2	1:A:63:ARG:N	2.37	0.78
1:A:350:GLU:CG	1:A:404:ARG:O	2.31	0.78
1:C:472:LYS:NZ	1:C:472:LYS:CB	2.39	0.78
1:D:205:ILE:O	1:D:205:ILE:HD13	1.84	0.78
1:C:38:LEU:O	1:C:41:LEU:HD12	1.84	0.78
1:A:404:ARG:HH22	1:A:414:ASN:ND2	1.80	0.78
1:C:308:HIS:CE1	1:C:458:LEU:HB2	2.19	0.78
1:D:62:LEU:HD23	1:D:63:ARG:CA	2.13	0.77
1:D:466:TYR:C	1:D:467:CYS:SG	2.66	0.77
1:D:275:LEU:O	1:D:275:LEU:CD1	2.25	0.77
1:A:177:THR:CG2	1:A:239:GLN:HG2	2.15	0.77
1:B:169:THR:HG22	1:B:173:ILE:CD1	2.12	0.77
1:B:409:LEU:O	1:B:410:GLU:HB3	1.84	0.77
1:B:128:LEU:HD11	1:B:287:LEU:CD2	2.15	0.77
1:B:294:THR:HG22	3:B:501:3QZ:CAA	2.15	0.77
1:C:88:ASP:HB2	1:C:89:PHE:CE1	2.19	0.77
1:C:105:CYS:O	1:C:106:GLN:HB2	1.84	0.77
1:B:214:LEU:HD21	1:B:216:PHE:CA	2.14	0.77
1:C:161:ILE:HD11	1:C:474:GLN:HA	1.66	0.77
1:D:168:LEU:HD23	1:D:292:THR:C	2.10	0.77
1:B:116:LEU:HD23	1:B:117:TRP:CA	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:GLU:O	1:D:168:LEU:HD11	1.82	0.77
1:B:41:LEU:O	1:B:42:GLN:CB	2.32	0.77
1:C:38:LEU:CB	1:C:41:LEU:CD1	2.63	0.77
1:C:85:LYS:HG3	1:C:88:ASP:OD2	1.83	0.77
1:D:66:LEU:CD1	1:D:66:LEU:N	2.47	0.77
1:A:38:LEU:O	1:A:41:LEU:CD1	2.32	0.77
1:A:372:ILE:O	1:A:372:ILE:CG2	2.32	0.77
1:A:30:LEU:HG	1:A:31:PRO:HD2	1.65	0.76
1:B:172:ILE:HD13	1:B:172:ILE:H	1.48	0.76
1:C:408:PHE:O	1:C:408:PHE:CD1	2.35	0.76
1:C:423:GLY:O	1:C:426:VAL:CG1	2.32	0.76
1:D:98:TYR:CD1	1:D:110:LEU:CD1	2.67	0.76
1:B:473:VAL:O	1:B:475:PRO:CD	2.32	0.76
1:C:472:LYS:NZ	1:C:473:VAL:N	2.33	0.76
1:D:98:TYR:CG	1:D:110:LEU:HD12	2.20	0.76
1:D:216:PHE:CD1	1:D:216:PHE:N	2.51	0.76
1:A:373:PHE:CD1	1:A:374:GLY:N	2.52	0.76
1:B:176:LEU:HA	1:B:255:MET:HB2	1.67	0.76
1:B:189:PHE:HE2	1:B:288:PHE:CE2	1.97	0.76
1:C:116:LEU:CD2	1:C:117:TRP:N	2.49	0.76
1:D:97:SER:CB	1:D:209:ASP:OD2	2.32	0.76
1:D:432:LEU:HD23	1:D:432:LEU:C	2.10	0.76
1:A:178:PHE:CB	1:A:243:HIS:HE1	1.97	0.76
1:A:451:LEU:CG	1:A:452:PRO:HD2	2.10	0.76
1:A:463:PRO:HG3	1:A:471:LEU:HB2	1.65	0.76
1:D:53:THR:HG22	1:D:54:GLN:N	2.00	0.76
1:A:37:PHE:C	1:A:38:LEU:HD23	2.11	0.76
1:A:332:ARG:CG	1:A:337:ASP:OD1	2.33	0.76
1:B:88:ASP:C	1:B:89:PHE:CD1	2.64	0.76
1:B:168:LEU:O	1:B:172:ILE:HD13	1.84	0.76
1:B:394:GLU:C	1:B:394:GLU:OE1	2.29	0.76
1:C:313:GLN:HE22	1:C:450:LEU:CB	1.99	0.76
1:D:116:LEU:HD23	1:D:117:TRP:CA	2.15	0.76
1:A:324:LEU:HD12	1:A:332:ARG:CG	2.13	0.76
1:B:408:PHE:CD2	1:B:408:PHE:O	2.39	0.76
1:D:208:LEU:HD23	1:D:208:LEU:H	1.51	0.76
1:C:407:ARG:O	1:C:413:ALA:CB	2.34	0.76
1:D:461:LEU:O	1:D:462:GLN:CB	2.33	0.76
1:C:40:LEU:C	1:C:40:LEU:CD1	2.52	0.75
1:A:38:LEU:O	1:A:41:LEU:CG	2.34	0.75
1:A:196:LEU:HD23	3:A:501:3QZ:CAI	2.13	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ASN:ND2	1:C:389:GLY:H	1.84	0.75
1:A:214:LEU:CG	1:A:216:PHE:N	2.46	0.75
1:C:473:VAL:CG1	1:C:474:GLN:OE1	2.35	0.75
1:D:372:ILE:O	1:D:373:PHE:CB	2.34	0.75
1:A:103:GLN:O	4:A:610:HOH:O	2.02	0.75
1:A:451:LEU:O	1:A:478:VAL:HG23	1.87	0.75
1:C:116:LEU:HD23	1:C:116:LEU:O	1.85	0.75
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.68	0.75
1:D:109:SER:C	1:D:110:LEU:HD22	2.11	0.75
1:D:117:TRP:HZ2	1:D:425:ARG:HD3	1.49	0.75
1:D:121:LYS:HD2	1:D:428:LEU:HD21	1.68	0.75
1:C:463:PRO:HB2	1:C:465:PRO:HD2	1.69	0.75
1:D:117:TRP:HE1	1:D:425:ARG:NH1	1.84	0.75
1:D:121:LYS:HE2	1:D:428:LEU:HD23	1.67	0.75
1:A:43:PRO:CB	1:A:44:ASN:OD1	2.34	0.75
1:A:332:ARG:C	1:A:333:VAL:CG2	2.53	0.75
1:D:98:TYR:CD1	1:D:110:LEU:HD12	2.22	0.75
1:B:289:ILE:CD1	1:B:289:ILE:N	2.50	0.75
1:D:106:GLN:HB3	1:D:279:HIS:NE2	1.99	0.75
1:A:41:LEU:O	1:A:42:GLN:HB3	1.86	0.75
1:A:45:LEU:O	1:A:45:LEU:HD23	1.86	0.75
1:A:50:LEU:C	1:A:53:THR:HG23	2.11	0.75
1:A:331:SER:O	1:A:333:VAL:CG2	2.35	0.75
1:D:111:GLY:O	1:D:425:ARG:CZ	2.35	0.75
1:D:447:ALA:HB3	1:D:448:PHE:HE2	1.51	0.75
1:D:463:PRO:HG3	1:D:471:LEU:HB2	1.59	0.75
1:A:329:SER:HG	1:A:330:CYS:HG	0.76	0.74
1:A:472:LYS:CE	1:A:473:VAL:HG23	2.14	0.74
1:B:408:PHE:O	1:B:408:PHE:CG	2.39	0.74
1:C:168:LEU:HD21	1:C:296:ALA:HB2	1.68	0.74
1:A:93:PRO:HD3	1:A:365:ARG:HB2	1.67	0.74
1:A:332:ARG:CD	1:A:337:ASP:OD1	2.35	0.74
1:B:40:LEU:O	1:B:40:LEU:CD1	2.36	0.74
1:C:181:LYS:O	1:C:181:LYS:CG	2.29	0.74
1:C:62:LEU:CD2	1:C:63:ARG:N	2.37	0.74
1:C:89:PHE:CZ	1:C:372:ILE:HD12	2.22	0.74
1:C:301:TRP:CZ2	1:C:472:LYS:HD2	2.22	0.74
1:D:211:VAL:O	1:D:211:VAL:CG1	2.33	0.74
1:D:404:ARG:O	1:D:404:ARG:CD	2.32	0.74
1:A:275:LEU:C	1:A:275:LEU:CD1	2.59	0.74
1:A:358:VAL:HG12	1:A:361:ALA:HA	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:THR:O	1:B:177:THR:CG2	2.33	0.74
1:C:59:VAL:O	1:C:59:VAL:HG12	1.86	0.74
1:C:159:VAL:HG12	1:C:476:PHE:CZ	2.21	0.74
1:B:461:LEU:HB2	4:B:604:HOH:O	1.86	0.74
1:C:159:VAL:HG23	1:C:159:VAL:O	1.86	0.74
1:A:285:VAL:CG1	1:A:286:ASP:OD1	2.35	0.74
1:D:214:LEU:CD2	1:D:216:PHE:HA	2.17	0.74
1:D:336:LYS:HG3	4:D:614:HOH:O	1.85	0.74
1:A:43:PRO:C	1:A:44:ASN:OD1	2.30	0.74
1:A:50:LEU:O	1:A:53:THR:CG2	2.36	0.74
1:A:106:GLN:HG2	1:A:116:LEU:HD22	1.70	0.74
1:B:104:ARG:O	1:B:105:CYS:SG	2.45	0.74
1:B:294:THR:HG22	3:B:501:3QZ:HAAA	1.65	0.74
1:A:62:LEU:HD23	1:A:63:ARG:CA	2.16	0.74
1:B:252:TRP:O	1:B:254:ASP:N	2.21	0.74
1:B:459:PRO:HB2	1:B:472:LYS:NZ	2.02	0.74
1:C:102:SER:OG	1:C:105:CYS:CA	2.36	0.74
1:C:420:PHE:CZ	2:C:500:HEM:HBB2	2.23	0.74
1:B:252:TRP:HB2	1:B:257:ASP:OD2	1.88	0.73
1:B:319:GLU:O	1:B:323:GLU:HB2	1.87	0.73
1:D:177:THR:CG2	1:D:239:GLN:HG2	2.17	0.73
1:B:409:LEU:O	1:B:409:LEU:CD2	2.34	0.73
1:C:30:LEU:HD11	1:C:378:PRO:HD3	1.70	0.73
1:C:151:MET:SD	1:C:163:LYS:HD2	2.29	0.73
1:D:95:ILE:HB	1:D:96:PRO:HD2	1.70	0.73
1:D:425:ARG:O	1:D:426:VAL:C	2.30	0.73
1:D:46:PRO:HG3	1:D:466:TYR:CD2	2.19	0.73
1:D:110:LEU:HD23	1:D:110:LEU:N	2.03	0.73
1:B:214:LEU:CD2	1:B:216:PHE:N	2.51	0.73
1:B:214:LEU:O	1:B:217:PHE:HE1	1.69	0.73
1:B:357:VAL:HG12	1:B:469:VAL:CG1	2.19	0.73
1:C:101:VAL:O	1:C:101:VAL:CG2	2.36	0.73
1:C:276:LEU:CD2	1:C:277:GLU:N	2.44	0.73
1:C:297:SER:CB	1:C:357:VAL:CG2	2.67	0.73
1:D:172:ILE:HD12	1:D:172:ILE:N	2.04	0.73
1:C:463:PRO:CG	1:C:471:LEU:CB	2.65	0.73
1:B:176:LEU:CD1	1:B:287:LEU:HD22	2.19	0.73
1:B:410:GLU:OE2	1:B:411:PRO:CG	2.35	0.73
1:A:177:THR:CG2	1:A:288:PHE:CZ	2.72	0.73
1:A:196:LEU:CD2	3:A:501:3QZ:HAI	2.17	0.73
1:D:81:ALA:HB2	1:D:372:ILE:HG12	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:O	1:A:159:VAL:CG2	2.37	0.73
1:C:246:SER:HB3	1:C:252:TRP:CZ2	2.24	0.73
1:C:307:LEU:HB3	1:C:458:LEU:HD22	1.69	0.73
1:A:214:LEU:CD2	1:A:216:PHE:CA	2.63	0.73
1:A:40:LEU:O	1:A:40:LEU:CD1	2.35	0.73
1:A:67:GLN:OE1	1:A:67:GLN:CA	2.36	0.73
1:B:285:VAL:HA	1:B:288:PHE:CB	2.15	0.73
1:B:420:PHE:CZ	2:B:500:HEM:HBB2	2.24	0.73
1:B:176:LEU:O	1:B:176:LEU:CD2	2.35	0.72
1:C:29:HIS:O	1:C:376:ASP:HB2	1.88	0.72
1:C:62:LEU:HD23	1:C:63:ARG:C	2.12	0.72
1:C:294:THR:CG2	3:C:501:3QZ:CAA	2.67	0.72
1:D:29:HIS:HA	1:D:375:TYR:HD1	1.52	0.72
1:D:205:ILE:O	1:D:205:ILE:CD1	2.37	0.72
1:D:350:GLU:HG3	1:D:404:ARG:C	2.14	0.72
1:A:472:LYS:HZ3	1:A:473:VAL:N	1.83	0.72
1:B:37:PHE:CE1	1:B:63:ARG:NE	2.57	0.72
1:B:214:LEU:O	1:B:215:ARG:CG	2.37	0.72
1:D:252:TRP:HB2	1:D:257:ASP:CG	2.14	0.72
1:D:462:GLN:CD	1:D:466:TYR:OH	2.32	0.72
1:A:275:LEU:O	1:A:275:LEU:CD1	2.37	0.72
1:B:37:PHE:HE1	1:B:63:ARG:NE	1.87	0.72
1:C:472:LYS:HZ3	1:C:472:LYS:CA	2.03	0.72
1:A:373:PHE:HD1	1:A:373:PHE:O	1.71	0.72
1:B:409:LEU:O	1:B:411:PRO:CD	2.36	0.72
1:B:459:PRO:CG	1:B:472:LYS:NZ	2.53	0.72
1:C:378:PRO:HG2	1:C:381:MET:HB2	1.69	0.72
1:C:472:LYS:HZ3	1:C:472:LYS:HB3	1.54	0.72
1:D:46:PRO:HD3	1:D:466:TYR:CD2	2.24	0.72
1:C:161:ILE:HG12	1:C:475:PRO:HD2	1.70	0.72
1:D:215:ARG:HH21	1:D:215:ARG:HG2	1.55	0.72
1:A:87:VAL:CG1	1:A:368:ARG:HH21	2.02	0.72
1:A:332:ARG:O	1:A:333:VAL:CG2	2.37	0.72
1:B:108:ILE:HD12	1:B:428:LEU:HD21	1.72	0.72
1:C:38:LEU:CB	1:C:41:LEU:HD11	2.20	0.72
1:A:87:VAL:HG11	1:A:368:ARG:HH21	1.55	0.72
1:D:313:GLN:HE21	1:D:445:LEU:HD11	1.54	0.72
1:B:63:ARG:NH2	4:B:617:HOH:O	1.77	0.72
1:C:470:ASN:C	1:C:470:ASN:OD1	2.33	0.72
1:D:208:LEU:HD13	1:D:214:LEU:HD22	1.70	0.72
1:C:41:LEU:O	1:C:42:GLN:CB	2.38	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ARG:HG3	1:D:407:ARG:NH1	1.96	0.72
1:B:40:LEU:O	1:B:40:LEU:HD13	1.89	0.71
1:C:53:THR:CG2	1:C:54:GLN:N	2.52	0.71
1:D:193:VAL:HG22	1:D:289:ILE:HG22	1.71	0.71
1:A:286:ASP:O	1:A:290:GLY:CA	2.38	0.71
1:B:104:ARG:C	1:B:105:CYS:SG	2.73	0.71
1:B:252:TRP:HB2	1:B:257:ASP:CG	2.15	0.71
1:B:285:VAL:O	1:B:289:ILE:N	2.21	0.71
1:C:105:CYS:HB2	1:C:106:GLN:NE2	2.04	0.71
1:C:178:PHE:CA	1:C:254:ASP:CG	2.63	0.71
1:D:196:LEU:CD2	3:D:501:3QZ:OAE	2.37	0.71
1:C:178:PHE:C	1:C:254:ASP:OD1	2.32	0.71
1:C:276:LEU:HD23	1:C:277:GLU:CA	2.20	0.71
1:D:432:LEU:O	1:D:432:LEU:CD2	2.36	0.71
1:A:461:LEU:O	1:A:461:LEU:CD2	2.36	0.71
1:B:196:LEU:HD23	3:B:501:3QZ:HAI	1.71	0.71
1:C:67:GLN:OE1	1:C:67:GLN:CA	2.36	0.71
1:D:214:LEU:CD2	1:D:216:PHE:CD1	2.54	0.71
1:D:62:LEU:CD2	1:D:63:ARG:N	2.38	0.71
1:B:88:ASP:HB3	1:B:89:PHE:CE1	2.26	0.71
1:C:69:VAL:HG13	1:C:382:VAL:HB	1.73	0.71
1:D:242:ARG:NH1	1:D:242:ARG:CG	2.34	0.71
1:A:337:ASP:O	1:A:340:ARG:HG2	1.89	0.71
1:B:127:ALA:HB1	1:B:255:MET:HG2	1.70	0.71
1:B:409:LEU:C	1:B:411:PRO:CD	2.63	0.71
1:D:123:LEU:HD11	1:D:262:GLY:O	1.91	0.71
1:A:309:HIS:HE1	1:A:403:PHE:HB3	1.54	0.71
1:C:161:ILE:HD11	1:C:475:PRO:HD2	1.73	0.71
1:C:474:GLN:O	1:C:474:GLN:CD	2.33	0.71
1:B:211:VAL:O	1:B:211:VAL:CG1	2.35	0.71
1:B:402:GLU:OE1	1:B:402:GLU:CA	2.33	0.71
1:B:407:ARG:CG	1:B:407:ARG:NH1	2.51	0.71
1:A:34:VAL:HG11	1:A:52:LEU:CD1	2.21	0.70
1:B:128:LEU:CG	1:B:287:LEU:CD2	2.66	0.70
1:C:219:ASN:CG	1:C:220:PRO:HD2	2.15	0.70
1:C:449:THR:OG1	1:C:480:LEU:O	2.08	0.70
1:B:410:GLU:O	1:B:410:GLU:HG2	1.90	0.70
1:B:418:LEU:N	1:B:418:LEU:CD1	2.36	0.70
1:D:168:LEU:HD22	1:D:292:THR:HB	1.74	0.70
1:D:172:ILE:N	1:D:172:ILE:CD1	2.54	0.70
1:D:262:GLY:O	1:D:263:VAL:HG23	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:HB3	1:A:422:CYS:O	1.91	0.70
1:A:104:ARG:C	1:A:105:CYS:SG	2.74	0.70
1:A:110:LEU:HD11	3:A:501:3QZ:HAH	1.73	0.70
1:A:374:GLY:C	1:A:375:TYR:CD2	2.69	0.70
1:A:375:TYR:N	1:A:375:TYR:HD2	1.90	0.70
1:B:33:LEU:CD1	1:B:34:VAL:O	2.38	0.70
1:D:150:ARG:HD2	1:D:163:LYS:HE3	1.72	0.70
1:A:420:PHE:CE1	2:A:500:HEM:HBB2	2.26	0.70
1:B:81:ALA:HB2	1:B:372:ILE:HG23	1.72	0.70
1:C:143:LEU:HD13	1:C:171:SER:HA	1.73	0.70
1:D:361:ALA:HB1	2:D:500:HEM:HAA2	1.73	0.70
1:D:466:TYR:O	1:D:467:CYS:SG	2.50	0.70
1:C:177:THR:HB	1:C:288:PHE:CE1	2.27	0.70
1:C:307:LEU:CD1	1:C:458:LEU:HD22	2.22	0.70
1:C:307:LEU:HB3	1:C:458:LEU:CD2	2.21	0.70
1:D:121:LYS:CE	1:D:428:LEU:HD23	2.21	0.70
1:A:332:ARG:NE	1:A:332:ARG:CA	2.38	0.70
1:B:176:LEU:C	1:B:176:LEU:CD2	2.62	0.70
1:B:459:PRO:CB	1:B:472:LYS:HZ1	2.04	0.70
1:C:37:PHE:N	4:C:601:HOH:O	2.20	0.70
1:C:161:ILE:HD11	1:C:474:GLN:CA	2.21	0.70
1:A:40:LEU:C	1:A:40:LEU:CD1	2.63	0.70
1:A:313:GLN:HE22	1:A:450:LEU:HD12	1.50	0.70
1:C:31:PRO:HA	1:C:375:TYR:CD1	2.26	0.70
1:D:101:VAL:HG12	1:D:229:ILE:HD12	1.71	0.70
1:B:74:SER:OG	1:B:77:THR:OG1	2.08	0.70
1:B:128:LEU:CD2	1:B:287:LEU:HD21	2.21	0.69
1:C:447:ALA:HB3	1:C:448:PHE:CD2	2.27	0.69
1:D:109:SER:OG	1:D:110:LEU:CD2	2.39	0.69
1:D:359:PRO:O	1:D:387:LEU:HB2	1.92	0.69
1:D:377:ILE:CG2	1:D:378:PRO:HD2	2.22	0.69
1:A:64:LEU:HD22	3:A:502:3QZ:CAB	2.21	0.69
1:A:160:THR:CG2	1:A:164:GLU:OE1	2.41	0.69
1:C:165:PHE:O	1:C:168:LEU:CD1	2.39	0.69
1:A:128:LEU:HD21	1:A:287:LEU:HD23	1.74	0.69
1:B:69:VAL:HG22	1:B:382:VAL:CG2	2.22	0.69
1:B:214:LEU:HD23	1:B:216:PHE:N	2.08	0.69
1:B:244:LYS:HG2	1:B:260:LEU:HD21	1.74	0.69
1:D:319:GLU:O	1:D:323:GLU:HB2	1.91	0.69
1:A:283:SER:O	1:A:287:LEU:HD12	1.93	0.69
1:B:340:ARG:HH21	1:C:340:ARG:HH21	1.38	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:VAL:O	1:B:427:CYS:HB2	1.91	0.69
1:C:307:LEU:HB3	1:C:458:LEU:HD13	1.74	0.69
1:C:313:GLN:NE2	1:C:450:LEU:HB2	2.08	0.69
1:C:426:VAL:O	1:C:427:CYS:HB2	1.92	0.69
1:C:161:ILE:CD1	1:C:475:PRO:HD2	2.23	0.69
1:C:342:PRO:HG2	1:C:343:LEU:H	1.58	0.69
1:D:459:PRO:HB3	1:D:473:VAL:HB	1.75	0.69
1:A:475:PRO:HG3	4:A:605:HOH:O	1.92	0.69
1:B:174:CYS:O	1:B:179:GLY:CA	2.34	0.69
1:B:180:ASN:ND2	1:B:185:LEU:HD13	2.08	0.69
1:B:307:LEU:HD21	1:B:477:GLN:HG3	1.73	0.69
1:C:45:LEU:HD21	1:C:64:LEU:HD21	1.75	0.69
1:A:185:LEU:HD11	1:A:239:GLN:HE22	1.58	0.69
1:B:216:PHE:CD2	1:B:216:PHE:N	2.53	0.69
1:B:301:TRP:CE3	1:B:472:LYS:HD3	2.28	0.69
1:D:104:ARG:O	1:D:105:CYS:HB2	1.92	0.69
1:B:136:MET:SD	1:B:175:TYR:CD2	2.86	0.69
1:C:357:VAL:HG12	1:C:358:VAL:N	2.08	0.69
1:D:62:LEU:CD2	1:D:63:ARG:C	2.66	0.69
1:B:112:ASP:CG	1:B:365:ARG:NH2	2.50	0.69
1:C:101:VAL:HG21	3:C:501:3QZ:HAG	1.75	0.69
1:C:418:LEU:HD13	1:C:418:LEU:O	1.94	0.68
1:D:212:PRO:O	1:D:216:PHE:HE1	1.77	0.68
1:D:376:ASP:O	1:D:377:ILE:HD12	1.94	0.68
1:C:276:LEU:HD23	1:C:278:GLY:H	1.54	0.68
1:D:168:LEU:CD2	1:D:292:THR:C	2.66	0.68
1:A:78:ILE:HD11	1:A:385:PRO:HB2	1.74	0.68
1:B:151:MET:HB3	1:B:479:ARG:NH1	2.08	0.68
1:B:284:VAL:C	1:B:288:PHE:CB	2.47	0.68
1:C:472:LYS:C	1:C:472:LYS:CE	2.66	0.68
1:D:471:LEU:HD13	1:D:472:LYS:CA	2.22	0.68
1:A:177:THR:HG21	1:A:288:PHE:CZ	2.27	0.68
1:A:294:THR:HG21	3:A:501:3QZ:HAAA	0.69	0.68
1:B:40:LEU:CD1	1:B:40:LEU:C	2.66	0.68
1:C:46:PRO:HB2	1:C:388:GLN:HG2	1.74	0.68
1:C:301:TRP:CE2	1:C:472:LYS:HD2	2.28	0.68
1:C:408:PHE:O	1:C:409:LEU:HB2	1.91	0.68
1:A:472:LYS:HZ3	1:A:472:LYS:HB3	1.58	0.68
1:C:34:VAL:HG11	1:C:52:LEU:HD13	1.75	0.68
1:C:313:GLN:HE21	1:C:445:LEU:CD1	2.07	0.68
1:A:41:LEU:O	1:A:42:GLN:CB	2.42	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD13	1:B:428:LEU:O	1.94	0.68
1:A:313:GLN:NE2	1:A:450:LEU:CB	2.56	0.68
1:C:161:ILE:HD11	1:C:475:PRO:CD	2.24	0.68
1:C:472:LYS:C	1:C:472:LYS:HE2	2.18	0.68
1:D:447:ALA:O	1:D:481:GLN:HB3	1.93	0.68
1:A:280:VAL:O	1:A:284:VAL:HG23	1.94	0.68
1:C:147:PHE:O	1:C:151:MET:HG2	1.94	0.68
1:C:159:VAL:HG13	1:C:476:PHE:CE2	2.29	0.68
1:A:44:ASN:OD1	1:A:44:ASN:N	2.26	0.67
1:A:284:VAL:HG12	1:A:288:PHE:HB2	1.75	0.67
1:A:477:GLN:CD	1:A:477:GLN:N	2.51	0.67
1:D:109:SER:C	1:D:110:LEU:CD2	2.67	0.67
1:B:360:LEU:O	1:B:361:ALA:CB	2.42	0.67
1:C:472:LYS:CA	1:C:472:LYS:NZ	2.57	0.67
1:D:54:GLN:CD	1:D:55:LYS:N	2.52	0.67
1:B:31:PRO:HG2	1:B:61:ARG:HG3	1.76	0.67
1:B:396:VAL:CG1	1:B:397:TRP:CD2	2.74	0.67
1:C:38:LEU:CB	1:C:41:LEU:HD12	2.24	0.67
1:D:410:GLU:HB3	1:D:411:PRO:C	2.20	0.67
1:A:45:LEU:N	1:A:46:PRO:HD2	2.09	0.67
1:A:252:TRP:HB2	1:A:257:ASP:CB	2.25	0.67
1:D:106:GLN:CG	1:D:116:LEU:HD11	2.23	0.67
1:A:130:LEU:HD13	1:A:134:SER:O	1.95	0.67
1:A:168:LEU:CD2	1:A:292:THR:O	2.43	0.67
1:C:472:LYS:NZ	1:C:473:VAL:O	2.27	0.67
1:D:108:ILE:CD1	1:D:124:THR:HG21	2.24	0.67
1:D:473:VAL:HG13	1:D:474:GLN:OE1	1.94	0.67
1:B:192:CYS:O	1:B:196:LEU:HB2	1.95	0.67
1:C:42:GLN:HG3	1:C:43:PRO:HD2	1.76	0.67
1:C:46:PRO:HG3	1:C:466:TYR:CZ	2.30	0.67
1:C:161:ILE:HD13	1:C:474:GLN:HA	1.77	0.67
1:C:176:LEU:HG	1:C:255:MET:HE3	1.75	0.67
1:D:56:LEU:CD2	1:D:56:LEU:N	2.57	0.67
1:D:117:TRP:CZ2	1:D:425:ARG:CD	2.77	0.67
1:C:425:ARG:C	4:C:606:HOH:O	2.36	0.67
1:D:214:LEU:CD2	1:D:216:PHE:CA	2.72	0.67
1:A:38:LEU:O	1:A:41:LEU:HD11	1.95	0.67
1:A:309:HIS:CE1	1:A:403:PHE:HB3	2.29	0.67
1:A:464:ASP:N	1:A:465:PRO:HD2	2.10	0.67
1:B:214:LEU:C	1:B:215:ARG:HG3	2.19	0.67
1:C:297:SER:CB	1:C:357:VAL:HG21	2.17	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:CD2	1:D:64:LEU:N	2.58	0.67
1:D:459:PRO:HD3	1:D:475:PRO:HB3	1.77	0.67
1:B:313:GLN:HE21	1:B:445:LEU:HD12	1.60	0.67
1:C:244:LYS:HG2	1:C:260:LEU:HD21	1.77	0.67
1:C:386:ASN:HD21	1:C:389:GLY:H	1.40	0.67
1:D:203:TRP:HA	1:D:206:GLN:CB	2.23	0.67
1:A:177:THR:HG22	1:A:239:GLN:HG2	1.76	0.67
1:D:38:LEU:CD1	1:D:41:LEU:HD11	2.25	0.67
1:D:313:GLN:CD	1:D:449:THR:O	2.37	0.67
1:B:301:TRP:CZ3	1:B:472:LYS:HD3	2.30	0.66
1:C:89:PHE:CD1	1:C:89:PHE:N	2.61	0.66
1:C:387:LEU:HD22	1:C:418:LEU:HD13	1.77	0.66
1:D:168:LEU:HD22	1:D:292:THR:CB	2.25	0.66
1:D:404:ARG:NH1	1:D:407:ARG:HB3	2.09	0.66
1:B:169:THR:O	1:B:173:ILE:CD1	2.43	0.66
1:B:178:PHE:H	1:B:254:ASP:HB2	1.61	0.66
1:A:357:VAL:CG1	1:A:469:VAL:CG1	2.69	0.66
1:A:449:THR:O	1:A:450:LEU:HB2	1.96	0.66
1:C:101:VAL:HG23	1:C:232:ARG:NH2	2.10	0.66
1:D:418:LEU:HD22	1:D:422:CYS:SG	2.35	0.66
1:A:214:LEU:HD21	1:A:216:PHE:N	2.04	0.66
1:C:276:LEU:HD21	1:C:278:GLY:N	2.05	0.66
1:C:473:VAL:HG13	1:C:474:GLN:OE1	1.94	0.66
1:D:54:GLN:C	1:D:54:GLN:CD	2.63	0.66
1:D:117:TRP:CE2	1:D:425:ARG:CZ	2.79	0.66
1:D:248:VAL:HG23	1:D:249:ALA:N	2.09	0.66
1:A:178:PHE:N	1:A:243:HIS:HE1	1.83	0.66
1:A:243:HIS:NE2	1:A:254:ASP:OD1	2.29	0.66
1:A:423:GLY:O	1:A:426:VAL:N	2.27	0.66
1:D:211:VAL:O	1:D:214:LEU:HB3	1.96	0.66
1:A:338:ARG:O	1:A:338:ARG:HG2	1.94	0.66
1:A:423:GLY:C	1:A:426:VAL:H	2.04	0.66
1:B:61:ARG:HH11	1:B:68:GLU:CD	2.02	0.66
1:D:192:CYS:O	1:D:196:LEU:HB2	1.96	0.66
1:D:447:ALA:C	1:D:481:GLN:HB3	2.20	0.66
1:C:89:PHE:CE2	1:C:372:ILE:HD13	2.31	0.66
1:C:192:CYS:O	1:C:196:LEU:HB2	1.96	0.66
1:C:196:LEU:HD11	1:C:229:ILE:HA	1.77	0.66
1:D:56:LEU:HD22	1:D:56:LEU:H	1.60	0.66
1:D:62:LEU:HD23	1:D:63:ARG:C	2.21	0.66
1:A:174:CYS:O	1:A:179:GLY:HA2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:SER:HB3	1:B:252:TRP:CH2	2.31	0.66
1:B:357:VAL:O	1:B:470:ASN:HB3	1.95	0.66
1:A:459:PRO:O	1:A:460:SER:CB	2.44	0.66
1:A:472:LYS:HE3	1:A:473:VAL:CG2	2.17	0.66
1:B:200:TRP:HD1	1:B:225:LEU:HD11	1.61	0.66
1:C:203:TRP:O	1:C:207:ILE:HG13	1.96	0.66
1:C:219:ASN:OD1	1:C:220:PRO:CD	2.34	0.66
1:D:176:LEU:HG	1:D:255:MET:SD	2.36	0.66
1:A:285:VAL:HG12	1:A:286:ASP:N	2.11	0.65
1:B:180:ASN:OD1	1:B:182:GLU:HB2	1.95	0.65
1:C:276:LEU:HD23	1:C:278:GLY:N	2.08	0.65
1:C:307:LEU:HB3	1:C:458:LEU:CD1	2.25	0.65
1:D:44:ASN:HB3	1:D:47:ILE:HG12	1.77	0.65
1:D:72:LEU:HD11	1:D:372:ILE:HD11	1.77	0.65
1:B:470:ASN:C	1:B:470:ASN:OD1	2.39	0.65
1:C:275:LEU:C	1:C:275:LEU:HD12	2.19	0.65
1:C:447:ALA:C	1:C:448:PHE:HD2	2.03	0.65
1:D:462:GLN:HG2	1:D:463:PRO:HD2	1.78	0.65
1:A:354:LEU:O	1:A:355:ARG:HD2	1.96	0.65
1:A:87:VAL:CB	1:A:368:ARG:HH21	2.10	0.65
1:D:392:LEU:HA	1:D:400:PRO:HB2	1.77	0.65
1:A:245:GLU:OE1	1:A:246:SER:N	2.29	0.65
1:B:121:LYS:HD2	1:B:428:LEU:HD22	1.77	0.65
1:C:444:LEU:HD22	1:C:450:LEU:HD11	1.79	0.65
1:A:192:CYS:O	1:A:196:LEU:HB2	1.96	0.65
1:A:212:PRO:C	1:A:214:LEU:H	2.03	0.65
1:A:313:GLN:HE22	1:A:450:LEU:HB3	1.62	0.65
1:B:161:ILE:H	1:B:161:ILE:HD12	1.61	0.65
1:B:189:PHE:CZ	1:B:288:PHE:CZ	2.66	0.65
1:C:277:GLU:O	1:C:280:VAL:HB	1.96	0.65
1:D:169:THR:HG21	1:D:190:HIS:HB2	1.78	0.65
1:D:471:LEU:HD13	1:D:472:LYS:O	1.96	0.65
1:A:69:VAL:HG13	1:A:382:VAL:HB	1.78	0.65
1:A:333:VAL:HA	4:A:622:HOH:O	1.95	0.65
1:C:38:LEU:HB3	1:C:41:LEU:HD11	1.77	0.65
1:C:464:ASP:N	1:C:465:PRO:CD	2.60	0.65
1:A:97:SER:HB2	1:A:209:ASP:OD1	1.95	0.65
1:A:294:THR:CG2	3:A:501:3QZ:HAAB	2.16	0.65
1:B:89:PHE:CE2	1:B:372:ILE:CD1	2.77	0.65
1:C:324:LEU:HG	1:C:340:ARG:HG3	1.76	0.65
1:D:376:ASP:N	1:D:376:ASP:OD1	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:PHE:CE1	2:D:500:HEM:HBB2	2.30	0.65
1:D:448:PHE:HD1	1:D:479:ARG:HB3	1.62	0.65
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.58	0.65
1:B:284:VAL:HG12	1:B:288:PHE:CG	2.30	0.65
1:D:33:LEU:HD22	1:D:34:VAL:H	1.61	0.65
1:D:52:LEU:O	1:D:56:LEU:CD2	2.37	0.65
1:A:38:LEU:N	4:A:601:HOH:O	2.22	0.64
1:C:420:PHE:CE1	2:C:500:HEM:HBB2	2.30	0.64
1:D:121:LYS:CE	1:D:428:LEU:CD2	2.75	0.64
1:D:172:ILE:CD1	1:D:172:ILE:H	2.10	0.64
1:D:197:MET:HE2	1:D:293:GLU:HG3	1.78	0.64
1:A:52:LEU:N	1:A:52:LEU:HD23	2.12	0.64
1:A:108:ILE:CD1	1:A:124:THR:HG21	2.26	0.64
1:A:429:GLY:HA3	2:A:500:HEM:HBC2	1.78	0.64
1:D:252:TRP:CE3	1:D:253:ARG:CD	2.78	0.64
1:D:426:VAL:HG23	1:D:427:CYS:H	1.62	0.64
1:B:31:PRO:HG2	1:B:61:ARG:CG	2.28	0.64
1:A:337:ASP:OD2	1:A:337:ASP:N	2.30	0.64
1:A:353:ARG:NH2	1:A:404:ARG:HD3	2.12	0.64
1:B:473:VAL:CG1	1:B:474:GLN:N	2.60	0.64
1:C:171:SER:HB3	1:C:175:TYR:OH	1.97	0.64
1:C:358:VAL:HG11	2:C:500:HEM:C4A	2.33	0.64
1:C:473:VAL:HG12	1:C:474:GLN:OE1	1.97	0.64
1:D:208:LEU:N	1:D:208:LEU:CD2	2.60	0.64
1:D:357:VAL:HG13	1:D:469:VAL:HG13	1.77	0.64
1:A:89:PHE:CE2	1:A:372:ILE:CG1	2.81	0.64
1:A:404:ARG:NH1	1:A:406:ASP:O	2.31	0.64
1:B:41:LEU:H	1:B:41:LEU:CD2	1.93	0.64
1:B:141:ASP:HA	1:B:439:VAL:HG11	1.80	0.64
1:B:286:ASP:O	1:B:290:GLY:N	2.31	0.64
1:B:386:ASN:C	1:B:386:ASN:HD22	2.06	0.64
1:D:44:ASN:OD1	1:D:462:GLN:NE2	2.31	0.64
1:A:205:ILE:HG13	1:A:225:LEU:HD13	1.78	0.64
1:B:324:LEU:HD22	1:C:336:LYS:HE2	1.78	0.64
1:A:333:VAL:HG11	1:A:443:ARG:NH1	2.12	0.64
1:B:197:MET:HE2	1:B:293:GLU:HG3	1.80	0.64
1:B:285:VAL:CA	1:B:288:PHE:CB	2.74	0.64
1:D:372:ILE:O	1:D:372:ILE:HG23	1.98	0.64
1:A:211:VAL:O	1:A:214:LEU:HB3	1.98	0.64
1:A:214:LEU:HD23	1:A:216:PHE:CD2	2.32	0.64
1:A:406:ASP:OD1	1:A:406:ASP:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLN:HE22	1:C:165:PHE:HB3	1.60	0.64
1:C:263:VAL:HG13	1:C:275:LEU:O	1.98	0.64
1:C:275:LEU:HD12	1:C:275:LEU:O	1.96	0.64
1:D:38:LEU:CB	1:D:41:LEU:CD1	2.74	0.64
1:D:110:LEU:N	1:D:110:LEU:HD22	2.13	0.64
1:C:38:LEU:HB3	1:C:41:LEU:HD12	1.76	0.64
1:C:62:LEU:HD21	1:C:64:LEU:N	2.12	0.64
1:C:279:HIS:ND1	4:C:608:HOH:O	2.29	0.64
1:D:205:ILE:CD1	1:D:205:ILE:C	2.70	0.64
1:A:214:LEU:CD2	1:A:216:PHE:HA	2.19	0.64
1:A:477:GLN:N	1:A:477:GLN:OE1	2.31	0.64
1:B:172:ILE:O	1:B:176:LEU:HB3	1.98	0.64
1:D:53:THR:CG2	1:D:54:GLN:N	2.60	0.64
1:D:430:GLU:OE1	1:D:434:ARG:NH1	2.29	0.64
1:A:74:SER:O	1:A:78:ILE:HG22	1.98	0.63
1:A:86:TRP:CH2	1:A:424:ALA:HA	2.34	0.63
1:D:202:HIS:O	1:D:206:GLN:N	2.30	0.63
1:A:97:SER:HB2	1:A:209:ASP:CG	2.24	0.63
1:A:193:VAL:CG2	1:A:289:ILE:HG22	2.18	0.63
1:B:91:GLY:C	1:B:365:ARG:HB3	2.23	0.63
1:D:30:LEU:CD1	1:D:31:PRO:HD2	2.28	0.63
1:A:42:GLN:OE1	1:A:48:HIS:ND1	2.32	0.63
1:B:30:LEU:CG	1:B:31:PRO:HD2	2.27	0.63
1:C:226:LYS:O	1:C:229:ILE:HG22	1.99	0.63
1:D:97:SER:HB2	1:D:209:ASP:CG	2.23	0.63
1:D:196:LEU:HD21	1:D:232:ARG:HD3	1.80	0.63
1:A:116:LEU:HD11	1:A:279:HIS:NE2	2.14	0.63
1:B:354:LEU:O	1:B:355:ARG:HD2	1.98	0.63
1:C:38:LEU:N	4:C:601:HOH:O	2.29	0.63
1:C:137:GLU:H	1:C:138:PRO:HD2	1.63	0.63
1:A:178:PHE:HD2	1:A:243:HIS:CE1	2.17	0.63
1:B:62:LEU:CD2	1:B:63:ARG:N	2.37	0.63
1:D:215:ARG:HB3	1:D:217:PHE:CD1	2.33	0.63
1:A:335:TYR:CD2	1:A:336:LYS:CA	2.81	0.63
1:C:37:PHE:CA	4:C:601:HOH:O	2.45	0.63
1:D:173:ILE:HD12	1:D:186:VAL:HG13	1.81	0.63
1:D:185:LEU:HD11	1:D:239:GLN:NE2	2.13	0.63
1:D:288:PHE:HB3	1:D:289:ILE:HD13	1.80	0.63
1:A:34:VAL:HG11	1:A:52:LEU:HD13	1.79	0.63
1:A:116:LEU:HD21	1:A:279:HIS:NE2	2.13	0.63
1:A:331:SER:O	1:A:333:VAL:HG23	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ASP:N	1:B:465:PRO:CD	2.61	0.63
1:C:239:GLN:HG3	1:C:243:HIS:CE1	2.34	0.63
1:C:459:PRO:O	1:C:460:SER:HB3	1.99	0.63
1:D:158:PRO:HD2	1:D:477:GLN:O	1.98	0.63
1:D:370:SER:OG	1:D:371:SER:N	2.31	0.63
1:A:38:LEU:CD2	1:A:65:GLY:O	2.47	0.63
1:A:248:VAL:HG23	1:A:249:ALA:N	2.14	0.63
1:B:69:VAL:HG22	1:B:382:VAL:HG23	1.80	0.63
1:B:284:VAL:HG12	1:B:288:PHE:HD1	1.30	0.63
1:C:159:VAL:CG1	1:C:476:PHE:CZ	2.81	0.63
1:A:475:PRO:HG2	1:A:477:GLN:NE2	2.14	0.62
1:D:37:PHE:O	1:D:38:LEU:HD23	1.99	0.62
1:D:56:LEU:CD2	1:D:56:LEU:H	2.11	0.62
1:D:215:ARG:CB	1:D:217:PHE:CE1	2.73	0.62
1:A:45:LEU:CD2	1:A:45:LEU:C	2.72	0.62
1:A:214:LEU:HD21	1:A:216:PHE:CG	2.33	0.62
