Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2021 – 11:27 AM EDT

PDB ID	:	1M57
Title	:	Structure of cytochrome c oxidase from Rhodobacter sphaeroides (EQ(I-286) mutant))
Authors	:	Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on	:	2002-07-08
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

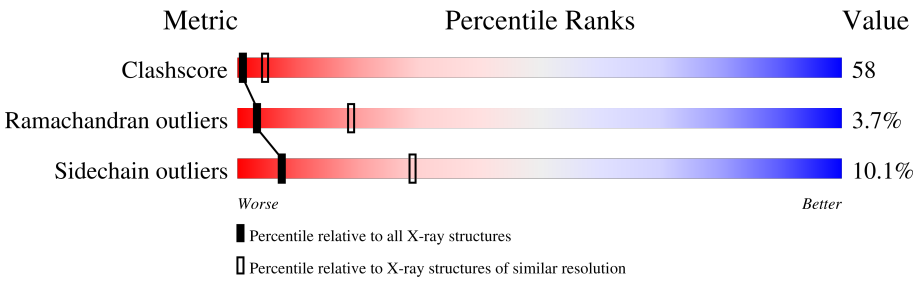
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	21% 53% 20% • •
1	G	566	20% 53% 20% • •
2	B	264	33% 48% 15% • •
2	H	264	29% 49% 19% • •
3	C	266	35% 51% 12% •
3	I	266	38% 48% 14% •
4	D	51	29% 41% 12% 18%
4	J	51	25% 47% 8% • 18%

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
8	HEA	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	X	-
8	HEA	G	1002	X	-	-	-
9	3PE	C	2010	-	-	X	-
9	3PE	C	2013	-	-	X	-
9	3PE	G	3012	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 18934 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4322	2892	685	714	31	0	0	0
1	G	547	4322	2892	685	714	31	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLN	GLU	engineered mutation	UNP P33517
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	286	GLN	GLU	engineered mutation	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	2046	1334	332	374	6	0	0	0
2	H	260	2046	1334	332	374	6	0	0	0

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	265	2139	1448	342	337	12	0	0	0
3	I	265	2139	1448	342	337	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	42	311	203	52	54	2	0	0	0
4	J	42	311	203	52	54	2	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
5	A	1	1	1	0	0
5	B	2	2	2	0	0
5	G	1	1	1	0	0
5	H	2	2	2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0

Continued on next page...

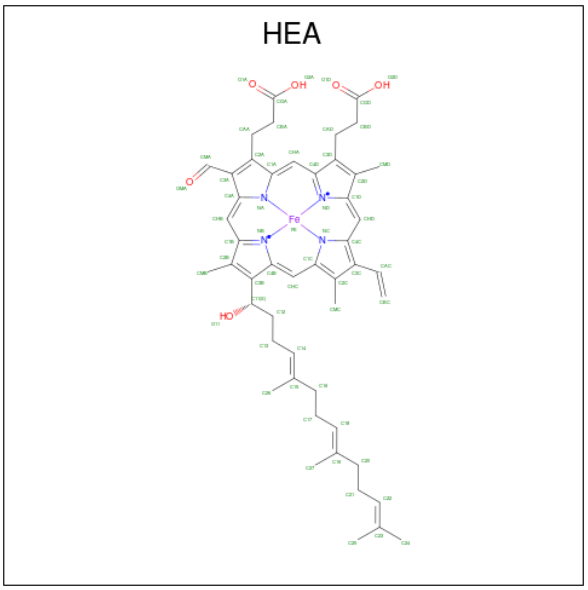
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	G	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

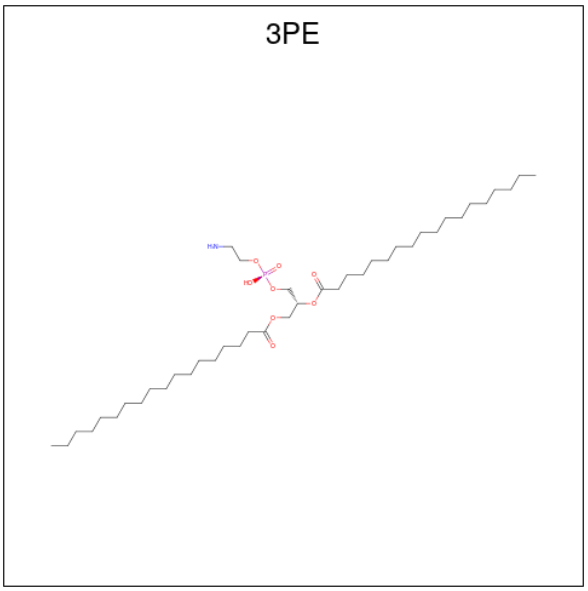
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	G	1	1	1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	51	41	1	8	1	0	0
9	A	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	D	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	J	1	51	41	1	8	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	97	97	97	0	0
			Total	O		
10	B	70	70	70	0	0
			Total	O		
10	C	38	38	38	0	0
			Total	O		
10	D	13	13	13	0	0
			Total	O		
10	G	107	107	107	0	0
			Total	O		
10	H	64	64	64	0	0
			Total	O		
10	I	37	37	37	0	0
			Total	O		
10	J	10	10	10	0	0

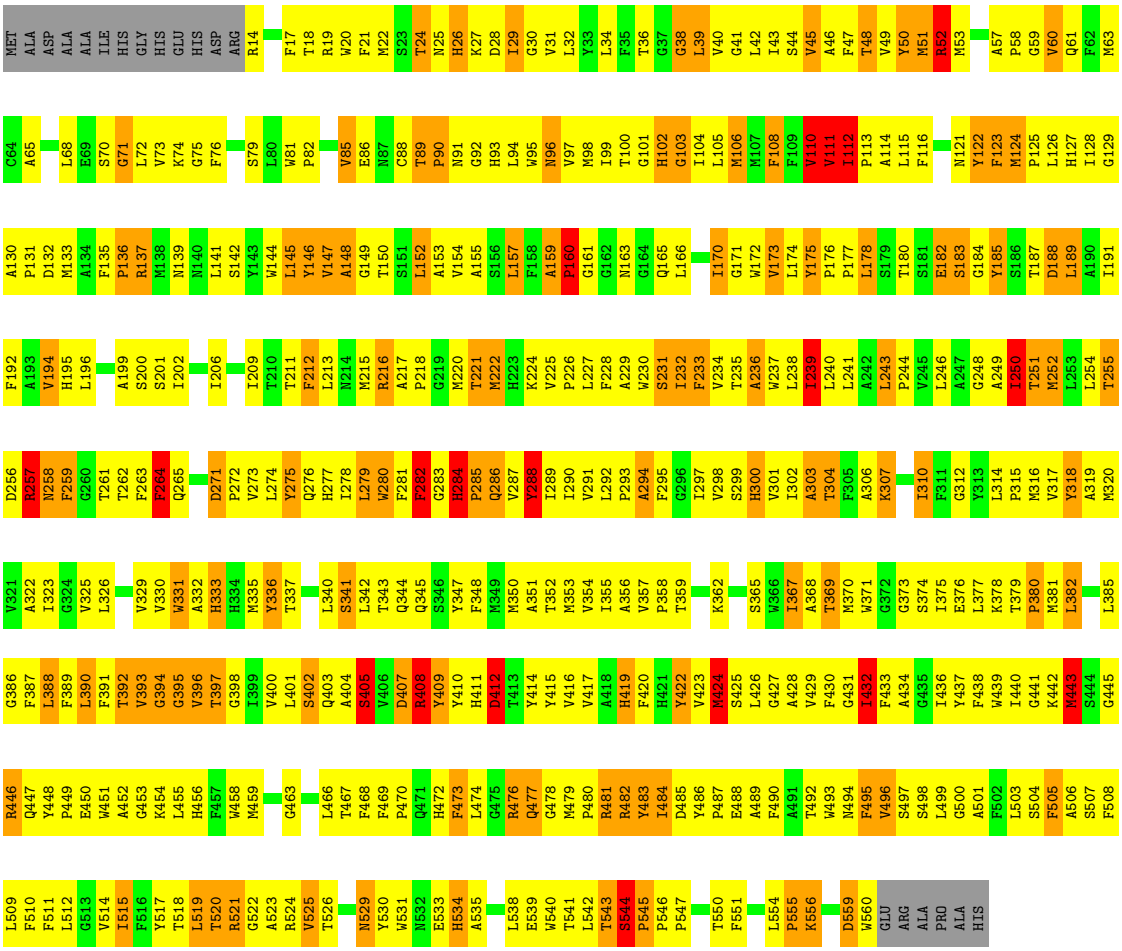
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

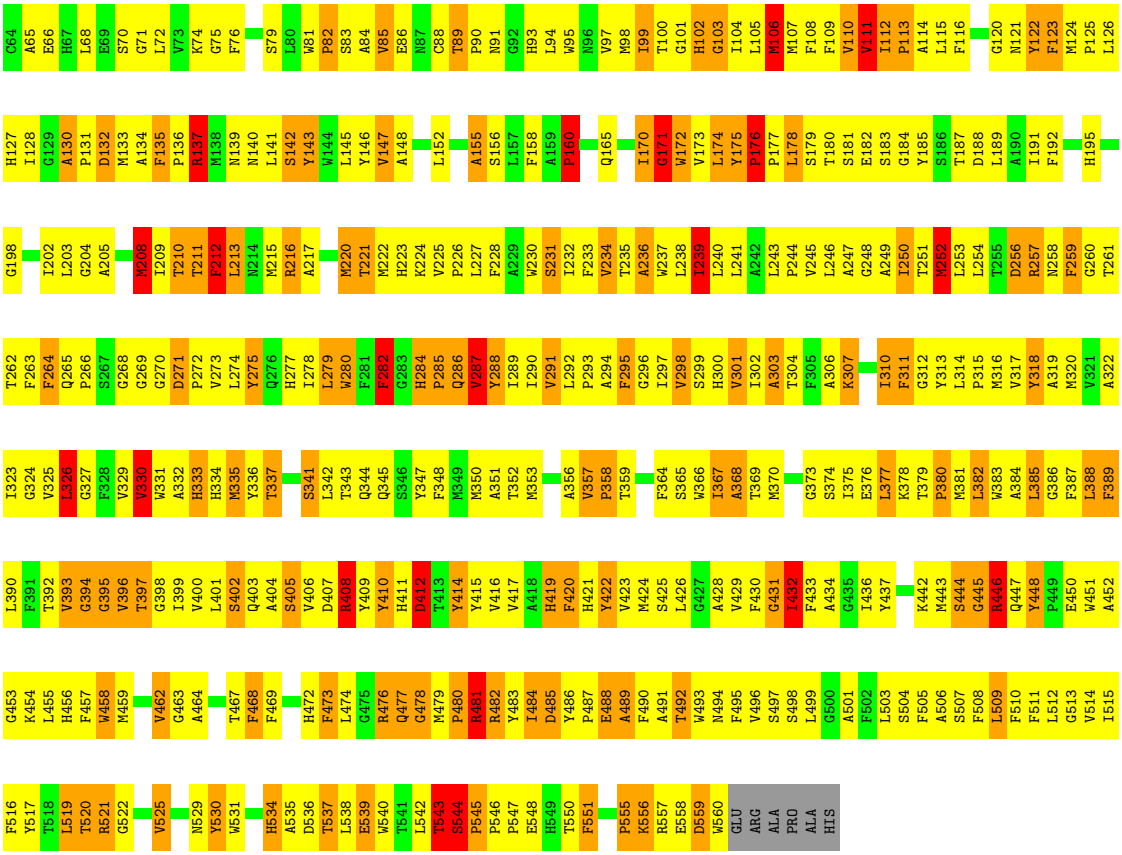
• Molecule 1: CYTOCHROME C OXIDASE

Chain A: 21% 53% 20%



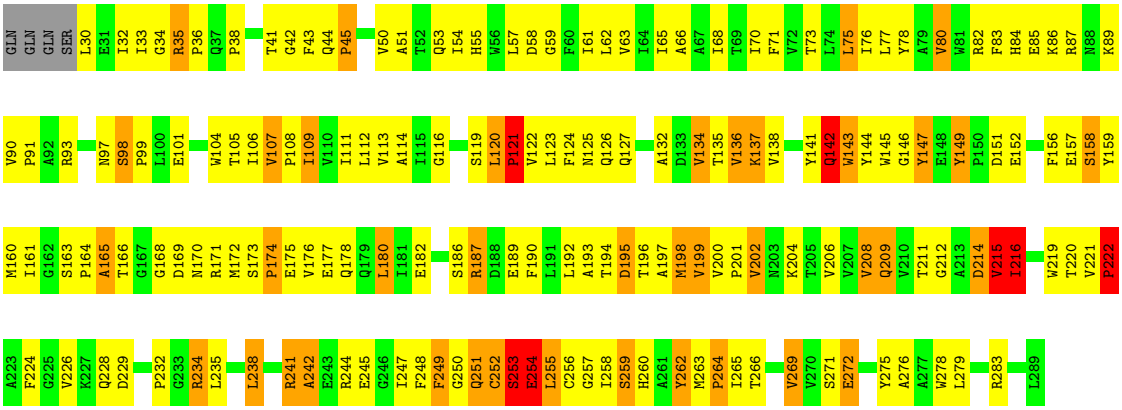
• Molecule 1: CYTOCHROME C OXIDASE

Chain G: 20% 53% 20%



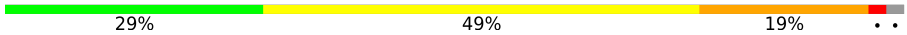
- Molecule 2: CYTOCHROME C OXIDASE

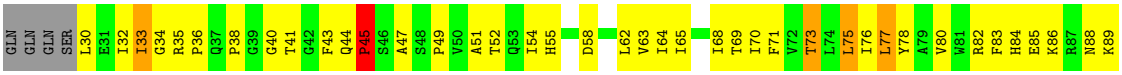
Chain B:

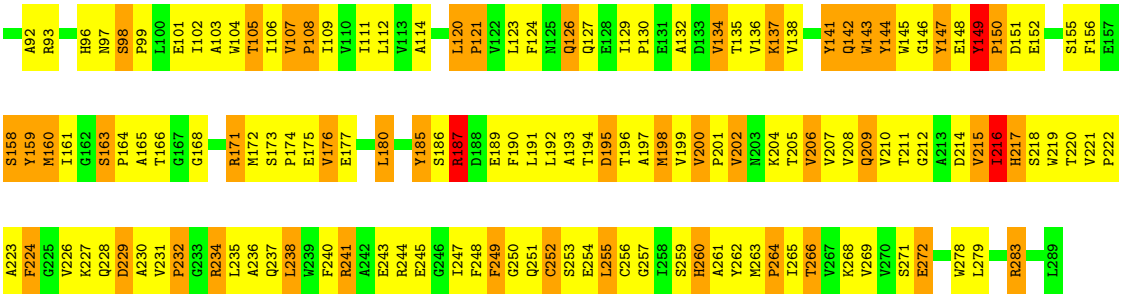


- Molecule 2: CYTOCHROME C OXIDASE

Chain H:

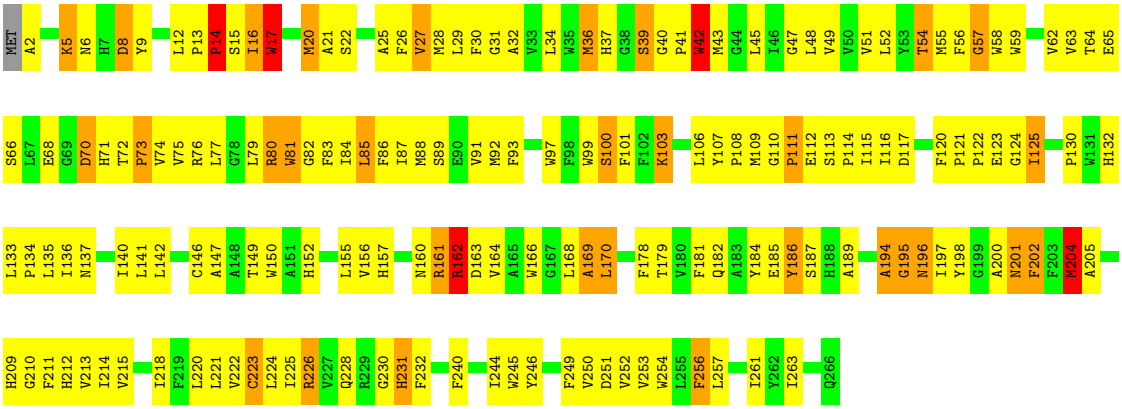






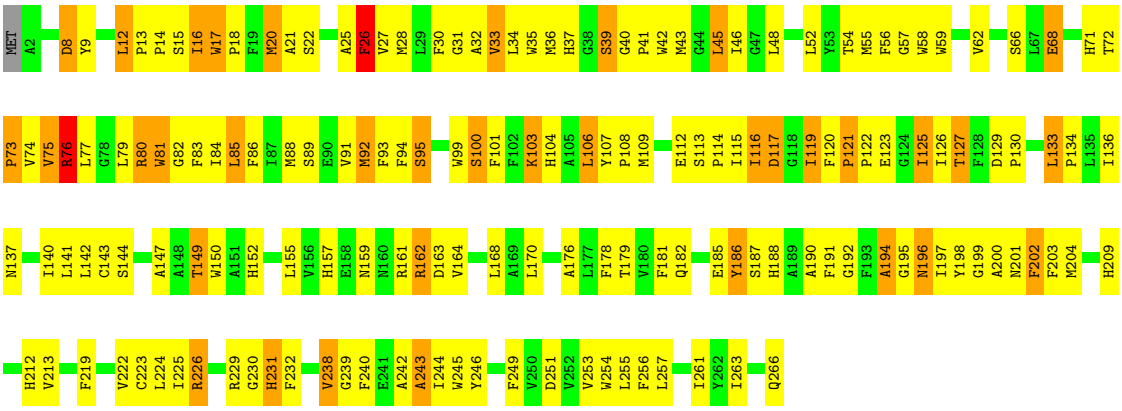
- Molecule 3: CYTOCHROME C OXIDASE

Chain C: 35% 51% 12%



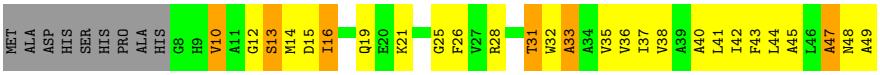
- Molecule 3: CYTOCHROME C OXIDASE

Chain I: 38% 48% 14%



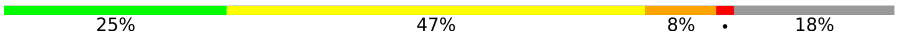
- Molecule 4: CYTOCHROME C OXIDASE

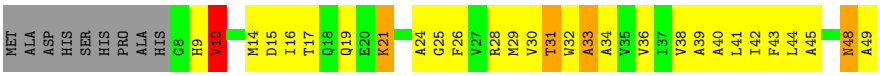
Chain D: 29% 41% 12% 18%



- Molecule 4: CYTOCHROME C OXIDASE

Chain J:


25%
47%
8%
•
18%


MET
ALA
ASP
HIS
SER
HIS
PRO
ALA
HIS
G8
H9
V10
M14
D15
I16
T17
Q18
Q19
E20
K21
A24
G25
F26
V27
R28
M29
V30
T31
W32
A33
A34
V35
V36
I37
V38
A39
A40
L41
I42
F43
L44
A45
N48
A49

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	340.72Å 340.72Å 89.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	4.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.293 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

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: CU, MG, CA, 3PE, HEA

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	0.73	0/4482	2.01	128/6114 (2.1%)
1	G	0.75	1/4482 (0.0%)	2.06	133/6114 (2.2%)
2	B	0.60	0/2105	1.93	56/2879 (1.9%)
2	H	0.65	0/2105	1.96	58/2879 (2.0%)
3	C	0.57	0/2232	1.66	33/3054 (1.1%)
3	I	0.59	0/2232	1.65	30/3054 (1.0%)
4	D	0.58	0/316	1.63	4/428 (0.9%)
4	J	0.60	0/316	1.63	4/428 (0.9%)
All	All	0.67	1/18270 (0.0%)	1.91	446/24950 (1.8%)

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	A	0	19
1	G	0	16
2	B	0	6
2	H	0	3
3	C	0	5
3	I	0	7
4	D	0	1
All	All	0	57

