



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:25 PM EDT

PDB ID : 1MYP / pdb_00001myp
Title : X-RAY CRYSTAL STRUCTURE OF CANINE MYELOPEROXIDASE AT
3 ANGSTROMS RESOLUTION
Authors : Fenna, R.E.; Zeng, J.
Deposited on : 1992-04-15
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

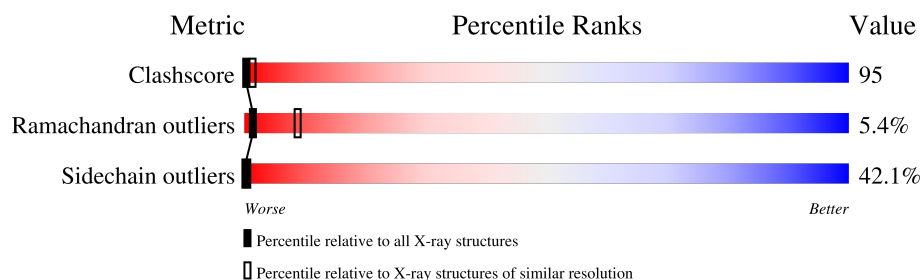
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	15% 35% 32% 14% .
1	B	108	15% 34% 29% 19% .
2	C	466	9% 37% 35% 19% .
2	D	466	12% 36% 35% 16% .
3	E	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	X	-	-	-
3	NAG	J	1	X	-	X	-
5	HEM	C	601	-	-	X	-
5	HEM	D	602	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9134 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			830	525	147	153	5			
1	B	104	Total	C	N	O	S	0	0	0
			830	525	147	153	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	462	Total	C	N	O	S	0	0	0
			3609	2289	648	647	25			
2	D	462	Total	C	N	O	S	0	0	0
			3609	2289	648	647	25			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

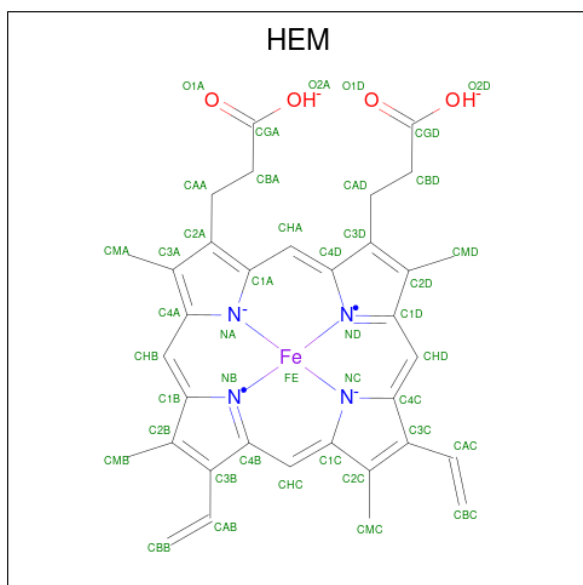
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



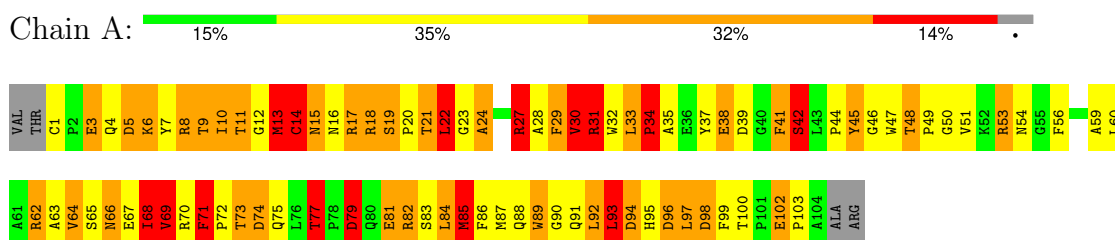
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

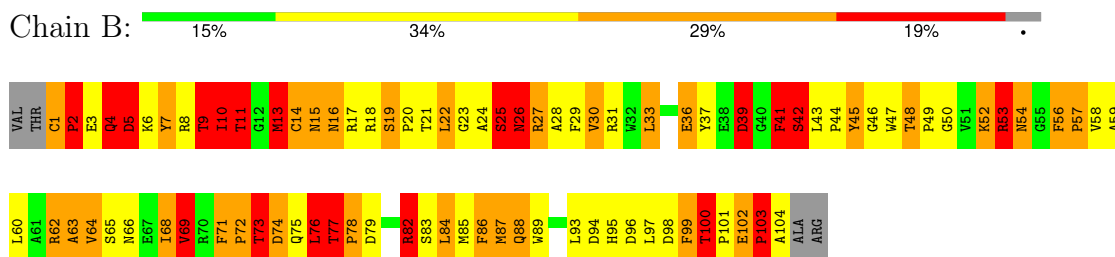
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

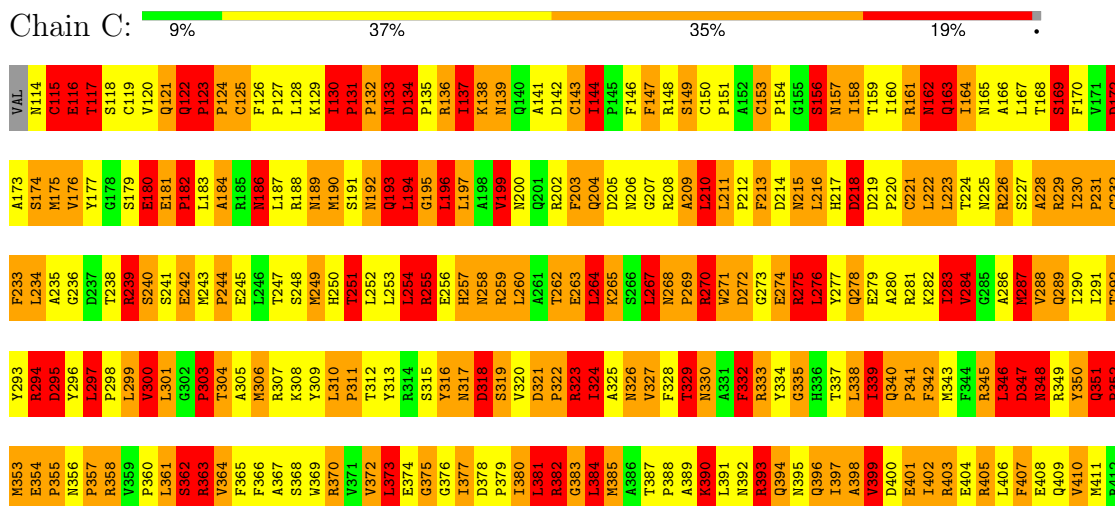
• Molecule 1: MYELOPEROXIDASE

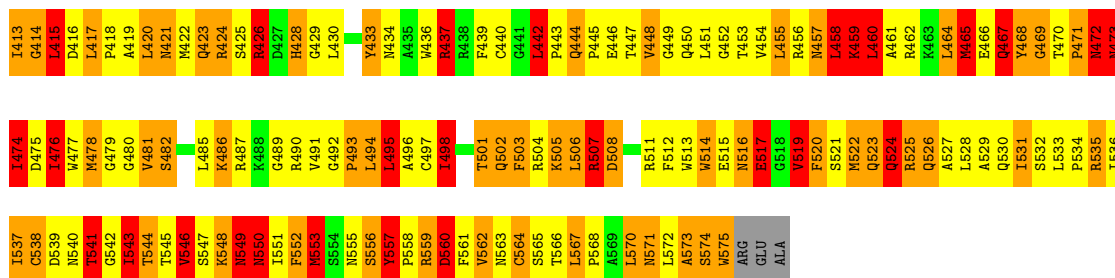


• Molecule 1: MYELOPEROXIDASE



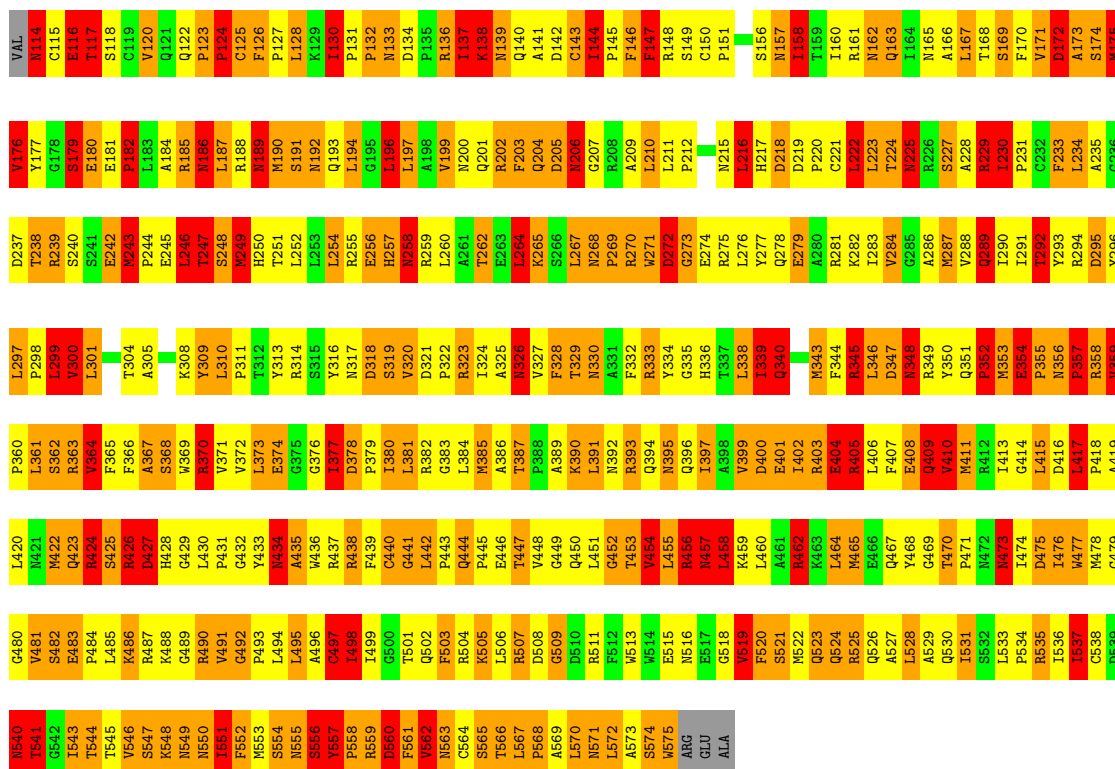
• Molecule 2: MYELOPEROXIDASE





• Molecule 2: MYELOPEROXIDASE

Chain D: 12% 36% 35% 16%



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.00Å 133.00Å 203.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.257 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	3/855 (0.4%)	2.41	57/1166 (4.9%)
1	B	1.80	13/854 (1.5%)	2.63	66/1163 (5.7%)
2	C	1.46	19/3695 (0.5%)	2.71	325/5030 (6.5%)
2	D	1.55	19/3695 (0.5%)	2.72	290/5030 (5.8%)
All	All	1.50	54/9099 (0.6%)	2.68	738/12389 (6.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	3
1	B	0	4
2	C	6	12
2	D	5	13
All	All	13	32

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	560	ASP	C-N	45.20	1.95	1.33
2	D	560	ASP	C-N	36.98	1.78	1.33
2	D	179	SER	C-N	34.10	1.81	1.33
2	C	516	ASN	C-N	32.65	1.72	1.33
2	D	203	PHE	C-N	29.20	1.74	1.33
2	C	228	ALA	C-N	24.76	1.66	1.33
2	C	347	ASP	C-N	21.29	1.63	1.33
2	D	184	ALA	C-N	21.10	1.65	1.33
2	D	574	SER	C-N	-20.58	1.04	1.33
2	D	347	ASP	C-N	18.32	1.60	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	ASP	C-N	17.94	1.59	1.33
1	B	26	ASN	C-N	17.03	1.57	1.33
2	D	557	TYR	C-N	16.75	1.73	1.33
1	B	14	CYS	CA-C	-16.50	1.30	1.52
2	D	556	SER	C-N	16.14	1.67	1.33
1	B	52	LYS	C-N	15.98	1.56	1.33
1	A	66	ASN	C-N	14.47	1.54	1.33
2	D	529	ALA	C-N	13.52	1.52	1.33
2	C	204	GLN	C-N	13.30	1.52	1.33
1	B	103	PRO	C-N	12.71	1.51	1.33
2	C	458	LEU	C-N	-12.37	1.19	1.33
1	B	101	PRO	C-N	12.14	1.52	1.32
1	B	54	ASN	C-N	11.69	1.50	1.33
1	B	53	ARG	C-N	11.68	1.49	1.33
2	D	199	VAL	C-N	-11.43	1.18	1.33
2	D	132	PRO	C-N	-11.21	1.17	1.33
2	D	275	ARG	C-N	-11.06	1.19	1.34
1	B	25	SER	C-N	10.99	1.49	1.33
2	C	522	MET	C-N	-10.02	1.21	1.33
2	D	348	ASN	C-N	9.87	1.47	1.33
2	C	133	ASN	C-N	9.52	1.51	1.33
1	B	52	LYS	CB-CG	-9.32	1.24	1.52
2	D	362	SER	C-N	8.97	1.46	1.33
2	D	348	ASN	N-CA	-8.90	1.34	1.46
2	C	517	GLU	C-N	8.47	1.45	1.33
1	B	84	LEU	C-N	8.44	1.45	1.33
2	C	350	TYR	C-N	8.41	1.50	1.33
2	C	362	SER	C-N	-8.27	1.21	1.33
1	B	4	GLN	C-N	8.21	1.45	1.33
1	A	3	GLU	C-N	8.18	1.45	1.33
2	C	346	LEU	C-N	-7.65	1.23	1.33
2	C	182	PRO	C-N	7.53	1.44	1.33
2	D	408	GLU	C-N	-7.50	1.23	1.33
2	D	354	GLU	C-N	7.48	1.51	1.33
2	C	348	ASN	C-N	-7.36	1.24	1.33
2	C	487	ARG	CB-CG	-6.92	1.31	1.52
2	C	132	PRO	C-N	6.89	1.46	1.34
2	C	180	GLU	C-N	6.63	1.47	1.33
1	A	67	GLU	C-N	-6.60	1.25	1.33
2	C	229	ARG	C-N	6.45	1.40	1.33
1	B	5	ASP	N-CA	5.53	1.52	1.46
2	D	575	TRP	NE1-CE2	-5.46	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	575	TRP	NE1-CE2	-5.43	1.31	1.37
2	D	271	TRP	NE1-CE2	-5.34	1.31	1.37