1:A:89:PHE:CE2	1:A:372:ILE:CD1	2.80	0.62
1:B:176:LEU:HD11	1:B:287:LEU:CB	2.27	0.62
1:B:461:LEU:O	1:B:462:GLN:HB3	1.98	0.62
1:C:307:LEU:CB	1:C:458:LEU:HD22	2.28	0.62
1:D:66:LEU:O	1:D:67:GLN:NE2	2.31	0.62
1:D:117:TRP:CE2	1:D:425:ARG:NH1	2.67	0.62
1:D:376:ASP:C	1:D:377:ILE:CD1	2.72	0.62
1:C:238:LYS:HE2	1:C:238:LYS:HA	1.80	0.62
1:C:429:GLY:HA3	2:C:500:HEM:HBC2	1.82	0.62
1:D:204:SER:OG	1:D:221:GLY:HA3	1.98	0.62
1:D:406:ASP:OD1	1:D:406:ASP:N	2.31	0.62
1:A:64:LEU:HD12	1:A:69:VAL:HB	1.81	0.62
1:A:462:GLN:CB	1:A:466:TYR:OH	2.46	0.62
1:B:61:ARG:NH1	1:B:68:GLU:OE1	2.32	0.62
1:B:97:SER:HB2	1:B:209:ASP:OD2	2.00	0.62
1:B:193:VAL:HG13	1:B:289:ILE:HG21	1.77	0.62
1:C:374:GLY:C	1:C:375:TYR:HD2	2.07	0.62
1:C:391:HIS:NE2	1:C:418:LEU:HD12	2.14	0.62
1:B:61:ARG:NH1	1:B:68:GLU:OE2	2.32	0.62
1:B:459:PRO:CB	1:B:472:LYS:NZ	2.63	0.62
1:C:44:ASN:C	1:C:46:PRO:HD2	2.25	0.62
1:A:85:LYS:HE3	1:A:371:SER:O	1.99	0.62
1:A:463:PRO:HB2	1:A:465:PRO:HD2	1.80	0.62
1:B:88:ASP:CB	1:B:89:PHE:CE1	2.82	0.62
1:B:243:HIS:O	1:B:247:MET:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASP:N	1:C:406:ASP:OD1	2.31	0.62
1:D:232:ARG:HH11	3:D:501:3QZ:CAQ	2.09	0.62
1:C:474:GLN:OE1	1:C:474:GLN:N	2.33	0.62
1:D:46:PRO:CD	1:D:466:TYR:CE2	2.82	0.62
1:A:275:LEU:C	1:A:275:LEU:HD13	2.25	0.62
1:C:165:PHE:O	1:C:168:LEU:HD11	1.99	0.62
1:A:71:VAL:O	1:A:72:LEU:HD23	1.99	0.62
1:A:396:VAL:HG13	1:A:415:PRO:HG2	1.80	0.62
1:B:112:ASP:OD2	1:B:365:ARG:CZ	2.47	0.62
1:B:357:VAL:CG1	1:B:469:VAL:CG1	2.77	0.62
1:C:373:PHE:CD1	1:C:373:PHE:C	2.78	0.62
1:A:332:ARG:NH1	1:A:337:ASP:OD1	2.32	0.61
1:B:41:LEU:O	1:B:42:GLN:HB3	1.99	0.61
1:B:301:TRP:CD2	1:B:472:LYS:HD3	2.35	0.61
1:C:241:ARG:HA	1:C:244:LYS:HB2	1.80	0.61
1:A:106:GLN:O	1:A:107:ASP:CB	2.43	0.61
1:A:423:GLY:H	1:A:426:VAL:CG1	2.12	0.61
1:B:473:VAL:HG12	1:B:474:GLN:N	2.14	0.61
1:C:161:ILE:CD1	1:C:474:GLN:CA	2.78	0.61
1:C:214:LEU:HD23	1:C:214:LEU:H	1.65	0.61
1:C:162:GLN:NE2	1:C:162:GLN:O	2.33	0.61
1:D:55:LYS:HG3	1:D:56:LEU:HD23	1.81	0.61
1:D:353:ARG:HH12	1:D:400:PRO:HA	1.65	0.61
1:A:298:THR:OG1	1:A:357:VAL:CG2	2.48	0.61
1:B:136:MET:SD	1:B:175:TYR:HD2	2.24	0.61
1:C:53:THR:O	1:C:57:GLY:N	2.31	0.61
1:C:392:LEU:HD23	1:C:401:HIS:NE2	2.16	0.61
1:D:72:LEU:CD1	1:D:372:ILE:CD1	2.78	0.61
1:B:211:VAL:HG12	1:B:214:LEU:HB2	1.83	0.61
1:B:304:ALA:CB	1:B:472:LYS:HE3	2.31	0.61
1:C:128:LEU:C	1:C:129:LEU:HD13	2.24	0.61
1:D:53:THR:O	1:D:57:GLY:N	2.30	0.61
1:D:161:ILE:HD12	1:D:161:ILE:H	1.66	0.61
1:D:202:HIS:O	1:D:205:ILE:CG2	2.33	0.61
1:A:38:LEU:HB2	1:A:41:LEU:HD21	1.81	0.61
1:D:448:PHE:CD1	1:D:479:ARG:O	2.53	0.61
1:D:461:LEU:CD2	1:D:462:GLN:O	2.33	0.61
1:A:46:PRO:HB2	1:A:388:GLN:HG2	1.83	0.61
1:A:358:VAL:HG11	1:A:361:ALA:HA	1.81	0.61
1:C:307:LEU:CB	1:C:458:LEU:HD13	2.31	0.61
1:D:104:ARG:O	1:D:105:CYS:CB	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LEU:HD13	1:D:344:LEU:HD12	1.82	0.61
1:B:185:LEU:HD11	1:B:239:GLN:NE2	2.15	0.61
1:D:66:LEU:C	1:D:67:GLN:HE21	2.09	0.61
1:A:147:PHE:O	1:A:151:MET:HG2	2.01	0.60
1:B:205:ILE:O	1:B:205:ILE:HD13	2.01	0.60
1:C:45:LEU:N	1:C:46:PRO:HD2	2.15	0.60
1:B:286:ASP:OD2	1:B:286:ASP:N	2.32	0.60
1:B:459:PRO:HG2	1:B:472:LYS:NZ	2.14	0.60
1:C:56:LEU:N	1:C:56:LEU:HD23	2.16	0.60
1:C:177:THR:CG2	1:C:239:GLN:HG2	2.32	0.60
1:C:472:LYS:NZ	1:C:472:LYS:HB3	2.13	0.60
1:D:135:SER:O	1:D:138:PRO:HD2	2.00	0.60
1:D:196:LEU:CD2	3:D:501:3QZ:CAI	2.67	0.60
1:D:463:PRO:CB	1:D:471:LEU:HD12	2.27	0.60
1:D:470:ASN:OD1	1:D:471:LEU:N	2.35	0.60
1:A:199:THR:O	1:A:225:LEU:HD12	2.00	0.60
1:A:334:THR:HG23	1:A:335:TYR:N	2.15	0.60
1:B:169:THR:O	1:B:173:ILE:HD11	2.01	0.60
1:C:104:ARG:O	1:C:105:CYS:CB	2.49	0.60
1:D:216:PHE:HD1	1:D:216:PHE:N	1.95	0.60
1:A:62:LEU:CD2	1:A:63:ARG:C	2.74	0.60
1:A:64:LEU:HD22	3:A:502:3QZ:HABA	1.83	0.60
1:C:386:ASN:C	1:C:386:ASN:HD22	2.08	0.60
1:D:36:GLY:O	1:D:63:ARG:HD3	2.01	0.60
1:D:463:PRO:CB	1:D:471:LEU:CD1	2.55	0.60
1:C:97:SER:HB2	1:C:209:ASP:OD1	2.01	0.60
1:C:196:LEU:HD21	1:C:232:ARG:HD3	1.83	0.60
1:D:72:LEU:HD21	1:D:372:ILE:HD12	1.84	0.60
1:D:81:ALA:HB2	1:D:372:ILE:CG1	2.31	0.60
1:D:252:TRP:C	1:D:254:ASP:H	2.09	0.60
1:B:280:VAL:O	1:B:284:VAL:HG23	2.02	0.60
1:C:391:HIS:NE2	1:C:418:LEU:CD1	2.65	0.60
1:D:98:TYR:CG	1:D:110:LEU:CD1	2.85	0.60
1:A:38:LEU:HD21	1:A:66:LEU:HD12	1.82	0.60
1:A:147:PHE:CE2	1:A:163:LYS:HB3	2.37	0.60
1:A:161:ILE:O	1:A:165:PHE:CB	2.43	0.60
1:A:423:GLY:H	1:A:426:VAL:HG13	1.67	0.60
1:C:31:PRO:HB3	1:C:375:TYR:HD1	1.65	0.60
1:C:108:ILE:HD11	1:C:121:LYS:HD2	1.83	0.60
1:D:212:PRO:O	1:D:216:PHE:CE1	2.55	0.60
1:A:34:VAL:HG21	1:A:62:LEU:HG	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:O	1:A:60:TYR:OH	2.19	0.60
1:A:104:ARG:O	1:A:105:CYS:CB	2.50	0.60
1:A:171:SER:O	1:A:175:TYR:CD1	2.54	0.60
1:B:216:PHE:HD2	1:B:216:PHE:N	1.97	0.60
1:D:214:LEU:O	1:D:215:ARG:HB2	2.02	0.60
1:A:178:PHE:CD2	1:A:243:HIS:CE1	2.90	0.60
1:C:40:LEU:O	1:C:40:LEU:CD1	2.37	0.60
1:C:275:LEU:C	1:C:275:LEU:CD1	2.75	0.60
1:C:418:LEU:CD1	1:C:418:LEU:O	2.49	0.60
1:D:205:ILE:CG2	1:D:206:GLN:N	2.64	0.60
1:D:410:GLU:H	1:D:412:GLY:H	1.50	0.60
1:A:331:SER:O	1:A:333:VAL:HG22	2.02	0.60
1:C:243:HIS:HD1	1:C:256:THR:HG21	1.67	0.60
1:D:50:LEU:O	1:D:53:THR:HB	2.00	0.60
1:D:248:VAL:CG2	1:D:249:ALA:N	2.65	0.60
1:A:214:LEU:O	1:A:215:ARG:CB	2.50	0.59
1:D:279:HIS:ND1	4:D:604:HOH:O	2.25	0.59
1:B:78:ILE:HD11	1:B:385:PRO:HB2	1.84	0.59
1:B:135:SER:C	1:B:136:MET:HE2	2.27	0.59
1:B:324:LEU:HD13	1:C:336:LYS:HG2	1.84	0.59
1:C:83:ILE:HG13	1:C:422:CYS:SG	2.42	0.59
1:C:124:THR:HG23	1:C:428:LEU:HD11	1.85	0.59
1:D:252:TRP:CZ3	1:D:253:ARG:NE	2.69	0.59
1:D:276:LEU:HG	1:D:277:GLU:N	2.15	0.59
1:D:374:GLY:O	1:D:375:TYR:CB	2.49	0.59
1:B:88:ASP:HB3	1:B:89:PHE:HE1	1.66	0.59
1:B:469:VAL:HG22	3:B:501:3QZ:HAAB	1.85	0.59
1:C:177:THR:HG23	1:C:239:GLN:HG2	1.84	0.59
1:A:160:THR:HG22	1:A:164:GLU:OE1	2.02	0.59
1:B:96:PRO:HG2	1:B:209:ASP:OD1	2.01	0.59
1:B:205:ILE:HG13	1:B:225:LEU:HD12	1.83	0.59
1:B:346:ALA:HB2	1:B:408:PHE:CD1	2.37	0.59
1:B:399:GLN:OE1	1:B:404:ARG:NH1	2.34	0.59
1:C:30:LEU:HD12	1:C:376:ASP:O	2.03	0.59
1:C:303:VAL:HG13	1:C:450:LEU:HD21	1.82	0.59
1:D:55:LYS:CD	1:D:56:LEU:HD22	2.23	0.59
1:D:173:ILE:HA	1:D:288:PHE:HE1	1.65	0.59
1:D:211:VAL:O	1:D:214:LEU:CB	2.50	0.59
1:D:301:TRP:CZ3	1:D:460:SER:HA	2.37	0.59
1:D:304:ALA:HA	1:D:307:LEU:HD12	1.84	0.59
1:D:425:ARG:HB3	2:D:500:HEM:O2D	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HG	1:A:340:ARG:HG3	1.84	0.59
1:B:178:PHE:H	1:B:254:ASP:CB	2.14	0.59
1:B:308:HIS:CE1	1:B:458:LEU:HB2	2.38	0.59
1:B:463:PRO:HB2	1:B:465:PRO:HD2	1.83	0.59
1:C:418:LEU:N	1:C:418:LEU:CD1	2.38	0.59
1:B:320:LEU:HA	1:B:341:LEU:CD2	2.33	0.59
1:B:387:LEU:HD22	1:B:418:LEU:HD13	1.83	0.59
1:C:62:LEU:HD21	1:C:63:ARG:C	2.26	0.59
1:A:44:ASN:O	1:A:47:ILE:HG12	2.03	0.59
1:A:168:LEU:HD21	1:A:292:THR:O	2.03	0.59
1:B:62:LEU:HD21	1:B:63:ARG:C	2.26	0.59
1:C:49:LEU:HD13	1:C:71:VAL:HG11	1.84	0.59
1:A:89:PHE:CZ	1:A:372:ILE:CD1	2.85	0.59
1:B:85:LYS:O	1:B:87:VAL:N	2.35	0.59
1:B:216:PHE:HD2	1:B:216:PHE:H	1.49	0.59
1:C:167:LEU:C	1:C:167:LEU:HD22	2.25	0.59
1:D:196:LEU:CD2	3:D:501:3QZ:CAQ	2.80	0.59
1:D:472:LYS:CD	1:D:473:VAL:H	2.13	0.59
1:A:60:TYR:HE1	1:A:73:ASN:ND2	2.00	0.59
1:A:408:PHE:HD1	1:A:408:PHE:O	1.86	0.59
1:B:97:SER:HB2	1:B:209:ASP:CG	2.27	0.59
1:B:420:PHE:HZ	2:B:500:HEM:HBB2	1.67	0.59
1:C:162:GLN:HE22	1:C:165:PHE:CB	2.16	0.59
1:C:294:THR:HG21	3:C:501:3QZ:CAA	2.22	0.59
1:D:463:PRO:CG	1:D:471:LEU:HB2	2.20	0.59
1:C:304:ALA:HA	1:C:307:LEU:HD12	1.84	0.59
1:D:280:VAL:O	1:D:284:VAL:HG23	2.03	0.59
1:C:193:VAL:HG22	1:C:289:ILE:HG22	1.84	0.58
1:D:252:TRP:CH2	1:D:253:ARG:NH1	2.70	0.58
1:A:31:PRO:HG2	1:A:61:ARG:HG3	1.85	0.58
1:A:391:HIS:CD2	1:A:417:ALA:HB1	2.38	0.58
1:A:423:GLY:C	1:A:425:ARG:N	2.56	0.58
1:B:406:ASP:C	1:B:408:PHE:H	2.10	0.58
1:D:215:ARG:HD3	1:D:217:PHE:CE1	2.38	0.58
1:B:313:GLN:HE22	1:B:450:LEU:HB2	1.68	0.58
1:C:56:LEU:HD23	1:C:56:LEU:H	1.68	0.58
1:C:106:GLN:O	1:C:107:ASP:HB3	2.03	0.58
1:D:376:ASP:C	1:D:377:ILE:HD13	2.28	0.58
1:D:387:LEU:HD22	1:D:418:LEU:O	2.03	0.58
1:A:461:LEU:O	1:A:462:GLN:CB	2.52	0.58
1:A:470:ASN:C	1:A:470:ASN:OD1	2.46	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TRP:CZ2	1:B:424:ALA:HA	2.39	0.58
1:B:203:TRP:O	1:B:207:ILE:HG13	2.03	0.58
1:C:357:VAL:O	1:C:359:PRO:HD3	2.03	0.58
1:D:215:ARG:CD	1:D:217:PHE:HE1	2.16	0.58
1:D:236:VAL:O	1:D:240:LEU:HB2	2.03	0.58
1:A:243:HIS:NE2	1:A:254:ASP:OD2	2.35	0.58
1:A:285:VAL:HG13	1:A:286:ASP:N	2.18	0.58
1:A:286:ASP:OD1	1:A:286:ASP:N	2.33	0.58
1:C:160:THR:HG22	1:C:477:GLN:HB2	1.84	0.58
1:C:169:THR:HG21	1:C:190:HIS:CB	2.30	0.58
1:D:40:LEU:C	1:D:40:LEU:CD1	2.72	0.58
1:D:252:TRP:HB2	1:D:257:ASP:CB	2.33	0.58
1:D:252:TRP:HZ3	1:D:253:ARG:CZ	2.13	0.58
1:A:143:LEU:HD13	1:A:171:SER:HA	1.84	0.58
1:C:54:GLN:HG2	1:C:55:LYS:N	2.19	0.58
1:C:101:VAL:HG21	1:C:232:ARG:HH12	1.68	0.58
1:D:208:LEU:HD23	1:D:208:LEU:N	2.16	0.58
1:A:284:VAL:HG12	1:A:288:PHE:CB	2.32	0.58
1:A:313:GLN:NE2	1:A:450:LEU:CD1	2.51	0.58
1:C:101:VAL:CG2	1:C:232:ARG:HH12	2.16	0.58
1:A:447:ALA:O	1:A:481:GLN:HB3	2.04	0.58
1:B:214:LEU:CD2	1:B:216:PHE:CA	2.82	0.58
1:B:473:VAL:CG1	1:B:474:GLN:OE1	2.52	0.58
1:A:62:LEU:HD23	1:A:63:ARG:C	2.27	0.58
1:B:40:LEU:O	1:B:40:LEU:HD12	2.04	0.58
1:B:73:ASN:N	1:B:73:ASN:ND2	2.33	0.58
1:B:449:THR:O	1:B:450:LEU:HB2	2.03	0.58
1:C:38:LEU:HB2	1:C:41:LEU:CD1	2.33	0.58
1:D:453:PRO:HB3	1:D:476:PHE:O	2.04	0.58
1:A:164:GLU:HA	1:A:167:LEU:HB2	1.85	0.58
1:A:180:ASN:OD1	1:A:182:GLU:HB2	2.03	0.58
1:A:404:ARG:HH22	1:A:414:ASN:CG	2.11	0.58
1:A:475:PRO:CG	1:A:477:GLN:HE21	2.17	0.58
1:B:113:TYR:CD2	1:B:114:SER:N	2.68	0.58
1:D:275:LEU:C	1:D:275:LEU:HD13	2.29	0.58
1:A:49:LEU:CA	1:A:60:TYR:OH	2.52	0.57
1:B:96:PRO:CG	1:B:209:ASP:HA	2.33	0.57
1:B:320:LEU:HA	1:B:341:LEU:HD21	1.85	0.57
1:C:85:LYS:CG	1:C:88:ASP:OD2	2.52	0.57
1:C:159:VAL:O	1:C:159:VAL:CG2	2.52	0.57
1:C:159:VAL:HG13	1:C:476:PHE:HE2	1.66	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:VAL:HG11	1:C:277:GLU:HA	1.85	0.57
1:C:477:GLN:HB3	1:C:479:ARG:HD2	1.85	0.57
1:C:165:PHE:O	1:C:168:LEU:HD12	2.04	0.57
1:D:46:PRO:CG	1:D:466:TYR:CD2	2.78	0.57
1:D:404:ARG:HD2	1:D:404:ARG:C	2.26	0.57
1:D:448:PHE:HB3	1:D:479:ARG:C	2.30	0.57
1:B:110:LEU:HD11	3:B:501:3QZ:HAH	1.85	0.57
1:B:210:MET:HG3	3:B:502:3QZ:HAG	1.81	0.57
1:C:112:ASP:HB2	1:C:365:ARG:NH2	2.20	0.57
1:C:288:PHE:HB3	1:C:289:ILE:HD13	1.86	0.57
1:D:141:ASP:HA	1:D:439:VAL:CG1	2.34	0.57
1:D:181:LYS:NZ	1:D:181:LYS:HB3	2.19	0.57
1:A:180:ASN:C	1:A:182:GLU:H	2.13	0.57
1:A:315:ARG:HH11	1:A:343:LEU:HD21	1.70	0.57
1:B:193:VAL:CG1	1:B:289:ILE:HG23	2.33	0.57
1:B:459:PRO:HB2	1:B:472:LYS:HZ3	1.70	0.57
1:C:60:TYR:C	1:C:60:TYR:CD2	2.82	0.57
1:C:97:SER:HB2	1:C:209:ASP:CG	2.29	0.57
1:D:75:LYS:HA	1:D:78:ILE:HG22	1.87	0.57
1:D:160:THR:OG1	1:D:477:GLN:HB2	2.04	0.57
1:D:212:PRO:C	1:D:214:LEU:N	2.54	0.57
1:D:359:PRO:HG2	1:D:360:LEU:H	1.68	0.57
1:A:40:LEU:HB2	1:A:64:LEU:O	2.04	0.57
1:A:45:LEU:HD23	1:A:45:LEU:C	2.29	0.57
1:B:37:PHE:CD1	1:B:63:ARG:HD3	2.39	0.57
1:C:59:VAL:HG21	1:C:372:ILE:CG2	2.32	0.57
1:D:340:ARG:HA	1:D:340:ARG:NE	2.19	0.57
1:A:89:PHE:CE2	1:A:372:ILE:HG13	2.39	0.57
1:A:407:ARG:HH11	1:A:407:ARG:CG	2.11	0.57
1:C:80:GLU:HG3	1:C:84:ARG:HD3	1.86	0.57
1:C:113:TYR:O	1:C:114:SER:CB	2.47	0.57
1:C:185:LEU:HD11	1:C:239:GLN:HE22	1.69	0.57
1:C:232:ARG:HH11	3:C:501:3QZ:CAG	2.18	0.57
1:D:177:THR:C	1:D:179:GLY:H	2.12	0.57
1:D:394:GLU:O	1:D:394:GLU:HG2	2.03	0.57
1:A:103:GLN:NE2	1:A:104:ARG:CD	2.64	0.57
1:B:214:LEU:C	1:B:215:ARG:CG	2.76	0.57
1:A:59:VAL:HG13	1:A:72:LEU:HD23	1.86	0.57
1:B:252:TRP:C	1:B:254:ASP:H	2.13	0.57
1:D:121:LYS:HE2	1:D:428:LEU:CD2	2.33	0.57
1:D:377:ILE:CD1	1:D:377:ILE:N	2.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:O	1:A:229:ILE:HG22	2.05	0.57
1:A:316:LEU:HD23	1:A:343:LEU:HB3	1.87	0.57
1:B:43:PRO:O	1:B:44:ASN:HB2	2.05	0.57
1:B:102:SER:OG	1:B:105:CYS:HA	2.05	0.57
1:B:168:LEU:HD12	1:B:168:LEU:N	2.20	0.57
1:B:324:LEU:HB2	1:B:340:ARG:HB3	1.86	0.57
1:C:137:GLU:N	1:C:138:PRO:HD2	2.19	0.57
1:C:215:ARG:O	1:C:216:PHE:C	2.48	0.57
1:C:232:ARG:NH1	3:C:501:3QZ:OAE	2.38	0.57
1:D:212:PRO:O	1:D:214:LEU:N	2.38	0.57
1:D:374:GLY:O	1:D:375:TYR:CG	2.58	0.57
1:B:136:MET:SD	1:B:175:TYR:CE2	2.98	0.56
1:B:426:VAL:O	1:B:427:CYS:CB	2.53	0.56
1:C:53:THR:HG22	1:C:54:GLN:N	2.19	0.56
1:C:161:ILE:CD1	1:C:474:GLN:CB	2.83	0.56
1:C:333:VAL:O	1:C:333:VAL:CG1	2.48	0.56
1:A:37:PHE:O	1:A:38:LEU:CD2	2.27	0.56
1:A:87:VAL:HB	1:A:368:ARG:HH21	1.69	0.56
1:A:252:TRP:H	1:A:257:ASP:HB3	1.70	0.56
1:D:176:LEU:HD11	1:D:287:LEU:HD23	1.87	0.56
1:D:358:VAL:CG1	1:D:361:ALA:HA	2.34	0.56
1:A:180:ASN:ND2	1:A:185:LEU:HD13	2.19	0.56
1:B:40:LEU:HD21	3:B:502:3QZ:HALA	1.87	0.56
1:B:178:PHE:HB2	1:B:243:HIS:NE2	2.19	0.56
1:B:275:LEU:HD22	1:B:279:HIS:HD2	1.70	0.56
1:C:324:LEU:HG	1:C:340:ARG:CG	2.35	0.56
1:C:361:ALA:C	1:C:362:LEU:HD22	2.30	0.56
1:D:72:LEU:CD1	1:D:372:ILE:HD11	2.35	0.56
1:D:116:LEU:HD23	1:D:116:LEU:O	2.03	0.56
1:D:141:ASP:HA	1:D:439:VAL:HG11	1.86	0.56
1:D:196:LEU:HD23	3:D:501:3QZ:CAQ	2.34	0.56
1:D:216:PHE:HD1	1:D:216:PHE:H	1.54	0.56
1:B:92:ARG:HE	1:B:425:ARG:HE	1.53	0.56
1:B:117:TRP:CH2	1:B:425:ARG:HG2	2.39	0.56
1:B:394:GLU:HA	1:B:397:TRP:O	2.04	0.56
1:C:116:LEU:O	1:C:120:HIS:N	2.38	0.56
1:A:459:PRO:O	1:A:460:SER:HB2	2.06	0.56
1:B:108:ILE:HD13	1:B:124:THR:HG21	1.88	0.56
1:B:459:PRO:HB2	1:B:472:LYS:HZ1	1.65	0.56
1:A:30:LEU:HD11	1:A:378:PRO:HD3	1.86	0.56
1:A:287:LEU:CD1	1:A:287:LEU:H	1.95	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:VAL:HG13	1:C:469:VAL:HG13	1.87	0.56
1:D:72:LEU:CD2	1:D:372:ILE:HD12	2.36	0.56
1:D:342:PRO:HG2	1:D:343:LEU:H	1.69	0.56
1:A:168:LEU:HD21	1:A:296:ALA:CB	2.35	0.56
1:B:97:SER:HB2	1:B:209:ASP:OD1	2.05	0.56
1:B:219:ASN:ND2	4:B:616:HOH:O	1.99	0.56
1:B:252:TRP:CB	1:B:257:ASP:CG	2.78	0.56
1:D:203:TRP:CA	1:D:206:GLN:HB2	2.34	0.56
1:D:313:GLN:HE22	1:D:450:LEU:HB2	1.71	0.56
1:A:243:HIS:CD2	1:A:254:ASP:OD2	2.59	0.56
1:B:189:PHE:O	1:B:193:VAL:HG23	2.06	0.56
1:B:472:LYS:HG3	1:B:473:VAL:N	2.19	0.56
1:C:44:ASN:HB3	1:C:47:ILE:HG12	1.88	0.56
1:C:112:ASP:HB2	1:C:365:ARG:HH22	1.70	0.56
1:C:116:LEU:HD23	1:C:117:TRP:CA	2.36	0.56
1:D:120:HIS:O	1:D:124:THR:HG22	2.05	0.56
1:D:313:GLN:HE22	1:D:450:LEU:HD13	1.71	0.56
1:A:311:GLU:HG3	1:A:312:ILE:H	1.71	0.56
1:A:464:ASP:N	1:A:465:PRO:CD	2.69	0.56
1:B:85:LYS:O	1:B:87:VAL:HG23	2.06	0.56
1:D:304:ALA:HB1	1:D:459:PRO:HG2	1.88	0.56
1:D:372:ILE:O	1:D:372:ILE:HG22	2.03	0.56
1:A:34:VAL:HG22	1:A:62:LEU:HA	1.87	0.56
1:C:60:TYR:HE2	1:C:62:LEU:HB2	1.69	0.56
1:D:168:LEU:HD21	1:D:292:THR:O	2.02	0.56
1:D:347:THR:HA	1:D:405:PRO:HB3	1.87	0.56
1:D:448:PHE:CD1	1:D:479:ARG:HB3	2.40	0.56
1:B:225:LEU:O	1:B:229:ILE:HB	2.06	0.55
1:B:469:VAL:HG12	1:B:470:ASN:N	2.21	0.55
1:D:425:ARG:HD2	2:D:500:HEM:O2D	2.07	0.55
1:B:450:LEU:HD23	1:B:479:ARG:HG2	1.89	0.55
1:C:160:THR:HG21	1:C:477:GLN:HB2	1.88	0.55
1:C:232:ARG:HD2	1:C:285:VAL:CG1	2.37	0.55
1:D:263:VAL:HG13	1:D:275:LEU:O	2.06	0.55
1:B:90:ALA:HB3	1:B:113:TYR:CE1	2.40	0.55
1:B:141:ASP:HA	1:B:439:VAL:CG1	2.37	0.55
1:C:85:LYS:CB	1:C:88:ASP:OD2	2.54	0.55
1:C:341:LEU:HD13	1:C:344:LEU:CD1	2.33	0.55
1:A:189:PHE:CE2	1:A:288:PHE:CE2	2.95	0.55
1:B:80:GLU:HA	1:B:84:ARG:HG3	1.87	0.55
1:B:181:LYS:HB3	1:B:181:LYS:NZ	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ALA:HA	1:B:307:LEU:HD12	1.88	0.55
1:C:128:LEU:O	1:C:129:LEU:HD12	2.04	0.55
1:D:34:VAL:HG22	1:D:62:LEU:HA	1.87	0.55
1:D:479:ARG:HB2	1:D:479:ARG:HH11	1.69	0.55
1:A:55:LYS:HB2	1:A:56:LEU:HD22	1.87	0.55
1:B:137:GLU:CD	1:B:334:THR:HG23	2.32	0.55
1:B:311:GLU:HG3	1:B:312:ILE:H	1.72	0.55
1:C:225:LEU:C	1:C:225:LEU:HD23	2.32	0.55
1:D:75:LYS:O	1:D:79:GLU:HB2	2.05	0.55
1:D:420:PHE:CG	1:D:430:GLU:HG3	2.41	0.55
1:B:165:PHE:CD2	1:B:296:ALA:HB1	2.41	0.55
1:D:106:GLN:CB	1:D:279:HIS:CD2	2.80	0.55
1:A:147:PHE:HE2	1:A:163:LYS:HB3	1.72	0.55
1:B:96:PRO:HG2	1:B:209:ASP:HA	1.88	0.55
1:C:444:LEU:CD2	1:C:450:LEU:HD11	2.37	0.55
1:D:323:GLU:HG2	1:D:340:ARG:O	2.07	0.55
1:A:176:LEU:HA	1:A:255:MET:HB2	1.89	0.55
1:A:404:ARG:CG	1:A:404:ARG:O	2.43	0.55
1:A:425:ARG:HB3	2:A:500:HEM:O2D	2.06	0.55
1:B:30:LEU:HD23	1:B:61:ARG:CZ	2.37	0.55
1:C:85:LYS:HG2	1:C:89:PHE:HE1	1.72	0.55
1:A:71:VAL:HG12	1:A:72:LEU:H	1.71	0.55
1:A:168:LEU:HD22	1:A:292:THR:O	2.07	0.55
1:B:42:GLN:OE1	1:B:48:HIS:CG	2.60	0.55
1:B:346:ALA:HB2	1:B:408:PHE:HD1	1.71	0.55
1:C:120:HIS:O	1:C:124:THR:HG22	2.07	0.55
1:C:127:ALA:HA	1:C:258:TYR:HD1	1.72	0.55
1:C:167:LEU:O	1:C:167:LEU:CD2	2.37	0.55
1:D:106:GLN:HG2	1:D:279:HIS:CE1	2.27	0.55
1:D:165:PHE:C	1:D:168:LEU:HD11	2.31	0.55
1:D:248:VAL:HG23	1:D:249:ALA:H	1.72	0.55
1:D:252:TRP:O	1:D:254:ASP:N	2.40	0.55
1:B:443:ARG:HA	1:B:446:GLN:HB3	1.89	0.55
1:C:88:ASP:CB	1:C:89:PHE:CE1	2.90	0.55
1:C:315:ARG:HH11	1:C:343:LEU:HD21	1.72	0.55
1:A:210:MET:C	1:A:212:PRO:HD3	2.32	0.54
1:A:304:ALA:HA	1:A:307:LEU:HD12	1.88	0.54
1:B:91:GLY:C	1:B:365:ARG:H	2.07	0.54
1:C:85:LYS:HE3	1:C:371:SER:O	2.07	0.54
1:C:88:ASP:HB2	1:C:89:PHE:HD1	1.71	0.54
1:C:122:LYS:O	1:C:126:SER:OG	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:PHE:N	1:C:243:HIS:NE2	2.55	0.54
1:C:205:ILE:O	1:C:205:ILE:HD13	2.06	0.54
1:D:200:TRP:O	1:D:205:ILE:HG21	2.07	0.54
1:D:425:ARG:HB3	2:D:500:HEM:CGD	2.36	0.54
1:A:113:TYR:OH	1:A:118:LYS:HE2	2.07	0.54
1:A:301:TRP:CH2	1:A:472:LYS:HD2	2.43	0.54
1:A:404:ARG:NH2	1:A:414:ASN:CG	2.66	0.54
1:B:117:TRP:CZ2	1:B:425:ARG:NH1	2.75	0.54
1:B:459:PRO:CB	1:B:473:VAL:HB	2.38	0.54
1:C:278:GLY:O	1:C:281:HIS:N	2.41	0.54
1:D:168:LEU:HD13	1:D:169:THR:H	1.71	0.54
1:A:45:LEU:CD2	1:A:45:LEU:O	2.55	0.54
1:C:451:LEU:N	1:C:451:LEU:CD1	2.70	0.54
1:D:147:PHE:HE2	1:D:163:LYS:HD2	1.71	0.54
1:A:475:PRO:HB2	1:A:477:GLN:CD	2.26	0.54
1:B:89:PHE:CE2	1:B:372:ILE:CG1	2.91	0.54
1:C:55:LYS:CD	1:C:56:LEU:HD21	2.37	0.54
1:C:200:TRP:HD1	1:C:225:LEU:HD11	1.71	0.54
1:C:307:LEU:CG	1:C:458:LEU:HD22	2.37	0.54
1:C:386:ASN:HD22	1:C:387:LEU:N	2.06	0.54
1:C:451:LEU:N	1:C:451:LEU:HD13	2.22	0.54
1:D:168:LEU:O	1:D:172:ILE:CD1	2.33	0.54
1:D:173:ILE:HG12	1:D:288:PHE:CZ	2.43	0.54
1:D:429:GLY:HA2	2:D:500:HEM:HBC2	1.90	0.54
1:B:70:VAL:HG13	1:B:383:VAL:HA	1.90	0.54
1:B:88:ASP:CB	1:B:89:PHE:HE1	2.20	0.54
1:C:161:ILE:O	1:C:165:PHE:HD2	1.90	0.54
1:C:461:LEU:HG	1:C:461:LEU:O	2.07	0.54
1:D:38:LEU:HD13	1:D:41:LEU:CD1	2.35	0.54
1:D:311:GLU:HG3	1:D:312:ILE:H	1.72	0.54
1:D:448:PHE:CB	1:D:479:ARG:O	2.51	0.54
1:B:386:ASN:ND2	1:B:389:GLY:N	2.54	0.54
1:D:137:GLU:N	1:D:138:PRO:HD2	2.23	0.54
1:D:145:GLN:HE21	1:D:443:ARG:HD3	1.71	0.54
1:D:169:THR:O	1:D:173:ILE:HG13	2.07	0.54
1:D:203:TRP:O	1:D:206:GLN:N	2.41	0.54
1:D:211:VAL:HG12	1:D:214:LEU:CB	2.35	0.54
1:D:294:THR:O	1:D:357:VAL:HG21	2.07	0.54
1:D:420:PHE:CB	1:D:430:GLU:HG3	2.38	0.54
1:D:440:VAL:O	1:D:444:LEU:HB2	2.07	0.54
1:A:137:GLU:N	1:A:138:PRO:HD2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:O	1:A:193:VAL:HG23	2.08	0.54
1:A:333:VAL:HG11	1:A:443:ARG:HH12	1.71	0.54
1:C:283:SER:O	1:C:287:LEU:HD13	2.08	0.54
1:D:322:ARG:NE	1:D:322:ARG:HA	2.23	0.54
1:B:92:ARG:HH12	1:B:362:LEU:C	2.16	0.54
1:B:128:LEU:HD11	1:B:287:LEU:CG	2.38	0.54
1:C:189:PHE:O	1:C:193:VAL:HG23	2.08	0.54
1:C:226:LYS:HA	1:C:229:ILE:HG22	1.89	0.54
1:C:463:PRO:CG	1:C:471:LEU:HB2	2.37	0.54
1:D:301:TRP:HZ3	1:D:460:SER:HA	1.73	0.54
1:A:49:LEU:HA	1:A:60:TYR:OH	2.08	0.54
1:B:89:PHE:CE2	1:B:372:ILE:HG12	2.43	0.54
1:B:301:TRP:CH2	1:B:472:LYS:HD3	2.43	0.54
1:C:177:THR:O	1:C:179:GLY:N	2.40	0.54
1:C:440:VAL:O	1:C:444:LEU:HB2	2.08	0.54
1:D:376:ASP:C	1:D:377:ILE:HD12	2.32	0.54
1:B:83:ILE:CG1	1:B:422:CYS:HB2	2.38	0.53
1:B:92:ARG:HE	1:B:425:ARG:NE	2.06	0.53
1:B:116:LEU:HD23	1:B:116:LEU:O	2.01	0.53
1:B:189:PHE:CD2	1:B:288:PHE:CE2	2.95	0.53
1:B:313:GLN:HE21	1:B:445:LEU:CD1	2.20	0.53
1:B:360:LEU:CB	3:B:502:3QZ:HAAA	2.39	0.53
1:C:479:ARG:HH11	1:C:479:ARG:HB2	1.74	0.53
1:D:193:VAL:CG2	1:D:289:ILE:HG22	2.36	0.53
1:D:420:PHE:CG	1:D:430:GLU:CG	2.91	0.53
1:A:43:PRO:C	1:A:44:ASN:CG	2.77	0.53
1:A:113:TYR:O	1:A:114:SER:CB	2.56	0.53
1:A:176:LEU:HD21	1:A:287:LEU:HD22	1.90	0.53
1:B:214:LEU:O	1:B:215:ARG:CB	2.55	0.53
1:C:311:GLU:HG3	1:C:312:ILE:H	1.73	0.53
1:C:320:LEU:HA	1:C:341:LEU:CD2	2.38	0.53
1:D:252:TRP:HB2	1:D:257:ASP:HB2	1.90	0.53
1:D:293:GLU:OE2	1:D:293:GLU:O	2.27	0.53
1:A:214:LEU:CD2	1:A:216:PHE:CG	2.90	0.53
1:A:313:GLN:NE2	1:A:450:LEU:HB2	2.24	0.53
1:A:326:PRO:HG2	1:D:336:LYS:HD3	1.90	0.53
1:B:41:LEU:O	1:B:42:GLN:HB2	2.07	0.53
1:B:62:LEU:HD21	1:B:64:LEU:N	2.21	0.53
1:B:341:LEU:CD1	1:B:344:LEU:HD12	2.37	0.53
1:B:40:LEU:C	1:B:40:LEU:HD12	2.32	0.53
1:B:151:MET:CB	1:B:479:ARG:HH22	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:SER:HB2	1:B:252:TRP:CZ3	2.44	0.53
1:C:177:THR:HB	1:C:288:PHE:CZ	2.43	0.53
1:C:447:ALA:CB	1:C:448:PHE:CD2	2.90	0.53
1:D:104:ARG:HH21	1:D:278:GLY:CA	2.21	0.53
1:D:143:LEU:HD13	1:D:171:SER:HA	1.90	0.53
1:D:307:LEU:HD11	1:D:477:GLN:CD	2.32	0.53
1:D:451:LEU:O	1:D:478:VAL:HG23	2.09	0.53
1:A:205:ILE:O	1:A:205:ILE:HD13	2.09	0.53
1:C:106:GLN:O	1:C:107:ASP:CB	2.57	0.53
1:D:215:ARG:CD	1:D:217:PHE:CE1	2.91	0.53
1:A:170:CYS:SG	1:A:186:VAL:HG11	2.49	0.53
1:B:88:ASP:CB	1:B:89:PHE:CD1	2.91	0.53
1:B:308:HIS:C	1:B:309:HIS:HD2	2.15	0.53
1:C:359:PRO:HG2	1:C:360:LEU:H	1.73	0.53
1:D:36:GLY:O	1:D:63:ARG:CD	2.56	0.53
1:D:117:TRP:NE1	1:D:425:ARG:HH12	2.01	0.53
1:C:29:HIS:O	1:C:376:ASP:CB	2.56	0.53
1:D:45:LEU:N	1:D:46:PRO:HD2	2.24	0.53
1:D:54:GLN:NE2	1:D:54:GLN:O	2.42	0.53
1:B:176:LEU:HD12	1:B:287:LEU:CD2	2.36	0.53
1:B:315:ARG:HH11	1:B:343:LEU:HD21	1.73	0.53
1:D:148:CYS:O	1:D:152:ARG:HB2	2.09	0.53
1:D:243:HIS:NE2	1:D:254:ASP:OD1	2.42	0.53
1:A:85:LYS:HB3	1:A:88:ASP:OD2	2.09	0.53
1:A:109:SER:OG	1:A:110:LEU:N	2.41	0.53
1:A:120:HIS:O	1:A:124:THR:HG22	2.09	0.53
1:B:289:ILE:HG22	1:B:289:ILE:O	2.09	0.53
1:D:41:LEU:O	1:D:42:GLN:HB3	2.09	0.53
1:D:117:TRP:CZ2	1:D:425:ARG:CZ	2.92	0.53
1:D:205:ILE:HG23	1:D:206:GLN:N	2.23	0.53
1:D:313:GLN:NE2	1:D:450:LEU:HB2	2.23	0.53
1:A:403:PHE:CD1	1:A:405:PRO:HD3	2.44	0.53
1:B:246:SER:CB	1:B:252:TRP:CH2	2.92	0.53
1:C:75:LYS:HG3	1:C:397:TRP:CH2	2.44	0.53
1:C:89:PHE:CZ	1:C:370:SER:OG	2.62	0.53
1:C:162:GLN:NE2	1:C:162:GLN:C	2.67	0.53
1:C:232:ARG:HD2	1:C:285:VAL:HG11	1.90	0.53
1:C:243:HIS:ND1	1:C:256:THR:HG21	2.24	0.53
1:D:316:LEU:HD23	1:D:343:LEU:HB3	1.89	0.53
1:D:418:LEU:CD2	1:D:422:CYS:HG	2.20	0.53
1:A:136:MET:O	1:A:140:VAL:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG23	1:A:165:PHE:CD2	2.43	0.52
1:A:315:ARG:NH1	1:A:343:LEU:HD21	2.24	0.52
1:B:324:LEU:HG	1:B:340:ARG:CD	2.39	0.52
1:D:102:SER:O	1:D:104:ARG:N	2.42	0.52
1:D:162:GLN:HA	1:D:165:PHE:HB2	1.90	0.52
1:D:207:ILE:O	1:D:208:LEU:C	2.52	0.52
1:D:315:ARG:NH1	1:D:343:LEU:HD21	2.24	0.52
1:A:298:THR:OG1	1:A:357:VAL:HG23	2.09	0.52
1:A:335:TYR:CD2	1:A:336:LYS:HA	2.45	0.52
1:B:74:SER:OG	1:B:77:THR:HG23	2.10	0.52
1:B:89:PHE:HE2	1:B:372:ILE:CG1	2.22	0.52
1:B:467:CYS:O	1:B:468:GLY:C	2.52	0.52
1:D:279:HIS:O	1:D:280:VAL:C	2.52	0.52