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	ILE	N-CA	5.08	1.56	1.46

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	52	ARG	NE-CZ-NH2	-24.46	108.07	120.30
2	B	171	ARG	NE-CZ-NH1	19.39	130.00	120.30
1	A	543	THR	C-N-CA	19.24	169.80	121.70
1	G	543	THR	C-N-CA	16.53	163.02	121.70
2	H	171	ARG	NE-CZ-NH1	15.75	128.17	120.30
2	B	35	ARG	NE-CZ-NH2	-14.49	113.05	120.30
1	G	172	TRP	CA-CB-CG	14.03	140.35	113.70
1	A	106	MET	CA-CB-CG	-13.99	89.52	113.30
1	A	172	TRP	CA-CB-CG	13.67	139.67	113.70
2	B	93	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	A	14	ARG	NE-CZ-NH2	13.53	127.06	120.30
2	H	214	ASP	CB-CG-OD1	13.25	130.22	118.30
1	G	175	TYR	CA-CB-CG	12.91	137.92	113.40
1	G	412	ASP	CB-CG-OD1	-12.85	106.73	118.30
1	G	106	MET	CA-CB-CG	-12.71	91.70	113.30
2	H	234	ARG	NE-CZ-NH1	-12.15	114.23	120.30
2	H	252	CYS	N-CA-CB	11.82	131.87	110.60
3	I	229	ARG	NE-CZ-NH2	-11.41	114.59	120.30
2	H	234	ARG	NE-CZ-NH2	11.38	125.99	120.30
2	H	93	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	G	545	PRO	N-CA-CB	11.24	116.79	103.30
3	I	226	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	G	476	ARG	NE-CZ-NH2	11.10	125.85	120.30
1	A	111	VAL	CA-C-N	11.09	141.59	117.20
3	C	226	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	G	110	VAL	CA-CB-CG2	10.83	127.15	110.90
2	B	171	ARG	CD-NE-CZ	10.71	138.59	123.60
1	A	146	TYR	CB-CG-CD1	10.65	127.39	121.00
2	H	82	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	G	123	PHE	CB-CG-CD2	-10.44	113.49	120.80
1	A	408	ARG	NE-CZ-NH1	-10.20	115.20	120.30
3	C	162	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	28	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	G	544	SER	CA-C-O	-9.96	99.18	120.10
1	G	123	PHE	CB-CG-CD1	9.85	127.69	120.80
1	A	256	ASP	CB-CG-OD2	9.69	127.02	118.30
2	B	107	VAL	CA-CB-CG1	9.64	125.36	110.90
1	A	476	ARG	NE-CZ-NH2	9.54	125.07	120.30
2	H	137	LYS	N-CA-CB	9.49	127.68	110.60
1	A	146	TYR	CB-CG-CD2	-9.48	115.31	121.00
2	B	143	TRP	CB-CA-C	9.39	129.19	110.40
2	H	58	ASP	CB-CG-OD2	9.37	126.73	118.30
1	G	143	TYR	CB-CG-CD1	-9.29	115.42	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	35	ARG	NH1-CZ-NH2	9.21	129.54	119.40
1	G	275	TYR	CB-CG-CD1	-9.20	115.48	121.00
1	A	544	SER	CA-C-O	-9.20	100.79	120.10
2	H	171	ARG	CD-NE-CZ	9.12	136.37	123.60
1	G	52	ARG	NH1-CZ-NH2	9.09	129.40	119.40
3	I	80	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	G	236	ALA	N-CA-CB	8.95	122.62	110.10
1	G	216	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	G	271	ASP	CB-CG-OD1	8.93	126.34	118.30
1	A	123	PHE	CB-CG-CD1	8.93	127.05	120.80
1	G	172	TRP	N-CA-CB	8.93	126.67	110.60
1	G	111	VAL	C-N-CA	-8.89	99.47	121.70
3	I	76	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	G	212	PHE	CB-CG-CD1	8.81	126.97	120.80
1	A	545	PRO	N-CA-CB	8.79	113.85	103.30
1	A	318	TYR	CB-CG-CD2	8.69	126.22	121.00
2	B	82	ARG	CD-NE-CZ	8.69	135.76	123.60
3	I	8	ASP	CB-CG-OD1	8.62	126.06	118.30
1	G	545	PRO	CA-N-CD	-8.61	99.45	111.50
1	G	468	PHE	CB-CG-CD1	8.60	126.82	120.80
1	A	229	ALA	N-CA-CB	8.59	122.13	110.10
1	G	446	ARG	NE-CZ-NH2	8.57	124.58	120.30
1	A	521	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	G	234	VAL	CA-CB-CG1	8.49	123.64	110.90
1	A	545	PRO	CA-N-CD	-8.47	99.64	111.50
1	G	534	HIS	CA-CB-CG	-8.46	99.22	113.60
1	A	175	TYR	CA-CB-CG	8.45	129.45	113.40
1	G	288	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	G	414	TYR	CB-CG-CD2	-8.34	116.00	121.00
4	J	28	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	A	284	HIS	CA-CB-CG	-8.31	99.47	113.60
3	C	204	MET	CG-SD-CE	8.25	113.40	100.20
3	C	223	CYS	CA-CB-SG	-8.20	99.25	114.00
1	A	412	ASP	CB-CG-OD1	-8.17	110.94	118.30
1	G	288	TYR	CA-CB-CG	-8.15	97.91	113.40
2	H	93	ARG	CD-NE-CZ	8.15	135.00	123.60
2	H	35	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	B	152	GLU	OE1-CD-OE2	-8.03	113.67	123.30
2	H	229	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	111	VAL	O-C-N	-7.97	109.95	122.70
1	A	19	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	G	318	TYR	CB-CG-CD2	7.93	125.76	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	162	ARG	NE-CZ-NH2	-7.91	116.34	120.30
2	B	58	ASP	CB-CG-OD2	7.90	125.41	118.30
2	B	82	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	G	14	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	A	123	PHE	CB-CG-CD2	-7.88	115.28	120.80
1	G	106	MET	CG-SD-CE	-7.88	87.60	100.20
1	A	481	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	H	159	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	A	280	TRP	CA-CB-CG	-7.78	98.91	113.70
1	G	279	LEU	CA-CB-CG	-7.73	97.51	115.30
2	B	195	ASP	CB-CG-OD1	7.71	125.24	118.30
1	G	383	TRP	CB-CG-CD2	7.70	136.60	126.60
1	G	170	ILE	CB-CA-C	-7.68	96.23	111.60
1	G	408	ARG	CG-CD-NE	-7.68	95.67	111.80
1	G	14	ARG	NE-CZ-NH2	7.66	124.13	120.30
3	C	204	MET	CA-CB-CG	7.63	126.27	113.30
2	B	195	ASP	CB-CG-OD2	-7.62	111.44	118.30
3	C	226	ARG	NE-CZ-NH1	7.61	124.10	120.30
3	I	119	ILE	CB-CA-C	-7.59	96.42	111.60
2	B	171	ARG	NH1-CZ-NH2	-7.58	111.07	119.40
1	G	335	MET	CA-CB-CG	7.55	126.13	113.30
1	G	172	TRP	NE1-CE2-CZ2	-7.52	122.12	130.40
2	H	58	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	A	257	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	288	TYR	N-CA-CB	7.46	124.02	110.60
1	G	333	HIS	CA-CB-CG	7.44	126.25	113.60
1	G	257	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	G	383	TRP	CB-CG-CD1	-7.42	117.36	127.00
1	A	285	PRO	O-C-N	-7.39	110.87	122.70
1	A	481	ARG	CD-NE-CZ	7.39	133.94	123.60
2	H	214	ASP	N-CA-CB	-7.38	97.31	110.60
1	A	473	PHE	CB-CG-CD1	-7.37	115.64	120.80
1	A	170	ILE	CB-CA-C	-7.36	96.88	111.60
3	I	202	PHE	CB-CG-CD2	-7.36	115.65	120.80
1	A	407	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	A	559	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	534	HIS	CA-CB-CG	-7.29	101.21	113.60
1	A	351	ALA	N-CA-CB	7.25	120.25	110.10
3	C	17	TRP	CB-CA-C	7.25	124.90	110.40
1	G	536	ASP	CB-CG-OD2	-7.21	111.81	118.30
2	B	252	CYS	N-CA-CB	7.17	123.51	110.60
1	G	257	ARG	NE-CZ-NH1	-7.16	116.72	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	107	VAL	CA-CB-CG1	7.14	121.61	110.90
1	A	303	ALA	CB-CA-C	-7.13	99.41	110.10
1	A	482	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	545	PRO	N-CD-CG	7.12	113.88	103.20
1	G	99	ILE	CB-CA-C	-7.11	97.38	111.60
2	H	185	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	G	135	PHE	CB-CG-CD2	7.10	125.77	120.80
1	G	482	ARG	CD-NE-CZ	7.07	133.50	123.60
2	B	262	TYR	CB-CG-CD2	-7.07	116.76	121.00
3	C	8	ASP	CB-CG-OD1	7.07	124.66	118.30
1	G	368	ALA	N-CA-CB	7.03	119.94	110.10
1	A	288	TYR	CA-CB-CG	-6.99	100.12	113.40
1	G	481	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	B	144	TYR	CB-CG-CD2	6.94	125.17	121.00
1	G	208	MET	CA-CB-CG	-6.94	101.50	113.30
2	B	262	TYR	CB-CG-CD1	6.94	125.16	121.00
3	C	186	TYR	CB-CG-CD1	6.93	125.16	121.00
1	A	468	PHE	CB-CG-CD2	-6.89	115.97	120.80
1	G	19	ARG	NE-CZ-NH2	-6.87	116.86	120.30
3	C	14	PRO	N-CA-CB	6.87	111.54	103.30
1	G	284	HIS	CA-CB-CG	-6.85	101.96	113.60
3	C	42	TRP	CA-CB-CG	-6.84	100.71	113.70
1	G	520	THR	CA-CB-CG2	6.83	121.96	112.40
1	G	368	ALA	CB-CA-C	-6.83	99.86	110.10
1	A	52	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	B	93	ARG	CD-NE-CZ	6.71	133.00	123.60
2	B	147	TYR	CB-CG-CD1	-6.71	116.97	121.00
1	A	188	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	36	THR	CA-CB-CG2	-6.68	103.05	112.40
3	I	8	ASP	OD1-CG-OD2	-6.66	110.64	123.30
2	H	187	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	G	412	ASP	OD1-CG-OD2	6.65	135.94	123.30
3	C	80	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	G	280	TRP	CA-CB-CG	-6.65	101.06	113.70
1	G	481	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	281	PHE	CB-CG-CD2	-6.65	116.15	120.80
1	G	172	TRP	CH2-CZ2-CE2	-6.64	110.76	117.40
1	G	555	PRO	N-CA-CB	6.63	111.26	103.30
1	A	318	TYR	CB-CG-CD1	-6.60	117.04	121.00
3	C	161	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	428	ALA	CB-CA-C	-6.58	100.22	110.10
3	I	186	TYR	CB-CG-CD2	-6.58	117.05	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	MET	CA-CB-CG	-6.56	102.15	113.30
1	A	336	TYR	CB-CG-CD1	6.56	124.93	121.00
2	H	217	HIS	CG-ND1-CE1	6.55	117.37	108.20
2	H	160	MET	CB-CA-C	-6.54	97.31	110.40
2	H	232	PRO	CA-C-N	6.54	129.28	116.20
3	C	195	GLY	N-CA-C	6.53	129.43	113.10
1	G	485	ASP	CB-CG-OD2	-6.53	112.42	118.30
3	I	42	TRP	CA-CB-CG	-6.53	101.29	113.70
2	H	214	ASP	O-C-N	-6.52	112.27	122.70
1	G	130	ALA	N-CA-CB	6.49	119.18	110.10
1	G	301	VAL	CA-CB-CG2	-6.48	101.18	110.90
1	A	236	ALA	N-CA-CB	6.47	119.16	110.10
1	A	476	ARG	NE-CZ-NH1	-6.44	117.08	120.30
3	I	76	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	H	143	TRP	CB-CA-C	6.43	123.25	110.40
1	A	482	ARG	CD-NE-CZ	6.42	132.58	123.60
1	G	295	PHE	CB-CG-CD1	6.40	125.28	120.80
1	G	26	HIS	CA-CB-CG	-6.39	102.74	113.60
1	A	26	HIS	CA-CB-CG	-6.38	102.76	113.60
1	G	108	PHE	CB-CG-CD1	6.37	125.26	120.80
1	G	408	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	G	318	TYR	CB-CG-CD1	-6.32	117.21	121.00
2	B	157	GLU	CG-CD-OE2	-6.31	105.68	118.30
1	G	256	ASP	CB-CG-OD2	6.31	123.98	118.30
4	D	28	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	477	GLN	C-N-CA	6.28	135.49	122.30
1	G	171	GLY	O-C-N	-6.28	112.65	122.70
2	B	208	VAL	CG1-CB-CG2	6.28	120.94	110.90
2	B	202	VAL	CA-CB-CG2	6.28	120.31	110.90
1	G	234	VAL	CG1-CB-CG2	-6.27	100.86	110.90
1	G	422	TYR	CB-CG-CD2	6.26	124.76	121.00
3	I	17	TRP	CB-CA-C	6.26	122.91	110.40
2	B	187	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	333	HIS	CA-CB-CG	6.24	124.21	113.60
1	G	54	GLU	OE1-CD-OE2	6.24	130.79	123.30
1	A	468	PHE	CB-CG-CD1	6.22	125.16	120.80
2	B	75	LEU	CA-CB-CG	6.22	129.61	115.30
2	B	252	CYS	CB-CA-C	-6.22	97.97	110.40
4	J	48	ASN	CA-CB-CG	-6.18	99.80	113.40
1	G	482	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	H	252	CYS	CB-CA-C	-6.18	98.05	110.40
1	A	282	PHE	CB-CG-CD1	-6.17	116.48	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	ASP	CA-CB-CG	6.16	126.96	113.40
1	G	545	PRO	N-CD-CG	6.16	112.44	103.20
1	G	484	ILE	CB-CA-C	-6.15	99.29	111.60
1	G	335	MET	CB-CG-SD	6.15	130.86	112.40
1	G	521	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	280	TRP	CE2-CD2-CG	6.12	112.20	107.30
1	A	555	PRO	N-CA-CB	6.11	110.64	103.30
1	G	295	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	G	287	VAL	CA-CB-CG2	-6.10	101.74	110.90
1	A	173	VAL	O-C-N	-6.09	112.95	122.70
1	G	282	PHE	CB-CG-CD2	6.08	125.05	120.80
2	B	215	VAL	CB-CA-C	-6.07	99.86	111.40
2	H	249	PHE	CB-CG-CD2	-6.05	116.56	120.80
2	H	249	PHE	CB-CG-CD1	6.05	125.03	120.80
3	I	186	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	279	LEU	CA-CB-CG	-6.05	101.39	115.30
1	A	449	PRO	N-CA-CB	6.05	110.56	103.30
1	G	520	THR	N-CA-CB	-6.03	98.84	110.30
1	G	216	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	216	ILE	CA-C-O	-6.00	107.50	120.10
3	C	198	TYR	CB-CG-CD2	-6.00	117.40	121.00
2	H	216	ILE	CA-C-O	-6.00	107.51	120.10
1	G	110	VAL	CA-CB-CG1	-5.98	101.93	110.90
1	A	185	TYR	CA-CB-CG	5.97	124.74	113.40
1	A	279	LEU	CB-CG-CD2	-5.95	100.88	111.00
3	I	121	PRO	N-CA-CB	5.94	110.43	103.30
1	A	106	MET	CG-SD-CE	-5.94	90.70	100.20
1	A	136	PRO	N-CA-CB	5.91	110.40	103.30
1	G	88	CYS	CA-CB-SG	-5.91	103.36	114.00
1	G	223	HIS	CA-CB-CG	-5.90	103.56	113.60
1	A	541	THR	CA-CB-OG1	-5.90	96.61	109.00
2	H	159	TYR	CB-CG-CD1	5.90	124.54	121.00
1	A	300	HIS	CA-CB-CG	-5.89	103.59	113.60
2	H	171	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	A	318	TYR	CB-CA-C	5.87	122.14	110.40
1	A	106	MET	N-CA-CB	-5.87	100.04	110.60
3	I	251	ASP	CB-CG-OD2	5.85	123.56	118.30
1	G	132	ASP	CB-CG-OD1	5.84	123.56	118.30
1	G	264	PHE	CB-CG-CD2	5.84	124.89	120.80
2	H	108	PRO	N-CA-CB	5.84	110.31	103.30
1	G	213	LEU	CA-C-O	5.84	132.36	120.10
3	C	27	VAL	CA-CB-CG2	-5.83	102.16	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	THR	N-CA-CB	5.82	121.35	110.30
1	A	50	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	331	TRP	CA-C-N	5.80	129.95	117.20
3	C	256	PHE	CB-CG-CD1	5.80	124.86	120.80
2	H	241	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	C	194	ALA	C-N-CA	5.79	134.46	122.30
2	B	35	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	159	ALA	CB-CA-C	5.78	118.76	110.10
1	G	259	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	38	GLY	CA-C-O	5.76	130.97	120.60
2	B	93	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
1	G	287	VAL	C-N-CA	-5.74	107.36	121.70
1	A	148	ALA	CB-CA-C	5.72	118.68	110.10
1	A	111	VAL	CA-C-O	-5.71	108.11	120.10
1	A	301	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	A	443	MET	CA-CB-CG	5.71	123.00	113.30
1	G	155	ALA	CB-CA-C	5.71	118.66	110.10
2	B	182	GLU	OE1-CD-OE2	-5.70	116.45	123.30
2	B	109	ILE	CA-CB-CG1	-5.70	100.17	111.00
2	B	63	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	G	419	HIS	CB-CA-C	-5.69	99.02	110.40
1	A	233	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	A	484	ILE	CB-CA-C	-5.68	100.24	111.60
2	B	251	GLN	CG-CD-OE1	-5.67	110.26	121.60
3	C	170	LEU	CA-CB-CG	5.65	128.30	115.30
2	B	149	TYR	CA-CB-CG	5.65	124.14	113.40
1	G	358	PRO	N-CA-CB	5.65	110.08	103.30
1	G	351	ALA	CB-CA-C	-5.65	101.63	110.10
1	G	422	TYR	CB-CG-CD1	-5.63	117.62	121.00
2	B	152	GLU	CG-CD-OE1	5.63	129.56	118.30
1	G	410	TYR	CB-CG-CD2	5.63	124.38	121.00
2	H	195	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	A	14	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	422	TYR	CB-CG-CD2	5.62	124.37	121.00
1	G	137	ARG	NE-CZ-NH1	-5.62	117.49	120.30
2	H	252	CYS	O-C-N	5.61	131.68	122.70
3	I	26	PHE	CB-CG-CD2	-5.61	116.88	120.80
2	H	185	TYR	CB-CG-CD1	5.61	124.36	121.00
2	B	135	THR	CA-CB-CG2	-5.60	104.56	112.40
1	G	14	ARG	N-CA-CB	-5.60	100.52	110.60
3	I	116	ILE	CB-CA-C	-5.60	100.39	111.60
2	H	224	PHE	CB-CG-CD1	-5.59	116.88	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	448	TYR	CA-CB-CG	-5.59	102.77	113.40
1	A	14	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	172	TRP	CB-CG-CD2	5.59	133.87	126.60
1	A	48	THR	CA-CB-OG1	5.58	120.72	109.00
1	A	282	PHE	CB-CG-CD2	5.58	124.70	120.80
2	H	259	SER	CB-CA-C	5.58	120.69	110.10
3	I	229	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	B	269	VAL	CB-CA-C	5.56	121.97	111.40
2	H	207	VAL	CA-CB-CG1	-5.56	102.56	110.90
1	G	213	LEU	O-C-N	-5.56	113.81	122.70
3	I	8	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	259	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	A	526	THR	CA-CB-CG2	-5.55	104.63	112.40
3	C	194	ALA	O-C-N	-5.54	113.78	123.20
3	C	5	LYS	CA-CB-CG	5.54	125.59	113.40
1	A	481	ARG	CA-CB-CG	5.54	125.59	113.40
3	I	191	PHE	CB-CG-CD1	-5.54	116.92	120.80
2	B	152	GLU	CB-CG-CD	5.54	129.15	114.20
3	C	169	ALA	N-CA-CB	5.53	117.84	110.10
1	A	194	VAL	O-C-N	5.52	131.54	122.70
2	H	149	TYR	CA-CB-CG	5.51	123.88	113.40
1	A	271	ASP	CB-CG-OD1	5.51	123.26	118.30
3	C	184	TYR	CB-CG-CD2	5.51	124.31	121.00
1	A	216	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	159	ALA	CA-C-O	5.49	131.63	120.10
2	B	242	ALA	N-CA-CB	5.49	117.79	110.10
2	B	80	VAL	CA-CB-CG1	-5.49	102.67	110.90
2	B	222	PRO	CA-C-N	5.49	129.28	117.20
1	A	250	ILE	CB-CG1-CD1	5.48	129.24	113.90
1	G	111	VAL	CA-CB-CG1	5.47	119.11	110.90
3	I	238	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	G	489	ALA	CB-CA-C	-5.47	101.90	110.10
2	H	144	TYR	N-CA-CB	5.46	120.43	110.60
3	C	54	THR	CA-CB-CG2	-5.46	104.76	112.40
1	G	228	PHE	CB-CG-CD2	-5.46	116.98	120.80
3	C	117	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	G	428	ALA	CB-CA-C	-5.46	101.92	110.10
1	A	520	THR	N-CA-CB	-5.45	99.94	110.30
1	A	438	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	G	419	HIS	C-N-CA	-5.44	108.09	121.70
1	G	458	TRP	CB-CA-C	5.44	121.29	110.40
1	G	326	LEU	CB-CG-CD1	-5.44	101.75	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	257	ARG	C-N-CA	-5.44	108.11	121.70
1	A	257	ARG	CB-CA-C	-5.43	99.53	110.40
1	G	205	ALA	CB-CA-C	-5.43	101.96	110.10
1	G	412	ASP	CA-CB-CG	-5.42	101.47	113.40
3	C	201	ASN	CB-CG-OD1	5.42	132.43	121.60
4	D	47	ALA	CB-CA-C	-5.40	102.00	110.10
3	I	127	THR	N-CA-CB	5.40	120.56	110.30
1	G	445	GLY	CA-C-O	-5.39	110.89	120.60
1	A	51	MET	N-CA-CB	5.39	120.30	110.60
1	A	110	VAL	CA-C-O	5.38	131.40	120.10
3	C	202	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	A	351	ALA	CA-C-O	-5.38	108.81	120.10
4	J	10	VAL	CG1-CB-CG2	-5.37	102.31	110.90
2	B	42	GLY	O-C-N	-5.36	114.12	122.70
2	B	165	ALA	N-CA-CB	-5.36	102.60	110.10
3	I	80	ARG	NH1-CZ-NH2	5.36	125.30	119.40
1	A	483	TYR	CB-CG-CD1	5.36	124.21	121.00
1	A	294	ALA	CB-CA-C	-5.35	102.07	110.10
2	H	147	TYR	CB-CG-CD1	-5.35	117.79	121.00
2	H	152	GLU	CB-CG-CD	5.35	128.65	114.20
2	H	206	VAL	CG1-CB-CG2	5.35	119.46	110.90
1	G	521	ARG	NE-CZ-NH2	5.34	122.97	120.30
2	H	73	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	257	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	G	446	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	H	141	TYR	O-C-N	5.32	131.21	122.70
2	B	256	CYS	N-CA-CB	-5.32	101.03	110.60
1	G	174	LEU	O-C-N	-5.32	114.19	122.70
1	G	357	VAL	CB-CA-C	5.31	121.50	111.40
2	B	143	TRP	CB-CG-CD2	5.30	133.50	126.60
2	B	234	ARG	O-C-N	5.29	131.17	122.70
1	A	264	PHE	CB-CG-CD2	5.29	124.50	120.80
1	G	337	THR	CA-CB-CG2	-5.29	105.00	112.40
2	H	75	LEU	N-CA-CB	5.28	120.96	110.40
1	A	159	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	392	THR	CA-CB-CG2	-5.28	105.01	112.40
1	G	543	THR	N-CA-C	-5.26	96.79	111.00
1	A	481	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
3	C	184	TYR	CB-CG-CD1	-5.25	117.85	121.00
3	I	162	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	60	VAL	CB-CA-C	-5.24	101.45	111.40
2	H	260	HIS	N-CA-CB	-5.23	101.19	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	260	HIS	CG-ND1-CE1	5.22	115.51	108.20
4	J	10	VAL	CA-C-O	5.21	131.04	120.10
2	B	208	VAL	CA-CB-CG1	-5.21	103.09	110.90
1	A	173	VAL	CA-C-O	5.21	131.03	120.10
1	A	232	ILE	CA-CB-CG1	-5.21	101.11	111.00
1	A	45	VAL	CA-CB-CG1	-5.20	103.09	110.90
1	A	189	LEU	CB-CA-C	5.20	120.09	110.20
1	A	112	ILE	C-N-CD	-5.20	109.16	120.60
1	A	173	VAL	N-CA-CB	-5.20	100.06	111.50
1	A	255	THR	CA-CB-OG1	-5.19	98.11	109.00
1	A	380	PRO	CB-CA-C	5.18	124.96	112.00
3	I	12	LEU	CB-CA-C	-5.18	100.35	110.20
2	B	254	GLU	O-C-N	-5.18	114.41	122.70
1	G	24	THR	N-CA-CB	5.18	120.14	110.30
3	I	92	MET	CA-CB-CG	-5.18	104.49	113.30
1	G	539	GLU	CB-CA-C	5.17	120.75	110.40
1	G	132	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	144	TRP	CA-CB-CG	-5.16	103.89	113.70
1	A	60	VAL	CA-CB-CG1	-5.16	103.16	110.90
1	G	422	TYR	N-CA-CB	5.16	119.89	110.60
3	I	117	ASP	CB-CA-C	-5.16	100.08	110.40
2	B	249	PHE	CB-CG-CD1	5.16	124.41	120.80
3	C	68	GLU	CA-CB-CG	5.15	124.73	113.40
2	H	92	ALA	N-CA-CB	5.15	117.31	110.10
2	B	58	ASP	CB-CG-OD1	-5.15	113.67	118.30
2	B	264	PRO	N-CA-CB	5.15	109.48	103.30
3	C	186	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	G	420	PHE	CA-CB-CG	5.14	126.25	113.90
1	A	280	TRP	NE1-CE2-CD2	-5.14	102.16	107.30
2	H	150	PRO	N-CA-CB	5.14	109.47	103.30
1	A	110	VAL	O-C-N	-5.14	114.48	122.70
2	B	241	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	187	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	405	SER	N-CA-CB	-5.12	102.82	110.50
2	H	266	THR	CA-CB-CG2	-5.12	105.24	112.40
1	G	351	ALA	N-CA-CB	5.11	117.26	110.10
2	H	283	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	G	275	TYR	CB-CG-CD2	5.10	124.06	121.00
2	H	176	VAL	CA-CB-CG1	-5.09	103.26	110.90
3	C	202	PHE	CB-CG-CD1	5.09	124.36	120.80
4	D	10	VAL	CG1-CB-CG2	-5.09	102.75	110.90
2	H	187	ARG	CD-NE-CZ	5.08	130.71	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	252	MET	CB-CG-SD	5.07	127.62	112.40
2	H	75	LEU	CA-CB-CG	5.07	126.97	115.30
1	G	311	PHE	CB-CG-CD2	5.07	124.35	120.80
1	G	478	GLY	N-CA-C	5.07	125.77	113.10
3	I	106	LEU	CA-CB-CG	-5.06	103.67	115.30
1	G	220	MET	N-CA-CB	5.05	119.70	110.60
1	G	264	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	A	281	PHE	CB-CG-CD1	5.04	124.33	120.80
2	B	137	LYS	CA-CB-CG	-5.04	102.32	113.40
2	B	142	GLN	N-CA-CB	5.03	119.66	110.60
3	I	92	MET	O-C-N	-5.03	114.65	122.70
1	A	505	PHE	CB-CG-CD1	5.03	124.32	120.80
2	H	144	TYR	CB-CG-CD2	5.03	124.02	121.00
1	A	175	TYR	CA-C-O	-5.03	109.54	120.10
1	G	160	PRO	CA-CB-CG	-5.03	94.45	104.00
1	G	291	VAL	O-C-N	5.03	130.74	122.70
2	H	88	ASN	N-CA-CB	5.03	119.65	110.60
3	C	146	CYS	CA-CB-SG	-5.02	104.96	114.00
4	D	47	ALA	N-CA-CB	-5.02	103.07	110.10
1	A	275	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	215	MET	CA-C-N	5.01	128.23	117.20
1	G	239	ILE	CA-CB-CG1	-5.01	101.48	111.00
2	H	77	LEU	CB-CA-C	5.01	119.72	110.20
3	C	70	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	A	61	GLN	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	114	ALA	Mainchain
1	A	124	MET	Mainchain
1	A	145	LEU	Mainchain
1	A	152	LEU	Mainchain
1	A	157	LEU	Mainchain
1	A	222	MET	Mainchain
1	A	257	ARG	Mainchain
1	A	258	ASN	Mainchain
1	A	261	THR	Mainchain
1	A	283	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	288	TYR	Mainchain
1	A	29	ILE	Mainchain
1	A	333	HIS	Mainchain
1	A	340	LEU	Mainchain
1	A	544	SER	Mainchain,Peptide
1	A	96	ASN	Mainchain
2	B	136	VAL	Mainchain
2	B	142	GLN	Mainchain
2	B	160	MET	Mainchain
2	B	222	PRO	Mainchain
2	B	253	SER	Mainchain
2	B	259	SER	Mainchain
3	C	162	ARG	Mainchain
3	C	17	TRP	Mainchain
3	C	194	ALA	Mainchain
3	C	36	MET	Mainchain
3	C	57	GLY	Mainchain
4	D	47	ALA	Mainchain
1	G	171	GLY	Mainchain
1	G	285	PRO	Mainchain
1	G	287	VAL	Mainchain
1	G	301	VAL	Mainchain
1	G	303	ALA	Mainchain
1	G	326	LEU	Mainchain
1	G	368	ALA	Mainchain
1	G	380	PRO	Mainchain
1	G	385	LEU	Mainchain
1	G	444	SER	Mainchain
1	G	473	PHE	Mainchain
1	G	481	ARG	Mainchain
1	G	488	GLU	Mainchain
1	G	544	SER	Mainchain,Peptide
1	G	66	GLU	Mainchain
2	H	105	THR	Mainchain
2	H	142	GLN	Mainchain
2	H	202	VAL	Mainchain
3	I	117	ASP	Mainchain
3	I	26	PHE	Mainchain
3	I	33	VAL	Mainchain
3	I	35	TRP	Mainchain
3	I	76	ARG	Mainchain
3	I	85	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	I	94	PHE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4322	0	4240	609	0
1	G	4322	0	4240	621	0
2	B	2046	0	2011	219	0
2	H	2046	0	2011	231	0
3	C	2139	0	2056	224	0
3	I	2139	0	2056	214	0
4	D	311	0	319	33	0
4	J	311	0	319	40	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	40	0
8	G	120	0	108	38	0
9	A	102	0	164	38	0
9	C	153	0	246	56	0
9	D	51	0	82	17	0
9	G	102	0	164	41	0
9	I	153	0	246	59	0
9	J	51	0	82	13	0
10	A	97	0	0	26	0
10	B	70	0	0	20	0
10	C	38	0	0	8	0
10	D	13	0	0	0	0
10	G	107	0	0	30	0
10	H	64	0	0	18	0
10	I	37	0	0	7	0
10	J	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18934	0	18452	2141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (2141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:THR:HB	1:G:380:PRO:HD3	1.18	1.17
1:A:106:MET:HG2	8:A:1001:HEA:HAC	1.17	1.16
9:C:2010:3PE:H3E2	9:C:2010:3PE:H3I2	1.22	1.13
9:I:3010:3PE:H3E2	9:I:3010:3PE:C3I	1.78	1.13
8:A:1002:HEA:HMC1	8:A:1002:HEA:HBC1	1.30	1.11
1:A:106:MET:HG2	8:A:1001:HEA:CAC	1.79	1.10
1:G:414:TYR:HA	1:G:417:VAL:HG23	1.31	1.10
1:A:177:PRO:HG2	2:B:215:VAL:HA	1.34	1.09
8:G:1002:HEA:HMC1	8:G:1002:HEA:HBC1	1.34	1.09
1:G:401:LEU:HD13	1:G:416:VAL:HG22	1.31	1.09
1:G:106:MET:HG2	8:G:1001:HEA:CAC	1.81	1.08
9:I:3010:3PE:C3E	9:I:3010:3PE:H3I2	1.80	1.08
1:G:106:MET:HG2	8:G:1001:HEA:HAC	1.23	1.08
1:G:127:HIS:HB3	1:G:226:PRO:HG3	1.29	1.08
1:A:279:LEU:HD23	1:A:279:LEU:C	1.73	1.05
1:A:379:THR:HB	1:A:380:PRO:HD3	1.35	1.04
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.40	1.04
1:G:243:LEU:N	1:G:244:PRO:HD2	1.74	1.02
9:A:2009:3PE:H392	9:A:2009:3PE:H291	1.42	1.01
9:I:3010:3PE:H3E2	9:I:3010:3PE:H3I2	1.07	1.01
1:A:284:HIS:NE2	1:A:288:TYR:HE2	1.58	1.00
2:B:98:SER:HB2	2:B:99:PRO:HD3	1.41	1.00
1:G:279:LEU:HD23	1:G:279:LEU:C	1.81	1.00
3:C:21:ALA:HB2	3:C:54:THR:HG21	1.42	1.00
1:G:222:MET:HG3	9:G:3012:3PE:H111	1.41	0.99
8:A:1002:HEA:HMC1	8:A:1002:HEA:CBC	1.87	0.98
1:G:249:ALA:HB2	1:G:278:ILE:HG22	1.46	0.98
1:A:401:LEU:HD13	1:A:416:VAL:HG22	1.45	0.97
3:C:8:ASP:HB3	3:C:72:THR:HG21	1.47	0.97
1:A:25:ASN:HD21	1:A:27:LYS:HZ3	1.05	0.97
2:H:62:LEU:HD12	2:H:65:ILE:HD11	1.46	0.96
2:B:107:VAL:HG13	2:B:108:PRO:HD3	1.46	0.96
9:C:2010:3PE:H3I2	9:C:2010:3PE:C3E	1.94	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2012:3PE:H2F1	9:D:2011:3PE:H2I2	1.44	0.96
1:A:243:LEU:H	1:A:244:PRO:HD2	1.32	0.95
1:G:345:GLN:HE22	1:G:408:ARG:HH22	1.07	0.95
2:H:98:SER:HB2	2:H:99:PRO:HD3	1.48	0.95
3:C:122:PRO:HG2	3:C:125:ILE:HG13	1.46	0.95
1:A:243:LEU:N	1:A:244:PRO:HD2	1.82	0.94
1:G:342:LEU:HD13	2:H:127:GLN:HB2	1.49	0.94
2:H:30:LEU:HD22	2:H:247:ILE:HD11	1.50	0.94
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.48	0.93
1:G:520:THR:HG22	1:G:521:ARG:HG2	1.51	0.93
1:A:342:LEU:HD13	2:B:127:GLN:HB2	1.51	0.93
1:A:25:ASN:HD21	1:A:27:LYS:NZ	1.67	0.93
3:I:21:ALA:HB2	3:I:54:THR:HG21	1.50	0.93
1:G:136:PRO:HG2	3:I:12:LEU:HD12	1.51	0.92
1:G:63:MET:HG2	1:G:94:LEU:HD23	1.48	0.92
1:G:432:ILE:HG21	8:G:1001:HEA:H252	1.52	0.92
1:G:284:HIS:HB3	1:G:285:PRO:HD3	1.48	0.92
1:G:396:VAL:HG11	2:H:65:ILE:HD13	1.51	0.92
3:I:253:VAL:HA	9:I:3010:3PE:H3H1	1.50	0.91
9:C:2010:3PE:H3E2	9:C:2010:3PE:C3I	1.99	0.91
2:B:30:LEU:HD22	2:B:247:ILE:HD11	1.52	0.90
9:I:3013:3PE:H261	9:I:3013:3PE:H3A2	1.54	0.89
2:B:62:LEU:HD12	2:B:65:ILE:HD11	1.55	0.89
9:G:3012:3PE:H2H1	9:I:3010:3PE:H2I3	1.53	0.89
1:A:345:GLN:NE2	1:A:408:ARG:HH22	1.70	0.89
1:G:445:GLY:HA2	1:G:525:VAL:HG12	1.55	0.88
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.53	0.88
1:G:25:ASN:HD21	1:G:27:LYS:NZ	1.69	0.88
1:A:135:PHE:HE1	3:C:79:LEU:HD23	1.38	0.87
1:A:284:HIS:HE2	1:A:288:TYR:HE2	1.15	0.87
3:I:8:ASP:H	4:J:14:MET:HE3	1.38	0.86
1:A:345:GLN:HE22	1:A:408:ARG:HH22	0.92	0.86
2:B:111:ILE:HG22	2:B:112:LEU:HD23	1.56	0.86
1:G:284:HIS:NE2	1:G:288:TYR:HE2	1.74	0.86
3:C:254:TRP:HA	3:C:257:LEU:HD12	1.57	0.85
9:C:2013:3PE:O14	9:C:2013:3PE:H121	1.75	0.85
8:A:1002:HEA:HBC1	8:A:1002:HEA:CMC	2.07	0.85
1:A:170:ILE:HG21	1:A:174:LEU:HA	1.59	0.85
9:I:3013:3PE:H3F2	9:I:3013:3PE:H2B2	1.57	0.84
1:A:243:LEU:HD21	10:A:2034:HOH:O	1.74	0.84
1:G:63:MET:HE1	1:G:95:TRP:HB2	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:161:ARG:HH12	3:I:230:GLY:HA2	1.42	0.84
1:G:55:LEU:HD11	10:G:3022:HOH:O	1.76	0.84
9:I:3010:3PE:C3I	9:I:3010:3PE:C3E	2.40	0.84
9:I:3013:3PE:H2D2	9:I:3013:3PE:C3G	2.06	0.84
1:A:100:THR:HG23	1:A:104:ILE:HD12	1.59	0.84
1:G:20:TRP:CE3	1:G:32:LEU:HD21	2.13	0.83
9:G:3009:3PE:H392	9:G:3009:3PE:H291	1.58	0.83
1:A:414:TYR:HA	1:A:417:VAL:HG23	1.58	0.83
1:G:127:HIS:HB3	1:G:226:PRO:CG	2.08	0.83
1:G:177:PRO:HG2	2:H:215:VAL:HA	1.60	0.83
9:I:3013:3PE:O14	9:I:3013:3PE:H121	1.78	0.83
3:I:59:TRP:HA	3:I:62:VAL:HG23	1.60	0.83
1:G:170:ILE:HD11	1:G:187:THR:OG1	1.77	0.83
1:G:379:THR:HB	1:G:380:PRO:CD	2.05	0.83
1:G:302:ILE:HG22	1:G:369:THR:HG21	1.59	0.82
8:G:1002:HEA:O11	8:G:1002:HEA:HHC	1.79	0.82
9:A:2009:3PE:H291	9:A:2009:3PE:C39	2.10	0.82
1:G:379:THR:CB	1:G:380:PRO:HD3	2.03	0.82
3:I:161:ARG:NH2	3:I:232:PHE:H	1.77	0.82
2:B:238:LEU:C	2:B:238:LEU:HD12	2.01	0.82
1:G:25:ASN:HD21	1:G:27:LYS:HZ3	1.24	0.81
9:I:3013:3PE:H3H2	9:I:3013:3PE:H2E1	1.61	0.81
1:G:243:LEU:H	1:G:244:PRO:HD2	1.38	0.81
1:G:547:PRO:HD2	1:G:550:THR:HG22	1.62	0.80
1:A:127:HIS:HB3	1:A:226:PRO:HG3	1.63	0.80
3:C:253:VAL:HA	9:C:2010:3PE:H3H1	1.62	0.80
1:G:180:THR:HA	1:G:257:ARG:HD2	1.63	0.80
1:G:505:PHE:O	1:G:509:LEU:HG	1.80	0.80
2:H:107:VAL:HG13	2:H:108:PRO:HD3	1.62	0.80
3:C:59:TRP:HA	3:C:62:VAL:HG23	1.64	0.80
4:D:14:MET:HG2	4:D:15:ASP:N	1.96	0.80
2:B:158:SER:HA	2:B:196:THR:HB	1.63	0.79
1:G:160:PRO:HG2	1:G:185:TYR:CE1	2.17	0.79
1:A:106:MET:CG	8:A:1001:HEA:HAC	2.08	0.79
1:G:115:LEU:HD22	1:G:293:PRO:HB2	1.63	0.79
3:I:103:LYS:HD3	3:I:103:LYS:C	2.02	0.79
9:C:2010:3PE:C3E	9:C:2010:3PE:C3I	2.55	0.78
1:A:379:THR:HB	1:A:380:PRO:CD	2.12	0.78
1:G:345:GLN:NE2	1:G:408:ARG:HH22	1.80	0.78
1:A:26:HIS:C	1:A:26:HIS:CD2	2.55	0.78
1:A:91:ASN:ND2	1:A:165:GLN:HE22	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:VAL:HG21	2:H:278:TRP:CE3	2.18	0.78
2:H:200:VAL:O	2:H:269:VAL:HA	1.84	0.78
1:A:222:MET:HG3	9:A:2012:3PE:H111	1.65	0.78
3:I:8:ASP:CB	3:I:72:THR:HG21	2.13	0.78
2:H:163:SER:HB2	2:H:165:ALA:HB3	1.65	0.77
4:J:45:ALA:HA	9:J:3011:3PE:H321	1.66	0.77
1:A:533:GLU:OE1	10:A:2107:HOH:O	2.03	0.77
3:I:62:VAL:HG11	9:I:3008:3PE:H31	1.67	0.77
1:A:345:GLN:HE22	1:A:408:ARG:NH2	1.76	0.77
3:C:9:TYR:HB3	10:C:2017:HOH:O	1.85	0.77
3:I:137:ASN:HA	3:I:140:ILE:HD12	1.67	0.77
1:G:63:MET:CG	1:G:94:LEU:HD23	2.15	0.76
1:G:387:PHE:CD1	1:G:387:PHE:C	2.57	0.76
1:A:74:LYS:H	1:A:74:LYS:HD2	1.50	0.76
1:A:529:ASN:C	1:A:529:ASN:OD1	2.24	0.76
3:C:161:ARG:HH12	3:C:230:GLY:HA2	1.48	0.76
1:G:18:THR:HA	1:G:22:MET:HE3	1.65	0.76
3:I:62:VAL:CG1	9:I:3008:3PE:H31	2.16	0.76
8:G:1002:HEA:HBC1	8:G:1002:HEA:CMC	2.15	0.76
1:A:367:ILE:HD13	2:B:75:LEU:HD22	1.66	0.76
9:A:2009:3PE:H261	3:C:55:MET:HG2	1.68	0.76
2:B:145:TRP:HB2	10:B:1049:HOH:O	1.85	0.76
1:A:505:PHE:O	1:A:509:LEU:HG	1.86	0.76
1:A:473:PHE:CD1	2:B:41:THR:HB	2.20	0.75
1:G:174:LEU:HD13	1:G:191:ILE:HD13	1.69	0.75
1:G:50:TYR:O	1:G:53:MET:HB2	1.86	0.75
1:G:401:LEU:CD1	1:G:416:VAL:HG22	2.14	0.75
3:C:13:PRO:HD3	10:C:2018:HOH:O	1.86	0.75
3:C:162:ARG:HG3	3:C:163:ASP:H	1.51	0.75
2:H:76:ILE:O	2:H:80:VAL:HG23	1.87	0.75
3:C:8:ASP:CB	3:C:72:THR:HG21	2.16	0.75
3:I:31:GLY:HA2	3:I:43:MET:SD	2.27	0.75
1:A:445:GLY:HA2	1:A:525:VAL:HG12	1.68	0.74
2:H:111:ILE:HG22	2:H:112:LEU:HD23	1.68	0.74
3:I:8:ASP:H	4:J:14:MET:CE	1.99	0.74
1:G:345:GLN:HE22	1:G:408:ARG:NH2	1.85	0.74
2:H:226:VAL:HA	10:H:1157:HOH:O	1.86	0.74
1:A:379:THR:HA	1:A:382:LEU:HD12	1.66	0.74
9:C:2010:3PE:H342	9:D:2011:3PE:H342	1.67	0.74
3:I:133:LEU:H	3:I:134:PRO:CD	2.00	0.74
1:A:417:VAL:HA	1:A:420:PHE:CE1	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:TYR:O	2:B:142:GLN:C	2.23	0.74
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3G1	1.70	0.74
1:G:429:VAL:HG13	8:G:1001:HEA:H273	1.69	0.74
2:H:132:ALA:HB1	2:H:134:VAL:O	1.87	0.74
1:A:112:ILE:H	1:A:113:PRO:CD	2.00	0.74
3:C:162:ARG:HG3	3:C:163:ASP:N	2.03	0.73
1:A:284:HIS:NE2	1:A:288:TYR:CE2	2.50	0.73
8:G:1002:HEA:HMC1	8:G:1002:HEA:CBC	2.09	0.73
3:I:123:GLU:HB2	10:I:3032:HOH:O	1.85	0.73
1:G:367:ILE:HD13	2:H:75:LEU:HB2	1.70	0.73
3:C:101:PHE:CE1	3:C:261:ILE:HG12	2.23	0.73
1:G:378:LYS:HE2	10:G:3035:HOH:O	1.88	0.73
1:A:93:HIS:HA	10:A:2026:HOH:O	1.86	0.73
1:A:425:SER:HA	1:A:429:VAL:HG21	1.70	0.73
1:A:240:LEU:HD21	3:C:85:LEU:HB3	1.69	0.73
1:G:455:LEU:HD23	1:G:510:PHE:CE2	2.22	0.73
1:A:403:GLN:O	1:A:404:ALA:C	2.27	0.73
3:C:122:PRO:HG2	3:C:125:ILE:CG1	2.18	0.73
1:G:376:GLU:HG2	1:G:378:LYS:HG2	1.70	0.73
1:A:63:MET:HG2	1:A:94:LEU:HD23	1.69	0.73
1:G:91:ASN:ND2	1:G:165:GLN:HE22	1.86	0.73
1:A:165:GLN:HB3	10:A:2044:HOH:O	1.88	0.72
1:A:378:LYS:HE2	10:A:2031:HOH:O	1.89	0.72
1:G:414:TYR:HA	1:G:417:VAL:CG2	2.15	0.72
9:A:2012:3PE:H2F1	9:D:2011:3PE:C2I	2.19	0.72
1:A:376:GLU:HG2	1:A:378:LYS:HG2	1.71	0.72
2:B:76:ILE:O	2:B:80:VAL:HG23	1.89	0.72
1:A:432:ILE:HG21	8:A:1001:HEA:H252	1.71	0.72
1:G:284:HIS:O	1:G:287:VAL:HG22	1.89	0.72
1:G:485:ASP:OD1	1:G:486:TYR:N	2.22	0.72
1:A:381:MET:HE3	1:A:385:LEU:HD21	1.72	0.72
9:C:2013:3PE:H261	9:C:2013:3PE:H3A2	1.70	0.72
1:G:170:ILE:HG21	1:G:174:LEU:HA	1.72	0.72
1:G:332:ALA:HB3	1:G:348:PHE:CD2	2.25	0.72
1:A:480:PRO:HG2	1:A:483:TYR:CE2	2.25	0.72
1:G:243:LEU:N	1:G:244:PRO:CD	2.52	0.72
1:G:386:GLY:O	1:G:390:LEU:HG	1.90	0.72
3:C:62:VAL:HG11	9:C:2008:3PE:H31	1.72	0.71
2:H:192:LEU:HB3	2:H:249:PHE:CD2	2.24	0.71
1:A:285:PRO:O	1:A:286:GLN:C	2.25	0.71
1:G:95:TRP:CZ2	1:G:99:ILE:HD11	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:LEU:O	1:G:204:GLY:C	2.29	0.71
1:G:246:LEU:HD22	1:G:282:PHE:CZ	2.24	0.71
1:G:432:ILE:HG22	1:G:436:ILE:HD11	1.71	0.71
9:G:3009:3PE:H242	9:G:3009:3PE:H371	1.71	0.71
2:H:145:TRP:NE1	2:H:263:MET:HE2	2.05	0.71
1:A:20:TRP:CE3	1:A:32:LEU:HD21	2.26	0.71
1:A:396:VAL:HG11	2:B:65:ILE:HD13	1.71	0.71
1:A:485:ASP:OD1	1:A:486:TYR:N	2.23	0.71
1:G:486:TYR:CD2	1:G:490:PHE:HB2	2.26	0.71
8:G:1002:HEA:HHA	10:G:3052:HOH:O	1.90	0.71
1:A:170:ILE:CG2	1:A:174:LEU:HA	2.20	0.71
3:C:226:ARG:HH21	3:C:231:HIS:HB3	1.55	0.71
1:G:489:ALA:CB	2:H:36:PRO:HB2	2.21	0.71
8:G:1002:HEA:H131	10:G:3026:HOH:O	1.90	0.71
1:A:112:ILE:H	1:A:113:PRO:HD2	1.55	0.71
8:A:1002:HEA:H131	10:A:2022:HOH:O	1.90	0.71
1:G:332:ALA:HB3	1:G:348:PHE:CG	2.25	0.71
3:C:249:PHE:O	3:C:253:VAL:HG23	1.89	0.71
1:G:24:THR:HG21	3:I:13:PRO:O	1.91	0.70
1:G:111:VAL:CG1	1:G:290:ILE:HG23	2.21	0.70
1:A:422:TYR:CD2	1:A:426:LEU:HD12	2.26	0.70
1:G:433:PHE:HA	1:G:436:ILE:HD12	1.72	0.70
2:H:208:VAL:HB	2:H:238:LEU:HG	1.73	0.70
1:G:350:MET:HA	1:G:353:MET:HE2	1.72	0.70
2:H:211:THR:HG22	2:H:212:GLY:H	1.57	0.70
2:H:211:THR:HG22	2:H:212:GLY:N	2.07	0.70
1:G:135:PHE:HE1	3:I:79:LEU:HD23	1.56	0.70
3:I:133:LEU:H	3:I:134:PRO:HD2	1.56	0.70
3:C:111:PRO:HA	4:J:10:VAL:HB	1.73	0.70
1:G:26:HIS:C	1:G:26:HIS:CD2	2.65	0.70
3:I:240:PHE:CE1	3:I:244:ILE:HD11	2.27	0.70
1:A:289:ILE:O	1:A:293:PRO:HD2	1.90	0.70
2:H:191:LEU:O	2:H:264:PRO:HG3	1.91	0.70
1:A:342:LEU:HD21	2:B:124:PHE:CD1	2.27	0.70
1:G:262:THR:HG22	10:I:3029:HOH:O	1.91	0.70
2:H:105:THR:O	2:H:109:ILE:HD12	1.91	0.70
1:A:99:ILE:HD12	8:A:1001:HEA:HBA2	1.73	0.69
9:G:3012:3PE:H2F1	9:J:3011:3PE:H2I2	1.74	0.69
2:H:201:PRO:HB2	2:H:204:LYS:HG3	1.75	0.69
3:I:137:ASN:HD21	3:I:181:PHE:HB3	1.57	0.69
1:A:217:ALA:HB1	10:A:2082:HOH:O	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:HIS:HB3	2:H:252:CYS:SG	2.32	0.69
2:H:234:ARG:NH1	3:I:114:PRO:HG3	2.08	0.69
1:A:299:SER:O	1:A:300:HIS:C	2.29	0.69
3:C:240:PHE:CE1	3:C:244:ILE:HD11	2.28	0.69
1:G:394:GLY:HA3	1:G:423:VAL:CG1	2.22	0.69
3:I:83:PHE:HE1	9:I:3008:3PE:H262	1.58	0.69
1:A:176:PRO:O	2:B:216:ILE:HD11	1.91	0.69
1:G:331:TRP:CD1	1:G:331:TRP:C	2.65	0.69
1:G:367:ILE:HD13	2:H:75:LEU:HD22	1.72	0.69
1:A:22:MET:HG2	3:C:16:ILE:HA	1.75	0.69
1:A:115:LEU:HD22	1:A:293:PRO:HB2	1.75	0.69
1:A:174:LEU:HD13	1:A:191:ILE:CD1	2.23	0.69
1:A:243:LEU:N	1:A:244:PRO:CD	2.55	0.69
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.27	0.69
2:B:132:ALA:HB1	2:B:134:VAL:O	1.93	0.69
1:G:136:PRO:CG	3:I:12:LEU:HD12	2.23	0.69
1:G:173:VAL:HG12	1:G:279:LEU:HD13	1.75	0.69
1:G:381:MET:HE3	1:G:385:LEU:HD21	1.74	0.69
2:H:199:VAL:HG11	2:H:278:TRP:CE2	2.28	0.69
3:I:194:ALA:O	3:I:196:ASN:N	2.26	0.69
2:B:158:SER:HB2	2:B:196:THR:O	1.93	0.69
1:A:99:ILE:CD1	8:A:1001:HEA:HBA2	2.24	0.68
1:G:50:TYR:OH	1:G:79:SER:HB3	1.93	0.68
3:I:162:ARG:HG3	3:I:163:ASP:N	2.08	0.68
1:A:115:LEU:CD1	1:A:432:ILE:HG12	2.23	0.68
1:A:509:LEU:HA	1:A:512:LEU:HD12	1.75	0.68
1:G:91:ASN:CG	1:G:165:GLN:HE22	1.97	0.68
2:H:201:PRO:HB2	2:H:204:LYS:CG	2.23	0.68
2:B:260:HIS:N	10:B:1034:HOH:O	2.26	0.68
3:I:104:HIS:HB2	10:I:3021:HOH:O	1.92	0.68
1:A:367:ILE:CD1	2:B:75:LEU:HB2	2.23	0.68
1:A:538:LEU:HD21	1:A:560:TRP:CE3	2.28	0.68
2:B:176:VAL:HG12	2:B:180:LEU:HD11	1.75	0.68
9:C:2013:3PE:H3F2	9:C:2013:3PE:H2B2	1.74	0.68
1:G:299:SER:HB3	1:G:310:ILE:HD13	1.76	0.68
1:G:403:GLN:O	1:G:404:ALA:C	2.30	0.68
2:H:199:VAL:O	2:H:200:VAL:HG23	1.92	0.68
1:A:127:HIS:HB3	1:A:226:PRO:CG	2.22	0.68
2:B:254:GLU:H	2:B:260:HIS:HE1	1.41	0.68
1:G:99:ILE:HD12	8:G:1001:HEA:HBA2	1.75	0.68
1:G:220:MET:HE2	1:G:225:VAL:HA	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:TRP:HZ2	2:H:257:GLY:HA3	1.58	0.68
1:G:65:ALA:O	1:G:68:LEU:HG	1.92	0.68
1:G:395:GLY:O	1:G:396:VAL:C	2.32	0.68
3:C:101:PHE:CZ	3:C:261:ILE:HG12	2.28	0.68
1:A:442:LYS:HD3	1:A:540:TRP:CZ3	2.28	0.68
2:B:200:VAL:O	2:B:269:VAL:HA	1.93	0.68
2:B:84:HIS:HD2	2:B:86:LYS:H	1.41	0.68
3:C:62:VAL:CG1	9:C:2008:3PE:H31	2.24	0.68
4:D:44:LEU:HD23	9:D:2011:3PE:H322	1.75	0.68
1:G:74:LYS:H	1:G:74:LYS:HD2	1.58	0.68
1:G:426:LEU:HD21	1:G:464:ALA:HB1	1.76	0.68
1:G:506:ALA:HA	1:G:509:LEU:HD12	1.76	0.68
2:H:158:SER:HB2	2:H:196:THR:O	1.94	0.67
2:B:199:VAL:HG11	2:B:278:TRP:CE2	2.29	0.67
1:A:202:ILE:HD11	1:A:244:PRO:HD3	1.76	0.67
1:A:373:GLY:O	2:B:83:PHE:HB3	1.94	0.67
1:A:489:ALA:CB	2:B:36:PRO:HB2	2.24	0.67
1:G:381:MET:CE	1:G:385:LEU:HD21	2.24	0.67
1:A:161:GLY:H	1:A:166:LEU:HA	1.60	0.67
1:A:424:MET:HB3	8:A:1001:HEA:HBC1	1.75	0.67
1:A:543:THR:HG23	1:A:546:PRO:HA	1.77	0.67
3:C:130:PRO:HA	3:C:134:PRO:HG2	1.77	0.67
3:C:152:HIS:HA	3:C:240:PHE:CE1	2.29	0.67
1:A:170:ILE:HD11	1:A:187:THR:OG1	1.95	0.67
1:A:393:VAL:O	1:A:394:GLY:C	2.33	0.67
1:G:165:GLN:HB3	10:G:3049:HOH:O	1.93	0.67
1:A:63:MET:CG	1:A:94:LEU:HD23	2.25	0.67
1:A:160:PRO:HG2	1:A:185:TYR:CE1	2.30	0.67
2:H:220:THR:O	2:H:250:GLY:HA3	1.95	0.67
1:A:132:ASP:OD1	1:A:133:MET:N	2.28	0.67
1:A:374:SER:HB2	2:B:85:GLU:HA	1.76	0.67
1:A:387:PHE:CD1	1:A:387:PHE:C	2.67	0.67
1:G:180:THR:HA	1:G:257:ARG:CD	2.24	0.67
1:G:211:THR:HG22	1:G:212:PHE:N	2.10	0.67
1:A:175:TYR:HB2	10:A:2056:HOH:O	1.95	0.67
1:A:350:MET:HA	1:A:353:MET:HE2	1.77	0.67
1:A:414:TYR:HA	1:A:417:VAL:CG2	2.24	0.67
9:G:3009:3PE:H291	9:G:3009:3PE:C39	2.25	0.67
3:I:161:ARG:NH1	3:I:230:GLY:HA2	2.10	0.67
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.77	0.66
1:G:473:PHE:CD1	2:H:41:THR:HB	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD22	1:A:282:PHE:CE2	2.30	0.66
2:B:156:PHE:HD2	2:B:196:THR:HG21	1.60	0.66
1:A:497:SER:O	1:A:498:SER:C	2.31	0.66
2:B:192:LEU:HB3	2:B:249:PHE:CD2	2.31	0.66
2:B:32:ILE:HD13	2:B:189:GLU:OE2	1.95	0.66
1:G:367:ILE:CD1	2:H:75:LEU:HB2	2.25	0.66
2:H:173:SER:O	2:H:174:PRO:C	2.33	0.66
1:A:177:PRO:HD2	2:B:216:ILE:HG12	1.77	0.66
1:G:213:LEU:HB3	3:I:81:TRP:CH2	2.31	0.66
9:I:3013:3PE:H3G1	9:I:3013:3PE:C2D	2.26	0.66
8:A:1002:HEA:O11	8:A:1002:HEA:HHC	1.96	0.66
3:C:124:GLY:HA2	1:G:557:ARG:HH12	1.60	0.66
3:I:253:VAL:HG13	9:I:3010:3PE:C3I	2.26	0.66
1:A:388:LEU:HD12	2:B:76:ILE:HD11	1.76	0.66
1:A:112:ILE:N	1:A:113:PRO:CD	2.53	0.65
1:A:367:ILE:HD13	2:B:75:LEU:HB2	1.78	0.65
2:H:224:PHE:HB2	2:H:226:VAL:HG22	1.77	0.65
3:I:21:ALA:HB2	3:I:54:THR:CG2	2.25	0.65
1:A:115:LEU:HD12	1:A:432:ILE:HD11	1.77	0.65
9:C:2010:3PE:H231	9:C:2010:3PE:H332	1.79	0.65
1:G:467:THR:HG21	8:G:1001:HEA:HMB2	1.78	0.65
2:H:245:GLU:HA	2:H:269:VAL:HG13	1.79	0.65
2:H:158:SER:HA	2:H:196:THR:HB	1.78	0.65
1:A:65:ALA:HB3	1:A:89:THR:HB	1.78	0.65
1:A:174:LEU:HD13	1:A:191:ILE:HD13	1.79	0.65
1:G:128:ILE:HD12	1:G:216:ARG:HA	1.76	0.65
1:G:249:ALA:HB2	1:G:278:ILE:CG2	2.23	0.65
1:G:380:PRO:HG3	1:G:437:TYR:HB3	1.78	0.65
1:G:433:PHE:O	1:G:436:ILE:N	2.29	0.65
1:G:529:ASN:OD1	1:G:531:TRP:N	2.30	0.65
3:I:101:PHE:CZ	3:I:261:ILE:HG12	2.31	0.65
1:A:433:PHE:HA	1:A:436:ILE:HD12	1.77	0.65
1:A:493:TRP:HA	1:A:493:TRP:CE3	2.29	0.65
9:C:2010:3PE:H231	9:C:2010:3PE:C33	2.26	0.65
2:B:120:LEU:O	2:B:123:LEU:N	2.29	0.65
1:A:202:ILE:HD11	1:A:243:LEU:HB2	1.78	0.65
1:A:332:ALA:HB3	1:A:348:PHE:CG	2.31	0.65
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.79	0.65
1:G:221:THR:HA	9:G:3012:3PE:H121	1.79	0.65
1:G:307:LYS:HA	1:G:534:HIS:CB	2.27	0.65