All (738) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	560	ASP	O-C-N	-25.81	88.26	122.59
2	C	560	ASP	O-C-N	-22.54	92.61	122.59
2	D	179	SER	CA-C-N	-22.20	87.73	122.59
2	D	179	SER	C-N-CA	-22.20	87.73	122.59
1	B	5	ASP	O-C-N	-20.75	99.04	123.31
2	D	202	ARG	O-C-N	-20.01	95.67	122.49
2	D	347	ASP	CA-C-N	-18.26	89.33	122.38
2	D	347	ASP	C-N-CA	-18.26	89.33	122.38
2	D	130	ILE	CA-C-N	18.22	132.78	119.66
2	D	130	ILE	C-N-CA	18.22	132.78	119.66
2	D	348	ASN	N-CA-CB	-17.63	83.46	110.44
2	C	132	PRO	CA-C-N	-17.51	99.57	123.03
2	C	132	PRO	C-N-CA	-17.51	99.57	123.03
2	D	272	ASP	CB-CA-C	-16.91	76.77	110.42
2	D	144	ILE	CB-CA-C	16.04	128.32	110.52
2	D	529	ALA	CA-C-N	-15.77	99.68	123.17
2	D	529	ALA	C-N-CA	-15.77	99.68	123.17
2	C	380	ILE	CB-CA-C	-15.20	97.00	111.44
2	D	557	TYR	CA-C-N	-15.05	101.03	119.84
2	D	557	TYR	C-N-CA	-15.05	101.03	119.84
2	C	574	SER	CA-C-N	14.84	148.41	121.70
2	C	574	SER	C-N-CA	14.84	148.41	121.70
2	D	300	VAL	N-CA-C	-14.68	96.58	110.82
2	D	356	ASN	CB-CA-C	14.67	139.06	110.17
2	C	557	TYR	CA-C-N	14.59	138.07	119.84
2	C	557	TYR	C-N-CA	14.59	138.07	119.84
2	D	348	ASN	CB-CA-C	-14.21	84.44	110.01
2	D	137	ILE	CB-CA-C	14.20	126.85	111.80
2	D	229	ARG	CB-CA-C	-14.08	89.30	111.83
2	D	357	PRO	O-C-N	-14.07	103.65	122.64
1	B	54	ASN	O-C-N	-14.05	106.92	122.09
2	C	516	ASN	CA-C-N	-13.91	96.54	122.27
2	C	516	ASN	C-N-CA	-13.91	96.54	122.27
2	C	574	SER	O-C-N	-13.79	104.25	122.59
2	D	199	VAL	O-C-N	-13.78	107.74	123.04
2	D	203	PHE	CA-C-N	-13.04	100.90	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	203	PHE	C-N-CA	-13.04	100.90	122.81
2	C	517	GLU	O-C-N	-12.83	103.35	122.08
2	D	519	VAL	N-CA-C	12.57	123.61	111.67
2	C	346	LEU	CA-C-N	12.50	141.99	120.87
2	C	346	LEU	C-N-CA	12.50	141.99	120.87
2	C	520	PHE	N-CA-C	-12.42	90.27	109.52
2	C	354	GLU	N-CA-C	12.31	137.02	109.81
1	B	30	VAL	CB-CA-C	-12.30	94.52	111.49
1	B	102	GLU	CA-C-N	-12.19	104.60	119.84
1	B	102	GLU	C-N-CA	-12.19	104.60	119.84
1	B	52	LYS	CA-C-N	-11.80	99.00	121.54
1	B	52	LYS	C-N-CA	-11.80	99.00	121.54
2	C	355	PRO	N-CA-C	-11.74	88.28	112.47
2	C	228	ALA	CA-C-N	-11.71	105.90	122.41
2	C	228	ALA	C-N-CA	-11.71	105.90	122.41
2	D	192	ASN	CB-CA-C	-11.53	88.88	110.56
2	D	143	CYS	CB-CA-C	-11.46	87.80	112.78
2	C	172	ASP	N-CA-C	-11.42	94.03	110.59
2	D	364	VAL	CB-CA-C	-11.41	99.91	110.63
2	D	179	SER	N-CA-CB	11.40	126.52	110.67
2	D	132	PRO	CA-C-N	-11.22	104.37	121.53
2	D	132	PRO	C-N-CA	-11.22	104.37	121.53
1	B	14	CYS	N-CA-CB	-10.87	92.12	110.49
2	C	122	GLN	CA-C-N	10.86	131.57	120.38
2	C	122	GLN	C-N-CA	10.86	131.57	120.38
2	C	428	HIS	CA-CB-CG	-10.81	102.99	113.80
1	A	14	CYS	N-CA-C	10.74	124.03	110.61
2	D	184	ALA	CA-C-N	-10.73	100.67	121.58
2	D	184	ALA	C-N-CA	-10.73	100.67	121.58
2	C	498	ILE	CB-CA-C	10.68	126.02	112.04
2	C	492	GLY	CA-C-N	-10.64	108.81	119.56
2	C	492	GLY	C-N-CA	-10.64	108.81	119.56
2	D	362	SER	CA-C-N	-10.55	101.40	121.54
2	D	362	SER	C-N-CA	-10.55	101.40	121.54
2	C	384	LEU	N-CA-C	-10.53	98.74	111.69
2	C	206	ASN	N-CA-C	-10.45	98.08	110.41
2	C	546	VAL	N-CA-CB	-10.43	99.15	112.60
2	D	518	GLY	CA-C-N	-10.40	110.26	122.63
2	D	518	GLY	C-N-CA	-10.40	110.26	122.63
2	D	230	ILE	O-C-N	10.38	132.93	121.10
2	D	427	ASP	CA-CB-CG	10.35	122.94	112.60
2	C	519	VAL	N-CA-C	10.34	120.85	110.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	144	ILE	CA-C-N	10.12	132.49	119.84
2	D	144	ILE	C-N-CA	10.12	132.49	119.84
2	C	218	ASP	CA-CB-CG	-10.09	102.51	112.60
2	D	395	ASN	CB-CA-C	-9.76	91.53	109.29
2	C	398	ALA	CA-C-N	-9.72	109.26	122.77
2	C	398	ALA	C-N-CA	-9.72	109.26	122.77
2	C	468	TYR	N-CA-C	9.72	124.88	112.92
1	B	50	GLY	N-CA-C	-9.69	102.16	114.37
2	C	550	ASN	N-CA-CB	9.68	126.85	110.49
1	B	13	MET	N-CA-C	9.57	125.46	111.96
1	A	66	ASN	CA-C-N	-9.54	104.27	120.58
1	A	66	ASN	C-N-CA	-9.54	104.27	120.58
2	C	180	GLU	CA-C-N	-9.53	98.54	121.80
2	C	180	GLU	C-N-CA	-9.53	98.54	121.80
2	D	168	THR	CB-CA-C	-9.53	93.47	109.48
2	D	458	LEU	N-CA-CB	9.46	126.31	110.41
1	B	45	TYR	N-CA-C	-9.43	97.20	110.50
2	C	442	LEU	CB-CA-C	9.35	124.23	109.37
2	D	415	LEU	N-CA-C	9.33	122.84	110.53
2	C	454	VAL	N-CA-C	9.30	119.84	110.82
1	B	77	THR	CB-CA-C	9.30	120.45	109.85
2	C	456	ARG	CG-CD-NE	-9.26	91.63	112.00
2	D	348	ASN	O-C-N	-9.18	109.70	122.37
2	D	199	VAL	N-CA-CB	-9.09	97.17	112.44
2	C	131	PRO	CB-CA-C	9.07	121.99	110.92
2	C	382	ARG	N-CA-CB	-9.04	96.57	110.77
2	D	179	SER	O-C-N	8.97	133.34	122.48
2	C	133	ASN	O-C-N	-8.94	108.85	122.61
2	C	350	TYR	N-CA-C	8.93	123.75	112.86
2	D	196	LEU	N-CA-CB	-8.92	96.75	111.20
2	D	462	ARG	CB-CA-C	8.85	125.48	110.79
1	B	99	PHE	CA-CB-CG	-8.83	104.97	113.80
2	C	458	LEU	CA-C-N	8.80	135.18	121.19
2	C	458	LEU	C-N-CA	8.80	135.18	121.19
1	A	89	TRP	N-CA-C	-8.79	102.73	113.97
2	C	363	ARG	CA-C-N	-8.77	111.11	122.16
2	C	363	ARG	C-N-CA	-8.77	111.11	122.16
1	A	71	PHE	N-CA-C	8.76	116.02	108.13
2	C	487	ARG	CA-CB-CG	8.76	131.62	114.10
2	D	191	SER	N-CA-C	-8.73	98.37	111.81
2	D	339	ILE	CB-CA-C	8.69	123.85	111.08
1	B	25	SER	CB-CA-C	-8.64	94.71	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	374	GLU	CA-C-N	-8.61	110.50	122.63
2	D	374	GLU	C-N-CA	-8.61	110.50	122.63
2	C	195	GLY	CA-C-O	-8.58	113.17	120.30
2	C	550	ASN	CA-CB-CG	-8.55	104.05	112.60
2	D	275	ARG	CA-C-N	8.53	132.57	120.28
2	D	275	ARG	C-N-CA	8.53	132.57	120.28
2	C	147	PHE	CB-CA-C	-8.50	96.42	110.19
1	B	76	LEU	CA-C-N	-8.47	108.62	121.83
1	B	76	LEU	C-N-CA	-8.47	108.62	121.83
2	C	130	ILE	CA-C-N	-8.46	111.66	120.38
2	C	130	ILE	C-N-CA	-8.46	111.66	120.38
1	A	39	ASP	N-CA-C	-8.46	103.47	113.88
2	D	557	TYR	CB-CA-C	-8.45	93.52	110.17
2	D	556	SER	CA-C-N	-8.43	101.23	121.80
2	D	556	SER	C-N-CA	-8.43	101.23	121.80
2	C	189	ASN	CB-CA-C	8.41	123.81	110.19
2	C	156	SER	CB-CA-C	8.39	124.72	109.37
2	C	442	LEU	N-CA-C	8.39	121.60	110.36
2	C	227	SER	CA-CB-OG	-8.37	94.36	111.10
1	B	14	CYS	CB-CA-C	8.35	127.03	110.42
1	B	14	CYS	N-CA-C	8.34	128.55	110.80
1	B	8	ARG	CB-CA-C	-8.32	92.61	109.68
2	D	141	ALA	CB-CA-C	8.31	124.97	110.01
2	D	498	ILE	CB-CA-C	8.30	122.51	111.88
1	B	78	PRO	N-CA-CB	8.30	108.79	103.23
2	C	132	PRO	O-C-N	8.30	133.47	122.27
2	C	221	CYS	CB-CA-C	8.26	126.29	110.27
2	D	227	SER	CA-C-N	8.26	137.31	121.54
2	D	227	SER	C-N-CA	8.26	137.31	121.54
2	C	540	ASN	N-CA-C	8.23	123.14	113.18
2	D	432	GLY	N-CA-C	8.22	124.74	112.41
2	C	116	GLU	N-CA-C	-8.22	102.20	112.72
2	C	557	TYR	N-CA-C	8.21	127.96	109.81
2	D	566	THR	N-CA-C	-8.21	103.77	113.21
2	D	273	GLY	O-C-N	-8.19	112.05	122.70
2	D	457	ASN	N-CA-C	8.19	121.74	107.49
2	D	139	ASN	CA-CB-CG	-8.17	104.43	112.60
2	D	538	CYS	CB-CA-C	-8.16	93.27	109.67
2	C	231	PRO	CB-CA-C	8.16	124.50	110.96
2	C	494	LEU	CA-C-N	8.15	132.70	120.31
2	C	494	LEU	C-N-CA	8.15	132.70	120.31
2	C	292	THR	N-CA-C	-8.14	103.49	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	297	LEU	CA-C-O	8.12	125.80	118.33
1	B	69	VAL	N-CA-C	8.08	120.14	111.58
2	D	320	VAL	CB-CA-C	8.07	122.41	111.19
2	C	407	PHE	CA-C-N	-8.07	109.43	122.26
2	C	407	PHE	C-N-CA	-8.07	109.43	122.26
2	C	350	TYR	CA-C-N	-8.02	102.23	121.80
2	C	350	TYR	C-N-CA	-8.02	102.23	121.80
1	A	69	VAL	N-CA-CB	7.99	123.91	110.56
2	D	561	PHE	CB-CA-C	-7.99	95.36	112.78
2	C	123	PRO	CB-CA-C	7.99	120.66	110.92
2	C	303	PRO	N-CA-C	-7.96	96.07	112.47
2	C	381	LEU	CA-C-O	7.95	129.11	120.20
2	D	525	ARG	CB-CA-C	-7.94	98.41	110.88
2	C	403	ARG	N-CA-C	-7.90	102.18	112.68
2	C	274	GLU	CA-C-N	-7.89	107.54	120.72
2	C	274	GLU	C-N-CA	-7.89	107.54	120.72
2	D	440	CYS	N-CA-CB	7.86	127.47	111.36
2	C	204	GLN	O-C-N	-7.84	113.51	122.68
2	D	222	LEU	N-CA-C	-7.82	103.76	113.38
1	A	30	VAL	CA-CB-CG2	-7.82	97.11	110.40
2	C	329	THR	CA-CB-OG1	-7.82	97.87	109.60
2	D	172	ASP	N-CA-C	-7.80	97.88	109.81
1	A	71	PHE	CB-CA-C	7.78	120.69	110.03
2	C	327	VAL	N-CA-C	7.78	117.89	110.42
2	D	246	LEU	N-CA-C	-7.77	102.81	111.28
2	C	134	ASP	CA-CB-CG	-7.73	104.87	112.60
2	C	216	LEU	N-CA-C	7.73	122.00	109.40
2	D	199	VAL	CA-C-N	7.73	131.71	120.82
2	D	199	VAL	C-N-CA	7.73	131.71	120.82
2	D	435	ALA	N-CA-C	-7.71	102.87	111.28
1	A	31	ARG	N-CA-CB	-7.68	98.35	110.87
1	B	42	SER	CB-CA-C	-7.66	95.18	110.42
2	C	276	LEU	CA-C-O	7.63	128.19	119.27
2	C	543	ILE	N-CA-C	7.63	119.58	109.21
2	D	503	PHE	N-CA-C	-7.63	103.97	113.28
1	A	4	GLN	CB-CA-C	-7.63	94.06	111.83
2	D	456	ARG	CA-C-N	7.63	132.99	121.40
2	D	456	ARG	C-N-CA	7.63	132.99	121.40
1	A	50	GLY	N-CA-C	-7.58	104.76	115.30
2	D	455	LEU	CA-C-N	-7.53	111.34	122.78
2	D	455	LEU	C-N-CA	-7.53	111.34	122.78
2	C	556	SER	N-CA-C	7.52	120.88	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	ASN	N-CA-C	-7.52	94.78	110.80
2	C	118	SER	N-CA-C	7.52	121.75	109.72
1	B	100	THR	N-CA-CB	-7.51	97.81	111.03
2	C	264	LEU	N-CA-C	-7.47	103.16	111.82
2	C	454	VAL	CB-CA-C	-7.46	102.27	112.04
2	D	202	ARG	CA-C-N	7.45	135.05	121.94
2	D	202	ARG	C-N-CA	7.45	135.05	121.94
2	C	341	PRO	CA-C-N	-7.43	110.21	122.39
2	C	341	PRO	C-N-CA	-7.43	110.21	122.39
1	A	27	ARG	N-CA-C	-7.42	98.12	109.85
2	C	227	SER	N-CA-C	7.42	120.01	111.11
2	C	383	GLY	N-CA-C	-7.41	95.61	113.18
2	D	188	ARG	N-CA-C	7.40	120.99	109.52
2	C	162	ASN	CA-CB-CG	-7.39	105.21	112.60
2	C	283	ILE	CA-C-N	-7.38	111.87	120.88
2	C	283	ILE	C-N-CA	-7.38	111.87	120.88
1	B	30	VAL	N-CA-CB	-7.36	97.78	111.91
2	D	425	SER	N-CA-C	-7.36	102.04	111.02
2	C	390	LYS	CA-C-N	-7.36	112.62	122.99
2	C	390	LYS	C-N-CA	-7.36	112.62	122.99
2	C	384	LEU	CA-C-N	7.34	133.99	121.14
2	C	384	LEU	C-N-CA	7.34	133.99	121.14
2	C	193	GLN	N-CA-C	-7.34	102.60	113.61
2	C	295	ASP	N-CA-C	7.33	121.94	112.92
1	A	64	VAL	CB-CA-C	7.32	122.05	112.24
1	A	50	GLY	CA-C-N	-7.31	113.23	122.37
1	A	50	GLY	C-N-CA	-7.31	113.23	122.37
2	C	557	TYR	N-CA-CB	7.31	123.38	110.37
2	C	227	SER	N-CA-CB	-7.31	99.05	109.94
1	A	93	LEU	CA-C-O	-7.25	113.19	120.80
2	C	324	ILE	N-CA-CB	7.25	118.43	110.53
2	D	216	LEU	N-CA-C	7.25	122.14	109.96
2	D	565	SER	N-CA-C	-7.24	105.36	114.56
2	C	156	SER	N-CA-CB	7.23	122.42	110.85
2	C	414	GLY	O-C-N	-7.22	113.31	122.70
2	C	218	ASP	CB-CG-OD1	-7.22	101.80	118.40
2	C	544	THR	CA-C-N	7.21	131.82	121.50
2	C	544	THR	C-N-CA	7.21	131.82	121.50
2	D	265	LYS	N-CA-CB	7.20	122.14	110.40
1	A	8	ARG	CB-CA-C	-7.20	94.50	110.19
2	C	115	CYS	N-CA-C	7.17	120.57	112.97
2	C	360	PRO	N-CA-CB	7.17	110.00	103.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	440	CYS	N-CA-C	-7.17	98.92	110.32
2	D	147	PHE	O-C-N	-7.16	114.31	122.68
2	C	209	ALA	N-CA-C	7.15	120.36	110.35
2	D	537	ILE	N-CA-CB	7.14	123.70	110.77
2	C	148	ARG	N-CA-C	7.13	119.94	110.53
2	C	251	THR	CB-CA-C	7.13	121.94	110.96
2	C	541	THR	CA-CB-OG1	-7.13	98.91	109.60
2	D	548	LYS	N-CA-CB	7.11	120.13	110.38
2	C	339	ILE	N-CA-C	7.11	118.75	109.58
2	D	400	ASP	CA-CB-CG	-7.11	105.49	112.60
1	B	48	THR	CA-C-N	7.11	128.72	119.84
1	B	48	THR	C-N-CA	7.11	128.72	119.84
2	C	459	LYS	O-C-N	-7.10	113.61	122.20
2	C	473	ASN	CB-CA-C	7.09	122.83	110.64
2	C	160	ILE	N-CA-CB	7.07	118.23	110.53
1	A	22	LEU	N-CA-C	7.06	120.48	109.96
2	D	199	VAL	N-CA-C	7.05	120.59	108.95
2	D	410	VAL	N-CA-C	7.05	118.04	112.12
1	A	18	ARG	CA-C-N	7.05	132.43	123.34
1	A	18	ARG	C-N-CA	7.05	132.43	123.34
2	D	196	LEU	N-CA-C	7.04	120.98	109.85
1	A	63	ALA	CA-C-N	-7.04	109.28	120.55
1	A	63	ALA	C-N-CA	-7.04	109.28	120.55
2	C	137	ILE	CB-CA-C	7.03	122.82	111.29
2	D	569	ALA	O-C-N	-7.01	115.26	123.25
2	D	551	ILE	N-CA-C	-7.01	102.29	111.05
2	D	215	ASN	N-CA-CB	-6.99	102.31	110.35
2	C	311	PRO	N-CA-C	-6.99	101.43	111.22
2	D	367	ALA	CA-C-O	-6.98	114.35	122.37
2	D	172	ASP	CA-C-N	-6.98	111.62	122.08
2	D	172	ASP	C-N-CA	-6.98	111.62	122.08
1	B	2	PRO	O-C-N	6.95	132.02	122.64
2	C	253	LEU	CB-CA-C	6.94	124.54	110.38
2	C	137	ILE	N-CA-C	6.94	123.78	109.34
1	B	48	THR	N-CA-CB	6.94	118.42	110.03
1	B	39	ASP	CB-CA-C	-6.92	100.30	110.96
2	D	447	THR	N-CA-CB	-6.92	100.43	111.43
2	C	340	GLN	OE1-CD-NE2	6.92	129.52	122.60
2	D	551	ILE	CB-CA-C	-6.91	101.44	112.16
2	D	205	ASP	N-CA-CB	6.91	120.02	110.01
1	B	9	THR	CA-CB-OG1	-6.89	99.26	109.60
2	C	119	CYS	N-CA-C	6.88	121.76	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	SER	N-CA-CB	-6.88	98.86	110.49
2	D	114	ASN	CA-CB-CG	-6.87	105.73	112.60
2	D	477	TRP	N-CA-C	6.86	119.63	111.33
2	C	505	LYS	N-CA-C	6.86	121.73	113.23
1	A	3	GLU	O-C-N	-6.86	113.47	122.59
2	C	357	PRO	N-CA-C	6.85	126.58	112.47
2	D	326	ASN	CA-CB-CG	6.85	119.45	112.60
2	C	323	ARG	O-C-N	6.84	130.65	122.85
2	D	434	ASN	CA-CB-CG	6.84	119.44	112.60
2	C	222	LEU	CA-C-O	6.83	126.65	119.14
2	C	407	PHE	O-C-N	-6.82	114.67	122.86
2	D	473	ASN	N-CA-C	6.78	120.86	112.59
1	A	29	PHE	CA-CB-CG	-6.78	107.02	113.80
2	C	517	GLU	CA-C-N	-6.78	108.13	121.41
2	C	517	GLU	C-N-CA	-6.78	108.13	121.41
2	D	535	ARG	NE-CZ-NH2	-6.77	113.10	119.20
1	B	72	PRO	N-CA-CB	6.77	110.36	103.25
2	C	257	HIS	CA-CB-CG	-6.76	107.04	113.80
2	D	547	SER	N-CA-CB	-6.75	100.03	110.29
2	C	216	LEU	CB-CA-C	6.75	122.27	109.37
2	D	564	CYS	CB-CA-C	-6.75	102.92	111.22
2	C	123	PRO	N-CA-C	6.75	118.93	110.70
2	D	358	ARG	N-CA-CB	-6.75	100.58	110.84
1	B	76	LEU	CB-CA-C	-6.73	100.35	109.71
2	C	150	CYS	O-C-N	6.73	127.44	121.18
2	D	122	GLN	O-C-N	6.70	126.63	121.88
2	C	190	MET	N-CA-CB	-6.68	101.49	111.25
2	D	424	ARG	N-CA-C	-6.67	104.09	111.82
2	C	240	SER	CA-C-N	-6.66	111.89	122.29
2	C	240	SER	C-N-CA	-6.66	111.89	122.29
2	D	117	THR	N-CA-CB	-6.65	101.44	111.15
2	D	339	ILE	N-CA-C	6.64	120.28	109.78
2	C	426	ARG	CA-C-O	6.63	127.60	119.97
2	C	407	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	98	ASP	N-CA-C	6.63	119.80	109.52
2	C	382	ARG	NE-CZ-NH2	-6.63	113.24	119.20
2	D	235	ALA	N-CA-C	6.62	117.02	108.34
2	D	407	PHE	CA-C-N	-6.62	111.85	122.24
2	D	407	PHE	C-N-CA	-6.62	111.85	122.24
2	D	516	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	15	ASN	N-CA-C	-6.59	103.58	111.69
2	D	137	ILE	N-CA-C	6.58	116.71	107.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	399	VAL	CA-C-N	6.57	129.41	120.54
2	C	399	VAL	C-N-CA	6.57	129.41	120.54
1	B	39	ASP	N-CA-C	-6.55	103.83	110.97
2	D	201	GLN	CB-CA-C	6.53	122.81	109.55
2	D	481	VAL	CA-C-N	-6.53	112.32	122.37
2	D	481	VAL	C-N-CA	-6.53	112.32	122.37
2	D	561	PHE	N-CA-C	6.52	116.85	108.24
2	D	289	GLN	CB-CA-C	-6.52	100.38	110.81
2	D	323	ARG	N-CA-CB	6.52	119.55	109.97
2	C	297	LEU	N-CA-C	6.51	122.50	113.45
2	D	556	SER	CA-C-O	-6.51	113.81	120.71
2	D	186	ASN	CA-CB-CG	6.50	119.11	112.60
2	C	312	THR	N-CA-C	6.50	118.41	110.41
1	A	45	TYR	N-CA-CB	6.50	119.81	110.06
2	D	224	THR	CA-CB-OG1	-6.50	99.86	109.60
2	D	395	ASN	OD1-CG-ND2	6.50	129.10	122.60
2	C	244	PRO	N-CA-C	-6.48	105.41	113.84
2	D	405	ARG	NE-CZ-NH1	6.48	127.98	121.50
2	D	318	ASP	CA-CB-CG	6.48	119.08	112.60
2	C	367	ALA	N-CA-C	6.46	118.28	109.11
1	B	22	LEU	N-CA-C	6.45	119.58	109.96
1	B	82	ARG	CD-NE-CZ	-6.44	115.38	124.40
2	D	498	ILE	N-CA-C	6.44	117.13	110.36
2	D	367	ALA	N-CA-C	6.43	119.75	108.56
2	C	272	ASP	N-CA-C	6.43	119.44	109.60
2	D	199	VAL	CB-CA-C	-6.42	100.78	110.55
1	A	77	THR	CA-C-O	6.42	128.95	120.16
2	D	509	GLY	O-C-N	6.41	128.35	122.19
1	B	49	PRO	CA-C-N	-6.41	114.43	123.08
1	B	49	PRO	C-N-CA	-6.41	114.43	123.08
2	C	466	GLU	CA-C-N	-6.40	111.73	120.44
2	C	466	GLU	C-N-CA	-6.40	111.73	120.44
2	C	267	LEU	N-CA-CB	6.39	119.93	110.53
2	C	346	LEU	O-C-N	-6.38	114.89	123.19
2	D	176	VAL	N-CA-CB	6.38	121.76	111.23
2	D	541	THR	N-CA-CB	6.38	120.40	109.10
2	C	458	LEU	O-C-N	-6.37	114.50	122.20
1	A	14	CYS	CA-C-O	-6.37	114.58	121.20
2	C	481	VAL	CB-CA-C	-6.36	102.31	112.16
2	C	121	GLN	CA-C-N	-6.35	106.30	121.80
2	C	121	GLN	C-N-CA	-6.35	106.30	121.80
2	C	150	CYS	CA-C-N	6.34	126.30	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	CYS	C-N-CA	6.34	126.30	120.03
2	C	516	ASN	O-C-N	6.34	130.34	122.86
2	C	284	VAL	N-CA-C	6.33	116.50	110.74
2	D	354	GLU	N-CA-C	6.32	123.78	109.81
2	C	153	CYS	CB-CA-C	6.31	118.43	110.98
1	A	79	ASP	N-CA-C	-6.29	98.29	108.41
2	C	407	PHE	CB-CA-C	-6.28	102.20	112.06
2	C	548	LYS	N-CA-C	6.28	118.81	110.53
2	D	348	ASN	CA-C-O	6.26	126.85	119.28
1	A	28	ALA	N-CA-C	6.24	118.58	110.53
2	D	549	ASN	CB-CA-C	6.23	122.82	110.42
2	C	138	LYS	N-CA-C	6.23	124.06	110.80
2	C	144	ILE	N-CA-C	-6.22	95.45	108.88
2	D	562	VAL	CB-CA-C	-6.22	101.09	111.29
2	D	483	GLU	N-CA-C	-6.21	102.05	110.36
2	D	525	ARG	CD-NE-CZ	-6.20	115.72	124.40
2	D	230	ILE	CA-C-N	-6.20	112.10	119.84
2	D	230	ILE	C-N-CA	-6.20	112.10	119.84
1	B	101	PRO	CA-C-N	-6.19	111.97	123.55
1	B	101	PRO	C-N-CA	-6.19	111.97	123.55
2	C	232	CYS	CB-CA-C	6.18	120.91	109.54
2	D	473	ASN	CB-CA-C	-6.17	101.08	111.02
2	C	559	ARG	CB-CA-C	-6.17	96.48	109.38
2	D	141	ALA	N-CA-CB	6.17	119.88	110.44
2	C	565	SER	CB-CA-C	6.16	119.37	109.02
2	D	301	LEU	N-CA-C	6.16	123.92	110.80
2	C	172	ASP	CA-C-N	-6.15	113.52	122.06
2	C	172	ASP	C-N-CA	-6.15	113.52	122.06
1	B	54	ASN	CA-C-N	6.14	133.45	121.41
1	B	54	ASN	C-N-CA	6.14	133.45	121.41
2	D	147	PHE	CA-C-N	-6.14	114.03	122.93
2	D	147	PHE	C-N-CA	-6.14	114.03	122.93
2	D	411	MET	CA-C-N	6.14	130.95	121.19
2	D	411	MET	C-N-CA	6.14	130.95	121.19
1	B	41	PHE	CA-CB-CG	6.13	119.93	113.80
2	D	218	ASP	CA-CB-CG	-6.13	106.47	112.60
2	C	520	PHE	CA-C-O	-6.12	114.28	121.44
1	B	11	THR	N-CA-CB	-6.12	101.04	110.46
2	C	153	CYS	N-CA-CB	-6.10	101.34	111.78
2	D	188	ARG	N-CA-CB	-6.10	100.93	111.55
2	D	363	ARG	CA-C-N	6.10	130.07	121.53
2	D	363	ARG	C-N-CA	6.10	130.07	121.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	328	PHE	N-CA-C	-6.10	103.94	111.75
2	D	345	ARG	CD-NE-CZ	-6.09	115.87	124.40
2	D	386	ALA	N-CA-C	6.09	120.03	112.59
2	D	182	PRO	O-C-N	-6.09	114.42	122.64
1	B	102	GLU	CB-CA-C	-6.09	100.83	109.96
2	D	407	PHE	CB-CA-C	-6.08	98.32	110.42
2	C	549	ASN	CB-CA-C	6.05	122.46	110.42
2	D	314	ARG	CB-CA-C	6.05	122.45	110.42
2	D	357	PRO	CA-C-N	6.04	131.43	122.86
2	D	357	PRO	C-N-CA	6.04	131.43	122.86
2	C	466	GLU	CB-CA-C	-6.03	97.31	109.55
2	C	421	ASN	CA-CB-CG	-6.03	106.58	112.60
2	D	521	SER	O-C-N	6.02	129.66	122.79
2	C	115	CYS	CA-C-N	-6.01	111.64	122.46
2	C	115	CYS	C-N-CA	-6.01	111.64	122.46
2	D	124	PRO	N-CA-CB	6.01	109.56	103.25
2	C	287	MET	N-CA-CB	6.01	118.95	110.12
2	C	301	LEU	CA-C-N	-6.01	112.44	121.87
2	C	301	LEU	C-N-CA	-6.01	112.44	121.87
1	B	69	VAL	CB-CA-C	5.99	119.49	111.94
2	D	520	PHE	N-CA-CB	-5.97	100.66	110.68
2	C	144	ILE	CB-CA-C	5.96	122.22	111.36
2	C	257	HIS	N-CA-CB	5.96	118.71	110.07
2	D	323	ARG	N-CA-C	5.96	119.10	110.28
2	C	317	ASN	CA-CB-CG	5.96	118.56	112.60
2	D	126	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	90	GLY	N-CA-C	-5.96	105.59	112.50
2	C	506	LEU	CA-C-N	5.95	130.52	120.88
2	C	506	LEU	C-N-CA	5.95	130.52	120.88
2	C	507	ARG	N-CA-CB	-5.95	101.32	110.07
2	D	563	ASN	CA-C-O	-5.95	114.70	121.72
2	C	517	GLU	CB-CA-C	5.94	119.17	111.50
2	D	317	ASN	OD1-CG-ND2	-5.94	116.66	122.60
2	D	404	GLU	CB-CG-CD	-5.92	102.53	112.60
1	A	69	VAL	N-CA-C	5.91	117.44	111.00
2	C	254	LEU	N-CA-C	-5.90	104.84	111.28
2	C	503	PHE	O-C-N	-5.90	115.86	122.12
2	D	225	ASN	OD1-CG-ND2	-5.90	116.70	122.60
2	D	270	ARG	CA-C-N	5.90	129.25	120.87
2	D	270	ARG	C-N-CA	5.90	129.25	120.87
2	D	538	CYS	N-CA-CB	5.90	119.19	110.33
1	A	13	MET	N-CA-C	5.90	123.37	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	440	CYS	CA-C-N	-5.89	109.86	121.41
2	C	440	CYS	C-N-CA	-5.89	109.86	121.41
2	C	372	VAL	N-CA-CB	-5.89	103.99	110.65
2	D	377	ILE	CB-CG1-CD1	-5.89	101.43	113.80
2	C	573	ALA	N-CA-C	-5.89	101.72	111.37
2	D	344	PHE	CA-CB-CG	5.89	119.69	113.80
2	C	420	LEU	CA-C-O	5.87	126.58	119.31
2	C	526	GLN	CA-C-N	-5.85	110.90	121.14
2	C	526	GLN	C-N-CA	-5.85	110.90	121.14
2	C	163	GLN	N-CA-CB	-5.85	101.84	110.85
2	C	254	LEU	CB-CA-C	-5.85	101.08	110.79
1	B	7	TYR	N-CA-C	5.84	119.19	110.14
1	A	96	ASP	CA-CB-CG	5.83	118.43	112.60
2	C	420	LEU	N-CA-C	-5.83	105.66	112.89
2	C	388	PRO	CB-CA-C	-5.82	104.24	111.64
2	D	536	ILE	N-CA-C	-5.82	104.84	110.72
2	C	549	ASN	N-CA-CB	5.82	120.33	110.49
2	D	189	ASN	CB-CA-C	-5.82	100.74	110.29
2	D	173	ALA	N-CA-C	-5.82	102.59	110.68
2	D	137	ILE	CA-CB-CG1	5.82	120.28	110.40
2	D	264	LEU	N-CA-C	-5.81	105.69	112.89
1	A	62	ARG	N-CA-CB	5.80	118.65	110.12
2	C	151	PRO	CA-N-CD	-5.80	103.88	112.00
2	C	318	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	521	SER	CA-C-N	5.77	128.81	120.38
2	D	521	SER	C-N-CA	5.77	128.81	120.38
2	D	260	LEU	N-CA-CB	5.76	118.36	110.01
2	C	410	VAL	CA-C-O	5.75	124.15	118.98
2	C	564	CYS	N-CA-C	5.75	119.37	112.93
2	C	474	ILE	CA-C-O	-5.74	114.28	121.11
2	D	367	ALA	O-C-N	5.73	129.28	122.46
2	D	367	ALA	CB-CA-C	-5.73	103.09	112.03
2	D	127	PRO	N-CA-C	5.72	121.11	111.32
2	D	233	PHE	CA-CB-CG	-5.72	108.08	113.80
2	D	140	GLN	CA-CB-CG	-5.71	102.67	114.10
2	C	456	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	C	241	SER	N-CA-C	-5.71	105.05	113.61
2	D	454	VAL	CB-CA-C	-5.70	104.40	111.70
2	C	321	ASP	CA-C-N	5.70	125.80	119.87
2	C	321	ASP	C-N-CA	5.70	125.80	119.87
2	D	300	VAL	O-C-N	5.70	129.31	121.90
2	D	354	GLU	CA-C-N	-5.70	112.72	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	354	GLU	C-N-CA	-5.70	112.72	119.84
2	C	194	LEU	N-CA-C	-5.69	101.22	109.59
2	D	116	GLU	N-CA-C	-5.68	105.69	113.30
1	B	86	PHE	CA-C-O	5.68	126.49	119.79
2	D	309	TYR	CA-CB-CG	-5.67	103.69	113.90
2	D	196	LEU	CA-C-N	-5.67	112.37	122.07
2	D	196	LEU	C-N-CA	-5.67	112.37	122.07
2	C	415	LEU	N-CA-C	5.67	122.87	110.80
2	C	437	ARG	N-CA-C	-5.67	105.24	111.82
2	D	410	VAL	O-C-N	-5.65	116.21	121.97
2	C	207	GLY	N-CA-C	-5.65	106.96	115.32
2	C	154	PRO	N-CA-C	-5.65	102.25	111.68
2	C	476	ILE	O-C-N	5.65	129.63	122.57
2	D	544	THR	N-CA-C	5.65	120.83	113.88
2	C	471	PRO	N-CA-C	-5.65	106.50	113.84
2	D	492	GLY	CA-C-N	5.65	125.76	119.32
2	D	492	GLY	C-N-CA	5.65	125.76	119.32
2	C	184	ALA	CA-C-N	5.64	132.31	121.54
2	C	184	ALA	C-N-CA	5.64	132.31	121.54
1	B	56	PHE	O-C-N	5.64	126.14	121.35
2	D	282	LYS	CA-C-N	-5.64	111.56	120.47
2	D	282	LYS	C-N-CA	-5.64	111.56	120.47
1	A	94	ASP	O-C-N	5.63	129.01	122.20
2	C	196	LEU	N-CA-C	5.63	117.67	108.55
1	A	51	VAL	CB-CA-C	5.63	117.77	110.96
2	D	299	LEU	CA-C-N	-5.62	112.71	120.74
2	D	299	LEU	C-N-CA	-5.62	112.71	120.74
2	C	136	ARG	N-CA-CB	5.61	119.98	110.49
2	D	363	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	C	495	LEU	N-CA-CB	-5.61	101.59	110.28
1	B	62	ARG	N-CA-C	-5.61	105.54	112.38
2	C	284	VAL	CB-CA-C	5.60	119.34	111.94
2	C	508	ASP	CA-CB-CG	-5.60	107.00	112.60
2	D	426	ARG	N-CA-C	5.60	117.39	111.28
2	C	472	ASN	CB-CA-C	5.60	121.59	110.17
2	C	229	ARG	CB-CA-C	-5.59	103.56	112.05
2	C	352	PRO	CA-C-N	5.59	128.77	120.95
2	C	352	PRO	C-N-CA	5.59	128.77	120.95
2	C	292	THR	CA-C-N	-5.58	112.27	121.92
2	C	292	THR	C-N-CA	-5.58	112.27	121.92
2	D	360	PRO	N-CA-CB	5.58	108.29	103.27
2	C	465	MET	CA-CB-CG	-5.58	102.95	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	191	SER	N-CA-C	-5.57	105.52	112.93
2	C	149	SER	N-CA-C	5.57	118.31	109.96
2	D	352	PRO	N-CA-CB	5.56	109.09	103.25
1	B	57	PRO	N-CA-C	-5.56	103.07	111.41
2	C	351	GLN	CB-CA-C	-5.56	99.22	110.17
1	B	41	PHE	CA-C-N	-5.56	110.92	121.54
1	B	41	PHE	C-N-CA	-5.56	110.92	121.54
2	C	173	ALA	CA-C-N	5.56	127.99	120.38
2	C	173	ALA	C-N-CA	5.56	127.99	120.38
2	C	433	TYR	CA-C-N	-5.56	112.31	121.92
2	C	433	TYR	C-N-CA	-5.56	112.31	121.92
2	D	378	ASP	CA-C-O	5.55	124.24	119.13
2	D	158	ILE	N-CA-CB	-5.55	102.08	111.23
2	C	210	LEU	CB-CA-C	5.54	120.67	110.24
2	C	176	VAL	N-CA-CB	5.54	120.55	110.86
2	C	295	ASP	N-CA-CB	5.54	118.65	110.56
2	C	143	CYS	N-CA-CB	-5.53	102.98	111.56
2	D	191	SER	O-C-N	5.53	129.44	121.97
1	A	14	CYS	CB-CA-C	5.53	120.86	111.35
2	D	497	CYS	N-CA-C	-5.52	104.95	110.97
2	C	372	VAL	N-CA-C	5.51	115.60	110.42
2	C	150	CYS	N-CA-C	5.50	119.39	109.44
2	C	380	ILE	O-C-N	5.49	126.87	121.98
2	D	309	TYR	CB-CA-C	5.49	121.59	110.38
2	C	199	VAL	CB-CA-C	-5.49	104.23	111.70
2	D	270	ARG	O-C-N	-5.49	115.29	122.59
2	D	361	LEU	CA-C-N	5.49	130.01	120.68
2	D	361	LEU	C-N-CA	5.49	130.01	120.68
1	B	82	ARG	CA-C-O	-5.48	114.91	121.11
2	D	229	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	D	475	ASP	CA-C-O	-5.48	115.17	121.19
2	D	427	ASP	CB-CA-C	5.47	121.75	110.31
2	C	313	TYR	N-CA-C	5.47	118.04	108.52
2	D	362	SER	CB-CA-C	-5.47	99.23	110.38
2	C	524	GLN	OE1-CD-NE2	5.46	128.06	122.60
2	D	138	LYS	N-CA-C	5.46	118.76	112.97
2	C	342	PHE	CB-CA-C	-5.46	100.26	113.19
2	C	355	PRO	N-CA-CB	5.45	108.98	103.25
2	C	426	ARG	N-CA-C	-5.45	105.50	111.82
2	C	553	MET	N-CA-CB	-5.45	102.60	110.56
2	D	191	SER	N-CA-CB	-5.45	103.30	111.25
1	B	46	GLY	N-CA-C	-5.44	100.28	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	374	GLU	CB-CG-CD	-5.44	103.35	112.60
2	C	210	LEU	N-CA-C	-5.44	101.49	109.81
2	D	191	SER	CA-CB-OG	-5.43	100.23	111.10
1	A	46	GLY	CA-C-N	-5.43	114.16	121.71
1	A	46	GLY	C-N-CA	-5.43	114.16	121.71
2	D	456	ARG	NE-CZ-NH2	5.43	124.09	119.20
2	D	374	GLU	CG-CD-OE1	-5.43	105.91	118.40
1	A	18	ARG	N-CA-C	5.43	120.00	112.45
2	C	271	TRP	CB-CA-C	-5.43	102.34	110.16
2	D	243	MET	CB-CA-C	-5.43	101.06	109.20
2	C	413	ILE	N-CA-C	-5.41	100.68	108.42
2	C	373	LEU	CB-CA-C	-5.41	99.89	110.11
1	B	76	LEU	N-CA-C	5.41	118.32	110.42
2	C	339	ILE	CB-CA-C	5.40	119.47	111.26
2	D	505	LYS	CB-CA-C	-5.40	100.30	110.67
2	C	229	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	C	228	ALA	O-C-N	-5.38	116.66	123.01
2	D	400	ASP	N-CA-C	5.38	118.63	111.75
2	C	300	VAL	N-CA-CB	-5.37	106.11	112.39
2	D	359	VAL	N-CA-C	5.37	114.00	107.61
2	C	523	GLN	CA-C-N	5.37	128.25	120.79
2	C	523	GLN	C-N-CA	5.37	128.25	120.79
2	D	204	GLN	CA-C-N	-5.36	113.47	120.44
2	D	204	GLN	C-N-CA	-5.36	113.47	120.44
2	C	505	LYS	CB-CA-C	-5.36	98.67	109.55
2	D	149	SER	CA-C-N	5.36	128.50	120.83
2	D	149	SER	C-N-CA	5.36	128.50	120.83
1	A	35	ALA	O-C-N	5.35	129.44	123.19
2	C	472	ASN	N-CA-C	5.35	119.43	113.01
2	D	462	ARG	CA-CB-CG	5.35	124.79	114.10
2	D	432	GLY	O-C-N	-5.34	117.81	122.88
2	D	247	THR	CA-CB-OG1	-5.34	101.59	109.60
2	C	409	GLN	CB-CA-C	5.33	120.56	109.95
2	C	557	TYR	O-C-N	-5.33	115.19	121.32
2	D	146	PHE	CB-CA-C	-5.33	101.94	110.14
2	C	215	ASN	CA-C-N	-5.32	114.96	122.94
2	C	215	ASN	C-N-CA	-5.32	114.96	122.94
2	C	460	LEU	N-CA-CB	5.32	119.22	110.39
2	D	146	PHE	N-CA-C	5.32	117.09	108.26
2	D	424	ARG	CA-C-O	5.32	126.08	119.97
2	C	308	LYS	N-CA-C	-5.31	106.93	113.41
2	D	361	LEU	CA-C-O	-5.31	112.92	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	265	LYS	N-CA-C	-5.30	106.32	112.89
2	D	292	THR	O-C-N	5.29	127.59	122.09
1	A	79	ASP	CA-CB-CG	-5.29	107.31	112.60
2	C	121	GLN	N-CA-CB	5.28	118.30	110.49
2	C	415	LEU	CA-C-O	5.28	128.06	120.51
2	D	225	ASN	CA-CB-CG	5.28	117.88	112.60
2	D	318	ASP	O-C-N	5.28	127.72	122.12
1	A	34	PRO	CA-C-N	-5.27	114.79	122.65
1	A	34	PRO	C-N-CA	-5.27	114.79	122.65
2	C	213	PHE	CA-C-N	-5.27	111.47	122.07
2	C	213	PHE	C-N-CA	-5.27	111.47	122.07
1	B	28	ALA	N-CA-C	5.27	117.34	110.43
2	D	540	ASN	CB-CA-C	5.27	119.62	110.72
2	D	158	ILE	CB-CG1-CD1	-5.27	102.74	113.80
2	C	393	ARG	CG-CD-NE	5.26	123.57	112.00
1	A	71	PHE	N-CA-CB	-5.26	106.33	111.27
2	D	140	GLN	N-CA-C	5.26	118.79	112.38
1	A	24	ALA	N-CA-C	5.25	117.11	110.33
2	C	255	ARG	NE-CZ-NH1	5.25	126.75	121.50
2	D	184	ALA	O-C-N	5.25	127.69	122.12
2	C	355	PRO	CA-C-N	5.25	134.62	121.80
2	C	355	PRO	C-N-CA	5.25	134.62	121.80
2	C	455	LEU	O-C-N	5.25	128.71	122.26
2	C	275	ARG	N-CA-CB	5.24	119.08	110.39
2	D	544	THR	N-CA-CB	-5.24	103.63	110.59
2	C	202	ARG	N-CA-CB	-5.23	101.74	110.79
2	C	186	ASN	CA-CB-CG	5.23	117.83	112.60
2	C	312	THR	CB-CA-C	5.22	121.58	110.19
2	C	467	GLN	O-C-N	5.22	127.73	122.09
2	D	552	PHE	CB-CA-C	5.22	120.28	110.63
2	D	222	LEU	CA-C-O	5.22	125.10	119.15
2	D	394	GLN	CA-C-O	5.21	125.83	119.05
2	D	556	SER	O-C-N	-5.21	116.59	123.21
2	D	559	ARG	CB-CA-C	-5.21	101.55	110.24
2	C	254	LEU	CA-C-O	5.20	126.06	120.55
2	C	284	VAL	N-CA-CB	5.20	116.88	110.64
1	A	79	ASP	O-C-N	5.18	129.15	122.93
1	B	1	CYS	CB-CA-C	-5.18	100.26	110.10
2	D	438	ARG	CB-CA-C	-5.18	102.52	110.81
2	C	496	ALA	N-CA-C	-5.18	105.72	111.36
2	C	258	ASN	CA-CB-CG	5.18	117.78	112.60
2	D	248	SER	CB-CA-C	5.18	120.21	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	VAL	N-CA-CB	5.17	116.89	111.00
2	D	456	ARG	O-C-N	5.17	129.88	123.32
1	B	53	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	C	134	ASP	CA-C-N	-5.17	113.38	119.84
2	C	134	ASP	C-N-CA	-5.17	113.38	119.84
2	D	138	LYS	N-CA-CB	-5.17	103.32	110.65
2	D	550	ASN	O-C-N	5.16	129.62	123.33
2	C	119	CYS	N-CA-CB	5.15	118.72	110.73
2	D	353	MET	N-CA-CB	5.15	119.20	110.49
2	C	322	PRO	N-CA-CB	-5.15	98.57	103.41
2	D	540	ASN	CA-C-N	-5.15	111.22	123.16
2	D	540	ASN	C-N-CA	-5.15	111.22	123.16
1	B	5	ASP	CB-CA-C	-5.14	100.39	109.70
2	C	233	PHE	CB-CA-C	-5.14	101.46	109.84
2	C	335	GLY	CA-C-O	5.14	125.26	119.09
1	B	10	ILE	N-CA-C	5.14	116.60	111.00
1	B	63	ALA	CA-C-N	-5.13	112.22	120.64
1	B	63	ALA	C-N-CA	-5.13	112.22	120.64
2	C	460	LEU	CB-CA-C	5.13	121.04	110.31
2	C	538	CYS	CA-C-O	5.13	127.81	120.16
2	C	115	CYS	N-CA-CB	5.13	117.94	110.65
2	C	552	PHE	CA-CB-CG	-5.13	108.67	113.80
2	D	565	SER	CA-C-O	5.12	124.39	118.55
1	B	76	LEU	CA-C-O	5.12	126.07	120.95
2	C	493	PRO	N-CA-CB	5.11	108.41	103.51
2	C	239	ARG	N-CA-C	5.11	116.54	109.54
2	D	249	MET	CA-CB-CG	-5.10	103.90	114.10
2	D	136	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	B	24	ALA	N-CA-C	5.09	117.76	109.86
1	A	49	PRO	N-CA-CB	5.09	108.12	102.72
1	A	68	ILE	N-CA-CB	-5.09	103.17	111.98
2	C	474	ILE	CA-CB-CG2	5.09	119.15	110.50
2	D	289	GLN	O-C-N	5.08	127.38	122.09
2	C	169	SER	N-CA-CB	-5.08	101.96	110.39
2	C	258	ASN	N-CA-C	-5.07	106.19	112.38
2	C	363	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	D	370	ARG	N-CA-CB	-5.07	102.38	109.94
2	C	190	MET	N-CA-C	5.07	119.62	111.81
2	C	357	PRO	N-CA-CB	5.06	108.57	103.25
2	C	240	SER	CA-C-O	5.06	125.92	119.95
2	D	340	GLN	CB-CA-C	5.06	116.42	108.63
2	D	376	GLY	CA-C-N	5.06	128.94	120.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	376	GLY	C-N-CA	5.06	128.94	120.64
2	C	502	GLN	N-CA-C	-5.06	105.67	111.14
2	C	375	GLY	CA-C-N	5.06	131.32	121.41
2	C	375	GLY	C-N-CA	5.06	131.32	121.41
2	C	332	PHE	N-CA-CB	5.05	118.91	110.32
1	A	97	LEU	CA-C-N	-5.05	114.66	122.59
1	A	97	LEU	C-N-CA	-5.05	114.66	122.59
2	D	217	HIS	CA-CB-CG	-5.05	108.75	113.80
2	D	435	ALA	O-C-N	5.05	127.47	122.12
2	C	226	ARG	CA-C-N	5.04	127.35	120.54
2	C	226	ARG	C-N-CA	5.04	127.35	120.54
2	D	238	THR	CA-C-N	-5.04	112.03	121.81
2	D	238	THR	C-N-CA	-5.04	112.03	121.81
2	C	147	PHE	CA-C-N	-5.04	111.80	120.97
2	C	147	PHE	C-N-CA	-5.04	111.80	120.97
1	A	70	ARG	N-CA-C	5.04	116.78	110.24
2	D	170	PHE	CA-C-N	-5.04	116.43	122.22
2	D	170	PHE	C-N-CA	-5.04	116.43	122.22
2	D	210	LEU	O-C-N	-5.03	117.43	123.27
2	D	143	CYS	O-C-N	5.03	128.50	122.72
2	C	117	THR	N-CA-CB	-5.02	101.97	110.41
2	C	315	SER	CB-CA-C	-5.02	100.44	110.42
1	A	11	THR	N-CA-C	-5.02	107.16	113.28
2	C	294	ARG	CA-C-N	-5.01	114.63	122.65
2	C	294	ARG	C-N-CA	-5.01	114.63	122.65
2	C	550	ASN	N-CA-C	-5.01	100.12	110.80
1	B	77	THR	N-CA-CB	5.01	117.33	110.01
2	D	185	ARG	CB-CA-C	5.01	119.91	109.95
2	C	349	ARG	CA-C-N	-5.00	115.19	123.05
2	C	349	ARG	C-N-CA	-5.00	115.19	123.05