1:A:335:TYR:HD2	1:A:336:LYS:CA	2.22	0.52
1:A:398:GLU:O	1:A:399:GLN:C	2.52	0.52
1:A:418:LEU:HD23	1:A:418:LEU:H	1.74	0.52
1:B:100:LEU:HD11	1:B:222:LEU:HD11	1.91	0.52
1:B:398:GLU:O	1:B:399:GLN:C	2.52	0.52
1:B:473:VAL:HG13	1:B:474:GLN:OE1	2.09	0.52
1:C:320:LEU:HA	1:C:341:LEU:HD21	1.91	0.52
1:D:432:LEU:CD2	1:D:436:GLU:HG3	2.40	0.52
1:B:314:ARG:O	1:B:318:GLU:HG3	2.09	0.52
1:D:172:ILE:HG21	1:D:288:PHE:HA	1.91	0.52
1:A:316:LEU:CD2	1:A:343:LEU:HB3	2.40	0.52
1:B:178:PHE:HD1	1:B:239:GLN:OE1	1.93	0.52
1:B:309:HIS:HE1	1:B:403:PHE:HB3	1.74	0.52
1:C:177:THR:OG1	1:C:239:GLN:HG2	2.09	0.52
1:D:226:LYS:O	1:D:229:ILE:HG22	2.08	0.52
1:D:254:ASP:OD2	1:D:256:THR:HB	2.09	0.52
1:A:243:HIS:CD2	1:A:256:THR:CB	2.90	0.52
1:A:460:SER:OG	1:A:461:LEU:N	2.38	0.52
1:C:97:SER:HB2	1:C:209:ASP:OD2	2.10	0.52
1:A:332:ARG:CZ	1:A:337:ASP:OD1	2.58	0.52
1:B:92:ARG:NH1	1:B:363:PRO:C	2.65	0.52
1:C:31:PRO:CA	1:C:375:TYR:HD1	2.23	0.52
1:C:172:ILE:HG21	1:C:287:LEU:O	2.09	0.52
1:C:316:LEU:HD23	1:C:343:LEU:HB3	1.91	0.52
1:D:189:PHE:O	1:D:193:VAL:HG23	2.09	0.52
1:D:189:PHE:CE2	1:D:235:MET:HB3	2.45	0.52
1:D:373:PHE:HD1	1:D:374:GLY:CA	2.22	0.52
1:A:332:ARG:O	1:A:333:VAL:CB	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:N	1:B:288:PHE:HB2	2.21	0.52
1:B:316:LEU:HD23	1:B:343:LEU:HB3	1.90	0.52
1:C:31:PRO:CB	1:C:375:TYR:HD1	2.23	0.52
1:C:37:PHE:O	1:C:65:GLY:O	2.28	0.52
1:C:173:ILE:HG23	1:C:288:PHE:HZ	1.75	0.52
1:C:315:ARG:NH1	1:C:343:LEU:HD21	2.25	0.52
1:C:463:PRO:HG2	1:C:471:LEU:HB2	1.91	0.52
1:D:350:GLU:OE2	1:D:407:ARG:HD3	2.10	0.52
1:A:408:PHE:N	1:A:408:PHE:CD1	2.75	0.52
1:B:62:LEU:HD21	1:B:64:LEU:HD23	1.92	0.52
1:B:247:MET:HG3	1:B:248:VAL:H	1.75	0.52
1:C:59:VAL:CG2	1:C:72:LEU:HD22	2.40	0.52
1:C:294:THR:HG23	3:C:501:3QZ:CAA	2.39	0.52
1:D:65:GLY:O	1:D:66:LEU:CD1	2.39	0.52
1:D:262:GLY:O	1:D:263:VAL:CG2	2.57	0.52
1:D:374:GLY:O	1:D:375:TYR:HB2	2.09	0.52
1:A:87:VAL:HG11	1:A:368:ARG:NH2	2.24	0.52
1:B:406:ASP:C	1:B:408:PHE:N	2.66	0.52
1:C:193:VAL:HG13	1:C:289:ILE:O	2.09	0.52
1:C:279:HIS:CE1	4:C:608:HOH:O	2.63	0.52
1:B:136:MET:O	1:B:140:VAL:HG23	2.10	0.51
1:B:205:ILE:HG13	1:B:225:LEU:CD1	2.40	0.51
1:B:285:VAL:C	1:B:288:PHE:HB3	2.34	0.51
1:C:465:PRO:CG	1:C:471:LEU:CD2	2.82	0.51
1:D:357:VAL:CG1	1:D:469:VAL:HG13	2.40	0.51
1:D:413:ALA:HA	4:D:601:HOH:O	2.10	0.51
1:A:97:SER:HB2	1:A:209:ASP:OD2	2.10	0.51
1:B:42:GLN:OE1	1:B:48:HIS:CD2	2.63	0.51
1:B:44:ASN:HB3	1:B:47:ILE:HG12	1.91	0.51
1:B:231:ASN:O	1:B:235:MET:HB2	2.10	0.51
1:B:423:GLY:C	1:B:425:ARG:N	2.61	0.51
1:C:176:LEU:HD11	1:C:287:LEU:HB3	1.91	0.51
1:C:373:PHE:CG	1:C:373:PHE:O	2.61	0.51
1:D:34:VAL:HG11	1:D:52:LEU:HD13	1.92	0.51
1:D:177:THR:HB	1:D:288:PHE:CZ	2.46	0.51
1:A:299:LEU:HD13	1:A:440:VAL:HG11	1.92	0.51
1:A:426:VAL:HG23	1:A:427:CYS:H	1.74	0.51
1:B:151:MET:HE1	1:B:163:LYS:HG3	1.93	0.51
1:D:172:ILE:CG2	1:D:288:PHE:HA	2.41	0.51
1:D:461:LEU:HD22	1:D:462:GLN:C	2.30	0.51
1:A:284:VAL:O	1:A:288:PHE:N	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:CG	1:A:336:LYS:N	2.71	0.51
1:B:92:ARG:HH12	1:B:363:PRO:C	2.18	0.51
1:B:145:GLN:HE21	1:B:443:ARG:HD3	1.75	0.51
1:D:65:GLY:C	1:D:66:LEU:HD13	2.35	0.51
1:D:116:LEU:HD23	1:D:117:TRP:HA	1.91	0.51
1:A:477:GLN:OE1	1:A:477:GLN:CA	2.56	0.51
1:B:128:LEU:CD2	1:B:432:LEU:HD12	2.40	0.51
1:C:36:GLY:HA3	1:C:39:HIS:CE1	2.46	0.51
1:C:38:LEU:HB2	1:C:41:LEU:HD11	1.92	0.51
1:C:42:GLN:HG3	1:C:43:PRO:CD	2.41	0.51
1:C:178:PHE:N	1:C:254:ASP:OD2	2.41	0.51
1:C:443:ARG:HA	1:C:446:GLN:HB3	1.92	0.51
1:C:453:PRO:HD3	1:C:476:PHE:O	2.10	0.51
1:D:66:LEU:N	1:D:66:LEU:HD13	2.24	0.51
1:D:165:PHE:CZ	1:D:293:GLU:OE2	2.60	0.51
1:D:189:PHE:CD1	1:D:288:PHE:HE2	2.28	0.51
1:D:315:ARG:HH11	1:D:343:LEU:HD21	1.74	0.51
1:A:64:LEU:HD22	3:A:502:3QZ:HABB	1.92	0.51
1:A:106:GLN:HG2	1:A:116:LEU:CD2	2.41	0.51
1:A:173:ILE:HD12	1:A:186:VAL:HG13	1.93	0.51
1:A:309:HIS:HE1	1:A:403:PHE:CB	2.22	0.51
1:B:223:TRP:HA	1:B:223:TRP:CE3	2.46	0.51
1:B:230:GLU:HG2	1:B:234:HIS:CD2	2.45	0.51
1:B:460:SER:N	1:B:472:LYS:HE2	2.24	0.51
1:C:70:VAL:HG12	1:C:383:VAL:HG13	1.91	0.51
1:C:307:LEU:HD11	1:C:477:GLN:CD	2.35	0.51
1:C:354:LEU:O	1:C:355:ARG:HD2	2.10	0.51
1:A:161:ILE:CG2	1:A:165:PHE:CE2	2.94	0.51
1:B:315:ARG:NH1	1:B:343:LEU:HD21	2.25	0.51
1:C:109:SER:O	1:C:110:LEU:HD23	2.10	0.51
1:D:354:LEU:O	1:D:355:ARG:HD2	2.11	0.51
1:A:214:LEU:HD21	1:A:216:PHE:CB	2.40	0.51
1:B:301:TRP:CE2	1:B:472:LYS:HD3	2.45	0.51
1:B:341:LEU:HD13	1:B:344:LEU:CD1	2.37	0.51
1:C:176:LEU:HD21	1:C:287:LEU:CD2	2.40	0.51
1:D:303:VAL:HG13	1:D:450:LEU:HD21	1.92	0.51
1:D:308:HIS:CE1	1:D:458:LEU:HB2	2.46	0.51
1:D:470:ASN:OD1	1:D:470:ASN:C	2.53	0.51
1:A:135:SER:O	1:A:138:PRO:HD2	2.11	0.51
1:A:301:TRP:CD2	1:A:472:LYS:HG2	2.44	0.51
1:A:470:ASN:OD1	1:A:471:LEU:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLU:N	1:B:138:PRO:HD2	2.26	0.51
1:B:252:TRP:H	1:B:257:ASP:HB3	1.76	0.51
1:B:459:PRO:HB2	1:B:473:VAL:HB	1.93	0.51
1:C:307:LEU:HD22	1:C:458:LEU:CD2	2.41	0.51
1:C:447:ALA:CB	1:C:448:PHE:HE2	2.07	0.51
1:D:202:HIS:CE1	1:D:203:TRP:NE1	2.79	0.51
1:A:121:LYS:HD2	1:A:428:LEU:HD13	1.93	0.51
1:B:117:TRP:O	1:B:120:HIS:N	2.43	0.51
1:C:426:VAL:HG23	1:C:427:CYS:H	1.74	0.51
1:D:297:SER:HA	1:D:300:SER:OG	2.11	0.51
1:A:197:MET:HE2	1:A:293:GLU:HG3	1.93	0.50
1:B:168:LEU:HD12	1:B:168:LEU:H	1.76	0.50
1:C:34:VAL:HG22	1:C:62:LEU:HA	1.92	0.50
1:C:53:THR:HG23	1:C:54:GLN:N	2.26	0.50
1:C:314:ARG:O	1:C:318:GLU:HG3	2.10	0.50
1:C:358:VAL:HG22	1:C:361:ALA:HA	1.93	0.50
1:C:383:VAL:O	1:C:385:PRO:HD3	2.11	0.50
1:D:176:LEU:HD11	1:D:287:LEU:HB3	1.93	0.50
1:D:176:LEU:HA	1:D:255:MET:H	1.76	0.50
1:D:220:PRO:O	1:D:224:ARG:HG3	2.11	0.50
1:D:407:ARG:CB	1:D:414:ASN:HB2	2.41	0.50
1:A:180:ASN:HD21	1:B:184:THR:HG23	1.76	0.50
1:A:449:THR:O	1:A:450:LEU:CB	2.58	0.50
1:B:58:PRO:HB3	1:B:74:SER:HB3	1.93	0.50
1:B:464:ASP:N	1:B:465:PRO:HD2	2.25	0.50
1:C:105:CYS:HB2	1:C:106:GLN:HE21	1.75	0.50
1:D:72:LEU:HD11	1:D:372:ILE:CD1	2.40	0.50
1:D:240:LEU:HD22	1:D:260:LEU:HD13	1.93	0.50
1:A:337:ASP:C	1:A:339:ALA:N	2.68	0.50
1:A:372:ILE:O	1:A:373:PHE:CB	2.50	0.50
1:B:223:TRP:HA	1:B:223:TRP:HE3	1.77	0.50
1:B:225:LEU:CD2	1:B:229:ILE:HD13	2.42	0.50
1:B:407:ARG:O	1:B:413:ALA:HB1	2.10	0.50
1:C:226:LYS:C	1:C:229:ILE:HG22	2.36	0.50
1:D:100:LEU:HD11	1:D:222:LEU:HD11	1.93	0.50
1:D:314:ARG:O	1:D:318:GLU:HG3	2.12	0.50
1:D:447:ALA:C	1:D:448:PHE:HD2	2.00	0.50
1:A:440:VAL:O	1:A:444:LEU:HB2	2.11	0.50
1:B:313:GLN:HB3	4:B:613:HOH:O	2.11	0.50
1:B:463:PRO:HG3	1:B:471:LEU:HB2	1.92	0.50
1:C:340:ARG:O	1:C:342:PRO:HD3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ASN:HD22	1:C:414:ASN:N	2.08	0.50
1:D:72:LEU:HD13	1:D:372:ILE:CD1	2.42	0.50
1:D:174:CYS:SG	1:D:181:LYS:HD3	2.51	0.50
1:A:30:LEU:CG	1:A:31:PRO:HD2	2.40	0.50
1:A:45:LEU:HD21	1:A:49:LEU:HG	1.92	0.50
1:A:148:CYS:O	1:A:152:ARG:HB2	2.11	0.50
1:A:286:ASP:O	1:A:290:GLY:N	2.45	0.50
1:A:407:ARG:CG	1:A:407:ARG:NH1	2.69	0.50
1:B:46:PRO:HD3	1:B:466:TYR:CE2	2.46	0.50
1:C:168:LEU:HD12	1:C:169:THR:H	1.76	0.50
1:C:177:THR:C	1:C:179:GLY:H	2.19	0.50
1:C:365:ARG:HG2	1:C:380:GLY:HA2	1.93	0.50
1:D:159:VAL:HG23	1:D:159:VAL:O	2.10	0.50
1:D:215:ARG:HG2	1:D:215:ARG:NH2	2.26	0.50
1:A:64:LEU:HD13	3:A:502:3QZ:HABB	1.94	0.50
1:A:312:ILE:HD12	1:A:405:PRO:HG2	1.93	0.50
1:A:314:ARG:O	1:A:318:GLU:HG3	2.10	0.50
1:A:462:GLN:CD	1:A:466:TYR:OH	2.55	0.50
1:A:463:PRO:CG	1:A:471:LEU:HB2	2.39	0.50
1:B:120:HIS:O	1:B:124:THR:HG22	2.11	0.50
1:B:218:PRO:HG2	1:B:218:PRO:O	2.12	0.50
1:B:226:LYS:O	1:B:229:ILE:HG22	2.11	0.50
1:C:313:GLN:NE2	1:C:450:LEU:CB	2.66	0.50
1:D:30:LEU:HD21	1:D:61:ARG:NH1	2.26	0.50
1:B:154:GLN:C	1:B:156:GLY:H	2.19	0.50
1:C:178:PHE:CE2	1:C:242:ARG:HB3	2.46	0.50
1:D:81:ALA:CB	1:D:372:ILE:HD11	2.42	0.50
1:A:102:SER:O	1:A:105:CYS:N	2.45	0.50
1:B:246:SER:CB	1:B:252:TRP:CZ3	2.95	0.50
1:C:33:LEU:HD22	1:C:34:VAL:N	2.25	0.50
1:C:85:LYS:HG3	1:C:88:ASP:CG	2.37	0.50
1:A:71:VAL:HG12	1:A:72:LEU:N	2.27	0.50
1:A:353:ARG:HH22	1:A:404:ARG:HD3	1.76	0.50
1:B:45:LEU:N	1:B:46:PRO:HD2	2.26	0.50
1:B:117:TRP:O	1:B:120:HIS:HB3	2.11	0.50
1:B:459:PRO:C	4:B:604:HOH:O	2.55	0.50
1:D:33:LEU:HD22	1:D:34:VAL:N	2.25	0.50
1:D:168:LEU:CD2	1:D:292:THR:CA	2.90	0.50
1:D:407:ARG:HB2	1:D:407:ARG:CZ	2.38	0.50
1:A:81:ALA:CB	1:A:372:ILE:HD13	2.42	0.49
1:A:425:ARG:O	1:A:426:VAL:C	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:GLU:N	1:B:411:PRO:CD	2.75	0.49
1:C:232:ARG:NH1	3:C:501:3QZ:CAQ	2.74	0.49
1:C:352:LEU:O	1:C:419:ALA:HB2	2.11	0.49
1:C:409:LEU:O	1:C:410:GLU:HB2	2.11	0.49
1:A:64:LEU:HD12	1:A:69:VAL:CB	2.42	0.49
1:A:284:VAL:O	1:A:288:PHE:HB2	2.13	0.49
1:A:373:PHE:CD1	1:A:374:GLY:HA3	2.47	0.49
1:B:62:LEU:HD11	1:B:64:LEU:HD23	1.95	0.49
1:B:394:GLU:OE1	1:B:394:GLU:O	2.29	0.49
1:C:309:HIS:ND1	1:C:403:PHE:HD2	2.10	0.49
1:D:316:LEU:CD2	1:D:343:LEU:HB3	2.42	0.49
1:D:370:SER:O	4:D:606:HOH:O	2.18	0.49
1:D:377:ILE:HD13	1:D:377:ILE:N	2.26	0.49
1:A:205:ILE:HG13	1:A:225:LEU:CD1	2.42	0.49
1:B:30:LEU:HD11	1:B:378:PRO:CD	2.40	0.49
1:B:410:GLU:CB	1:B:411:PRO:HD3	2.42	0.49
1:C:127:ALA:HA	1:C:258:TYR:CD1	2.47	0.49
1:D:257:ASP:O	1:D:261:GLN:HB2	2.13	0.49
1:A:141:ASP:HA	1:A:439:VAL:HG11	1.93	0.49
1:A:168:LEU:N	1:A:168:LEU:HD12	2.27	0.49
1:A:231:ASN:O	1:A:235:MET:HB2	2.12	0.49
1:A:337:ASP:C	1:A:339:ALA:H	2.19	0.49
1:B:218:PRO:O	1:B:218:PRO:CG	2.60	0.49
1:D:283:SER:O	1:D:287:LEU:HD13	2.12	0.49
1:D:463:PRO:CG	1:D:463:PRO:O	2.61	0.49
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.18	0.49
1:A:434:ARG:HG3	1:A:434:ARG:HH11	1.77	0.49
1:B:316:LEU:CD2	1:B:343:LEU:HB3	2.42	0.49
1:C:89:PHE:HE2	1:C:372:ILE:HD13	1.76	0.49
1:C:154:GLN:C	1:C:156:GLY:H	2.21	0.49
1:C:301:TRP:HZ3	1:C:460:SER:OG	1.96	0.49
1:D:109:SER:O	1:D:110:LEU:HD22	2.11	0.49
1:A:168:LEU:HD22	1:A:292:THR:HA	1.95	0.49
1:A:418:LEU:HD22	4:A:607:HOH:O	2.12	0.49
1:C:178:PHE:N	1:C:254:ASP:OD1	2.46	0.49
1:D:196:LEU:CD1	1:D:229:ILE:HA	2.40	0.49
1:D:463:PRO:O	1:D:463:PRO:HG2	2.13	0.49
1:A:110:LEU:HD11	3:A:501:3QZ:CAH	2.41	0.49
1:A:225:LEU:HD23	1:A:225:LEU:C	2.38	0.49
1:B:128:LEU:HG	1:B:287:LEU:CD2	2.35	0.49
1:B:346:ALA:HB1	1:B:405:PRO:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:TYR:CG	1:C:336:LYS:N	2.79	0.49
1:D:29:HIS:HA	1:D:375:TYR:CD1	2.42	0.49
1:A:60:TYR:CE1	1:A:73:ASN:ND2	2.81	0.49
1:A:78:ILE:CD1	1:A:387:LEU:HD23	2.42	0.49
1:A:263:VAL:HG21	1:A:280:VAL:HG22	1.95	0.49
1:A:313:GLN:HE22	1:A:450:LEU:CG	2.25	0.49
1:B:30:LEU:HD12	1:B:376:ASP:O	2.13	0.49
1:B:55:LYS:HG3	1:B:56:LEU:HD22	1.94	0.49
1:B:211:VAL:HG12	1:B:214:LEU:CB	2.41	0.49
1:B:473:VAL:O	1:B:475:PRO:HD2	2.12	0.49
1:D:459:PRO:O	1:D:460:SER:HB3	2.12	0.49
1:A:242:ARG:NH2	1:B:187:HIS:ND1	2.60	0.49
1:B:193:VAL:HG11	1:B:292:THR:OG1	2.12	0.49
1:B:440:VAL:O	1:B:444:LEU:HB2	2.13	0.49
1:C:173:ILE:HG23	1:C:288:PHE:CZ	2.48	0.49
1:C:197:MET:HE2	1:C:293:GLU:HG3	1.93	0.49
1:C:205:ILE:HG13	1:C:225:LEU:CD1	2.42	0.49
1:D:42:GLN:HG3	1:D:43:PRO:HD2	1.94	0.49
1:D:173:ILE:HG23	1:D:288:PHE:HZ	1.77	0.49
1:D:409:LEU:HD13	1:D:410:GLU:HB2	1.94	0.49
1:A:108:ILE:HD12	1:A:428:LEU:HD22	1.94	0.49
1:A:285:VAL:HG12	1:A:286:ASP:H	1.78	0.49
1:A:373:PHE:CD1	1:A:374:GLY:CA	2.96	0.49
1:A:373:PHE:CE1	1:A:374:GLY:HA3	2.48	0.49
1:B:148:CYS:O	1:B:448:PHE:HZ	1.96	0.49
1:C:177:THR:O	1:C:177:THR:HG22	2.12	0.49
1:C:214:LEU:CD2	1:C:216:PHE:CD2	2.96	0.49
1:C:280:VAL:O	1:C:284:VAL:HG23	2.13	0.49
1:C:470:ASN:OD1	1:C:471:LEU:O	2.31	0.49
1:D:233:ASP:HB3	1:D:237:GLU:OE2	2.13	0.49
1:D:459:PRO:CG	1:D:472:LYS:HE3	2.43	0.49
1:A:168:LEU:HD12	1:A:168:LEU:H	1.79	0.48
1:A:304:ALA:HB2	4:A:605:HOH:O	2.12	0.48
1:B:406:ASP:O	1:B:408:PHE:N	2.46	0.48
1:C:59:VAL:HG22	1:C:72:LEU:CD2	2.43	0.48
1:C:75:LYS:HG3	1:C:397:TRP:HH2	1.78	0.48
1:C:208:LEU:HD23	1:C:214:LEU:HD11	1.94	0.48
1:C:211:VAL:O	1:C:214:LEU:HD22	2.12	0.48
1:C:225:LEU:HD23	1:C:225:LEU:O	2.13	0.48
1:D:117:TRP:CH2	1:D:425:ARG:HD3	2.48	0.48
1:D:316:LEU:HG	1:D:343:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLN:HE21	1:A:443:ARG:HD3	1.78	0.48
1:B:211:VAL:CG1	1:B:214:LEU:HB2	2.42	0.48
1:B:236:VAL:HG22	1:B:288:PHE:CZ	2.48	0.48
1:C:50:LEU:O	1:C:53:THR:HG22	2.13	0.48
1:C:160:THR:O	1:C:161:ILE:C	2.54	0.48
1:C:185:LEU:HD11	1:C:239:GLN:NE2	2.28	0.48
1:C:218:PRO:HD3	4:C:622:HOH:O	2.13	0.48
1:C:414:ASN:HB3	1:C:415:PRO:CD	2.43	0.48
1:D:101:VAL:HA	1:D:229:ILE:HD11	1.94	0.48
1:D:223:TRP:CE3	1:D:223:TRP:HA	2.48	0.48
1:D:462:GLN:OE1	1:D:466:TYR:OH	2.31	0.48
1:A:49:LEU:C	1:A:60:TYR:HH	2.18	0.48
1:C:66:LEU:O	1:C:67:GLN:OE1	2.31	0.48
1:C:220:PRO:O	1:C:224:ARG:HG3	2.13	0.48
1:C:299:LEU:O	1:C:303:VAL:HG23	2.14	0.48
1:C:407:ARG:CG	1:C:407:ARG:NH1	2.36	0.48
1:C:414:ASN:HB3	1:C:415:PRO:HD2	1.96	0.48
1:D:38:LEU:CD1	1:D:41:LEU:CD1	2.91	0.48
1:A:106:GLN:CB	1:A:279:HIS:CE1	2.96	0.48
1:A:284:VAL:CG1	1:A:288:PHE:HB2	2.41	0.48
1:A:332:ARG:HD3	1:A:337:ASP:OD1	2.13	0.48
1:A:354:LEU:C	1:A:355:ARG:HD3	2.39	0.48
1:A:462:GLN:CG	1:A:466:TYR:OH	2.61	0.48
1:A:472:LYS:CA	1:A:472:LYS:NZ	2.74	0.48
1:B:85:LYS:CG	1:B:88:ASP:OD2	2.62	0.48
1:B:129:LEU:O	1:B:130:LEU:HD23	2.13	0.48
1:D:39:HIS:O	1:D:41:LEU:O	2.31	0.48
1:A:34:VAL:HG11	1:A:52:LEU:HD12	1.95	0.48
1:A:138:PRO:O	1:A:142:GLN:HG3	2.14	0.48
1:A:423:GLY:C	1:A:425:ARG:H	2.21	0.48
1:B:409:LEU:H	1:B:413:ALA:HB2	1.79	0.48
1:C:33:LEU:HD13	1:C:33:LEU:C	2.38	0.48
1:C:85:LYS:O	1:C:86:TRP:CB	2.61	0.48
1:D:121:LYS:HD2	1:D:428:LEU:CD2	2.39	0.48
1:D:173:ILE:CD1	1:D:186:VAL:HA	2.43	0.48
1:D:420:PHE:HB3	1:D:430:GLU:HG3	1.94	0.48
1:D:471:LEU:CD1	1:D:472:LYS:N	2.68	0.48
1:A:104:ARG:H	1:A:104:ARG:HG2	1.43	0.48
1:A:108:ILE:HG22	2:A:500:HEM:O1D	2.14	0.48
1:B:42:GLN:OE1	1:B:48:HIS:CE1	2.66	0.48
1:B:61:ARG:HH12	1:B:68:GLU:CD	2.19	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:HD3	1:B:391:HIS:O	2.14	0.48
1:D:172:ILE:HD13	1:D:172:ILE:H	1.77	0.48
1:D:219:ASN:HD21	1:D:222:LEU:HB2	1.78	0.48
1:D:313:GLN:HE22	1:D:450:LEU:CD1	2.26	0.48
1:D:470:ASN:OD1	1:D:471:LEU:O	2.31	0.48
1:A:96:PRO:HG2	1:A:209:ASP:HA	1.96	0.48
1:A:216:PHE:O	1:A:217:PHE:C	2.56	0.48
1:A:334:THR:O	1:A:335:TYR:C	2.56	0.48
1:A:334:THR:O	1:A:337:ASP:OD2	2.31	0.48
1:B:168:LEU:CD2	1:B:292:THR:O	2.62	0.48
1:B:225:LEU:HD21	1:B:229:ILE:HD13	1.95	0.48
1:C:378:PRO:HG3	1:C:381:MET:HE2	1.95	0.48
1:C:386:ASN:ND2	1:C:386:ASN:C	2.69	0.48
1:D:168:LEU:N	1:D:168:LEU:HD13	2.23	0.48
1:D:214:LEU:O	1:D:215:ARG:CB	2.61	0.48
1:D:365:ARG:HG2	1:D:366:THR:N	2.29	0.48
1:D:429:GLY:O	1:D:433:ALA:N	2.28	0.48
1:A:112:ASP:CG	1:A:113:TYR:H	2.21	0.48
1:A:144:THR:HA	1:A:167:LEU:HD21	1.96	0.48
1:A:149:GLU:O	1:A:153:VAL:HG13	2.14	0.48
1:A:150:ARG:O	1:A:153:VAL:HG22	2.14	0.48
1:A:212:PRO:C	1:A:214:LEU:N	2.68	0.48
1:A:298:THR:OG1	1:A:357:VAL:HG21	2.14	0.48
1:B:29:HIS:O	1:B:375:TYR:HB3	2.14	0.48
1:B:243:HIS:CD2	1:B:256:THR:HB	2.48	0.48
1:D:87:VAL:CG1	1:D:88:ASP:N	2.72	0.48
1:A:284:VAL:O	1:A:288:PHE:CB	2.62	0.48
1:B:85:LYS:NZ	1:B:371:SER:O	2.44	0.48
1:B:151:MET:HB2	1:B:479:ARG:HH22	1.77	0.48
1:B:394:GLU:O	1:B:397:TRP:O	2.32	0.48
1:C:316:LEU:CD2	1:C:343:LEU:HB3	2.44	0.48
1:C:470:ASN:OD1	1:C:470:ASN:O	2.32	0.48
1:D:81:ALA:HB2	1:D:372:ILE:CD1	2.43	0.48
1:A:423:GLY:O	1:A:426:VAL:HG22	2.14	0.48
1:A:437:LEU:HD11	2:A:500:HEM:HBB1	1.96	0.48
1:A:461:LEU:CD2	1:A:462:GLN:O	2.62	0.48
1:A:477:GLN:CD	1:A:477:GLN:H	2.22	0.48
1:B:62:LEU:CD1	1:B:64:LEU:CD2	2.92	0.48
1:B:178:PHE:HB2	1:B:243:HIS:HE1	1.71	0.48
1:B:286:ASP:O	1:B:290:GLY:CA	2.62	0.48
1:B:298:THR:OG1	1:B:357:VAL:CG2	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD13	1:B:418:LEU:O	2.14	0.48
1:D:168:LEU:HD23	1:D:292:THR:CA	2.44	0.48
1:D:200:TRP:HD1	1:D:225:LEU:HD11	1.79	0.48
1:D:449:THR:O	1:D:450:LEU:CB	2.48	0.48
1:A:465:PRO:O	1:A:471:LEU:HD11	2.13	0.47
1:B:53:THR:HB	1:B:57:GLY:O	2.14	0.47
1:B:62:LEU:HD13	1:B:64:LEU:HD21	1.96	0.47
1:C:177:THR:CG2	1:C:177:THR:O	2.61	0.47
1:C:189:PHE:CD1	1:C:288:PHE:HE2	2.31	0.47
1:C:307:LEU:HD13	1:C:458:LEU:CD2	2.35	0.47
1:D:447:ALA:CB	1:D:448:PHE:CE2	2.94	0.47
1:A:50:LEU:O	1:A:53:THR:OG1	2.31	0.47
1:A:252:TRP:HB2	1:A:257:ASP:OD2	2.08	0.47
1:A:334:THR:O	1:A:337:ASP:N	2.47	0.47
1:A:461:LEU:HD23	1:A:462:GLN:N	2.23	0.47
1:A:475:PRO:O	1:A:476:PHE:CD2	2.67	0.47
1:B:313:GLN:NE2	1:B:450:LEU:HB2	2.29	0.47
1:B:445:LEU:HD11	1:B:450:LEU:HD12	1.96	0.47
1:B:464:ASP:H	1:B:465:PRO:CD	2.27	0.47
1:C:31:PRO:CA	1:C:375:TYR:CD1	2.95	0.47
1:C:85:LYS:HG2	1:C:89:PHE:CE1	2.48	0.47
1:D:151:MET:HA	1:D:154:GLN:HG2	1.96	0.47
1:D:252:TRP:C	1:D:254:ASP:N	2.68	0.47
1:A:78:ILE:HD13	1:A:387:LEU:HD23	1.96	0.47
1:A:103:GLN:C	4:A:610:HOH:O	2.56	0.47
1:A:196:LEU:HD21	3:A:501:3QZ:OAE	2.13	0.47
1:A:350:GLU:HG3	1:A:404:ARG:C	2.38	0.47
1:B:39:HIS:ND1	1:B:62:LEU:HG	2.30	0.47
1:B:313:GLN:HE22	1:B:450:LEU:HD12	1.79	0.47
1:C:128:LEU:HD22	1:C:128:LEU:HA	1.68	0.47
1:D:429:GLY:CA	2:D:500:HEM:HBC2	2.43	0.47
1:A:109:SER:HA	1:A:425:ARG:HH21	1.79	0.47
1:A:113:TYR:CD2	1:A:114:SER:N	2.75	0.47
1:C:161:ILE:H	1:C:161:ILE:HG13	1.55	0.47
1:D:176:LEU:O	1:D:176:LEU:HD23	2.13	0.47
1:B:301:TRP:CZ3	1:B:472:LYS:CD	2.96	0.47
1:C:138:PRO:O	1:C:142:GLN:HG3	2.15	0.47
1:D:352:LEU:O	1:D:419:ALA:HB2	2.14	0.47
1:B:342:PRO:HB2	1:B:408:PHE:CZ	2.50	0.47
1:C:173:ILE:HD13	1:C:186:VAL:HA	1.96	0.47
1:D:121:LYS:CD	1:D:428:LEU:HD21	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASN:HB2	1:D:220:PRO:HD2	1.96	0.47
1:A:42:GLN:OE1	1:A:48:HIS:CD2	2.67	0.47
1:A:62:LEU:CD2	1:A:64:LEU:N	2.77	0.47
1:A:449:THR:H	1:A:480:LEU:C	2.21	0.47
1:B:62:LEU:CD2	1:B:64:LEU:HD23	2.44	0.47
1:C:103:GLN:C	1:C:105:CYS:N	2.70	0.47
1:C:205:ILE:HG13	1:C:225:LEU:HD13	1.97	0.47
1:C:412:GLY:C	4:C:604:HOH:O	2.32	0.47
1:C:474:GLN:OE1	1:C:474:GLN:O	2.32	0.47
1:D:170:CYS:SG	1:D:186:VAL:HG11	2.55	0.47
1:D:177:THR:O	1:D:177:THR:HG22	2.14	0.47
1:A:263:VAL:HG21	1:A:280:VAL:CG2	2.45	0.47
1:A:342:PRO:HG2	1:A:343:LEU:H	1.80	0.47
1:A:399:GLN:N	1:A:400:PRO:CD	2.78	0.47
1:B:71:VAL:HG12	1:B:73:ASN:ND2	2.17	0.47
1:B:108:ILE:HG13	1:B:286:ASP:OD1	2.14	0.47
1:B:164:GLU:C	1:B:166:SER:H	2.21	0.47
1:B:169:THR:HG23	1:B:292:THR:HG21	1.97	0.47
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.51	0.47
1:D:252:TRP:CH2	1:D:253:ARG:CZ	2.96	0.47
1:D:387:LEU:CD2	1:D:418:LEU:HB2	2.44	0.47
1:D:459:PRO:CD	1:D:475:PRO:HB3	2.45	0.47
1:A:42:GLN:HA	1:A:43:PRO:HD2	1.72	0.47
1:A:64:LEU:HD12	1:A:69:VAL:CG2	2.45	0.47
1:A:178:PHE:CB	1:A:243:HIS:CE1	2.88	0.47
1:A:263:VAL:HG13	1:A:275:LEU:O	2.14	0.47
1:C:350:GLU:HG3	1:C:405:PRO:HA	1.96	0.47
1:D:247:MET:HG3	1:D:257:ASP:OD1	2.14	0.47
1:A:319:GLU:OE1	1:A:343:LEU:HB2	2.15	0.47
1:A:373:PHE:O	1:A:375:TYR:N	2.40	0.47
1:B:168:LEU:HD21	1:B:296:ALA:CB	2.35	0.47
1:B:197:MET:HE2	1:B:293:GLU:CG	2.45	0.47
1:B:350:GLU:CD	1:B:404:ARG:O	2.58	0.47
1:B:463:PRO:HA	4:B:625:HOH:O	2.15	0.47
1:C:72:LEU:HD12	1:C:78:ILE:HA	1.96	0.47
1:C:81:ALA:HB2	1:C:372:ILE:CG1	2.41	0.47
1:C:316:LEU:HG	1:C:343:LEU:HD12	1.97	0.47
1:C:474:GLN:CD	1:C:474:GLN:C	2.82	0.47
1:D:137:GLU:CD	1:D:334:THR:HG23	2.40	0.47
1:D:205:ILE:HD13	1:D:205:ILE:C	2.33	0.47
1:A:472:LYS:NZ	1:A:473:VAL:C	2.72	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:HD2	1:B:114:SER:N	2.02	0.46
1:B:138:PRO:O	1:B:142:GLN:HG3	2.15	0.46
1:B:168:LEU:HD21	1:B:292:THR:O	2.15	0.46
1:B:252:TRP:C	1:B:254:ASP:N	2.70	0.46
1:B:288:PHE:CG	1:B:289:ILE:CD1	2.90	0.46
1:B:473:VAL:CG1	1:B:474:GLN:H	2.27	0.46
1:C:87:VAL:CG1	1:C:368:ARG:HH12	2.18	0.46
1:C:171:SER:O	1:C:175:TYR:CZ	2.68	0.46
1:C:425:ARG:HB3	2:C:500:HEM:O2D	2.14	0.46
1:D:108:ILE:C	1:D:110:LEU:H	2.22	0.46
1:D:203:TRP:O	1:D:207:ILE:N	2.36	0.46
1:D:232:ARG:HD2	1:D:285:VAL:CG1	2.44	0.46
1:A:62:LEU:O	1:A:69:VAL:N	2.43	0.46
1:A:259:MET:O	1:A:263:VAL:HG23	2.16	0.46
1:A:444:LEU:HD21	1:A:479:ARG:NH1	2.30	0.46
1:C:316:LEU:O	1:C:320:LEU:HB2	2.16	0.46
1:C:350:GLU:CG	1:C:405:PRO:HA	2.46	0.46
1:D:180:ASN:C	1:D:182:GLU:H	2.21	0.46
1:D:215:ARG:HH21	1:D:215:ARG:CG	2.26	0.46
1:D:322:ARG:HA	1:D:322:ARG:HE	1.79	0.46
1:A:154:GLN:C	1:A:156:GLY:H	2.23	0.46
1:A:358:VAL:HG12	1:A:361:ALA:CA	2.41	0.46
1:B:174:CYS:HB2	1:B:181:LYS:HB2	1.97	0.46
1:B:177:THR:O	1:B:178:PHE:HB3	2.16	0.46
1:B:308:HIS:C	1:B:309:HIS:CD2	2.94	0.46
1:B:379:GLU:C	1:B:381:MET:H	2.24	0.46
1:D:52:LEU:O	1:D:55:LYS:HG3	2.16	0.46
1:D:58:PRO:HG3	1:D:76:ARG:NH2	2.20	0.46
1:D:148:CYS:O	1:D:152:ARG:N	2.43	0.46
1:D:207:ILE:O	1:D:210:MET:N	2.49	0.46
1:D:347:THR:HG23	1:D:403:PHE:HZ	1.81	0.46
1:A:45:LEU:N	1:A:46:PRO:CD	2.77	0.46
1:A:174:CYS:SG	1:A:181:LYS:HB2	2.56	0.46
1:B:83:ILE:HD11	1:B:422:CYS:HB2	1.96	0.46
1:C:62:LEU:HD22	1:C:64:LEU:HG	1.98	0.46
1:C:80:GLU:CD	1:C:372:ILE:O	2.59	0.46
1:D:94:GLN:HE22	1:D:99:LYS:NZ	2.13	0.46
1:D:101:VAL:HB	1:D:232:ARG:HH12	1.80	0.46
1:D:178:PHE:HA	1:D:243:HIS:CE1	2.51	0.46
1:A:333:VAL:CG1	1:A:443:ARG:HH12	2.29	0.46
1:B:128:LEU:HD23	1:B:432:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LYS:HB3	1:D:88:ASP:HB2	1.96	0.46
1:D:313:GLN:HE21	1:D:445:LEU:CD1	2.25	0.46
1:D:397:TRP:O	1:D:400:PRO:HD3	2.15	0.46
1:A:141:ASP:HA	1:A:439:VAL:CG1	2.45	0.46
1:B:75:LYS:O	1:B:79:GLU:HB2	2.16	0.46
1:B:180:ASN:HB3	1:B:185:LEU:HD22	1.97	0.46
1:B:323:GLU:HG2	1:B:340:ARG:O	2.16	0.46
1:C:298:THR:HG21	1:C:437:LEU:HD11	1.97	0.46
1:D:217:PHE:CD1	1:D:217:PHE:N	2.84	0.46
1:D:276:LEU:HG	1:D:277:GLU:H	1.80	0.46
1:A:50:LEU:CA	1:A:53:THR:HG23	2.46	0.46
1:A:316:LEU:HG	1:A:343:LEU:HD12	1.98	0.46
1:B:82:MET:SD	1:B:364:HIS:CE1	3.09	0.46
1:B:92:ARG:NH1	1:B:362:LEU:O	2.44	0.46
1:B:285:VAL:O	1:B:288:PHE:HB3	2.16	0.46
1:C:43:PRO:O	1:C:44:ASN:HB2	2.15	0.46
1:C:178:PHE:CA	1:C:254:ASP:OD1	2.63	0.46
1:D:71:VAL:C	1:D:72:LEU:HD23	2.40	0.46
1:D:165:PHE:CA	1:D:168:LEU:HD11	2.46	0.46
1:D:313:GLN:NE2	1:D:449:THR:O	2.49	0.46
1:D:428:LEU:HG	2:D:500:HEM:CMD	2.46	0.46
1:A:136:MET:HE2	1:A:136:MET:HB3	1.84	0.46
1:A:148:CYS:O	1:A:448:PHE:HZ	1.99	0.46
1:A:169:THR:HG21	1:A:190:HIS:CB	2.38	0.46
1:A:232:ARG:HD2	1:A:285:VAL:HG21	1.98	0.46
1:A:248:VAL:HG23	1:A:250:GLY:H	1.81	0.46
1:B:69:VAL:HG22	1:B:382:VAL:HG21	1.96	0.46
1:C:55:LYS:HG2	1:C:56:LEU:N	2.31	0.46
1:C:168:LEU:HD22	1:C:292:THR:HA	1.98	0.46
1:C:324:LEU:HD12	1:C:332:ARG:CB	2.45	0.46
1:D:471:LEU:HD13	1:D:472:LYS:H	1.77	0.46
1:D:111:GLY:C	1:D:425:ARG:HH22	2.19	0.46
1:D:193:VAL:HG13	1:D:289:ILE:O	2.16	0.46
1:D:214:LEU:CG	1:D:216:PHE:H	2.28	0.46
1:D:333:VAL:N	4:D:602:HOH:O	2.49	0.46
1:D:353:ARG:HD3	1:D:391:HIS:O	2.16	0.46
1:D:407:ARG:HB2	1:D:414:ASN:HB2	1.97	0.46
1:A:189:PHE:CD2	1:A:289:ILE:HD13	2.51	0.46
1:A:227:GLN:OE1	1:B:224:ARG:HG2	2.16	0.46
1:A:451:LEU:HG	1:A:452:PRO:CD	2.17	0.46
1:B:301:TRP:CH2	1:B:472:LYS:CD	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PRO:O	1:B:387:LEU:HB2	2.16	0.46
1:C:226:LYS:O	1:C:230:GLU:HG3	2.16	0.46
1:C:246:SER:HB3	1:C:252:TRP:CH2	2.50	0.46
1:D:177:THR:C	1:D:179:GLY:N	2.74	0.46
1:D:202:HIS:HE1	1:D:203:TRP:NE1	2.14	0.46
1:A:282:MET:O	1:A:285:VAL:HG12	2.16	0.45
1:B:112:ASP:CG	1:B:365:ARG:CZ	2.88	0.45
1:B:193:VAL:CG2	1:B:289:ILE:CG2	2.79	0.45
1:C:154:GLN:O	1:C:155:ALA:HB3	2.16	0.45
1:C:474:GLN:O	1:C:474:GLN:NE2	2.50	0.45