1:A:135:PHE:CE1	3:C:79:LEU:HD23	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:ILE:HG21	2:H:75:LEU:HD22	1.77	0.65
1:A:211:THR:HG22	1:A:212:PHE:N	2.12	0.64
1:G:46:ALA:O	1:G:49:VAL:HG12	1.97	0.64
1:G:357:VAL:HB	1:G:358:PRO:HD3	1.79	0.64
1:G:509:LEU:HA	1:G:512:LEU:HD12	1.79	0.64
3:I:133:LEU:N	3:I:134:PRO:CD	2.59	0.64
2:B:59:GLY:HA2	10:B:1017:HOH:O	1.98	0.64
4:D:45:ALA:HA	9:D:2011:3PE:H321	1.79	0.64
1:G:246:LEU:HD22	1:G:282:PHE:CE2	2.32	0.64
3:I:176:ALA:O	3:I:179:THR:HB	1.97	0.64
1:A:483:TYR:OH	2:B:251:GLN:HB3	1.97	0.64
1:G:48:THR:HA	1:G:51:MET:SD	2.38	0.64
1:G:493:TRP:CE3	1:G:493:TRP:HA	2.30	0.64
1:G:520:THR:CG2	1:G:521:ARG:HG2	2.26	0.64
3:C:133:LEU:H	3:C:134:PRO:HD2	1.61	0.64
1:G:481:ARG:NH1	10:G:3018:HOH:O	2.26	0.64
2:B:98:SER:HB2	2:B:99:PRO:CD	2.21	0.64
1:G:284:HIS:HE2	1:G:288:TYR:HE2	1.44	0.64
3:I:103:LYS:HE2	3:I:107:TYR:HB2	1.79	0.64
2:B:105:THR:O	2:B:109:ILE:HD12	1.97	0.64
3:C:123:GLU:HB2	10:C:2031:HOH:O	1.96	0.64
1:G:300:HIS:HB3	10:G:3023:HOH:O	1.97	0.64
1:G:393:VAL:O	1:G:394:GLY:C	2.34	0.64
3:C:82:GLY:HA2	3:C:85:LEU:HD12	1.80	0.64
1:A:25:ASN:ND2	1:A:27:LYS:NZ	2.45	0.64
1:A:511:PHE:CZ	1:A:515:ILE:HD11	2.33	0.64
1:G:127:HIS:NE2	1:G:539:GLU:OE1	2.31	0.64
1:G:284:HIS:H	1:G:285:PRO:CD	2.11	0.64
2:H:238:LEU:C	2:H:238:LEU:HD12	2.18	0.64
1:A:235:THR:OG1	1:A:293:PRO:HD3	1.97	0.64
1:A:456:HIS:CE1	1:A:511:PHE:HB2	2.33	0.64
4:D:40:ALA:O	4:D:41:LEU:C	2.35	0.64
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3H2	1.80	0.63
1:A:286:GLN:HA	1:A:289:ILE:HD12	1.80	0.63
1:G:176:PRO:HD2	10:G:3016:HOH:O	1.98	0.63
4:J:15:ASP:OD1	4:J:16:ILE:N	2.30	0.63
1:A:287:VAL:HG23	1:A:288:TYR:N	2.14	0.63
1:G:284:HIS:CB	1:G:285:PRO:HD3	2.21	0.63
2:H:200:VAL:HG12	2:H:269:VAL:HG23	1.80	0.63
2:B:199:VAL:HG21	2:B:278:TRP:CE3	2.33	0.63
1:A:126:LEU:O	1:A:129:GLY:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:HZ3	3:C:88:MET:HE3	1.64	0.63
1:A:467:THR:HG21	8:A:1001:HEA:HMB2	1.80	0.63
3:C:59:TRP:HA	3:C:62:VAL:CG2	2.28	0.63
3:C:152:HIS:HA	3:C:240:PHE:HE1	1.63	0.63
1:G:86:GLU:O	2:H:171:ARG:NH1	2.31	0.63
2:B:201:PRO:HB2	2:B:204:LYS:HG3	1.80	0.63
1:G:287:VAL:HA	1:G:290:ILE:HD12	1.81	0.63
3:I:68:GLU:HB2	10:I:3014:HOH:O	1.99	0.63
3:C:210:GLY:O	3:C:211:PHE:C	2.35	0.63
1:A:290:ILE:HA	10:A:2024:HOH:O	1.99	0.63
1:G:95:TRP:HB2	1:G:484:ILE:HG13	1.81	0.63
1:G:176:PRO:HA	1:G:177:PRO:C	2.19	0.63
3:I:34:LEU:HB3	3:I:39:SER:OG	1.98	0.62
1:A:27:LYS:O	1:A:31:VAL:HG23	1.99	0.62
1:A:287:VAL:HB	8:A:1002:HEA:CBC	2.29	0.62
1:A:529:ASN:OD1	1:A:531:TRP:N	2.32	0.62
1:G:116:PHE:CD1	1:G:235:THR:HG21	2.33	0.62
1:G:274:LEU:O	1:G:277:HIS:N	2.32	0.62
2:H:32:ILE:HD13	2:H:189:GLU:OE2	1.99	0.62
9:A:2012:3PE:H2H1	9:C:2010:3PE:H2I3	1.81	0.62
1:G:65:ALA:HB3	1:G:89:THR:HB	1.81	0.62
2:H:136:VAL:HG11	2:H:198:MET:HE3	1.81	0.62
1:A:439:TRP:O	1:A:443:MET:HG3	1.99	0.62
2:B:278:TRP:HZ2	10:B:1028:HOH:O	1.81	0.62
3:C:56:PHE:O	3:C:57:GLY:C	2.35	0.62
1:G:141:LEU:HB2	3:I:18:PRO:HB3	1.80	0.62
1:G:152:LEU:HD23	3:I:26:PHE:CE2	2.34	0.62
1:G:390:LEU:N	1:G:390:LEU:HD23	2.14	0.62
2:H:252:CYS:HB2	2:H:263:MET:SD	2.40	0.62
9:I:3013:3PE:H3H2	9:I:3013:3PE:C2E	2.28	0.62
1:A:95:TRP:HB2	1:A:484:ILE:HG13	1.82	0.62
2:B:141:TYR:HE1	2:B:146:GLY:HA3	1.64	0.62
2:H:220:THR:HB	2:H:227:LYS:HG3	1.82	0.62
3:I:59:TRP:HA	3:I:62:VAL:CG2	2.30	0.62
1:A:115:LEU:HD11	1:A:432:ILE:HG12	1.80	0.62
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.82	0.62
1:A:455:LEU:HD23	1:A:510:PHE:CE2	2.33	0.62
1:G:284:HIS:N	1:G:285:PRO:CD	2.63	0.62
1:G:401:LEU:HD13	1:G:416:VAL:CG2	2.19	0.62
1:A:221:THR:HG23	1:A:224:LYS:HD2	1.81	0.62
1:G:307:LYS:HD3	1:G:374:SER:OG	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3013:3PE:H2D2	9:I:3013:3PE:C3H	2.29	0.62
2:B:245:GLU:HA	2:B:269:VAL:HG13	1.81	0.62
3:C:150:TRP:NE1	3:C:163:ASP:OD1	2.31	0.62
3:C:161:ARG:NH2	3:C:232:PHE:H	1.98	0.62
1:G:474:LEU:HD13	10:G:3047:HOH:O	1.98	0.62
1:A:279:LEU:HD23	1:A:279:LEU:O	1.99	0.61
1:A:376:GLU:O	1:A:378:LYS:N	2.32	0.61
2:B:211:THR:HG22	2:B:212:GLY:N	2.15	0.61
2:H:176:VAL:HG12	2:H:180:LEU:HD11	1.82	0.61
1:A:44:SER:O	1:A:45:VAL:C	2.37	0.61
1:G:307:LYS:HA	1:G:534:HIS:CG	2.34	0.61
1:G:325:VAL:O	1:G:326:LEU:C	2.37	0.61
1:G:342:LEU:HD21	2:H:124:PHE:CD1	2.35	0.61
2:H:271:SER:HA	10:H:1091:HOH:O	2.00	0.61
1:A:65:ALA:O	1:A:68:LEU:HG	1.99	0.61
1:A:407:ASP:O	1:A:408:ARG:C	2.39	0.61
3:C:152:HIS:CG	3:C:244:ILE:HD13	2.35	0.61
1:G:51:MET:O	1:G:52:ARG:C	2.39	0.61
3:I:80:ARG:HH12	9:I:3013:3PE:H111	1.65	0.61
1:A:48:THR:HA	1:A:51:MET:SD	2.40	0.61
1:A:170:ILE:HG22	1:A:171:GLY:N	2.15	0.61
1:G:404:ALA:O	1:G:407:ASP:N	2.34	0.61
1:G:442:LYS:NZ	1:G:542:LEU:O	2.31	0.61
2:H:164:PRO:HB3	10:H:1122:HOH:O	2.00	0.61
1:A:70:SER:HB2	1:A:74:LYS:HB2	1.82	0.61
1:A:81:TRP:CD2	1:A:82:PRO:HD2	2.36	0.61
2:B:107:VAL:CG1	2:B:108:PRO:HD3	2.25	0.61
2:B:136:VAL:HG11	2:B:198:MET:HE3	1.81	0.61
2:B:151:ASP:HB2	10:B:1025:HOH:O	1.99	0.61
3:C:133:LEU:N	3:C:134:PRO:CD	2.64	0.61
1:G:99:ILE:CD1	8:G:1001:HEA:HBA2	2.30	0.61
1:G:130:ALA:HB1	1:G:131:PRO:HD2	1.80	0.61
1:G:560:TRP:C	1:G:560:TRP:CD1	2.73	0.61
3:I:186:TYR:O	3:I:187:SER:C	2.39	0.61
1:G:170:ILE:O	2:H:255:LEU:HD23	2.01	0.61
1:G:222:MET:HG3	9:G:3012:3PE:C11	2.26	0.61
3:I:9:TYR:HB3	10:I:3018:HOH:O	1.99	0.61
1:A:520:THR:CG2	1:A:521:ARG:HG2	2.29	0.61
1:G:463:GLY:N	1:G:503:LEU:HD23	2.16	0.61
2:H:248:PHE:HE2	2:H:269:VAL:CG1	2.14	0.61
3:I:253:VAL:CA	9:I:3010:3PE:H3H1	2.27	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:HB3	1:A:348:PHE:CD2	2.35	0.61
1:A:422:TYR:HH	1:A:469:PHE:HD1	1.47	0.61
2:B:173:SER:O	2:B:174:PRO:C	2.39	0.61
1:G:265:GLN:H	1:G:270:GLY:HA3	1.65	0.61
2:H:173:SER:HG	2:H:175:GLU:HB2	1.66	0.61
1:A:92:GLY:HA2	1:A:484:ILE:HD12	1.83	0.61
1:A:128:ILE:HD12	1:A:216:ARG:HA	1.82	0.61
1:A:397:THR:O	1:A:400:VAL:N	2.34	0.61
3:I:73:PRO:HB2	4:J:16:ILE:HD11	1.82	0.61
4:J:16:ILE:HG22	4:J:19:GLN:HB2	1.81	0.61
1:G:264:PHE:HB3	1:G:272:PRO:HA	1.83	0.61
1:G:417:VAL:HA	1:G:420:PHE:CE1	2.36	0.61
1:G:543:THR:HG23	1:G:546:PRO:HA	1.83	0.61
2:H:43:PHE:CD2	2:H:55:HIS:CD2	2.89	0.61
2:H:250:GLY:O	2:H:265:ILE:N	2.33	0.61
1:A:447:GLN:HG3	1:A:448:TYR:N	2.15	0.60
1:A:543:THR:CG2	1:A:547:PRO:HD3	2.31	0.60
2:B:234:ARG:NH1	3:C:114:PRO:HG3	2.16	0.60
1:G:176:PRO:HB2	1:G:177:PRO:HA	1.82	0.60
1:G:302:ILE:HG22	1:G:369:THR:CG2	2.30	0.60
3:I:162:ARG:HG3	3:I:163:ASP:H	1.65	0.60
1:A:284:HIS:H	1:A:285:PRO:HD2	1.66	0.60
3:C:133:LEU:N	3:C:134:PRO:HD2	2.15	0.60
1:G:202:ILE:HD11	1:G:243:LEU:HB2	1.81	0.60
3:I:21:ALA:CB	3:I:54:THR:HG21	2.26	0.60
1:G:28:ASP:O	1:G:32:LEU:HG	2.02	0.60
2:H:98:SER:HB2	2:H:99:PRO:CD	2.28	0.60
3:I:152:HIS:HA	3:I:240:PHE:CE1	2.35	0.60
4:J:14:MET:HG2	4:J:15:ASP:N	2.17	0.60
1:A:65:ALA:H	1:A:89:THR:HB	1.67	0.60
1:A:432:ILE:O	1:A:436:ILE:HG13	2.01	0.60
2:B:199:VAL:O	2:B:200:VAL:HG23	2.00	0.60
1:G:323:ILE:HD11	1:G:359:THR:OG1	2.01	0.60
2:H:103:ALA:O	2:H:107:VAL:HG12	2.00	0.60
3:I:239:GLY:H	9:I:3008:3PE:H11	1.66	0.60
1:A:29:ILE:HD13	1:A:139:ASN:ND2	2.15	0.60
1:G:451:TRP:O	1:G:452:ALA:C	2.40	0.60
1:G:538:LEU:HD21	1:G:560:TRP:CE3	2.37	0.60
3:I:120:PHE:HA	3:I:121:PRO:C	2.22	0.60
1:A:192:PHE:CZ	1:A:254:LEU:HD21	2.37	0.60
1:A:213:LEU:HB3	3:C:81:TRP:CH2	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD12	1:A:426:LEU:HB3	1.84	0.60
9:A:2012:3PE:H2I3	9:C:2010:3PE:H2H1	1.83	0.60
2:B:228:GLN:NE2	2:B:229:ASP:H	1.99	0.60
2:H:228:GLN:HB2	10:H:1069:HOH:O	2.02	0.60
1:A:50:TYR:OH	1:A:79:SER:HB3	2.02	0.60
1:A:357:VAL:HG21	2:B:109:ILE:HD11	1.83	0.60
1:A:390:LEU:HD23	1:A:390:LEU:N	2.16	0.60
1:A:503:LEU:O	1:A:506:ALA:HB3	2.01	0.60
1:A:367:ILE:HG21	2:B:75:LEU:HD22	1.83	0.60
2:B:235:LEU:HD21	4:J:9:HIS:HB2	1.84	0.60
9:C:2013:3PE:H2I3	4:D:35:VAL:HG21	1.84	0.60
1:G:394:GLY:HA3	1:G:423:VAL:HG12	1.82	0.60
3:I:77:LEU:HA	3:I:80:ARG:HD3	1.83	0.60
1:G:442:LYS:HD3	1:G:540:TRP:CZ3	2.36	0.60
1:A:52:ARG:HD3	1:A:498:SER:HA	1.84	0.60
1:A:60:VAL:HG21	1:A:90:PRO:HB3	1.84	0.60
1:A:390:LEU:HA	1:A:393:VAL:HG23	1.83	0.60
1:A:466:LEU:O	1:A:470:PRO:HD2	2.02	0.60
3:C:76:ARG:O	3:C:80:ARG:HG3	2.01	0.60
1:G:40:VAL:O	1:G:41:GLY:C	2.40	0.60
4:J:49:ALA:O	9:J:3011:3PE:H122	2.02	0.60
1:G:486:TYR:HB2	1:G:487:PRO:HD2	1.83	0.59
1:A:106:MET:HE3	1:A:110:VAL:HB	1.83	0.59
3:C:133:LEU:H	3:C:134:PRO:CD	2.15	0.59
3:C:253:VAL:HG22	9:C:2010:3PE:H3I1	1.83	0.59
1:G:432:ILE:CG2	8:G:1001:HEA:H252	2.31	0.59
2:H:197:ALA:HB2	2:H:268:LYS:NZ	2.17	0.59
3:C:209:HIS:NE2	3:C:254:TRP:HB2	2.18	0.59
1:A:489:ALA:HB3	2:B:36:PRO:HB2	1.82	0.59
2:B:175:GLU:O	2:B:178:GLN:HG2	2.03	0.59
3:C:149:THR:O	3:C:152:HIS:HB3	2.03	0.59
1:G:106:MET:HE1	1:G:110:VAL:HG11	1.85	0.59
1:G:357:VAL:CB	1:G:358:PRO:HD3	2.32	0.59
1:G:491:ALA:HB1	10:G:3036:HOH:O	2.02	0.59
2:H:160:MET:CE	2:H:262:TYR:HB3	2.32	0.59
3:I:155:LEU:HB2	3:I:164:VAL:HG21	1.84	0.59
3:I:212:HIS:O	3:I:213:VAL:C	2.39	0.59
1:A:38:GLY:HA2	8:A:1001:HEA:H22	1.84	0.59
9:C:2010:3PE:H2I1	9:C:2013:3PE:H2B2	1.84	0.59
1:A:65:ALA:CB	1:A:89:THR:HB	2.32	0.59
1:A:299:SER:HB3	1:A:310:ILE:HD13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TYR:HB2	1:A:487:PRO:HD2	1.84	0.59
2:B:200:VAL:HG12	2:B:269:VAL:HG23	1.83	0.59
2:B:228:GLN:HB2	10:B:1014:HOH:O	2.02	0.59
3:I:92:MET:O	3:I:93:PHE:C	2.36	0.59
1:A:380:PRO:HG3	1:A:437:TYR:HB3	1.83	0.59
1:G:91:ASN:HD21	1:G:165:GLN:CD	2.06	0.59
1:G:268:GLY:O	3:I:197:ILE:HG23	2.02	0.59
2:B:208:VAL:HB	2:B:238:LEU:HG	1.84	0.59
1:G:40:VAL:HG12	1:G:110:VAL:HG22	1.85	0.59
1:A:17:PHE:O	1:A:21:PHE:HB2	2.03	0.59
1:G:178:LEU:HD12	1:G:178:LEU:O	2.02	0.59
1:A:98:MET:O	1:A:99:ILE:C	2.42	0.58
1:A:262:THR:HG22	10:C:2028:HOH:O	2.02	0.58
1:G:106:MET:HE3	1:G:110:VAL:HB	1.85	0.58
1:G:486:TYR:HD2	1:G:490:PHE:HB2	1.67	0.58
2:H:279:LEU:O	2:H:283:ARG:HG2	2.03	0.58
1:A:279:LEU:C	1:A:279:LEU:CD2	2.53	0.58
1:G:63:MET:SD	1:G:94:LEU:HD23	2.43	0.58
1:G:93:HIS:HA	10:G:3030:HOH:O	2.02	0.58
3:I:74:VAL:HG12	4:J:16:ILE:HG23	1.85	0.58
4:J:15:ASP:OD1	4:J:15:ASP:C	2.41	0.58
1:A:287:VAL:HG11	8:A:1002:HEA:CHD	2.33	0.58
2:B:51:ALA:HA	2:B:54:ILE:HD12	1.85	0.58
3:I:85:LEU:O	3:I:88:MET:N	2.36	0.58
1:A:18:THR:HA	1:A:22:MET:HE3	1.83	0.58
1:A:70:SER:HB2	1:A:74:LYS:CB	2.32	0.58
1:A:227:LEU:O	1:A:230:TRP:N	2.36	0.58
1:G:125:PRO:HG3	1:G:133:MET:SD	2.43	0.58
1:G:407:ASP:O	1:G:408:ARG:C	2.41	0.58
2:B:200:VAL:HG22	2:B:201:PRO:HD2	1.85	0.58
1:G:91:ASN:ND2	1:G:165:GLN:NE2	2.51	0.58
1:G:112:ILE:N	1:G:113:PRO:CD	2.66	0.58
1:A:342:LEU:HD13	2:B:127:GLN:CB	2.30	0.58
1:A:95:TRP:CZ2	1:A:99:ILE:HD11	2.38	0.58
2:B:252:CYS:HB2	2:B:263:MET:CG	2.34	0.58
1:G:456:HIS:CE1	1:G:511:PHE:HB2	2.38	0.58
1:G:474:LEU:HD21	1:G:494:ASN:HD22	1.68	0.58
1:G:279:LEU:C	1:G:279:LEU:CD2	2.55	0.58
1:G:336:TYR:HD2	1:G:407:ASP:OD2	1.87	0.58
1:G:379:THR:CB	1:G:380:PRO:CD	2.76	0.58
3:I:127:THR:OG1	3:I:266:GLN:HG3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ALA:CB	3:I:170:LEU:HD23	2.33	0.58
1:A:38:GLY:O	1:A:39:LEU:C	2.41	0.58
1:A:108:PHE:CE2	1:A:194:VAL:HG13	2.39	0.58
1:A:160:PRO:O	1:A:184:GLY:HA3	2.03	0.58
1:A:330:VAL:HG11	1:A:352:THR:HA	1.86	0.58
1:A:495:PHE:O	1:A:496:VAL:C	2.42	0.58
3:I:130:PRO:O	3:I:134:PRO:HB2	2.03	0.58
1:A:24:THR:HG23	3:C:14:PRO:HA	1.85	0.57
1:A:264:PHE:HB3	1:A:272:PRO:HA	1.86	0.57
1:G:63:MET:HE1	1:G:95:TRP:HE3	1.69	0.57
1:G:185:TYR:HB3	3:I:37:HIS:CD2	2.39	0.57
1:G:284:HIS:H	1:G:285:PRO:HD2	1.69	0.57
1:G:482:ARG:HD2	10:G:3111:HOH:O	2.03	0.57
1:A:22:MET:HG2	3:C:16:ILE:CA	2.34	0.57
1:A:212:PHE:CD1	1:A:213:LEU:HD23	2.39	0.57
1:G:27:LYS:O	1:G:31:VAL:HG23	2.04	0.57
1:G:131:PRO:HG2	3:I:9:TYR:HD2	1.69	0.57
1:G:295:PHE:O	1:G:298:VAL:HB	2.04	0.57
1:G:389:PHE:O	1:G:392:THR:N	2.38	0.57
2:B:43:PHE:CD2	2:B:55:HIS:CD2	2.92	0.57
1:G:253:LEU:HD21	1:G:275:TYR:CE1	2.39	0.57
9:G:3009:3PE:H381	9:G:3009:3PE:H251	1.86	0.57
2:H:145:TRP:CD1	2:H:263:MET:HE2	2.40	0.57
3:I:240:PHE:CD1	3:I:244:ILE:HD11	2.38	0.57
3:I:249:PHE:O	3:I:253:VAL:HG23	2.05	0.57
1:A:41:GLY:O	1:A:45:VAL:N	2.35	0.57
1:A:128:ILE:HD12	1:A:216:ARG:CA	2.35	0.57
1:G:350:MET:O	1:G:353:MET:HB2	2.05	0.57
1:G:420:PHE:O	1:G:421:HIS:C	2.43	0.57
1:G:432:ILE:O	1:G:436:ILE:HG13	2.04	0.57
3:I:161:ARG:HH21	3:I:232:PHE:H	1.52	0.57
1:A:246:LEU:HD22	1:A:282:PHE:CZ	2.39	0.57
2:H:120:LEU:O	2:H:123:LEU:N	2.35	0.57
1:A:357:VAL:CB	1:A:358:PRO:HD3	2.35	0.57
2:B:228:GLN:HG3	2:B:229:ASP:N	2.19	0.57
1:G:217:ALA:HB1	10:G:3090:HOH:O	2.04	0.57
2:H:86:LYS:HE3	10:H:1179:HOH:O	2.03	0.57
2:H:278:TRP:HZ2	10:H:1115:HOH:O	1.87	0.57
3:I:141:LEU:HD11	3:I:178:PHE:CE2	2.40	0.57
1:A:551:PHE:CE1	1:A:555:PRO:HG3	2.40	0.57
3:C:17:TRP:O	3:C:20:MET:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:LYS:HB3	1:G:534:HIS:CD2	2.40	0.57
3:I:92:MET:O	3:I:95:SER:N	2.38	0.57
1:A:508:PHE:CD1	1:A:512:LEU:HD11	2.39	0.57
1:A:99:ILE:O	1:A:102:HIS:HB3	2.05	0.57
1:G:249:ALA:O	1:G:252:MET:HG3	2.05	0.57
1:G:341:SER:OG	1:G:344:GLN:HG3	2.05	0.57
1:A:111:VAL:HG13	1:A:111:VAL:O	2.04	0.57
1:A:425:SER:HA	1:A:429:VAL:CG2	2.35	0.57
9:C:2013:3PE:H2G2	4:D:35:VAL:CG2	2.35	0.57
1:G:212:PHE:C	1:G:212:PHE:CD1	2.78	0.57
2:H:120:LEU:CB	2:H:121:PRO:CD	2.83	0.57
2:H:147:TYR:HE1	10:H:1159:HOH:O	1.87	0.57
1:A:147:VAL:O	1:A:148:ALA:C	2.43	0.56
1:A:222:MET:H	9:A:2012:3PE:H111	1.70	0.56
1:A:228:PHE:CE1	1:A:297:ILE:HG13	2.40	0.56
1:A:284:HIS:H	1:A:285:PRO:CD	2.18	0.56
1:A:379:THR:O	1:A:380:PRO:C	2.42	0.56
1:G:198:GLY:HA2	1:G:243:LEU:HD13	1.87	0.56
1:G:212:PHE:CD1	1:G:213:LEU:HD23	2.40	0.56
1:G:402:SER:OG	1:G:403:GLN:NE2	2.34	0.56
1:G:450:GLU:O	1:G:454:LYS:HG3	2.04	0.56
3:I:130:PRO:HB3	3:I:263:ILE:HD13	1.87	0.56
9:I:3010:3PE:C33	9:I:3010:3PE:H231	2.35	0.56
1:A:452:ALA:HB1	1:A:514:VAL:HG21	1.87	0.56
3:I:72:THR:O	3:I:75:VAL:HG23	2.06	0.56
1:A:26:HIS:HB3	1:A:132:ASP:OD1	2.05	0.56
1:A:63:MET:HE1	1:A:95:TRP:HE3	1.69	0.56
1:G:34:LEU:HD23	1:G:114:ALA:HB1	1.86	0.56
1:G:145:LEU:HD23	3:I:22:SER:OG	2.05	0.56
1:G:222:MET:H	9:G:3012:3PE:H111	1.69	0.56
1:G:463:GLY:CA	1:G:503:LEU:HD23	2.35	0.56
1:G:480:PRO:HG2	1:G:483:TYR:CE2	2.40	0.56
3:I:99:TRP:CD1	9:I:3010:3PE:H352	2.41	0.56
1:A:40:VAL:CG1	1:A:105:LEU:HD22	2.36	0.56
1:A:40:VAL:O	1:A:41:GLY:C	2.43	0.56
3:C:70:ASP:O	3:C:75:VAL:HG21	2.06	0.56
3:I:81:TRP:O	3:I:84:ILE:N	2.34	0.56
3:I:245:TRP:HE1	9:I:3013:3PE:H322	1.71	0.56
1:A:176:PRO:HD2	10:A:2013:HOH:O	2.06	0.56
1:A:396:VAL:HG13	2:B:65:ILE:HG21	1.87	0.56
4:D:16:ILE:HA	4:D:19:GLN:OE1	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ILE:HD11	1:G:289:ILE:HG21	1.88	0.56
1:G:251:THR:O	1:G:254:LEU:N	2.37	0.56
1:G:503:LEU:O	1:G:506:ALA:HB3	2.06	0.56
3:I:101:PHE:CE1	3:I:261:ILE:HG12	2.40	0.56
3:I:125:ILE:CD1	3:I:198:TYR:HB3	2.36	0.56
1:A:336:TYR:HD2	1:A:407:ASP:OD2	1.89	0.56
2:B:259:SER:HB3	2:B:262:TYR:HB2	1.86	0.56
3:C:84:ILE:HG23	9:C:2013:3PE:H272	1.88	0.56
3:I:99:TRP:O	3:I:100:SER:C	2.44	0.56
1:A:170:ILE:O	2:B:255:LEU:HD23	2.05	0.56
1:A:319:ALA:O	1:A:322:ALA:HB3	2.04	0.56
1:A:511:PHE:CE1	1:A:515:ILE:HD11	2.41	0.56
2:B:224:PHE:HB2	2:B:226:VAL:HG22	1.86	0.56
3:C:226:ARG:NH2	3:C:231:HIS:HB3	2.21	0.56
1:G:63:MET:HE1	1:G:95:TRP:CB	2.33	0.56
1:G:137:ARG:HH21	9:G:3009:3PE:C11	2.19	0.56
1:G:287:VAL:HG23	1:G:288:TYR:N	2.20	0.56
1:A:394:GLY:HA3	1:A:423:VAL:HG13	1.88	0.56
1:G:231:SER:N	1:G:320:MET:HE1	2.20	0.56
1:G:314:LEU:HB3	1:G:315:PRO:HD3	1.88	0.56
9:G:3012:3PE:H261	4:J:29:MET:SD	2.46	0.56
2:H:196:THR:O	2:H:196:THR:HG22	2.06	0.56
2:H:221:VAL:HB	2:H:224:PHE:HD2	1.71	0.56
1:A:176:PRO:HB2	1:A:177:PRO:HA	1.86	0.56
2:B:263:MET:HG3	2:B:263:MET:O	2.04	0.56
3:C:86:PHE:CZ	9:C:2008:3PE:H2A1	2.41	0.56
1:A:27:LYS:HG2	1:A:122:TYR:CE1	2.40	0.56
1:A:63:MET:HE1	1:A:95:TRP:HB2	1.88	0.56
1:A:298:VAL:O	1:A:299:SER:C	2.44	0.56
1:A:481:ARG:NH1	10:A:2015:HOH:O	2.23	0.56
1:A:520:THR:HG22	1:A:521:ARG:N	2.20	0.56
1:G:91:ASN:HD21	1:G:165:GLN:NE2	2.04	0.56
1:G:423:VAL:HG21	8:G:1002:HEA:C3C	2.35	0.56
1:A:46:ALA:O	1:A:49:VAL:HG12	2.05	0.55
1:A:390:LEU:CD1	1:A:426:LEU:HB3	2.36	0.55
2:B:33:ILE:HD11	10:B:1042:HOH:O	2.06	0.55
1:G:101:GLY:HA2	10:G:3027:HOH:O	2.05	0.55
2:H:255:LEU:N	10:H:1052:HOH:O	2.39	0.55
1:A:284:HIS:HB3	1:A:285:PRO:CD	2.32	0.55
1:A:402:SER:OG	1:A:403:GLN:NE2	2.38	0.55
1:G:18:THR:HA	1:G:22:MET:CE	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:ILE:CG2	1:G:377:LEU:HD23	2.37	0.55
2:H:194:THR:HG22	2:H:266:THR:HB	1.88	0.55
1:A:106:MET:HG2	8:A:1001:HEA:C3C	2.33	0.55
1:A:239:ILE:O	1:A:240:LEU:C	2.43	0.55
2:B:271:SER:HA	10:B:1024:HOH:O	2.05	0.55
3:C:222:VAL:HG11	9:C:2008:3PE:H351	1.87	0.55
1:G:557:ARG:NH1	10:G:3015:HOH:O	2.39	0.55
2:H:45:PRO:HB3	2:H:244:ARG:NH2	2.21	0.55
2:H:217:HIS:CE1	2:H:256:CYS:HB2	2.41	0.55
4:J:45:ALA:CA	9:J:3011:3PE:H321	2.34	0.55
1:A:173:VAL:HG12	1:A:279:LEU:HD13	1.87	0.55
1:A:411:HIS:CD2	1:A:412:ASP:HB2	2.42	0.55
1:A:431:GLY:O	1:A:432:ILE:C	2.43	0.55
3:C:31:GLY:HA2	3:C:43:MET:SD	2.46	0.55
1:G:24:THR:HG23	3:I:14:PRO:HA	1.88	0.55
1:G:38:GLY:HA2	8:G:1001:HEA:H22	1.88	0.55
1:G:433:PHE:O	1:G:434:ALA:C	2.45	0.55
3:I:81:TRP:O	3:I:82:GLY:C	2.45	0.55
1:A:137:ARG:HB2	9:A:2009:3PE:O14	2.06	0.55
3:C:124:GLY:CA	1:G:557:ARG:HH12	2.19	0.55
2:H:220:THR:HB	2:H:227:LYS:CG	2.37	0.55
1:A:91:ASN:HD21	1:A:165:GLN:NE2	2.05	0.55
1:A:228:PHE:CD1	1:A:297:ILE:HG13	2.42	0.55
1:A:237:TRP:CZ2	9:A:2012:3PE:H282	2.42	0.55
1:A:284:HIS:O	1:A:287:VAL:HG22	2.07	0.55
1:A:539:GLU:HG2	1:A:540:TRP:H	1.72	0.55
3:C:34:LEU:HB3	3:C:39:SER:OG	2.07	0.55
1:G:29:ILE:HD13	1:G:139:ASN:ND2	2.22	0.55
1:G:175:TYR:HB3	10:G:3016:HOH:O	2.07	0.55
1:G:269:GLY:O	3:I:109:MET:HG3	2.07	0.55
1:G:289:ILE:O	1:G:293:PRO:HD2	2.07	0.55
1:G:294:ALA:O	1:G:295:PHE:C	2.44	0.55
1:G:450:GLU:OE2	1:G:454:LYS:HE3	2.07	0.55
1:A:76:PHE:O	1:A:79:SER:HB2	2.07	0.55
2:B:78:TYR:CD1	2:B:78:TYR:C	2.80	0.55
1:G:192:PHE:CZ	1:G:254:LEU:HD21	2.41	0.55
1:G:402:SER:HA	8:G:1002:HEA:OMA	2.07	0.55
1:A:116:PHE:CD1	1:A:235:THR:HG21	2.42	0.55
1:A:381:MET:O	1:A:382:LEU:C	2.43	0.55
1:A:473:PHE:HB3	2:B:41:THR:HA	1.88	0.55
3:C:52:LEU:HD22	9:C:2008:3PE:H3C2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:VAL:HG11	1:G:290:ILE:HG23	1.88	0.55
1:A:386:GLY:O	1:A:390:LEU:HG	2.07	0.55
1:A:474:LEU:HD13	10:A:2042:HOH:O	2.06	0.55
1:G:235:THR:OG1	1:G:293:PRO:HD3	2.06	0.55
2:H:33:ILE:HG22	2:H:34:GLY:N	2.21	0.55
1:A:52:ARG:CD	1:A:498:SER:HA	2.37	0.55
1:A:159:ALA:HB1	1:A:160:PRO:HD2	1.89	0.55
1:A:220:MET:HE2	1:A:225:VAL:HA	1.89	0.55
8:A:1002:HEA:C22	2:B:68:ILE:HD13	2.37	0.55
2:H:176:VAL:O	2:H:180:LEU:HG	2.07	0.55
2:H:195:ASP:OD1	2:H:196:THR:N	2.40	0.55
1:A:274:LEU:HD21	3:C:100:SER:HA	1.89	0.54
1:A:329:VAL:HG23	1:A:329:VAL:O	2.05	0.54
1:A:396:VAL:O	1:A:397:THR:C	2.45	0.54
1:A:494:ASN:O	1:A:495:PHE:C	2.45	0.54
1:G:15:GLY:O	1:G:18:THR:HB	2.07	0.54
2:H:210:VAL:N	2:H:236:ALA:O	2.34	0.54
3:C:186:TYR:O	3:C:187:SER:C	2.45	0.54
1:G:284:HIS:HB3	1:G:285:PRO:CD	2.30	0.54
1:G:411:HIS:CD2	1:G:412:ASP:HB2	2.43	0.54
1:A:295:PHE:CD2	1:A:362:LYS:HE2	2.43	0.54
1:A:304:THR:OG1	1:A:535:ALA:HA	2.08	0.54
1:G:210:THR:O	1:G:211:THR:C	2.46	0.54
9:G:3009:3PE:H2C2	9:G:3009:3PE:H3B2	1.89	0.54
3:I:152:HIS:HA	3:I:240:PHE:HE1	1.70	0.54
1:A:41:GLY:O	1:A:42:LEU:C	2.44	0.54
1:A:292:LEU:HB2	1:A:293:PRO:HD3	1.90	0.54
3:C:161:ARG:NH1	3:C:230:GLY:HA2	2.18	0.54
1:G:394:GLY:HA3	1:G:423:VAL:HG13	1.89	0.54
1:G:459:MET:O	1:G:462:VAL:HB	2.07	0.54
2:H:73:THR:HG22	2:H:77:LEU:HG	1.89	0.54
1:A:96:ASN:O	1:A:97:VAL:C	2.46	0.54
3:C:137:ASN:HA	3:C:140:ILE:HD12	1.89	0.54
9:I:3010:3PE:H342	9:J:3011:3PE:H342	1.88	0.54
1:A:188:ASP:CG	1:A:257:ARG:HH12	2.11	0.54
1:A:390:LEU:HD23	1:A:390:LEU:H	1.72	0.54
1:G:70:SER:HB2	1:G:74:LYS:HB2	1.90	0.54
2:H:161:ILE:HG13	2:H:193:ALA:O	2.08	0.54
4:J:40:ALA:O	4:J:41:LEU:C	2.44	0.54
1:A:401:LEU:CD1	1:A:416:VAL:HG22	2.29	0.54
1:A:407:ASP:OD1	1:A:411:HIS:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:GLY:HA2	10:J:1118:HOH:O	2.07	0.54
4:D:15:ASP:C	4:D:15:ASP:OD1	2.46	0.54
1:G:63:MET:CE	1:G:95:TRP:HE3	2.21	0.54
1:G:137:ARG:HH21	9:G:3009:3PE:H112	1.72	0.54
1:A:124:MET:SD	1:A:125:PRO:HD3	2.47	0.54
1:A:424:MET:SD	8:A:1002:HEA:HAC	2.47	0.54
3:C:130:PRO:O	3:C:134:PRO:HB2	2.08	0.54
1:G:25:ASN:ND2	1:G:27:LYS:NZ	2.50	0.54
1:G:176:PRO:HA	1:G:178:LEU:N	2.23	0.54
1:G:318:TYR:O	1:G:319:ALA:C	2.46	0.54
2:H:62:LEU:CD1	2:H:65:ILE:HD11	2.28	0.54
3:I:226:ARG:HH21	3:I:231:HIS:HB3	1.72	0.54
1:A:452:ALA:O	1:A:453:GLY:C	2.46	0.54
2:B:65:ILE:C	2:B:65:ILE:HD12	2.28	0.54
3:I:31:GLY:CA	3:I:43:MET:SD	2.96	0.54
1:A:91:ASN:ND2	1:A:165:GLN:NE2	2.51	0.54
1:A:178:LEU:O	1:A:178:LEU:HD12	2.07	0.54
2:B:201:PRO:HB2	2:B:204:LYS:CG	2.38	0.54
1:G:127:HIS:CE1	1:G:300:HIS:CE1	2.96	0.54
1:G:176:PRO:O	2:H:216:ILE:HD11	2.08	0.54
1:G:191:ILE:HD12	1:G:250:ILE:HB	1.90	0.54
1:G:263:PHE:HE1	3:I:201:ASN:ND2	2.06	0.54
1:G:396:VAL:O	1:G:397:THR:C	2.46	0.54
1:A:27:LYS:HG2	1:A:122:TYR:CD1	2.43	0.53
1:A:441:GLY:O	1:A:442:LYS:C	2.46	0.53
3:C:152:HIS:CA	3:C:240:PHE:HE1	2.21	0.53
1:G:473:PHE:HB3	2:H:41:THR:HA	1.90	0.53
2:H:211:THR:CG2	2:H:212:GLY:H	2.20	0.53
3:I:222:VAL:HA	3:I:225:ILE:HD12	1.89	0.53
1:A:115:LEU:HD12	1:A:432:ILE:CD1	2.38	0.53
1:A:227:LEU:O	1:A:228:PHE:C	2.47	0.53
1:A:300:HIS:O	1:A:303:ALA:HB3	2.08	0.53
1:A:312:GLY:O	1:A:316:MET:HG2	2.08	0.53
1:A:329:VAL:HG12	9:D:2011:3PE:H2B2	1.88	0.53
2:B:142:GLN:O	2:B:143:TRP:HB2	2.08	0.53
3:C:120:PHE:CD1	3:C:120:PHE:C	2.82	0.53
1:G:102:HIS:O	1:G:103:GLY:C	2.47	0.53
2:H:143:TRP:CZ2	2:H:257:GLY:HA3	2.40	0.53
3:I:125:ILE:HD12	3:I:198:TYR:HB3	1.89	0.53
3:I:161:ARG:HH22	3:I:232:PHE:H	1.55	0.53
1:A:315:PRO:O	1:A:316:MET:C	2.45	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TYR:HD2	1:A:490:PHE:HB2	1.71	0.53
3:C:152:HIS:O	3:C:156:VAL:HG23	2.07	0.53
2:H:78:TYR:C	2:H:78:TYR:CD1	2.82	0.53
3:I:108:PRO:HA	10:I:3016:HOH:O	2.07	0.53
1:A:279:LEU:HD23	1:A:280:TRP:N	2.20	0.53
2:B:248:PHE:HE2	2:B:269:VAL:CG1	2.20	0.53
1:G:106:MET:HE1	1:G:110:VAL:CG1	2.38	0.53
1:G:235:THR:HG22	1:G:236:ALA:N	2.19	0.53
2:H:71:PHE:O	2:H:75:LEU:HD12	2.07	0.53
3:I:256:PHE:CZ	9:J:3011:3PE:H391	2.43	0.53
8:A:1002:HEA:H202	8:A:1002:HEA:H253	1.91	0.53
2:B:143:TRP:N	2:B:143:TRP:CD1	2.75	0.53
1:G:314:LEU:O	1:G:315:PRO:C	2.47	0.53
1:G:489:ALA:HB3	2:H:36:PRO:HB2	1.90	0.53
1:G:547:PRO:O	1:G:548:GLU:C	2.44	0.53
3:I:192:GLY:O	3:I:199:GLY:HA3	2.07	0.53
4:J:36:VAL:O	4:J:39:ALA:HB3	2.08	0.53
1:A:152:LEU:HD23	3:C:26:PHE:CE2	2.44	0.53
1:A:437:TYR:O	1:A:440:ILE:HG22	2.08	0.53
9:A:2012:3PE:H361	9:A:2012:3PE:H291	1.90	0.53
9:A:2012:3PE:H2D1	9:D:2011:3PE:H2I1	1.90	0.53
3:C:74:VAL:HG23	3:C:75:VAL:N	2.24	0.53
1:G:538:LEU:HD21	1:G:560:TRP:HE3	1.73	0.53
9:G:3009:3PE:H251	9:G:3009:3PE:C38	2.38	0.53
1:A:451:TRP:O	1:A:452:ALA:C	2.47	0.53
1:A:493:TRP:O	1:A:494:ASN:C	2.47	0.53
3:C:66:SER:HB2	3:C:71:HIS:CE1	2.42	0.53
1:G:273:VAL:O	1:G:274:LEU:C	2.45	0.53
1:G:425:SER:HA	1:G:429:VAL:HG21	1.91	0.53
2:H:148:GLU:HG2	2:H:155:SER:OG	2.09	0.53
2:H:200:VAL:O	2:H:269:VAL:HG23	2.09	0.53
3:I:59:TRP:CE3	9:I:3008:3PE:H361	2.43	0.53
1:A:277:HIS:CD2	1:A:335:MET:HE1	2.44	0.53
1:A:401:LEU:HD21	1:A:415:TYR:CD1	2.43	0.53
1:A:482:ARG:N	8:A:1001:HEA:O2A	2.41	0.53
2:B:176:VAL:O	2:B:180:LEU:HG	2.09	0.53
3:C:8:ASP:OD2	4:D:14:MET:HB3	2.09	0.53
1:G:259:PHE:O	1:G:260:GLY:C	2.48	0.53
1:G:260:GLY:O	3:I:194:ALA:HA	2.08	0.53
1:G:286:GLN:HA	1:G:289:ILE:HD12	1.91	0.53
1:G:376:GLU:O	1:G:378:LYS:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:462:VAL:HG12	1:G:503:LEU:CD2	2.39	0.53
2:H:197:ALA:HB2	2:H:268:LYS:HZ3	1.73	0.53
1:A:404:ALA:O	1:A:407:ASP:N	2.41	0.53
1:A:469:PHE:O	1:A:470:PRO:C	2.46	0.53
2:B:33:ILE:HG22	2:B:34:GLY:N	2.23	0.53
2:B:57:LEU:HG	2:B:61:ILE:HD12	1.90	0.53
2:B:221:VAL:HB	2:B:224:PHE:HD2	1.74	0.53
1:G:160:PRO:O	1:G:184:GLY:HA3	2.09	0.53
2:H:263:MET:HG3	2:H:263:MET:O	2.09	0.53
3:I:141:LEU:O	3:I:142:LEU:C	2.47	0.53
1:A:237:TRP:O	1:A:238:LEU:C	2.47	0.53
10:A:2079:HOH:O	2:B:44:GLN:HG2	2.09	0.53
3:I:56:PHE:O	3:I:57:GLY:C	2.45	0.53
3:I:182:GLN:O	3:I:185:GLU:HB2	2.09	0.53
1:A:325:VAL:HG22	9:A:2012:3PE:H3B2	1.91	0.52
1:A:411:HIS:HD1	8:A:1002:HEA:CGA	2.21	0.52
2:B:234:ARG:HG2	3:C:114:PRO:HD3	1.92	0.52
4:D:43:PHE:O	4:D:44:LEU:C	2.47	0.52
1:G:22:MET:HG2	3:I:16:ILE:HA	1.91	0.52
1:G:63:MET:HE1	1:G:95:TRP:CE3	2.44	0.52
1:G:127:HIS:HE1	1:G:300:HIS:CE1	2.27	0.52
1:G:254:LEU:O	1:G:258:ASN:N	2.38	0.52
2:H:137:LYS:HG2	2:H:138:VAL:N	2.19	0.52
1:A:378:LYS:O	1:A:379:THR:C	2.45	0.52
2:B:141:TYR:O	2:B:143:TRP:N	2.42	0.52
1:G:191:ILE:HG23	1:G:250:ILE:HG13	1.91	0.52
1:G:333:HIS:ND1	1:G:352:THR:OG1	2.39	0.52
1:G:422:TYR:OH	1:G:469:PHE:HB2	2.08	0.52
2:H:156:PHE:HD1	2:H:196:THR:HG21	1.72	0.52
2:H:215:VAL:O	2:H:232:PRO:HD3	2.10	0.52
3:I:133:LEU:N	3:I:134:PRO:HD2	2.21	0.52
1:A:394:GLY:O	1:A:395:GLY:C	2.46	0.52
9:A:2012:3PE:H3E1	9:D:2011:3PE:H2I3	1.91	0.52
3:C:220:LEU:O	3:C:221:LEU:C	2.48	0.52
1:G:385:LEU:O	1:G:388:LEU:HB2	2.08	0.52
1:G:430:PHE:O	1:G:431:GLY:C	2.47	0.52
1:G:493:TRP:HA	1:G:493:TRP:HE3	1.73	0.52
1:A:287:VAL:HB	8:A:1002:HEA:CAC	2.40	0.52
1:A:356:ALA:O	1:A:357:VAL:C	2.47	0.52
1:A:534:HIS:HA	10:A:2043:HOH:O	2.08	0.52
1:A:550:THR:O	1:A:551:PHE:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2009:3PE:C26	3:C:55:MET:HG2	2.38	0.52
2:B:177:GLU:HA	2:B:180:LEU:HD12	1.91	0.52
3:C:133:LEU:HD23	3:C:185:GLU:HG3	1.92	0.52
1:G:103:GLY:HA2	8:G:1001:HEA:HMD3	1.90	0.52
1:G:364:PHE:O	1:G:365:SER:C	2.46	0.52
1:G:558:GLU:O	1:G:560:TRP:N	2.42	0.52
2:H:211:THR:CG2	2:H:212:GLY:N	2.73	0.52
2:H:226:VAL:HG12	10:H:1157:HOH:O	2.08	0.52
3:I:62:VAL:HG12	9:I:3008:3PE:H31	1.92	0.52
3:I:72:THR:HG22	3:I:74:VAL:H	1.73	0.52
3:I:253:VAL:HG13	9:I:3010:3PE:H3I1	1.92	0.52
4:J:38:VAL:HG12	4:J:42:ILE:HD12	1.91	0.52
1:A:202:ILE:CD1	1:A:244:PRO:HD3	2.38	0.52
1:A:493:TRP:HA	1:A:493:TRP:HE3	1.74	0.52
2:B:158:SER:CA	2:B:196:THR:HB	2.35	0.52
1:G:378:LYS:O	1:G:379:THR:C	2.48	0.52
1:G:380:PRO:HG3	1:G:437:TYR:CB	2.39	0.52
1:G:506:ALA:O	1:G:509:LEU:N	2.42	0.52
2:H:201:PRO:CB	2:H:204:LYS:HG3	2.39	0.52
3:I:106:LEU:O	3:I:108:PRO:HD3	2.10	0.52
3:I:150:TRP:NE1	3:I:163:ASP:OD1	2.31	0.52
3:I:155:LEU:O	3:I:155:LEU:HG	2.08	0.52
3:I:196:ASN:HD21	3:I:199:GLY:HA3	1.75	0.52
3:I:245:TRP:NE1	9:I:3013:3PE:H322	2.24	0.52
1:A:213:LEU:CB	3:C:81:TRP:CH2	2.93	0.52
1:A:262:THR:OG1	1:A:265:GLN:HB2	2.10	0.52
3:C:72:THR:HG22	3:C:74:VAL:H	1.75	0.52
1:G:330:VAL:HG11	1:G:352:THR:HA	1.90	0.52
1:G:477:GLN:NE2	1:G:477:GLN:HA	2.25	0.52
2:H:84:HIS:HD2	2:H:86:LYS:H	1.57	0.52
2:H:234:ARG:HG2	3:I:114:PRO:HD3	1.91	0.52
1:A:251:THR:HG22	3:C:97:TRP:HH2	1.75	0.52
3:C:72:THR:O	3:C:73:PRO:C	2.48	0.52
1:G:230:TRP:O	1:G:233:PHE:HB3	2.09	0.52
1:G:381:MET:O	1:G:382:LEU:C	2.48	0.52
1:A:292:LEU:O	1:A:293:PRO:C	2.46	0.52
1:A:302:ILE:HG22	1:A:369:THR:HG21	1.91	0.52
1:G:188:ASP:CG	1:G:257:ARG:HH12	2.13	0.52
1:G:198:GLY:HA2	1:G:243:LEU:CD1	2.39	0.52
1:G:253:LEU:HD21	1:G:275:TYR:CD1	2.45	0.52
2:H:176:VAL:O	2:H:177:GLU:C	2.48	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:CG	1:A:165:GLN:HE22	2.12	0.52
2:B:238:LEU:C	2:B:238:LEU:CD1	2.74	0.52
1:G:221:THR:HG23	1:G:224:LYS:HD2	1.92	0.52
1:G:237:TRP:CG	9:G:3012:3PE:H382	2.45	0.52
2:H:159:TYR:O	2:H:194:THR:OG1	2.23	0.52
2:H:173:SER:OG	2:H:175:GLU:HB2	2.10	0.52
3:I:254:TRP:HA	3:I:257:LEU:HD12	1.92	0.52
9:I:3013:3PE:H3H2	9:I:3013:3PE:C2D	2.40	0.52
1:A:221:THR:H	1:A:224:LYS:HB2	1.75	0.52
2:B:71:PHE:CE1	2:B:75:LEU:HD11	2.45	0.52
2:B:147:TYR:HE1	10:B:1049:HOH:O	1.93	0.52
3:C:253:VAL:CA	9:C:2010:3PE:H3H1	2.36	0.52
4:D:37:ILE:O	4:D:38:VAL:C	2.46	0.52
1:G:123:PHE:O	1:G:124:MET:C	2.47	0.52
2:H:144:TYR:HB2	2:H:158:SER:O	2.09	0.52
4:J:44:LEU:O	4:J:45:ALA:C	2.49	0.52
1:A:202:ILE:O	1:A:206:ILE:HG13	2.10	0.51
1:G:212:PHE:HD1	1:G:213:LEU:HD23	1.74	0.51
1:G:404:ALA:O	1:G:405:SER:C	2.48	0.51
1:A:196:LEU:O	1:A:199:ALA:HB3	2.11	0.51
1:G:237:TRP:CH2	9:G:3012:3PE:H282	2.44	0.51
1:G:373:GLY:O	2:H:83:PHE:HB3	2.10	0.51
9:G:3009:3PE:H221	3:I:58:TRP:CE2	2.46	0.51
10:G:3087:HOH:O	2:H:44:GLN:HG2	2.11	0.51
2:H:45:PRO:HB3	2:H:244:ARG:HH21	1.75	0.51
2:H:219:TRP:CD1	2:H:265:ILE:HD13	2.45	0.51
3:I:202:PHE:CD1	3:I:202:PHE:C	2.83	0.51
1:A:63:MET:SD	1:A:94:LEU:HD23	2.50	0.51
1:A:367:ILE:HD11	2:B:75:LEU:HB2	1.91	0.51
2:B:84:HIS:C	2:B:84:HIS:CD2	2.83	0.51
1:G:132:ASP:OD1	1:G:133:MET:N	2.44	0.51
1:G:291:VAL:O	1:G:294:ALA:HB3	2.11	0.51
2:H:236:ALA:HB2	10:H:1128:HOH:O	2.09	0.51
3:I:30:PHE:CD2	3:I:43:MET:HE1	2.45	0.51
1:G:234:VAL:HG12	1:G:292:LEU:HD11	1.93	0.51
1:G:291:VAL:O	1:G:291:VAL:HG22	2.10	0.51
2:H:40:GLY:HA2	10:H:1216:HOH:O	2.09	0.51
1:A:154:VAL:HA	1:A:157:LEU:HD12	1.93	0.51
1:G:127:HIS:CE1	1:G:300:HIS:HE1	2.29	0.51
3:I:125:ILE:HD12	3:I:198:TYR:CB	2.40	0.51
1:A:222:MET:HG3	9:A:2012:3PE:C11	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HA	1:A:534:HIS:CG	2.45	0.51
3:C:74:VAL:HG23	3:C:75:VAL:H	1.76	0.51
3:C:99:TRP:CZ2	9:C:2010:3PE:H222	2.44	0.51
1:G:128:ILE:HD12	1:G:216:ARG:CA	2.40	0.51
1:G:128:ILE:HB	1:G:216:ARG:HG2	1.92	0.51
2:H:106:ILE:O	2:H:107:VAL:C	2.48	0.51
3:I:71:HIS:O	3:I:76:ARG:HG3	2.11	0.51
1:A:263:PHE:HE1	3:C:201:ASN:ND2	2.09	0.51
1:A:390:LEU:HA	1:A:393:VAL:CG2	2.41	0.51
1:G:367:ILE:HA	1:G:370:MET:CE	2.41	0.51
2:H:143:TRP:NE1	2:H:256:CYS:O	2.42	0.51
1:A:74:LYS:HD2	1:A:74:LYS:N	2.22	0.51
1:A:136:PRO:HG2	3:C:12:LEU:HD12	1.93	0.51
1:A:237:TRP:CZ3	3:C:88:MET:HE3	2.45	0.51
1:A:508:PHE:CE1	1:A:512:LEU:HD21	2.46	0.51
1:G:189:LEU:HD23	3:I:33:VAL:HG21	1.93	0.51
1:G:233:PHE:O	1:G:234:VAL:C	2.47	0.51
3:I:119:ILE:HG22	3:I:120:PHE:N	2.26	0.51
9:I:3013:3PE:H2D2	9:I:3013:3PE:C3F	2.39	0.51
1:A:307:LYS:HA	1:A:534:HIS:CB	2.41	0.51
3:C:256:PHE:CZ	9:D:2011:3PE:H391	2.46	0.51
1:G:284:HIS:NE2	1:G:288:TYR:CE2	2.66	0.51
1:G:425:SER:HA	1:G:429:VAL:CG2	2.40	0.51
1:G:535:ALA:HB1	1:G:540:TRP:CD1	2.46	0.51
2:H:84:HIS:CD2	2:H:85:GLU:HG2	2.46	0.51
2:H:200:VAL:HG22	2:H:201:PRO:HD2	1.93	0.51
1:A:478:GLY:O	1:A:480:PRO:HD3	2.11	0.51
1:G:41:GLY:O	1:G:45:VAL:HG23	2.11	0.51
1:G:177:PRO:HD3	1:G:272:PRO:HG3	1.93	0.51
1:G:325:VAL:HG22	9:G:3012:3PE:H3D1	1.92	0.51
9:G:3012:3PE:H2G2	9:I:3010:3PE:H2E2	1.93	0.51
3:I:147:ALA:HB1	3:I:170:LEU:HD23	1.91	0.51
1:A:127:HIS:NE2	1:A:539:GLU:OE1	2.44	0.50
1:A:307:LYS:HB3	1:A:534:HIS:CD2	2.46	0.50
1:A:424:MET:HE1	8:A:1002:HEA:HMD3	1.92	0.50
2:B:254:GLU:H	2:B:260:HIS:CE1	2.26	0.50
9:C:2013:3PE:H3F2	9:C:2013:3PE:H2D2	1.93	0.50
1:G:416:VAL:HG21	8:G:1002:HEA:CBA	2.40	0.50
3:I:209:HIS:NE2	3:I:254:TRP:HB2	2.26	0.50
1:A:75:GLY:O	1:A:76:PHE:C	2.50	0.50
1:A:112:ILE:HB	1:A:113:PRO:HD3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:MET:N	1:A:125:PRO:HD2	2.25	0.50
1:A:154:VAL:HA	1:A:157:LEU:CD1	2.42	0.50
2:B:86:LYS:HA	2:B:89:LYS:HE2	1.93	0.50
1:G:99:ILE:HD12	8:G:1001:HEA:CBA	2.40	0.50
9:I:3013:3PE:H3F2	9:I:3013:3PE:H2D2	1.93	0.50
4:J:33:ALA:O	4:J:36:VAL:N	2.44	0.50
1:A:433:PHE:CD1	1:A:436:ILE:HD12	2.46	0.50
2:B:62:LEU:O	2:B:66:ALA:N	2.44	0.50
2:B:169:ASP:O	2:B:170:ASN:HB2	2.10	0.50
3:C:122:PRO:O	3:C:125:ILE:HB	2.12	0.50
1:G:180:THR:HG22	1:G:257:ARG:HG3	1.93	0.50
1:G:482:ARG:N	8:G:1001:HEA:O2A	2.45	0.50
2:H:164:PRO:HA	2:H:168:GLY:O	2.10	0.50
3:I:107:TYR:OH	4:J:49:ALA:HA	2.11	0.50
1:A:52:ARG:O	1:A:53:MET:C	2.49	0.50
1:A:63:MET:HE1	1:A:95:TRP:CE3	2.47	0.50
1:A:123:PHE:O	1:A:124:MET:C	2.49	0.50
1:A:189:LEU:HD21	3:C:30:PHE:CD1	2.46	0.50
1:A:442:LYS:HE2	1:A:539:GLU:O	2.12	0.50
2:B:50:VAL:HG12	2:B:54:ILE:HD11	1.93	0.50
9:C:2013:3PE:H2D2	9:C:2013:3PE:H3H2	1.92	0.50
2:H:136:VAL:HG11	2:H:198:MET:CE	2.41	0.50
1:A:99:ILE:HD12	8:A:1001:HEA:CBA	2.39	0.50
1:A:180:THR:HA	1:A:257:ARG:HD2	1.94	0.50
1:A:231:SER:HA	1:A:320:MET:HE3	1.94	0.50
1:A:248:GLY:O	1:A:249:ALA:C	2.50	0.50
2:B:108:PRO:O	2:B:111:ILE:HB	2.12	0.50
1:G:38:GLY:O	1:G:39:LEU:C	2.50	0.50
2:H:161:ILE:HD11	2:H:193:ALA:HB1	1.93	0.50
1:A:22:MET:SD	3:C:16:ILE:HB	2.51	0.50
1:A:136:PRO:HA	10:A:2049:HOH:O	2.12	0.50
1:A:325:VAL:HG22	9:A:2012:3PE:H3D1	1.94	0.50
3:C:100:SER:O	3:C:101:PHE:C	2.50	0.50
1:G:396:VAL:HG13	2:H:65:ILE:HG21	1.94	0.50
2:H:120:LEU:O	2:H:121:PRO:C	2.49	0.50
2:H:250:GLY:O	2:H:265:ILE:HB	2.12	0.50
3:I:152:HIS:CG	3:I:244:ILE:HD13	2.47	0.50
1:A:354:VAL:O	1:A:355:ILE:C	2.49	0.50
1:A:517:TYR:O	1:A:521:ARG:N	2.40	0.50
2:B:120:LEU:HB2	2:B:121:PRO:CD	2.42	0.50
3:C:72:THR:HG23	4:D:12:GLY:HA2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:GLY:O	4:D:26:PHE:C	2.48	0.50
1:G:311:PHE:CZ	2:H:96:HIS:HA	2.47	0.50
1:G:424:MET:HB3	8:G:1001:HEA:HBC1	1.93	0.50
1:G:534:HIS:HA	10:G:3048:HOH:O	2.10	0.50
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2I3	1.94	0.50
2:H:200:VAL:O	2:H:200:VAL:HG12	2.10	0.50
3:I:254:TRP:O	3:I:257:LEU:HB2	2.11	0.50
1:A:42:LEU:O	1:A:43:ILE:C	2.49	0.50
2:B:156:PHE:CD2	2:B:196:THR:HG21	2.42	0.50
1:G:124:MET:N	1:G:125:PRO:HD2	2.27	0.50
1:G:134:ALA:H	1:G:211:THR:HG1	1.57	0.50
1:G:240:LEU:HD21	3:I:85:LEU:HB3	1.94	0.50
2:H:197:ALA:HB1	2:H:268:LYS:HG3	1.92	0.50
1:A:24:THR:HG21	3:C:13:PRO:O	2.12	0.50
9:A:2009:3PE:H2G1	9:A:2009:3PE:H3F2	1.93	0.50
2:B:279:LEU:O	2:B:283:ARG:HG2	2.11	0.50
1:G:121:ASN:O	1:G:125:PRO:HG2	2.12	0.50
1:G:529:ASN:OD1	1:G:529:ASN:C	2.50	0.50
2:H:160:MET:HE1	2:H:262:TYR:HB3	1.94	0.50
2:H:209:GLN:CG	2:H:235:LEU:HD22	2.42	0.50
2:H:217:HIS:O	2:H:230:ALA:N	2.42	0.50
1:A:420:PHE:HB2	8:A:1002:HEA:HMD3	1.94	0.49
1:A:425:SER:OG	1:A:426:LEU:HD23	2.11	0.49
3:C:132:HIS:O	3:C:136:ILE:HG12	2.12	0.49
1:G:52:ARG:HD3	1:G:498:SER:HA	1.93	0.49
1:G:147:VAL:O	1:G:148:ALA:C	2.49	0.49
1:G:291:VAL:HG22	1:G:295:PHE:CE1	2.47	0.49
3:I:256:PHE:O	3:I:257:LEU:C	2.51	0.49
1:A:318:TYR:O	1:A:319:ALA:C	2.49	0.49
2:B:209:GLN:CG	2:B:235:LEU:HD22	2.42	0.49
1:G:256:ASP:OD1	1:G:261:THR:OG1	2.20	0.49
2:H:192:LEU:HD13	2:H:249:PHE:CD2	2.47	0.49
1:A:18:THR:HA	1:A:22:MET:CE	2.42	0.49
1:A:148:ALA:O	1:A:149:GLY:C	2.50	0.49
3:C:32:ALA:O	3:C:36:MET:HG3	2.12	0.49
9:C:2010:3PE:H231	9:C:2010:3PE:H331	1.94	0.49
1:G:221:THR:O	1:G:222:MET:C	2.48	0.49
1:G:244:PRO:O	1:G:247:ALA:N	2.45	0.49
1:G:244:PRO:O	1:G:245:VAL:C	2.50	0.49
3:I:130:PRO:HA	3:I:134:PRO:HG2	1.93	0.49
1:A:137:ARG:HH21	9:A:2009:3PE:H112	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:HD1	1:A:213:LEU:HD23	1.77	0.49
1:A:213:LEU:HB3	3:C:81:TRP:HH2	1.76	0.49
1:A:331:TRP:CD1	1:A:331:TRP:C	2.84	0.49
2:B:113:VAL:O	2:B:116:GLY:N	2.46	0.49
2:B:196:THR:O	2:B:196:THR:HG22	2.09	0.49
3:C:245:TRP:NE1	9:C:2013:3PE:H322	2.28	0.49
4:D:37:ILE:HG22	4:D:38:VAL:N	2.27	0.49
1:G:227:LEU:O	1:G:230:TRP:N	2.44	0.49
2:H:151:ASP:HB2	10:H:1112:HOH:O	2.11	0.49
1:A:325:VAL:HG22	9:A:2012:3PE:C3D	2.42	0.49
1:A:446:ARG:NH1	1:A:522:GLY:O	2.46	0.49
2:B:161:ILE:HD11	2:B:193:ALA:HB1	1.95	0.49
3:C:115:ILE:H	3:C:115:ILE:HD12	1.77	0.49
3:C:147:ALA:HB1	3:C:170:LEU:HD23	1.93	0.49
3:C:155:LEU:O	3:C:155:LEU:HG	2.10	0.49
4:D:38:VAL:HG12	4:D:42:ILE:HD12	1.95	0.49
1:G:95:TRP:CE2	1:G:99:ILE:HD11	2.47	0.49
2:H:137:LYS:HB3	2:H:148:GLU:HB2	1.94	0.49
2:H:143:TRP:CD1	2:H:143:TRP:N	2.79	0.49
2:H:156:PHE:CD1	2:H:196:THR:HG21	2.46	0.49
3:I:238:VAL:HG12	9:I:3008:3PE:O21	2.11	0.49
1:A:163:ASN:CG	2:B:258:ILE:HD11	2.33	0.49
1:A:173:VAL:O	1:A:174:LEU:HB2	2.12	0.49
1:A:538:LEU:HD21	1:A:560:TRP:HE3	1.77	0.49
4:D:44:LEU:HD21	9:D:2011:3PE:H31	1.94	0.49
1:G:274:LEU:HD21	3:I:100:SER:HA	1.93	0.49
1:G:323:ILE:HG22	1:G:324:GLY:N	2.28	0.49
9:G:3009:3PE:H261	3:I:55:MET:HG2	1.94	0.49
1:A:126:LEU:O	1:A:127:HIS:C	2.51	0.49
8:A:1002:HEA:HAD2	10:A:2047:HOH:O	2.10	0.49
1:G:231:SER:O	1:G:232:ILE:C	2.49	0.49
1:G:422:TYR:HH	1:G:469:PHE:HD1	1.59	0.49
1:G:431:GLY:O	1:G:432:ILE:C	2.50	0.49
2:H:141:TYR:HE1	2:H:146:GLY:HA3	1.76	0.49
1:A:49:VAL:O	1:A:50:TYR:C	2.51	0.49
1:A:175:TYR:HB3	10:A:2013:HOH:O	2.11	0.49
1:A:176:PRO:O	10:A:2013:HOH:O	2.20	0.49
1:A:316:MET:SD	1:A:365:SER:CB	3.01	0.49
1:A:547:PRO:HD2	1:A:550:THR:HG22	1.94	0.49
2:H:248:PHE:HE2	2:H:269:VAL:HG12	1.77	0.49
1:A:131:PRO:HG2	3:C:9:TYR:HD2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:CD1	1:A:212:PHE:C	2.85	0.49
2:B:228:GLN:CG	2:B:229:ASP:N	2.76	0.49
1:G:178:LEU:HD12	1:G:178:LEU:C	2.33	0.49
1:G:292:LEU:HB2	1:G:293:PRO:HD3	1.95	0.49
2:H:136:VAL:HG12	2:H:137:LYS:N	2.27	0.49
3:I:52:LEU:HD22	9:I:3008:3PE:H3C2	1.95	0.49
3:I:122:PRO:HG2	3:I:125:ILE:HD12	1.95	0.49
1:A:26:HIS:HD2	1:A:122:TYR:HA	1.77	0.49
1:A:91:ASN:O	1:A:92:GLY:C	2.51	0.49
1:A:291:VAL:HG22	1:A:295:PHE:CE1	2.48	0.49
1:A:381:MET:CE	1:A:385:LEU:HD21	2.41	0.49
1:A:145:LEU:HD23	3:C:22:SER:OG	2.13	0.48
1:A:185:TYR:HB3	3:C:37:HIS:CD2	2.48	0.48
1:A:359:THR:HG22	8:A:1002:HEA:H172	1.95	0.48
2:B:224:PHE:HE1	2:B:242:ALA:HB2	1.77	0.48
2:B:275:TYR:O	2:B:278:TRP:HB3	2.12	0.48
3:C:155:LEU:HB2	3:C:164:VAL:HG21	1.94	0.48
3:C:228:GLN:OE1	3:C:228:GLN:HA	2.12	0.48
3:I:212:HIS:HD2	3:I:246:TYR:OH	1.96	0.48
1:A:106:MET:HE1	1:A:110:VAL:HG11	1.95	0.48
1:A:128:ILE:HB	1:A:216:ARG:HG2	1.95	0.48
1:A:380:PRO:HG3	1:A:437:TYR:CB	2.43	0.48
2:B:70:ILE:O	2:B:71:PHE:C	2.50	0.48
2:B:137:LYS:HG2	2:B:138:VAL:N	2.22	0.48
2:B:221:VAL:HG11	2:B:224:PHE:CD2	2.48	0.48
2:B:221:VAL:CB	2:B:224:PHE:HD2	2.26	0.48
1:G:106:MET:CG	8:G:1001:HEA:CAC	2.73	0.48
3:I:133:LEU:HD11	3:I:181:PHE:CD2	2.49	0.48
2:B:106:ILE:O	2:B:107:VAL:C	2.51	0.48
2:B:142:GLN:O	2:B:143:TRP:CB	2.61	0.48
3:C:130:PRO:HD2	10:C:2037:HOH:O	2.13	0.48
3:C:214:ILE:O	3:C:218:ILE:HG12	2.12	0.48
1:G:41:GLY:N	1:G:110:VAL:HG22	2.27	0.48
1:G:107:MET:HE1	1:G:424:MET:SD	2.53	0.48
1:G:487:PRO:HG2	1:G:490:PHE:HE2	1.79	0.48
3:I:72:THR:HB	3:I:75:VAL:HG23	1.95	0.48
1:A:277:HIS:CE1	1:A:335:MET:HE2	2.49	0.48
1:A:477:GLN:HA	1:A:477:GLN:NE2	2.28	0.48
2:B:220:THR:O	2:B:250:GLY:HA3	2.13	0.48
4:D:15:ASP:OD1	4:D:16:ILE:N	2.46	0.48
1:G:329:VAL:HB	1:G:347:TYR:OH	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:PRO:HG2	1:G:490:PHE:CE2	2.48	0.48
8:G:1002:HEA:O11	8:G:1002:HEA:CHC	2.49	0.48
2:H:142:GLN:NE2	10:H:1015:HOH:O	2.36	0.48
3:I:242:ALA:O	3:I:243:ALA:C	2.52	0.48
2:B:195:ASP:OD1	2:B:196:THR:N	2.46	0.48
3:C:123:GLU:HG3	1:G:557:ARG:NH2	2.29	0.48
3:C:141:LEU:HD12	3:C:254:TRP:CD1	2.49	0.48
3:C:150:TRP:CD1	3:C:150:TRP:C	2.87	0.48
1:G:377:LEU:HD21	2:H:80:VAL:CG1	2.42	0.48
1:G:408:ARG:HG3	2:H:126:GLN:OE1	2.13	0.48
1:G:416:VAL:HG11	10:G:3018:HOH:O	2.13	0.48
2:H:159:TYR:O	2:H:194:THR:HA	2.14	0.48
2:H:161:ILE:HD11	2:H:193:ALA:CB	2.44	0.48
2:H:194:THR:CG2	2:H:266:THR:HB	2.44	0.48
3:I:112:GLU:CB	3:I:116:ILE:HB	2.44	0.48
1:A:314:LEU:O	1:A:317:VAL:N	2.47	0.48
2:B:220:THR:OG1	2:B:221:VAL:N	2.46	0.48
2:B:252:CYS:HB2	2:B:263:MET:SD	2.53	0.48
3:C:147:ALA:CB	3:C:170:LEU:HD23	2.42	0.48
1:G:23:SER:O	1:G:140:ASN:HB2	2.14	0.48
3:I:126:ILE:HB	3:I:190:ALA:HB1	1.94	0.48
1:A:509:LEU:O	1:A:510:PHE:C	2.50	0.48
2:B:163:SER:O	2:B:166:THR:OG1	2.31	0.48
2:B:226:VAL:HG12	10:B:1047:HOH:O	2.12	0.48
1:G:130:ALA:HB1	1:G:131:PRO:CD	2.44	0.48
1:G:287:VAL:HG11	8:G:1002:HEA:CHD	2.44	0.48
1:G:313:TYR:O	1:G:314:LEU:C	2.52	0.48
2:H:108:PRO:O	2:H:111:ILE:HB	2.13	0.48
3:I:122:PRO:HG2	3:I:125:ILE:CG1	2.44	0.48
1:A:209:ILE:HG21	3:C:85:LEU:HD22	1.96	0.48
1:A:398:GLY:O	1:A:402:SER:N	2.43	0.48
3:C:55:MET:O	3:C:56:PHE:C	2.51	0.48
1:G:26:HIS:HD2	1:G:122:TYR:HA	1.79	0.48
1:G:41:GLY:O	1:G:45:VAL:N	2.31	0.48