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	CYS	CA
1	A	69	VAL	CA
2	C	137	ILE	CA
2	C	156	SER	CA
2	C	460	LEU	CA
2	C	472	ASN	CA
2	C	473	ASN	CA
2	C	549	ASN	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	D	123	PRO	CA
2	D	141	ALA	CA
2	D	356	ASN	CA
2	D	458	LEU	CA
2	D	549	ASN	CA

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	GLU	Mainchain
1	A	6	LYS	Mainchain
1	A	79	ASP	Sidechain
1	B	102	GLU	Mainchain
1	B	25	SER	Mainchain
1	B	5	ASP	Mainchain
1	B	54	ASN	Mainchain
2	C	122	GLN	Mainchain
2	C	133	ASN	Mainchain
2	C	180	GLU	Mainchain
2	C	182	PRO	Mainchain
2	C	203	PHE	Mainchain,Peptide
2	C	204	GLN	Mainchain
2	C	351	GLN	Mainchain
2	C	363	ARG	Mainchain
2	C	459	LYS	Mainchain
2	C	517	GLU	Mainchain
2	C	557	TYR	Peptide
2	D	114	ASN	Sidechain
2	D	182	PRO	Mainchain
2	D	185	ARG	Mainchain
2	D	230	ILE	Mainchain
2	D	348	ASN	Mainchain
2	D	355	PRO	Peptide
2	D	357	PRO	Mainchain
2	D	363	ARG	Sidechain,Mainchain
2	D	409	GLN	Mainchain
2	D	427	ASP	Sidechain
2	D	557	TYR	Sidechain
2	D	558	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	830	0	785	206	0
1	B	830	0	784	189	0
2	C	3609	0	3531	881	0
2	D	3609	0	3529	627	0
3	E	28	0	25	2	0
3	F	28	0	25	1	0
3	G	28	0	25	6	0
3	H	28	0	25	1	0
3	I	28	0	25	6	0
3	J	28	0	25	7	0
4	A	1	0	0	1	0
4	D	1	0	0	0	0
5	C	43	0	30	35	0
5	D	43	0	30	33	0
All	All	9134	0	8839	1703	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 95.