1:D:219:ASN:ND2	1:D:222:LEU:H	2.13	0.45
1:D:309:HIS:HE1	1:D:403:PHE:HB3	1.81	0.45
1:A:50:LEU:HA	1:A:53:THR:CG2	2.46	0.45
1:A:151:MET:O	1:A:154:GLN:HB2	2.15	0.45
1:A:301:TRP:CZ2	1:A:472:LYS:HG2	2.50	0.45
1:A:335:TYR:O	1:A:338:ARG:CB	2.64	0.45
1:B:107:ASP:HB2	1:B:282:MET:HB3	1.98	0.45
1:B:176:LEU:CD1	1:B:287:LEU:CD2	2.92	0.45
1:B:214:LEU:CG	1:B:216:PHE:H	2.27	0.45
1:B:286:ASP:O	1:B:290:GLY:HA3	2.16	0.45
1:B:426:VAL:HG23	1:B:427:CYS:H	1.80	0.45
1:B:470:ASN:OD1	1:B:470:ASN:O	2.34	0.45
1:C:176:LEU:HD21	1:C:287:LEU:HD22	1.98	0.45
1:C:181:LYS:NZ	1:C:181:LYS:HB3	2.32	0.45
1:D:41:LEU:O	1:D:42:GLN:CB	2.64	0.45
1:A:76:ARG:HH11	1:A:76:ARG:HB2	1.80	0.45
1:A:128:LEU:CD2	1:A:287:LEU:HD23	2.45	0.45
1:A:202:HIS:O	1:A:203:TRP:C	2.59	0.45
1:B:42:GLN:HG3	1:B:43:PRO:HD2	1.97	0.45
1:B:307:LEU:HD11	1:B:477:GLN:CD	2.40	0.45
1:B:309:HIS:ND1	1:B:403:PHE:HD1	2.14	0.45
1:B:313:GLN:NE2	1:B:445:LEU:HD12	2.31	0.45
1:B:354:LEU:C	1:B:355:ARG:HD3	2.41	0.45
1:C:128:LEU:HB3	1:C:129:LEU:CD1	2.46	0.45
1:C:252:TRP:HB2	1:C:257:ASP:CG	2.41	0.45
1:C:378:PRO:CG	1:C:381:MET:HE2	2.47	0.45
1:C:410:GLU:C	1:C:412:GLY:N	2.73	0.45
1:D:205:ILE:O	1:D:205:ILE:HD12	2.14	0.45
1:D:432:LEU:C	1:D:432:LEU:HD22	2.41	0.45
1:A:44:ASN:C	1:A:46:PRO:HD2	2.42	0.45
1:A:243:HIS:CD2	1:A:256:THR:CG2	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD11	1:B:422:CYS:CB	2.46	0.45
1:B:109:SER:OG	1:B:110:LEU:HG	2.16	0.45
1:B:172:ILE:HG21	1:B:287:LEU:O	2.16	0.45
1:C:144:THR:O	1:C:147:PHE:HB3	2.16	0.45
1:C:257:ASP:O	1:C:261:GLN:HB2	2.17	0.45
1:D:178:PHE:CA	1:D:243:HIS:CE1	3.00	0.45
1:D:316:LEU:O	1:D:320:LEU:HB2	2.16	0.45
1:A:177:THR:OG1	1:A:288:PHE:CD1	2.58	0.45
1:B:88:ASP:HB2	1:B:89:PHE:CE1	2.50	0.45
1:B:316:LEU:HG	1:B:343:LEU:HD12	1.99	0.45
1:B:319:GLU:OE1	1:B:343:LEU:HB2	2.16	0.45
1:B:423:GLY:O	1:B:424:ALA:C	2.59	0.45
1:C:89:PHE:N	1:C:89:PHE:HD1	2.11	0.45
1:C:178:PHE:C	1:C:180:ASN:H	2.25	0.45
1:C:432:LEU:O	1:C:436:GLU:HG3	2.17	0.45
1:D:173:ILE:HD13	1:D:186:VAL:HA	1.98	0.45
1:D:324:LEU:HG	1:D:340:ARG:CG	2.43	0.45
1:B:360:LEU:HB3	3:B:502:3QZ:HAAA	1.99	0.45
1:B:434:ARG:HH11	1:B:434:ARG:HG3	1.81	0.45
1:C:127:ALA:HB1	1:C:255:MET:HG2	1.99	0.45
1:C:356:PRO:HG2	1:C:356:PRO:O	2.16	0.45
1:D:116:LEU:O	1:D:120:HIS:N	2.49	0.45
1:A:344:LEU:C	1:A:346:ALA:N	2.74	0.45
1:A:423:GLY:O	1:A:426:VAL:CG1	2.58	0.45
1:B:78:ILE:HD13	1:B:387:LEU:HD23	1.98	0.45
1:B:95:ILE:HB	1:B:96:PRO:HD2	1.98	0.45
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.69	0.45
1:B:154:GLN:OE1	1:B:158:PRO:HB3	2.16	0.45
1:B:208:LEU:CD2	1:B:214:LEU:HD22	2.47	0.45
1:C:173:ILE:HD12	1:C:186:VAL:HG13	1.98	0.45
1:C:246:SER:CB	1:C:252:TRP:CH2	3.00	0.45
1:D:152:ARG:HG2	1:D:152:ARG:HH11	1.82	0.45
1:D:391:HIS:NE2	1:D:417:ALA:HB1	2.32	0.45
1:D:471:LEU:CD1	1:D:472:LYS:C	2.84	0.45
1:D:471:LEU:CD1	1:D:472:LYS:O	2.63	0.45
1:A:214:LEU:HD11	1:A:216:PHE:HA	1.99	0.45
1:D:46:PRO:HD3	1:D:466:TYR:HD2	1.77	0.45
1:A:89:PHE:CZ	1:A:372:ILE:HD11	2.45	0.45
1:A:103:GLN:HE21	1:A:104:ARG:H	1.65	0.45
1:B:144:THR:O	1:B:147:PHE:HB3	2.16	0.45
1:B:152:ARG:HG2	1:B:152:ARG:HH11	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:SER:H	1:B:472:LYS:NZ	2.15	0.45
1:C:284:VAL:O	1:C:288:PHE:HB2	2.17	0.45
1:D:29:HIS:O	1:D:30:LEU:HB2	2.17	0.45
1:D:278:GLY:O	1:D:281:HIS:HB3	2.17	0.45
1:A:324:LEU:HG	1:A:340:ARG:CG	2.47	0.45
1:B:40:LEU:HD23	3:B:502:3QZ:HAJ	1.99	0.45
1:B:372:ILE:O	1:B:372:ILE:HG22	2.17	0.45
1:C:359:PRO:HG3	1:C:466:TYR:CE2	2.52	0.45
1:C:464:ASP:O	1:C:466:TYR:N	2.50	0.45
1:D:44:ASN:CB	1:D:47:ILE:HG12	2.44	0.45
1:D:217:PHE:HB3	1:D:218:PRO:HD2	1.99	0.45
1:A:42:GLN:OE1	1:A:48:HIS:CE1	2.70	0.44
1:C:55:LYS:C	1:C:56:LEU:HD22	2.42	0.44
1:C:145:GLN:HE21	1:C:443:ARG:HD3	1.82	0.44
1:C:214:LEU:C	1:C:216:PHE:H	2.25	0.44
1:A:45:LEU:HD22	1:A:49:LEU:HG	1.98	0.44
1:A:70:VAL:O	1:A:70:VAL:HG13	2.17	0.44
1:A:316:LEU:O	1:A:320:LEU:HB2	2.17	0.44
1:B:301:TRP:CZ2	1:B:472:LYS:HD3	2.52	0.44
1:C:177:THR:C	1:C:179:GLY:N	2.74	0.44
1:C:247:MET:C	1:C:248:VAL:HG13	2.41	0.44
1:C:323:GLU:HG2	1:C:340:ARG:O	2.17	0.44
1:D:94:GLN:OE1	1:D:99:LYS:NZ	2.50	0.44
1:A:180:ASN:HB3	1:A:185:LEU:HD22	1.98	0.44
1:A:214:LEU:HD22	1:A:216:PHE:CD2	2.46	0.44
1:A:447:ALA:HB3	1:A:448:PHE:CE2	2.53	0.44
1:B:72:LEU:HD22	1:B:372:ILE:HG21	1.98	0.44
1:B:107:ASP:HB2	1:B:282:MET:CB	2.47	0.44
1:B:152:ARG:HH21	1:C:133:ARG:NH2	2.15	0.44
1:B:168:LEU:HD12	1:B:169:THR:H	1.82	0.44
1:B:432:LEU:O	1:B:436:GLU:HG3	2.16	0.44
1:C:62:LEU:HD22	1:C:64:LEU:N	2.26	0.44
1:D:301:TRP:CE2	1:D:355:ARG:HG2	2.53	0.44
1:D:426:VAL:O	1:D:427:CYS:HB2	2.17	0.44
1:A:214:LEU:CD2	1:A:216:PHE:HD2	2.22	0.44
1:A:332:ARG:NH1	1:A:337:ASP:OD2	2.51	0.44
1:A:404:ARG:HH21	1:A:414:ASN:ND2	2.10	0.44
1:B:181:LYS:O	1:B:181:LYS:HG2	2.16	0.44
1:B:459:PRO:HG3	1:B:475:PRO:HB3	1.99	0.44
1:C:301:TRP:CE2	1:C:472:LYS:CD	2.99	0.44
1:D:117:TRP:CZ2	1:D:425:ARG:NE	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:PRO:O	1:D:142:GLN:HG3	2.16	0.44
1:A:40:LEU:CB	1:A:64:LEU:O	2.64	0.44
1:A:178:PHE:O	1:A:179:GLY:C	2.61	0.44
1:A:254:ASP:OD2	1:A:256:THR:HB	2.18	0.44
1:B:200:TRP:CE3	3:B:501:3QZ:CAB	3.00	0.44
1:B:316:LEU:O	1:B:320:LEU:HB2	2.16	0.44
1:B:386:ASN:HD21	1:B:389:GLY:N	2.16	0.44
1:B:410:GLU:HB3	1:B:411:PRO:HD3	1.98	0.44
1:C:66:LEU:HA	1:C:66:LEU:HD12	1.53	0.44
1:C:252:TRP:HB2	1:C:257:ASP:CB	2.47	0.44
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.64	0.44
1:D:72:LEU:HD13	1:D:372:ILE:HD13	1.99	0.44
1:D:109:SER:C	1:D:110:LEU:HD23	2.40	0.44
1:D:284:VAL:O	1:D:288:PHE:HB2	2.18	0.44
1:A:168:LEU:HD12	1:A:169:THR:H	1.82	0.44
1:A:311:GLU:HG3	1:A:312:ILE:N	2.32	0.44
1:B:62:LEU:HD11	1:B:64:LEU:CD2	2.48	0.44
1:B:148:CYS:O	1:B:152:ARG:HB2	2.18	0.44
1:B:469:VAL:HG12	1:B:470:ASN:H	1.81	0.44
1:C:263:VAL:HG21	1:C:280:VAL:HG23	2.00	0.44
1:D:30:LEU:CG	1:D:31:PRO:HD2	2.47	0.44
1:D:55:LYS:HG3	1:D:56:LEU:H	1.83	0.44
1:D:319:GLU:OE1	1:D:343:LEU:HB2	2.17	0.44
1:D:368:ARG:NH1	1:D:368:ARG:HB3	2.33	0.44
1:A:332:ARG:NH1	1:A:337:ASP:CG	2.76	0.44
1:A:449:THR:HG22	1:A:450:LEU:N	2.32	0.44
1:C:324:LEU:C	1:C:326:PRO:HD3	2.42	0.44
1:D:108:ILE:HG22	1:D:109:SER:N	2.33	0.44
1:D:136:MET:H	1:D:136:MET:HG3	1.49	0.44
1:D:242:ARG:H	1:D:242:ARG:HD3	1.81	0.44
1:A:414:ASN:OD1	1:A:415:PRO:HD2	2.18	0.44
1:A:470:ASN:OD1	1:A:471:LEU:N	2.50	0.44
1:B:104:ARG:O	1:B:105:CYS:CB	2.66	0.44
1:C:214:LEU:HG	1:C:216:PHE:H	1.83	0.44
1:D:105:CYS:C	4:D:613:HOH:O	2.60	0.44
1:D:193:VAL:O	1:D:197:MET:HG2	2.18	0.44
1:A:60:TYR:HE1	1:A:73:ASN:HD21	1.64	0.44
1:A:89:PHE:CG	1:A:372:ILE:HD11	2.52	0.44
1:A:103:GLN:CA	4:A:610:HOH:O	2.58	0.44
1:A:210:MET:O	1:A:212:PRO:HD3	2.18	0.44
1:A:334:THR:HG23	1:A:335:TYR:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:THR:N	1:A:480:LEU:O	2.46	0.44
1:B:70:VAL:CG1	1:B:383:VAL:HG22	2.48	0.44
1:B:104:ARG:C	1:B:105:CYS:HG	2.16	0.44
1:B:350:GLU:HG3	1:B:404:ARG:C	2.39	0.44
1:C:77:THR:C	1:C:79:GLU:H	2.26	0.44
1:C:208:LEU:CD2	1:C:214:LEU:HD11	2.48	0.44
1:C:218:PRO:N	4:C:622:HOH:O	2.51	0.44
1:C:247:MET:C	1:C:248:VAL:CG1	2.91	0.44
1:D:31:PRO:HA	4:D:605:HOH:O	2.17	0.44
1:A:38:LEU:HD22	1:A:38:LEU:HA	1.69	0.43
1:A:231:ASN:HD22	1:A:235:MET:CE	2.31	0.43
1:A:354:LEU:C	1:A:355:ARG:CD	2.91	0.43
1:A:386:ASN:ND2	1:A:389:GLY:H	2.16	0.43
1:B:37:PHE:CE1	1:B:63:ARG:HD3	2.53	0.43
1:B:40:LEU:HB2	1:B:64:LEU:O	2.18	0.43
1:B:85:LYS:HG2	1:B:88:ASP:OD2	2.18	0.43
1:B:339:ALA:C	1:B:341:LEU:H	2.25	0.43
1:C:193:VAL:CG2	1:C:289:ILE:HG22	2.48	0.43
1:C:214:LEU:HD23	1:C:216:PHE:CD2	2.53	0.43
1:D:37:PHE:O	1:D:65:GLY:O	2.36	0.43
1:B:37:PHE:CE1	1:B:63:ARG:CD	3.01	0.43
1:B:169:THR:OG1	1:B:292:THR:HB	2.18	0.43
1:B:178:PHE:CG	1:B:178:PHE:O	2.71	0.43
1:C:161:ILE:HD11	1:C:474:GLN:CB	2.47	0.43
1:C:172:ILE:O	1:C:176:LEU:HB2	2.17	0.43
1:C:176:LEU:HA	1:C:255:MET:H	1.83	0.43
1:C:425:ARG:HB3	1:C:425:ARG:HE	1.30	0.43
1:C:480:LEU:O	1:C:480:LEU:HD12	2.18	0.43
1:D:167:LEU:HD23	1:D:167:LEU:O	2.18	0.43
1:A:80:GLU:O	1:A:84:ARG:HB2	2.19	0.43
1:A:95:ILE:HB	1:A:96:PRO:HD2	2.00	0.43
1:A:173:ILE:CD1	1:A:186:VAL:HA	2.48	0.43
1:C:162:GLN:O	1:C:165:PHE:HB2	2.18	0.43
1:C:325:GLY:N	1:C:326:PRO:HD3	2.32	0.43
1:C:434:ARG:HH11	1:C:434:ARG:HG3	1.82	0.43
1:D:144:THR:O	1:D:147:PHE:HB3	2.17	0.43
1:D:169:THR:HG21	1:D:190:HIS:CB	2.47	0.43
1:D:404:ARG:CD	1:D:404:ARG:C	2.88	0.43
1:D:462:GLN:CG	1:D:463:PRO:HD2	2.47	0.43
1:A:294:THR:HG22	3:A:501:3QZ:CAA	2.25	0.43
1:A:313:GLN:NE2	1:A:450:LEU:HB3	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:O	1:A:338:ARG:N	2.52	0.43
1:B:218:PRO:HB2	1:B:223:TRP:HE1	1.84	0.43
1:B:322:ARG:HA	1:B:322:ARG:NE	2.33	0.43
1:C:124:THR:HG23	1:C:428:LEU:CD1	2.47	0.43
1:C:353:ARG:HH12	1:C:400:PRO:HA	1.83	0.43
1:D:391:HIS:CE1	1:D:417:ALA:HB1	2.54	0.43
1:A:85:LYS:O	1:A:87:VAL:N	2.46	0.43
1:A:144:THR:O	1:A:147:PHE:HB3	2.18	0.43
1:A:151:MET:HE1	1:A:163:LYS:HG3	2.00	0.43
1:A:203:TRP:O	1:A:207:ILE:HG13	2.18	0.43
1:A:267:ARG:O	1:A:268:VAL:HB	2.19	0.43
1:A:354:LEU:O	1:A:355:ARG:CD	2.64	0.43
1:A:432:LEU:O	1:A:436:GLU:HG3	2.18	0.43
1:B:164:GLU:C	1:B:166:SER:N	2.75	0.43
1:D:72:LEU:CD2	1:D:372:ILE:CD1	2.97	0.43
1:D:75:LYS:HE3	1:D:79:GLU:OE1	2.19	0.43
1:D:123:LEU:HD21	1:D:259:MET:HA	2.01	0.43
1:D:217:PHE:N	1:D:217:PHE:HD1	2.15	0.43
1:D:475:PRO:HA	4:D:610:HOH:O	2.19	0.43
1:A:174:CYS:O	1:A:179:GLY:CA	2.64	0.43
1:A:374:GLY:HA3	1:A:375:TYR:CD2	2.53	0.43
1:B:40:LEU:HD13	1:B:40:LEU:C	2.37	0.43
1:B:136:MET:CB	1:B:175:TYR:CE2	2.93	0.43
1:B:216:PHE:O	1:B:217:PHE:C	2.56	0.43
1:C:80:GLU:OE2	1:C:372:ILE:O	2.37	0.43
1:C:178:PHE:C	1:C:180:ASN:N	2.75	0.43
1:C:358:VAL:HG12	2:C:500:HEM:HHB	2.00	0.43
1:C:472:LYS:HA	1:C:472:LYS:HD2	1.80	0.43
1:D:106:GLN:CG	1:D:116:LEU:CD1	2.96	0.43
1:D:324:LEU:C	1:D:326:PRO:HD3	2.43	0.43
1:D:407:ARG:O	1:D:413:ALA:HB1	2.19	0.43
1:A:113:TYR:O	1:A:114:SER:HB2	2.19	0.43
1:A:447:ALA:HB3	1:A:448:PHE:CD2	2.54	0.43
1:B:154:GLN:C	1:B:156:GLY:N	2.76	0.43
1:B:308:HIS:HE1	1:B:458:LEU:HB2	1.82	0.43
1:B:357:VAL:CG1	1:B:469:VAL:HG13	2.29	0.43
1:C:226:LYS:HA	1:C:229:ILE:CG2	2.48	0.43
1:C:226:LYS:CA	1:C:229:ILE:HG22	2.48	0.43
1:C:319:GLU:OE1	1:C:343:LEU:HB2	2.18	0.43
1:C:322:ARG:NE	1:C:322:ARG:HA	2.34	0.43
1:C:359:PRO:HG3	1:C:466:TYR:HE2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:THR:OG1	1:C:480:LEU:C	2.61	0.43
1:D:242:ARG:N	1:D:242:ARG:CD	2.82	0.43
1:D:357:VAL:HG13	1:D:469:VAL:CG1	2.46	0.43
1:A:473:VAL:O	1:A:475:PRO:HD3	2.18	0.43
1:B:152:ARG:HH21	1:C:133:ARG:HH21	1.67	0.43
1:C:44:ASN:HB3	1:C:47:ILE:HG23	2.00	0.43
1:C:128:LEU:O	1:C:136:MET:HE3	2.18	0.43
1:D:39:HIS:HB2	1:D:62:LEU:HD21	2.01	0.43
1:A:478:VAL:O	1:A:479:ARG:HB2	2.19	0.43
1:B:62:LEU:CD1	1:B:64:LEU:HD23	2.49	0.43
1:B:116:LEU:HD11	1:B:279:HIS:NE2	2.34	0.43
1:C:95:ILE:HB	1:C:96:PRO:HD2	2.01	0.43
1:C:468:GLY:HA2	3:C:502:3QZ:OAE	2.19	0.43
1:D:75:LYS:HA	1:D:78:ILE:CG2	2.49	0.43
1:D:178:PHE:HA	1:D:243:HIS:NE2	2.34	0.43
1:A:65:GLY:C	1:A:66:LEU:HD12	2.44	0.43
1:A:208:LEU:HD22	1:A:216:PHE:HD2	1.84	0.43
1:A:372:ILE:HB	1:A:377:ILE:HG13	1.99	0.43
1:B:168:LEU:CD1	1:B:169:THR:H	2.31	0.43
1:B:344:LEU:C	1:B:346:ALA:N	2.76	0.43
1:B:454:PRO:C	1:B:456:GLY:N	2.77	0.43
1:C:178:PHE:HB2	1:C:243:HIS:NE2	2.34	0.43
1:C:276:LEU:HD23	1:C:277:GLU:C	2.44	0.43
1:C:361:ALA:HB1	2:C:500:HEM:HAA2	2.00	0.43
1:D:81:ALA:HB2	1:D:372:ILE:HD11	2.01	0.43
1:A:34:VAL:CG1	1:A:52:LEU:HD13	2.49	0.42
1:A:37:PHE:N	4:A:601:HOH:O	2.46	0.42
1:A:44:ASN:HD22	1:A:47:ILE:CD1	2.31	0.42
1:A:72:LEU:HD11	1:A:383:VAL:CG1	2.48	0.42
1:A:77:THR:C	1:A:79:GLU:H	2.28	0.42
1:C:162:GLN:NE2	1:C:165:PHE:HB2	2.34	0.42
1:C:168:LEU:HD12	1:C:168:LEU:N	2.34	0.42
1:C:214:LEU:CD2	1:C:216:PHE:HD2	2.33	0.42
1:C:222:LEU:HD11	1:C:226:LYS:HE3	2.01	0.42
1:C:303:VAL:HG13	1:C:450:LEU:CD2	2.48	0.42
1:D:98:TYR:OH	1:D:363:PRO:HG3	2.19	0.42
1:D:151:MET:HB3	1:D:479:ARG:HH12	1.84	0.42
1:D:310:PRO:O	1:D:314:ARG:HG2	2.18	0.42
1:D:427:CYS:SG	2:D:500:HEM:ND	2.92	0.42
1:D:448:PHE:HD1	1:D:479:ARG:O	2.00	0.42
1:D:473:VAL:HG13	1:D:474:GLN:N	2.10	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HB2	3:A:502:3QZ:OAD	2.19	0.42
1:A:252:TRP:H	1:A:257:ASP:CB	2.32	0.42
1:B:58:PRO:HG2	1:B:373:PHE:CE1	2.54	0.42
1:B:113:TYR:O	1:B:114:SER:CB	2.45	0.42
1:B:169:THR:HG21	1:B:190:HIS:HB2	2.01	0.42
1:B:208:LEU:HD23	1:B:214:LEU:HD22	2.00	0.42
1:B:459:PRO:HB3	1:B:473:VAL:HB	2.00	0.42
1:C:96:PRO:HG2	1:C:209:ASP:OD1	2.19	0.42
1:C:162:GLN:NE2	1:C:165:PHE:CB	2.80	0.42
1:A:49:LEU:HB3	1:A:60:TYR:OH	2.19	0.42
1:A:109:SER:CA	1:A:425:ARG:HH21	2.32	0.42
1:B:85:LYS:HG3	1:B:88:ASP:OD2	2.20	0.42
1:B:116:LEU:CD2	1:B:117:TRP:CA	2.90	0.42
1:D:121:LYS:CD	1:D:428:LEU:CD2	2.98	0.42
1:D:128:LEU:HD23	1:D:255:MET:HE1	2.00	0.42
1:D:151:MET:SD	1:D:163:LYS:HG3	2.59	0.42
1:D:344:LEU:C	1:D:346:ALA:N	2.76	0.42
1:D:478:VAL:O	1:D:479:ARG:HB2	2.19	0.42
1:A:308:HIS:CE1	1:A:458:LEU:HB2	2.54	0.42
1:A:409:LEU:HG	4:A:609:HOH:O	2.18	0.42
1:B:244:LYS:CG	1:B:260:LEU:HD21	2.48	0.42
1:B:325:GLY:N	1:B:326:PRO:HD3	2.34	0.42
1:B:420:PHE:CE1	2:B:500:HEM:HBB2	2.54	0.42
1:D:117:TRP:HE1	1:D:425:ARG:HH12	1.60	0.42
1:D:178:PHE:CB	1:D:243:HIS:HE1	2.33	0.42
1:D:335:TYR:CG	1:D:336:LYS:N	2.87	0.42
1:A:45:LEU:CD2	1:A:49:LEU:CG	2.87	0.42
1:A:96:PRO:CG	1:A:209:ASP:HA	2.49	0.42
1:A:180:ASN:O	1:A:182:GLU:N	2.53	0.42
1:A:261:GLN:C	1:A:263:VAL:H	2.28	0.42
1:B:37:PHE:CE1	1:B:63:ARG:CZ	3.03	0.42
1:B:159:VAL:HG23	1:B:162:GLN:HB2	2.00	0.42
1:B:361:ALA:C	1:B:362:LEU:HD13	2.45	0.42
1:C:463:PRO:C	1:C:465:PRO:HD2	2.42	0.42
1:D:77:THR:C	1:D:79:GLU:H	2.27	0.42
1:D:106:GLN:CB	1:D:279:HIS:ND1	2.70	0.42
1:D:396:VAL:O	1:D:415:PRO:HG2	2.19	0.42
1:D:459:PRO:CB	1:D:473:VAL:HB	2.47	0.42
1:B:107:ASP:CG	1:B:108:ILE:N	2.76	0.42
1:B:178:PHE:CD2	1:B:252:TRP:HZ3	2.16	0.42
1:C:216:PHE:CD2	1:C:216:PHE:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:CG2	1:A:176:LEU:HD13	2.49	0.42
1:B:91:GLY:HA3	1:B:365:ARG:HB3	2.02	0.42
1:C:88:ASP:CB	1:C:89:PHE:CD1	2.93	0.42
1:D:97:SER:N	1:D:209:ASP:OD1	2.52	0.42
1:A:80:GLU:CG	1:A:84:ARG:HD3	2.42	0.42
1:A:93:PRO:CD	1:A:365:ARG:HB2	2.41	0.42
1:A:125:ARG:HA	1:A:128:LEU:HD12	2.02	0.42
1:A:337:ASP:O	1:A:338:ARG:C	2.61	0.42
1:A:461:LEU:HD23	1:A:462:GLN:HG2	1.97	0.42
1:B:148:CYS:O	1:B:152:ARG:N	2.53	0.42
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.70	0.42
1:C:106:GLN:C	1:C:107:ASP:OD1	2.63	0.42
1:C:171:SER:O	1:C:175:TYR:CE1	2.73	0.42
1:C:297:SER:HB3	1:C:357:VAL:CG2	2.48	0.42
1:C:311:GLU:HG3	1:C:312:ILE:N	2.34	0.42
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.75	0.42
1:D:179:GLY:O	1:D:180:ASN:C	2.62	0.42
1:D:189:PHE:CG	1:D:288:PHE:HE2	2.38	0.42
1:D:413:ALA:CA	4:D:601:HOH:O	2.67	0.42
1:A:34:VAL:CG2	1:A:62:LEU:HA	2.49	0.42
1:B:333:VAL:HB	1:B:443:ARG:HH12	1.84	0.42
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.84	0.42
1:C:458:LEU:H	1:C:458:LEU:HG	1.67	0.42
1:C:463:PRO:HB2	1:C:465:PRO:CD	2.46	0.42
1:D:177:THR:O	1:D:179:GLY:N	2.53	0.42
1:D:231:ASN:HB3	1:D:235:MET:CE	2.38	0.42
1:D:292:THR:OG1	1:D:293:GLU:N	2.50	0.42
1:D:311:GLU:HG3	1:D:312:ILE:N	2.34	0.42
1:D:353:ARG:HH12	1:D:400:PRO:CA	2.29	0.42
1:A:39:HIS:O	1:A:41:LEU:O	2.37	0.42
1:A:83:ILE:HD11	1:A:422:CYS:HB2	2.02	0.42
1:A:89:PHE:CD2	1:A:383:VAL:HG21	2.55	0.42
1:A:196:LEU:HD21	1:A:232:ARG:HD3	2.02	0.42
1:A:475:PRO:HG2	1:A:477:GLN:HE21	1.81	0.42
1:B:309:HIS:CE1	1:B:403:PHE:HB3	2.53	0.42
1:B:391:HIS:NE2	1:B:417:ALA:HB1	2.35	0.42
1:B:470:ASN:HA	1:B:471:LEU:HD12	2.01	0.42
1:C:260:LEU:HA	1:C:280:VAL:HG21	2.02	0.42
1:C:375:TYR:CD2	1:C:375:TYR:N	2.88	0.42
1:D:180:ASN:ND2	1:D:185:LEU:HD13	2.35	0.42
1:D:396:VAL:HG12	1:D:415:PRO:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:THR:C	1:B:79:GLU:H	2.26	0.41
1:B:246:SER:HB3	1:B:252:TRP:CZ2	2.55	0.41
1:B:339:ALA:C	1:B:341:LEU:N	2.78	0.41
1:C:31:PRO:HG2	1:C:61:ARG:CG	2.40	0.41
1:C:126:SER:C	1:C:128:LEU:N	2.75	0.41
1:C:173:ILE:HG12	1:C:288:PHE:CZ	2.55	0.41
1:C:199:THR:O	1:C:225:LEU:HD12	2.20	0.41
1:C:336:LYS:HG3	1:C:336:LYS:O	2.20	0.41
1:D:141:ASP:OD1	1:D:443:ARG:CZ	2.68	0.41
1:D:189:PHE:CZ	1:D:235:MET:HB3	2.55	0.41
1:D:298:THR:OG1	1:D:357:VAL:CG2	2.68	0.41
1:D:423:GLY:C	1:D:426:VAL:H	2.27	0.41
1:A:178:PHE:CZ	1:A:242:ARG:HB3	2.56	0.41
1:A:180:ASN:C	1:A:182:GLU:N	2.78	0.41
1:B:62:LEU:CD1	1:B:64:LEU:HD21	2.50	0.41
1:B:116:LEU:HD23	1:B:117:TRP:HA	1.95	0.41
1:B:210:MET:C	1:B:212:PRO:HD3	2.45	0.41
1:B:464:ASP:H	1:B:465:PRO:HD3	1.85	0.41
1:C:98:TYR:CD1	1:C:110:LEU:HD22	2.55	0.41
1:C:141:ASP:HA	1:C:439:VAL:HG11	2.02	0.41
1:C:162:GLN:C	1:C:162:GLN:CD	2.89	0.41
1:D:168:LEU:CD2	1:D:292:THR:CB	2.97	0.41
1:D:298:THR:OG1	1:D:357:VAL:HG23	2.20	0.41
1:D:313:GLN:HE22	1:D:450:LEU:CB	2.32	0.41
1:A:129:LEU:O	1:A:130:LEU:C	2.63	0.41
1:A:263:VAL:CG1	1:A:275:LEU:HD12	2.40	0.41
1:A:335:TYR:O	1:A:338:ARG:HB3	2.21	0.41
1:B:180:ASN:O	1:B:181:LYS:HB3	2.20	0.41
1:C:280:VAL:HG12	1:C:281:HIS:N	2.32	0.41
1:D:75:LYS:CA	1:D:78:ILE:HG22	2.50	0.41
1:D:212:PRO:CD	1:D:213:PHE:H	2.33	0.41
1:D:245:GLU:O	1:D:245:GLU:HG3	2.13	0.41
1:D:374:GLY:C	1:D:375:TYR:CD2	2.98	0.41
1:D:393:ASP:C	1:D:395:THR:H	2.27	0.41
1:D:414:ASN:HD22	1:D:414:ASN:HA	1.66	0.41
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.85	0.41
1:B:92:ARG:NH1	1:B:362:LEU:C	2.78	0.41
1:B:215:ARG:HE	1:B:215:ARG:HB3	1.68	0.41
1:B:298:THR:OG1	1:B:357:VAL:HG23	2.20	0.41
1:B:473:VAL:HG13	1:B:474:GLN:H	1.85	0.41
1:C:108:ILE:C	1:C:110:LEU:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD22	1:C:168:LEU:N	2.35	0.41
1:C:182:GLU:O	1:C:186:VAL:HG23	2.20	0.41
1:C:219:ASN:CB	1:C:220:PRO:HD2	2.51	0.41
1:C:462:GLN:CD	1:C:463:PRO:HD2	2.45	0.41
1:D:100:LEU:HD11	1:D:222:LEU:CD1	2.50	0.41
1:D:112:ASP:OD2	1:D:365:ARG:NH1	2.53	0.41
1:D:387:LEU:HD21	1:D:418:LEU:HB2	2.02	0.41
1:D:396:VAL:HB	1:D:397:TRP:CE3	2.55	0.41
1:A:172:ILE:HG21	1:A:287:LEU:O	2.20	0.41
1:A:361:ALA:C	1:A:362:LEU:HD22	2.45	0.41
1:B:185:LEU:HD11	1:B:239:GLN:HE22	1.84	0.41
1:C:79:GLU:HG2	1:C:83:ILE:HD12	2.02	0.41
1:C:85:LYS:HB3	1:C:88:ASP:OD2	2.20	0.41
1:C:214:LEU:HD21	1:C:216:PHE:CD2	2.54	0.41
1:C:373:PHE:CD1	1:C:373:PHE:O	2.73	0.41
1:D:181:LYS:HG2	1:D:181:LYS:O	2.20	0.41
1:D:182:GLU:C	1:D:184:THR:N	2.79	0.41
1:D:199:THR:O	1:D:225:LEU:HD12	2.19	0.41
1:D:364:HIS:CD2	1:D:385:PRO:HG3	2.56	0.41
1:A:43:PRO:O	1:A:44:ASN:C	2.60	0.41
1:B:37:PHE:O	1:B:65:GLY:O	2.39	0.41
1:B:208:LEU:CD1	1:B:222:LEU:HD13	2.50	0.41
1:B:354:LEU:O	1:B:355:ARG:CD	2.66	0.41
1:C:473:VAL:O	1:C:475:PRO:HD3	2.21	0.41
1:D:61:ARG:HA	1:D:70:VAL:HA	2.03	0.41
1:D:76:ARG:HG3	1:D:77:THR:N	2.36	0.41
1:D:215:ARG:NH2	1:D:215:ARG:CG	2.83	0.41
1:A:89:PHE:CE1	1:A:372:ILE:CG1	2.86	0.41
1:A:112:ASP:CG	1:A:113:TYR:N	2.79	0.41
1:A:154:GLN:C	1:A:156:GLY:N	2.78	0.41
1:B:74:SER:HG	1:B:77:THR:CB	2.33	0.41
1:B:324:LEU:CB	1:B:340:ARG:HB3	2.48	0.41
1:B:369:PRO:HD3	1:B:379:GLU:OE2	2.20	0.41
1:B:373:PHE:CD1	1:B:373:PHE:C	2.98	0.41
1:B:408:PHE:CD2	1:B:410:GLU:N	2.69	0.41
1:C:45:LEU:N	1:C:46:PRO:CD	2.82	0.41
1:C:278:GLY:O	1:C:281:HIS:HB3	2.21	0.41
1:D:240:LEU:CD2	1:D:260:LEU:HD13	2.50	0.41
1:A:30:LEU:HD12	1:A:376:ASP:O	2.21	0.41
1:A:341:LEU:HD13	1:A:344:LEU:CD1	2.40	0.41
1:A:344:LEU:C	1:A:346:ALA:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.93	0.41
1:B:311:GLU:HG3	1:B:312:ILE:N	2.34	0.41
1:B:336:LYS:HD3	1:C:326:PRO:HG2	2.02	0.41
1:B:354:LEU:C	1:B:355:ARG:CD	2.94	0.41
1:C:108:ILE:HD11	1:C:121:LYS:CD	2.50	0.41
1:C:307:LEU:HD11	1:C:477:GLN:NE2	2.35	0.41
1:D:299:LEU:O	1:D:303:VAL:HG23	2.21	0.41
1:D:374:GLY:O	1:D:375:TYR:HD2	1.99	0.41
1:A:33:LEU:HD13	1:A:33:LEU:C	2.46	0.41
1:A:182:GLU:C	1:A:184:THR:H	2.28	0.41
1:A:337:ASP:HA	1:A:340:ARG:HG2	2.02	0.41
1:A:374:GLY:HA3	1:A:375:TYR:CE2	2.56	0.41
1:A:463:PRO:O	1:A:466:TYR:HD1	1.90	0.41
1:A:463:PRO:C	1:A:465:PRO:HD2	2.45	0.41
1:A:467:CYS:HB3	1:A:468:GLY:H	1.72	0.41
1:A:473:VAL:HG12	1:A:474:GLN:OE1	2.21	0.41
1:B:76:ARG:H	1:B:76:ARG:HG2	1.62	0.41
1:B:78:ILE:CD1	1:B:385:PRO:HB2	2.51	0.41
1:B:100:LEU:HD23	1:B:100:LEU:O	2.20	0.41
1:B:136:MET:HE2	1:B:136:MET:N	2.36	0.41
1:C:69:VAL:HG13	1:C:382:VAL:CB	2.48	0.41
1:C:69:VAL:HG12	1:C:70:VAL:N	2.35	0.41
1:C:77:THR:C	1:C:79:GLU:N	2.78	0.41
1:C:173:ILE:HA	1:C:288:PHE:CZ	2.53	0.41
1:D:137:GLU:OE1	1:D:334:THR:HG23	2.21	0.41
1:D:202:HIS:CE1	1:D:203:TRP:CD1	3.09	0.41
1:D:211:VAL:CG1	1:D:214:LEU:HB2	2.38	0.41
1:D:232:ARG:HD2	1:D:285:VAL:HG11	2.01	0.41
1:D:420:PHE:CG	1:D:430:GLU:HG2	2.56	0.41
1:A:41:LEU:HG	1:A:41:LEU:H	1.21	0.41
1:A:189:PHE:CD2	1:A:289:ILE:CD1	3.04	0.41
1:B:243:HIS:NE2	1:B:256:THR:HB	2.36	0.41
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.36	0.41
1:C:62:LEU:HD21	1:C:64:LEU:CA	2.51	0.41
1:C:159:VAL:HG12	1:C:476:PHE:CD2	2.41	0.41
1:D:472:LYS:HZ3	1:D:472:LYS:HG3	1.63	0.41
1:A:70:VAL:HG12	1:A:381:MET:HG3	2.04	0.40
1:A:77:THR:C	1:A:79:GLU:N	2.79	0.40
1:A:143:LEU:HD13	1:A:171:SER:CA	2.51	0.40
1:A:143:LEU:HD21	1:A:181:LYS:HD2	2.03	0.40
1:B:212:PRO:C	1:B:214:LEU:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LEU:HD11	2:B:500:HEM:HBB1	2.02	0.40
1:C:160:THR:OG1	1:C:161:ILE:N	2.53	0.40
1:D:77:THR:C	1:D:79:GLU:N	2.79	0.40
1:D:320:LEU:HD23	1:D:320:LEU:C	2.46	0.40
1:A:214:LEU:HD21	1:A:216:PHE:HD2	1.78	0.40
1:A:233:ASP:O	1:A:237:GLU:HG3	2.21	0.40
1:A:475:PRO:C	1:A:476:PHE:CD2	3.00	0.40
1:B:77:THR:C	1:B:79:GLU:N	2.79	0.40
1:B:151:MET:CE	1:B:163:LYS:HG3	2.51	0.40
1:B:291:GLY:O	1:B:295:THR:OG1	2.40	0.40
1:B:413:ALA:O	1:B:414:ASN:C	2.63	0.40
1:C:352:LEU:HD13	1:C:420:PHE:HE2	1.86	0.40
1:C:374:GLY:C	1:C:375:TYR:CD2	2.95	0.40
1:D:304:ALA:HB2	1:D:472:LYS:HE3	2.02	0.40
1:D:322:ARG:NH2	1:D:326:PRO:HB3	2.36	0.40
1:A:50:LEU:O	1:A:53:THR:CB	2.68	0.40
1:A:78:ILE:CG2	1:A:418:LEU:HD11	2.51	0.40
1:A:263:VAL:C	1:A:265:ARG:H	2.30	0.40
1:A:329:SER:O	1:A:331:SER:OG	2.37	0.40
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.37	0.40
1:A:472:LYS:HZ1	1:A:473:VAL:C	2.25	0.40
1:B:125:ARG:HH12	1:B:426:VAL:CG2	2.34	0.40
1:B:432:LEU:O	1:B:432:LEU:HD23	2.21	0.40
1:C:59:VAL:HG22	1:C:72:LEU:HD22	2.02	0.40
1:C:177:THR:HG23	1:C:239:GLN:CG	2.51	0.40
1:C:213:PHE:C	1:C:215:ARG:H	2.29	0.40
1:C:338:ARG:HA	1:C:438:PHE:CZ	2.56	0.40
1:D:98:TYR:C	1:D:100:LEU:H	2.29	0.40
1:D:178:PHE:N	1:D:243:HIS:NE2	2.69	0.40
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.86	0.40
1:A:187:HIS:CE1	1:B:238:LYS:HE2	2.57	0.40
1:B:299:LEU:O	1:B:303:VAL:HG23	2.21	0.40
1:B:299:LEU:HD13	1:B:440:VAL:HG11	2.03	0.40
1:B:400:PRO:HD2	1:B:401:HIS:H	1.86	0.40
1:B:471:LEU:CD1	1:B:471:LEU:N	2.33	0.40
1:C:31:PRO:HA	1:C:375:TYR:HD1	1.77	0.40
1:C:69:VAL:HG22	1:C:382:VAL:HB	2.04	0.40
1:D:180:ASN:C	1:D:182:GLU:N	2.79	0.40
1:D:376:ASP:HA	4:D:606:HOH:O	2.20	0.40
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.87	0.40
1:A:64:LEU:HD12	1:A:69:VAL:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HB2	1:A:76:ARG:NH1	2.36	0.40
1:A:267:ARG:O	1:A:268:VAL:CB	2.70	0.40
1:B:44:ASN:C	1:B:46:PRO:HD2	2.46	0.40
1:B:74:SER:OG	1:B:77:THR:CB	2.70	0.40
1:B:291:GLY:HA2	2:B:500:HEM:HMC3	2.03	0.40
1:B:418:LEU:CD1	1:B:418:LEU:C	2.91	0.40