1:G:292:LEU:CB	1:G:293:PRO:HD3	2.43	0.48
1:G:300:HIS:CD2	1:G:300:HIS:N	2.81	0.48
1:G:474:LEU:HD21	1:G:494:ASN:ND2	2.29	0.48
2:H:84:HIS:CD2	2:H:85:GLU:N	2.81	0.48
2:H:220:THR:OG1	2:H:227:LYS:HB2	2.13	0.48
3:I:152:HIS:CD2	9:I:3013:3PE:H332	2.48	0.48
1:A:128:ILE:CD1	1:A:216:ARG:HA	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:CG	9:A:2012:3PE:H382	2.49	0.48
1:A:370:MET:O	1:A:371:TRP:C	2.49	0.48
1:A:392:THR:O	1:A:393:VAL:C	2.51	0.48
2:B:200:VAL:O	2:B:269:VAL:HG23	2.14	0.48
3:C:30:PHE:HB3	3:C:43:MET:HE2	1.96	0.48
3:C:111:PRO:HA	4:J:10:VAL:CB	2.42	0.48
1:G:139:ASN:O	1:G:140:ASN:C	2.51	0.48
1:G:181:SER:O	1:G:182:GLU:C	2.50	0.48
1:G:279:LEU:HD23	1:G:279:LEU:O	2.10	0.48
1:G:463:GLY:H	1:G:503:LEU:HD23	1.77	0.48
1:G:489:ALA:O	2:H:38:PRO:HA	2.14	0.48
3:I:45:LEU:O	3:I:46:ILE:C	2.51	0.48
1:A:213:LEU:HD12	3:C:81:TRP:CZ2	2.49	0.48
1:A:452:ALA:HB1	1:A:514:VAL:CG2	2.44	0.48
1:A:497:SER:O	1:A:500:GLY:N	2.47	0.48
1:A:539:GLU:HG2	1:A:540:TRP:N	2.28	0.48
8:A:1001:HEA:H122	8:A:1001:HEA:HMB1	1.94	0.48
2:B:258:ILE:HG22	2:B:259:SER:N	2.26	0.48
2:H:201:PRO:HB2	2:H:204:LYS:HB2	1.96	0.48
3:I:91:VAL:HG11	9:I:3010:3PE:H2H1	1.95	0.48
3:I:143:CYS:O	3:I:144:SER:C	2.53	0.48
2:B:194:THR:HG22	2:B:266:THR:HB	1.96	0.47
3:C:28:MET:HG2	3:C:29:LEU:HD23	1.96	0.47
1:G:123:PHE:O	1:G:126:LEU:N	2.47	0.47
1:G:263:PHE:CZ	3:I:200:ALA:HB1	2.49	0.47
1:G:277:HIS:CD2	1:G:335:MET:HE1	2.48	0.47
1:A:302:ILE:HG22	1:A:369:THR:CG2	2.45	0.47
3:C:212:HIS:HD2	3:C:246:TYR:OH	1.97	0.47
1:G:52:ARG:CD	1:G:498:SER:HA	2.44	0.47
4:J:16:ILE:HA	4:J:19:GLN:OE1	2.15	0.47
1:A:176:PRO:CB	1:A:177:PRO:HA	2.44	0.47
1:A:248:GLY:O	1:A:251:THR:N	2.47	0.47
1:A:402:SER:HA	8:A:1002:HEA:OMA	2.14	0.47
2:B:254:GLU:O	2:B:255:LEU:C	2.53	0.47
3:C:120:PHE:HA	3:C:121:PRO:C	2.35	0.47
9:C:2013:3PE:O14	9:C:2013:3PE:C12	2.53	0.47
1:G:112:ILE:HB	1:G:113:PRO:HD3	1.95	0.47
3:I:74:VAL:HG23	3:I:75:VAL:N	2.29	0.47
1:A:213:LEU:HD21	1:A:233:PHE:CZ	2.49	0.47
2:B:45:PRO:HB3	2:B:244:ARG:NH2	2.29	0.47
2:B:120:LEU:CB	2:B:121:PRO:CD	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:GLN:HG3	10:B:1016:HOH:O	2.13	0.47
4:D:16:ILE:HG22	4:D:19:GLN:HB2	1.95	0.47
1:G:81:TRP:CD2	1:G:82:PRO:HD2	2.49	0.47
1:G:230:TRP:O	1:G:231:SER:C	2.52	0.47
1:G:232:ILE:HA	1:G:232:ILE:HD13	1.71	0.47
1:G:293:PRO:O	1:G:294:ALA:C	2.53	0.47
1:G:341:SER:OG	1:G:344:GLN:N	2.34	0.47
1:G:433:PHE:HE1	1:G:511:PHE:CZ	2.32	0.47
1:G:547:PRO:O	1:G:550:THR:HG23	2.15	0.47
1:A:91:ASN:HD21	1:A:165:GLN:CD	2.17	0.47
1:A:231:SER:OG	1:A:293:PRO:HA	2.14	0.47
1:A:234:VAL:O	1:A:235:THR:C	2.52	0.47
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.85	0.47
1:A:543:THR:HG23	1:A:547:PRO:HD3	1.96	0.47
2:B:86:LYS:HD2	2:B:89:LYS:HZ1	1.78	0.47
3:C:212:HIS:O	3:C:213:VAL:C	2.53	0.47
1:G:106:MET:SD	8:G:1001:HEA:CMC	3.03	0.47
2:H:249:PHE:HE1	2:H:266:THR:HG1	1.62	0.47
2:H:254:GLU:H	2:H:260:HIS:HE1	1.62	0.47
3:I:74:VAL:HG13	4:J:16:ILE:HG12	1.96	0.47
1:A:59:GLY:HA2	1:A:485:ASP:OD2	2.15	0.47
1:A:112:ILE:CB	1:A:113:PRO:HD3	2.43	0.47
1:A:300:HIS:H	1:A:300:HIS:CD2	2.32	0.47
1:G:231:SER:OG	1:G:232:ILE:N	2.48	0.47
1:G:444:SER:OG	1:G:445:GLY:N	2.46	0.47
3:I:72:THR:O	3:I:73:PRO:C	2.53	0.47
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.83	0.47
1:A:316:MET:O	1:A:317:VAL:C	2.53	0.47
1:A:404:ALA:HB3	2:B:123:LEU:HD13	1.97	0.47
2:B:84:HIS:CD2	2:B:85:GLU:HG2	2.50	0.47
2:B:112:LEU:O	2:B:113:VAL:C	2.51	0.47
3:C:245:TRP:HE1	9:C:2013:3PE:H322	1.79	0.47
4:D:44:LEU:O	4:D:45:ALA:C	2.53	0.47
1:G:140:ASN:ND2	10:G:3041:HOH:O	2.32	0.47
1:G:155:ALA:HB1	10:G:3088:HOH:O	2.13	0.47
1:G:171:GLY:O	1:G:172:TRP:C	2.53	0.47
1:G:332:ALA:HB3	1:G:348:PHE:CD1	2.50	0.47
1:G:387:PHE:HD1	1:G:388:LEU:N	2.13	0.47
1:G:479:MET:HG2	1:G:480:PRO:O	2.15	0.47
1:G:550:THR:O	1:G:551:PHE:HB2	2.14	0.47
3:I:72:THR:O	3:I:72:THR:HG22	2.10	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:92:MET:HE2	9:J:3011:3PE:H2H2	1.96	0.47
3:I:196:ASN:O	3:I:196:ASN:CG	2.53	0.47
1:A:243:LEU:N	1:A:243:LEU:HD23	2.29	0.47
1:A:294:ALA:O	1:A:295:PHE:C	2.53	0.47
1:G:356:ALA:O	1:G:357:VAL:C	2.52	0.47
1:G:446:ARG:NH1	1:G:522:GLY:O	2.48	0.47
2:H:217:HIS:ND1	2:H:256:CYS:HB2	2.29	0.47
2:H:231:VAL:O	2:H:232:PRO:C	2.53	0.47
1:A:124:MET:SD	1:A:125:PRO:CD	3.03	0.47
1:A:173:VAL:O	1:A:174:LEU:CB	2.62	0.47
1:A:307:LYS:O	2:B:91:PRO:HB3	2.15	0.47
1:A:337:THR:HG22	1:A:408:ARG:HH11	1.79	0.47
9:A:2009:3PE:H291	9:A:2009:3PE:C3A	2.45	0.47
2:B:172:MET:HE1	2:B:187:ARG:O	2.15	0.47
3:C:91:VAL:HG11	9:C:2010:3PE:H2H1	1.97	0.47
3:C:99:TRP:HZ2	9:C:2010:3PE:H222	1.80	0.47
1:G:180:THR:HA	1:G:257:ARG:CG	2.45	0.47
9:G:3009:3PE:H221	3:I:58:TRP:CZ2	2.50	0.47
3:I:103:LYS:HD3	3:I:103:LYS:O	2.14	0.47
9:I:3010:3PE:H231	9:I:3010:3PE:H332	1.97	0.47
4:J:15:ASP:OD1	4:J:17:THR:N	2.37	0.47
1:A:273:VAL:O	1:A:274:LEU:C	2.51	0.47
2:B:86:LYS:HD2	2:B:89:LYS:NZ	2.30	0.47
2:B:136:VAL:HG12	2:B:137:LYS:N	2.29	0.47
2:B:250:GLY:O	2:B:265:ILE:N	2.48	0.47
3:C:72:THR:O	3:C:75:VAL:HG23	2.15	0.47
1:G:274:LEU:HD13	3:I:103:LYS:HG3	1.97	0.47
1:G:489:ALA:HA	2:H:38:PRO:HG3	1.97	0.47
1:G:517:TYR:O	1:G:521:ARG:N	2.46	0.47
2:H:221:VAL:O	2:H:222:PRO:C	2.52	0.47
9:A:2012:3PE:H3F1	9:D:2011:3PE:H2D1	1.96	0.46
2:B:97:ASN:O	2:B:101:GLU:HG3	2.15	0.46
1:G:84:ALA:O	1:G:85:VAL:C	2.53	0.46
1:G:188:ASP:O	1:G:189:LEU:C	2.54	0.46
1:G:424:MET:HB3	8:G:1001:HEA:CBC	2.45	0.46
1:G:517:TYR:O	1:G:520:THR:HB	2.15	0.46
2:H:49:PRO:HD3	2:H:243:GLU:OE2	2.14	0.46
2:H:107:VAL:N	2:H:108:PRO:HD2	2.31	0.46
1:A:249:ALA:HB2	1:A:278:ILE:CG2	2.44	0.46
1:A:291:VAL:O	1:A:292:LEU:C	2.54	0.46
1:A:302:ILE:CD1	1:A:381:MET:HE3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PRO:HA	1:A:473:PHE:CD2	2.51	0.46
3:C:226:ARG:NH2	9:C:2008:3PE:H121	2.31	0.46
1:G:306:ALA:O	1:G:307:LYS:C	2.53	0.46
1:G:508:PHE:CD2	1:G:512:LEU:HD11	2.50	0.46
1:G:519:LEU:N	1:G:519:LEU:HD23	2.30	0.46
8:G:1002:HEA:OMA	8:G:1002:HEA:HHB	2.15	0.46
9:G:3012:3PE:H232	4:J:29:MET:HE3	1.96	0.46
3:I:115:ILE:HD12	3:I:115:ILE:H	1.80	0.46
1:A:127:HIS:CE1	1:A:300:HIS:CE1	3.03	0.46
1:A:136:PRO:CG	3:C:12:LEU:HD12	2.46	0.46
1:A:141:LEU:HD12	1:A:141:LEU:O	2.16	0.46
1:A:292:LEU:CB	1:A:293:PRO:HD3	2.44	0.46
1:A:299:SER:O	1:A:302:ILE:N	2.48	0.46
1:A:389:PHE:HB3	1:A:390:LEU:HD23	1.96	0.46
3:C:83:PHE:HE1	9:C:2008:3PE:H262	1.80	0.46
3:C:240:PHE:CD1	3:C:244:ILE:HD11	2.50	0.46
4:D:32:TRP:O	4:D:33:ALA:C	2.54	0.46
1:G:71:GLY:CA	1:G:74:LYS:HD3	2.46	0.46
1:G:296:GLY:O	1:G:297:ILE:C	2.54	0.46
1:G:300:HIS:CD2	1:G:300:HIS:H	2.33	0.46
1:G:316:MET:O	1:G:320:MET:HG3	2.15	0.46
1:G:365:SER:O	1:G:366:TRP:C	2.53	0.46
1:G:375:ILE:CG2	1:G:376:GLU:N	2.78	0.46
4:J:9:HIS:O	4:J:10:VAL:HG23	2.16	0.46
4:J:21:LYS:O	4:J:24:ALA:HB3	2.15	0.46
1:G:72:LEU:O	1:G:76:PHE:HB2	2.15	0.46
1:G:237:TRP:HZ3	3:I:88:MET:HE3	1.80	0.46
1:G:451:TRP:CD2	1:G:452:ALA:N	2.83	0.46
8:G:1001:HEA:H252	8:G:1001:HEA:H212	1.77	0.46
2:H:136:VAL:CG1	2:H:137:LYS:N	2.78	0.46
3:I:120:PHE:C	3:I:120:PHE:CD1	2.89	0.46
1:A:225:VAL:HG13	1:A:226:PRO:HD2	1.97	0.46
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.59	0.46
1:A:288:TYR:O	1:A:292:LEU:HG	2.15	0.46
1:A:538:LEU:HG	10:A:2076:HOH:O	2.15	0.46
2:B:161:ILE:HD12	2:B:180:LEU:HD23	1.97	0.46
2:B:250:GLY:O	2:B:265:ILE:HB	2.14	0.46
1:G:91:ASN:OD1	1:G:93:HIS:HB3	2.15	0.46
1:G:112:ILE:N	1:G:113:PRO:HD2	2.30	0.46
1:A:71:GLY:HA3	1:A:74:LYS:HD3	1.98	0.46
1:A:127:HIS:CE1	1:A:300:HIS:HE1	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:HG22	2:B:77:LEU:HG	1.98	0.46
3:C:109:MET:HG2	10:C:2014:HOH:O	2.14	0.46
3:C:161:ARG:HH21	3:C:232:PHE:H	1.64	0.46
3:C:226:ARG:HH22	9:C:2008:3PE:H121	1.80	0.46
1:G:93:HIS:O	1:G:97:VAL:HG23	2.16	0.46
1:G:173:VAL:CG1	1:G:279:LEU:HD22	2.45	0.46
1:G:307:LYS:HD3	1:G:374:SER:HG	1.80	0.46
3:I:113:SER:HA	3:I:114:PRO:HA	1.59	0.46
3:I:122:PRO:HG2	3:I:125:ILE:HG13	1.97	0.46
3:I:253:VAL:O	3:I:257:LEU:HG	2.15	0.46
1:A:86:GLU:HA	1:A:86:GLU:OE1	2.15	0.46
1:A:122:TYR:CD1	1:A:122:TYR:C	2.89	0.46
1:A:300:HIS:CD2	1:A:300:HIS:N	2.78	0.46
1:A:432:ILE:HG22	1:A:436:ILE:HD11	1.97	0.46
1:A:543:THR:O	1:A:546:PRO:HA	2.16	0.46
1:A:543:THR:HG22	1:A:547:PRO:HD3	1.98	0.46
3:C:122:PRO:HA	10:C:2045:HOH:O	2.15	0.46
3:C:256:PHE:HE1	9:D:2011:3PE:H3B1	1.81	0.46
1:G:342:LEU:HD11	2:H:124:PHE:HD1	1.81	0.46
1:G:375:ILE:HG22	1:G:377:LEU:HD23	1.97	0.46
1:G:390:LEU:HD13	1:G:426:LEU:HD13	1.98	0.46
1:G:494:ASN:O	1:G:495:PHE:C	2.53	0.46
9:G:3009:3PE:H341	3:I:86:PHE:CD2	2.51	0.46
2:H:98:SER:CB	2:H:99:PRO:HD3	2.31	0.46
1:A:442:LYS:HD3	1:A:540:TRP:CE3	2.50	0.46
3:C:141:LEU:HD21	3:C:178:PHE:CD2	2.51	0.46
3:C:253:VAL:HG13	9:C:2010:3PE:C3I	2.45	0.46
1:G:20:TRP:HE3	1:G:32:LEU:HD21	1.74	0.46
1:G:134:ALA:O	1:G:136:PRO:HD3	2.16	0.46
1:G:179:SER:O	1:G:257:ARG:HD2	2.16	0.46
1:A:112:ILE:HG12	10:A:2024:HOH:O	2.16	0.46
1:A:241:LEU:HD13	9:D:2011:3PE:C2H	2.46	0.46
1:A:395:GLY:O	1:A:396:VAL:C	2.52	0.46
2:B:90:VAL:HG13	2:B:91:PRO:HD2	1.98	0.46
2:B:235:LEU:HD11	4:J:9:HIS:N	2.31	0.46
1:G:234:VAL:O	1:G:235:THR:C	2.54	0.46
1:G:292:LEU:HD23	1:G:292:LEU:HA	1.81	0.46
2:H:101:GLU:O	2:H:102:ILE:C	2.54	0.46
2:H:202:VAL:HG12	2:H:269:VAL:HG22	1.97	0.46
1:A:433:PHE:O	1:A:434:ALA:C	2.54	0.46
2:B:111:ILE:O	2:B:114:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:THR:HB	3:C:75:VAL:HG23	1.97	0.46
1:G:107:MET:CE	1:G:424:MET:SD	3.04	0.46
1:G:124:MET:SD	1:G:125:PRO:HD3	2.56	0.46
1:G:189:LEU:CD2	3:I:33:VAL:HG21	2.46	0.46
1:G:203:LEU:O	1:G:204:GLY:O	2.34	0.46
2:H:171:ARG:HD2	10:H:1142:HOH:O	2.16	0.46
3:I:202:PHE:CD1	3:I:202:PHE:O	2.69	0.46
4:J:31:THR:HG22	4:J:32:TRP:N	2.31	0.46
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.79	0.45
1:A:188:ASP:OD2	1:A:258:ASN:ND2	2.37	0.45
3:C:8:ASP:HB3	3:C:72:THR:CG2	2.31	0.45
3:C:58:TRP:O	3:C:62:VAL:HG23	2.16	0.45
3:C:103:LYS:C	3:C:103:LYS:HD3	2.37	0.45
3:C:136:ILE:HG21	3:C:181:PHE:CE2	2.51	0.45
1:G:310:ILE:HG23	1:G:310:ILE:O	2.16	0.45
1:G:551:PHE:CE1	1:G:555:PRO:HG3	2.51	0.45
10:G:3031:HOH:O	3:I:104:HIS:HE1	1.99	0.45
2:H:252:CYS:HB2	2:H:263:MET:CG	2.47	0.45
1:A:189:LEU:HD21	3:C:30:PHE:HD1	1.80	0.45
1:A:389:PHE:CD2	1:A:390:LEU:HD23	2.51	0.45
2:B:211:THR:CG2	2:B:212:GLY:N	2.79	0.45
1:G:298:VAL:O	1:G:299:SER:C	2.54	0.45
1:G:431:GLY:O	1:G:434:ALA:HB3	2.16	0.45
9:G:3012:3PE:H232	4:J:29:MET:CE	2.46	0.45
2:H:211:THR:HG23	2:H:234:ARG:O	2.16	0.45
1:A:137:ARG:N	9:A:2009:3PE:O12	2.49	0.45
1:A:251:THR:HG22	3:C:97:TRP:CH2	2.51	0.45
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.16	0.45
3:C:54:THR:O	3:C:55:MET:C	2.54	0.45
1:G:238:LEU:O	1:G:239:ILE:C	2.53	0.45
1:G:314:LEU:O	1:G:317:VAL:N	2.49	0.45
1:G:396:VAL:O	1:G:399:ILE:N	2.47	0.45
2:H:206:VAL:HB	2:H:240:PHE:CE1	2.52	0.45
1:A:237:TRP:HZ3	3:C:88:MET:CE	2.29	0.45
1:A:409:TYR:C	1:A:409:TYR:CD1	2.88	0.45
1:A:486:TYR:HB2	1:A:487:PRO:CD	2.45	0.45
8:A:1001:HEA:H201	8:A:1001:HEA:H253	1.99	0.45
2:B:120:LEU:HD23	2:B:120:LEU:HA	1.85	0.45
9:C:2010:3PE:H3F1	9:C:2010:3PE:H3I3	1.49	0.45
9:C:2010:3PE:H2H2	9:C:2013:3PE:H3F1	1.99	0.45
1:G:74:LYS:HD2	1:G:74:LYS:N	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:LEU:HD23	1:G:280:TRP:N	2.28	0.45
1:G:337:THR:HG22	1:G:408:ARG:HH11	1.81	0.45
3:I:238:VAL:HB	9:I:3008:3PE:P	2.56	0.45
3:I:245:TRP:CZ2	9:I:3013:3PE:H231	2.51	0.45
1:A:47:PHE:HB3	1:A:98:MET:HE3	1.99	0.45
1:A:286:GLN:O	1:A:289:ILE:HB	2.16	0.45
2:B:219:TRP:CD1	2:B:265:ILE:HD13	2.52	0.45
1:G:131:PRO:HG2	3:I:9:TYR:CD2	2.50	0.45
1:G:381:MET:O	1:G:384:ALA:HB3	2.16	0.45
9:G:3012:3PE:H2I3	3:I:91:VAL:HG11	1.99	0.45
2:H:68:ILE:HG22	2:H:69:THR:N	2.29	0.45
1:A:24:THR:O	1:A:136:PRO:HB3	2.17	0.45
1:A:51:MET:O	1:A:52:ARG:C	2.54	0.45
1:A:275:TYR:O	1:A:276:GLN:C	2.54	0.45
1:A:282:PHE:CD2	1:A:282:PHE:C	2.82	0.45
1:A:284:HIS:N	1:A:285:PRO:CD	2.78	0.45
9:A:2009:3PE:H381	9:A:2009:3PE:H251	1.97	0.45
1:G:52:ARG:O	1:G:53:MET:C	2.55	0.45
1:G:141:LEU:CB	3:I:18:PRO:HB3	2.45	0.45
1:G:231:SER:HA	1:G:320:MET:HE3	1.99	0.45
1:G:400:VAL:HG11	10:G:3109:HOH:O	2.16	0.45
2:H:84:HIS:CD2	2:H:84:HIS:C	2.90	0.45
2:H:134:VAL:CG1	2:H:135:THR:N	2.80	0.45
2:H:209:GLN:HB2	2:H:237:GLN:HG2	1.97	0.45
4:J:30:VAL:O	4:J:33:ALA:HB3	2.17	0.45
1:A:110:VAL:HG12	1:A:111:VAL:N	2.32	0.45
1:A:135:PHE:CD1	9:A:2009:3PE:H11	2.52	0.45
1:A:359:THR:HG21	1:A:391:PHE:HE2	1.79	0.45
2:B:61:ILE:HG22	10:B:1031:HOH:O	2.16	0.45
2:B:276:ALA:HA	2:B:279:LEU:CD1	2.46	0.45
3:C:71:HIS:O	3:C:76:ARG:HG3	2.17	0.45
3:C:92:MET:O	3:C:93:PHE:C	2.55	0.45
3:C:245:TRP:CZ2	9:C:2013:3PE:H231	2.52	0.45
9:C:2013:3PE:C31	9:C:2013:3PE:H351	2.46	0.45
4:D:44:LEU:HD23	9:D:2011:3PE:C32	2.45	0.45
1:G:18:THR:HG22	1:G:19:ARG:N	2.30	0.45
9:G:3009:3PE:H242	9:G:3009:3PE:C37	2.44	0.45
2:H:120:LEU:HB2	2:H:121:PRO:CD	2.47	0.45
9:I:3010:3PE:H231	9:I:3010:3PE:H331	1.97	0.45
1:A:88:CYS:SG	1:A:89:THR:N	2.90	0.45
1:A:92:GLY:HA2	1:A:484:ILE:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:HA2	8:A:1001:HEA:HMD3	1.99	0.45
1:A:337:THR:HG22	1:A:408:ARG:NH1	2.32	0.45
1:A:425:SER:O	1:A:429:VAL:HB	2.16	0.45
1:A:535:ALA:HB1	1:A:540:TRP:NE1	2.32	0.45
4:D:41:LEU:O	4:D:44:LEU:HB3	2.16	0.45
3:I:226:ARG:HH12	9:I:3008:3PE:H12	1.82	0.45
1:A:74:LYS:H	1:A:74:LYS:CD	2.24	0.45
1:A:237:TRP:CH2	9:A:2012:3PE:H282	2.52	0.45
1:A:291:VAL:CG2	1:A:295:PHE:CE1	3.00	0.45
1:A:442:LYS:NZ	1:A:542:LEU:O	2.40	0.45
1:A:463:GLY:CA	1:A:503:LEU:HD23	2.47	0.45
1:A:486:TYR:N	1:A:486:TYR:CD1	2.85	0.45
2:B:226:VAL:HA	10:B:1047:HOH:O	2.16	0.45
3:C:40:GLY:HA2	3:C:41:PRO:HD2	1.78	0.45
1:G:63:MET:CE	1:G:95:TRP:HB2	2.40	0.45
1:G:176:PRO:CB	1:G:177:PRO:HA	2.47	0.45
2:H:111:ILE:O	2:H:114:ALA:HB3	2.17	0.45
1:A:50:TYR:O	1:A:53:MET:HB2	2.17	0.45
1:A:147:VAL:HG12	1:A:148:ALA:N	2.32	0.45
1:A:323:ILE:HD11	1:A:359:THR:OG1	2.16	0.45
1:A:390:LEU:H	1:A:390:LEU:CD2	2.30	0.45
1:A:419:HIS:CD2	1:A:419:HIS:C	2.89	0.45
1:A:470:PRO:O	1:A:473:PHE:N	2.50	0.45
1:A:489:ALA:O	2:B:38:PRO:HA	2.16	0.45
2:B:190:PHE:CD1	2:B:190:PHE:C	2.89	0.45
1:G:390:LEU:O	1:G:393:VAL:HB	2.17	0.45
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2F1	1.99	0.45
9:I:3013:3PE:O14	9:I:3013:3PE:C12	2.55	0.45
4:J:44:LEU:HD23	9:J:3011:3PE:H322	1.99	0.45
1:A:48:THR:HG22	1:A:102:HIS:CE1	2.52	0.44
1:A:178:LEU:HD12	1:A:178:LEU:C	2.36	0.44
1:A:195:HIS:CD2	1:A:250:ILE:HD11	2.52	0.44
1:A:239:ILE:HD11	1:A:289:ILE:HG21	1.99	0.44
1:A:423:VAL:HG21	8:A:1002:HEA:C2C	2.47	0.44
1:A:433:PHE:HE1	1:A:511:PHE:CZ	2.36	0.44
1:A:523:ALA:O	1:A:524:ARG:C	2.56	0.44
1:A:547:PRO:O	1:A:550:THR:HG23	2.17	0.44
2:B:109:ILE:O	2:B:113:VAL:HG23	2.17	0.44
3:C:137:ASN:HD21	3:C:181:PHE:HB3	1.82	0.44
3:C:249:PHE:O	3:C:250:VAL:C	2.55	0.44
3:C:252:VAL:HG12	9:C:2010:3PE:C3H	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:ILE:HD11	1:G:140:ASN:HA	1.98	0.44
1:G:264:PHE:HA	1:G:271:ASP:N	2.31	0.44
1:G:302:ILE:CG2	1:G:369:THR:HG21	2.40	0.44
1:G:447:GLN:HG3	1:G:448:TYR:N	2.31	0.44
1:G:458:TRP:O	1:G:459:MET:C	2.56	0.44
2:H:249:PHE:HE1	2:H:266:THR:OG1	2.00	0.44
3:I:129:ASP:O	3:I:134:PRO:HG2	2.17	0.44
1:A:115:LEU:HD12	1:A:432:ILE:CG1	2.47	0.44
9:A:2009:3PE:H3B2	9:A:2009:3PE:H2C2	1.98	0.44
1:G:112:ILE:H	1:G:113:PRO:HD2	1.82	0.44
1:G:195:HIS:CD2	1:G:250:ILE:HD11	2.52	0.44
1:G:243:LEU:HD21	10:G:3038:HOH:O	2.17	0.44
9:G:3012:3PE:H2I3	9:I:3010:3PE:H2H1	1.99	0.44
2:H:107:VAL:CG1	2:H:108:PRO:HD3	2.43	0.44
2:H:173:SER:O	2:H:174:PRO:O	2.35	0.44
2:H:205:THR:O	2:H:205:THR:HG22	2.16	0.44
2:H:221:VAL:CB	2:H:224:PHE:HD2	2.30	0.44
4:J:10:VAL:O	4:J:10:VAL:HG12	2.18	0.44
1:A:145:LEU:O	1:A:146:TYR:C	2.55	0.44
1:A:235:THR:HG22	1:A:236:ALA:N	2.32	0.44
1:A:342:LEU:HD11	2:B:123:LEU:HG	1.98	0.44
3:C:63:VAL:O	3:C:64:THR:C	2.56	0.44
3:C:81:TRP:O	3:C:84:ILE:N	2.51	0.44
3:C:130:PRO:HB3	3:C:263:ILE:HD13	1.98	0.44
1:G:213:LEU:HD21	1:G:233:PHE:CZ	2.52	0.44
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.70	0.44
1:G:247:ALA:HB2	9:G:3009:3PE:H3H2	1.99	0.44
1:G:429:VAL:HG22	8:G:1001:HEA:H272	1.99	0.44
1:G:436:ILE:HD11	8:G:1001:HEA:H251	1.99	0.44
1:G:478:GLY:O	1:G:479:MET:C	2.55	0.44
3:I:59:TRP:HD1	3:I:62:VAL:HG21	1.81	0.44
3:I:74:VAL:O	3:I:77:LEU:N	2.51	0.44
1:A:307:LYS:HD3	1:A:374:SER:OG	2.18	0.44
8:A:1002:HEA:HHA	10:A:2047:HOH:O	2.17	0.44
2:B:201:PRO:CB	2:B:204:LYS:HG3	2.47	0.44
3:C:182:GLN:O	3:C:185:GLU:HB2	2.17	0.44
3:C:231:HIS:O	9:C:2008:3PE:H121	2.18	0.44
1:G:24:THR:O	1:G:136:PRO:HB3	2.17	0.44
1:G:104:ILE:O	1:G:105:LEU:C	2.55	0.44
1:G:539:GLU:O	1:G:542:LEU:HD12	2.17	0.44
3:I:74:VAL:O	3:I:75:VAL:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:OG1	1:A:292:LEU:HB2	2.17	0.44
1:A:390:LEU:HD13	1:A:426:LEU:HD13	1.99	0.44
2:B:253:SER:O	2:B:254:GLU:HB2	2.17	0.44
3:C:2:ALA:HB3	3:C:5:LYS:NZ	2.31	0.44
3:C:25:ALA:HA	3:C:28:MET:HB3	2.00	0.44
3:C:74:VAL:HG12	4:D:16:ILE:HG23	1.98	0.44
3:C:211:PHE:O	3:C:215:VAL:HG23	2.17	0.44
1:G:52:ARG:HD3	1:G:498:SER:OG	2.18	0.44
1:G:212:PHE:HE1	1:G:222:MET:CE	2.31	0.44
1:G:243:LEU:HD22	1:G:282:PHE:CE1	2.53	0.44
1:G:406:VAL:HG12	1:G:410:TYR:CE2	2.52	0.44
9:G:3009:3PE:H221	3:I:58:TRP:NE1	2.33	0.44
9:G:3009:3PE:O22	3:I:59:TRP:NE1	2.45	0.44
2:H:51:ALA:HA	2:H:54:ILE:HD12	2.00	0.44
2:H:192:LEU:HD23	2:H:192:LEU:HA	1.69	0.44
3:I:106:LEU:C	3:I:108:PRO:HD3	2.37	0.44
1:A:70:SER:C	1:A:71:GLY:O	2.53	0.44
1:A:98:MET:O	1:A:101:GLY:N	2.50	0.44
1:A:234:VAL:HG12	1:A:292:LEU:HD11	1.98	0.44
1:A:367:ILE:HG22	1:A:368:ALA:N	2.31	0.44
1:A:379:THR:HA	1:A:382:LEU:CD1	2.42	0.44
1:A:504:SER:HB3	8:A:1001:HEA:H262	1.99	0.44
9:A:2009:3PE:H291	9:A:2009:3PE:H3A1	2.00	0.44
9:A:2012:3PE:C3E	9:D:2011:3PE:H2F1	2.48	0.44
2:B:255:LEU:HB3	10:B:1011:HOH:O	2.18	0.44
1:G:34:LEU:O	1:G:38:GLY:N	2.47	0.44
2:H:209:GLN:HG3	2:H:235:LEU:HD22	2.00	0.44
1:A:341:SER:OG	1:A:344:GLN:HG3	2.18	0.44
1:A:367:ILE:HG13	2:B:76:ILE:HD13	1.99	0.44
1:A:442:LYS:O	1:A:546:PRO:HD3	2.18	0.44
2:B:120:LEU:O	2:B:121:PRO:C	2.56	0.44
2:B:142:GLN:NE2	10:B:1006:HOH:O	2.44	0.44
2:B:211:THR:HG22	2:B:212:GLY:O	2.17	0.44
1:G:37:GLY:O	1:G:110:VAL:HG13	2.18	0.44
1:G:91:ASN:OD1	1:G:165:GLN:NE2	2.49	0.44
1:G:120:GLY:O	1:G:121:ASN:C	2.55	0.44
1:G:390:LEU:CD1	1:G:426:LEU:HB3	2.48	0.44
1:G:496:VAL:O	1:G:497:SER:C	2.56	0.44
1:G:509:LEU:O	1:G:510:PHE:C	2.56	0.44
8:G:1001:HEA:HAA1	8:G:1001:HEA:HMA	1.80	0.44
2:H:77:LEU:O	2:H:78:TYR:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:133:LEU:O	3:I:136:ILE:HB	2.18	0.44
9:I:3013:3PE:H282	9:I:3013:3PE:H2B1	1.72	0.44
1:A:209:ILE:HG21	3:C:85:LEU:CD2	2.48	0.44
1:A:322:ALA:HB3	1:A:358:PRO:HB3	2.00	0.44
3:C:28:MET:CA	3:C:47:GLY:HA3	2.48	0.44
3:C:112:GLU:O	3:C:115:ILE:HD12	2.17	0.44
3:C:226:ARG:HH22	9:C:2008:3PE:C12	2.30	0.44
1:G:75:GLY:O	1:G:76:PHE:C	2.56	0.44
1:G:332:ALA:HB3	1:G:348:PHE:CE2	2.52	0.44
1:G:390:LEU:HD23	1:G:390:LEU:H	1.83	0.44
1:G:537:THR:HG21	10:G:3070:HOH:O	2.17	0.44
3:I:26:PHE:O	3:I:27:VAL:C	2.56	0.44
3:I:66:SER:HB2	3:I:71:HIS:CE1	2.53	0.44
1:A:487:PRO:HG2	1:A:490:PHE:HE2	1.83	0.44
1:A:499:LEU:O	1:A:500:GLY:C	2.56	0.44
8:A:1001:HEA:HMB1	8:A:1001:HEA:C12	2.48	0.44
9:A:2009:3PE:H361	9:C:2008:3PE:H292	1.99	0.44
3:C:31:GLY:CA	3:C:43:MET:SD	3.06	0.44
3:C:80:ARG:HH12	9:C:2013:3PE:H111	1.83	0.44
4:D:31:THR:HG22	4:D:32:TRP:N	2.32	0.44
1:G:208:MET:O	1:G:209:ILE:C	2.57	0.44
1:G:374:SER:HB2	2:H:85:GLU:HA	1.99	0.44
2:H:272:GLU:HG3	10:H:1091:HOH:O	2.18	0.44
3:I:17:TRP:O	3:I:20:MET:HB3	2.17	0.44
9:I:3010:3PE:H3I3	9:I:3010:3PE:H3F1	1.60	0.44
1:A:102:HIS:CE1	8:A:1001:HEA:NC	2.85	0.43
1:A:397:THR:HG21	10:A:2072:HOH:O	2.17	0.43
2:B:113:VAL:O	2:B:114:ALA:C	2.55	0.43
3:C:48:LEU:O	3:C:49:VAL:C	2.56	0.43
1:G:65:ALA:CB	1:G:89:THR:HB	2.46	0.43
1:G:106:MET:CE	1:G:110:VAL:HB	2.46	0.43
1:G:299:SER:HB3	1:G:310:ILE:CD1	2.46	0.43
1:G:496:VAL:O	1:G:499:LEU:HB2	2.18	0.43
1:G:498:SER:O	1:G:499:LEU:C	2.56	0.43
8:G:1001:HEA:HBA1	10:G:3059:HOH:O	2.17	0.43
3:I:8:ASP:HB3	3:I:72:THR:CG2	2.29	0.43
1:A:178:LEU:HD23	2:B:255:LEU:O	2.17	0.43
1:A:217:ALA:O	1:A:218:PRO:C	2.56	0.43
1:A:367:ILE:HD13	2:B:75:LEU:CB	2.48	0.43
1:A:506:ALA:HA	1:A:509:LEU:HD12	1.98	0.43
8:A:1001:HEA:HMA	8:A:1001:HEA:HAA1	1.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2009:3PE:C36	9:C:2008:3PE:H292	2.48	0.43
2:B:84:HIS:O	2:B:87:ARG:N	2.46	0.43
2:B:164:PRO:HA	2:B:168:GLY:O	2.18	0.43
3:C:112:GLU:HB2	3:C:116:ILE:HB	2.00	0.43
1:G:341:SER:N	1:G:344:GLN:OE1	2.45	0.43
1:G:481:ARG:O	1:G:482:ARG:HB2	2.18	0.43
4:J:33:ALA:O	4:J:34:ALA:C	2.56	0.43
1:A:72:LEU:O	1:A:73:VAL:C	2.56	0.43
1:A:404:ALA:O	1:A:405:SER:C	2.57	0.43
2:B:98:SER:CB	2:B:99:PRO:HD3	2.28	0.43
2:B:143:TRP:HZ2	2:B:257:GLY:HA3	1.82	0.43
2:B:276:ALA:HA	2:B:279:LEU:HD12	2.01	0.43
3:C:133:LEU:HD11	3:C:181:PHE:CD2	2.54	0.43
3:C:201:ASN:HD22	3:C:201:ASN:HA	1.48	0.43
1:G:71:GLY:HA3	1:G:74:LYS:HD3	2.01	0.43
1:G:135:PHE:CE1	3:I:79:LEU:HD23	2.43	0.43
9:G:3009:3PE:H271	9:G:3009:3PE:H382	1.99	0.43
10:G:3065:HOH:O	2:H:260:HIS:HB3	2.17	0.43
2:H:241:ARG:HH21	2:H:243:GLU:HG2	1.83	0.43
3:I:100:SER:O	3:I:101:PHE:C	2.57	0.43
3:I:239:GLY:N	9:I:3008:3PE:H11	2.30	0.43
2:B:248:PHE:HE2	2:B:269:VAL:HG12	1.82	0.43
3:C:225:ILE:O	3:C:226:ARG:C	2.56	0.43
1:G:17:PHE:O	1:G:21:PHE:HB2	2.17	0.43
1:G:170:ILE:HG22	1:G:171:GLY:N	2.31	0.43
1:G:277:HIS:CG	1:G:335:MET:HE1	2.53	0.43
1:G:384:ALA:O	1:G:388:LEU:HD23	2.19	0.43
1:G:385:LEU:O	1:G:386:GLY:C	2.57	0.43
2:H:190:PHE:CD1	2:H:190:PHE:C	2.90	0.43
3:I:48:LEU:O	3:I:48:LEU:HG	2.16	0.43
1:A:122:TYR:C	1:A:122:TYR:HD1	2.22	0.43
1:A:300:HIS:HB3	10:A:2020:HOH:O	2.17	0.43
1:A:433:PHE:HD1	1:A:436:ILE:HD12	1.83	0.43
2:B:71:PHE:O	2:B:75:LEU:HD12	2.19	0.43
2:B:142:GLN:HG3	2:B:214:ASP:OD2	2.18	0.43
3:C:73:PRO:HG2	4:D:12:GLY:HA2	2.00	0.43
3:C:136:ILE:HG21	3:C:181:PHE:HE2	1.83	0.43
3:C:141:LEU:O	3:C:142:LEU:C	2.56	0.43
3:C:161:ARG:HH22	3:C:230:GLY:HA2	1.83	0.43
9:C:2013:3PE:H2D2	9:C:2013:3PE:C3G	2.49	0.43
4:D:33:ALA:O	4:D:36:VAL:HB	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ILE:CG1	1:G:289:ILE:HG12	2.48	0.43
1:G:314:LEU:HA	1:G:314:LEU:HD12	1.70	0.43
2:H:177:GLU:HA	2:H:180:LEU:HD12	2.00	0.43
3:I:112:GLU:HB2	3:I:116:ILE:HB	2.01	0.43
1:A:271:ASP:HB2	3:C:109:MET:SD	2.58	0.43
1:A:387:PHE:CD1	1:A:388:LEU:N	2.87	0.43
9:A:2009:3PE:H221	3:C:58:TRP:CZ2	2.53	0.43
1:G:22:MET:HG2	3:I:16:ILE:CA	2.48	0.43
1:G:33:TYR:OH	1:G:142:SER:HB2	2.18	0.43
1:G:44:SER:O	1:G:45:VAL:C	2.57	0.43
1:G:170:ILE:CG2	1:G:174:LEU:HA	2.47	0.43
3:I:226:ARG:HE	3:I:231:HIS:CD2	2.36	0.43
3:I:256:PHE:CE1	9:J:3011:3PE:H391	2.53	0.43
4:J:42:ILE:O	4:J:43:PHE:C	2.57	0.43
1:A:22:MET:SD	3:C:16:ILE:HD12	2.59	0.43
1:A:95:TRP:HB2	1:A:484:ILE:CG1	2.47	0.43
1:A:284:HIS:O	1:A:285:PRO:C	2.56	0.43
1:A:419:HIS:O	1:A:419:HIS:CG	2.71	0.43
1:A:442:LYS:HD2	1:A:442:LYS:HA	1.70	0.43
2:B:35:ARG:HG3	2:B:36:PRO:HD2	2.00	0.43
2:B:108:PRO:HA	2:B:111:ILE:HD12	2.01	0.43
3:C:220:LEU:O	3:C:223:CYS:N	2.52	0.43
1:G:98:MET:O	1:G:101:GLY:N	2.51	0.43
1:G:195:HIS:O	1:G:198:GLY:N	2.51	0.43
1:G:291:VAL:O	1:G:291:VAL:CG2	2.67	0.43
1:G:509:LEU:HG	1:G:509:LEU:H	1.56	0.43
2:H:163:SER:O	2:H:166:THR:OG1	2.37	0.43
2:H:173:SER:H	2:H:176:VAL:HB	1.82	0.43
1:A:31:VAL:O	1:A:32:LEU:C	2.56	0.43
1:A:141:LEU:HD11	1:A:145:LEU:HD11	2.00	0.43
1:A:325:VAL:CG2	9:A:2012:3PE:H3B2	2.49	0.43
1:A:367:ILE:HG13	2:B:76:ILE:CD1	2.49	0.43
1:A:375:ILE:HD12	2:B:80:VAL:HA	2.01	0.43
1:A:407:ASP:O	1:A:411:HIS:N	2.38	0.43
3:C:85:LEU:HD23	3:C:88:MET:CE	2.48	0.43
1:G:93:HIS:CD2	1:G:165:GLN:HB2	2.54	0.43
2:H:120:LEU:HD23	2:H:120:LEU:HA	1.77	0.43
2:H:129:ILE:HA	2:H:130:PRO:HD3	1.64	0.43
2:H:192:LEU:HB3	2:H:249:PHE:CE2	2.54	0.43
3:I:25:ALA:HA	3:I:28:MET:HB3	2.00	0.43
1:A:150:THR:O	1:A:153:ALA:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB1	10:A:2080:HOH:O	2.18	0.43
1:A:519:LEU:N	1:A:519:LEU:HD23	2.33	0.43
1:A:556:LYS:O	1:A:559:ASP:HB2	2.19	0.43
3:C:72:THR:HG22	3:C:72:THR:O	2.15	0.43
1:G:237:TRP:CZ3	9:G:3012:3PE:H2A1	2.54	0.43
1:G:318:TYR:HD1	1:G:318:TYR:HA	1.65	0.43
1:G:342:LEU:HD11	2:H:123:LEU:HG	2.01	0.43
1:G:451:TRP:CG	1:G:452:ALA:N	2.87	0.43
2:H:135:THR:O	2:H:150:PRO:HD2	2.19	0.43
2:H:229:ASP:OD2	10:H:1050:HOH:O	2.21	0.43
3:I:147:ALA:HB2	3:I:170:LEU:HD23	2.00	0.43
1:A:243:LEU:CD2	1:A:282:PHE:CE1	3.01	0.43
1:A:271:ASP:OD2	3:C:103:LYS:NZ	2.51	0.43
1:A:530:TYR:CE2	1:A:531:TRP:NE1	2.87	0.43
2:B:161:ILE:CD1	2:B:180:LEU:HD23	2.49	0.43
3:C:72:THR:HG22	3:C:74:VAL:N	2.34	0.43
3:C:196:ASN:O	3:C:197:ILE:C	2.57	0.43
1:G:292:LEU:O	1:G:295:PHE:HB2	2.19	0.43
1:G:342:LEU:HD21	2:H:124:PHE:CE1	2.54	0.43
1:G:342:LEU:HD11	2:H:124:PHE:CD1	2.54	0.43
1:G:423:VAL:HG21	8:G:1002:HEA:C2C	2.48	0.43
1:G:431:GLY:O	1:G:434:ALA:N	2.52	0.43
1:G:433:PHE:CD1	1:G:436:ILE:HD12	2.53	0.43
1:G:472:HIS:O	1:G:476:ARG:HG3	2.19	0.43
2:H:194:THR:HG22	2:H:266:THR:OG1	2.18	0.43
4:J:25:GLY:O	4:J:26:PHE:C	2.57	0.43
1:A:70:SER:HB2	1:A:74:LYS:HB3	2.01	0.42
1:A:408:ARG:HG3	2:B:126:GLN:OE1	2.19	0.42
1:A:535:ALA:HB1	1:A:540:TRP:CD1	2.54	0.42
2:B:228:GLN:NE2	2:B:229:ASP:N	2.67	0.42
2:B:283:ARG:HG3	2:B:283:ARG:HH11	1.83	0.42
3:C:202:PHE:CD1	3:C:202:PHE:C	2.92	0.42
1:G:48:THR:HG22	1:G:102:HIS:CE1	2.54	0.42
1:G:155:ALA:O	1:G:158:PHE:N	2.39	0.42
1:G:263:PHE:O	1:G:270:GLY:HA2	2.19	0.42
1:G:312:GLY:O	1:G:313:TYR:C	2.56	0.42
2:H:172:MET:HE1	2:H:187:ARG:O	2.19	0.42
3:I:197:ILE:HG13	3:I:198:TYR:N	2.34	0.42
3:I:219:PHE:HE1	9:I:3008:3PE:H342	1.84	0.42
1:A:29:ILE:HG21	1:A:139:ASN:HD21	1.83	0.42
1:A:249:ALA:O	1:A:252:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PHE:CZ	3:C:200:ALA:HB1	2.54	0.42
2:B:202:VAL:HG12	2:B:269:VAL:HG22	2.02	0.42
3:C:135:LEU:HD12	3:C:135:LEU:HA	1.89	0.42
1:G:104:ILE:HG13	1:G:172:TRP:HA	2.00	0.42
1:G:419:HIS:CD2	1:G:419:HIS:C	2.87	0.42
1:G:422:TYR:O	1:G:426:LEU:HB2	2.19	0.42
2:H:33:ILE:HD11	10:H:1146:HOH:O	2.19	0.42
2:H:220:THR:HB	2:H:227:LYS:CB	2.48	0.42
3:I:57:GLY:O	3:I:58:TRP:C	2.58	0.42
1:A:115:LEU:CD1	1:A:432:ILE:CG1	2.95	0.42
1:A:427:GLY:O	1:A:430:PHE:HB2	2.20	0.42
9:C:2010:3PE:H391	9:C:2010:3PE:H362	1.74	0.42
1:G:26:HIS:NE2	1:G:27:LYS:HG3	2.34	0.42
1:G:300:HIS:O	1:G:303:ALA:HB3	2.19	0.42
1:G:325:VAL:O	1:G:327:GLY:N	2.52	0.42
3:I:40:GLY:HA2	3:I:41:PRO:HD2	1.76	0.42
1:A:72:LEU:O	1:A:76:PHE:HB2	2.19	0.42
1:A:99:ILE:HG21	1:A:482:ARG:HG2	2.00	0.42
1:A:390:LEU:O	1:A:393:VAL:N	2.52	0.42
2:B:136:VAL:CG1	2:B:137:LYS:N	2.82	0.42
2:B:163:SER:HB2	2:B:165:ALA:HB3	2.00	0.42
3:C:79:LEU:O	3:C:80:ARG:C	2.57	0.42
1:G:100:THR:HG23	1:G:104:ILE:HD12	2.02	0.42
1:G:124:MET:O	1:G:125:PRO:C	2.58	0.42
1:G:189:LEU:HD21	3:I:30:PHE:HD1	1.85	0.42
1:G:398:GLY:O	1:G:402:SER:HB3	2.18	0.42
1:G:448:TYR:HD1	1:G:448:TYR:H	1.61	0.42
1:G:454:LYS:O	1:G:457:PHE:N	2.52	0.42
2:H:218:SER:HA	2:H:229:ASP:HA	2.01	0.42
1:A:222:MET:O	1:A:224:LYS:N	2.52	0.42
1:A:389:PHE:O	1:A:392:THR:N	2.46	0.42
2:B:77:LEU:O	2:B:78:TYR:C	2.57	0.42
3:C:74:VAL:O	3:C:75:VAL:C	2.58	0.42
4:D:10:VAL:HG12	4:D:13:SER:HB3	2.02	0.42
1:G:61:GLN:O	1:G:83:SER:HB3	2.20	0.42
1:G:70:SER:HB2	1:G:74:LYS:CB	2.49	0.42
1:G:177:PRO:O	1:G:178:LEU:C	2.57	0.42
2:H:123:LEU:O	2:H:126:GLN:HG2	2.19	0.42
2:H:283:ARG:HG3	2:H:283:ARG:HH11	1.84	0.42
9:I:3013:3PE:H322	9:I:3013:3PE:H351	1.84	0.42
1:A:130:ALA:HA	1:A:131:PRO:HD3	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TRP:O	1:A:496:VAL:HB	2.20	0.42
2:B:159:TYR:O	2:B:194:THR:HA	2.19	0.42
3:C:83:PHE:O	3:C:86:PHE:HB3	2.19	0.42
1:G:56:MET:HG3	1:G:495:PHE:CD1	2.54	0.42
1:G:174:LEU:HD13	1:G:191:ILE:CD1	2.45	0.42
1:G:401:LEU:HD21	1:G:415:TYR:CD1	2.55	0.42
1:A:473:PHE:O	1:A:476:ARG:N	2.53	0.42
2:B:197:ALA:HB2	10:B:1022:HOH:O	2.20	0.42
3:C:107:TYR:OH	4:D:49:ALA:HA	2.19	0.42
1:G:126:LEU:HD23	10:G:3051:HOH:O	2.20	0.42
1:G:225:VAL:HA	1:G:226:PRO:HD2	1.78	0.42
1:G:390:LEU:HB2	1:G:426:LEU:O	2.19	0.42
1:G:407:ASP:O	1:G:410:TYR:N	2.53	0.42
1:G:515:ILE:O	1:G:516:PHE:C	2.58	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.66	0.42
1:A:243:LEU:O	1:A:244:PRO:C	2.58	0.42
1:A:304:THR:OG1	1:A:535:ALA:CA	2.67	0.42
1:A:424:MET:HB3	8:A:1001:HEA:CBC	2.45	0.42
2:B:98:SER:CB	2:B:99:PRO:CD	2.91	0.42
2:B:221:VAL:O	2:B:222:PRO:C	2.56	0.42
2:B:235:LEU:HD11	4:J:9:HIS:H	1.84	0.42
3:C:101:PHE:CZ	3:C:261:ILE:HA	2.55	0.42
3:C:178:PHE:O	3:C:179:THR:C	2.58	0.42
9:C:2010:3PE:H3F2	9:C:2010:3PE:H3C1	1.78	0.42
1:G:29:ILE:HG22	1:G:30:GLY:N	2.35	0.42
1:G:233:PHE:HE2	9:G:3012:3PE:H351	1.84	0.42
1:G:237:TRP:O	1:G:238:LEU:C	2.58	0.42
1:G:467:THR:OG1	1:G:501:ALA:N	2.53	0.42
1:G:483:TYR:OH	2:H:251:GLN:HB3	2.19	0.42
8:G:1002:HEA:HAD2	10:G:3052:HOH:O	2.20	0.42
9:G:3012:3PE:H2D2	4:J:33:ALA:CB	2.50	0.42
2:H:136:VAL:HG11	2:H:147:TYR:HD2	1.84	0.42
2:H:202:VAL:CG1	2:H:269:VAL:HG22	2.50	0.42
1:A:71:GLY:CA	1:A:74:LYS:HD3	2.50	0.42
1:A:137:ARG:NH2	3:C:65:GLU:OE1	2.49	0.42
1:A:200:SER:O	1:A:201:SER:C	2.58	0.42
1:A:277:HIS:CG	1:A:335:MET:HE1	2.55	0.42
1:A:306:ALA:O	1:A:307:LYS:C	2.57	0.42
2:B:84:HIS:CD2	2:B:86:LYS:H	2.30	0.42
2:B:136:VAL:HG21	2:B:198:MET:HE3	2.02	0.42
2:B:173:SER:HG	2:B:175:GLU:HB2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:GLU:HG3	1:G:557:ARG:CZ	2.50	0.42
1:G:111:VAL:HG13	1:G:290:ILE:HG23	1.98	0.42
1:G:530:TYR:CE2	1:G:531:TRP:NE1	2.88	0.42
2:H:175:GLU:O	2:H:176:VAL:C	2.58	0.42
3:I:32:ALA:O	3:I:36:MET:HG3	2.20	0.42
9:I:3010:3PE:H322	9:J:3011:3PE:O32	2.19	0.42
1:A:396:VAL:HG11	2:B:65:ILE:CD1	2.47	0.42
9:A:2009:3PE:H221	3:C:58:TRP:CE2	2.54	0.42
9:A:2009:3PE:H372	9:A:2009:3PE:H3A2	1.68	0.42
2:B:192:LEU:HD13	2:B:249:PHE:CB	2.50	0.42
2:B:206:VAL:O	2:B:206:VAL:HG12	2.13	0.42
2:B:272:GLU:HG3	10:B:1024:HOH:O	2.19	0.42
4:D:42:ILE:O	4:D:43:PHE:C	2.57	0.42
1:G:94:LEU:O	1:G:97:VAL:N	2.53	0.42
1:G:147:VAL:HG12	1:G:148:ALA:N	2.35	0.42
1:G:282:PHE:CD2	1:G:282:PHE:C	2.86	0.42
1:G:442:LYS:HD3	1:G:540:TRP:CE3	2.55	0.42
2:H:126:GLN:O	2:H:127:GLN:NE2	2.53	0.42
4:J:32:TRP:O	4:J:33:ALA:C	2.58	0.42
1:A:52:ARG:HD3	1:A:498:SER:OG	2.20	0.41
1:A:57:ALA:HA	10:A:2032:HOH:O	2.19	0.41
1:A:329:VAL:HB	1:A:347:TYR:OH	2.20	0.41
1:A:458:TRP:O	1:A:459:MET:C	2.59	0.41
1:G:22:MET:SD	3:I:16:ILE:HB	2.60	0.41
1:G:130:ALA:HB2	1:G:215:MET:O	2.20	0.41
1:G:137:ARG:NE	9:G:3009:3PE:O14	2.46	0.41
1:G:248:GLY:O	1:G:249:ALA:C	2.58	0.41
1:G:344:GLN:O	1:G:345:GLN:C	2.57	0.41
2:H:98:SER:CB	2:H:99:PRO:CD	2.94	0.41
3:I:152:HIS:CA	3:I:240:PHE:HE1	2.32	0.41
1:A:29:ILE:O	1:A:30:GLY:C	2.59	0.41
1:A:40:VAL:HG11	1:A:105:LEU:HD22	2.01	0.41
1:A:137:ARG:HB2	1:A:137:ARG:HE	1.63	0.41
1:A:472:HIS:O	1:A:473:PHE:C	2.58	0.41
1:A:496:VAL:O	1:A:497:SER:C	2.58	0.41
2:B:119:SER:O	2:B:120:LEU:C	2.59	0.41
2:B:142:GLN:HB3	2:B:143:TRP:CD2	2.55	0.41
9:C:2013:3PE:H2B1	9:C:2013:3PE:H3D2	2.02	0.41
1:G:302:ILE:CG2	1:G:369:THR:CG2	2.97	0.41
1:A:85:VAL:O	1:A:88:CYS:N	2.49	0.41
1:A:255:THR:HA	1:A:259:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:O	1:A:356:ALA:N	2.53	0.41
1:A:504:SER:O	1:A:507:SER:N	2.53	0.41
1:A:517:TYR:O	1:A:520:THR:HB	2.20	0.41
1:A:560:TRP:CD1	1:A:560:TRP:C	2.94	0.41
3:C:113:SER:HA	3:C:114:PRO:HA	1.64	0.41
4:D:43:PHE:C	4:D:43:PHE:CD1	2.93	0.41
1:G:62:PHE:CE2	1:G:82:PRO:HD3	2.55	0.41
1:G:286:GLN:CA	1:G:286:GLN:HE21	2.33	0.41
2:H:75:LEU:O	2:H:76:ILE:C	2.58	0.41
2:H:164:PRO:CA	2:H:168:GLY:O	2.68	0.41
2:H:173:SER:OG	2:H:176:VAL:HG23	2.19	0.41
2:H:272:GLU:HG3	2:H:272:GLU:H	1.55	0.41
3:I:72:THR:HG22	3:I:74:VAL:N	2.34	0.41
3:I:133:LEU:HA	3:I:136:ILE:HG12	2.02	0.41
3:I:141:LEU:HD21	3:I:178:PHE:CD2	2.56	0.41
3:I:149:THR:HG22	3:I:150:TRP:N	2.33	0.41
1:A:182:GLU:HG3	1:A:183:SER:N	2.35	0.41
1:G:26:HIS:CD2	1:G:27:LYS:N	2.89	0.41
1:G:116:PHE:HD1	1:G:235:THR:HG21	1.83	0.41
8:G:1001:HEA:HMB1	8:G:1001:HEA:C12	2.50	0.41
1:A:29:ILE:HG21	1:A:139:ASN:ND2	2.35	0.41
1:A:161:GLY:N	1:A:165:GLN:O	2.53	0.41
1:A:330:VAL:CG1	1:A:352:THR:HA	2.50	0.41
1:A:476:ARG:O	2:B:43:PHE:HA	2.20	0.41
1:A:498:SER:O	1:A:499:LEU:C	2.58	0.41
2:B:68:ILE:O	2:B:71:PHE:HB3	2.20	0.41
2:B:161:ILE:HG21	2:B:180:LEU:HD23	2.01	0.41
4:D:41:LEU:O	4:D:42:ILE:C	2.58	0.41
1:G:15:GLY:N	1:G:18:THR:HB	2.35	0.41
1:G:139:ASN:O	1:G:142:SER:N	2.50	0.41
1:G:442:LYS:HA	1:G:442:LYS:HD2	1.86	0.41
2:H:70:ILE:O	2:H:73:THR:N	2.49	0.41
2:H:206:VAL:HB	2:H:240:PHE:CD1	2.56	0.41
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.51	0.41
1:A:407:ASP:O	1:A:410:TYR:N	2.53	0.41
1:A:408:ARG:NE	2:B:126:GLN:OE1	2.53	0.41
1:A:479:MET:HA	1:A:480:PRO:HD3	1.89	0.41
3:C:27:VAL:O	3:C:28:MET:C	2.58	0.41
3:C:36:MET:HB2	3:C:36:MET:HE3	1.91	0.41
3:C:106:LEU:O	3:C:108:PRO:HD3	2.21	0.41
3:C:108:PRO:HA	10:C:2014:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:LEU:O	3:C:136:ILE:HB	2.21	0.41
1:G:76:PHE:O	1:G:79:SER:HB2	2.21	0.41
1:G:160:PRO:HG2	1:G:185:TYR:HE1	1.79	0.41
1:G:556:LYS:N	1:G:559:ASP:OD2	2.51	0.41
2:H:47:ALA:HB2	2:H:223:ALA:HB1	2.03	0.41
2:H:144:TYR:HD2	2:H:145:TRP:O	2.02	0.41
3:I:122:PRO:HG2	3:I:125:ILE:CD1	2.50	0.41
1:A:81:TRP:CG	1:A:82:PRO:HD2	2.55	0.41
1:A:379:THR:CA	1:A:382:LEU:HD12	2.45	0.41
2:B:221:VAL:HG11	2:B:224:PHE:CE2	2.56	0.41
3:C:186:TYR:O	3:C:189:ALA:N	2.54	0.41
3:C:250:VAL:O	3:C:251:ASP:C	2.58	0.41
3:C:256:PHE:HZ	9:D:2011:3PE:H391	1.83	0.41
1:G:243:LEU:HD22	1:G:282:PHE:HE1	1.86	0.41
1:G:453:GLY:O	1:G:454:LYS:C	2.59	0.41
2:H:194:THR:HG22	2:H:266:THR:CB	2.49	0.41
2:H:209:GLN:HA	2:H:236:ALA:O	2.20	0.41
3:I:83:PHE:CE2	3:I:242:ALA:HB1	2.56	0.41
3:I:99:TRP:CZ2	9:I:3010:3PE:H222	2.55	0.41
9:I:3010:3PE:H3C1	9:I:3010:3PE:H3F2	1.59	0.41
1:A:232:ILE:HD13	1:A:232:ILE:HA	1.80	0.41
3:C:25:ALA:O	3:C:26:PHE:C	2.57	0.41
1:G:49:VAL:O	1:G:50:TYR:C	2.59	0.41
1:G:56:MET:HG3	1:G:495:PHE:HD1	1.84	0.41
1:G:316:MET:SD	1:G:365:SER:HB2	2.61	0.41
1:G:367:ILE:HD13	2:H:75:LEU:CB	2.46	0.41
1:G:556:LYS:O	1:G:559:ASP:HB2	2.21	0.41
2:H:145:TRP:HB2	10:H:1159:HOH:O	2.20	0.41
3:I:253:VAL:HG22	9:I:3010:3PE:C3H	2.51	0.41
9:I:3010:3PE:H362	9:I:3010:3PE:H391	1.81	0.41
1:A:20:TRP:HE3	1:A:32:LEU:HD21	1.81	0.41
1:A:26:HIS:CB	1:A:133:MET:HG2	2.50	0.41
1:A:63:MET:CE	1:A:95:TRP:HE3	2.34	0.41
1:A:221:THR:HA	9:A:2012:3PE:H121	2.03	0.41
1:A:326:LEU:O	1:A:330:VAL:HG22	2.21	0.41
1:A:429:VAL:O	1:A:430:PHE:C	2.57	0.41
2:B:75:LEU:O	2:B:76:ILE:C	2.58	0.41
2:B:202:VAL:HG22	10:B:1024:HOH:O	2.20	0.41
2:B:235:LEU:HG	4:J:9:HIS:O	2.21	0.41
3:C:41:PRO:O	3:C:42:TRP:C	2.59	0.41
3:C:160:ASN:O	3:C:164:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HB2	3:C:224:LEU:HD13	2.03	0.41
3:C:169:ALA:O	3:C:170:LEU:C	2.59	0.41
3:C:204:MET:O	3:C:205:ALA:C	2.59	0.41
3:C:222:VAL:HG11	9:C:2008:3PE:C35	2.50	0.41
3:C:253:VAL:HG22	9:C:2010:3PE:C3I	2.51	0.41
9:C:2013:3PE:H261	9:C:2013:3PE:C3A	2.45	0.41
4:D:38:VAL:HG12	4:D:42:ILE:CD1	2.51	0.41
4:D:44:LEU:HD21	9:D:2011:3PE:C3	2.50	0.41
1:G:213:LEU:CB	3:I:81:TRP:CH2	3.02	0.41
1:G:237:TRP:CZ2	9:G:3012:3PE:H282	2.56	0.41
1:G:277:HIS:N	1:G:335:MET:HE1	2.36	0.41
1:G:280:TRP:CZ3	1:G:334:HIS:CE1	3.09	0.41
1:G:325:VAL:HG22	9:G:3012:3PE:C3D	2.51	0.41
1:G:342:LEU:HD13	2:H:127:GLN:CB	2.35	0.41
1:G:396:VAL:HG11	2:H:65:ILE:CD1	2.35	0.41
1:G:422:TYR:CD2	1:G:426:LEU:HD12	2.56	0.41
1:G:504:SER:O	1:G:507:SER:HB2	2.21	0.41
8:G:1001:HEA:H11	8:G:1001:HEA:HHC	1.80	0.41
8:G:1002:HEA:H241	2:H:112:LEU:HD21	2.03	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.89	0.41
2:B:53:GLN:OE1	2:B:122:VAL:HG13	2.21	0.41
2:B:97:ASN:C	2:B:97:ASN:OD1	2.59	0.41
2:B:272:GLU:HG3	2:B:272:GLU:H	1.68	0.41
3:C:51:VAL:O	3:C:54:THR:HB	2.21	0.41
1:G:26:HIS:HB3	1:G:132:ASP:OD1	2.20	0.41
1:G:74:LYS:H	1:G:74:LYS:CD	2.31	0.41
1:G:252:MET:HB3	1:G:263:PHE:CD2	2.56	0.41
1:G:423:VAL:O	1:G:423:VAL:HG23	2.21	0.41
1:G:459:MET:HB3	1:G:507:SER:OG	2.21	0.41
2:H:97:ASN:C	2:H:97:ASN:OD1	2.60	0.41
3:I:168:LEU:HB2	3:I:224:LEU:HD13	2.01	0.41
3:I:245:TRP:CE2	9:I:3013:3PE:H231	2.55	0.41
3:I:255:LEU:HD23	3:I:255:LEU:HA	1.73	0.41
1:A:387:PHE:HD1	1:A:388:LEU:N	2.19	0.40
1:A:447:GLN:O	1:A:518:THR:HG23	2.21	0.40
1:A:477:GLN:HA	1:A:477:GLN:HE21	1.86	0.40
10:A:2037:HOH:O	2:B:143:TRP:HH2	2.03	0.40
2:B:192:LEU:HD13	2:B:249:PHE:HB3	2.03	0.40
3:C:28:MET:HA	3:C:47:GLY:HA3	2.03	0.40
3:C:77:LEU:HA	3:C:80:ARG:HD3	2.03	0.40
3:C:87:ILE:O	3:C:91:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:ARG:HA	3:C:164:VAL:HB	2.03	0.40
1:G:292:LEU:O	1:G:293:PRO:C	2.59	0.40
1:G:387:PHE:CD1	1:G:388:LEU:N	2.87	0.40
1:G:454:LYS:O	1:G:457:PHE:HB3	2.20	0.40
1:G:494:ASN:ND2	10:G:3047:HOH:O	2.44	0.40
2:H:86:LYS:HD2	2:H:89:LYS:HZ1	1.86	0.40
2:H:149:TYR:HA	2:H:150:PRO:HD2	1.83	0.40
3:I:199:GLY:O	3:I:203:PHE:HB2	2.21	0.40
1:A:95:TRP:HB2	1:A:484:ILE:CD1	2.51	0.40
1:A:243:LEU:HD22	1:A:243:LEU:HA	1.89	0.40
1:A:554:LEU:H	3:C:6:ASN:HD21	1.68	0.40
2:B:61:ILE:CG2	10:B:1031:HOH:O	2.69	0.40
3:C:256:PHE:O	3:C:257:LEU:C	2.59	0.40
9:C:2013:3PE:H3H2	9:C:2013:3PE:H2E1	2.02	0.40
1:G:109:PHE:HA	1:G:146:TYR:HE1	1.86	0.40
1:G:189:LEU:HD21	3:I:30:PHE:CD1	2.56	0.40
1:G:234:VAL:CG1	1:G:292:LEU:HD11	2.51	0.40
1:G:241:LEU:HD13	9:J:3011:3PE:H2I1	2.03	0.40
1:G:421:HIS:HB3	1:G:468:PHE:CE2	2.57	0.40
1:G:445:GLY:HA2	1:G:525:VAL:CG1	2.38	0.40
1:G:483:TYR:CE1	2:H:261:ALA:HA	2.56	0.40
1:G:513:GLY:O	1:G:516:PHE:N	2.54	0.40
9:G:3009:3PE:C38	9:G:3009:3PE:H271	2.52	0.40
2:H:219:TRP:CD1	2:H:265:ILE:CD1	3.04	0.40
3:I:83:PHE:CE1	9:I:3008:3PE:H262	2.47	0.40
1:A:52:ARG:HG3	1:A:501:ALA:CB	2.51	0.40
1:A:121:ASN:O	1:A:125:PRO:HG3	2.21	0.40
1:A:152:LEU:O	1:A:155:ALA:N	2.54	0.40
1:A:316:MET:HG2	1:A:316:MET:H	1.71	0.40
1:A:488:GLU:O	1:A:490:PHE:N	2.54	0.40
2:B:192:LEU:HB3	2:B:249:PHE:CG	2.55	0.40
2:B:260:HIS:HB3	10:B:1034:HOH:O	2.20	0.40
3:C:152:HIS:CD2	9:C:2013:3PE:H332	2.56	0.40
1:G:33:TYR:CE1	1:G:143:TYR:HB2	2.56	0.40
1:G:106:MET:CE	1:G:110:VAL:CB	3.00	0.40
1:G:319:ALA:O	1:G:322:ALA:N	2.54	0.40
1:G:488:GLU:O	1:G:490:PHE:N	2.55	0.40
1:G:493:TRP:O	1:G:496:VAL:HB	2.21	0.40
2:H:211:THR:OG1	2:H:235:LEU:HD23	2.22	0.40
3:I:122:PRO:HA	10:I:3045:HOH:O	2.19	0.40
3:I:223:CYS:O	3:I:224:LEU:C	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HA	1:A:48:THR:HG23	2.03	0.40
1:A:124:MET:SD	1:A:124:MET:C	2.99	0.40
1:A:316:MET:SD	1:A:365:SER:HB2	2.61	0.40
1:A:375:ILE:HD13	1:A:375:ILE:HG21	1.90	0.40
1:A:424:MET:CE	8:A:1002:HEA:HMD3	2.51	0.40
3:C:85:LEU:O	3:C:88:MET:N	2.53	0.40
1:G:396:VAL:HG12	1:G:397:THR:N	2.36	0.40
3:I:72:THR:O	3:I:75:VAL:N	2.54	0.40
3:I:84:ILE:O	3:I:85:LEU:C	2.59	0.40
1:G:266:PRO:HG2	2:H:232:PRO:C	2.42	0.40
1:G:266:PRO:HG2	2:H:232:PRO:O	2.22	0.40
1:G:322:ALA:O	1:G:326:LEU:HG	2.21	0.40
1:G:385:LEU:O	1:G:388:LEU:N	2.54	0.40
1:G:507:SER:O	1:G:510:PHE:N	2.54	0.40
2:H:185:TYR:HE1	2:H:247:ILE:HD13	1.86	0.40
3:I:79:LEU:O	3:I:80:ARG:C	2.60	0.40
9:I:3010:3PE:H381	9:I:3010:3PE:H3B1	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	545/566 (96%)	416 (76%)	106 (19%)	23 (4%)	3 16
1	G	545/566 (96%)	403 (74%)	112 (21%)	30 (6%)	2 10
2	B	258/264 (98%)	203 (79%)	47 (18%)	8 (3%)	4 23
2	H	258/264 (98%)	206 (80%)	44 (17%)	8 (3%)	4 23
3	C	263/266 (99%)	217 (82%)	41 (16%)	5 (2%)	8 36
3	I	263/266 (99%)	209 (80%)	49 (19%)	5 (2%)	8 36
4	D	40/51 (78%)	26 (65%)	13 (32%)	1 (2%)	5 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	J	40/51 (78%)	26 (65%)	12 (30%)	2 (5%)	2 12
All	All	2212/2294 (96%)	1706 (77%)	424 (19%)	82 (4%)	3 19