All (1703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:557:TYR:C	2:D:558:PRO:N	1.73	1.47
2:C:516:ASN:C	2:C:517:GLU:N	1.72	1.46
2:D:203:PHE:C	2:D:204:GLN:N	1.74	1.43
2:C:560:ASP:H	2:C:561:PHE:N	1.17	1.42
2:D:560:ASP:C	2:D:561:PHE:N	1.78	1.41
2:D:179:SER:C	2:D:180:GLU:N	1.81	1.36
1:B:4:GLN:NE2	1:B:17:ARG:HH22	1.26	1.29
1:B:3:GLU:O	1:B:4:GLN:HB2	1.21	1.26
2:C:243:MET:SD	5:C:601:HEM:HMC3	1.77	1.24
2:C:560:ASP:C	2:C:561:PHE:N	1.95	1.24
2:D:365:PHE:CE1	5:D:602:HEM:HBC1	1.74	1.21
2:C:560:ASP:N	2:C:561:PHE:N	1.89	1.20
1:B:3:GLU:O	1:B:4:GLN:CB	1.91	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:ASN:HA	2:C:382:ARG:HH22	1.00	1.17
1:B:94:ASP:OD2	5:D:602:HEM:HMA3	1.45	1.17
2:D:557:TYR:HB3	2:D:558:PRO:N	1.59	1.16
1:B:4:GLN:NE2	1:B:17:ARG:NH2	1.92	1.16
2:D:136:ARG:HG2	2:D:137:ILE:HG22	1.25	1.15
2:C:478:MET:HE3	2:C:478:MET:HA	1.22	1.13
2:C:544:THR:HG23	2:C:545:THR:H	1.13	1.13
2:C:244:PRO:HB2	2:C:343:MET:HE1	1.31	1.12
2:C:230:ILE:HG21	2:C:372:VAL:HG21	1.32	1.11
1:A:31:ARG:HH11	2:C:162:ASN:ND2	1.50	1.10
1:A:85:MET:HE1	2:C:533:LEU:HD21	1.23	1.09
1:A:22:LEU:HD11	2:C:323:ARG:HD2	1.29	1.08
2:C:467:GLN:HE21	2:C:467:GLN:HA	1.15	1.08
2:C:491:VAL:HG13	2:C:495:LEU:HB3	1.28	1.08
2:D:356:ASN:OD1	2:D:357:PRO:HD3	1.54	1.08
2:D:365:PHE:HE1	5:D:602:HEM:HBC1	0.92	1.07
1:B:30:VAL:HG22	2:D:323:ARG:HG3	1.36	1.07
2:D:381:LEU:HA	2:D:384:LEU:HD12	1.35	1.07
2:D:179:SER:C	2:D:180:GLU:CA	2.29	1.06
2:C:541:THR:HB	2:C:543:ILE:HD13	1.37	1.06
2:C:122:GLN:HG3	2:C:123:PRO:HD2	1.27	1.06
2:D:192:ASN:HD22	2:D:194:LEU:HB2	1.13	1.06
1:B:3:GLU:C	1:B:4:GLN:HB2	1.81	1.05
2:C:446:GLU:H	2:C:450:GLN:NE2	1.55	1.05
2:C:229:ARG:O	2:C:229:ARG:HG3	1.31	1.05
2:C:447:THR:HB	2:C:450:GLN:HG3	1.05	1.04
3:J:1:NAG:H61	3:J:2:NAG:HN2	1.15	1.04
2:D:567:LEU:HD12	2:D:568:PRO:HD2	1.40	1.04
2:C:290:ILE:HG21	2:C:531:ILE:HD11	1.38	1.04
2:C:442:LEU:HB2	2:C:443:PRO:HD2	1.37	1.04
1:A:66:ASN:HD22	2:C:403:ARG:NH1	1.54	1.03
5:C:601:HEM:HH1	5:C:601:HEM:HBB2	1.40	1.03
2:C:382:ARG:HA	2:C:385:MET:HE2	1.40	1.03
1:A:30:VAL:HG21	2:C:323:ARG:HG3	1.41	1.02
2:C:348:ASN:HA	2:C:382:ARG:NH2	1.74	1.02
2:C:534:PRO:HG3	2:C:551:ILE:HD11	1.40	1.02
2:C:434:ASN:HD21	2:C:445:PRO:HD2	1.21	1.01
1:A:6:LYS:HG3	1:A:7:TYR:CE1	1.96	1.01
1:B:30:VAL:CG2	2:D:323:ARG:HG3	1.90	1.01
1:B:79:ASP:HB2	2:D:391:LEU:HB2	1.43	1.01
2:D:447:THR:HG22	2:D:449:GLY:H	1.25	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:MET:HE1	2:D:471:PRO:HD3	1.40	1.00
2:C:136:ARG:HG3	2:C:137:ILE:HG22	1.42	1.00
1:B:30:VAL:HB	2:D:325:ALA:HA	1.43	1.00
2:D:540:ASN:N	2:D:540:ASN:HD22	1.55	1.00
2:C:415:LEU:HB3	2:C:420:LEU:HD11	1.43	1.00
1:A:99:PHE:HB3	2:C:167:LEU:HD13	1.44	1.00
1:A:77:THR:HG21	2:C:393:ARG:HD3	1.01	0.99
2:C:267:LEU:HD11	2:C:575:TRP:O	1.62	0.99
2:C:393:ARG:HG3	2:C:396:GLN:NE2	1.78	0.98
2:D:560:ASP:CA	2:D:561:PHE:N	2.26	0.98
1:A:77:THR:CG2	2:C:393:ARG:HD3	1.93	0.98
2:C:306:MET:HE3	2:C:310:LEU:HD23	1.45	0.98
2:D:136:ARG:HE	2:D:404:GLU:HB3	1.27	0.98
1:A:30:VAL:CG2	2:C:323:ARG:HG3	1.93	0.98
1:A:87:MET:HE1	2:C:243:MET:HE1	1.46	0.97
5:D:602:HEM:HHC	5:D:602:HEM:HBB2	1.43	0.97
1:A:66:ASN:ND2	2:C:403:ARG:HH12	1.61	0.97
5:C:601:HEM:HMC2	5:C:601:HEM:HBC2	1.46	0.97
1:B:4:GLN:HE21	1:B:17:ARG:HH22	0.98	0.96
2:C:447:THR:HG22	2:C:449:GLY:N	1.81	0.96
1:A:77:THR:HG21	2:C:393:ARG:CD	1.95	0.96
1:B:87:MET:SD	5:D:602:HEM:HBB1	2.05	0.96
2:D:130:ILE:HG21	2:D:137:ILE:HD11	1.43	0.96
2:C:390:LYS:HG3	2:C:391:LEU:N	1.80	0.95
2:C:516:ASN:C	2:C:517:GLU:CA	2.39	0.95
2:C:447:THR:HG22	2:C:449:GLY:H	1.26	0.95
2:C:229:ARG:O	2:C:229:ARG:CG	2.11	0.94
2:C:544:THR:HG23	2:C:545:THR:HG22	1.47	0.94
2:C:491:VAL:CG1	2:C:495:LEU:HB3	1.96	0.94
1:B:4:GLN:HE22	1:B:17:ARG:NH2	1.65	0.94
2:D:555:ASN:N	2:D:560:ASP:OD1	1.99	0.94
2:D:557:TYR:CB	2:D:558:PRO:N	2.30	0.94
2:C:221:CYS:HB3	2:C:366:PHE:HB3	1.48	0.94
2:C:177:TYR:HE2	2:C:281:ARG:HA	1.31	0.94
2:D:216:LEU:HD22	2:D:216:LEU:H	1.33	0.94
2:C:348:ASN:CA	2:C:382:ARG:HH22	1.81	0.93
2:D:267:LEU:HD12	2:D:268:ASN:ND2	1.82	0.93
2:D:348:ASN:OD1	2:D:348:ASN:N	1.94	0.93
2:D:242:GLU:OE1	5:D:602:HEM:HBC2	1.69	0.93
1:B:77:THR:HG21	2:D:393:ARG:HH11	1.31	0.92
2:D:179:SER:C	2:D:180:GLU:HA	1.94	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:541:THR:CB	2:C:543:ILE:HD13	2.00	0.92
2:C:240:SER:HB2	2:C:250:HIS:CD2	2.05	0.92
2:D:353:MET:C	2:D:355:PRO:HD2	1.95	0.92
2:C:242:GLU:OE2	5:C:601:HEM:CAC	2.18	0.91
2:C:186:ASN:C	2:C:187:LEU:HD12	1.95	0.91
2:C:303:PRO:O	2:C:306:MET:HB3	1.70	0.91
2:D:557:TYR:O	2:D:558:PRO:C	2.12	0.91
2:C:244:PRO:CB	2:C:343:MET:HE1	1.98	0.91
2:C:297:LEU:HA	2:C:300:VAL:CG1	2.00	0.91
1:B:100:THR:HG21	2:D:428:HIS:HE1	1.35	0.91
2:D:197:LEU:H	2:D:258:ASN:HD21	1.12	0.91
2:C:557:TYR:HB2	2:C:561:PHE:CE1	2.06	0.91
1:A:31:ARG:NH1	2:C:162:ASN:ND2	2.19	0.91
2:C:478:MET:HA	2:C:478:MET:CE	2.01	0.91
2:C:560:ASP:CA	2:C:561:PHE:N	2.34	0.91
2:D:556:SER:HB2	2:D:560:ASP:OD2	1.69	0.91
2:D:284:VAL:HA	2:D:287:MET:HG3	1.52	0.90
2:C:211:LEU:HD13	2:C:233:PHE:CD2	2.07	0.90
2:D:171:VAL:CG1	2:D:289:GLN:HG3	2.01	0.90
2:C:225:ASN:OD1	3:G:1:NAG:O5	1.83	0.90
1:A:13:MET:O	1:A:14:CYS:HB3	1.70	0.90
1:A:62:ARG:NH2	2:C:136:ARG:HG2	1.87	0.89
2:C:139:ASN:HD22	2:C:141:ALA:H	1.20	0.89
2:C:477:TRP:O	2:C:481:VAL:HG22	1.73	0.89
2:D:320:VAL:HG13	2:D:509:GLY:HA2	1.52	0.89
1:B:85:MET:HE1	2:D:249:MET:SD	2.13	0.89
2:D:267:LEU:HD12	2:D:268:ASN:HD21	1.32	0.89
2:C:181:GLU:N	2:C:182:PRO:CD	2.35	0.89
2:D:197:LEU:H	2:D:258:ASN:ND2	1.69	0.89
2:D:458:LEU:HD22	2:D:462:ARG:HH11	1.36	0.88
2:C:213:PHE:CE2	2:C:231:PRO:HD2	2.07	0.88
1:B:3:GLU:C	1:B:4:GLN:N	2.32	0.88
1:B:79:ASP:HB2	2:D:391:LEU:CB	2.03	0.88
1:A:85:MET:HE1	2:C:533:LEU:CD2	2.04	0.88
2:D:557:TYR:C	2:D:558:PRO:CA	2.45	0.88
2:C:350:TYR:HB2	2:C:557:TYR:CE2	2.08	0.87
2:D:365:PHE:HE1	5:D:602:HEM:CBC	1.83	0.87
2:D:385:MET:HE1	2:D:546:VAL:HA	1.56	0.87
2:D:192:ASN:ND2	2:D:194:LEU:HB2	1.89	0.87
2:D:292:THR:O	2:D:297:LEU:HD22	1.74	0.87
2:D:465:MET:CE	2:D:470:THR:HA	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:GLN:HA	2:C:467:GLN:NE2	1.77	0.87
2:D:175:MET:HB2	2:D:250:HIS:HE1	1.37	0.87
2:D:229:ARG:O	2:D:230:ILE:HD13	1.75	0.87
2:D:415:LEU:H	2:D:415:LEU:HD12	1.38	0.87
2:C:136:ARG:HH12	2:C:414:GLY:CA	1.86	0.87
2:C:342:PHE:CD1	2:C:358:ARG:HD3	2.09	0.87
1:A:27:ARG:NH2	1:B:41:PHE:HB3	1.90	0.86
2:D:203:PHE:C	2:D:204:GLN:CA	2.48	0.86
2:C:243:MET:SD	5:C:601:HEM:CMC	2.63	0.86
2:C:557:TYR:CD1	2:C:557:TYR:C	2.51	0.86
2:C:348:ASN:H	2:C:348:ASN:HD22	1.24	0.86
3:I:1:NAG:H61	3:I:2:NAG:O5	1.76	0.85
2:C:541:THR:HB	2:C:543:ILE:CD1	2.06	0.85
1:B:64:VAL:HG21	2:D:422:MET:HE1	1.58	0.85
2:D:290:ILE:HG21	2:D:531:ILE:HD11	1.59	0.84
2:C:415:LEU:H	2:C:415:LEU:HD22	1.41	0.84
1:B:103:PRO:O	1:B:104:ALA:O	1.94	0.84
2:C:122:GLN:CG	2:C:123:PRO:HD2	2.06	0.84
2:C:130:ILE:HG21	2:C:137:ILE:HD11	1.60	0.84
2:C:351:GLN:HB3	2:C:352:PRO:HD2	1.60	0.84
1:B:71:PHE:HZ	1:B:76:LEU:HD12	1.39	0.84
2:D:422:MET:O	2:D:425:SER:HB3	1.76	0.84
1:A:95:HIS:CE1	2:C:239:ARG:HE	1.96	0.84
1:B:99:PHE:HB3	2:D:167:LEU:HD13	1.57	0.84
2:C:556:SER:HB2	2:C:560:ASP:OD2	1.78	0.83
2:D:130:ILE:HD12	2:D:137:ILE:HG12	1.59	0.83
2:D:353:MET:O	2:D:355:PRO:HD2	1.77	0.83
2:D:383:GLY:O	2:D:387:THR:HG23	1.78	0.83
1:A:31:ARG:NH2	2:C:428:HIS:O	2.09	0.83
2:C:348:ASN:H	2:C:348:ASN:ND2	1.75	0.83
2:D:372:VAL:HG12	2:D:373:LEU:HD13	1.60	0.83
2:D:130:ILE:HD12	2:D:137:ILE:CG1	2.08	0.83
2:C:249:MET:HE2	2:C:381:LEU:HD11	1.58	0.83
2:C:321:ASP:OD1	2:C:323:ARG:HD3	1.79	0.83
1:B:85:MET:O	1:B:85:MET:HG3	1.76	0.82
2:D:313:TYR:CD1	2:D:507:ARG:HD3	2.14	0.82
1:A:22:LEU:CD1	2:C:323:ARG:HD2	2.08	0.82
2:C:407:PHE:CD2	2:C:415:LEU:HD23	2.13	0.82
2:C:491:VAL:HG13	2:C:495:LEU:CB	2.09	0.82
2:C:139:ASN:ND2	2:C:141:ALA:H	1.76	0.82
2:C:346:LEU:HA	2:C:353:MET:HB2	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:458:LEU:HD22	2:D:462:ARG:NH1	1.94	0.82
2:C:256:GLU:HG2	2:C:287:MET:HE3	1.62	0.82
1:A:27:ARG:HH21	1:B:41:PHE:HB3	1.45	0.82
1:A:30:VAL:HG23	2:C:324:ILE:O	1.80	0.82
2:C:291:ILE:CG2	2:C:292:THR:N	2.42	0.82
2:D:251:THR:HG23	2:D:377:ILE:HD11	1.62	0.82
1:B:56:PHE:CD2	2:D:469:GLY:HA3	2.14	0.81
2:D:177:TYR:CD2	2:D:281:ARG:HG2	2.14	0.81
2:C:291:ILE:HG23	2:C:292:THR:N	1.92	0.81
2:C:196:LEU:CD1	2:C:258:ASN:HA	2.10	0.81
2:C:519:VAL:HG23	2:C:520:PHE:N	1.92	0.81
2:C:248:SER:O	2:C:377:ILE:HD11	1.79	0.81
2:C:474:ILE:HD11	2:C:478:MET:HB3	1.60	0.81
1:B:99:PHE:HB2	2:D:167:LEU:HD22	1.60	0.81
2:C:365:PHE:HE2	2:C:406:LEU:HD12	1.45	0.81
2:C:544:THR:HG23	2:C:545:THR:N	1.96	0.81
1:A:84:LEU:HB3	2:C:384:LEU:CD2	2.10	0.81
2:C:541:THR:CB	2:C:543:ILE:CD1	2.58	0.81
2:D:528:LEU:O	2:D:531:ILE:HG23	1.80	0.81
1:A:77:THR:CG2	2:C:393:ARG:HH11	1.94	0.81
2:D:567:LEU:HD12	2:D:568:PRO:CD	2.11	0.81
1:B:94:ASP:CG	5:D:602:HEM:HMA3	2.06	0.80
2:D:557:TYR:C	2:D:558:PRO:C	2.46	0.80
2:D:559:ARG:CG	2:D:560:ASP:N	2.44	0.80
1:B:3:GLU:O	1:B:4:GLN:N	2.14	0.80
1:A:42:SER:HB2	2:C:161:ARG:HD2	1.64	0.80
2:D:175:MET:HB2	2:D:250:HIS:CE1	2.17	0.80
2:C:513:TRP:HE1	2:C:515:GLU:HB2	1.43	0.80
2:C:177:TYR:CE2	2:C:281:ARG:HA	2.15	0.80
2:C:403:ARG:O	2:C:416:ASP:HA	1.81	0.80
2:D:229:ARG:C	2:D:230:ILE:HD13	2.06	0.80
2:C:346:LEU:HD12	2:C:353:MET:H	1.47	0.79
2:C:458:LEU:HD11	2:C:462:ARG:HE	1.44	0.79
1:A:99:PHE:HA	5:C:601:HEM:O2A	1.82	0.79
2:C:446:GLU:N	2:C:450:GLN:NE2	2.29	0.79
1:A:30:VAL:HG21	2:C:323:ARG:CG	2.11	0.79
5:C:601:HEM:HBC2	5:C:601:HEM:CMC	2.10	0.79
2:C:197:LEU:H	2:C:258:ASN:ND2	1.81	0.79
2:C:350:TYR:CD1	2:C:557:TYR:HE2	2.00	0.79
1:B:97:LEU:HB3	2:D:324:ILE:CD1	2.13	0.78
2:D:177:TYR:CE2	2:D:281:ARG:HG2	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:560:ASP:O	2:D:561:PHE:N	2.14	0.78
2:C:289:GLN:HE22	2:C:513:TRP:HA	1.46	0.78
2:C:532:SER:C	2:C:534:PRO:HD2	2.08	0.78
1:B:66:ASN:HA	2:D:403:ARG:HH12	1.46	0.78
1:B:10:ILE:HG23	1:B:11:THR:HG22	1.65	0.78
2:D:430:LEU:HD13	2:D:476:ILE:HD11	1.64	0.78
1:A:99:PHE:HB2	2:C:167:LEU:HD22	1.64	0.78
1:A:77:THR:O	2:C:391:LEU:HB3	1.83	0.78
2:C:522:MET:HA	2:C:525:ARG:HD3	1.65	0.78
2:C:306:MET:CE	2:C:310:LEU:HD23	2.13	0.78
2:D:130:ILE:HG21	2:D:137:ILE:CD1	2.12	0.78
2:C:519:VAL:CG2	2:C:520:PHE:N	2.47	0.77
2:C:195:GLY:O	2:C:196:LEU:HD13	1.85	0.77
2:D:187:LEU:HD12	2:D:234:LEU:HD21	1.65	0.77
2:C:330:ASN:O	2:C:333:ARG:HG2	1.84	0.77
2:C:467:GLN:HE21	2:C:467:GLN:CA	1.84	0.77
2:D:171:VAL:HG12	2:D:289:GLN:HG3	1.67	0.77
2:D:385:MET:CE	2:D:546:VAL:HA	2.15	0.77
2:C:446:GLU:C	2:C:450:GLN:HE21	1.93	0.77
1:B:16:ASN:ND2	1:B:19:SER:H	1.82	0.77
1:B:93:LEU:HD21	2:D:503:PHE:CZ	2.20	0.77
2:C:513:TRP:NE1	2:C:515:GLU:HB2	1.99	0.77
1:B:2:PRO:HB2	1:B:4:GLN:N	2.00	0.77
2:D:346:LEU:O	2:D:382:ARG:HD2	1.85	0.77
2:C:177:TYR:HE2	2:C:281:ARG:CA	1.97	0.77
2:C:365:PHE:CE2	2:C:406:LEU:HD12	2.19	0.77
2:C:417:LEU:HB3	2:C:418:PRO:HD3	1.67	0.77
1:B:103:PRO:C	1:B:104:ALA:O	2.27	0.77
2:D:320:VAL:HG13	2:D:509:GLY:CA	2.15	0.77
2:C:136:ARG:NH1	2:C:414:GLY:O	2.18	0.77
1:B:3:GLU:O	1:B:4:GLN:CA	2.32	0.77
1:B:29:PHE:HE2	1:B:100:THR:HG23	1.50	0.77
1:B:77:THR:HG21	2:D:393:ARG:NH1	1.99	0.77
2:D:557:TYR:HB3	2:D:558:PRO:CD	2.14	0.77
2:C:211:LEU:HD13	2:C:233:PHE:CG	2.20	0.76
2:C:330:ASN:HA	2:C:333:ARG:HD3	1.67	0.76
2:C:294:ARG:HG2	2:C:295:ASP:N	1.99	0.76
2:C:306:MET:HE3	2:C:310:LEU:HB2	1.67	0.76
1:A:66:ASN:HA	2:C:403:ARG:HH12	1.48	0.76
2:C:176:VAL:HG23	2:C:177:TYR:CD1	2.21	0.76
2:C:347:ASP:N	2:C:353:MET:HG3	1.99	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:HG21	2:C:393:ARG:HH11	1.47	0.76
2:D:320:VAL:CG1	2:D:509:GLY:HA2	2.14	0.76
2:D:223:LEU:N	2:D:223:LEU:HD13	1.99	0.76
2:D:465:MET:HE3	2:D:470:THR:HA	1.67	0.76
2:C:333:ARG:HD2	5:C:601:HEM:C3A	2.21	0.76
2:D:247:THR:O	2:D:251:THR:HG22	1.86	0.76
3:G:2:NAG:O7	3:G:2:NAG:O3	2.01	0.76
2:D:381:LEU:HD12	2:D:384:LEU:CD1	2.15	0.76
1:A:102:GLU:HG2	2:C:147:PHE:HB2	1.68	0.76
2:C:407:PHE:CZ	5:C:601:HEM:HMD2	2.21	0.76
2:C:434:ASN:HB2	2:C:472:ASN:HB3	1.68	0.75
2:C:447:THR:HB	2:C:450:GLN:CG	2.01	0.75
2:D:445:PRO:O	2:D:471:PRO:HG2	1.87	0.75
2:D:118:SER:OG	2:D:120:VAL:HG12	1.87	0.75
3:J:1:NAG:O7	3:J:1:NAG:O3	2.04	0.75
2:C:289:GLN:O	2:C:292:THR:HG22	1.85	0.75
2:C:382:ARG:CA	2:C:385:MET:HE2	2.16	0.75
2:C:457:ASN:OD1	2:C:460:LEU:N	2.20	0.75
1:B:16:ASN:C	1:B:16:ASN:HD22	1.94	0.75
2:D:123:PRO:O	2:D:125:CYS:N	2.20	0.75
2:D:528:LEU:O	2:D:531:ILE:HD13	1.87	0.75
2:C:175:MET:HB2	2:C:250:HIS:HE1	1.52	0.74
1:A:22:LEU:HD11	2:C:323:ARG:CD	2.13	0.74
2:C:485:LEU:HD23	2:C:490:ARG:HD3	1.68	0.74
1:B:87:MET:HG3	1:B:88:GLN:N	2.02	0.74
2:C:447:THR:CB	2:C:450:GLN:HG3	2.01	0.74
2:C:544:THR:CG2	2:C:545:THR:H	1.94	0.74
1:A:66:ASN:ND2	2:C:403:ARG:HH22	1.85	0.74
1:A:84:LEU:HD12	2:C:389:ALA:HA	1.67	0.74
1:A:95:HIS:CD2	2:C:239:ARG:HH21	2.06	0.74
2:C:256:GLU:HG3	2:C:260:LEU:HD22	1.68	0.74
2:C:338:LEU:O	2:C:390:LYS:HB3	1.87	0.74
2:C:399:VAL:CG2	2:C:400:ASP:N	2.51	0.74
2:C:196:LEU:HD12	2:C:258:ASN:HA	1.69	0.74
1:A:29:PHE:CE1	2:C:165:ASN:HB2	2.23	0.74
1:A:96:ASP:OD1	4:A:201:CA:CA	1.64	0.74
2:C:199:VAL:HG12	2:C:209:ALA:HB1	1.70	0.74
2:C:377:ILE:HD13	2:C:381:LEU:CD2	2.18	0.74
2:C:407:PHE:HD2	2:C:415:LEU:HD23	1.53	0.74
2:D:194:LEU:HB3	2:D:196:LEU:HD22	1.69	0.74
2:D:415:LEU:HD12	2:D:415:LEU:N	2.01	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:ILE:HD11	2:D:158:ILE:HD12	1.70	0.74
2:C:229:ARG:C	2:C:230:ILE:HD13	2.13	0.73
2:D:224:THR:HG21	2:D:367:ALA:HB2	1.70	0.73
2:D:332:PHE:CE1	2:D:334:TYR:HE1	2.06	0.73
3:J:1:NAG:H61	3:J:2:NAG:N2	1.97	0.73
2:C:369:TRP:HB2	2:C:373:LEU:HD23	1.70	0.73
2:C:399:VAL:HG22	2:C:400:ASP:N	2.02	0.73
1:B:26:ASN:N	1:B:26:ASN:HD22	1.87	0.73
2:C:333:ARG:NH2	5:C:601:HEM:O1D	2.21	0.73
2:C:434:ASN:ND2	2:C:444:GLN:HB3	2.04	0.73
2:C:474:ILE:HD11	2:C:479:GLY:N	2.03	0.73
2:D:189:ASN:OD1	3:I:1:NAG:N2	2.22	0.73
2:D:278:GLN:O	2:D:281:ARG:HB2	1.89	0.73
1:A:31:ARG:NH1	2:C:326:ASN:OD1	2.21	0.73
2:C:434:ASN:ND2	2:C:445:PRO:HD2	2.01	0.73
2:C:566:THR:O	2:C:567:LEU:HD13	1.88	0.73
2:D:171:VAL:HG11	2:D:289:GLN:HG3	1.69	0.73
2:D:221:CYS:HB3	2:D:366:PHE:O	1.88	0.73
2:C:136:ARG:CZ	2:C:414:GLY:O	2.35	0.73
1:B:94:ASP:OD2	5:D:602:HEM:CMA	2.31	0.73
2:D:540:ASN:HD22	2:D:540:ASN:H	1.33	0.73
2:C:164:ILE:HD11	2:D:158:ILE:CD1	2.18	0.73
2:C:251:THR:HG23	2:C:377:ILE:HD11	1.71	0.73
2:C:252:LEU:HD11	2:C:537:ILE:HA	1.71	0.73
2:C:296:TYR:O	2:C:300:VAL:HG12	1.89	0.73
2:C:497:CYS:O	2:C:501:THR:HG23	1.88	0.73
1:B:66:ASN:HD22	2:D:403:ARG:NH1	1.87	0.73
1:A:94:ASP:OD1	5:C:601:HEM:CMA	2.37	0.73
1:B:99:PHE:CB	2:D:167:LEU:HD13	2.19	0.73
1:A:6:LYS:C	1:A:7:TYR:CD1	2.67	0.72
2:C:264:LEU:CB	2:C:276:LEU:HD11	2.19	0.72
2:C:311:PRO:O	2:C:507:ARG:NH2	2.16	0.72
2:D:335:GLY:HA2	2:D:338:LEU:HD22	1.70	0.72
1:A:15:ASN:HD21	2:C:511:ARG:H	1.37	0.72
1:A:42:SER:HB2	2:C:161:ARG:CD	2.19	0.72
1:B:64:VAL:HG21	2:D:422:MET:CE	2.20	0.72
2:C:406:LEU:HD21	5:C:601:HEM:HMD3	1.72	0.72
1:A:99:PHE:HB2	2:C:167:LEU:CD2	2.20	0.72
1:B:39:ASP:HB3	1:B:41:PHE:CD1	2.25	0.72
1:B:65:SER:HA	1:B:69:VAL:HG13	1.72	0.72
2:C:169:SER:HB3	2:C:324:ILE:HD12	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:345:ARG:NH2	2:C:374:GLU:OE1	2.23	0.71
2:D:287:MET:O	2:D:291:ILE:HG13	1.89	0.71
2:C:153:CYS:SG	2:C:156:SER:HB2	2.31	0.71
2:C:447:THR:CG2	2:C:449:GLY:H	2.02	0.71
1:B:29:PHE:CE2	1:B:100:THR:HG23	2.25	0.71
2:D:365:PHE:O	2:D:409:GLN:NE2	2.23	0.71
2:D:454:VAL:HG12	2:D:455:LEU:N	2.05	0.71
1:A:53:ARG:HD2	2:C:473:ASN:HB2	1.72	0.71
2:C:223:LEU:HD23	2:C:410:VAL:HG23	1.71	0.71
1:A:99:PHE:CB	2:C:167:LEU:HD13	2.19	0.71
1:A:9:THR:OG1	1:A:10:ILE:N	2.23	0.71
2:C:306:MET:HE3	2:C:310:LEU:CD2	2.20	0.71
2:C:423:GLN:HE21	2:C:423:GLN:HA	1.54	0.71
2:C:572:LEU:O	2:C:575:TRP:HB2	1.91	0.71
2:C:337:THR:O	2:C:390:LYS:HE3	1.91	0.71
2:C:478:MET:HE3	2:C:478:MET:CA	2.14	0.71
2:D:321:ASP:OD2	2:D:323:ARG:NH1	2.24	0.71
2:C:131:PRO:HB2	2:C:132:PRO:CD	2.20	0.71
1:A:10:ILE:HG21	2:C:181:GLU:HG3	1.70	0.70
2:C:248:SER:O	2:C:251:THR:HG23	1.91	0.70
2:C:260:LEU:O	2:C:264:LEU:HD22	1.91	0.70
1:B:15:ASN:HD21	2:D:511:ARG:H	1.37	0.70
2:D:572:LEU:HA	2:D:575:TRP:CE3	2.25	0.70
2:C:131:PRO:HD2	2:C:134:ASP:OD2	1.91	0.70
2:D:244:PRO:O	2:D:247:THR:HG22	1.91	0.70
2:C:380:ILE:O	2:C:384:LEU:HB2	1.91	0.70
2:C:415:LEU:N	2:C:415:LEU:HD13	2.06	0.70
2:D:416:ASP:HB3	2:D:419:ALA:HB3	1.74	0.70
1:A:97:LEU:HB3	2:C:324:ILE:HD11	1.73	0.70
2:C:350:TYR:CB	2:C:557:TYR:CE2	2.74	0.70
2:C:533:LEU:O	2:C:537:ILE:HG22	1.92	0.70
2:D:257:HIS:O	2:D:258:ASN:ND2	2.22	0.70
2:C:562:VAL:HG23	2:C:563:ASN:N	2.06	0.70
2:D:257:HIS:O	2:D:257:HIS:ND1	2.24	0.70
2:D:571:ASN:HD22	2:D:573:ALA:H	1.40	0.70
1:A:66:ASN:HA	2:C:403:ARG:NH1	2.07	0.70
1:B:77:THR:CG2	2:D:396:GLN:HE22	2.05	0.70
2:D:224:THR:HG23	2:D:409:GLN:OE1	1.91	0.70
1:A:29:PHE:CE2	1:A:100:THR:HG22	2.26	0.70
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.27	0.70
1:B:4:GLN:HE21	1:B:4:GLN:HA	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:350:TYR:CG	2:C:557:TYR:CE2	2.80	0.69
1:B:26:ASN:HD22	1:B:26:ASN:H	1.37	0.69
1:B:45:TYR:CE2	1:B:53:ARG:HA	2.27	0.69
2:D:428:HIS:O	2:D:430:LEU:N	2.25	0.69
2:C:128:LEU:HD12	2:C:128:LEU:N	2.07	0.69
2:C:337:THR:O	2:C:390:LYS:HG2	1.91	0.69
2:C:534:PRO:CG	2:C:551:ILE:HD11	2.21	0.69
1:B:79:ASP:OD2	2:D:490:ARG:NH1	2.25	0.69
2:D:540:ASN:N	2:D:540:ASN:ND2	2.30	0.69
2:C:130:ILE:HG21	2:C:137:ILE:CD1	2.22	0.69
2:C:333:ARG:NH1	5:C:601:HEM:HAA2	2.07	0.69
1:B:85:MET:O	1:B:85:MET:CG	2.40	0.69
2:D:130:ILE:HD11	2:D:139:ASN:O	1.92	0.69
2:C:442:LEU:H	2:C:442:LEU:HD22	1.55	0.69
2:D:557:TYR:CA	2:D:558:PRO:N	2.53	0.69
2:C:126:PHE:O	2:C:146:PHE:HB3	1.92	0.69
2:C:181:GLU:N	2:C:182:PRO:HD2	2.04	0.69
2:C:223:LEU:CD2	2:C:410:VAL:HG23	2.23	0.69
2:D:348:ASN:C	2:D:350:TYR:H	1.97	0.69
2:D:535:ARG:O	2:D:535:ARG:HG3	1.93	0.69
1:A:77:THR:HB	2:C:393:ARG:NH1	2.08	0.69
2:C:329:THR:O	5:C:601:HEM:HMA1	1.92	0.69
1:A:66:ASN:ND2	2:C:403:ARG:NH1	2.28	0.69
2:C:242:GLU:OE2	5:C:601:HEM:HAC	1.91	0.69
1:B:16:ASN:ND2	1:B:18:ARG:N	2.41	0.69
2:D:200:ASN:ND2	2:D:203:PHE:H	1.91	0.69
1:A:66:ASN:HD22	2:C:403:ARG:HH12	0.78	0.69
1:A:84:LEU:O	1:A:87:MET:N	2.26	0.69
2:C:245:GLU:OE1	2:C:343:MET:HE3	1.91	0.69
2:C:342:PHE:CE1	2:C:358:ARG:HD3	2.28	0.69
2:C:549:ASN:ND2	2:C:550:ASN:H	1.90	0.69
2:D:237:ASP:OD2	2:D:239:ARG:HG2	1.92	0.69
2:D:428:HIS:O	2:D:430:LEU:HG	1.93	0.69
5:C:601:HEM:HBB2	5:C:601:HEM:CHC	2.17	0.69
1:A:29:PHE:CZ	1:A:100:THR:HG22	2.28	0.69
1:A:68:ILE:HD12	2:C:464:LEU:HD13	1.75	0.69
1:B:5:ASP:OD1	1:B:5:ASP:N	2.26	0.69
1:B:71:PHE:CZ	1:B:76:LEU:HD12	2.25	0.69
2:D:415:LEU:H	2:D:415:LEU:CD1	2.06	0.69
2:C:309:TYR:O	2:C:311:PRO:HD2	1.92	0.68
2:C:321:ASP:CG	2:C:323:ARG:HD3	2.18	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:HB2	2:C:126:PHE:CZ	2.29	0.68
2:C:385:MET:HE1	2:C:537:ILE:HD11	1.75	0.68
2:C:197:LEU:N	2:C:258:ASN:HD21	1.92	0.68
2:C:335:GLY:HA2	2:C:338:LEU:HD22	1.75	0.68
2:D:251:THR:O	2:D:255:ARG:HG3	1.91	0.68
1:A:99:PHE:CD1	2:C:239:ARG:NH1	2.62	0.68
2:D:392:ASN:OD1	2:D:392:ASN:C	2.35	0.68
2:C:200:ASN:HD21	2:C:213:PHE:HE1	1.40	0.68
2:C:370:ARG:HG3	2:C:374:GLU:OE1	1.93	0.68
2:C:197:LEU:N	2:C:258:ASN:ND2	2.41	0.68
2:C:434:ASN:HB2	2:C:472:ASN:CB	2.23	0.68
2:D:565:SER:C	2:D:567:LEU:H	1.99	0.68
1:A:5:ASP:OD1	1:A:5:ASP:N	2.25	0.68
1:A:87:MET:HE1	2:C:243:MET:CE	2.21	0.68
2:C:139:ASN:HD22	2:C:139:ASN:C	2.02	0.68
2:C:248:SER:OG	2:C:381:LEU:HD22	1.94	0.68
2:C:262:THR:O	2:C:265:LYS:HB3	1.93	0.68
1:B:66:ASN:HD22	2:D:403:ARG:HH12	1.40	0.67
2:C:136:ARG:NH2	2:C:414:GLY:O	2.27	0.67
2:C:350:TYR:CD2	2:C:557:TYR:HD2	2.13	0.67
1:A:94:ASP:OD1	5:C:601:HEM:HMA3	1.94	0.67
2:C:434:ASN:HD22	2:C:444:GLN:HB3	1.59	0.67
2:C:229:ARG:O	2:C:231:PRO:HD3	1.93	0.67
2:C:330:ASN:HD22	2:C:333:ARG:HD3	1.59	0.67
2:C:368:SER:O	2:C:372:VAL:HG23	1.94	0.67
2:D:242:GLU:OE1	5:D:602:HEM:CBC	2.42	0.67
2:D:251:THR:HG23	2:D:377:ILE:CD1	2.25	0.67
2:D:521:SER:O	2:D:525:ARG:HG2	1.94	0.67
2:C:228:ALA:HB2	3:G:1:NAG:H61	1.75	0.67
1:A:30:VAL:HG22	2:C:323:ARG:HG3	1.76	0.67
2:C:164:ILE:CD1	2:D:158:ILE:HD12	2.25	0.67
2:C:193:GLN:NE2	2:C:273:GLY:H	1.91	0.67
2:C:345:ARG:HA	2:C:379:PRO:O	1.94	0.67
1:A:77:THR:CB	2:C:393:ARG:HH11	2.07	0.67
2:D:362:SER:HA	2:D:365:PHE:CE2	2.29	0.67
1:B:94:ASP:OD1	5:D:602:HEM:HMA2	1.95	0.67
2:C:123:PRO:HB2	2:C:124:PRO:HD3	1.76	0.67
1:A:71:PHE:HD1	1:A:72:PRO:HD2	1.59	0.66
2:C:142:ASP:OD1	2:C:143:CYS:N	2.28	0.66
2:D:434:ASN:ND2	2:D:444:GLN:HB3	2.09	0.66
2:D:465:MET:HE1	2:D:471:PRO:CD	2.21	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:THR:O	2:C:307:ARG:N	2.27	0.66
1:A:7:TYR:CD2	2:C:278:GLN:HB3	2.30	0.66
2:C:415:LEU:H	2:C:415:LEU:CD2	2.00	0.66
2:D:256:GLU:OE2	2:D:259:ARG:HD3	1.95	0.66
1:A:16:ASN:HD22	1:A:19:SER:H	1.41	0.66
2:C:297:LEU:HA	2:C:300:VAL:HG11	1.76	0.66
2:C:114:ASN:OD1	2:C:115:CYS:N	2.29	0.66
2:C:282:LYS:HB3	2:C:520:PHE:HZ	1.60	0.66
1:B:19:SER:HB3	1:B:22:LEU:HD13	1.77	0.66
1:B:44:PRO:HD3	2:D:148:ARG:NH2	2.11	0.66
2:D:197:LEU:N	2:D:258:ASN:HD21	1.89	0.66
1:A:98:ASP:C	2:C:167:LEU:HD22	2.21	0.66
2:D:347:ASP:O	2:D:382:ARG:HD3	1.96	0.66
1:A:84:LEU:O	1:A:86:PHE:N	2.29	0.66
2:C:370:ARG:NE	2:C:374:GLU:OE1	2.27	0.66
1:B:3:GLU:N	1:B:4:GLN:N	2.42	0.66
2:D:492:GLY:O	2:D:496:ALA:HB2	1.96	0.66
2:C:123:PRO:O	2:C:124:PRO:C	2.35	0.66
2:C:196:LEU:HD11	2:C:258:ASN:HA	1.77	0.66
2:C:325:ALA:H	2:C:502:GLN:HE22	1.42	0.65
2:C:442:LEU:HB2	2:C:443:PRO:CD	2.22	0.65
2:C:393:ARG:CG	2:C:396:GLN:NE2	2.58	0.65
1:B:45:TYR:HE2	1:B:53:ARG:HA	1.59	0.65
2:D:385:MET:HE3	2:D:547:SER:H	1.60	0.65
1:B:97:LEU:HB3	2:D:324:ILE:HD11	1.77	0.65
2:D:381:LEU:HD12	2:D:384:LEU:HD12	1.77	0.65
2:D:406:LEU:HD21	5:D:602:HEM:HMD3	1.77	0.65
1:A:97:LEU:HB3	2:C:324:ILE:CD1	2.27	0.65
2:D:523:GLN:H	2:D:523:GLN:HE21	1.44	0.65
2:D:523:GLN:HE21	2:D:523:GLN:N	1.94	0.65
1:B:94:ASP:OD1	5:D:602:HEM:CMA	2.45	0.65
1:A:85:MET:CE	2:C:533:LEU:HD21	2.14	0.65
2:C:350:TYR:CD1	2:C:557:TYR:CE2	2.84	0.65
2:C:350:TYR:CG	2:C:557:TYR:CD2	2.85	0.65
2:C:378:ASP:HB2	2:C:379:PRO:HD3	1.79	0.65
2:C:254:LEU:O	2:C:254:LEU:HG	1.88	0.65
2:C:434:ASN:HD21	2:C:445:PRO:CD	2.02	0.65
2:D:311:PRO:O	2:D:507:ARG:NH2	2.30	0.65
2:C:404:GLU:O	2:C:405:ARG:HD3	1.96	0.65
2:C:507:ARG:HD2	2:C:508:ASP:OD1	1.97	0.65
2:D:347:ASP:OD1	2:D:351:GLN:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2:NAG:O7	3:I:2:NAG:O3	2.08	0.65
1:A:31:ARG:NH1	2:C:162:ASN:HD22	1.92	0.64
2:C:144:ILE:CD1	2:C:416:ASP:H	2.11	0.64
2:C:244:PRO:CG	2:C:343:MET:HE1	2.26	0.64
1:A:31:ARG:HH11	2:C:162:ASN:HD21	1.44	0.64
1:A:92:LEU:HD13	2:C:175:MET:HE3	1.80	0.64
2:C:221:CYS:CB	2:C:366:PHE:HB3	2.25	0.64
1:A:71:PHE:CD2	2:C:396:GLN:HA	2.33	0.64
2:C:556:SER:O	2:C:561:PHE:CE1	2.50	0.64
2:D:405:ARG:CG	2:D:405:ARG:HH11	2.10	0.64
2:C:433:TYR:CD1	2:C:494:LEU:HD22	2.33	0.64
2:D:479:GLY:O	2:D:483:GLU:HG3	1.96	0.64
2:C:516:ASN:C	2:C:517:GLU:HA	2.22	0.64
2:D:220:PRO:HA	2:D:223:LEU:HD22	1.79	0.64
2:D:244:PRO:HB2	2:D:343:MET:HE3	1.78	0.64
1:A:66:ASN:ND2	2:C:403:ARG:NH2	2.46	0.64
1:A:87:MET:SD	2:C:339:ILE:HG22	2.38	0.64
2:D:216:LEU:HD22	2:D:216:LEU:N	2.08	0.64
2:D:345:ARG:HH22	2:D:374:GLU:CD	2.06	0.64
1:A:10:ILE:HG21	2:C:181:GLU:CG	2.27	0.64
1:B:4:GLN:HE21	1:B:17:ARG:NH2	1.73	0.64
2:C:346:LEU:CA	2:C:353:MET:HB2	2.27	0.63
2:C:383:GLY:O	2:C:387:THR:HG22	1.98	0.63
1:B:13:MET:HG3	1:B:14:CYS:N	1.97	0.63
2:D:406:LEU:HD11	5:D:602:HEM:HAC	1.79	0.63
2:D:546:VAL:HG13	2:D:547:SER:N	2.13	0.63
2:C:177:TYR:OH	2:C:284:VAL:HG11	1.98	0.63
2:C:364:VAL:HG13	2:C:364:VAL:O	1.98	0.63
1:B:15:ASN:O	2:D:511:ARG:NE	2.26	0.63
2:D:362:SER:O	2:D:409:GLN:HG2	1.99	0.63
2:C:240:SER:HB2	2:C:250:HIS:HD2	1.62	0.63
2:C:382:ARG:HB2	2:C:385:MET:CE	2.28	0.63
1:B:16:ASN:HD21	1:B:19:SER:H	1.45	0.63
1:B:88:GLN:HA	1:B:88:GLN:OE1	1.98	0.63
2:D:453:THR:HG22	2:D:454:VAL:N	2.11	0.63
2:C:405:ARG:HG3	2:C:408:GLU:CD	2.23	0.63
1:B:4:GLN:NE2	1:B:4:GLN:HA	2.12	0.63
2:C:144:ILE:HD12	2:C:416:ASP:H	1.62	0.63
2:C:220:PRO:HB3	2:C:410:VAL:HG21	1.79	0.63
2:C:527:ALA:O	2:C:530:GLN:HB2	1.98	0.63
2:D:165:ASN:HD22	2:D:166:ALA:N	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:428:HIS:N	2:C:428:HIS:CD2	2.63	0.63
2:D:465:MET:CE	2:D:471:PRO:HD3	2.21	0.63
2:C:256:GLU:OE2	2:C:260:LEU:HD11	1.98	0.63
2:C:291:ILE:HD11	2:C:533:LEU:HB2	1.80	0.63
2:C:535:ARG:HD2	2:C:568:PRO:O	1.99	0.63
2:D:313:TYR:HD1	2:D:507:ARG:HD3	1.62	0.63
1:A:30:VAL:HG13	2:C:323:ARG:CZ	2.29	0.63
1:A:7:TYR:CE1	2:C:279:GLU:OE2	2.52	0.62
2:D:171:VAL:HG12	2:D:171:VAL:O	1.98	0.62
1:A:59:ALA:O	2:C:426:ARG:NH2	2.32	0.62
2:C:251:THR:O	2:C:254:LEU:HB3	1.98	0.62
1:B:33:LEU:HD22	2:D:436:TRP:CZ3	2.35	0.62
2:D:132:PRO:HD2	2:D:133:ASN:OD1	2.00	0.62
2:D:200:ASN:ND2	2:D:203:PHE:N	2.47	0.62
1:B:9:THR:HG21	1:B:13:MET:H	1.65	0.62
2:D:242:GLU:OE2	5:D:602:HEM:C3C	2.52	0.62
2:D:364:VAL:HG23	2:D:364:VAL:O	1.95	0.62
2:D:406:LEU:CD1	5:D:602:HEM:HAC	2.29	0.62
2:D:434:ASN:HD21	2:D:445:PRO:HD2	1.64	0.62
2:C:264:LEU:HB3	2:C:276:LEU:HD11	1.79	0.62
2:C:458:LEU:CD1	2:C:462:ARG:HE	2.10	0.62