All (5) 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:B:404:ARG:NH2	4:A:618:HOH:O[2_556]	1.67	0.53
1:A:39:HIS:NE2	1:D:35:PRO:O[1_556]	2.07	0.13
1:D:38:LEU:N	4:A:601:HOH:O[1_554]	2.13	0.07
1:B:35:PRO:O	1:C:35:PRO:O[1_556]	2.14	0.06
1:B:38:LEU:N	4:C:601:HOH:O[1_556]	2.14	0.06

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	437/496 (88%)	369 (84%)	49 (11%)	19 (4%)	2	12
1	B	428/496 (86%)	357 (83%)	53 (12%)	18 (4%)	2	13
1	C	429/496 (86%)	361 (84%)	50 (12%)	18 (4%)	2	13
1	D	426/496 (86%)	361 (85%)	42 (10%)	23 (5%)	1	9
All	All	1720/1984 (87%)	1448 (84%)	194 (11%)	78 (4%)	2	12

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	A	114	SER
1	A	335	TYR
1	A	338	ARG
1	A	426	VAL
1	A	460	SER
1	A	482	PRO
1	B	114	SER
1	B	324	LEU
1	B	335	TYR
1	B	410	GLU
1	B	411	PRO
1	B	474	GLN
1	B	482	PRO
1	C	107	ASP
1	C	114	SER
1	C	178	PHE
1	C	335	TYR
1	C	409	LEU
1	C	410	GLU
1	C	459	PRO
1	C	475	PRO
1	D	103	GLN
1	D	114	SER
1	D	335	TYR
1	D	375	TYR
1	D	426	VAL
1	A	105	CYS
1	A	373	PHE
1	B	42	GLN
1	B	253	ARG
1	B	361	ALA
1	B	427	CYS
1	B	459	PRO
1	C	86	TRP
1	C	333	VAL
1	D	253	ARG
1	D	324	LEU
1	D	427	CYS
1	D	462	GLN
1	A	42	GLN
1	A	109	SER
1	A	359	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	407	ARG
1	A	461	LEU
1	B	359	PRO
1	C	105	CYS
1	C	203	TRP
1	C	427	CYS
1	C	462	GLN
1	D	105	CYS
1	D	178	PHE
1	D	342	PRO
1	D	450	LEU
1	D	459	PRO
1	A	462	GLN
1	B	429	GLY
1	B	450	LEU
1	B	462	GLN
1	C	42	GLN
1	C	342	PRO
1	A	106	GLN
1	A	333	VAL
1	C	359	PRO
1	D	86	TRP
1	D	373	PHE
1	A	324	LEU
1	B	203	TRP
1	B	455	VAL
1	D	42	GLN
1	D	359	PRO
1	D	465	PRO
1	A	374	GLY
1	C	429	GLY
1	D	463	PRO
1	D	473	VAL
1	D	357	VAL
1	D	410	GLU