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	160	PRO
1	A	544	SER
1	A	545	PRO
2	B	254	GLU
2	B	264	PRO
3	C	73	PRO
3	C	195	GLY
1	G	58	PRO
1	G	102	HIS
1	G	160	PRO
1	G	544	SER
1	G	559	ASP
3	I	195	GLY
1	A	58	PRO
1	A	110	VAL
1	A	395	GLY
1	A	496	VAL
2	B	45	PRO
2	B	255	LEU
1	G	90	PRO
1	G	298	VAL
1	G	394	GLY
1	G	395	GLY
1	G	396	VAL
1	G	432	ILE
1	G	545	PRO
1	G	551	PHE
3	I	73	PRO
3	I	194	ALA
4	J	33	ALA
1	A	90	PRO
1	A	103	GLY
3	C	42	TRP
1	G	103	GLY
1	G	176	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	211	THR
1	G	239	ILE
1	G	377	LEU
1	G	405	SER
1	G	462	VAL
2	H	45	PRO
1	A	71	GLY
1	A	394	GLY
1	A	405	SER
1	A	408	ARG
1	A	495	PHE
3	C	14	PRO
1	G	210	THR
1	G	393	VAL
1	G	408	ARG
2	H	120	LEU
2	H	187	ARG
2	H	255	LEU
2	H	264	PRO
3	I	243	ALA
4	J	10	VAL
1	A	39	LEU
1	A	284	HIS
1	A	377	LEU
1	A	393	VAL
2	B	121	PRO
4	D	33	ALA
1	G	82	PRO
1	G	156	SER
1	G	389	PHE
2	H	215	VAL
2	B	120	LEU
2	B	174	PRO
1	G	492	THR
2	H	121	PRO
1	A	239	ILE
2	B	215	VAL
3	C	111	PRO
1	G	431	GLY
1	G	480	PRO
1	A	111	VAL
1	A	432	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	33	ILE
1	A	396	VAL
1	G	330	VAL
3	I	133	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	446/459 (97%)	397 (89%)	49 (11%)	6	25
1	G	446/459 (97%)	397 (89%)	49 (11%)	6	25
2	B	216/220 (98%)	195 (90%)	21 (10%)	8	31
2	H	216/220 (98%)	196 (91%)	20 (9%)	9	33
3	C	215/216 (100%)	198 (92%)	17 (8%)	12	41
3	I	215/216 (100%)	195 (91%)	20 (9%)	9	33
4	D	30/37 (81%)	25 (83%)	5 (17%)	2	11
4	J	30/37 (81%)	27 (90%)	3 (10%)	7	29
All	All	1814/1864 (97%)	1630 (90%)	184 (10%)	7	29