2:D:192:ASN:ND2	2:D:194:LEU:HD22	2.14	0.62
2:D:445:PRO:CG	2:D:451:LEU:HD13	2.29	0.62
2:C:283:ILE:O	2:C:287:MET:HG2	2.00	0.62
1:B:29:PHE:HE2	1:B:100:THR:CG2	2.12	0.62
2:D:355:PRO:O	2:D:356:ASN:HB2	1.98	0.62
2:D:390:LYS:HG3	2:D:390:LYS:O	1.97	0.62
2:D:570:LEU:HD23	2:D:571:ASN:H	1.64	0.62
1:A:99:PHE:CB	2:C:167:LEU:HD22	2.29	0.62
2:C:544:THR:CG2	2:C:545:THR:HG22	2.27	0.62
2:D:136:ARG:HE	2:D:404:GLU:CB	2.07	0.62
2:D:519:VAL:CG2	2:D:520:PHE:N	2.62	0.62
2:C:557:TYR:HB2	2:C:561:PHE:CD1	2.34	0.62
1:B:13:MET:O	1:B:20:PRO:O	2.17	0.62
2:C:303:PRO:O	2:C:306:MET:CB	2.46	0.62
2:C:303:PRO:HD2	2:C:304:THR:HG22	1.82	0.62
2:D:326:ASN:HD21	2:D:428:HIS:HB3	1.64	0.62
2:C:131:PRO:HB2	2:C:132:PRO:HD2	1.82	0.61
2:C:264:LEU:HB2	2:C:276:LEU:HD11	1.80	0.61
1:B:71:PHE:CD2	2:D:396:GLN:HB3	2.35	0.61
2:D:219:ASP:HB3	2:D:222:LEU:HD23	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PHE:HB2	2:D:167:LEU:CD2	2.30	0.61
2:C:407:PHE:HD2	2:C:415:LEU:CD2	2.12	0.61
1:B:53:ARG:N	1:B:56:PHE:O	2.33	0.61
2:C:548:LYS:CG	2:C:560:ASP:O	2.47	0.61
2:C:290:ILE:HD12	2:C:514:TRP:CZ2	2.36	0.61
2:C:430:LEU:CD1	2:C:476:ILE:HD11	2.30	0.61
2:C:501:THR:O	2:C:505:LYS:HG3	2.00	0.61
1:B:79:ASP:OD2	1:B:82:ARG:HB2	2.01	0.61
2:D:544:THR:HG23	2:D:545:THR:HG23	1.81	0.61
2:C:269:PRO:O	2:C:271:TRP:N	2.34	0.61
2:C:393:ARG:HG3	2:C:396:GLN:HE21	1.62	0.61
2:C:468:TYR:O	2:C:470:THR:N	2.32	0.61
1:B:36:GLU:CD	2:D:431:PRO:HB3	2.25	0.61
1:B:94:ASP:CG	5:D:602:HEM:CMA	2.73	0.61
2:C:262:THR:HG22	2:C:263:GLU:N	2.16	0.61
1:B:98:ASP:OD1	5:D:602:HEM:HBA1	2.01	0.61
2:C:361:LEU:HB2	2:C:401:GLU:HG2	1.82	0.60
2:D:524:GLN:HG2	2:D:575:TRP:CE2	2.36	0.60
2:D:533:LEU:O	2:D:537:ILE:HG23	2.00	0.60
2:C:251:THR:HG23	2:C:377:ILE:CD1	2.31	0.60
2:C:350:TYR:CB	2:C:557:TYR:CD2	2.84	0.60
2:C:490:ARG:O	2:C:491:VAL:HG23	2.02	0.60
1:A:81:GLU:C	1:A:82:ARG:HG2	2.26	0.60
2:D:187:LEU:CD1	2:D:234:LEU:HD21	2.31	0.60
2:C:121:GLN:HG3	2:C:127:PRO:HD2	1.84	0.60
2:C:345:ARG:C	2:C:346:LEU:HD13	2.26	0.60
2:C:350:TYR:CG	2:C:557:TYR:HE2	2.20	0.60
1:B:30:VAL:HG12	1:B:31:ARG:N	2.14	0.60
2:C:300:VAL:HG22	2:C:300:VAL:O	2.00	0.60
2:C:380:ILE:C	2:C:382:ARG:N	2.56	0.60
2:C:524:GLN:CA	2:C:524:GLN:HE21	2.13	0.60
2:D:128:LEU:CB	2:D:144:ILE:HG12	2.30	0.60
2:D:248:SER:HA	2:D:251:THR:HG22	1.82	0.60
2:D:405:ARG:HH11	2:D:405:ARG:HG3	1.67	0.60
1:A:85:MET:HE3	2:C:249:MET:HE1	1.84	0.60
2:C:181:GLU:N	2:C:182:PRO:HD3	2.14	0.60
2:D:179:SER:CA	2:D:180:GLU:N	2.63	0.60
2:C:543:ILE:HD13	2:C:543:ILE:H	1.66	0.60
2:D:138:LYS:O	2:D:138:LYS:HG2	2.00	0.60
2:D:415:LEU:HD23	2:D:420:LEU:HD21	1.83	0.60
1:A:65:SER:O	2:C:403:ARG:NH1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:ASN:O	2:C:187:LEU:HD12	2.01	0.60
2:C:365:PHE:HE2	2:C:406:LEU:CD1	2.13	0.60
2:C:480:GLY:C	2:C:495:LEU:HD22	2.27	0.60
2:D:165:ASN:HD22	2:D:165:ASN:C	2.10	0.60
2:C:183:LEU:CD1	2:C:187:LEU:HD11	2.32	0.59
2:C:418:PRO:HB3	2:C:477:TRP:CH2	2.37	0.59
2:C:220:PRO:O	2:C:223:LEU:HB2	2.02	0.59
2:C:309:TYR:O	2:C:310:LEU:HD13	2.02	0.59
1:B:1:CYS:O	1:B:2:PRO:O	2.20	0.59
1:B:100:THR:HG21	2:D:428:HIS:CE1	2.27	0.59
2:C:136:ARG:HH12	2:C:414:GLY:N	2.00	0.59
2:D:256:GLU:OE2	2:D:259:ARG:NH1	2.33	0.59
2:D:267:LEU:O	2:D:269:PRO:HD3	2.02	0.59
2:D:332:PHE:HE1	2:D:334:TYR:HE1	1.50	0.59
1:A:53:ARG:HD2	2:C:473:ASN:CB	2.32	0.59
2:D:478:MET:O	2:D:482:SER:HB3	2.02	0.59
2:D:497:CYS:O	2:D:501:THR:OG1	2.16	0.59
2:C:193:GLN:HE22	2:C:273:GLY:H	1.48	0.59
1:B:16:ASN:HD21	1:B:18:ARG:N	1.99	0.59
2:C:345:ARG:HH22	2:C:374:GLU:CD	2.11	0.59
2:C:533:LEU:N	2:C:534:PRO:CD	2.66	0.59
1:B:62:ARG:NH2	2:D:134:ASP:OD2	2.33	0.59
2:D:362:SER:HA	2:D:365:PHE:HE2	1.68	0.59
2:D:545:THR:HG22	2:D:563:ASN:HA	1.85	0.59
1:A:75:GLN:O	2:C:396:GLN:OE1	2.20	0.59
2:C:229:ARG:O	2:C:230:ILE:HD13	2.02	0.59
2:C:375:GLY:O	2:C:379:PRO:HG2	2.03	0.59
2:C:458:LEU:HD11	2:C:462:ARG:NE	2.16	0.59
1:B:83:SER:OG	2:D:551:ILE:O	2.17	0.59
2:D:336:HIS:NE2	5:D:602:HEM:NB	2.51	0.59
2:C:327:VAL:HG23	2:C:476:ILE:CD1	2.32	0.59
2:C:486:LYS:HD3	2:C:493:PRO:HD3	1.82	0.59
2:D:243:MET:SD	5:D:602:HEM:HMC3	2.43	0.59
2:C:114:ASN:OD1	2:C:114:ASN:C	2.45	0.58
2:C:399:VAL:CG2	2:C:400:ASP:H	2.14	0.58
2:D:203:PHE:C	2:D:204:GLN:HA	2.27	0.58
2:D:326:ASN:ND2	2:D:430:LEU:HD21	2.17	0.58
1:A:84:LEU:C	1:A:86:PHE:N	2.60	0.58
2:C:243:MET:HB3	2:C:245:GLU:HG2	1.85	0.58
2:C:560:ASP:O	2:C:561:PHE:N	2.36	0.58
1:B:10:ILE:CG2	1:B:11:THR:HG22	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:LEU:HB2	2:D:144:ILE:HG12	1.85	0.58
2:D:157:ASN:HB3	2:D:158:ILE:HG23	1.85	0.58
2:D:381:LEU:HD23	2:D:541:THR:HG21	1.85	0.58
2:C:457:ASN:OD1	2:C:460:LEU:HD12	2.03	0.58
2:D:437:ARG:NH1	2:D:443:PRO:O	2.37	0.58
2:D:557:TYR:C	2:D:559:ARG:N	2.61	0.58
1:A:94:ASP:CG	5:C:601:HEM:HMA3	2.29	0.58
2:D:326:ASN:HD22	2:D:326:ASN:C	2.11	0.58
2:D:328:PHE:CZ	2:D:332:PHE:CD2	2.91	0.58
2:D:460:LEU:HG	2:D:464:LEU:HD22	1.86	0.58
2:C:175:MET:HB2	2:C:250:HIS:CE1	2.38	0.58
2:C:244:PRO:HA	2:C:247:THR:HG22	1.85	0.58
2:C:328:PHE:HB2	2:C:502:GLN:HE21	1.69	0.58
1:B:97:LEU:HB3	2:D:324:ILE:HD13	1.83	0.58
2:D:430:LEU:CD1	2:D:476:ILE:HD11	2.33	0.58
2:D:434:ASN:HA	2:D:437:ARG:HB2	1.84	0.58
2:D:439:PHE:O	3:E:2:NAG:O3	2.21	0.58
2:C:187:LEU:HD12	2:C:187:LEU:N	2.15	0.58
2:C:280:ALA:O	2:C:284:VAL:HG12	2.04	0.58
2:D:502:GLN:O	2:D:502:GLN:HG3	2.03	0.58
1:B:83:SER:O	1:B:86:PHE:HB3	2.03	0.58
2:D:355:PRO:O	2:D:356:ASN:CB	2.52	0.58
2:D:395:ASN:CB	2:D:396:GLN:HG3	2.34	0.58
2:D:258:ASN:O	2:D:262:THR:HB	2.03	0.57
2:C:242:GLU:CD	5:C:601:HEM:CAC	2.77	0.57
1:B:29:PHE:HB3	2:D:326:ASN:HB2	1.86	0.57
2:D:174:SER:O	2:D:177:TYR:O	2.22	0.57
2:D:385:MET:HE3	2:D:546:VAL:HG22	1.86	0.57
2:C:128:LEU:CD1	2:C:146:PHE:HB2	2.35	0.57
2:C:345:ARG:O	2:C:346:LEU:HD13	2.04	0.57
2:C:436:TRP:HA	2:C:439:PHE:HB3	1.84	0.57
2:D:422:MET:HE2	2:D:468:TYR:OH	2.04	0.57
2:C:256:GLU:HG2	2:C:287:MET:CE	2.32	0.57
2:D:177:TYR:OH	2:D:257:HIS:CD2	2.58	0.57
1:A:74:ASP:OD1	1:A:74:ASP:N	2.28	0.57
1:B:66:ASN:HA	2:D:403:ARG:NH1	2.18	0.57
2:D:162:ASN:HD22	2:D:163:GLN:H	1.52	0.57
1:A:6:LYS:HE3	2:C:282:LYS:NZ	2.20	0.57
2:C:306:MET:HE3	2:C:310:LEU:CB	2.34	0.57
2:C:460:LEU:HD22	2:C:464:LEU:HD22	1.85	0.57
2:D:179:SER:O	2:D:180:GLU:HA	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:LEU:N	2:D:298:PRO:HD2	2.19	0.57
2:C:168:THR:HG23	2:C:179:SER:HB2	1.85	0.57
2:C:474:ILE:CD1	2:C:478:MET:HB3	2.33	0.57
2:D:572:LEU:HA	2:D:575:TRP:HE3	1.68	0.57
2:C:130:ILE:HG23	2:C:142:ASP:O	2.05	0.57
2:C:418:PRO:HB3	2:C:477:TRP:CZ3	2.39	0.57
2:C:382:ARG:HA	2:C:385:MET:CE	2.25	0.57
2:D:248:SER:HA	2:D:251:THR:CG2	2.35	0.57
3:I:1:NAG:H61	3:I:2:NAG:O6	2.05	0.57
2:C:131:PRO:CB	2:C:132:PRO:CD	2.83	0.57
2:C:205:ASP:HB2	2:C:210:LEU:HD13	1.85	0.57
2:C:244:PRO:CD	2:C:364:VAL:HG13	2.35	0.57
2:D:370:ARG:O	2:D:374:GLU:HB3	2.04	0.57
2:D:433:TYR:CE1	2:D:437:ARG:CG	2.88	0.57
1:A:77:THR:HB	2:C:393:ARG:HH11	1.68	0.56
1:A:93:LEU:HD23	2:C:296:TYR:HE2	1.70	0.56
2:C:321:ASP:OD2	2:C:323:ARG:NH1	2.33	0.56
2:D:177:TYR:OH	2:D:257:HIS:HD2	1.88	0.56
1:A:84:LEU:HB3	2:C:384:LEU:HD23	1.84	0.56
2:D:174:SER:O	2:D:176:VAL:N	2.37	0.56
2:D:291:ILE:HD13	2:D:533:LEU:HB2	1.87	0.56
2:D:378:ASP:O	2:D:379:PRO:C	2.47	0.56
1:A:82:ARG:HB3	2:C:552:PHE:O	2.06	0.56
1:A:89:TRP:O	1:A:93:LEU:HB2	2.04	0.56
2:C:162:ASN:ND2	2:C:163:GLN:H	2.04	0.56
2:C:230:ILE:HG13	2:C:369:TRP:HA	1.87	0.56
2:C:351:GLN:HB3	2:C:352:PRO:CD	2.34	0.56
2:C:410:VAL:O	2:C:410:VAL:HG22	2.05	0.56
2:C:422:MET:CE	2:C:478:MET:HB2	2.36	0.56
1:B:4:GLN:HE22	1:B:17:ARG:CZ	2.18	0.56
2:D:157:ASN:C	2:D:158:ILE:CG2	2.79	0.56
2:D:209:ALA:O	2:D:255:ARG:NH2	2.39	0.56
2:D:251:THR:CG2	2:D:377:ILE:HD11	2.32	0.56
2:D:309:TYR:O	2:D:504:ARG:HD3	2.05	0.56
2:D:350:TYR:HB2	2:D:557:TYR:CZ	2.41	0.56
2:C:556:SER:O	2:C:561:PHE:HE1	1.88	0.56
2:D:222:LEU:C	2:D:223:LEU:HD13	2.30	0.56
2:C:351:GLN:CB	2:C:352:PRO:CD	2.83	0.56
1:B:47:TRP:HD1	1:B:48:THR:HG23	1.71	0.56
2:D:247:THR:HG21	2:D:371:VAL:HG21	1.88	0.56
5:D:602:HEM:HHC	5:D:602:HEM:CBB	2.28	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:SER:OG	2:C:363:ARG:NH1	2.38	0.56
2:D:566:THR:O	2:D:567:LEU:HD13	2.06	0.56
2:C:262:THR:O	2:C:265:LYS:N	2.39	0.56
2:C:478:MET:HE3	2:C:481:VAL:CG2	2.36	0.56
2:D:399:VAL:HG22	2:D:401:GLU:H	1.70	0.56
2:D:465:MET:O	2:D:468:TYR:O	2.24	0.56
2:C:288:VAL:O	2:C:291:ILE:HG22	2.05	0.56
2:C:532:SER:CB	2:C:534:PRO:HD2	2.35	0.56
2:D:321:ASP:OD1	2:D:323:ARG:HG2	2.06	0.56
2:D:395:ASN:HB3	2:D:396:GLN:HG3	1.86	0.56
2:C:523:GLN:OE1	2:C:523:GLN:N	2.28	0.56
2:C:234:LEU:HG	2:C:235:ALA:N	2.20	0.56
2:C:326:ASN:O	2:C:329:THR:HB	2.06	0.56
2:C:333:ARG:HB3	5:C:601:HEM:C4A	2.41	0.56
2:C:248:SER:OG	2:C:377:ILE:HG12	2.06	0.55
2:C:249:MET:HE2	2:C:381:LEU:CD1	2.34	0.55
2:C:400:ASP:O	2:C:402:ILE:N	2.39	0.55
2:C:433:TYR:HD1	2:C:494:LEU:HD22	1.70	0.55
1:B:103:PRO:HD2	2:D:148:ARG:O	2.06	0.55
2:D:434:ASN:ND2	2:D:444:GLN:CB	2.68	0.55
1:A:27:ARG:NH2	1:B:41:PHE:CB	2.68	0.55
2:C:177:TYR:CD2	2:C:281:ARG:HD2	2.41	0.55
2:C:177:TYR:CD2	2:C:281:ARG:HG3	2.41	0.55
2:C:348:ASN:CA	2:C:382:ARG:NH2	2.55	0.55
2:C:400:ASP:HA	2:C:403:ARG:HB3	1.87	0.55
2:C:468:TYR:CD1	2:C:474:ILE:HA	2.42	0.55
5:C:601:HEM:HHC	5:C:601:HEM:CBB	2.22	0.55
2:D:548:LYS:HB3	2:D:562:VAL:HG22	1.88	0.55
3:J:1:NAG:HO3	3:J:1:NAG:C7	2.14	0.55
1:A:88:GLN:OE1	1:A:91:GLN:NE2	2.40	0.55
2:C:123:PRO:O	2:C:125:CYS:N	2.39	0.55
2:C:571:ASN:C	2:C:573:ALA:N	2.60	0.55
1:B:95:HIS:CE1	2:D:239:ARG:HG3	2.41	0.55
2:D:137:ILE:HD12	2:D:413:ILE:HD11	1.87	0.55
2:D:308:LYS:HD3	2:D:309:TYR:CZ	2.41	0.55
2:C:240:SER:CB	2:C:250:HIS:CD2	2.87	0.55
2:C:361:LEU:O	2:C:401:GLU:HG3	2.07	0.55
2:D:242:GLU:OE2	5:D:602:HEM:C4C	2.60	0.55
1:A:88:GLN:O	1:A:88:GLN:HG3	2.05	0.55
2:C:229:ARG:C	2:C:231:PRO:HD3	2.32	0.55
2:C:305:ALA:O	2:C:309:TYR:N	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:519:VAL:HG23	2:D:520:PHE:N	2.20	0.55
1:A:77:THR:CB	2:C:393:ARG:NH1	2.67	0.55
2:C:123:PRO:HB2	2:C:124:PRO:CD	2.36	0.55
2:C:264:LEU:HD11	2:C:572:LEU:HB3	1.88	0.55
2:C:296:TYR:HB2	2:C:552:PHE:CE2	2.41	0.55
2:C:399:VAL:HG22	2:C:401:GLU:H	1.72	0.55
2:C:407:PHE:CZ	5:C:601:HEM:CMD	2.88	0.55
1:B:16:ASN:ND2	1:B:16:ASN:C	2.57	0.55
2:D:181:GLU:CD	2:D:181:GLU:H	2.14	0.55
1:A:79:ASP:CG	2:C:490:ARG:HH12	2.14	0.55
2:C:208:ARG:NH2	2:C:542:GLY:CA	2.70	0.55
2:C:299:LEU:HD21	2:C:550:ASN:ND2	2.22	0.55
2:C:522:MET:CB	2:C:523:GLN:OE1	2.55	0.55
2:D:199:VAL:HG13	2:D:209:ALA:HB1	1.87	0.55
2:D:355:PRO:O	2:D:356:ASN:ND2	2.40	0.55
2:D:408:GLU:C	2:D:410:VAL:N	2.64	0.55
2:D:433:TYR:CE1	2:D:494:LEU:HD22	2.42	0.55
2:C:256:GLU:HG3	2:C:260:LEU:CD2	2.37	0.55
1:B:7:TYR:OH	2:D:279:GLU:OE1	2.24	0.55
2:C:534:PRO:HG3	2:C:551:ILE:CD1	2.27	0.55
2:D:279:GLU:O	2:D:283:ILE:HD12	2.07	0.55
2:D:345:ARG:NH2	2:D:374:GLU:HG2	2.22	0.55
2:C:136:ARG:HH22	2:C:414:GLY:C	2.14	0.54
2:C:165:ASN:C	2:C:165:ASN:ND2	2.63	0.54
2:C:347:ASP:OD1	2:C:351:GLN:N	2.40	0.54
2:C:415:LEU:HD22	2:C:415:LEU:N	2.18	0.54
2:C:474:ILE:CD1	2:C:479:GLY:N	2.69	0.54
1:B:56:PHE:CG	2:D:469:GLY:HA3	2.41	0.54
2:D:242:GLU:CD	5:D:602:HEM:CBC	2.81	0.54
2:C:363:ARG:N	2:C:363:ARG:CD	2.69	0.54
2:D:297:LEU:O	2:D:298:PRO:C	2.49	0.54
2:D:353:MET:HG2	2:D:355:PRO:HD3	1.89	0.54
2:C:181:GLU:H	2:C:182:PRO:HD3	1.72	0.54
2:C:534:PRO:HA	2:C:537:ILE:HG23	1.88	0.54
2:D:447:THR:HG22	2:D:449:GLY:N	2.10	0.54
1:A:13:MET:O	1:A:20:PRO:O	2.26	0.54
2:C:183:LEU:HD12	2:C:187:LEU:HD11	1.88	0.54
2:C:380:ILE:C	2:C:382:ARG:H	2.15	0.54
2:C:495:LEU:HA	2:C:498:ILE:HG22	1.89	0.54
1:A:84:LEU:C	1:A:86:PHE:H	2.16	0.54
1:A:94:ASP:OD2	5:C:601:HEM:HMA3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:414:GLY:O	2:C:415:LEU:C	2.48	0.54
1:B:41:PHE:CD1	1:B:41:PHE:N	2.76	0.54
2:D:480:GLY:O	2:D:495:LEU:HD22	2.08	0.54
2:C:114:ASN:OD1	2:C:116:GLU:N	2.41	0.54
2:C:244:PRO:HG2	2:C:364:VAL:HG22	1.89	0.54
1:B:62:ARG:HE	2:D:134:ASP:CG	2.16	0.54
2:D:272:ASP:O	2:D:276:LEU:HB2	2.08	0.54
2:C:282:LYS:HB3	2:C:520:PHE:CZ	2.42	0.54
2:D:278:GLN:O	2:D:281:ARG:N	2.41	0.54
2:C:197:LEU:HD22	2:C:257:HIS:CG	2.43	0.54
2:C:519:VAL:CG2	2:C:520:PHE:H	2.19	0.54
2:D:326:ASN:ND2	2:D:326:ASN:O	2.26	0.54
2:D:523:GLN:H	2:D:523:GLN:NE2	2.04	0.54
2:D:567:LEU:O	2:D:568:PRO:O	2.26	0.54
3:J:1:NAG:O3	3:J:1:NAG:C7	2.54	0.54
1:B:93:LEU:HD21	2:D:503:PHE:HZ	1.71	0.54
2:D:181:GLU:HB2	2:D:182:PRO:HD3	1.89	0.54
1:A:22:LEU:HD12	1:A:23:GLY:N	2.23	0.54
1:A:72:PRO:O	1:A:74:ASP:N	2.41	0.54
2:C:157:ASN:OD1	2:C:158:ILE:HG23	2.08	0.54
2:C:304:THR:HG23	2:C:305:ALA:H	1.72	0.54
2:C:339:ILE:HD12	5:C:601:HEM:CMC	2.38	0.54
2:C:461:ALA:O	2:C:465:MET:HB2	2.08	0.54
2:C:534:PRO:O	2:C:537:ILE:HG23	2.08	0.54
2:C:136:ARG:HH12	2:C:414:GLY:HA3	1.69	0.53
2:C:361:LEU:HB3	2:C:401:GLU:HG3	1.89	0.53
2:C:452:GLY:O	2:C:453:THR:C	2.51	0.53
5:C:601:HEM:HMC2	5:C:601:HEM:CBC	2.27	0.53
2:D:565:SER:C	2:D:567:LEU:N	2.65	0.53
1:A:21:THR:O	1:A:24:ALA:HB3	2.09	0.53
1:A:66:ASN:CA	2:C:403:ARG:HH12	2.19	0.53
2:C:347:ASP:N	2:C:353:MET:CG	2.70	0.53
2:D:200:ASN:ND2	2:D:202:ARG:H	2.06	0.53
2:D:267:LEU:CD1	2:D:268:ASN:HD21	2.14	0.53
2:D:486:LYS:HB2	2:D:491:VAL:O	2.08	0.53
5:D:602:HEM:HBB2	5:D:602:HEM:CHC	2.21	0.53
2:C:146:PHE:CE2	2:C:424:ARG:NH1	2.76	0.53
2:C:286:ALA:O	2:C:290:ILE:HG22	2.08	0.53
2:D:439:PHE:O	2:D:439:PHE:CG	2.60	0.53
2:D:559:ARG:CG	2:D:560:ASP:HB3	2.38	0.53
2:C:244:PRO:HG2	2:C:343:MET:HE1	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:TYR:HH	2:C:284:VAL:CG1	2.21	0.53
2:C:213:PHE:CE2	2:C:231:PRO:CD	2.86	0.53
2:D:251:THR:HG21	2:D:377:ILE:HG13	1.89	0.53
2:D:416:ASP:O	2:D:419:ALA:HB3	2.09	0.53
2:C:377:ILE:HD13	2:C:381:LEU:HD22	1.91	0.53
2:C:423:GLN:HE21	2:C:423:GLN:CA	2.17	0.53
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.91	0.53
2:C:290:ILE:HD11	2:C:529:ALA:HA	1.91	0.53
2:C:428:HIS:N	2:C:428:HIS:HD2	2.04	0.53
2:C:470:THR:OG1	2:C:471:PRO:HD2	2.09	0.53
2:D:385:MET:HE1	2:D:546:VAL:CG2	2.39	0.53
2:C:136:ARG:NH2	2:C:413:ILE:HG12	2.24	0.53
2:C:570:LEU:HD13	2:C:572:LEU:HD11	1.90	0.53
1:B:14:CYS:O	2:D:511:ARG:NH2	2.42	0.53
2:C:127:PRO:C	2:C:128:LEU:HD12	2.34	0.53
2:C:193:GLN:HE22	2:C:272:ASP:HB2	1.72	0.53
2:C:391:LEU:HD12	2:C:392:ASN:N	2.24	0.53
2:C:446:GLU:CA	2:C:450:GLN:NE2	2.72	0.53
2:C:220:PRO:CB	2:C:410:VAL:HG21	2.38	0.53
2:C:293:TYR:CD2	2:C:513:TRP:HZ3	2.27	0.53
1:B:45:TYR:CE2	1:B:53:ARG:HG3	2.43	0.53
2:D:327:VAL:O	2:D:330:ASN:N	2.26	0.53
2:D:354:GLU:O	2:D:356:ASN:ND2	2.42	0.53
1:A:71:PHE:CZ	2:C:396:GLN:HG2	2.43	0.52
2:C:136:ARG:HH12	2:C:414:GLY:C	2.18	0.52
2:C:287:MET:O	2:C:290:ILE:HG22	2.09	0.52
2:C:350:TYR:CD2	2:C:557:TYR:CD2	2.96	0.52
2:C:556:SER:HB2	2:C:560:ASP:CG	2.33	0.52
1:B:19:SER:CB	1:B:22:LEU:HD13	2.39	0.52
2:D:157:ASN:C	2:D:158:ILE:HG23	2.34	0.52
2:D:223:LEU:HB2	2:D:410:VAL:HG22	1.91	0.52
2:D:533:LEU:N	2:D:534:PRO:HD2	2.23	0.52
2:C:330:ASN:HD22	2:C:333:ARG:CD	2.21	0.52
2:C:446:GLU:N	2:C:450:GLN:HE21	2.06	0.52
1:B:71:PHE:CD1	1:B:71:PHE:C	2.86	0.52
1:B:82:ARG:NH2	2:D:299:LEU:HD12	2.24	0.52
2:D:224:THR:CG2	2:D:369:TRP:HE1	2.22	0.52
2:D:555:ASN:H	2:D:560:ASP:CG	2.16	0.52
1:A:11:THR:HG23	1:A:13:MET:H	1.74	0.52
1:A:71:PHE:HD1	1:A:72:PRO:CD	2.21	0.52
2:D:167:LEU:CD1	2:D:167:LEU:N	2.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:560:ASP:N	2:D:561:PHE:N	2.56	0.52
1:A:66:ASN:ND2	2:C:403:ARG:CZ	2.72	0.52
1:A:96:ASP:OD2	2:C:172:ASP:O	2.28	0.52
2:C:177:TYR:HD2	2:C:281:ARG:CD	2.22	0.52
2:C:260:LEU:HD21	2:C:287:MET:CE	2.40	0.52
2:C:300:VAL:HG23	2:C:334:TYR:OH	2.09	0.52
2:C:415:LEU:HB3	2:C:420:LEU:CD1	2.30	0.52
2:D:216:LEU:H	2:D:216:LEU:CD2	2.14	0.52
1:A:72:PRO:HG2	1:A:75:GLN:OE1	2.10	0.52
1:A:79:ASP:HB2	2:C:391:LEU:HB2	1.90	0.52
2:C:416:ASP:OD1	2:C:418:PRO:HD2	2.10	0.52
1:A:27:ARG:NH2	1:B:41:PHE:CG	2.77	0.52
2:C:259:ARG:NH2	2:C:539:ASP:HB3	2.24	0.52
2:C:430:LEU:HD12	2:C:476:ILE:HD11	1.92	0.52
1:B:60:LEU:HB3	1:B:63:ALA:HB2	1.91	0.52
2:D:131:PRO:C	2:D:133:ASN:H	2.17	0.52
1:A:5:ASP:OD2	2:C:511:ARG:NH2	2.41	0.52
2:C:128:LEU:N	2:C:128:LEU:CD1	2.72	0.52
2:C:139:ASN:HD22	2:C:141:ALA:N	2.01	0.52
2:C:248:SER:HA	2:C:251:THR:CG2	2.40	0.52
2:C:342:PHE:CE1	2:C:358:ARG:CD	2.93	0.52
2:C:521:SER:OG	2:C:523:GLN:HB2	2.10	0.52
2:D:497:CYS:SG	2:D:498:ILE:N	2.82	0.52
2:C:165:ASN:ND2	2:C:166:ALA:N	2.58	0.52
2:C:180:GLU:C	2:C:182:PRO:HD2	2.35	0.52
2:C:369:TRP:HB2	2:C:373:LEU:CD2	2.39	0.52
1:A:41:PHE:HD1	1:A:41:PHE:H	1.58	0.52
2:C:301:LEU:HG	2:C:305:ALA:HB3	1.91	0.52
2:C:361:LEU:CB	2:C:401:GLU:HG2	2.40	0.52
2:C:524:GLN:HG3	2:C:575:TRP:CZ3	2.45	0.52
2:D:203:PHE:O	2:D:204:GLN:HA	2.09	0.52
2:D:416:ASP:O	2:D:420:LEU:HD12	2.10	0.52
1:A:38:GLU:OE2	1:A:48:THR:OG1	2.27	0.52
2:C:139:ASN:HD21	2:C:141:ALA:HB3	1.75	0.52
2:C:348:ASN:HD22	2:C:348:ASN:N	2.01	0.52
2:D:143:CYS:O	2:D:413:ILE:HD13	2.10	0.52
2:C:197:LEU:HD22	2:C:257:HIS:ND1	2.25	0.51
2:C:211:LEU:HB2	2:C:233:PHE:HB3	1.93	0.51
2:C:293:TYR:CD2	2:C:513:TRP:CZ3	2.98	0.51
2:C:399:VAL:HG23	2:C:400:ASP:H	1.75	0.51
1:B:87:MET:SD	2:D:339:ILE:HG22	2.49	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:423:GLN:HA	2:D:426:ARG:HD3	1.92	0.51
2:D:533:LEU:HB3	2:D:551:ILE:HD11	1.92	0.51
2:C:269:PRO:C	2:C:271:TRP:H	2.18	0.51
2:C:327:VAL:O	2:C:330:ASN:N	2.39	0.51
2:C:430:LEU:HD13	2:C:476:ILE:HD11	1.90	0.51
2:C:516:ASN:CA	2:C:517:GLU:N	2.65	0.51
2:D:347:ASP:OD1	2:D:351:GLN:HB2	2.10	0.51
2:D:440:CYS:O	2:D:442:LEU:HD13	2.11	0.51
2:C:196:LEU:HD11	2:C:258:ASN:CA	2.41	0.51
2:C:290:ILE:HG23	2:C:291:ILE:N	2.25	0.51
1:B:68:ILE:CG2	2:D:460:LEU:HD11	2.39	0.51
1:B:71:PHE:CE2	2:D:396:GLN:HB3	2.46	0.51
2:D:240:SER:HA	2:D:246:LEU:HD13	1.91	0.51
2:D:433:TYR:CE1	2:D:437:ARG:HG2	2.46	0.51
2:D:446:GLU:H	2:D:450:GLN:NE2	2.08	0.51
1:A:95:HIS:HA	2:C:239:ARG:NH2	2.26	0.51
2:C:541:THR:OG1	2:C:543:ILE:CD1	2.59	0.51
1:B:62:ARG:NE	2:D:134:ASP:OD1	2.43	0.51
2:D:136:ARG:NE	2:D:404:GLU:HB3	2.10	0.51
2:D:417:LEU:O	2:D:420:LEU:N	2.44	0.51
2:C:209:ALA:O	2:C:210:LEU:HD12	2.11	0.51
2:C:244:PRO:CG	2:C:364:VAL:HG22	2.41	0.51
2:C:300:VAL:O	2:C:300:VAL:CG2	2.58	0.51
2:C:348:ASN:ND2	2:C:348:ASN:N	2.51	0.51
2:C:482:SER:O	2:C:482:SER:OG	2.26	0.51
1:A:91:GLN:O	1:A:95:HIS:HB2	2.11	0.51
2:C:197:LEU:H	2:C:258:ASN:HD22	1.55	0.51
2:C:208:ARG:NH2	2:C:542:GLY:HA3	2.26	0.51
2:C:391:LEU:HD12	2:C:392:ASN:H	1.74	0.51
2:C:400:ASP:O	2:C:401:GLU:C	2.51	0.51
2:C:571:ASN:HD22	2:C:573:ALA:CB	2.22	0.51
1:B:87:MET:SD	5:D:602:HEM:CBB	2.91	0.51
2:D:128:LEU:HD23	2:D:144:ILE:HD11	1.92	0.51
2:C:165:ASN:HD22	2:C:166:ALA:N	2.07	0.51
2:C:196:LEU:HD12	2:C:258:ASN:HD22	1.75	0.51
2:C:268:ASN:HB2	2:C:271:TRP:CD2	2.45	0.51
1:B:9:THR:OG1	1:B:10:ILE:N	2.41	0.51
2:D:128:LEU:HD22	2:D:144:ILE:CG1	2.40	0.51
2:D:200:ASN:HD22	2:D:203:PHE:H	1.56	0.51
2:D:300:VAL:CG1	2:D:334:TYR:OH	2.59	0.51
1:A:17:ARG:HH11	2:C:511:ARG:NH1	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:446:GLU:CA	2:C:450:GLN:HE21	2.23	0.51
2:C:556:SER:O	2:C:560:ASP:CB	2.59	0.51
2:D:287:MET:HE2	2:D:531:ILE:HG21	1.92	0.51
2:D:436:TRP:HA	2:D:436:TRP:CE3	2.45	0.51
2:C:192:ASN:CG	2:C:194:LEU:HB2	2.36	0.51
2:C:397:ILE:HG22	2:C:398:ALA:N	2.26	0.51
2:C:537:ILE:O	2:C:543:ILE:HD11	2.11	0.51
1:B:22:LEU:HD23	2:D:322:PRO:CD	2.41	0.51
2:D:424:ARG:NH1	5:D:602:HEM:O2D	2.45	0.51
2:D:247:THR:HG22	2:D:248:SER:N	2.26	0.50
2:D:494:LEU:O	2:D:498:ILE:HB	2.11	0.50
1:A:99:PHE:HB2	2:C:239:ARG:HH12	1.74	0.50
2:D:385:MET:CE	2:D:546:VAL:HG22	2.41	0.50
2:D:465:MET:HE3	2:D:470:THR:CA	2.39	0.50
2:C:533:LEU:HD12	2:C:536:ILE:HB	1.92	0.50
2:C:549:ASN:ND2	2:C:550:ASN:N	2.58	0.50
1:A:15:ASN:ND2	2:C:511:ARG:H	2.07	0.50
1:A:32:TRP:CE2	2:C:325:ALA:HB2	2.47	0.50
2:C:400:ASP:C	2:C:402:ILE:N	2.69	0.50
2:C:442:LEU:HD22	2:C:442:LEU:N	2.21	0.50
2:D:205:ASP:OD1	2:D:205:ASP:O	2.30	0.50
2:D:257:HIS:NE2	2:D:277:TYR:CD1	2.80	0.50
2:D:345:ARG:HH22	2:D:374:GLU:CG	2.24	0.50
2:C:468:TYR:CE1	2:C:474:ILE:HA	2.46	0.50
2:C:534:PRO:HA	2:C:537:ILE:CG2	2.40	0.50
2:D:350:TYR:CE2	2:D:561:PHE:CZ	3.00	0.50
2:D:440:CYS:O	2:D:442:LEU:N	2.44	0.50
1:A:41:PHE:CD1	1:A:41:PHE:N	2.79	0.50
2:C:445:PRO:O	2:C:471:PRO:HG2	2.12	0.50
2:D:244:PRO:HB2	2:D:343:MET:CE	2.41	0.50
2:C:144:ILE:HD12	2:C:416:ASP:N	2.26	0.50
2:C:146:PHE:CZ	2:C:423:GLN:HG3	2.46	0.50
2:C:248:SER:C	2:C:377:ILE:HD11	2.36	0.50
2:C:476:ILE:O	2:C:480:GLY:N	2.38	0.50
2:D:417:LEU:HB3	2:D:418:PRO:CD	2.41	0.50
1:A:84:LEU:O	1:A:85:MET:C	2.55	0.50
2:C:175:MET:HG2	2:C:176:VAL:N	2.26	0.50
2:C:270:ARG:HH11	2:C:270:ARG:CG	2.25	0.50
2:C:343:MET:SD	2:C:364:VAL:HG21	2.52	0.50
2:C:489:GLY:C	2:C:490:ARG:HG2	2.37	0.50
2:D:114:ASN:HD22	2:D:117:THR:HB	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:TYR:HE2	2:C:281:ARG:CB	2.25	0.50
2:C:247:THR:O	2:C:251:THR:HG22	2.12	0.50
1:B:44:PRO:CB	2:D:126:PHE:CE2	2.94	0.50
1:A:72:PRO:O	1:A:73:THR:C	2.54	0.49
2:C:339:ILE:HD12	5:C:601:HEM:HMC1	1.94	0.49
2:C:351:GLN:CB	2:C:352:PRO:HD2	2.27	0.49
2:C:422:MET:HE2	2:C:478:MET:HB2	1.94	0.49
2:D:165:ASN:ND2	2:D:167:LEU:H	2.08	0.49
2:D:200:ASN:ND2	2:D:202:ARG:N	2.59	0.49
2:D:491:VAL:HG22	2:D:495:LEU:HB3	1.93	0.49
2:C:177:TYR:CE2	2:C:281:ARG:CB	2.95	0.49
2:C:260:LEU:HD21	2:C:287:MET:HE2	1.94	0.49
2:C:334:TYR:CG	2:C:335:GLY:N	2.80	0.49
2:C:382:ARG:CB	2:C:385:MET:CE	2.91	0.49
1:B:10:ILE:HG23	1:B:11:THR:N	2.26	0.49
1:A:81:GLU:O	2:C:553:MET:HG2	2.12	0.49
2:C:224:THR:HG21	2:C:369:TRP:HE1	1.77	0.49
1:B:39:ASP:HB3	1:B:41:PHE:H	1.78	0.49
2:D:136:ARG:HH21	2:D:404:GLU:HA	1.77	0.49
2:D:233:PHE:CE2	2:D:368:SER:HB3	2.48	0.49
2:D:293:TYR:HA	2:D:297:LEU:HD23	1.94	0.49
2:D:447:THR:HG22	2:D:448:VAL:N	2.27	0.49
2:C:177:TYR:OH	2:C:257:HIS:CD2	2.66	0.49
2:C:382:ARG:CA	2:C:385:MET:CE	2.88	0.49
2:C:406:LEU:HD11	5:C:601:HEM:HAC	1.93	0.49
1:B:47:TRP:CD1	1:B:48:THR:HG23	2.47	0.49
2:D:350:TYR:CZ	2:D:561:PHE:CE2	3.00	0.49
2:D:361:LEU:O	2:D:365:PHE:CE2	2.66	0.49
2:D:524:GLN:O	2:D:527:ALA:HB3	2.13	0.49
2:C:136:ARG:CG	2:C:137:ILE:HG22	2.28	0.49
2:C:187:LEU:N	2:C:187:LEU:CD1	2.76	0.49
1:B:16:ASN:ND2	1:B:18:ARG:H	2.09	0.49
2:D:130:ILE:HD12	2:D:137:ILE:CD1	2.42	0.49
2:D:287:MET:HE1	2:D:570:LEU:HD12	1.95	0.49
2:D:408:GLU:C	2:D:410:VAL:H	2.17	0.49
2:D:455:LEU:O	2:D:456:ARG:HB2	2.13	0.49
1:A:9:THR:HG23	1:A:12:GLY:HA2	1.94	0.49
2:C:378:ASP:N	2:C:379:PRO:HD2	2.28	0.49
1:A:69:VAL:HG23	1:A:69:VAL:O	2.13	0.49
2:C:247:THR:HG23	2:C:248:SER:N	2.28	0.49
2:C:347:ASP:CA	2:C:353:MET:HG3	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:ARG:HE	2:C:374:GLU:CD	2.19	0.49
1:B:44:PRO:HD3	2:D:148:ARG:CZ	2.41	0.49
2:D:556:SER:O	2:D:557:TYR:C	2.51	0.49
2:C:297:LEU:HA	2:C:300:VAL:HG12	1.92	0.49
2:C:434:ASN:ND2	2:C:444:GLN:HA	2.28	0.49
2:D:174:SER:O	2:D:175:MET:C	2.54	0.49
2:D:560:ASP:HA	2:D:561:PHE:N	2.23	0.49
1:A:30:VAL:CG1	2:C:323:ARG:CZ	2.91	0.49
1:A:37:TYR:CE1	2:C:429:GLY:HA3	2.48	0.49
2:C:433:TYR:HD1	2:C:494:LEU:CD2	2.24	0.49
2:D:356:ASN:CG	2:D:357:PRO:HD3	2.31	0.49
2:D:424:ARG:O	2:D:425:SER:C	2.54	0.49
2:C:131:PRO:CB	2:C:132:PRO:HD3	2.43	0.49
2:C:220:PRO:HD2	2:C:232:CYS:SG	2.52	0.49
2:C:395:ASN:O	2:C:396:GLN:HG3	2.13	0.49
2:C:434:ASN:HD21	2:C:444:GLN:HA	1.78	0.49
2:D:378:ASP:O	2:D:380:ILE:N	2.46	0.49
2:C:284:VAL:O	2:C:287:MET:N	2.46	0.48
1:A:89:TRP:CZ2	2:C:291:ILE:HG21	2.48	0.48
2:C:480:GLY:C	2:C:495:LEU:CD2	2.86	0.48
2:C:556:SER:O	2:C:561:PHE:CD1	2.65	0.48
2:C:571:ASN:ND2	2:C:573:ALA:HB2	2.28	0.48
2:D:422:MET:HG2	2:D:475:ASP:OD2	2.12	0.48
2:D:440:CYS:O	2:D:441:GLY:C	2.56	0.48
2:D:521:SER:OG	2:D:524:GLN:NE2	2.46	0.48
2:D:554:SER:CA	2:D:560:ASP:OD1	2.61	0.48
1:A:98:ASP:OD1	5:C:601:HEM:HBA1	2.13	0.48
2:C:130:ILE:CG2	2:C:137:ILE:HD11	2.37	0.48
2:C:136:ARG:HH22	2:C:414:GLY:N	2.12	0.48
2:C:216:LEU:HD11	2:C:219:ASP:HA	1.95	0.48
2:C:329:THR:O	2:C:333:ARG:HD3	2.12	0.48
2:C:546:VAL:O	2:C:561:PHE:HB3	2.12	0.48
1:B:47:TRP:CD1	1:B:47:TRP:C	2.91	0.48
1:B:87:MET:CE	2:D:339:ILE:HG22	2.43	0.48
2:D:297:LEU:O	2:D:301:LEU:HB2	2.13	0.48
2:D:554:SER:C	2:D:560:ASP:OD1	2.56	0.48
1:A:10:ILE:HG21	2:C:181:GLU:CD	2.38	0.48
2:C:230:ILE:CG2	2:C:372:VAL:HG21	2.22	0.48
2:C:382:ARG:HA	2:C:385:MET:HB2	1.94	0.48
2:C:220:PRO:HA	2:C:223:LEU:HD22	1.95	0.48
1:B:79:ASP:CG	2:D:490:ARG:NH1	2.72	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:PHE:N	2:D:147:PHE:CD1	2.81	0.48
2:D:247:THR:CG2	2:D:248:SER:N	2.72	0.48
1:A:77:THR:HG22	2:C:396:GLN:OE1	2.13	0.48
1:A:86:PHE:CD1	2:C:552:PHE:HB3	2.48	0.48
1:A:93:LEU:HD23	2:C:296:TYR:CE2	2.48	0.48
2:C:175:MET:O	2:C:236:GLY:HA3	2.14	0.48
2:C:297:LEU:N	2:C:298:PRO:CD	2.76	0.48
1:B:37:TYR:O	1:B:45:TYR:HE1	1.97	0.48
1:B:84:LEU:HD13	2:D:389:ALA:HA	1.95	0.48
2:D:116:GLU:HA	2:D:145:PRO:HB3	1.96	0.48
1:A:79:ASP:CG	2:C:490:ARG:NH1	2.71	0.48
2:C:385:MET:CE	2:C:537:ILE:HD11	2.41	0.48
2:C:571:ASN:HD22	2:C:573:ALA:HB2	1.77	0.48
2:D:197:LEU:O	2:D:199:VAL:HG23	2.14	0.48
2:D:330:ASN:HD21	2:D:477:TRP:HB2	1.78	0.48
2:C:221:CYS:SG	2:C:232:CYS:N	2.87	0.48
2:C:333:ARG:NH1	5:C:601:HEM:CAA	2.75	0.48
2:C:533:LEU:O	2:C:536:ILE:N	2.47	0.48