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	393/430 (91%)	298 (76%)	95 (24%)	1	4
1	B	387/430 (90%)	306 (79%)	81 (21%)	1	7
1	C	386/430 (90%)	300 (78%)	86 (22%)	1	5
1	D	385/430 (90%)	299 (78%)	86 (22%)	1	5
All	All	1551/1720 (90%)	1203 (78%)	348 (22%)	1	5

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	40	LEU
1	A	41	LEU
1	A	42	GLN
1	A	44	ASN
1	A	45	LEU
1	A	52	LEU
1	A	56	LEU
1	A	61	ARG
1	A	62	LEU
1	A	67	GLN
1	A	69	VAL
1	A	85	LYS
1	A	92	ARG
1	A	100	LEU
1	A	101	VAL
1	A	102	SER
1	A	103	GLN
1	A	104	ARG
1	A	106	GLN
1	A	108	ILE
1	A	134	SER
1	A	159	VAL
1	A	165	PHE
1	A	167	LEU
1	A	168	LEU
1	A	176	LEU
1	A	178	PHE
1	A	181	LYS
1	A	182	GLU
1	A	191	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	GLN
1	A	196	LEU
1	A	198	LYS
1	A	205	ILE
1	A	213	PHE
1	A	214	LEU
1	A	215	ARG
1	A	217	PHE
1	A	226	LYS
1	A	244	LYS
1	A	245	GLU
1	A	246	SER
1	A	247	MET
1	A	252	TRP
1	A	253	ARG
1	A	257	ASP
1	A	275	LEU
1	A	276	LEU
1	A	285	VAL
1	A	286	ASP
1	A	287	LEU
1	A	289	ILE
1	A	292	THR
1	A	295	THR
1	A	323	GLU
1	A	324	LEU
1	A	330	CYS
1	A	331	SER
1	A	332	ARG
1	A	333	VAL
1	A	334	THR
1	A	335	TYR
1	A	336	LYS
1	A	337	ASP
1	A	343	LEU
1	A	366	THR
1	A	371	SER
1	A	372	ILE
1	A	373	PHE
1	A	375	TYR
1	A	392	LEU
1	A	394	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	404	ARG
1	A	405	PRO
1	A	406	ASP
1	A	407	ARG
1	A	408	PHE
1	A	418	LEU
1	A	422	CYS
1	A	426	VAL
1	A	428	LEU
1	A	445	LEU
1	A	446	GLN
1	A	449	THR
1	A	451	LEU
1	A	458	LEU
1	A	461	LEU
1	A	471	LEU
1	A	472	LYS
1	A	473	VAL
1	A	474	GLN
1	A	477	GLN
1	A	480	LEU
1	A	482	PRO
1	B	37	PHE
1	B	40	LEU
1	B	41	LEU
1	B	45	LEU
1	B	62	LEU
1	B	66	LEU
1	B	72	LEU
1	B	73	ASN
1	B	76	ARG
1	B	84	ARG
1	B	87	VAL
1	B	89	PHE
1	B	102	SER
1	B	103	GLN
1	B	105	CYS
1	B	107	ASP
1	B	110	LEU
1	B	115	LEU
1	B	116	LEU
1	B	161	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	167	LEU
1	B	168	LEU
1	B	170	CYS
1	B	172	ILE
1	B	173	ILE
1	B	177	THR
1	B	181	LYS
1	B	184	THR
1	B	194	GLN
1	B	196	LEU
1	B	198	LYS
1	B	205	ILE
1	B	211	VAL
1	B	213	PHE
1	B	214	LEU
1	B	215	ARG
1	B	216	PHE
1	B	218	PRO
1	B	219	ASN
1	B	231	ASN
1	B	241	ARG
1	B	247	MET
1	B	248	VAL
1	B	257	ASP
1	B	275	LEU
1	B	276	LEU
1	B	286	ASP
1	B	287	LEU
1	B	289	ILE
1	B	292	THR
1	B	295	THR
1	B	323	GLU
1	B	324	LEU
1	B	343	LEU
1	B	358	VAL
1	B	362	LEU
1	B	373	PHE
1	B	375	TYR
1	B	382	VAL
1	B	392	LEU
1	B	395	THR
1	B	396	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	402	GLU
1	B	404	ARG
1	B	407	ARG
1	B	408	PHE
1	B	410	GLU
1	B	416	SER
1	B	418	LEU
1	B	422	CYS
1	B	426	VAL
1	B	428	LEU
1	B	461	LEU
1	B	464	ASP
1	B	466	TYR
1	B	470	ASN
1	B	471	LEU
1	B	474	GLN
1	B	477	GLN
1	B	480	LEU
1	B	482	PRO
1	C	33	LEU
1	C	40	LEU
1	C	41	LEU
1	C	45	LEU
1	C	53	THR
1	C	54	GLN
1	C	55	LYS
1	C	56	LEU
1	C	59	VAL
1	C	62	LEU
1	C	66	LEU
1	C	67	GLN
1	C	70	VAL
1	C	89	PHE
1	C	101	VAL
1	C	102	SER
1	C	104	ARG
1	C	105	CYS
1	C	106	GLN
1	C	108	ILE
1	C	116	LEU
1	C	125	ARG
1	C	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	128	LEU
1	C	129	LEU
1	C	160	THR
1	C	161	ILE
1	C	162	GLN
1	C	165	PHE
1	C	167	LEU
1	C	168	LEU
1	C	169	THR
1	C	176	LEU
1	C	177	THR
1	C	180	ASN
1	C	181	LYS
1	C	194	GLN
1	C	196	LEU
1	C	198	LYS
1	C	205	ILE
1	C	217	PHE
1	C	219	ASN
1	C	239	GLN
1	C	247	MET
1	C	252	TRP
1	C	253	ARG
1	C	257	ASP
1	C	275	LEU
1	C	276	LEU
1	C	277	GLU
1	C	280	VAL
1	C	289	ILE
1	C	295	THR
1	C	323	GLU
1	C	324	LEU
1	C	334	THR
1	C	343	LEU
1	C	354	LEU
1	C	357	VAL
1	C	366	THR
1	C	371	SER
1	C	372	ILE
1	C	373	PHE
1	C	388	GLN
1	C	404	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	406	ASP
1	C	407	ARG
1	C	408	PHE
1	C	409	LEU
1	C	418	LEU
1	C	425	ARG
1	C	426	VAL
1	C	428	LEU
1	C	448	PHE
1	C	449	THR
1	C	450	LEU
1	C	451	LEU
1	C	458	LEU
1	C	466	TYR
1	C	470	ASN
1	C	472	LYS
1	C	474	GLN
1	C	476	PHE
1	C	477	GLN
1	C	479	ARG
1	C	480	LEU
1	D	40	LEU
1	D	45	LEU
1	D	53	THR
1	D	54	GLN
1	D	55	LYS
1	D	56	LEU
1	D	62	LEU
1	D	87	VAL
1	D	103	GLN
1	D	106	GLN
1	D	110	LEU
1	D	113	TYR
1	D	114	SER
1	D	115	LEU
1	D	116	LEU
1	D	136	MET
1	D	160	THR
1	D	162	GLN
1	D	163	LYS
1	D	168	LEU
1	D	169	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	172	ILE
1	D	176	LEU
1	D	177	THR
1	D	180	ASN
1	D	181	LYS
1	D	194	GLN
1	D	196	LEU
1	D	198	LYS
1	D	202	HIS
1	D	205	ILE
1	D	208	LEU
1	D	211	VAL
1	D	213	PHE
1	D	214	LEU
1	D	215	ARG
1	D	216	PHE
1	D	242	ARG
1	D	244	LYS
1	D	245	GLU
1	D	247	MET
1	D	248	VAL
1	D	252	TRP
1	D	253	ARG
1	D	257	ASP
1	D	275	LEU
1	D	276	LEU
1	D	289	ILE
1	D	292	THR
1	D	293	GLU
1	D	294	THR
1	D	297	SER
1	D	323	GLU
1	D	324	LEU
1	D	333	VAL
1	D	334	THR
1	D	337	ASP
1	D	343	LEU
1	D	372	ILE
1	D	373	PHE
1	D	376	ASP
1	D	377	ILE
1	D	382	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	402	GLU
1	D	404	ARG
1	D	406	ASP
1	D	407	ARG
1	D	408	PHE
1	D	409	LEU
1	D	410	GLU
1	D	414	ASN
1	D	418	LEU
1	D	422	CYS
1	D	426	VAL
1	D	430	GLU
1	D	432	LEU
1	D	434	ARG
1	D	448	PHE
1	D	449	THR
1	D	450	LEU
1	D	451	LEU
1	D	461	LEU
1	D	472	LYS
1	D	474	GLN
1	D	477	GLN
1	D	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	142	GLN
1	A	145	GLN
1	A	187	HIS
1	A	190	HIS
1	A	202	HIS
1	A	231	ASN
1	A	239	GLN
1	A	243	HIS
1	A	266	GLN
1	A	279	HIS
1	A	309	HIS
1	A	313	GLN
1	A	317	GLN
1	A	345	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386	ASN
1	A	388	GLN
1	A	401	HIS
1	A	414	ASN
1	A	477	GLN
1	B	39	HIS
1	B	73	ASN
1	B	103	GLN
1	B	106	GLN
1	B	142	GLN
1	B	145	GLN
1	B	162	GLN
1	B	202	HIS
1	B	206	GLN
1	B	219	ASN
1	B	231	ASN
1	B	234	HIS
1	B	239	GLN
1	B	274	GLN
1	B	309	HIS
1	B	313	GLN
1	B	317	GLN
1	B	345	ASN
1	B	386	ASN
1	B	414	ASN
1	B	481	GLN
1	C	39	HIS
1	C	48	HIS
1	C	54	GLN
1	C	106	GLN
1	C	142	GLN
1	C	145	GLN
1	C	162	GLN
1	C	180	ASN
1	C	202	HIS
1	C	239	GLN
1	C	308	HIS
1	C	313	GLN
1	C	317	GLN
1	C	345	ASN
1	C	386	ASN
1	C	388	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	414	ASN
1	C	446	GLN
1	C	481	GLN
1	D	54	GLN
1	D	67	GLN
1	D	103	GLN
1	D	106	GLN
1	D	142	GLN
1	D	145	GLN
1	D	180	ASN
1	D	187	HIS
1	D	231	ASN
1	D	308	HIS
1	D	309	HIS
1	D	313	GLN
1	D	345	ASN
1	D	386	ASN
1	D	401	HIS
1	D	446	GLN
1	D	481	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3QZ	D	501	-	27,27,27	1.30	3 (11%)	44,45,45	1.40	8 (18%)
3	3QZ	C	502	-	27,27,27	1.14	2 (7%)	44,45,45	1.19	6 (13%)
2	HEM	A	500	1	50,50,50	1.62	9 (18%)	67,82,82	0.89	4 (5%)
3	3QZ	B	501	-	27,27,27	1.20	3 (11%)	44,45,45	1.36	9 (20%)
3	3QZ	A	502	-	27,27,27	1.11	3 (11%)	44,45,45	1.20	7 (15%)
3	3QZ	D	502	-	27,27,27	1.33	2 (7%)	44,45,45	1.18	4 (9%)
3	3QZ	A	501	-	27,27,27	1.21	3 (11%)	44,45,45	1.35	10 (22%)
3	3QZ	B	502	-	27,27,27	1.12	3 (11%)	44,45,45	1.22	6 (13%)
2	HEM	D	500	-	50,50,50	1.67	10 (20%)	67,82,82	0.84	3 (4%)
2	HEM	B	500	-	50,50,50	1.65	10 (20%)	67,82,82	0.87	3 (4%)
2	HEM	C	500	-	50,50,50	1.66	12 (24%)	67,82,82	0.84	3 (4%)
3	3QZ	C	501	-	27,27,27	1.09	4 (14%)	44,45,45	1.29	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3QZ	D	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	C	502	-	-	0/6/68/68	0/4/4/4
2	HEM	A	500	1	-	8/14/54/54	-
3	3QZ	B	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	A	502	-	-	0/6/68/68	0/4/4/4
3	3QZ	D	502	-	-	0/6/68/68	0/4/4/4
3	3QZ	A	501	-	-	0/6/68/68	0/4/4/4
3	3QZ	B	502	-	-	0/6/68/68	0/4/4/4
2	HEM	D	500	-	-	8/14/54/54	-
2	HEM	B	500	-	-	8/14/54/54	-
2	HEM	C	500	-	-	6/14/54/54	-
3	3QZ	C	501	-	-	0/6/68/68	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	CBC-CAC	5.24	1.55	1.30
2	B	500	HEM	CBC-CAC	5.08	1.54	1.30
2	C	500	HEM	CBC-CAC	5.05	1.54	1.30
2	B	500	HEM	CBB-CAB	5.03	1.54	1.30
2	A	500	HEM	CBC-CAC	4.95	1.54	1.30
2	A	500	HEM	CBB-CAB	4.80	1.53	1.30
2	C	500	HEM	CBB-CAB	4.78	1.53	1.30
2	D	500	HEM	CBB-CAB	4.71	1.53	1.30
3	D	502	3QZ	CAG-CAR	4.41	1.40	1.34
3	D	501	3QZ	CAG-CAR	4.04	1.40	1.34
3	A	501	3QZ	CAG-CAR	3.40	1.39	1.34
3	C	502	3QZ	CAG-CAR	3.38	1.39	1.34
3	D	501	3QZ	CAG-CAQ	-3.29	1.38	1.45
2	A	500	HEM	FE-NB	3.25	2.04	1.94
3	D	502	3QZ	CAG-CAQ	-3.22	1.39	1.45
3	B	501	3QZ	CAG-CAR	3.21	1.39	1.34
2	B	500	HEM	FE-NB	3.18	2.04	1.94
3	A	502	3QZ	CAG-CAR	3.04	1.38	1.34
2	C	500	HEM	FE-NB	3.02	2.04	1.94
3	B	502	3QZ	CAG-CAR	2.99	1.38	1.34
2	D	500	HEM	CAC-C3C	2.90	1.55	1.47
3	B	501	3QZ	CAG-CAQ	-2.83	1.39	1.45
3	A	501	3QZ	CAG-CAQ	-2.80	1.39	1.45
2	D	500	HEM	FE-NB	2.77	2.03	1.94
3	C	502	3QZ	CAG-CAQ	-2.77	1.39	1.45
2	A	500	HEM	FE-NC	2.70	2.04	1.95
2	B	500	HEM	FE-NC	2.70	2.04	1.95
2	D	500	HEM	CAB-C3B	2.69	1.54	1.47
2	C	500	HEM	CAC-C3C	2.69	1.54	1.47
2	D	500	HEM	CMC-C2C	2.68	1.56	1.50
3	B	502	3QZ	CAG-CAQ	-2.62	1.40	1.45
3	A	502	3QZ	CAG-CAQ	-2.54	1.40	1.45
2	B	500	HEM	CAC-C3C	2.54	1.54	1.47
2	C	500	HEM	CMC-C2C	2.53	1.56	1.50
3	C	501	3QZ	CAG-CAR	2.53	1.38	1.34
2	C	500	HEM	FE-NA	2.43	2.03	1.95
2	A	500	HEM	CAC-C3C	2.38	1.53	1.47
3	C	501	3QZ	CAG-CAQ	-2.31	1.40	1.45
3	A	501	3QZ	CAX-CAW	-2.29	1.53	1.56
2	B	500	HEM	CMD-C2D	2.28	1.55	1.50
2	C	500	HEM	O2A-CGA	-2.27	1.23	1.30
3	D	501	3QZ	CAX-CAW	-2.27	1.53	1.56
2	D	500	HEM	O2A-CGA	-2.27	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	FE-NA	2.26	2.02	1.95
2	B	500	HEM	CAB-C3B	2.26	1.53	1.47
2	B	500	HEM	O1A-CGA	2.26	1.29	1.22
3	B	501	3QZ	CAX-CAW	-2.21	1.53	1.56
2	C	500	HEM	O1A-CGA	2.21	1.29	1.22
2	D	500	HEM	CMD-C2D	2.20	1.55	1.50
2	D	500	HEM	O1A-CGA	2.18	1.29	1.22
3	C	501	3QZ	CAX-CAW	-2.16	1.53	1.56
2	A	500	HEM	CAB-C3B	2.15	1.53	1.47
2	A	500	HEM	CMD-C2D	2.15	1.55	1.50
2	C	500	HEM	CAB-C3B	2.14	1.53	1.47
2	B	500	HEM	O2A-CGA	-2.13	1.23	1.30
3	A	502	3QZ	CAH-CAR	2.10	1.53	1.50
3	B	502	3QZ	CAH-CAR	2.09	1.53	1.50
2	C	500	HEM	FE-NC	2.07	2.02	1.95
2	C	500	HEM	CAA-C2A	2.07	1.56	1.51
2	A	500	HEM	FE-NA	2.06	2.02	1.95
2	A	500	HEM	O1A-CGA	2.06	1.28	1.22
2	B	500	HEM	FE-NA	2.03	2.01	1.95
2	C	500	HEM	CMA-C3A	2.02	1.54	1.50
3	C	501	3QZ	CAH-CAR	2.02	1.53	1.50