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	85	VAL
1	A	89	THR
1	A	111	VAL
1	A	122	TYR
1	A	137	ARG
1	A	142	SER
1	A	147	VAL
1	A	160	PRO
1	A	178	LEU
1	A	182	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	SER
1	A	212	PHE
1	A	221	THR
1	A	231	SER
1	A	239	ILE
1	A	243	LEU
1	A	250	ILE
1	A	251	THR
1	A	252	MET
1	A	264	PHE
1	A	282	PHE
1	A	286	GLN
1	A	304	THR
1	A	307	LYS
1	A	310	ILE
1	A	341	SER
1	A	343	THR
1	A	367	ILE
1	A	369	THR
1	A	382	LEU
1	A	388	LEU
1	A	390	LEU
1	A	397	THR
1	A	402	SER
1	A	409	TYR
1	A	412	ASP
1	A	419	HIS
1	A	424	MET
1	A	432	ILE
1	A	443	MET
1	A	446	ARG
1	A	477	GLN
1	A	492	THR
1	A	515	ILE
1	A	519	LEU
1	A	525	VAL
1	A	529	ASN
1	A	556	LYS
2	B	98	SER
2	B	104	TRP
2	B	121	PRO
2	B	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	134	VAL
2	B	149	TYR
2	B	158	SER
2	B	180	LEU
2	B	186	SER
2	B	198	MET
2	B	199	VAL
2	B	209	GLN
2	B	214	ASP
2	B	215	VAL
2	B	216	ILE
2	B	222	PRO
2	B	232	PRO
2	B	238	LEU
2	B	241	ARG
2	B	253	SER
2	B	272	GLU
3	C	15	SER
3	C	16	ILE
3	C	20	MET
3	C	39	SER
3	C	45	LEU
3	C	81	TRP
3	C	85	LEU
3	C	89	SER
3	C	100	SER
3	C	103	LYS
3	C	125	ILE
3	C	157	HIS
3	C	162	ARG
3	C	166	TRP
3	C	196	ASN
3	C	204	MET
3	C	231	HIS
4	D	13	SER
4	D	16	ILE
4	D	21	LYS
4	D	31	THR
4	D	48	ASN
1	G	25	ASN
1	G	52	ARG
1	G	85	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	89	THR
1	G	106	MET
1	G	111	VAL
1	G	113	PRO
1	G	122	TYR
1	G	137	ARG
1	G	142	SER
1	G	147	VAL
1	G	160	PRO
1	G	176	PRO
1	G	178	LEU
1	G	183	SER
1	G	208	MET
1	G	212	PHE
1	G	221	THR
1	G	231	SER
1	G	239	ILE
1	G	250	ILE
1	G	252	MET
1	G	282	PHE
1	G	286	GLN
1	G	304	THR
1	G	307	LYS
1	G	310	ILE
1	G	330	VAL
1	G	341	SER
1	G	343	THR
1	G	367	ILE
1	G	382	LEU
1	G	388	LEU
1	G	397	THR
1	G	402	SER
1	G	409	TYR
1	G	412	ASP
1	G	432	ILE
1	G	443	MET
1	G	446	ARG
1	G	492	THR
1	G	509	LEU
1	G	514	VAL
1	G	519	LEU
1	G	525	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	530	TYR
1	G	537	THR
1	G	543	THR
1	G	556	LYS
2	H	45	PRO
2	H	52	THR
2	H	63	VAL
2	H	64	ILE
2	H	98	SER
2	H	104	TRP
2	H	126	GLN
2	H	134	VAL
2	H	149	TYR
2	H	158	SER
2	H	163	SER
2	H	180	LEU
2	H	186	SER
2	H	198	MET
2	H	200	VAL
2	H	209	GLN
2	H	216	ILE
2	H	238	LEU
2	H	253	SER
2	H	272	GLU
3	I	15	SER
3	I	16	ILE
3	I	20	MET
3	I	39	SER
3	I	45	LEU
3	I	68	GLU
3	I	75	VAL
3	I	81	TRP
3	I	89	SER
3	I	95	SER
3	I	100	SER
3	I	103	LYS
3	I	125	ILE
3	I	149	THR
3	I	157	HIS
3	I	159	ASN
3	I	188	HIS
3	I	196	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	204	MET
3	I	231	HIS
4	J	21	LYS
4	J	31	THR
4	J	48	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	26	HIS
1	A	91	ASN
1	A	96	ASN
1	A	165	GLN
1	A	286	GLN
1	A	345	GLN
1	A	494	ASN
2	B	55	HIS
2	B	84	HIS
2	B	125	ASN
2	B	209	GLN
2	B	237	GLN
3	C	10	HIS
3	C	37	HIS
3	C	159	ASN
3	C	201	ASN
3	C	231	HIS
1	G	25	ASN
1	G	26	HIS
1	G	91	ASN
1	G	165	GLN
1	G	286	GLN
1	G	345	GLN
1	G	494	ASN
2	H	55	HIS
2	H	84	HIS
2	H	125	ASN
2	H	209	GLN
2	H	237	GLN
3	I	37	HIS
3	I	71	HIS
3	I	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	159	ASN
3	I	201	ASN
3	I	212	HIS
3	I	231	HIS
4	J	9	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	3PE	C	2010	-	50,50,50	1.53	2 (4%)	53,55,55	1.14	3 (5%)
9	3PE	J	3011	-	50,50,50	1.70	2 (4%)	53,55,55	1.51	7 (13%)
9	3PE	I	3013	-	50,50,50	1.63	3 (6%)	53,55,55	1.18	3 (5%)
9	3PE	D	2011	-	50,50,50	1.49	3 (6%)	53,55,55	1.29	7 (13%)
9	3PE	G	3009	-	50,50,50	1.49	3 (6%)	53,55,55	0.98	2 (3%)
9	3PE	C	2013	-	50,50,50	1.58	3 (6%)	53,55,55	1.29	2 (3%)
9	3PE	A	2009	-	50,50,50	1.61	3 (6%)	53,55,55	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	HEA	G	1001	1	44,67,67	1.73	8 (18%)	37,103,103	2.59	19 (51%)
9	3PE	C	2008	-	50,50,50	1.58	2 (4%)	53,55,55	1.18	6 (11%)
8	HEA	G	1002	1	44,67,67	1.60	8 (18%)	37,103,103	2.04	14 (37%)
9	3PE	I	3008	-	50,50,50	1.64	2 (4%)	53,55,55	1.13	3 (5%)
9	3PE	G	3012	-	50,50,50	1.62	3 (6%)	53,55,55	1.23	5 (9%)
9	3PE	I	3010	-	50,50,50	1.60	4 (8%)	53,55,55	1.03	2 (3%)
9	3PE	A	2012	-	50,50,50	1.61	3 (6%)	53,55,55	1.39	6 (11%)
8	HEA	A	1002	1	44,67,67	1.76	8 (18%)	37,103,103	2.13	9 (24%)
8	HEA	A	1001	1	44,67,67	1.74	7 (15%)	37,103,103	2.52	21 (56%)