2:C:571:ASN:C	2:C:573:ALA:H	2.21	0.48
2:D:300:VAL:HG11	2:D:334:TYR:OH	2.13	0.48
2:D:434:ASN:ND2	2:D:445:PRO:HD2	2.28	0.48
2:D:483:GLU:HB3	2:D:484:PRO:HD2	1.95	0.48
1:A:62:ARG:HH21	2:C:136:ARG:HG2	1.72	0.48
1:A:96:ASP:OD1	2:C:174:SER:OG	2.32	0.48
2:C:244:PRO:HG2	2:C:343:MET:CE	2.43	0.48
2:C:383:GLY:O	2:C:387:THR:CG2	2.60	0.48
2:D:400:ASP:C	2:D:402:ILE:H	2.22	0.48
2:D:490:ARG:HD3	2:D:490:ARG:HA	1.60	0.48
1:A:7:TYR:CZ	2:C:279:GLU:OE2	2.67	0.48
2:C:139:ASN:ND2	2:C:139:ASN:C	2.72	0.48
2:C:338:LEU:HD12	2:C:338:LEU:HA	1.47	0.48
2:C:437:ARG:O	2:C:442:LEU:HD23	2.13	0.48
2:C:544:THR:O	2:C:564:CYS:SG	2.71	0.48
1:A:82:ARG:HA	2:C:553:MET:HA	1.95	0.47
2:C:284:VAL:C	2:C:286:ALA:N	2.71	0.47
2:C:486:LYS:HA	2:C:486:LYS:HD2	1.51	0.47
2:C:521:SER:HG	2:C:524:GLN:H	1.61	0.47
1:B:18:ARG:HH21	2:D:318:ASP:HB3	1.79	0.47
1:B:60:LEU:HB3	1:B:63:ALA:CB	2.44	0.47
2:D:424:ARG:HG3	5:D:602:HEM:O1D	2.13	0.47
2:D:433:TYR:CG	2:D:433:TYR:O	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:457:ASN:HD22	2:D:457:ASN:HA	1.40	0.47
2:D:471:PRO:HA	2:D:474:ILE:HD12	1.96	0.47
1:A:22:LEU:HD13	1:A:22:LEU:HA	1.61	0.47
2:C:177:TYR:CD2	2:C:281:ARG:CG	2.97	0.47
2:C:244:PRO:HD3	2:C:364:VAL:HG13	1.95	0.47
2:C:533:LEU:N	2:C:534:PRO:HD2	2.29	0.47
2:C:537:ILE:O	2:C:541:THR:OG1	2.31	0.47
2:D:190:MET:HE2	2:D:190:MET:HB3	1.68	0.47
2:C:417:LEU:HB3	2:C:418:PRO:CD	2.40	0.47
2:D:433:TYR:CD1	2:D:494:LEU:HD22	2.49	0.47
2:C:262:THR:CG2	2:C:263:GLU:N	2.76	0.47
2:C:345:ARG:NH2	2:C:374:GLU:CD	2.72	0.47
2:C:424:ARG:HA	2:C:424:ARG:HD3	1.63	0.47
2:D:293:TYR:OH	2:D:503:PHE:O	2.26	0.47
2:D:340:GLN:HE21	2:D:340:GLN:HB2	1.53	0.47
2:D:385:MET:CE	2:D:546:VAL:CG2	2.92	0.47
2:D:493:PRO:O	2:D:497:CYS:HB3	2.14	0.47
1:A:29:PHE:CZ	2:C:165:ASN:HB2	2.49	0.47
2:C:177:TYR:OH	2:C:284:VAL:CG1	2.62	0.47
2:C:338:LEU:HD13	2:C:338:LEU:N	2.29	0.47
2:C:562:VAL:HG23	2:C:566:THR:OG1	2.14	0.47
1:B:9:THR:HG21	1:B:13:MET:N	2.29	0.47
1:B:96:ASP:OD2	2:D:172:ASP:O	2.32	0.47
2:D:199:VAL:CG1	2:D:209:ALA:HB1	2.44	0.47
2:D:571:ASN:O	2:D:575:TRP:HZ3	1.98	0.47
1:A:99:PHE:CB	2:C:167:LEU:CD1	2.90	0.47
2:C:177:TYR:CE2	2:C:281:ARG:HG3	2.49	0.47
2:C:234:LEU:O	2:C:235:ALA:HB2	2.15	0.47
2:C:350:TYR:CE2	2:C:561:PHE:CE2	3.03	0.47
2:C:433:TYR:O	2:C:437:ARG:HB2	2.15	0.47
2:C:437:ARG:HD3	2:C:443:PRO:O	2.15	0.47
2:C:513:TRP:CD1	2:C:515:GLU:HB2	2.49	0.47
1:B:9:THR:CG2	1:B:13:MET:H	2.26	0.47
2:D:435:ALA:O	2:D:438:ARG:HB3	2.15	0.47
1:A:1:CYS:SG	1:A:20:PRO:HB3	2.55	0.47
1:A:29:PHE:HE2	1:A:100:THR:HG22	1.77	0.47
1:A:32:TRP:CZ2	2:C:325:ALA:HB2	2.50	0.47
1:A:41:PHE:HD2	1:B:27:ARG:HH22	1.61	0.47
1:A:44:PRO:CB	2:C:126:PHE:CE2	2.97	0.47
2:C:139:ASN:ND2	2:C:141:ALA:N	2.55	0.47
2:C:177:TYR:OH	2:C:257:HIS:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:VAL:CG1	2:C:209:ALA:HB1	2.43	0.47
2:C:211:LEU:HD12	2:C:211:LEU:H	1.79	0.47
2:C:221:CYS:HB2	2:C:366:PHE:O	2.15	0.47
1:B:100:THR:OG1	5:D:602:HEM:O2A	2.27	0.47
2:D:385:MET:HE1	2:D:546:VAL:HG23	1.96	0.47
1:A:85:MET:HE3	2:C:249:MET:CE	2.44	0.47
2:C:136:ARG:NH2	2:C:414:GLY:C	2.73	0.47
2:C:541:THR:OG1	2:C:543:ILE:HD11	2.14	0.47
1:B:64:VAL:O	1:B:64:VAL:HG23	2.12	0.47
1:A:13:MET:O	1:A:13:MET:SD	2.73	0.47
2:C:214:ASP:OD1	2:C:215:ASN:N	2.43	0.47
2:C:267:LEU:HD12	2:C:268:ASN:ND2	2.30	0.47
2:C:282:LYS:CG	2:C:520:PHE:CZ	2.97	0.47
2:C:356:ASN:HD22	2:C:356:ASN:HA	1.36	0.47
2:D:225:ASN:OD1	2:D:369:TRP:CE2	2.68	0.47
1:A:91:GLN:O	1:A:92:LEU:C	2.55	0.47
2:C:249:MET:CE	2:C:381:LEU:CD1	2.93	0.47
2:C:249:MET:CE	2:C:381:LEU:HD11	2.37	0.47
2:C:267:LEU:HD12	2:C:267:LEU:O	2.14	0.47
2:C:387:THR:HG23	2:C:387:THR:O	2.15	0.47
2:C:556:SER:O	2:C:560:ASP:HB3	2.14	0.47
2:D:295:ASP:HB2	2:D:552:PHE:HE2	1.81	0.47
2:D:310:LEU:HD11	2:D:504:ARG:HA	1.97	0.47
1:A:56:PHE:CD1	2:C:469:GLY:HA3	2.49	0.46
2:C:294:ARG:HE	2:C:295:ASP:CG	2.22	0.46
2:C:299:LEU:HD21	2:C:550:ASN:CG	2.39	0.46
2:C:470:THR:C	2:C:472:ASN:N	2.72	0.46
2:C:559:ARG:CG	2:C:560:ASP:N	2.78	0.46
1:B:72:PRO:C	1:B:74:ASP:H	2.23	0.46
1:B:103:PRO:O	1:B:104:ALA:C	2.58	0.46
2:D:350:TYR:HB2	2:D:557:TYR:CE1	2.50	0.46
2:D:353:MET:HG2	2:D:355:PRO:CD	2.44	0.46
1:A:41:PHE:HD1	1:A:41:PHE:N	2.12	0.46
2:C:457:ASN:OD1	2:C:460:LEU:CA	2.62	0.46
2:C:531:ILE:H	2:C:531:ILE:HG23	1.29	0.46
2:D:177:TYR:CE1	2:D:197:LEU:HD21	2.50	0.46
1:A:86:PHE:HD1	2:C:552:PHE:HB3	1.80	0.46
2:C:177:TYR:CD1	2:C:177:TYR:N	2.82	0.46
2:C:321:ASP:OD2	2:C:323:ARG:HD3	2.15	0.46
2:C:439:PHE:HA	3:H:2:NAG:O7	2.16	0.46
2:C:551:ILE:CD1	2:C:551:ILE:N	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PHE:CD1	1:B:100:THR:N	2.83	0.46
2:D:192:ASN:ND2	2:D:194:LEU:CD2	2.79	0.46
1:A:94:ASP:OD1	5:C:601:HEM:HHB	2.16	0.46
2:C:176:VAL:HG23	2:C:177:TYR:CE1	2.51	0.46
1:B:66:ASN:ND2	2:D:403:ARG:HH12	2.09	0.46
1:B:71:PHE:HZ	1:B:76:LEU:CD1	2.19	0.46
2:D:405:ARG:CG	2:D:405:ARG:NH1	2.73	0.46
2:D:489:GLY:O	2:D:490:ARG:NE	2.48	0.46
1:A:87:MET:HB3	2:C:338:LEU:HB3	1.96	0.46
2:C:175:MET:C	2:C:236:GLY:HA3	2.41	0.46
2:C:309:TYR:C	2:C:311:PRO:HD2	2.41	0.46
1:B:68:ILE:HD12	2:D:464:LEU:HD13	1.98	0.46
2:D:327:VAL:CG1	2:D:328:PHE:N	2.79	0.46
2:D:395:ASN:C	2:D:396:GLN:HG3	2.39	0.46
2:C:458:LEU:C	2:C:458:LEU:HD12	2.40	0.46
2:D:216:LEU:N	2:D:216:LEU:CD2	2.76	0.46
2:D:327:VAL:C	2:D:329:THR:N	2.72	0.46
2:D:336:HIS:CD2	5:D:602:HEM:NB	2.83	0.46
2:D:348:ASN:O	2:D:350:TYR:N	2.49	0.46
1:A:8:ARG:HG2	2:C:512:PHE:CD2	2.51	0.46
1:A:77:THR:HG21	2:C:393:ARG:NH1	2.23	0.46
2:C:422:MET:HE1	2:C:478:MET:SD	2.56	0.46
2:D:194:LEU:N	2:D:194:LEU:CD1	2.77	0.46
2:D:212:PRO:O	2:D:233:PHE:HA	2.16	0.46
2:D:310:LEU:CD1	2:D:504:ARG:HA	2.46	0.46
2:D:380:ILE:HG22	2:D:381:LEU:N	2.31	0.46
2:D:392:ASN:OD1	2:D:393:ARG:N	2.48	0.46
2:D:417:LEU:O	2:D:418:PRO:C	2.56	0.46
2:D:492:GLY:O	2:D:496:ALA:CB	2.63	0.46
1:A:99:PHE:O	2:C:165:ASN:ND2	2.47	0.46
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.47	0.46
2:C:306:MET:O	2:C:310:LEU:N	2.48	0.46
2:C:498:ILE:HD13	2:C:498:ILE:HG21	1.63	0.46
2:D:136:ARG:CZ	2:D:414:GLY:O	2.63	0.46
2:D:320:VAL:CG1	2:D:509:GLY:CA	2.87	0.46
2:D:338:LEU:HD13	2:D:338:LEU:N	2.31	0.46
2:D:350:TYR:CG	2:D:557:TYR:CE1	3.04	0.46
2:D:433:TYR:CE1	2:D:437:ARG:HG3	2.50	0.46
1:A:62:ARG:HH22	2:C:136:ARG:HG2	1.72	0.46
2:C:158:ILE:HA	1:B:27:ARG:NH2	2.30	0.46
2:C:269:PRO:C	2:C:271:TRP:N	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:361:LEU:HB3	2:C:401:GLU:CG	2.46	0.46
2:C:571:ASN:ND2	2:C:573:ALA:CB	2.78	0.46
2:D:345:ARG:NH2	2:D:374:GLU:CG	2.79	0.46
2:D:385:MET:CE	2:D:546:VAL:CA	2.92	0.46
1:A:79:ASP:OD2	1:A:82:ARG:CG	2.63	0.45
2:C:485:LEU:CD1	2:C:485:LEU:N	2.79	0.45
1:B:77:THR:CG2	2:D:396:GLN:NE2	2.78	0.45
2:D:405:ARG:HG3	2:D:405:ARG:NH1	2.31	0.45
2:D:531:ILE:HG23	2:D:531:ILE:HD13	1.69	0.45
2:D:537:ILE:O	2:D:541:THR:HG23	2.16	0.45
1:B:44:PRO:HB2	2:D:126:PHE:CE2	2.51	0.45
2:D:336:HIS:ND1	2:D:417:LEU:HG	2.32	0.45
2:D:533:LEU:N	2:D:534:PRO:CD	2.79	0.45
2:C:434:ASN:ND2	2:C:444:GLN:CB	2.77	0.45
2:C:460:LEU:HD22	2:C:464:LEU:CD2	2.46	0.45
2:C:465:MET:HE2	2:C:465:MET:HB3	1.86	0.45
2:D:571:ASN:HD22	2:D:571:ASN:C	2.24	0.45
2:C:213:PHE:CD2	2:C:231:PRO:HD2	2.50	0.45
2:C:420:LEU:O	2:C:424:ARG:N	2.48	0.45
2:C:422:MET:HG2	2:C:475:ASP:HB2	1.99	0.45
2:D:123:PRO:O	2:D:124:PRO:C	2.59	0.45
2:D:333:ARG:NH2	5:D:602:HEM:HHA	2.32	0.45
1:A:71:PHE:CD1	1:A:72:PRO:N	2.85	0.45
2:C:316:TYR:CD2	2:C:511:ARG:HA	2.51	0.45
2:C:346:LEU:C	2:C:353:MET:HB2	2.42	0.45
2:C:442:LEU:CB	2:C:443:PRO:HD2	2.22	0.45
2:C:557:TYR:O	2:C:557:TYR:CG	2.67	0.45
2:C:570:LEU:HD13	2:C:572:LEU:CD1	2.47	0.45
2:C:572:LEU:CD1	2:C:572:LEU:N	2.78	0.45
2:D:257:HIS:NE2	2:D:277:TYR:HD1	2.14	0.45
2:D:372:VAL:HG12	2:D:373:LEU:CD1	2.39	0.45
2:D:424:ARG:CG	2:D:424:ARG:HH11	2.28	0.45
2:C:262:THR:HG22	2:C:263:GLU:H	1.80	0.45
1:B:66:ASN:ND2	2:D:403:ARG:NH1	2.60	0.45
2:D:400:ASP:C	2:D:402:ILE:N	2.74	0.45
2:C:165:ASN:HD21	2:C:167:LEU:H	1.65	0.45
2:C:291:ILE:HG23	2:C:292:THR:CA	2.47	0.45
2:C:339:ILE:HD12	2:C:339:ILE:HG21	1.74	0.45
2:C:365:PHE:N	2:C:365:PHE:CD1	2.84	0.45
2:D:471:PRO:C	2:D:473:ASN:N	2.74	0.45
2:C:170:PHE:HB2	2:C:172:ASP:OD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:248:SER:CB	2:C:377:ILE:HG12	2.47	0.45
2:C:297:LEU:HD21	2:C:503:PHE:CG	2.51	0.45
2:C:333:ARG:HD2	5:C:601:HEM:CMA	2.47	0.45
2:C:339:ILE:HD11	2:C:402:ILE:HD12	1.99	0.45
2:D:163:GLN:HG3	2:D:428:HIS:ND1	2.32	0.45
2:D:437:ARG:HH11	2:D:437:ARG:HD2	1.59	0.45
2:C:350:TYR:CG	2:C:557:TYR:HD2	2.30	0.45
2:C:415:LEU:N	2:C:415:LEU:CD1	2.68	0.45
2:C:541:THR:CB	2:C:543:ILE:HD11	2.46	0.45
2:D:223:LEU:HB2	2:D:410:VAL:CG2	2.46	0.45
2:D:292:THR:C	2:D:297:LEU:HD22	2.39	0.45
2:D:477:TRP:O	2:D:481:VAL:HG22	2.17	0.45
2:D:543:ILE:HG23	2:D:543:ILE:HD13	1.61	0.45
3:I:1:NAG:C6	3:I:2:NAG:O5	2.56	0.45
2:C:264:LEU:HD12	2:C:264:LEU:HA	1.50	0.45
2:D:400:ASP:O	2:D:402:ILE:N	2.50	0.45
1:A:87:MET:O	5:C:601:HEM:HBB1	2.17	0.44
2:C:167:LEU:CD1	2:C:167:LEU:N	2.79	0.44
2:C:213:PHE:HE2	2:C:231:PRO:CD	2.25	0.44
2:C:270:ARG:NH1	2:C:270:ARG:HG2	2.31	0.44
2:C:295:ASP:CB	2:C:550:ASN:ND2	2.80	0.44
2:C:378:ASP:O	2:C:382:ARG:HB3	2.17	0.44
2:C:382:ARG:HB2	2:C:385:MET:HE1	1.99	0.44
1:B:36:GLU:OE2	2:D:431:PRO:HB3	2.17	0.44
2:D:126:PHE:C	2:D:126:PHE:CD1	2.91	0.44
2:D:223:LEU:HA	2:D:223:LEU:HD12	1.41	0.44
2:D:381:LEU:HA	2:D:384:LEU:CD1	2.24	0.44
2:D:546:VAL:O	2:D:561:PHE:HD2	1.99	0.44
1:A:41:PHE:O	2:C:161:ARG:HB2	2.18	0.44
1:A:98:ASP:O	2:C:167:LEU:HD22	2.16	0.44
2:C:165:ASN:ND2	2:C:167:LEU:H	2.15	0.44
2:C:421:ASN:HD22	2:C:421:ASN:HA	1.41	0.44
2:D:174:SER:C	2:D:176:VAL:N	2.75	0.44
2:D:179:SER:N	2:D:180:GLU:N	2.65	0.44
2:D:211:LEU:HB2	2:D:233:PHE:CD1	2.52	0.44
2:D:242:GLU:OE2	5:D:602:HEM:CHD	2.65	0.44
2:D:493:PRO:HA	2:D:496:ALA:HB3	1.98	0.44
1:A:83:SER:O	1:A:86:PHE:HB3	2.17	0.44
1:A:83:SER:C	2:C:389:ALA:HB2	2.42	0.44
2:C:317:ASN:C	2:C:319:SER:H	2.25	0.44
2:C:399:VAL:O	2:C:403:ARG:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:LEU:H	2:C:415:LEU:CD1	2.30	0.44
1:B:3:GLU:C	1:B:4:GLN:CB	2.67	0.44
2:D:200:ASN:ND2	2:D:202:ARG:C	2.76	0.44
1:A:44:PRO:HB2	2:C:126:PHE:CE2	2.52	0.44
2:C:244:PRO:HA	2:C:247:THR:CG2	2.47	0.44
2:C:406:LEU:HD21	5:C:601:HEM:CMD	2.43	0.44
2:D:336:HIS:CD2	5:D:602:HEM:C4B	3.05	0.44
2:D:451:LEU:O	2:D:452:GLY:C	2.59	0.44
1:A:99:PHE:HD2	2:C:166:ALA:HB3	1.82	0.44
1:B:56:PHE:HA	1:B:57:PRO:HD3	1.85	0.44
2:D:142:ASP:OD1	2:D:143:CYS:N	2.46	0.44
2:D:294:ARG:HG2	2:D:295:ASP:OD1	2.18	0.44
2:D:332:PHE:CD1	2:D:334:TYR:HE1	2.34	0.44
2:D:543:ILE:HG21	2:D:543:ILE:HD12	1.66	0.44
2:C:208:ARG:HH22	2:C:542:GLY:HA3	1.83	0.44
2:C:297:LEU:O	2:C:300:VAL:HG13	2.17	0.44
2:C:317:ASN:O	2:C:319:SER:N	2.51	0.44
2:C:326:ASN:HD21	2:C:428:HIS:HB3	1.83	0.44
2:C:521:SER:HG	2:C:523:GLN:HB2	1.82	0.44
2:C:537:ILE:O	2:C:537:ILE:CG1	2.65	0.44
2:D:248:SER:C	2:D:251:THR:HG22	2.42	0.44
2:D:301:LEU:HA	2:D:301:LEU:HD12	1.66	0.44
2:D:403:ARG:HG2	2:D:416:ASP:OD1	2.17	0.44
2:C:130:ILE:HD13	2:C:137:ILE:O	2.18	0.44
2:C:216:LEU:HD12	2:C:218:ASP:H	1.82	0.44
2:C:267:LEU:CD2	2:C:572:LEU:O	2.66	0.44
2:C:278:GLN:HE21	2:C:278:GLN:HB2	1.30	0.44
2:C:310:LEU:HD11	2:C:504:ARG:HA	2.00	0.44
1:B:41:PHE:N	1:B:41:PHE:HD1	2.16	0.44
2:D:128:LEU:CD2	2:D:144:ILE:HD11	2.48	0.44
1:A:29:PHE:CE2	1:A:100:THR:CG2	2.99	0.44
2:C:230:ILE:HG21	2:C:372:VAL:CG2	2.23	0.44
2:C:270:ARG:HH11	2:C:270:ARG:HG2	1.82	0.44
2:C:346:LEU:HA	2:C:346:LEU:HD12	1.68	0.44
1:B:68:ILE:CG2	2:D:460:LEU:CD1	2.96	0.44
1:B:87:MET:HE1	2:D:243:MET:HE1	1.99	0.44
2:D:150:CYS:HA	2:D:151:PRO:HD3	1.77	0.44
2:D:182:PRO:O	2:D:186:ASN:HB2	2.17	0.44
2:D:347:ASP:HA	2:D:382:ARG:NH1	2.33	0.44
2:D:362:SER:OG	2:D:401:GLU:OE1	2.31	0.44
1:A:44:PRO:O	1:A:47:TRP:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:350:TYR:HB2	2:C:557:TYR:HE2	1.76	0.44
2:C:514:TRP:HA	2:C:519:VAL:HG21	2.00	0.44
2:C:519:VAL:HG22	2:C:520:PHE:H	1.81	0.44
2:D:225:ASN:OD1	3:J:1:NAG:N2	2.51	0.44
2:D:264:LEU:HD12	2:D:264:LEU:HA	1.86	0.44
2:D:320:VAL:O	2:D:322:PRO:HD3	2.18	0.44
2:D:327:VAL:HG13	2:D:328:PHE:N	2.33	0.44
2:D:513:TRP:CD1	2:D:515:GLU:HB2	2.53	0.44
1:B:72:PRO:C	1:B:74:ASP:N	2.75	0.43
2:D:206:ASN:HD22	2:D:206:ASN:HA	1.39	0.43
2:D:286:ALA:O	2:D:287:MET:C	2.58	0.43
2:D:297:LEU:O	2:D:301:LEU:N	2.51	0.43
2:D:377:ILE:HG21	2:D:377:ILE:HD12	1.38	0.43
2:D:422:MET:O	2:D:426:ARG:HD3	2.18	0.43
2:D:447:THR:CG2	2:D:448:VAL:N	2.81	0.43
2:D:498:ILE:HG21	2:D:498:ILE:HD13	1.71	0.43
1:A:94:ASP:HB3	1:A:95:HIS:HD2	1.83	0.43
2:C:363:ARG:N	2:C:363:ARG:HD3	2.32	0.43
2:C:378:ASP:CB	2:C:379:PRO:HD3	2.48	0.43
2:C:474:ILE:HD11	2:C:479:GLY:H	1.82	0.43
2:D:177:TYR:CE2	2:D:281:ARG:CG	2.96	0.43
2:D:385:MET:SD	2:D:537:ILE:HD11	2.58	0.43
2:D:447:THR:HB	2:D:450:GLN:HB2	1.98	0.43
1:A:72:PRO:C	1:A:74:ASP:N	2.75	0.43
1:A:77:THR:O	2:C:391:LEU:N	2.52	0.43
2:C:162:ASN:ND2	2:C:163:GLN:N	2.67	0.43
2:C:260:LEU:HA	2:C:260:LEU:HD12	1.72	0.43
2:C:264:LEU:CD1	2:C:572:LEU:HD23	2.48	0.43
2:C:297:LEU:CA	2:C:300:VAL:CG1	2.86	0.43
1:B:13:MET:HE3	1:B:14:CYS:SG	2.58	0.43
1:B:72:PRO:HB2	1:B:75:GLN:HG3	1.99	0.43
2:D:199:VAL:O	2:D:200:ASN:C	2.61	0.43
2:D:321:ASP:CG	2:D:323:ARG:HH11	2.27	0.43
2:D:385:MET:HE3	2:D:547:SER:N	2.28	0.43
2:D:471:PRO:C	2:D:473:ASN:H	2.26	0.43
3:G:2:NAG:O3	3:G:2:NAG:C7	2.65	0.43
2:C:199:VAL:CG1	2:C:209:ALA:CB	2.96	0.43
2:C:223:LEU:HD22	2:C:410:VAL:HG23	1.99	0.43
2:C:317:ASN:C	2:C:319:SER:N	2.76	0.43
2:C:378:ASP:N	2:C:379:PRO:CD	2.81	0.43
1:B:11:THR:CG2	2:D:181:GLU:OE2	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:ARG:O	2:D:374:GLU:CB	2.67	0.43
2:C:480:GLY:CA	2:C:495:LEU:HD22	2.48	0.43
1:B:22:LEU:HD23	2:D:322:PRO:HD2	1.99	0.43
1:B:68:ILE:H	1:B:68:ILE:HG12	1.54	0.43
1:B:79:ASP:CB	2:D:391:LEU:HB2	2.31	0.43
2:D:193:GLN:O	2:D:273:GLY:HA2	2.19	0.43
2:D:291:ILE:O	2:D:295:ASP:N	2.45	0.43
2:D:436:TRP:CE3	2:D:498:ILE:HD11	2.54	0.43
2:D:544:THR:HG23	2:D:545:THR:N	2.31	0.43
3:E:1:NAG:O4	3:E:2:NAG:O7	2.36	0.43
1:A:47:TRP:CE3	2:C:121:GLN:OE1	2.72	0.43
1:A:71:PHE:CD1	1:A:71:PHE:C	2.97	0.43
1:A:94:ASP:OD1	5:C:601:HEM:CHB	2.67	0.43
2:C:287:MET:HA	2:C:531:ILE:HD11	2.01	0.43
1:B:85:MET:HG3	2:D:552:PHE:CE1	2.53	0.43
2:D:264:LEU:HD12	2:D:267:LEU:HD11	2.00	0.43
2:D:491:VAL:HG11	2:D:496:ALA:HA	2.00	0.43
2:C:162:ASN:HD22	2:C:162:ASN:HA	1.24	0.43
2:C:551:ILE:N	2:C:551:ILE:HD12	2.33	0.43
2:D:377:ILE:HG23	2:D:377:ILE:HD13	1.43	0.43
2:D:486:LYS:HA	2:D:486:LYS:HD2	1.68	0.43
2:D:534:PRO:HB3	2:D:546:VAL:CG1	2.49	0.43
1:A:68:ILE:HD11	2:C:467:GLN:HG3	2.00	0.43
1:A:84:LEU:CB	2:C:384:LEU:HD23	2.48	0.43
2:C:130:ILE:CG2	2:C:137:ILE:CD1	2.96	0.43
2:C:437:ARG:O	2:C:442:LEU:CD2	2.66	0.43
2:D:486:LYS:HZ3	2:D:486:LYS:HG3	1.14	0.43
2:D:550:ASN:O	2:D:553:MET:N	2.46	0.43
2:D:557:TYR:O	2:D:558:PRO:CA	2.59	0.43
2:C:524:GLN:HG3	2:C:575:TRP:CH2	2.54	0.43
1:B:72:PRO:O	1:B:74:ASP:N	2.52	0.43
2:D:196:LEU:HD12	2:D:258:ASN:HA	2.00	0.43
2:D:334:TYR:CD2	2:D:334:TYR:C	2.95	0.43
2:D:467:GLN:NE2	2:D:467:GLN:HA	2.34	0.43
2:C:503:PHE:O	2:C:504:ARG:C	2.61	0.43
2:C:528:LEU:HD12	2:C:528:LEU:HA	1.72	0.43
2:C:528:LEU:O	2:C:531:ILE:HG23	2.19	0.43
1:B:10:ILE:HG23	1:B:11:THR:CG2	2.44	0.43
1:B:13:MET:CG	1:B:14:CYS:N	2.73	0.43
1:B:22:LEU:HD23	2:D:322:PRO:HD3	2.00	0.43
2:D:200:ASN:HD22	2:D:202:ARG:N	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:ASN:OD1	2:D:271:TRP:CZ3	2.72	0.43
2:D:350:TYR:CZ	2:D:561:PHE:HE2	2.37	0.43
1:A:6:LYS:HE3	2:C:282:LYS:HZ2	1.83	0.42
2:C:417:LEU:O	2:C:420:LEU:N	2.46	0.42
2:D:251:THR:CG2	2:D:377:ILE:CD1	2.93	0.42
2:D:422:MET:O	2:D:426:ARG:CD	2.67	0.42
2:D:457:ASN:HB3	2:D:460:LEU:HB3	2.00	0.42
2:C:361:LEU:CB	2:C:401:GLU:CG	2.96	0.42
2:C:516:ASN:HB3	2:C:519:VAL:CG1	2.49	0.42
2:C:538:CYS:O	2:C:539:ASP:C	2.60	0.42
2:D:224:THR:HG21	2:D:367:ALA:CB	2.46	0.42
2:D:257:HIS:CE1	2:D:277:TYR:HD1	2.37	0.42
1:A:13:MET:HE3	1:A:13:MET:HB3	1.93	0.42
1:A:84:LEU:CD1	2:C:389:ALA:HA	2.41	0.42
1:A:87:MET:HE3	1:A:88:GLN:NE2	2.34	0.42
1:A:91:GLN:C	1:A:93:LEU:N	2.75	0.42
2:C:183:LEU:HD11	2:C:187:LEU:HD11	2.00	0.42
2:C:264:LEU:HD13	2:C:572:LEU:HD23	2.01	0.42
2:C:513:TRP:CD1	2:C:515:GLU:H	2.37	0.42
2:D:219:ASP:HB3	2:D:222:LEU:CD2	2.48	0.42
2:D:557:TYR:HB3	2:D:558:PRO:HD3	1.95	0.42
2:C:183:LEU:HG	2:C:184:ALA:N	2.34	0.42
2:C:383:GLY:H	2:C:385:MET:H	1.68	0.42
2:C:474:ILE:CD1	2:C:479:GLY:H	2.32	0.42
2:C:567:LEU:HD12	2:C:567:LEU:HA	1.87	0.42
2:D:433:TYR:CD1	2:D:494:LEU:CD2	3.03	0.42
3:G:2:NAG:C7	3:G:2:NAG:HO3	2.23	0.42
2:C:158:ILE:HD12	2:C:158:ILE:HG21	1.71	0.42
2:C:361:LEU:HD13	2:C:365:PHE:CE1	2.54	0.42
2:C:434:ASN:ND2	2:C:444:GLN:CA	2.83	0.42
2:C:485:LEU:HG	2:C:490:ARG:HA	2.02	0.42
2:D:370:ARG:HA	2:D:374:GLU:HB2	2.02	0.42
2:C:350:TYR:HE1	2:C:545:THR:HG23	1.84	0.42
2:C:417:LEU:C	2:C:419:ALA:N	2.77	0.42
2:C:447:THR:CG2	2:C:448:VAL:N	2.78	0.42
2:C:567:LEU:HA	2:C:568:PRO:HD2	1.94	0.42
2:D:297:LEU:O	2:D:299:LEU:N	2.52	0.42
2:D:339:ILE:HG23	2:D:339:ILE:HD13	1.68	0.42
2:D:487:ARG:O	2:D:488:LYS:HB3	2.19	0.42
2:D:507:ARG:HD2	2:D:508:ASP:OD1	2.18	0.42
1:A:18:ARG:HD3	2:C:318:ASP:OD2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:THR:H	2:C:117:THR:HG22	1.35	0.42
2:C:146:PHE:HZ	2:C:424:ARG:HA	1.84	0.42
2:C:169:SER:CB	2:C:324:ILE:HD12	2.46	0.42
2:C:177:TYR:CD2	2:C:281:ARG:CD	2.99	0.42
2:C:274:GLU:OE1	2:C:278:GLN:NE2	2.38	0.42
2:C:321:ASP:HA	2:C:322:PRO:HD3	1.63	0.42
2:C:422:MET:O	2:C:426:ARG:HD3	2.20	0.42
2:C:544:THR:HG23	2:C:545:THR:CG2	2.35	0.42
1:B:71:PHE:CD2	2:D:396:GLN:HA	2.54	0.42
2:D:144:ILE:HD12	2:D:144:ILE:HG21	1.58	0.42
2:D:243:MET:SD	5:D:602:HEM:CMC	3.07	0.42
2:D:534:PRO:CB	2:D:546:VAL:HG11	2.50	0.42
2:C:225:ASN:OD1	3:G:1:NAG:C5	2.68	0.42
1:B:10:ILE:CG2	1:B:11:THR:CG2	2.98	0.42
2:D:197:LEU:HD12	2:D:197:LEU:HA	1.44	0.42
2:D:295:ASP:OD1	2:D:295:ASP:N	2.50	0.42
2:D:339:ILE:HD12	2:D:339:ILE:HG21	1.82	0.42
2:C:321:ASP:CG	2:C:323:ARG:HH11	2.26	0.42
2:C:535:ARG:O	2:C:536:ILE:C	2.61	0.42
1:B:23:GLY:HA2	2:D:169:SER:OG	2.20	0.42
1:B:76:LEU:O	1:B:78:PRO:HD3	2.20	0.42
2:D:163:GLN:HG3	2:D:428:HIS:CG	2.55	0.42
2:D:403:ARG:HG3	2:D:418:PRO:HG2	2.00	0.42
2:D:458:LEU:O	2:D:462:ARG:HD2	2.20	0.42
1:A:99:PHE:CB	2:C:239:ARG:HH12	2.33	0.42
2:C:287:MET:HA	2:C:531:ILE:CD1	2.50	0.42
1:B:16:ASN:ND2	1:B:19:SER:N	2.61	0.42
1:B:53:ARG:CB	2:D:473:ASN:HD21	2.33	0.42
1:B:56:PHE:CD1	1:B:56:PHE:N	2.88	0.42
2:D:144:ILE:HA	2:D:145:PRO:HD2	1.58	0.42
2:D:297:LEU:O	2:D:301:LEU:CB	2.68	0.42
2:D:480:GLY:C	2:D:495:LEU:HD22	2.45	0.42
2:D:537:ILE:HG23	2:D:537:ILE:HD13	1.67	0.42
2:D:557:TYR:O	2:D:558:PRO:O	2.38	0.42
2:C:225:ASN:O	2:C:226:ARG:C	2.62	0.41
2:C:300:VAL:HG12	2:C:300:VAL:H	1.53	0.41
2:C:444:GLN:HA	2:C:445:PRO:HD3	1.85	0.41
2:C:537:ILE:HD13	2:C:537:ILE:HG21	1.89	0.41
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.61	0.41
2:D:177:TYR:CE1	2:D:257:HIS:CD2	3.07	0.41
2:D:199:VAL:HG12	2:D:200:ASN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:225:ASN:CG	3:J:1:NAG:HN2	2.28	0.41
2:D:230:ILE:HA	2:D:231:PRO:HD2	1.83	0.41
2:D:406:LEU:HB3	2:D:415:LEU:HB2	2.02	0.41
2:D:494:LEU:HA	2:D:494:LEU:HD12	1.83	0.41
1:A:29:PHE:HZ	1:A:100:THR:HG22	1.80	0.41
1:A:44:PRO:O	1:A:47:TRP:HB3	2.20	0.41
1:A:85:MET:SD	2:C:551:ILE:HG21	2.59	0.41
1:A:89:TRP:HD1	2:C:296:TYR:CD2	2.37	0.41
2:C:197:LEU:HD23	2:C:257:HIS:HB3	2.02	0.41
2:C:216:LEU:HD12	2:C:216:LEU:C	2.45	0.41
2:C:244:PRO:HD2	2:C:364:VAL:CG1	2.50	0.41
2:C:316:TYR:HB3	2:C:516:ASN:OD1	2.20	0.41
2:C:407:PHE:HB2	2:C:415:LEU:CD2	2.50	0.41
1:B:31:ARG:HH11	2:D:162:ASN:ND2	2.18	0.41
2:D:171:VAL:HG11	2:D:289:GLN:HA	2.01	0.41
2:D:177:TYR:HE1	2:D:197:LEU:HD21	1.84	0.41
2:D:299:LEU:HD21	2:D:553:MET:CE	2.50	0.41
2:D:299:LEU:HD21	2:D:553:MET:HE3	2.02	0.41
2:D:547:SER:HB3	2:D:551:ILE:HG23	2.02	0.41
1:A:10:ILE:HG23	1:A:11:THR:N	2.36	0.41
1:A:33:LEU:O	1:A:34:PRO:O	2.39	0.41
1:A:83:SER:O	1:A:86:PHE:CB	2.69	0.41
2:C:244:PRO:HD2	2:C:364:VAL:HG13	2.01	0.41
2:C:267:LEU:CD1	2:C:268:ASN:HD21	2.33	0.41
2:C:287:MET:C	2:C:290:ILE:HG22	2.44	0.41
2:C:369:TRP:O	2:C:373:LEU:HB2	2.20	0.41
2:C:447:THR:N	2:C:450:GLN:HE21	2.19	0.41
1:B:26:ASN:N	1:B:26:ASN:ND2	2.56	0.41
1:B:88:GLN:O	1:B:89:TRP:C	2.61	0.41
2:D:146:PHE:CZ	2:D:424:ARG:CZ	3.04	0.41
2:D:292:THR:HA	2:D:296:TYR:HB3	2.02	0.41
2:D:445:PRO:HA	2:D:450:GLN:HB3	2.02	0.41
2:D:451:LEU:HD12	2:D:451:LEU:HA	1.88	0.41
3:F:1:NAG:H61	3:F:2:NAG:O5	2.19	0.41
2:C:264:LEU:HD11	2:C:572:LEU:CG	2.51	0.41
2:C:485:LEU:HD23	2:C:490:ARG:CD	2.45	0.41
2:C:520:PHE:HD1	2:C:520:PHE:HA	1.79	0.41
2:C:570:LEU:HD23	2:C:570:LEU:HA	1.77	0.41
1:B:62:ARG:NH2	2:D:136:ARG:HB3	2.36	0.41
1:B:77:THR:HG23	2:D:396:GLN:NE2	2.36	0.41
2:D:346:LEU:HD12	2:D:352:PRO:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:MET:HE2	2:D:470:THR:HA	1.94	0.41
2:C:213:PHE:HE2	2:C:231:PRO:N	2.18	0.41
2:C:255:ARG:C	2:C:257:HIS:N	2.79	0.41
2:C:316:TYR:CD1	2:C:316:TYR:C	2.98	0.41
2:C:332:PHE:HD1	2:C:332:PHE:HA	1.81	0.41
1:B:31:ARG:NH1	2:D:162:ASN:ND2	2.69	0.41
2:D:130:ILE:HD12	2:D:137:ILE:HD11	2.02	0.41
2:D:194:LEU:N	2:D:194:LEU:HD13	2.35	0.41
2:D:447:THR:H	2:D:450:GLN:HB2	1.85	0.41
2:D:458:LEU:CD2	2:D:462:ARG:NH1	2.75	0.41
1:A:17:ARG:NH1	2:C:511:ARG:NH1	2.67	0.41
2:C:196:LEU:HD12	2:C:196:LEU:HA	1.74	0.41
2:C:244:PRO:CA	2:C:247:THR:HG22	2.51	0.41
1:B:95:HIS:O	2:D:167:LEU:HD23	2.21	0.41
2:D:177:TYR:HH	2:D:284:VAL:HG11	1.84	0.41
2:D:531:ILE:O	2:D:531:ILE:HG12	2.10	0.41
1:A:87:MET:CB	2:C:338:LEU:HB3	2.51	0.41
2:C:223:LEU:HA	2:C:223:LEU:HD12	1.78	0.41
2:C:287:MET:O	2:C:290:ILE:CG2	2.69	0.41
2:D:173:ALA:HB1	2:D:176:VAL:HG13	2.01	0.41
2:D:177:TYR:OH	2:D:284:VAL:HG11	2.20	0.41
2:D:248:SER:CA	2:D:251:THR:HG22	2.49	0.41
2:D:491:VAL:HG21	2:D:499:ILE:HD12	2.02	0.41
2:D:550:ASN:C	2:D:553:MET:H	2.28	0.41
1:A:94:ASP:OD1	5:C:601:HEM:HMA2	2.18	0.41
2:C:177:TYR:HD2	2:C:281:ARG:HG3	1.83	0.41
2:C:243:MET:C	2:C:245:GLU:N	2.76	0.41
1:B:42:SER:O	1:B:42:SER:OG	2.28	0.41
2:D:130:ILE:CD1	2:D:137:ILE:HG12	2.42	0.41
2:D:175:MET:SD	2:D:175:MET:N	2.94	0.41
2:D:433:TYR:CE1	2:D:483:GLU:OE2	2.74	0.41
2:D:528:LEU:HD12	2:D:528:LEU:HA	1.72	0.41
2:D:544:THR:CG2	2:D:545:THR:N	2.84	0.41
2:D:567:LEU:HD12	2:D:567:LEU:HA	1.47	0.41
1:A:41:PHE:CD1	1:A:42:SER:N	2.88	0.41
2:C:282:LYS:HE2	2:C:520:PHE:CE1	2.56	0.41
2:C:291:ILE:HG22	2:C:292:THR:N	2.30	0.41
2:C:297:LEU:C	2:C:300:VAL:HG12	2.46	0.41
2:C:321:ASP:OD1	2:C:322:PRO:CD	2.69	0.41
2:C:322:PRO:HD2	2:C:323:ARG:H	1.85	0.41
2:C:385:MET:HG2	2:C:547:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:O	1:B:53:ARG:O	2.38	0.41
2:D:189:ASN:OD1	3:I:1:NAG:C2	2.69	0.41
2:D:197:LEU:HB3	2:D:254:LEU:CD1	2.51	0.41
2:D:244:PRO:HD2	2:D:364:VAL:HG21	2.03	0.41
2:D:417:LEU:HD12	2:D:417:LEU:HA	1.81	0.41
2:D:567:LEU:C	2:D:568:PRO:O	2.63	0.41
1:A:7:TYR:OH	2:C:279:GLU:OE2	2.23	0.41
1:A:10:ILE:CG2	2:C:181:GLU:CD	2.94	0.41
2:C:177:TYR:HD2	2:C:281:ARG:HD2	1.83	0.41
2:C:196:LEU:HD12	2:C:258:ASN:ND2	2.36	0.41
2:C:197:LEU:HB3	2:C:254:LEU:HD12	2.03	0.41
2:C:293:TYR:CE2	2:C:513:TRP:HZ3	2.39	0.41
2:C:448:VAL:H	2:C:448:VAL:HG12	1.57	0.41
1:B:30:VAL:HG22	2:D:323:ARG:CG	2.26	0.41
1:B:73:THR:H	1:B:73:THR:HG22	1.63	0.41
2:D:137:ILE:HD12	2:D:137:ILE:HG21	1.63	0.41
2:D:237:ASP:CG	2:D:239:ARG:HH11	2.29	0.41
2:C:271:TRP:NE1	2:C:275:ARG:NH1	2.69	0.40
2:C:290:ILE:CG2	2:C:291:ILE:N	2.84	0.40
2:C:381:LEU:HD13	2:C:381:LEU:HA	1.66	0.40
1:B:10:ILE:CG2	1:B:11:THR:N	2.84	0.40
1:B:18:ARG:NH2	2:D:319:SER:OG	2.51	0.40
2:D:224:THR:HG21	2:D:369:TRP:HE1	1.86	0.40
2:D:295:ASP:O	2:D:552:PHE:CD2	2.74	0.40
2:D:304:THR:HG23	2:D:305:ALA:N	2.36	0.40
2:D:345:ARG:HH11	2:D:345:ARG:HD3	1.48	0.40
2:D:353:MET:C	2:D:355:PRO:CD	2.81	0.40
2:C:224:THR:CG2	2:C:369:TRP:HE1	2.34	0.40
2:C:327:VAL:C	2:C:329:THR:N	2.78	0.40
1:B:79:ASP:HB3	2:D:389:ALA:O	2.22	0.40
2:D:522:MET:HA	2:D:525:ARG:HG3	2.03	0.40
1:A:82:ARG:HA	2:C:552:PHE:O	2.22	0.40
2:C:137:ILE:O	2:C:137:ILE:HG12	2.19	0.40
2:C:248:SER:CA	2:C:377:ILE:HD11	2.52	0.40
2:C:290:ILE:HD12	2:C:514:TRP:CH2	2.56	0.40
2:C:346:LEU:HD12	2:C:353:MET:N	2.24	0.40
2:D:128:LEU:HB3	2:D:144:ILE:HG12	2.03	0.40
2:D:295:ASP:HB2	2:D:552:PHE:CE2	2.56	0.40
2:D:403:ARG:HH21	2:D:404:GLU:CD	2.30	0.40
1:A:102:GLU:OE2	2:C:424:ARG:NH2	2.55	0.40
2:C:177:TYR:HD2	2:C:281:ARG:CG	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:ARG:HH11	2:C:281:ARG:HD3	1.60	0.40
2:C:327:VAL:O	2:C:328:PHE:C	2.64	0.40
2:C:393:ARG:CD	2:C:396:GLN:HE22	2.34	0.40
2:C:476:ILE:HD13	2:C:476:ILE:HG21	1.84	0.40
2:D:330:ASN:HA	2:D:333:ARG:HD2	2.02	0.40
2:D:343:MET:HB3	2:D:359:VAL:HG13	2.03	0.40
2:C:519:VAL:H	2:C:519:VAL:HG13	1.65	0.40
2:C:532:SER:C	2:C:534:PRO:CD	2.85	0.40
2:D:252:LEU:HD21	2:D:537:ILE:HG22	2.03	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	102/108 (94%)	75 (74%)	22 (22%)	5 (5%)	1	10
1	B	100/108 (93%)	80 (80%)	13 (13%)	7 (7%)	1	4
2	C	460/466 (99%)	349 (76%)	84 (18%)	27 (6%)	1	7
2	D	460/466 (99%)	356 (77%)	82 (18%)	22 (5%)	2	11
All	All	1122/1148 (98%)	860 (77%)	201 (18%)	61 (5%)	1	9