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	3QZ	CAX-CAW-CAU	-3.29	96.30	99.93
3	B	501	3QZ	CAX-CAW-CAU	-3.23	96.36	99.93
3	D	501	3QZ	CAJ-CAS-CAU	-3.09	106.94	112.08
3	D	501	3QZ	CAX-CAW-CAU	-2.96	96.66	99.93
3	D	501	3QZ	CAL-CAU-CAS	-2.93	114.42	119.10
3	C	501	3QZ	CAL-CAU-CAS	-2.85	114.55	119.10
3	A	502	3QZ	CAL-CAU-CAW	-2.79	100.13	103.70
3	B	501	3QZ	CAL-CAU-CAS	-2.76	114.69	119.10
3	C	501	3QZ	CAJ-CAS-CAU	-2.74	107.52	112.08
2	A	500	HEM	CBC-CAC-C3C	-2.74	113.84	127.53
3	C	501	3QZ	CAX-CAW-CAU	-2.73	96.92	99.93
2	B	500	HEM	CBB-CAB-C3B	-2.70	114.03	127.53
2	A	500	HEM	CBB-CAB-C3B	-2.68	114.11	127.53
3	C	502	3QZ	CAL-CAU-CAS	-2.68	114.83	119.10
3	B	502	3QZ	CAC-CAW-CAX	2.65	112.41	109.11
3	B	502	3QZ	CAL-CAU-CAS	-2.64	114.88	119.10
3	B	501	3QZ	CAC-CAW-CAX	2.64	112.40	109.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CBB-CAB-C3B	-2.63	114.37	127.53
3	C	502	3QZ	CAC-CAW-CAX	2.62	112.38	109.11
3	B	502	3QZ	CAJ-CAS-CAU	-2.62	107.73	112.08
2	B	500	HEM	CBC-CAC-C3C	-2.61	114.46	127.53
3	D	501	3QZ	CAO-CAL-CAU	-2.61	99.53	104.69
3	A	501	3QZ	CAL-CAU-CAS	-2.59	114.96	119.10
2	C	500	HEM	CBC-CAC-C3C	-2.58	114.66	127.53
2	D	500	HEM	CBC-CAC-C3C	-2.54	114.83	127.53
3	D	501	3QZ	CAC-CAW-CAX	2.52	112.25	109.11
3	B	501	3QZ	CAJ-CAS-CAU	-2.49	107.94	112.08
3	A	501	3QZ	CAJ-CAS-CAU	-2.48	107.95	112.08
2	D	500	HEM	CBB-CAB-C3B	-2.48	115.13	127.53
3	A	502	3QZ	CAJ-CAS-CAU	-2.46	107.99	112.08
2	C	500	HEM	O1A-CGA-CBA	-2.46	115.30	123.09
3	C	501	3QZ	CAL-CAU-CAW	-2.43	100.59	103.70
3	D	501	3QZ	CAH-CAR-CAG	-2.40	117.02	120.86
2	A	500	HEM	O1A-CGA-CBA	-2.40	115.49	123.09
2	D	500	HEM	O1A-CGA-CBA	-2.40	115.49	123.09
3	C	502	3QZ	CAL-CAU-CAW	-2.37	100.67	103.70
3	D	502	3QZ	CAL-CAU-CAW	-2.36	100.68	103.70
3	C	501	3QZ	CAO-CAL-CAU	-2.32	100.11	104.69
2	B	500	HEM	O1A-CGA-CBA	-2.32	115.75	123.09
3	D	502	3QZ	CAL-CAU-CAS	-2.31	115.42	119.10
3	B	502	3QZ	CAX-CAW-CAU	-2.31	97.39	99.93
3	B	501	3QZ	CAO-CAL-CAU	-2.29	100.17	104.69
3	C	501	3QZ	CAC-CAW-CAX	2.26	111.92	109.11
3	A	501	3QZ	CAO-CAL-CAU	-2.24	100.26	104.69
3	D	501	3QZ	CAL-CAU-CAW	-2.23	100.84	103.70
3	A	501	3QZ	CAC-CAW-CAX	2.20	111.85	109.11
3	A	502	3QZ	CAC-CAW-CAX	2.18	111.83	109.11
3	B	501	3QZ	CAI-CAQ-CAG	2.18	120.05	116.73
3	A	502	3QZ	CAO-CAL-CAU	-2.16	100.42	104.69
3	D	502	3QZ	CAC-CAW-CAX	2.15	111.79	109.11
3	B	501	3QZ	CAL-CAU-CAW	-2.15	100.94	103.70
3	B	502	3QZ	CAH-CAR-CAG	-2.15	117.43	120.86
3	A	502	3QZ	CAL-CAU-CAS	-2.14	115.69	119.10
3	D	501	3QZ	CAH-CAR-CAV	2.13	120.52	116.76
3	A	501	3QZ	CAO-CAX-CAW	2.11	105.17	103.24
3	A	501	3QZ	CAH-CAR-CAG	-2.10	117.50	120.86
3	A	501	3QZ	CAL-CAU-CAW	-2.10	101.01	103.70
3	C	502	3QZ	CAK-CAN-CAW	-2.08	109.25	112.85
3	B	501	3QZ	CAH-CAR-CAV	2.08	120.43	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	3QZ	CAX-CAW-CAU	-2.07	97.64	99.93
2	A	500	HEM	CHD-C4C-NC	-2.07	122.20	124.45
3	B	502	3QZ	CAL-CAU-CAW	-2.07	101.05	103.70
3	B	501	3QZ	CAH-CAR-CAG	-2.07	117.55	120.86
3	C	502	3QZ	CAJ-CAS-CAU	-2.07	108.64	112.08
3	C	502	3QZ	CAX-CAW-CAU	-2.04	97.68	99.93
3	C	501	3QZ	CAK-CAN-CAW	-2.04	109.33	112.85
3	A	502	3QZ	CAI-CAQ-CAG	2.03	119.81	116.73
3	C	501	3QZ	CAH-CAR-CAG	-2.03	117.62	120.86
3	A	501	3QZ	CAH-CAR-CAV	2.01	120.31	116.76
3	A	502	3QZ	CAH-CAR-CAG	-2.01	117.65	120.86
3	A	501	3QZ	CAK-CAN-CAW	-2.01	109.39	112.85

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2B-C3B-CAB-CBB
2	A	500	HEM	C4B-C3B-CAB-CBB
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2B-C3B-CAB-CBB
2	B	500	HEM	C4B-C3B-CAB-CBB
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C2B-C3B-CAB-CBB
2	C	500	HEM	C4B-C3B-CAB-CBB
2	C	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C2B-C3B-CAB-CBB
2	D	500	HEM	C4B-C3B-CAB-CBB
2	D	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

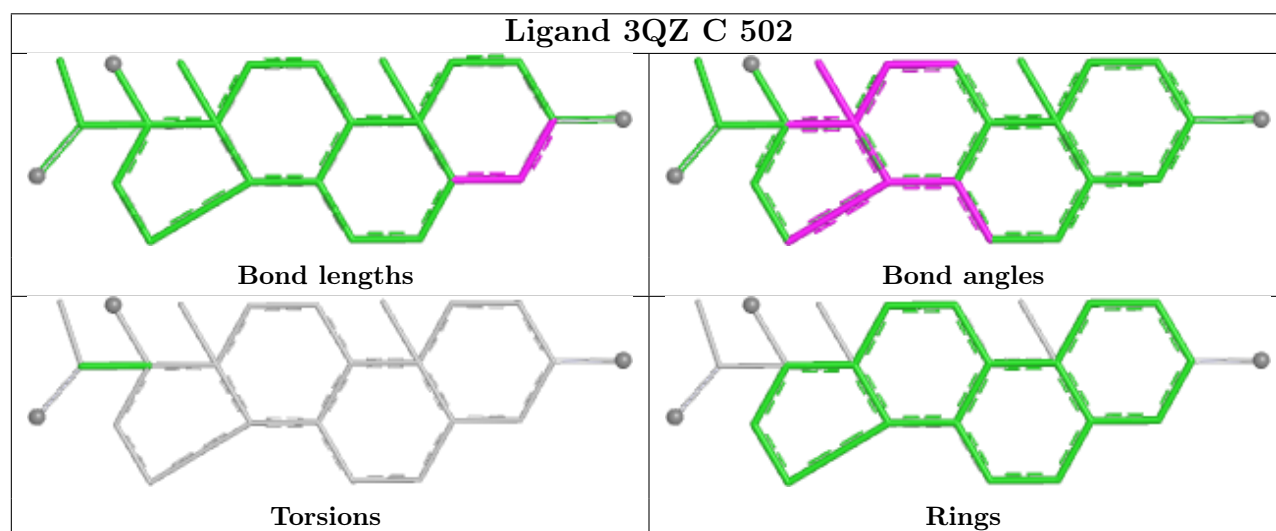
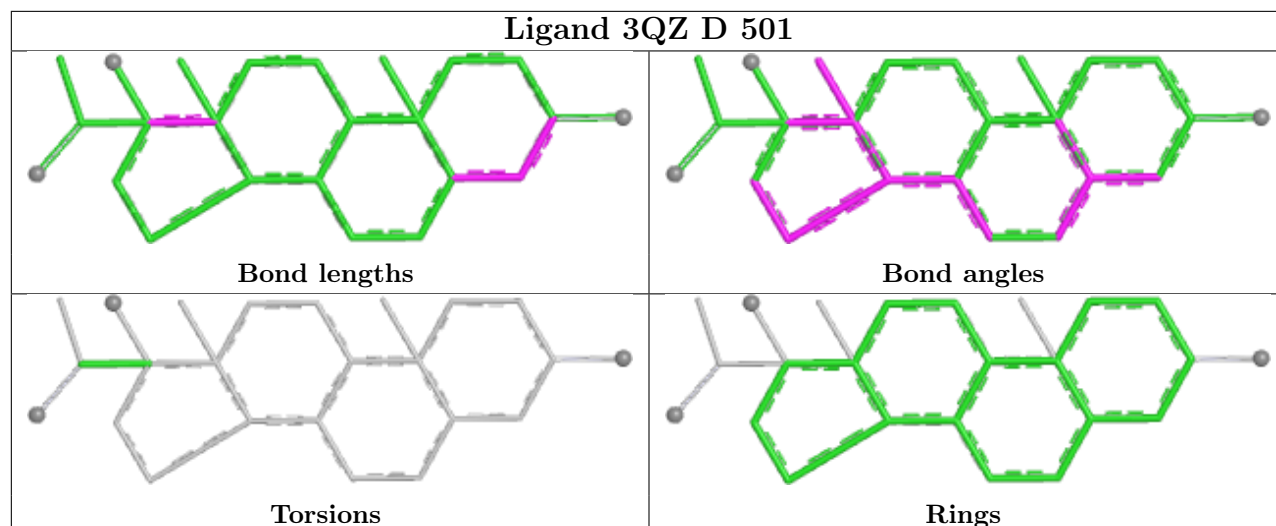
Mol	Chain	Res	Type	Atoms
2	C	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O1D
2	D	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A

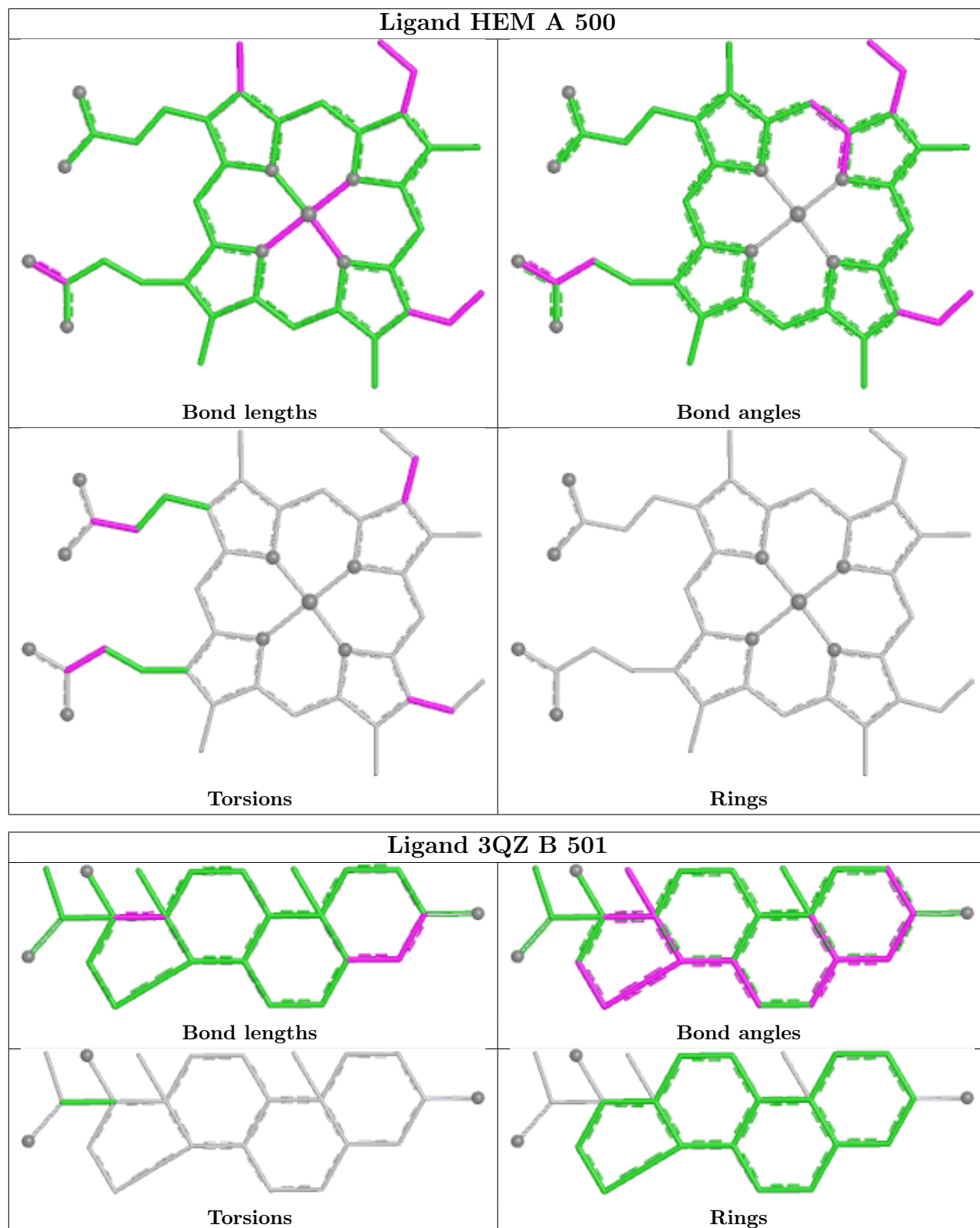
There are no ring outliers.

11 monomers are involved in 97 short contacts:

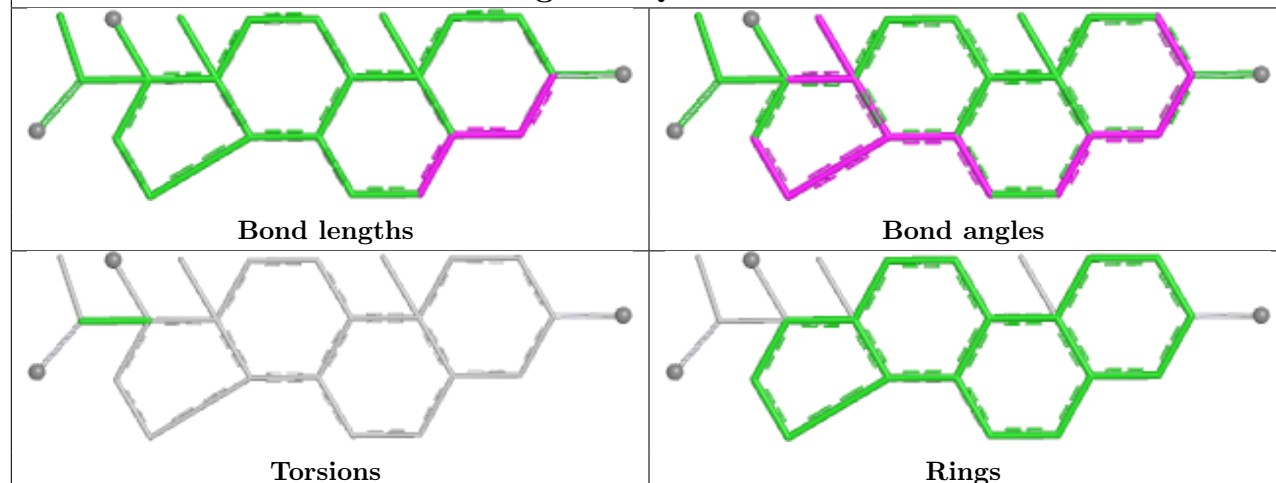
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	3QZ	10	0
3	C	502	3QZ	1	0
2	A	500	HEM	6	0
3	B	501	3QZ	12	0
3	A	502	3QZ	5	0
3	A	501	3QZ	14	0
3	B	502	3QZ	8	0
2	D	500	HEM	11	0
2	B	500	HEM	5	0
2	C	500	HEM	13	0
3	C	501	3QZ	12	0