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
9	3PE	C	2010	-	-	23/54/54/54	-
9	3PE	J	3011	-	-	22/54/54/54	-
9	3PE	I	3013	-	-	29/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-
9	3PE	G	3009	-	-	29/54/54/54	-
9	3PE	C	2013	-	-	27/54/54/54	-
9	3PE	A	2009	-	-	29/54/54/54	-
8	HEA	G	1001	1	3/3/7/16	9/24/76/76	-
9	3PE	C	2008	-	-	37/54/54/54	-
8	HEA	G	1002	1	3/3/7/16	2/24/76/76	-
9	3PE	I	3008	-	-	34/54/54/54	-
9	3PE	G	3012	-	-	22/54/54/54	-
9	3PE	I	3010	-	-	29/54/54/54	-
9	3PE	A	2012	-	-	22/54/54/54	-
8	HEA	A	1002	1	3/3/7/16	3/24/76/76	-
8	HEA	A	1001	1	3/3/7/16	10/24/76/76	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	3011	3PE	O21-C21	8.34	1.57	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	3013	3PE	O31-C31	7.69	1.55	1.33
9	A	2009	3PE	O21-C21	7.64	1.55	1.34
9	I	3008	3PE	O21-C21	7.64	1.55	1.34
9	C	2010	3PE	O21-C21	7.56	1.55	1.34
9	G	3012	3PE	O31-C31	7.54	1.55	1.33
9	C	2013	3PE	O31-C31	7.49	1.55	1.33
9	A	2012	3PE	O31-C31	7.45	1.55	1.33
9	I	3008	3PE	O31-C31	7.45	1.55	1.33
9	I	3010	3PE	O31-C31	7.41	1.55	1.33
9	G	3012	3PE	O21-C21	7.41	1.55	1.34
9	I	3013	3PE	O21-C21	7.38	1.55	1.34
9	C	2008	3PE	O21-C21	7.27	1.54	1.34
9	C	2008	3PE	O31-C31	7.26	1.54	1.33
9	C	2013	3PE	O21-C21	7.26	1.54	1.34
9	D	2011	3PE	O21-C21	7.23	1.54	1.34
9	J	3011	3PE	O31-C31	7.21	1.54	1.33
9	I	3010	3PE	O21-C21	7.17	1.54	1.34
9	A	2012	3PE	O21-C21	7.10	1.54	1.34
9	A	2009	3PE	O31-C31	6.94	1.53	1.33
9	G	3009	3PE	O21-C21	6.80	1.53	1.34
9	G	3009	3PE	O31-C31	6.80	1.53	1.33
9	C	2010	3PE	O31-C31	6.67	1.52	1.33
9	D	2011	3PE	O31-C31	6.51	1.52	1.33
8	A	1002	HEA	C3A-C2A	-5.86	1.32	1.40
8	A	1002	HEA	C3C-C2C	-5.46	1.32	1.40
8	A	1001	HEA	C3C-C2C	-5.09	1.33	1.40
8	G	1001	HEA	C3C-C2C	-5.05	1.33	1.40
8	G	1001	HEA	C3C-CAC	-4.79	1.38	1.47
8	A	1001	HEA	C3C-CAC	-4.65	1.38	1.47
8	G	1002	HEA	C3A-C2A	-4.38	1.34	1.40
8	G	1001	HEA	C3A-C2A	-4.24	1.34	1.40
8	G	1002	HEA	C3C-C2C	-4.09	1.34	1.40
8	A	1002	HEA	C3C-CAC	-4.00	1.39	1.47
8	A	1001	HEA	C3A-C2A	-3.54	1.35	1.40
8	G	1002	HEA	C3C-CAC	-3.46	1.40	1.47
8	A	1001	HEA	C16-C15	-3.28	1.44	1.51
8	G	1002	HEA	C3B-C11	-3.04	1.50	1.52
8	G	1001	HEA	CAD-C3D	2.91	1.56	1.52
8	G	1001	HEA	C3B-C2B	-2.90	1.31	1.41
8	A	1002	HEA	C3B-C11	-2.89	1.50	1.52
9	A	2012	3PE	O21-C2	-2.67	1.39	1.46
8	G	1001	HEA	C3B-C11	-2.58	1.50	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1002	HEA	C3A-CMA	2.45	1.52	1.46
8	A	1001	HEA	C3B-C2B	-2.45	1.33	1.41
8	G	1002	HEA	C1C-CHC	-2.42	1.34	1.41
9	I	3010	3PE	O32-C31	2.27	1.29	1.22
9	D	2011	3PE	O21-C2	-2.25	1.41	1.46
8	A	1002	HEA	C3B-C2B	-2.24	1.34	1.41
8	G	1002	HEA	C3B-C2B	-2.24	1.34	1.41
9	I	3013	3PE	O32-C31	2.21	1.29	1.22
8	G	1001	HEA	C22-C23	2.19	1.38	1.32
8	A	1001	HEA	C1C-CHC	-2.16	1.35	1.41
8	G	1002	HEA	C1A-C2A	2.16	1.47	1.42
9	G	3009	3PE	O21-C2	-2.15	1.41	1.46
8	A	1002	HEA	C4C-NC	-2.15	1.31	1.36
8	A	1002	HEA	C4C-CHD	-2.10	1.35	1.41
9	I	3010	3PE	C32-C31	2.06	1.56	1.50
9	C	2013	3PE	O32-C31	2.05	1.28	1.22
8	G	1001	HEA	C4C-NC	-2.05	1.31	1.36
8	A	1001	HEA	C22-C23	2.03	1.38	1.32
9	A	2009	3PE	C32-C31	2.02	1.56	1.50
9	G	3012	3PE	O21-C2	-2.01	1.41	1.46
8	A	1002	HEA	C14-C15	2.00	1.37	1.33

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	1001	HEA	CBA-CAA-C2A	6.88	125.16	112.48
9	C	2013	3PE	C2-O21-C21	-6.44	101.93	117.79
9	J	3011	3PE	C2-O21-C21	-6.23	102.44	117.79
8	A	1002	HEA	C13-C14-C15	-6.19	112.75	127.66
8	G	1002	HEA	C13-C14-C15	-5.49	114.44	127.66
9	I	3013	3PE	C2-O21-C21	-5.42	104.44	117.79
9	I	3008	3PE	C2-O21-C21	-4.92	105.67	117.79
8	G	1001	HEA	CMB-C2B-C1B	4.82	135.88	128.46
8	A	1002	HEA	CMC-C2C-C1C	4.81	135.85	128.46
9	A	2012	3PE	C3-C2-C1	-4.39	101.41	111.79
8	A	1001	HEA	C27-C19-C18	-4.37	112.47	123.68
8	A	1001	HEA	CMB-C2B-C1B	4.29	135.06	128.46
9	A	2012	3PE	O21-C21-O22	4.22	133.91	123.70
8	G	1002	HEA	CMB-C2B-C1B	4.09	134.75	128.46
8	A	1001	HEA	CAA-C2A-C3A	-4.00	116.99	126.86
8	A	1002	HEA	C3C-C4C-NC	4.00	114.38	109.21
8	G	1001	HEA	C16-C17-C18	-3.99	98.77	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	3012	3PE	O21-C21-O22	3.94	133.24	123.70
9	G	3009	3PE	C3-C2-C1	-3.92	102.52	111.79
9	C	2008	3PE	C2-O21-C21	-3.91	108.17	117.79
8	A	1001	HEA	C21-C22-C23	-3.90	114.41	127.75
9	D	2011	3PE	C3-C2-C1	-3.88	102.61	111.79
8	G	1001	HEA	C21-C22-C23	-3.82	114.68	127.75
8	G	1001	HEA	C13-C14-C15	-3.69	118.77	127.66
8	A	1001	HEA	CAD-CBD-CGD	3.67	118.83	112.67
8	A	1002	HEA	CMC-C2C-C3C	-3.67	117.81	124.68
8	A	1001	HEA	CBA-CAA-C2A	3.66	119.23	112.48
8	G	1001	HEA	OMA-CMA-C3A	3.62	132.81	124.91
9	J	3011	3PE	C3-C2-C1	-3.62	103.23	111.79
8	G	1001	HEA	C27-C19-C20	3.61	121.34	115.27
8	A	1002	HEA	CBA-CAA-C2A	3.60	119.12	112.48
9	A	2009	3PE	C3-C2-C1	-3.57	103.35	111.79
9	A	2012	3PE	O21-C2-C1	3.44	120.85	108.40
8	A	1001	HEA	C16-C17-C18	-3.42	100.64	111.88
8	G	1001	HEA	C3C-C4C-NC	3.34	113.53	109.21
8	A	1001	HEA	C27-C19-C20	3.31	120.83	115.27
8	A	1001	HEA	C13-C12-C11	3.27	119.26	114.35
8	A	1001	HEA	CMB-C2B-C3B	-3.26	118.30	124.69
8	G	1002	HEA	CBA-CAA-C2A	3.21	118.39	112.48
8	G	1001	HEA	C25-C23-C22	-3.18	113.45	122.65
8	A	1001	HEA	CMC-C2C-C3C	3.15	130.57	124.68
9	A	2012	3PE	O21-C21-C22	-3.09	104.85	111.50
8	G	1001	HEA	CMB-C2B-C3B	-3.08	118.65	124.69
8	G	1002	HEA	C27-C19-C20	3.07	120.43	115.27
8	G	1001	HEA	CBD-CAD-C3D	-3.02	106.92	112.49
8	A	1001	HEA	C16-C15-C14	3.01	127.21	121.12
8	A	1001	HEA	C4B-C3B-C2B	-2.99	104.78	106.87
9	G	3012	3PE	C3-O31-C31	-2.92	106.31	117.12
8	A	1002	HEA	CBD-CAD-C3D	2.91	117.86	112.49
9	D	2011	3PE	C2-O21-C21	-2.90	110.65	117.79
8	A	1002	HEA	C17-C16-C15	-2.89	103.48	112.98
9	C	2010	3PE	O21-C21-O22	2.86	130.62	123.70
8	G	1002	HEA	C1B-C2B-C3B	-2.85	105.01	107.00
8	A	1001	HEA	C13-C14-C15	-2.84	120.82	127.66
9	C	2008	3PE	C3-O31-C31	-2.83	106.64	117.12
8	G	1002	HEA	C12-C13-C14	2.83	119.70	112.23
8	G	1002	HEA	O11-C11-C3B	-2.78	103.98	112.00
8	G	1001	HEA	C17-C18-C19	-2.77	120.99	127.66
8	A	1001	HEA	C26-C15-C14	-2.76	116.61	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	HEA	C20-C19-C18	2.76	126.69	121.12
9	C	2010	3PE	C2-O21-C21	-2.73	111.08	117.79
9	A	2012	3PE	C3-O31-C31	-2.72	107.05	117.12
8	G	1001	HEA	CAA-C2A-C3A	-2.64	120.34	126.86
9	I	3010	3PE	O31-C31-O32	2.61	130.19	123.59
8	G	1001	HEA	C4B-C3B-C2B	-2.61	105.05	106.87
8	A	1002	HEA	CMB-C2B-C1B	2.60	132.47	128.46
8	G	1001	HEA	C27-C19-C18	-2.59	117.04	123.68
8	G	1001	HEA	C24-C23-C22	2.59	130.13	122.65
9	G	3012	3PE	C3-C2-C1	-2.57	105.72	111.79
8	A	1001	HEA	C3C-C4C-NC	2.50	112.44	109.21
8	A	1002	HEA	C12-C13-C14	2.49	118.81	112.23
9	A	2009	3PE	C33-C32-C31	-2.46	104.69	113.62
8	G	1001	HEA	CAD-CBD-CGD	2.45	116.78	112.67
9	G	3012	3PE	C2-O21-C21	-2.45	111.77	117.79
9	C	2013	3PE	C23-C22-C21	-2.43	104.78	113.62
9	D	2011	3PE	C2D-C2C-C2B	-2.42	102.14	114.42
9	C	2010	3PE	O21-C2-C3	-2.42	99.66	108.40
8	G	1002	HEA	C16-C17-C18	-2.40	103.99	111.88
8	G	1001	HEA	C16-C15-C14	2.40	125.97	121.12
8	G	1002	HEA	CAA-CBA-CGA	-2.39	108.66	112.67
8	A	1001	HEA	CMC-C2C-C1C	-2.39	124.80	128.46
9	I	3008	3PE	O31-C3-C2	2.37	115.34	108.43
8	G	1002	HEA	C17-C16-C15	-2.37	105.17	112.98
9	A	2009	3PE	O31-C31-O32	2.36	129.55	123.59
8	A	1001	HEA	CAA-CBA-CGA	2.33	116.58	112.67
8	G	1002	HEA	CMB-C2B-C3B	-2.32	120.14	124.69
9	J	3011	3PE	P-O13-C11	-2.31	110.23	121.59
9	C	2008	3PE	O21-C2-C3	-2.27	100.17	108.40
9	C	2008	3PE	O21-C21-O22	2.27	129.19	123.70
9	J	3011	3PE	C2D-C2C-C2B	-2.26	102.94	114.42
9	J	3011	3PE	O21-C21-O22	-2.24	118.28	123.70
9	I	3010	3PE	C2-O21-C21	-2.23	112.30	117.79
8	G	1002	HEA	C17-C18-C19	-2.22	122.31	127.66
9	D	2011	3PE	C2E-C2D-C2C	-2.22	103.15	114.42
9	D	2011	3PE	O32-C31-C32	-2.22	115.07	123.73
9	A	2012	3PE	C2E-C2D-C2C	-2.21	103.20	114.42
8	G	1001	HEA	C1B-C2B-C3B	-2.20	105.46	107.00
9	I	3008	3PE	C3-O31-C31	-2.20	108.96	117.12
9	J	3011	3PE	P-O11-C1	-2.20	108.77	121.68
8	A	1001	HEA	C17-C16-C15	2.20	120.21	112.98
9	G	3009	3PE	O21-C21-C22	2.19	116.23	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	HEA	C24-C23-C22	2.17	128.91	122.65
9	D	2011	3PE	P-O13-C11	-2.12	111.13	121.59
9	C	2008	3PE	O31-C3-C2	2.12	114.61	108.43
9	I	3013	3PE	O31-C3-C2	2.11	114.58	108.43
9	J	3011	3PE	O22-C21-C22	2.08	131.85	123.73
8	G	1002	HEA	C20-C19-C18	-2.07	116.92	121.12
9	G	3012	3PE	O21-C2-C1	2.07	115.89	108.40
9	C	2008	3PE	O22-C21-C22	-2.05	115.72	123.73
9	I	3013	3PE	C23-C22-C21	-2.04	106.20	113.62
9	D	2011	3PE	P-O11-C1	-2.04	109.74	121.68
8	G	1002	HEA	CAD-CBD-CGD	2.03	116.07	112.67

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1001	HEA	ND
8	A	1001	HEA	NA
8	A	1001	HEA	NB
8	A	1002	HEA	ND
8	A	1002	HEA	NA
8	A	1002	HEA	NB
8	G	1001	HEA	ND
8	G	1001	HEA	NA
8	G	1001	HEA	NB
8	G	1002	HEA	ND
8	G	1002	HEA	NA
8	G	1002	HEA	NB

All (349) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C1A-C2A-CAA-CBA
8	A	1001	HEA	C3A-C2A-CAA-CBA
8	A	1001	HEA	C3B-C11-C12-C13
8	A	1001	HEA	O11-C11-C12-C13
8	A	1001	HEA	C11-C12-C13-C14
8	G	1001	HEA	C1A-C2A-CAA-CBA
8	G	1001	HEA	C3A-C2A-CAA-CBA
8	G	1001	HEA	C3B-C11-C12-C13
8	G	1001	HEA	O11-C11-C12-C13
8	G	1001	HEA	C11-C12-C13-C14
9	A	2009	3PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	2009	3PE	C1-O11-P-O13
9	A	2009	3PE	C1-O11-P-O14
9	A	2009	3PE	C11-O13-P-O12
9	A	2009	3PE	C11-O13-P-O14
9	A	2009	3PE	O13-C11-C12-N
9	A	2012	3PE	C1-O11-P-O14
9	C	2008	3PE	C1-O11-P-O12
9	C	2008	3PE	O13-C11-C12-N
9	C	2010	3PE	C1-O11-P-O12
9	C	2010	3PE	C1-O11-P-O13
9	C	2010	3PE	C1-O11-P-O14
9	C	2010	3PE	O13-C11-C12-N
9	C	2013	3PE	C12-C11-O13-P
9	C	2013	3PE	O13-C11-C12-N
9	C	2013	3PE	O22-C21-O21-C2
9	C	2013	3PE	C22-C21-O21-C2
9	D	2011	3PE	C11-O13-P-O12
9	G	3009	3PE	C11-O13-P-O12
9	G	3009	3PE	C11-O13-P-O14
9	G	3009	3PE	O13-C11-C12-N
9	G	3012	3PE	C1-O11-P-O14
9	G	3012	3PE	O13-C11-C12-N
9	G	3012	3PE	O11-C1-C2-O21
9	I	3008	3PE	C1-O11-P-O12
9	I	3008	3PE	O13-C11-C12-N
9	I	3010	3PE	C1-O11-P-O12
9	I	3010	3PE	C1-O11-P-O14
9	I	3010	3PE	O13-C11-C12-N
9	I	3013	3PE	C12-C11-O13-P
9	I	3013	3PE	O13-C11-C12-N
9	I	3013	3PE	C22-C21-O21-C2
9	J	3011	3PE	C11-O13-P-O12
9	I	3008	3PE	O32-C31-O31-C3
9	I	3013	3PE	O22-C21-O21-C2
9	C	2008	3PE	O32-C31-O31-C3
9	C	2010	3PE	C38-C39-C3A-C3B
9	C	2008	3PE	C32-C31-O31-C3
9	I	3008	3PE	C32-C31-O31-C3
9	I	3010	3PE	C38-C39-C3A-C3B
9	C	2013	3PE	C32-C33-C34-C35
9	I	3013	3PE	C32-C33-C34-C35
8	A	1001	HEA	C27-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	1001	HEA	C27-C19-C20-C21
8	A	1001	HEA	C18-C19-C20-C21
8	G	1001	HEA	C18-C19-C20-C21
9	A	2009	3PE	C3B-C3C-C3D-C3E
9	G	3009	3PE	C3B-C3C-C3D-C3E
9	D	2011	3PE	C31-C32-C33-C34
9	D	2011	3PE	C21-C22-C23-C24
9	J	3011	3PE	C21-C22-C23-C24
9	A	2009	3PE	C11-O13-P-O11
9	C	2008	3PE	C1-O11-P-O13
9	C	2013	3PE	C1-O11-P-O13
9	D	2011	3PE	C11-O13-P-O11
9	G	3009	3PE	C1-O11-P-O13
9	G	3009	3PE	C11-O13-P-O11
9	G	3012	3PE	C1-O11-P-O13
9	I	3010	3PE	C1-O11-P-O13
9	I	3013	3PE	C1-O11-P-O13
9	J	3011	3PE	C11-O13-P-O11
9	C	2010	3PE	C21-C22-C23-C24
9	G	3009	3PE	C31-C32-C33-C34
9	D	2011	3PE	C28-C29-C2A-C2B
9	A	2009	3PE	C25-C26-C27-C28
9	A	2009	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C36-C37-C38-C39
9	C	2008	3PE	C2D-C2E-C2F-C2G
9	G	3012	3PE	C26-C27-C28-C29
9	A	2009	3PE	C24-C25-C26-C27
9	C	2008	3PE	C26-C27-C28-C29
9	C	2013	3PE	C22-C23-C24-C25
9	A	2012	3PE	C23-C24-C25-C26
9	D	2011	3PE	C26-C27-C28-C29
9	G	3012	3PE	C23-C24-C25-C26
9	C	2013	3PE	C3D-C3E-C3F-C3G
9	I	3008	3PE	C3A-C3B-C3C-C3D
9	I	3008	3PE	C26-C27-C28-C29
9	J	3011	3PE	C26-C27-C28-C29
9	A	2009	3PE	C39-C3A-C3B-C3C
9	G	3009	3PE	C25-C26-C27-C28
9	I	3008	3PE	C38-C39-C3A-C3B
9	C	2008	3PE	C27-C28-C29-C2A
9	I	3008	3PE	C27-C28-C29-C2A
9	I	3010	3PE	C2E-C2F-C2G-C2H

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	J	3011	3PE	C31-C32-C33-C34
9	A	2009	3PE	C3D-C3E-C3F-C3G
9	A	2009	3PE	C3E-C3F-C3G-C3H
9	C	2013	3PE	C39-C3A-C3B-C3C
9	G	3009	3PE	C24-C25-C26-C27
9	G	3009	3PE	C29-C2A-C2B-C2C
9	I	3013	3PE	C22-C23-C24-C25
9	C	2008	3PE	C3A-C3B-C3C-C3D
9	C	2013	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C2A-C2B-C2C-C2D
9	I	3010	3PE	C26-C27-C28-C29
9	C	2008	3PE	C36-C37-C38-C39
9	C	2008	3PE	C23-C24-C25-C26
9	D	2011	3PE	C36-C37-C38-C39
9	G	3009	3PE	C3D-C3E-C3F-C3G
9	G	3009	3PE	C23-C24-C25-C26
9	I	3010	3PE	C2A-C2B-C2C-C2D
9	J	3011	3PE	C33-C34-C35-C36
9	I	3008	3PE	C2A-C2B-C2C-C2D
9	I	3013	3PE	C36-C37-C38-C39
9	A	2012	3PE	O13-C11-C12-N
9	C	2008	3PE	C24-C25-C26-C27
9	G	3012	3PE	C3B-C3C-C3D-C3E
9	I	3008	3PE	C32-C33-C34-C35
9	I	3008	3PE	C24-C25-C26-C27
9	J	3011	3PE	C27-C28-C29-C2A
9	G	3009	3PE	C39-C3A-C3B-C3C
9	I	3013	3PE	C2C-C2D-C2E-C2F
9	A	2012	3PE	C26-C27-C28-C29
9	A	2012	3PE	C28-C29-C2A-C2B
9	C	2013	3PE	C36-C37-C38-C39
9	G	3009	3PE	C3E-C3F-C3G-C3H
9	I	3013	3PE	C3D-C3E-C3F-C3G
8	G	1001	HEA	C26-C15-C16-C17
9	I	3008	3PE	C2E-C2F-C2G-C2H
9	A	2009	3PE	C36-C37-C38-C39
9	C	2013	3PE	C2C-C2D-C2E-C2F
9	I	3010	3PE	C3F-C3G-C3H-C3I
9	A	2009	3PE	C2B-C2C-C2D-C2E
9	C	2010	3PE	C3F-C3G-C3H-C3I
9	D	2011	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	2011	3PE	C2B-C2C-C2D-C2E
9	G	3009	3PE	C2E-C2F-C2G-C2H
9	C	2010	3PE	C36-C37-C38-C39
9	C	2010	3PE	C26-C27-C28-C29
9	D	2011	3PE	C27-C28-C29-C2A
9	I	3013	3PE	C39-C3A-C3B-C3C
9	I	3010	3PE	C21-C22-C23-C24
9	C	2013	3PE	C2E-C2F-C2G-C2H
9	I	3008	3PE	C2D-C2E-C2F-C2G
9	G	3012	3PE	C28-C29-C2A-C2B
9	G	3009	3PE	C21-C22-C23-C24
9	D	2011	3PE	C33-C34-C35-C36
9	C	2008	3PE	C38-C39-C3A-C3B
9	C	2010	3PE	C2E-C2F-C2G-C2H
9	A	2009	3PE	C23-C24-C25-C26
9	I	3008	3PE	C34-C35-C36-C37
9	I	3010	3PE	C22-C21-O21-C2
9	A	2012	3PE	O11-C1-C2-O21
9	A	2009	3PE	C2E-C2F-C2G-C2H
9	A	2012	3PE	C3B-C3C-C3D-C3E
9	C	2008	3PE	C32-C33-C34-C35
9	J	3011	3PE	C36-C37-C38-C39
9	J	3011	3PE	C2B-C2C-C2D-C2E
9	C	2008	3PE	C34-C35-C36-C37
9	G	3009	3PE	C2B-C2C-C2D-C2E
8	G	1001	HEA	C14-C15-C16-C17
9	I	3010	3PE	C28-C29-C2A-C2B
9	I	3013	3PE	C25-C26-C27-C28
9	C	2010	3PE	C2A-C2B-C2C-C2D
9	I	3013	3PE	C37-C38-C39-C3A
9	J	3011	3PE	C3E-C3F-C3G-C3H
9	A	2012	3PE	C1-O11-P-O13
9	I	3008	3PE	C1-O11-P-O13
9	G	3012	3PE	C34-C35-C36-C37
9	A	2012	3PE	O11-C1-C2-C3
9	C	2008	3PE	O11-C1-C2-C3
9	C	2013	3PE	O11-C1-C2-C3
9	I	3013	3PE	O11-C1-C2-C3
9	A	2012	3PE	C3E-C3F-C3G-C3H
9	G	3012	3PE	C31-C32-C33-C34
9	I	3008	3PE	C29-C2A-C2B-C2C
9	I	3010	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	2008	3PE	C22-C21-O21-C2
9	C	2008	3PE	C29-C2A-C2B-C2C
9	A	2009	3PE	C1-C2-C3-O31
9	C	2013	3PE	C1-C2-C3-O31
9	G	3009	3PE	C1-C2-C3-O31
9	G	3009	3PE	C36-C37-C38-C39
9	G	3012	3PE	C1-C2-C3-O31
9	I	3013	3PE	C1-C2-C3-O31
9	J	3011	3PE	C3F-C3G-C3H-C3I
9	I	3013	3PE	C2E-C2F-C2G-C2H
9	C	2010	3PE	C28-C29-C2A-C2B
9	C	2010	3PE	C23-C24-C25-C26
9	A	2012	3PE	C34-C35-C36-C37
9	D	2011	3PE	C3B-C3C-C3D-C3E
9	D	2011	3PE	C3E-C3F-C3G-C3H
9	D	2011	3PE	C32-C31-O31-C3
9	C	2013	3PE	C29-C2A-C2B-C2C
9	A	2009	3PE	C22-C21-O21-C2
9	I	3008	3PE	C2F-C2G-C2H-C2I
9	A	2009	3PE	O21-C2-C3-O31
9	I	3013	3PE	C3B-C3C-C3D-C3E
9	J	3011	3PE	C3B-C3C-C3D-C3E
9	J	3011	3PE	C29-C2A-C2B-C2C
9	I	3010	3PE	C32-C33-C34-C35
9	C	2008	3PE	C2E-C2F-C2G-C2H
9	D	2011	3PE	C3F-C3G-C3H-C3I
9	G	3009	3PE	C22-C21-O21-C2
9	C	2013	3PE	C25-C26-C27-C28
9	G	3012	3PE	O11-C1-C2-C3
9	I	3008	3PE	O11-C1-C2-C3
8	A	1002	HEA	C15-C16-C17-C18
8	G	1002	HEA	C15-C16-C17-C18
9	G	3012	3PE	C24-C25-C26-C27
9	C	2010	3PE	C32-C31-O31-C3
9	C	2008	3PE	C2F-C2G-C2H-C2I
9	G	3012	3PE	C29-C2A-C2B-C2C
9	G	3012	3PE	C3E-C3F-C3G-C3H
8	A	1001	HEA	C26-C15-C16-C17
9	A	2012	3PE	C37-C38-C39-C3A
9	C	2008	3PE	O11-C1-C2-O21
9	I	3008	3PE	O11-C1-C2-O21
9	I	3010	3PE	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	I	3013	3PE	O11-C1-C2-O21
9	D	2011	3PE	O32-C31-O31-C3
9	I	3013	3PE	C35-C36-C37-C38
9	C	2013	3PE	C3B-C3C-C3D-C3E
9	C	2008	3PE	O21-C2-C3-O31
9	G	3009	3PE	O21-C2-C3-O31
9	C	2008	3PE	C3C-C3D-C3E-C3F
9	C	2008	3PE	O22-C21-O21-C2
9	G	3009	3PE	O22-C21-O21-C2
9	C	2010	3PE	O32-C31-O31-C3
9	I	3013	3PE	C34-C35-C36-C37
9	A	2009	3PE	O22-C21-O21-C2
9	G	3012	3PE	C27-C28-C29-C2A
9	A	2012	3PE	C24-C25-C26-C27
9	C	2010	3PE	C32-C33-C34-C35
9	D	2011	3PE	C3A-C3B-C3C-C3D
9	C	2013	3PE	C33-C34-C35-C36
9	C	2013	3PE	C35-C36-C37-C38
9	J	3011	3PE	C32-C31-O31-C3
9	A	2012	3PE	C29-C2A-C2B-C2C
9	C	2010	3PE	O11-C1-C2-O21
9	C	2013	3PE	O11-C1-C2-O21
9	A	2012	3PE	C27-C28-C29-C2A
9	I	3013	3PE	O21-C2-C3-O31
9	I	3013	3PE	C33-C34-C35-C36
9	A	2009	3PE	C38-C39-C3A-C3B
9	C	2008	3PE	C3B-C3C-C3D-C3E
9	J	3011	3PE	O32-C31-O31-C3
9	C	2008	3PE	C2C-C2D-C2E-C2F
9	C	2013	3PE	C34-C35-C36-C37
8	A	1001	HEA	C14-C15-C16-C17
9	A	2012	3PE	C1-O11-P-O12
9	C	2008	3PE	C1-O11-P-O14
9	C	2013	3PE	C1-O11-P-O14
9	G	3009	3PE	C1-O11-P-O12
9	G	3009	3PE	C1-O11-P-O14
9	G	3012	3PE	C1-O11-P-O12
9	I	3008	3PE	C1-O11-P-O14
9	I	3013	3PE	C1-O11-P-O14
9	A	2009	3PE	O11-C1-C2-C3
9	I	3010	3PE	O11-C1-C2-C3
9	I	3008	3PE	C2C-C2D-C2E-C2F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	J	3011	3PE	C24-C25-C26-C27
9	G	3009	3PE	C38-C39-C3A-C3B
9	I	3013	3PE	C3A-C3B-C3C-C3D
9	A	2009	3PE	C33-C34-C35-C36
9	A	2012	3PE	C31-C32-C33-C34
9	I	3010	3PE	C23-C24-C25-C26
9	G	3012	3PE	C39-C3A-C3B-C3C
9	G	3009	3PE	C34-C35-C36-C37
9	I	3008	3PE	C3C-C3D-C3E-C3F
9	C	2008	3PE	C1-C2-C3-O31
9	C	2013	3PE	O21-C2-C3-O31
9	I	3008	3PE	O21-C2-C3-O31
9	A	2012	3PE	C39-C3A-C3B-C3C
9	I	3013	3PE	C31-C32-C33-C34
9	I	3010	3PE	C32-C31-O31-C3
9	C	2010	3PE	C22-C21-O21-C2
9	A	2012	3PE	C38-C39-C3A-C3B
9	J	3011	3PE	C3A-C3B-C3C-C3D
9	G	3009	3PE	C33-C34-C35-C36
9	G	3012	3PE	C37-C38-C39-C3A
9	C	2010	3PE	O22-C21-O21-C2
9	I	3010	3PE	O32-C31-O31-C3
9	D	2011	3PE	C2A-C2B-C2C-C2D
9	G	3012	3PE	C38-C39-C3A-C3B
8	A	1002	HEA	C11-C12-C13-C14
9	I	3010	3PE	C3C-C3D-C3E-C3F
9	I	3010	3PE	C36-C37-C38-C39
9	C	2008	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C11-O13-P-O11
9	C	2013	3PE	C11-O13-P-O11
9	I	3008	3PE	C11-O13-P-O11
9	I	3013	3PE	C11-O13-P-O11
9	I	3008	3PE	C1-C2-C3-O31
9	G	3009	3PE	O11-C1-C2-C3
9	A	2009	3PE	C34-C35-C36-C37
9	G	3012	3PE	C2D-C2E-C2F-C2G
9	G	3012	3PE	C36-C37-C38-C39
9	J	3011	3PE	C2D-C2E-C2F-C2G
9	I	3010	3PE	C1-C2-C3-O31
9	A	2012	3PE	C2A-C2B-C2C-C2D
9	I	3008	3PE	C3F-C3G-C3H-C3I
9	I	3013	3PE	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	2008	3PE	C1-C2-O21-C21
9	C	2008	3PE	C3-C2-O21-C21
9	I	3008	3PE	C3-C2-O21-C21
9	J	3011	3PE	C23-C24-C25-C26
9	I	3010	3PE	C2C-C2D-C2E-C2F
9	C	2013	3PE	C3A-C3B-C3C-C3D
9	I	3008	3PE	O22-C21-O21-C2
9	I	3008	3PE	C3B-C3C-C3D-C3E
9	D	2011	3PE	C34-C35-C36-C37
9	J	3011	3PE	C28-C29-C2A-C2B
9	C	2008	3PE	C3F-C3G-C3H-C3I
8	G	1002	HEA	C26-C15-C16-C17
9	I	3013	3PE	C29-C2A-C2B-C2C
9	J	3011	3PE	C2A-C2B-C2C-C2D
9	I	3010	3PE	O31-C31-C32-C33
9	A	2009	3PE	C37-C38-C39-C3A
9	A	2009	3PE	C31-C32-C33-C34
9	C	2008	3PE	C21-C22-C23-C24
9	I	3008	3PE	C22-C21-O21-C2
8	A	1002	HEA	C20-C21-C22-C23
9	I	3010	3PE	O21-C2-C3-O31
9	I	3010	3PE	C31-C32-C33-C34
9	I	3008	3PE	C37-C38-C39-C3A
9	C	2010	3PE	O31-C31-C32-C33
9	I	3010	3PE	O21-C21-C22-C23
9	I	3010	3PE	O32-C31-C32-C33
9	D	2011	3PE	C24-C25-C26-C27
9	G	3009	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C11-O13-P-O14
9	C	2013	3PE	C11-O13-P-O14
9	A	2012	3PE	C12-C11-O13-P
9	A	2012	3PE	C36-C37-C38-C39
9	C	2010	3PE	O21-C21-C22-C23
9	D	2011	3PE	O21-C21-C22-C23
9	J	3011	3PE	O21-C21-C22-C23
8	A	1001	HEA	C16-C17-C18-C19
9	A	2009	3PE	O11-C1-C2-O21
9	C	2010	3PE	C25-C26-C27-C28
9	C	2010	3PE	O32-C31-C32-C33
9	I	3010	3PE	O22-C21-C22-C23
9	C	2008	3PE	O21-C21-C22-C23
9	I	3008	3PE	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	2011	3PE	O22-C21-C22-C23
9	I	3013	3PE	C2B-C2C-C2D-C2E

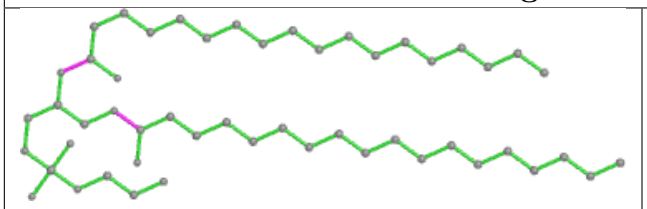
There are no ring outliers.