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	123	PRO
2	C	303	PRO
2	C	352	PRO
2	C	376	GLY
2	C	560	ASP
2	D	123	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	124	PRO
2	D	354	GLU
2	D	429	GLY
2	D	555	ASN
2	D	568	PRO
1	A	73	THR
1	A	85	MET
2	C	135	PRO
2	C	218	ASP
2	C	270	ARG
2	C	354	GLU
2	C	362	SER
2	C	397	ILE
2	C	469	GLY
2	C	550	ASN
2	C	558	PRO
1	B	53	ARG
1	B	59	ALA
1	B	73	THR
2	D	175	MET
2	D	270	ARG
2	D	441	GLY
1	A	42	SER
2	C	269	PRO
2	C	394	GLN
2	C	415	LEU
2	C	457	ASN
1	B	26	ASN
1	B	42	SER
2	D	206	ASN
2	D	207	GLY
2	D	258	ASN
2	D	434	ASN
1	A	34	PRO
1	A	103	PRO
2	C	514	TRP
2	D	228	ALA
2	D	349	ARG
2	D	352	PRO
2	D	397	ILE
2	C	212	PRO
2	C	355	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	401	GLU
1	B	103	PRO
2	D	401	GLU
2	D	549	ASN
2	C	417	LEU
1	B	2	PRO
2	C	341	PRO
2	C	131	PRO
2	C	124	PRO
2	C	357	PRO
2	D	417	LEU
2	D	269	PRO
2	D	452	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/93 (95%)	54 (61%)	34 (39%)	0	1
1	B	88/93 (95%)	56 (64%)	32 (36%)	0	1
2	C	386/411 (94%)	220 (57%)	166 (43%)	0	0
2	D	386/411 (94%)	219 (57%)	167 (43%)	0	0
All	All	948/1008 (94%)	549 (58%)	399 (42%)	0	0