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

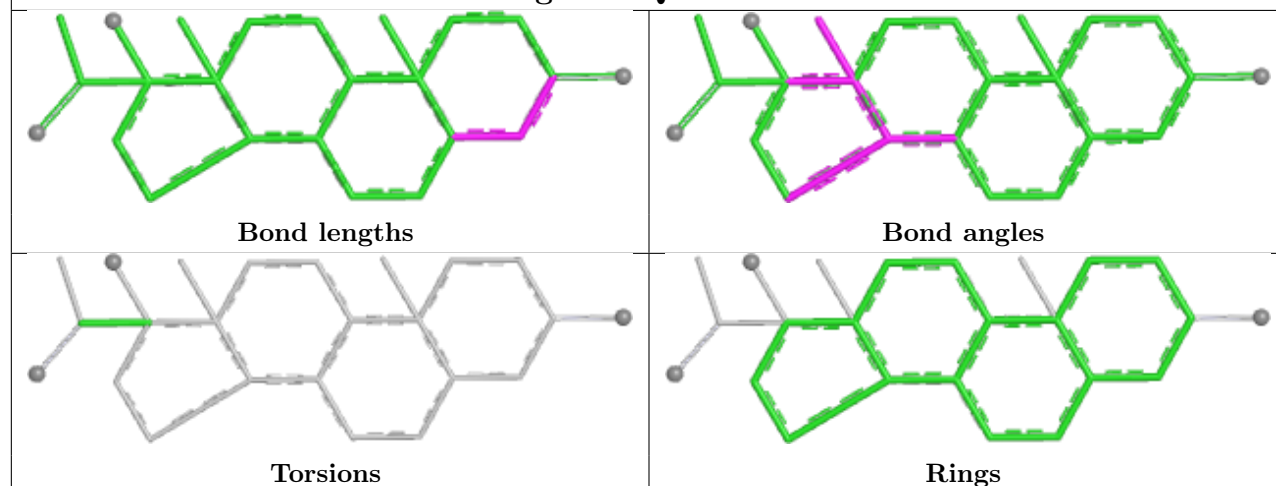




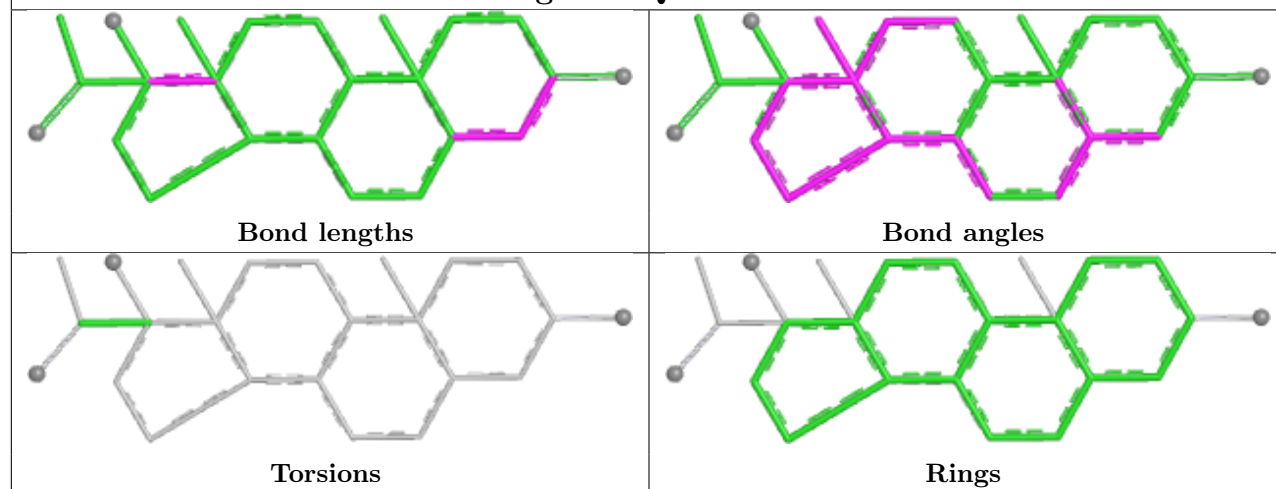
Ligand 3QZ A 502



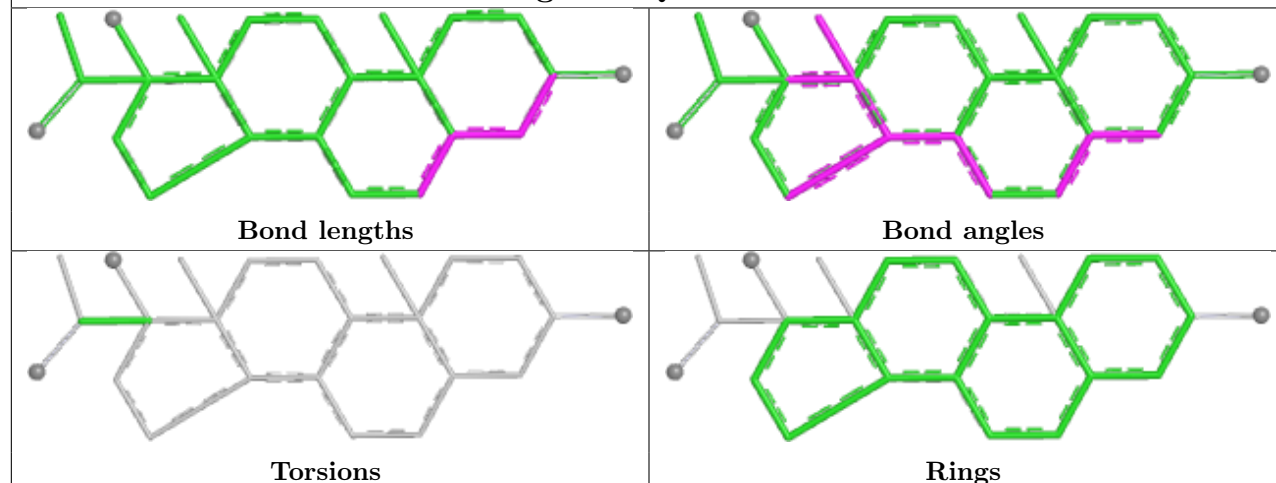
Ligand 3QZ D 502



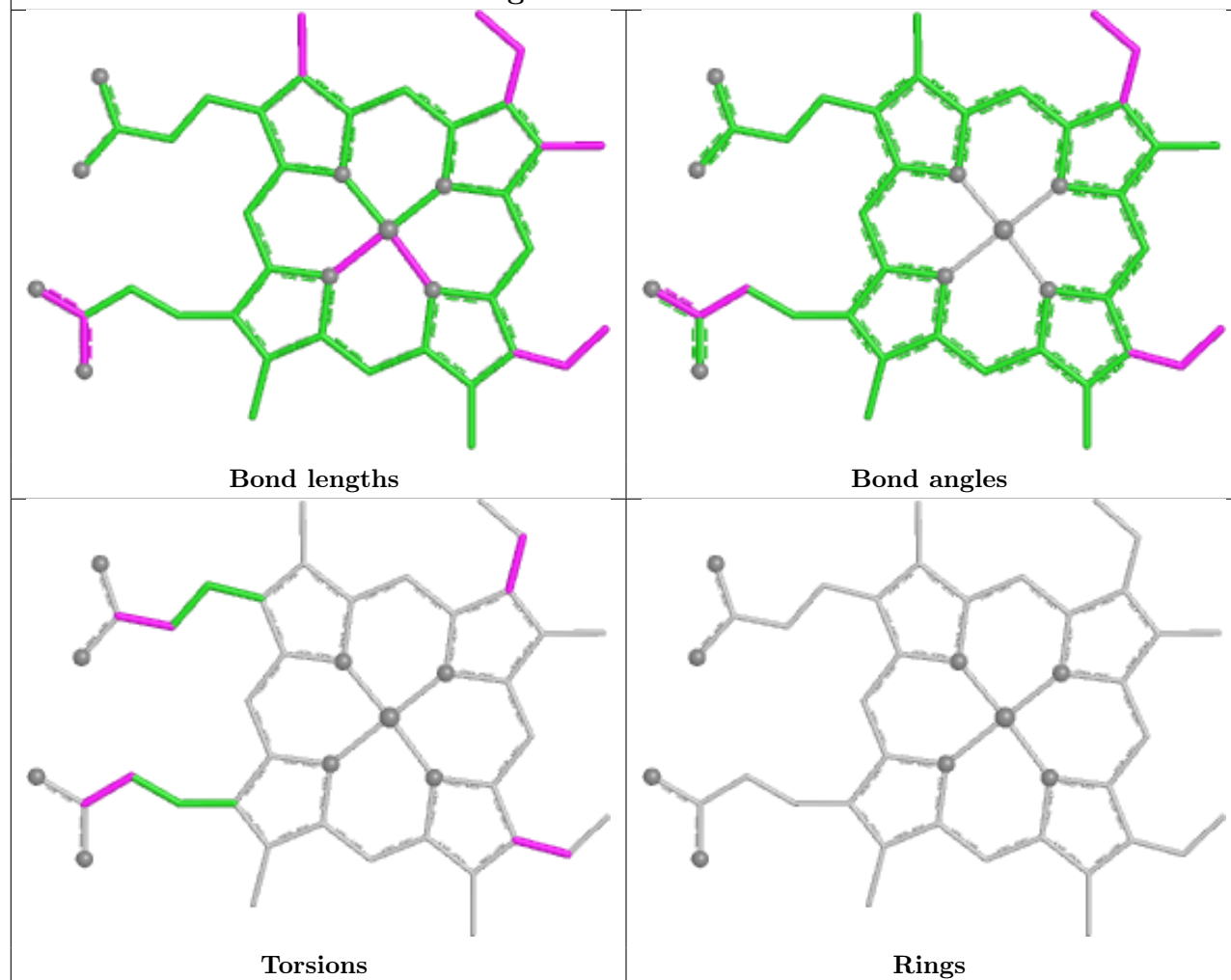
Ligand 3QZ A 501

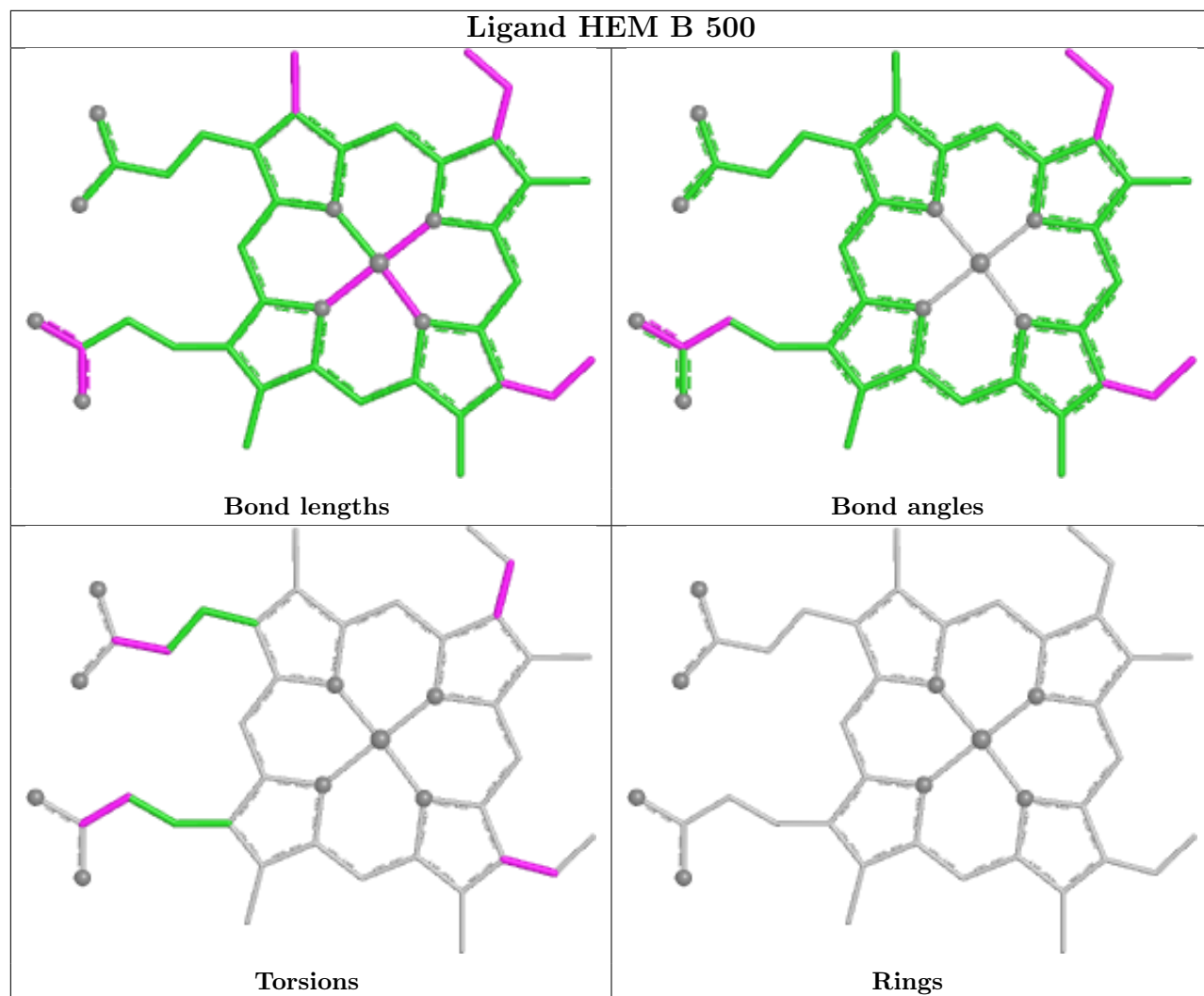


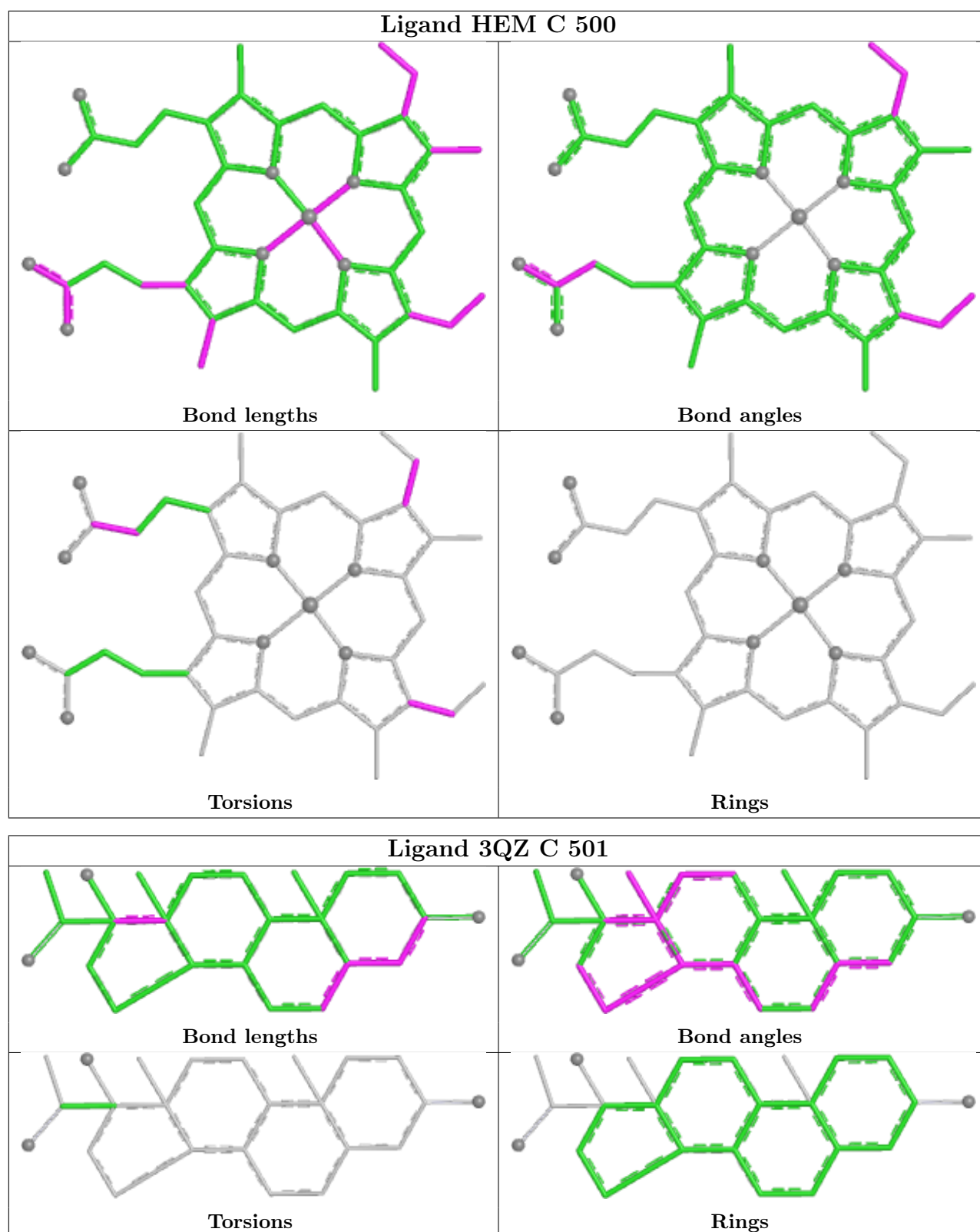
Ligand 3QZ B 502



Ligand HEM D 500







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	445/496 (89%)	-1.32	0 100 100	61, 112, 161, 252	0
1	B	436/496 (87%)	-1.32	0 100 100	61, 113, 169, 252	0
1	C	437/496 (88%)	-1.26	0 100 100	61, 117, 177, 252	0
1	D	434/496 (87%)	-1.29	0 100 100	61, 116, 175, 252	0
All	All	1752/1984 (88%)	-1.30	0 100 100	61, 115, 171, 252	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3QZ	A	501	24/24	0.98	0.06	54,79,87,91	0
3	3QZ	A	502	24/24	0.98	0.05	76,86,93,93	0
3	3QZ	C	501	24/24	0.98	0.07	54,82,101,101	0
3	3QZ	D	502	24/24	0.98	0.05	83,88,91,110	0

Continued on next page...

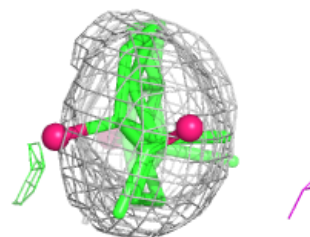
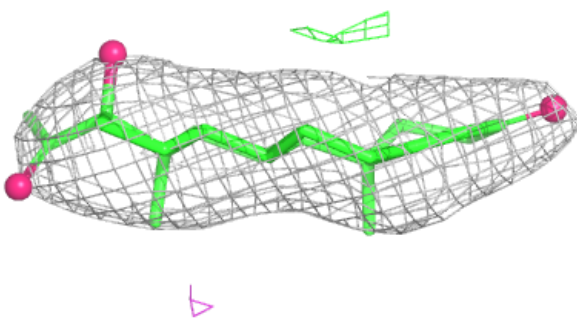
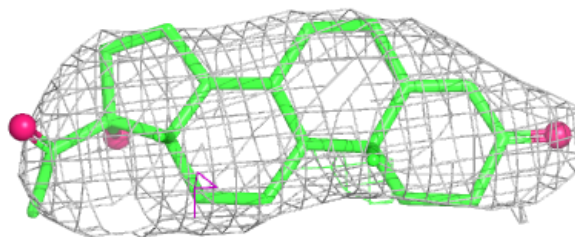
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	500	43/43	0.99	0.05	51,105,127,139	0
3	3QZ	B	501	24/24	0.99	0.06	54,87,104,137	0
3	3QZ	B	502	24/24	0.99	0.08	75,84,91,91	24
2	HEM	C	500	43/43	0.99	0.05	51,95,132,162	0
3	3QZ	C	502	24/24	0.99	0.05	82,86,91,92	0
3	3QZ	D	501	24/24	0.99	0.06	59,96,103,111	0
2	HEM	A	500	43/43	0.99	0.05	51,77,92,113	0
2	HEM	D	500	43/43	1.00	0.04	51,96,125,140	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

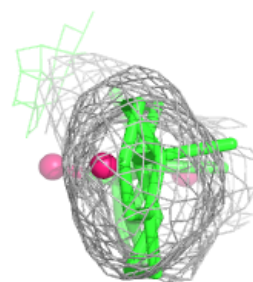
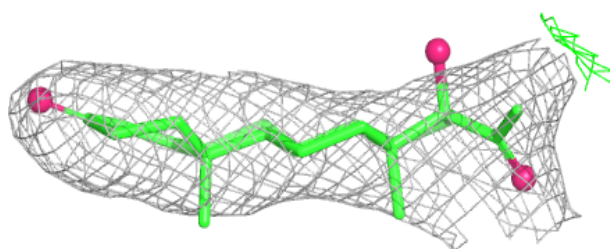
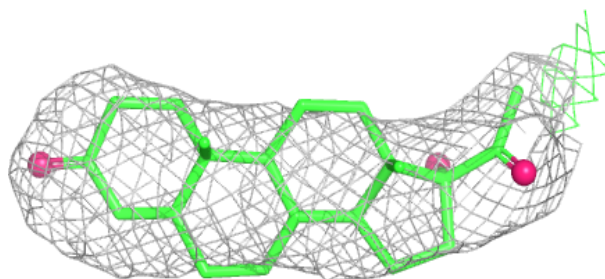
Electron density around 3QZ A 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

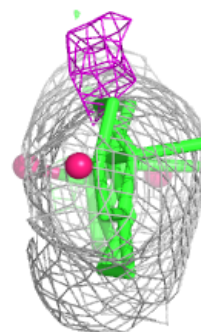
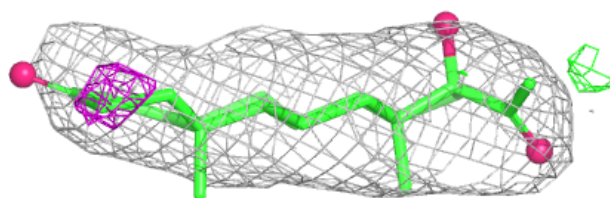
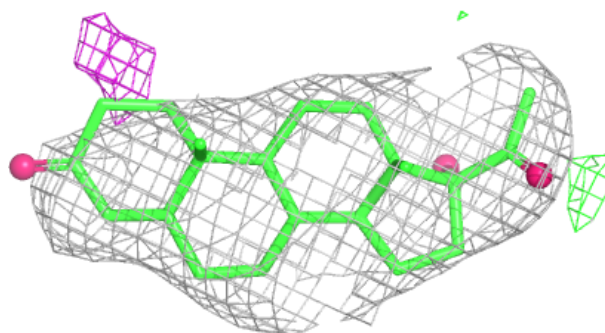


Electron density around 3QZ A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

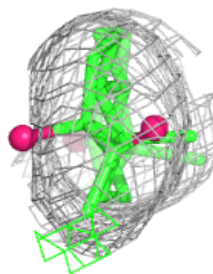
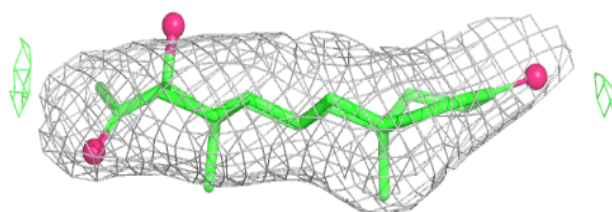
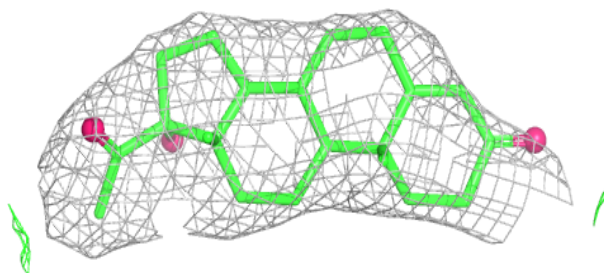
**Electron density around 3QZ C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

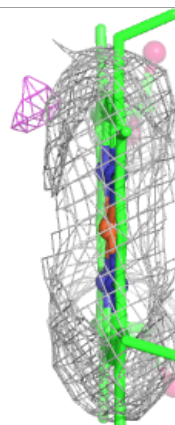
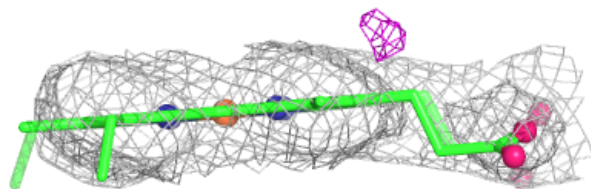
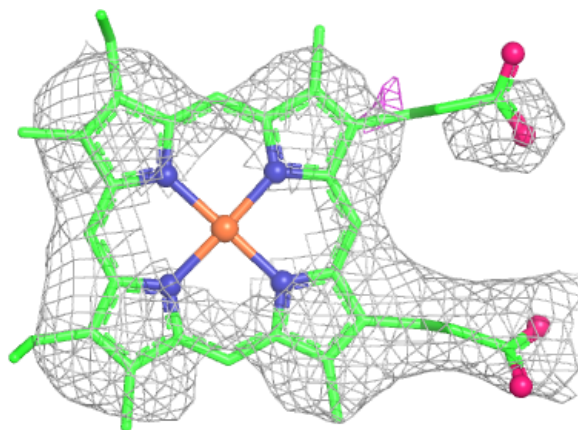


Electron density around 3QZ D 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

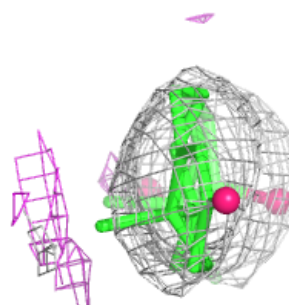
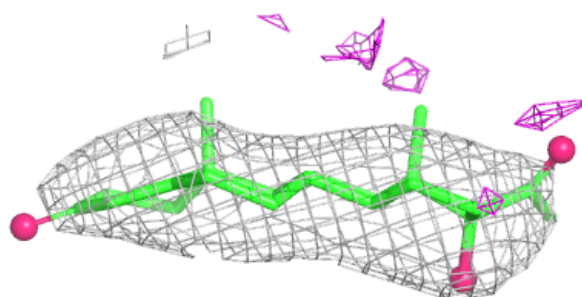
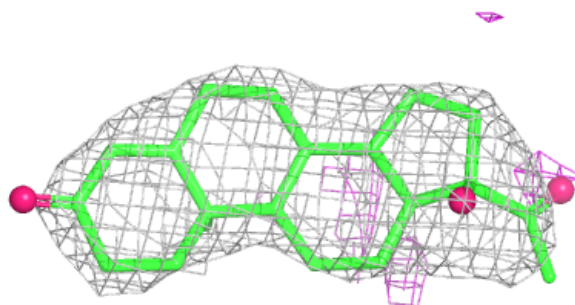
**Electron density around HEM B 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

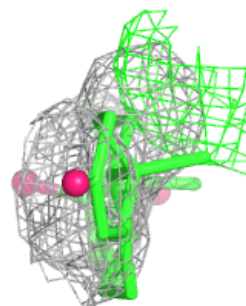
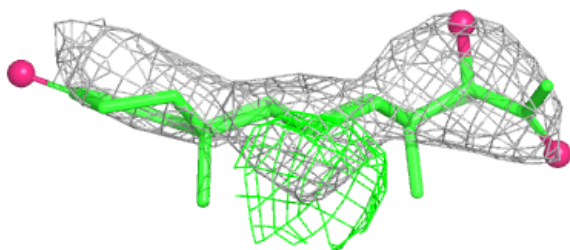
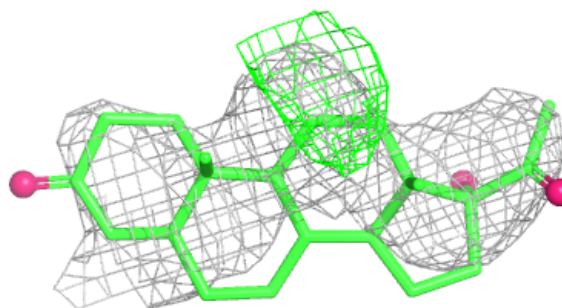


Electron density around 3QZ B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

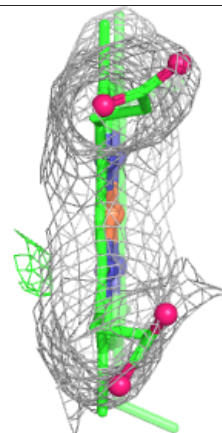
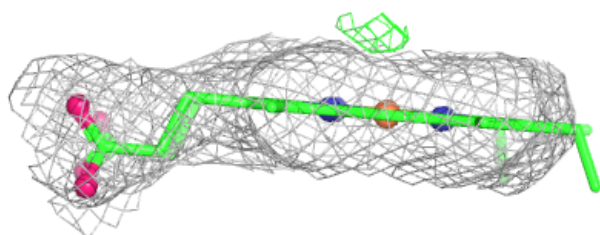
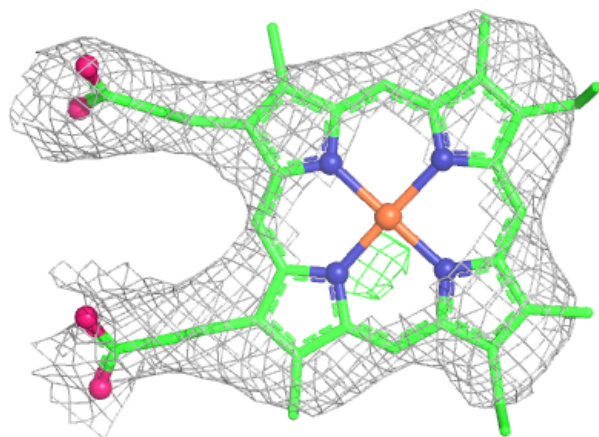
**Electron density around 3QZ B 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

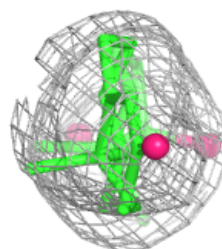
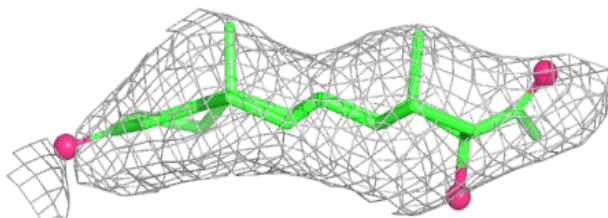
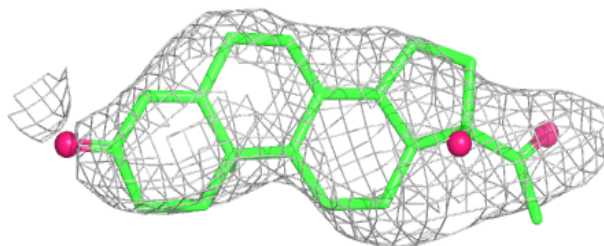


Electron density around HEM C 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

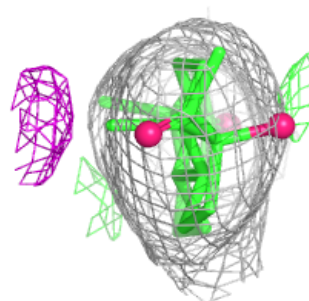
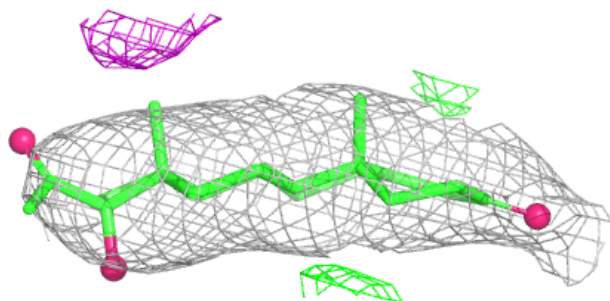
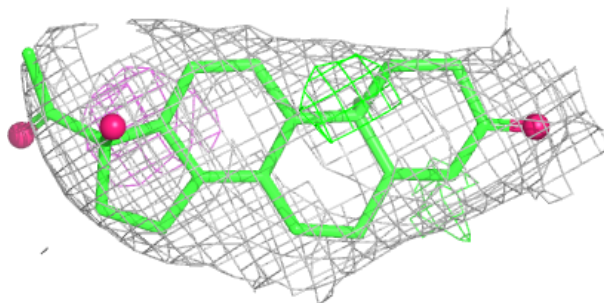
**Electron density around 3QZ C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

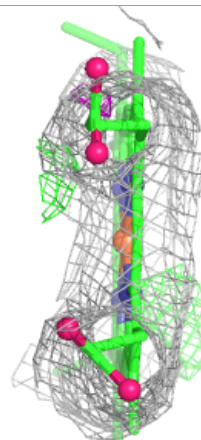
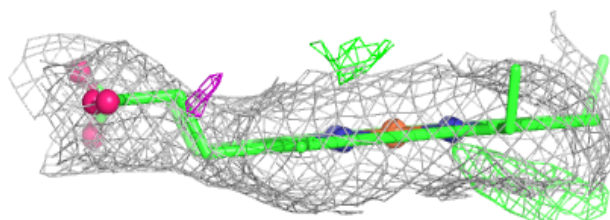
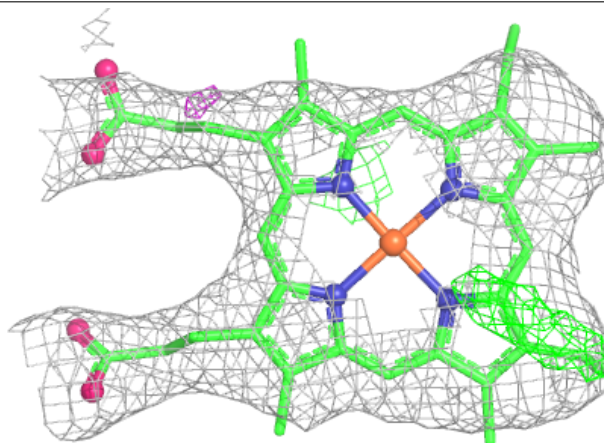


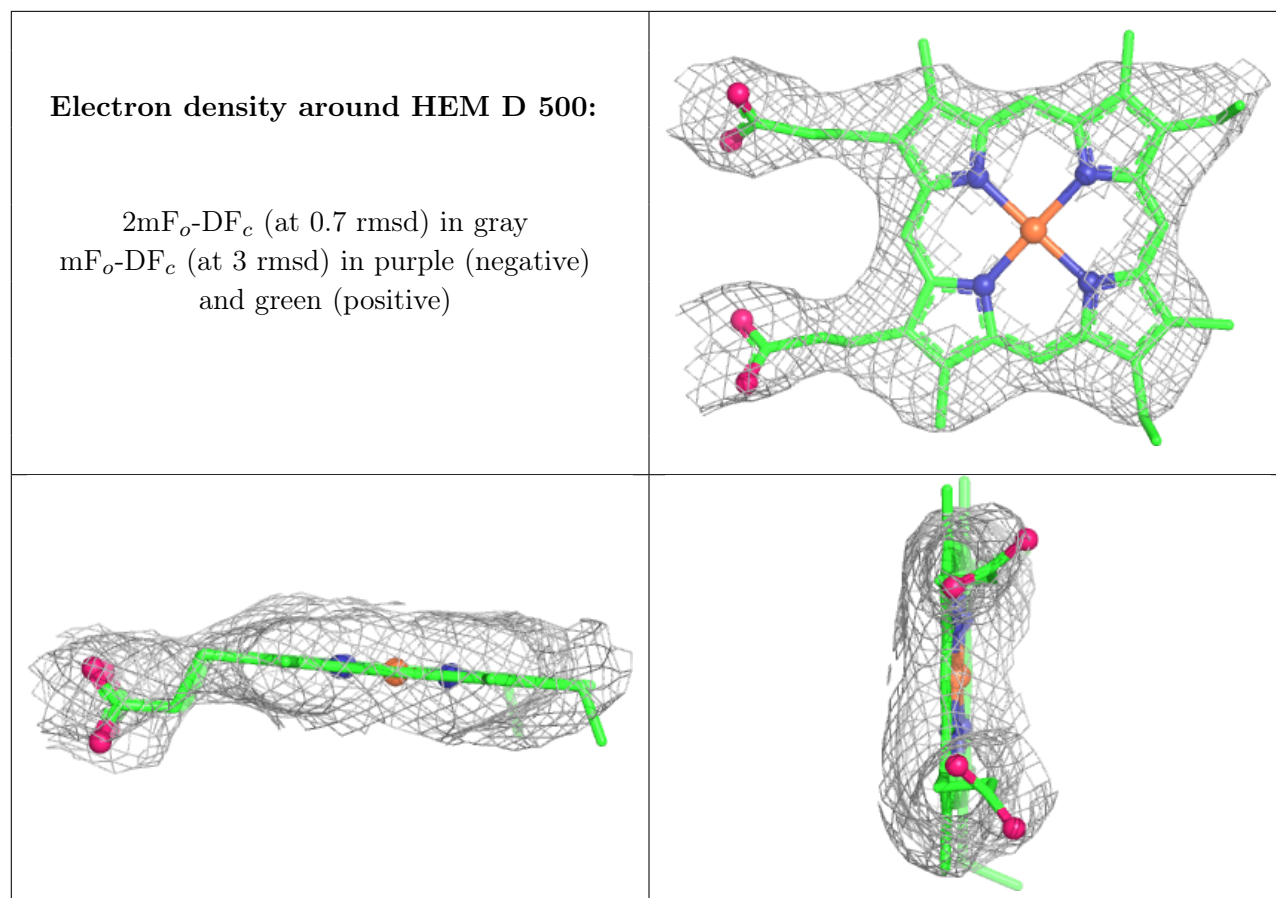
Electron density around 3QZ D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HEM A 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.