16 monomers are involved in 283 short contacts:

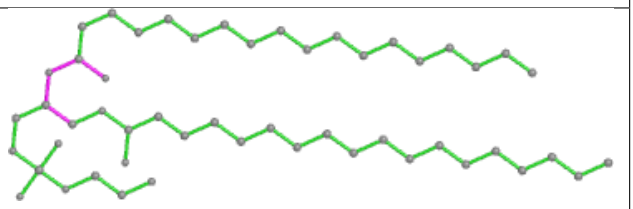
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2010	3PE	24	0
9	J	3011	3PE	13	0
9	I	3013	3PE	22	0
9	D	2011	3PE	17	0
9	G	3009	3PE	19	0
9	C	2013	3PE	21	0
9	A	2009	3PE	18	0
8	G	1001	HEA	23	0
9	C	2008	3PE	13	0
8	G	1002	HEA	15	0
9	I	3008	3PE	13	0
9	G	3012	3PE	22	0
9	I	3010	3PE	24	0
9	A	2012	3PE	20	0
8	A	1002	HEA	20	0
8	A	1001	HEA	20	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 then 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.

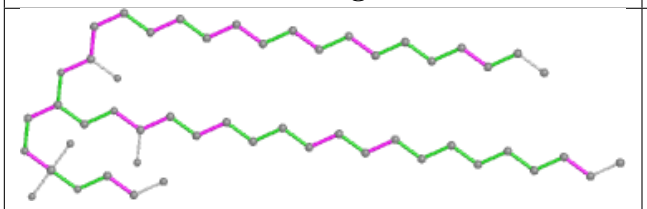
Ligand 3PE C 2010



Bond lengths



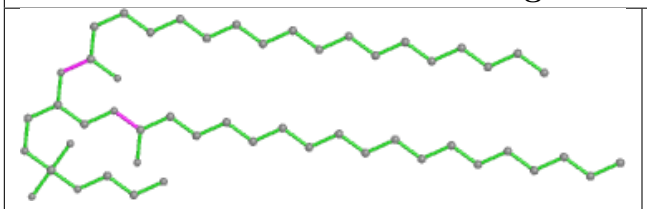
Bond angles



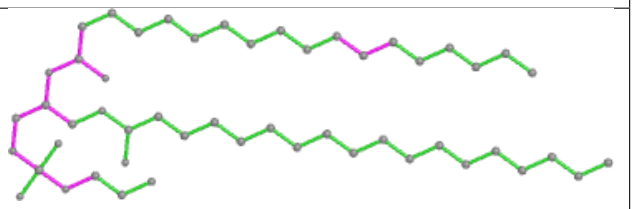
Torsions

Rings

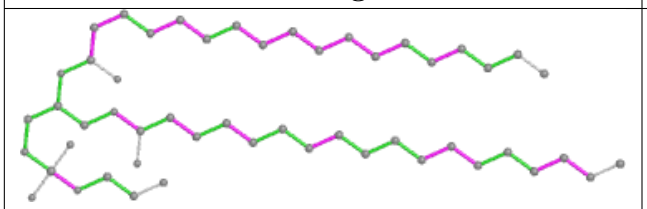
Ligand 3PE J 3011



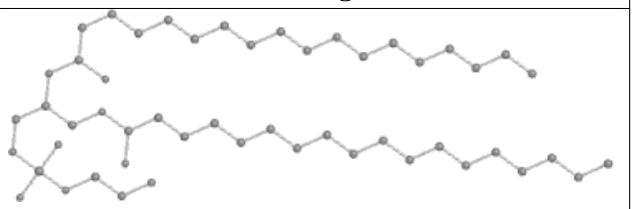
Bond lengths



Bond angles

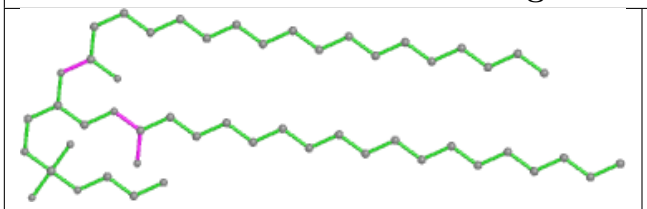


Torsions

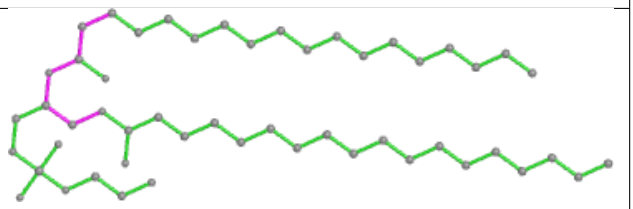


Rings

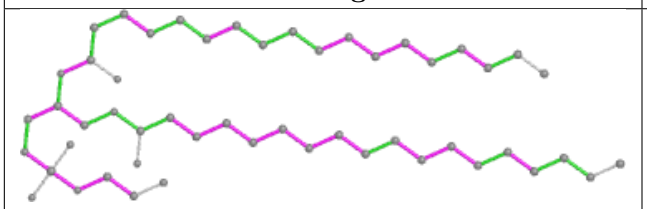
Ligand 3PE I 3013



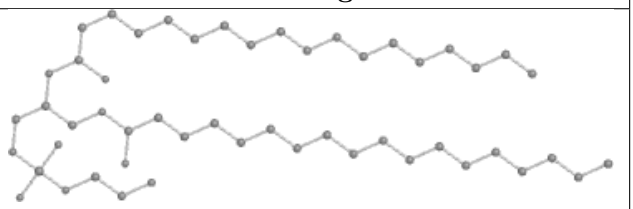
Bond lengths



Bond angles

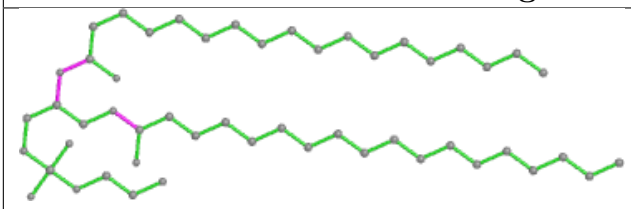


Torsions

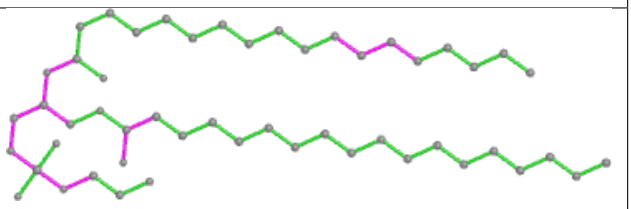


Rings

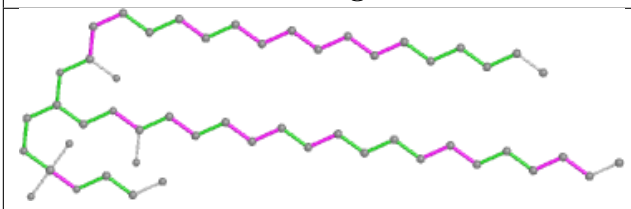
Ligand 3PE D 2011



Bond lengths



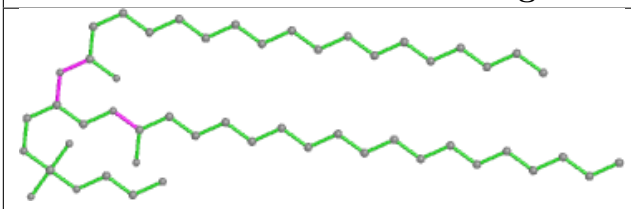
Bond angles



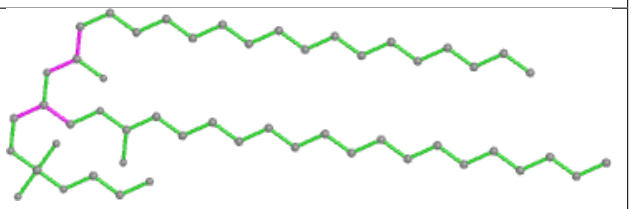
Torsions

Rings

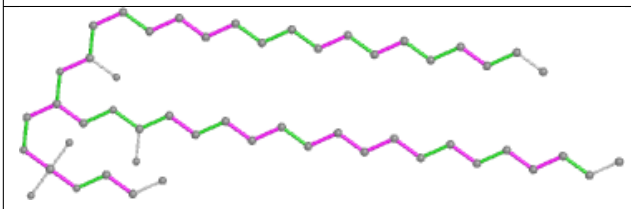
Ligand 3PE G 3009



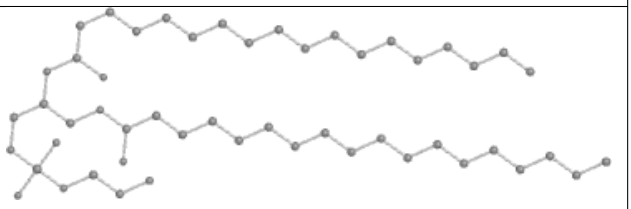
Bond lengths



Bond angles

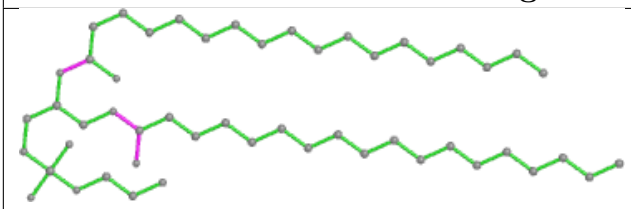


Torsions

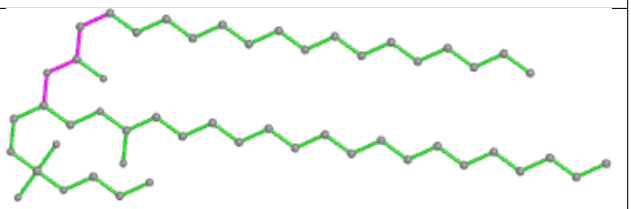


Rings

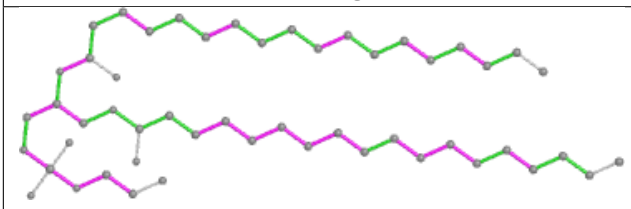
Ligand 3PE C 2013



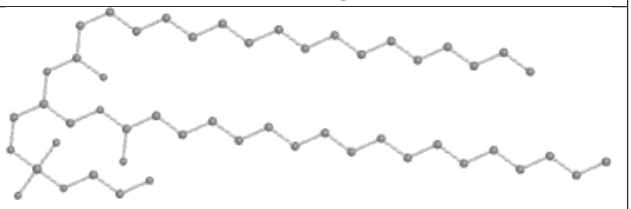
Bond lengths



Bond angles

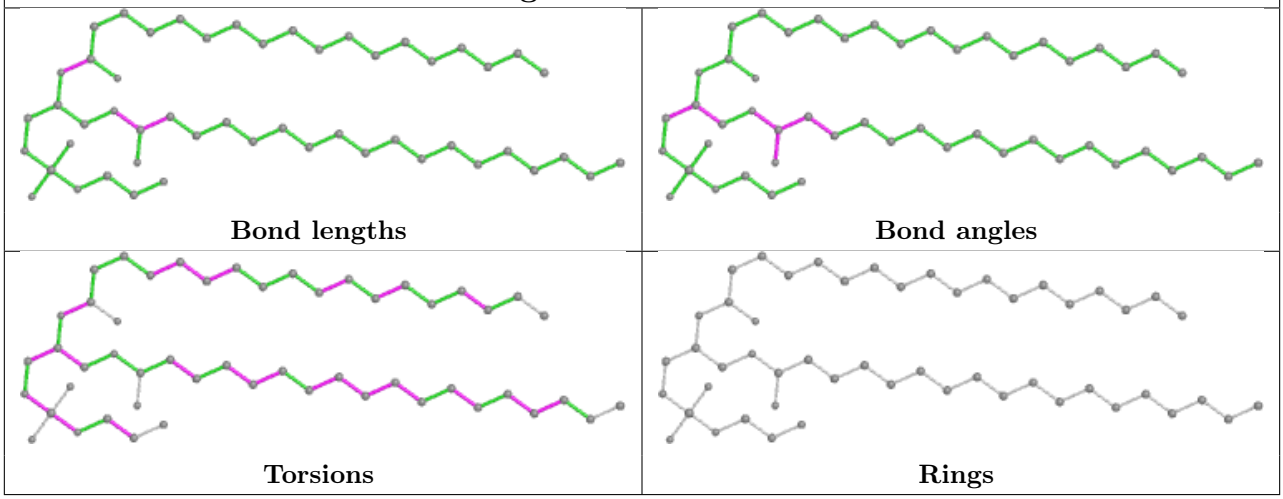


Torsions

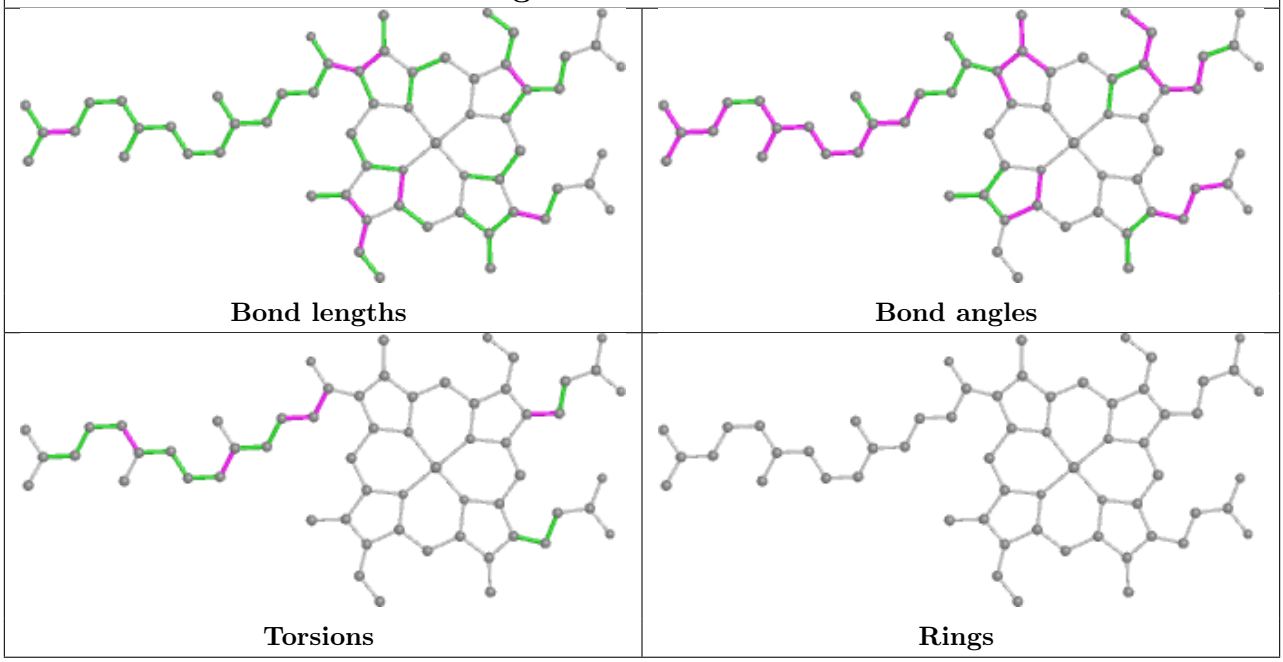


Rings

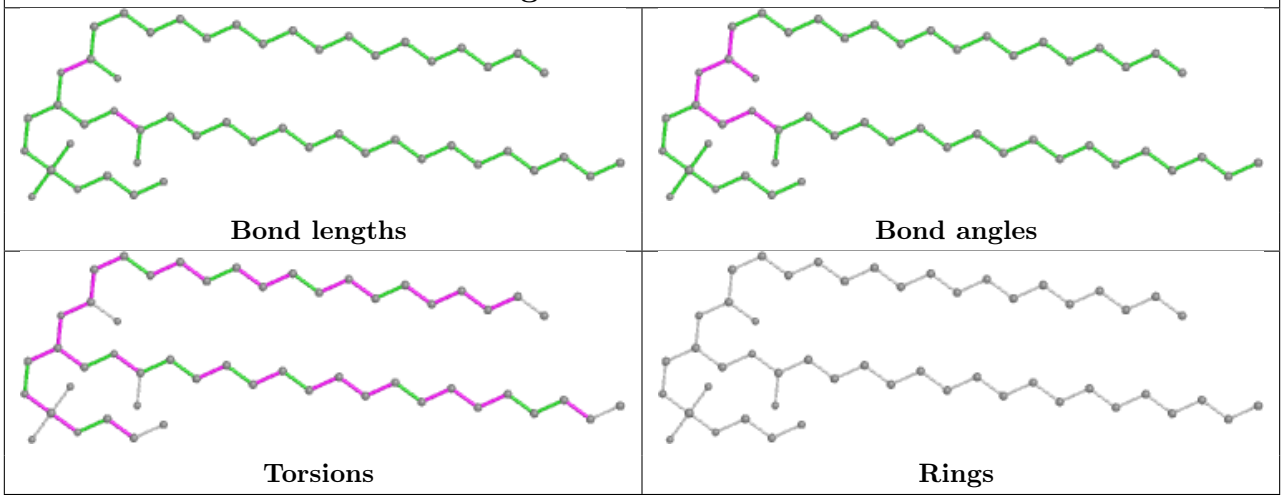
Ligand 3PE A 2009



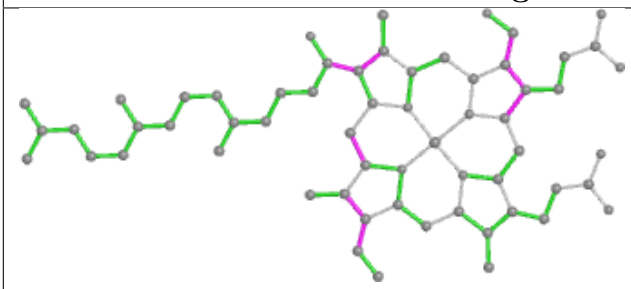
Ligand HEA G 1001



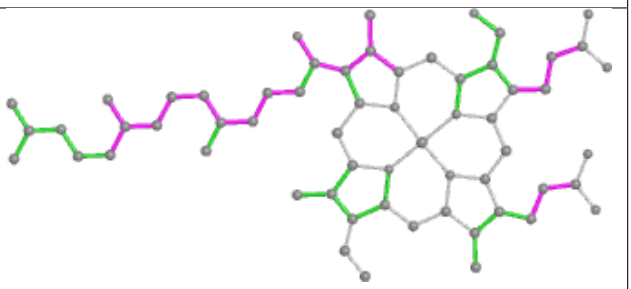
Ligand 3PE C 2008



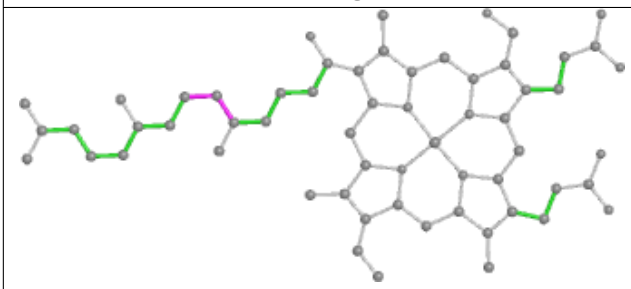
Ligand HEA G 1002



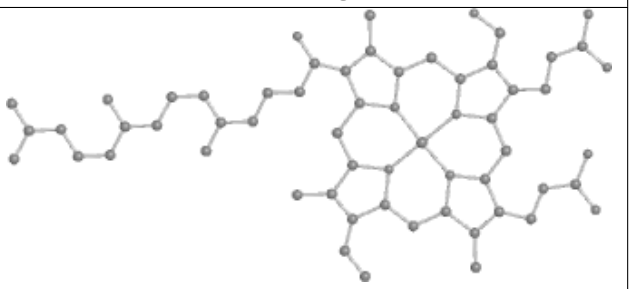
Bond lengths



Bond angles

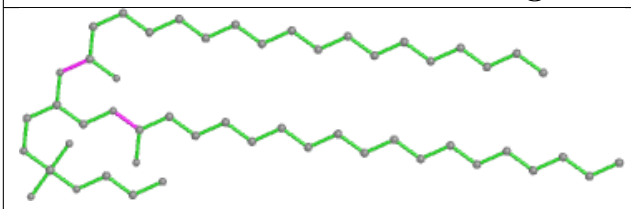


Torsions

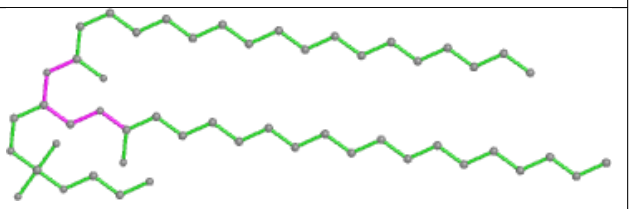


Rings

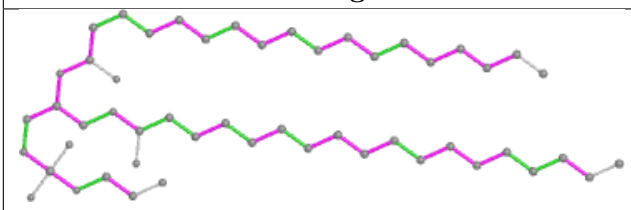
Ligand 3PE I 3008



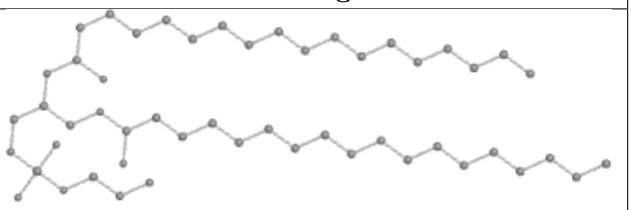
Bond lengths



Bond angles

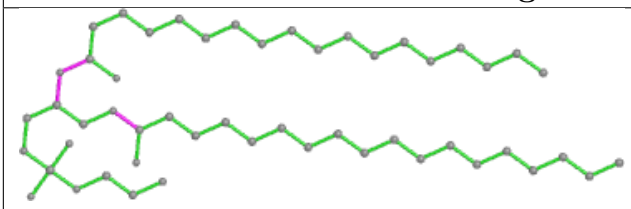


Torsions

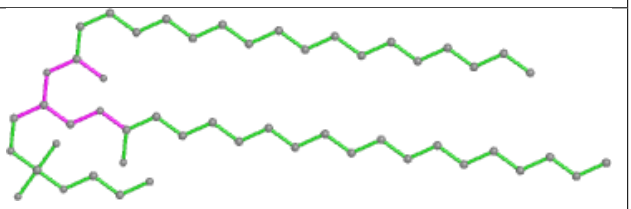


Rings

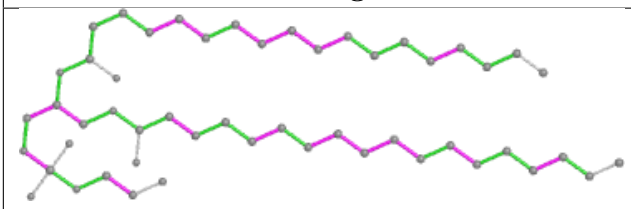
Ligand 3PE G 3012



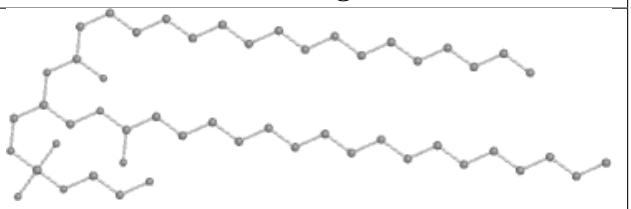
Bond lengths



Bond angles

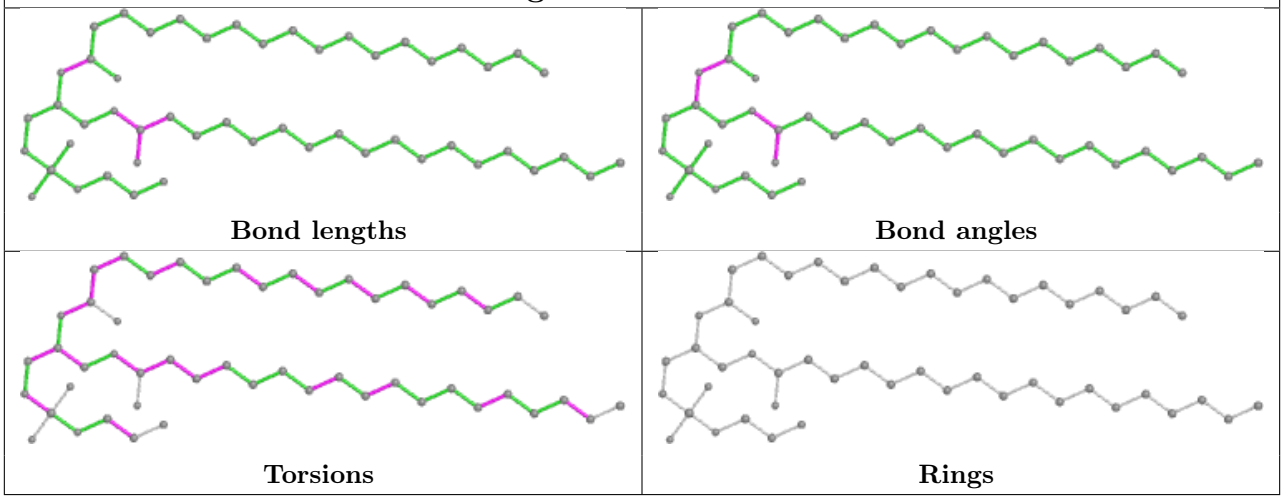


Torsions

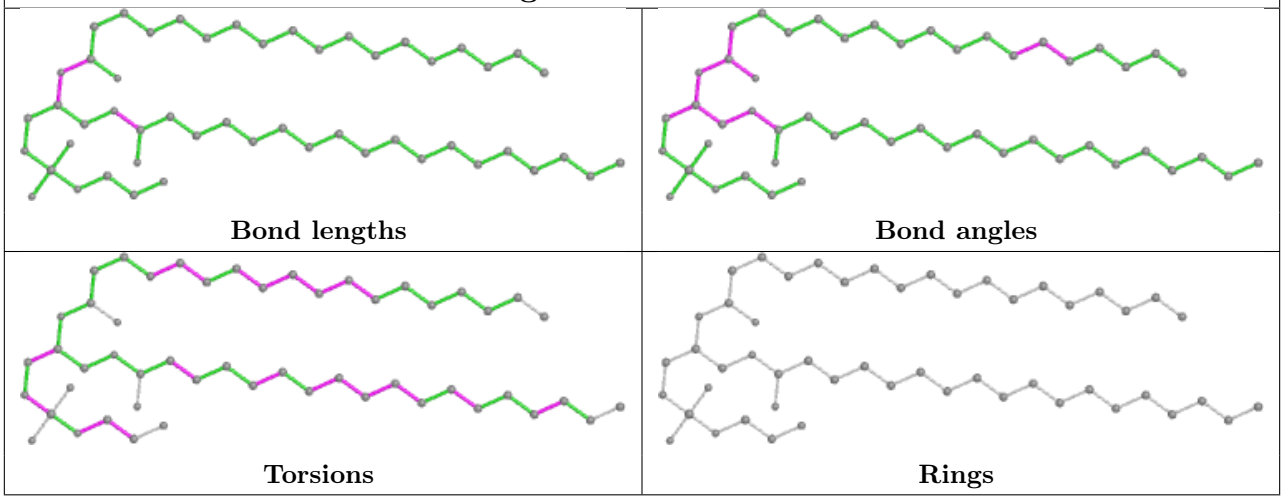


Rings

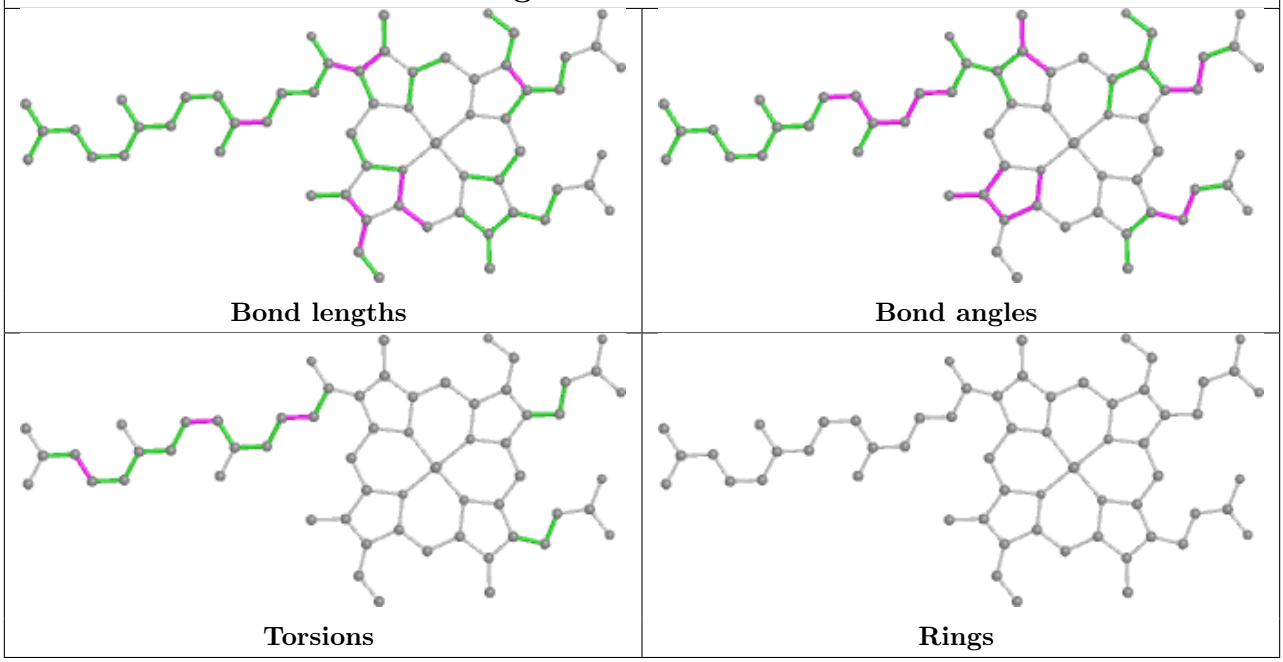
Ligand 3PE I 3010

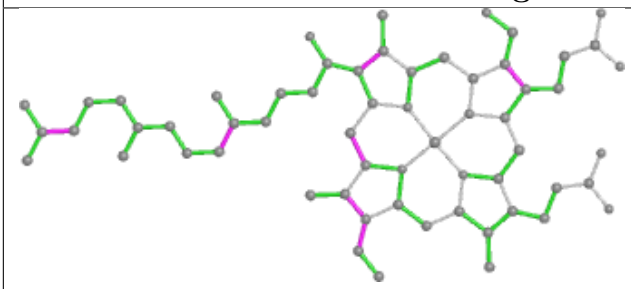
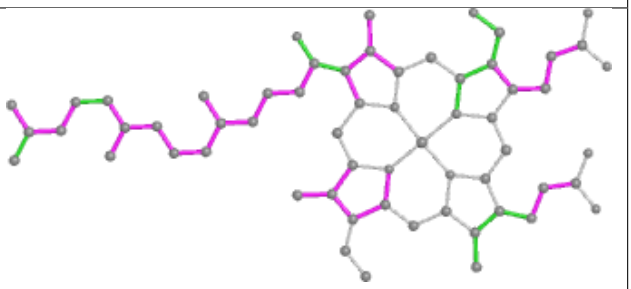
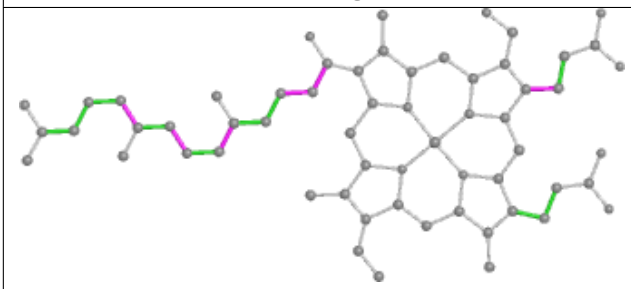
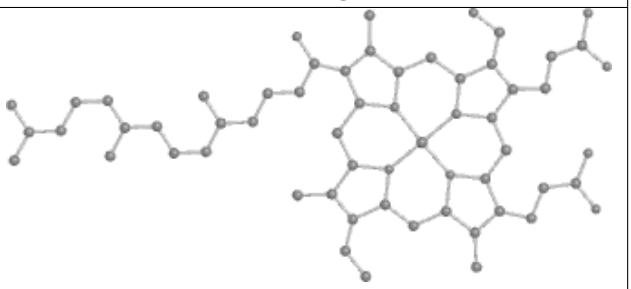


Ligand 3PE A 2012



Ligand HEA A 1002



Ligand HEA A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.