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	9	THR
1	A	10	ILE
1	A	13	MET
1	A	14	CYS
1	A	17	ARG
1	A	19	SER
1	A	21	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	22	LEU
1	A	27	ARG
1	A	30	VAL
1	A	31	ARG
1	A	33	LEU
1	A	38	GLU
1	A	41	PHE
1	A	42	SER
1	A	45	TYR
1	A	48	THR
1	A	53	ARG
1	A	54	ASN
1	A	60	LEU
1	A	64	VAL
1	A	68	ILE
1	A	69	VAL
1	A	71	PHE
1	A	74	ASP
1	A	77	THR
1	A	81	GLU
1	A	82	ARG
1	A	84	LEU
1	A	85	MET
1	A	92	LEU
1	A	93	LEU
1	A	102	GLU
2	C	115	CYS
2	C	116	GLU
2	C	117	THR
2	C	120	VAL
2	C	122	GLN
2	C	125	CYS
2	C	129	LYS
2	C	130	ILE
2	C	133	ASN
2	C	134	ASP
2	C	137	ILE
2	C	138	LYS
2	C	139	ASN
2	C	144	ILE
2	C	149	SER
2	C	156	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	157	ASN
2	C	158	ILE
2	C	159	THR
2	C	161	ARG
2	C	162	ASN
2	C	163	GLN
2	C	164	ILE
2	C	169	SER
2	C	172	ASP
2	C	174	SER
2	C	175	MET
2	C	181	GLU
2	C	186	ASN
2	C	188	ARG
2	C	189	ASN
2	C	190	MET
2	C	192	ASN
2	C	193	GLN
2	C	194	LEU
2	C	196	LEU
2	C	197	LEU
2	C	199	VAL
2	C	203	PHE
2	C	210	LEU
2	C	211	LEU
2	C	217	HIS
2	C	218	ASP
2	C	222	LEU
2	C	223	LEU
2	C	230	ILE
2	C	234	LEU
2	C	238	THR
2	C	239	ARG
2	C	242	GLU
2	C	249	MET
2	C	251	THR
2	C	254	LEU
2	C	255	ARG
2	C	259	ARG
2	C	260	LEU
2	C	262	THR
2	C	263	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	264	LEU
2	C	265	LYS
2	C	267	LEU
2	C	268	ASN
2	C	270	ARG
2	C	275	ARG
2	C	276	LEU
2	C	277	TYR
2	C	278	GLN
2	C	283	ILE
2	C	284	VAL
2	C	287	MET
2	C	288	VAL
2	C	289	GLN
2	C	294	ARG
2	C	295	ASP
2	C	297	LEU
2	C	299	LEU
2	C	300	VAL
2	C	304	THR
2	C	306	MET
2	C	310	LEU
2	C	316	TYR
2	C	318	ASP
2	C	319	SER
2	C	320	VAL
2	C	323	ARG
2	C	324	ILE
2	C	326	ASN
2	C	329	THR
2	C	330	ASN
2	C	332	PHE
2	C	333	ARG
2	C	338	LEU
2	C	339	ILE
2	C	340	GLN
2	C	345	ARG
2	C	346	LEU
2	C	347	ASP
2	C	348	ASN
2	C	351	GLN
2	C	353	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	358	ARG
2	C	361	LEU
2	C	364	VAL
2	C	370	ARG
2	C	373	LEU
2	C	377	ILE
2	C	381	LEU
2	C	382	ARG
2	C	384	LEU
2	C	385	MET
2	C	390	LYS
2	C	393	ARG
2	C	394	GLN
2	C	396	GLN
2	C	399	VAL
2	C	402	ILE
2	C	405	ARG
2	C	411	MET
2	C	415	LEU
2	C	423	GLN
2	C	424	ARG
2	C	425	SER
2	C	426	ARG
2	C	437	ARG
2	C	442	LEU
2	C	444	GLN
2	C	448	VAL
2	C	451	LEU
2	C	455	LEU
2	C	458	LEU
2	C	459	LYS
2	C	460	LEU
2	C	464	LEU
2	C	465	MET
2	C	467	GLN
2	C	472	ASN
2	C	473	ASN
2	C	474	ILE
2	C	476	ILE
2	C	478	MET
2	C	482	SER
2	C	486	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	495	LEU
2	C	498	ILE
2	C	501	THR
2	C	506	LEU
2	C	507	ARG
2	C	519	VAL
2	C	524	GLN
2	C	525	ARG
2	C	526	GLN
2	C	531	ILE
2	C	535	ARG
2	C	537	ILE
2	C	541	THR
2	C	543	ILE
2	C	546	VAL
2	C	549	ASN
2	C	553	MET
2	C	555	ASN
2	C	560	ASP
2	C	562	VAL
2	C	567	LEU
2	C	570	LEU
2	C	571	ASN
2	C	574	SER
1	B	4	GLN
1	B	5	ASP
1	B	6	LYS
1	B	9	THR
1	B	10	ILE
1	B	11	THR
1	B	13	MET
1	B	15	ASN
1	B	16	ASN
1	B	19	SER
1	B	21	THR
1	B	25	SER
1	B	26	ASN
1	B	27	ARG
1	B	33	LEU
1	B	36	GLU
1	B	39	ASP
1	B	41	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	LEU
1	B	58	VAL
1	B	64	VAL
1	B	68	ILE
1	B	69	VAL
1	B	71	PHE
1	B	73	THR
1	B	74	ASP
1	B	76	LEU
1	B	77	THR
1	B	82	ARG
1	B	87	MET
1	B	88	GLN
1	B	100	THR
2	D	115	CYS
2	D	116	GLU
2	D	117	THR
2	D	120	VAL
2	D	125	CYS
2	D	128	LEU
2	D	130	ILE
2	D	133	ASN
2	D	137	ILE
2	D	138	LYS
2	D	144	ILE
2	D	147	PHE
2	D	156	SER
2	D	157	ASN
2	D	158	ILE
2	D	160	ILE
2	D	161	ARG
2	D	162	ASN
2	D	163	GLN
2	D	167	LEU
2	D	169	SER
2	D	171	VAL
2	D	172	ASP
2	D	174	SER
2	D	175	MET
2	D	176	VAL
2	D	179	SER
2	D	180	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	186	ASN
2	D	187	LEU
2	D	189	ASN
2	D	190	MET
2	D	191	SER
2	D	194	LEU
2	D	196	LEU
2	D	197	LEU
2	D	206	ASN
2	D	210	LEU
2	D	216	LEU
2	D	218	ASP
2	D	222	LEU
2	D	223	LEU
2	D	225	ASN
2	D	227	SER
2	D	229	ARG
2	D	230	ILE
2	D	234	LEU
2	D	238	THR
2	D	239	ARG
2	D	242	GLU
2	D	243	MET
2	D	245	GLU
2	D	246	LEU
2	D	247	THR
2	D	249	MET
2	D	254	LEU
2	D	256	GLU
2	D	257	HIS
2	D	258	ASN
2	D	262	THR
2	D	264	LEU
2	D	265	LYS
2	D	267	LEU
2	D	268	ASN
2	D	272	ASP
2	D	274	GLU
2	D	279	GLU
2	D	284	VAL
2	D	287	MET
2	D	288	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	289	GLN
2	D	292	THR
2	D	295	ASP
2	D	297	LEU
2	D	299	LEU
2	D	300	VAL
2	D	310	LEU
2	D	316	TYR
2	D	319	SER
2	D	326	ASN
2	D	329	THR
2	D	330	ASN
2	D	333	ARG
2	D	338	LEU
2	D	339	ILE
2	D	340	GLN
2	D	343	MET
2	D	345	ARG
2	D	346	LEU
2	D	348	ASN
2	D	358	ARG
2	D	359	VAL
2	D	364	VAL
2	D	368	SER
2	D	370	ARG
2	D	373	LEU
2	D	377	ILE
2	D	380	ILE
2	D	381	LEU
2	D	385	MET
2	D	387	THR
2	D	390	LYS
2	D	391	LEU
2	D	393	ARG
2	D	397	ILE
2	D	399	VAL
2	D	402	ILE
2	D	403	ARG
2	D	404	GLU
2	D	405	ARG
2	D	409	GLN
2	D	410	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	411	MET
2	D	417	LEU
2	D	422	MET
2	D	423	GLN
2	D	424	ARG
2	D	426	ARG
2	D	427	ASP
2	D	434	ASN
2	D	442	LEU
2	D	444	GLN
2	D	453	THR
2	D	454	VAL
2	D	456	ARG
2	D	457	ASN
2	D	458	LEU
2	D	459	LYS
2	D	462	ARG
2	D	464	LEU
2	D	465	MET
2	D	470	THR
2	D	473	ASN
2	D	476	ILE
2	D	482	SER
2	D	485	LEU
2	D	486	LYS
2	D	490	ARG
2	D	491	VAL
2	D	495	LEU
2	D	497	CYS
2	D	498	ILE
2	D	505	LYS
2	D	506	LEU
2	D	507	ARG
2	D	519	VAL
2	D	523	GLN
2	D	524	GLN
2	D	526	GLN
2	D	528	LEU
2	D	530	GLN
2	D	531	ILE
2	D	537	ILE
2	D	540	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	541	THR
2	D	543	ILE
2	D	546	VAL
2	D	551	ILE
2	D	554	SER
2	D	556	SER
2	D	560	ASP
2	D	562	VAL
2	D	567	LEU
2	D	570	LEU
2	D	571	ASN
2	D	572	LEU
2	D	574	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	ASN
1	A	54	ASN
1	A	66	ASN
1	A	95	HIS
2	C	121	GLN
2	C	133	ASN
2	C	139	ASN
2	C	162	ASN
2	C	163	GLN
2	C	165	ASN
2	C	192	ASN
2	C	193	GLN
2	C	217	HIS
2	C	250	HIS
2	C	257	HIS
2	C	258	ASN
2	C	278	GLN
2	C	289	GLN
2	C	330	ASN
2	C	348	ASN
2	C	356	ASN
2	C	392	ASN
2	C	394	GLN
2	C	421	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	423	GLN
2	C	434	ASN
2	C	444	GLN
2	C	450	GLN
2	C	467	GLN
2	C	502	GLN
2	C	524	GLN
2	C	540	ASN
2	C	549	ASN
2	C	550	ASN
2	C	571	ASN
1	B	4	GLN
1	B	15	ASN
1	B	16	ASN
1	B	26	ASN
1	B	66	ASN
1	B	95	HIS
2	D	121	GLN
2	D	139	ASN
2	D	162	ASN
2	D	163	GLN
2	D	165	ASN
2	D	192	ASN
2	D	200	ASN
2	D	206	ASN
2	D	250	HIS
2	D	258	ASN
2	D	268	ASN
2	D	289	GLN
2	D	326	ASN
2	D	330	ASN
2	D	340	GLN
2	D	394	GLN
2	D	395	ASN
2	D	396	GLN
2	D	423	GLN
2	D	434	ASN
2	D	450	GLN
2	D	457	ASN
2	D	523	GLN
2	D	524	GLN
2	D	540	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	550	ASN
2	D	571	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,2	14,14,15	1.10	1 (7%)	17,19,21	1.77	4 (23%)
3	NAG	E	2	3	14,14,15	1.76	2 (14%)	17,19,21	0.94	0
3	NAG	F	1	3,2	14,14,15	1.05	1 (7%)	17,19,21	1.55	3 (17%)
3	NAG	F	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.01	2 (11%)
3	NAG	G	1	3,2	14,14,15	1.01	1 (7%)	17,19,21	1.76	2 (11%)
3	NAG	G	2	3	14,14,15	1.13	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	H	1	3,2	14,14,15	1.17	2 (14%)	17,19,21	1.55	3 (17%)
3	NAG	H	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	I	1	3,2	14,14,15	0.99	1 (7%)	17,19,21	1.65	2 (11%)
3	NAG	I	2	3	14,14,15	0.93	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	J	1	3,2	14,14,15	1.08	1 (7%)	17,19,21	1.52	4 (23%)
3	NAG	J	2	3	14,14,15	0.98	1 (7%)	17,19,21	0.84	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O4-C4	5.48	1.56	1.43
3	F	2	NAG	C8-C7	3.46	1.57	1.50
3	E	1	NAG	C8-C7	3.37	1.57	1.50
3	F	1	NAG	C8-C7	3.37	1.57	1.50
3	H	1	NAG	C8-C7	3.37	1.57	1.50
3	G	1	NAG	C8-C7	3.36	1.57	1.50
3	J	2	NAG	C8-C7	3.36	1.57	1.50
3	E	2	NAG	C8-C7	3.34	1.57	1.50
3	I	2	NAG	C8-C7	3.34	1.57	1.50
3	I	1	NAG	C8-C7	3.32	1.57	1.50
3	G	2	NAG	C8-C7	3.32	1.57	1.50
3	H	2	NAG	C8-C7	3.24	1.57	1.50
3	J	1	NAG	C8-C7	3.23	1.57	1.50
3	H	1	NAG	O5-C5	2.04	1.47	1.43
3	G	2	NAG	C1-C2	2.04	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O4-C4-C5	-5.91	94.78	109.32
3	I	1	NAG	O4-C4-C5	5.81	123.63	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O4-C4-C5	4.90	121.39	109.32
3	E	1	NAG	O4-C4-C5	-4.79	97.53	109.32
3	H	1	NAG	O5-C5-C6	-4.39	99.11	107.66
3	E	1	NAG	O5-C5-C6	-3.76	100.34	107.66
3	J	1	NAG	O4-C4-C5	3.72	118.48	109.32
3	H	2	NAG	C1-O5-C5	2.66	115.75	112.19
3	H	1	NAG	O5-C1-C2	-2.66	107.18	111.29
3	J	1	NAG	O5-C5-C6	-2.64	102.53	107.66
3	G	1	NAG	O5-C5-C6	2.52	112.56	107.66
3	H	1	NAG	C1-O5-C5	2.36	115.35	112.19
3	E	1	NAG	O5-C1-C2	-2.36	107.64	111.29
3	G	2	NAG	C1-O5-C5	2.35	115.34	112.19
3	J	1	NAG	C1-O5-C5	2.35	115.33	112.19
3	F	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	F	2	NAG	C1-O5-C5	2.24	115.19	112.19
3	F	1	NAG	O5-C5-C6	-2.23	103.32	107.66
3	J	1	NAG	O5-C1-C2	-2.21	107.87	111.29
3	E	1	NAG	C1-O5-C5	2.20	115.14	112.19
3	I	1	NAG	C1-O5-C5	2.20	115.14	112.19
3	J	2	NAG	O4-C4-C5	-2.10	104.16	109.32
3	F	2	NAG	O3-C3-C4	-2.08	105.46	110.38
3	I	2	NAG	C1-O5-C5	2.05	114.93	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1	NAG	C1
3	J	1	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C3-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

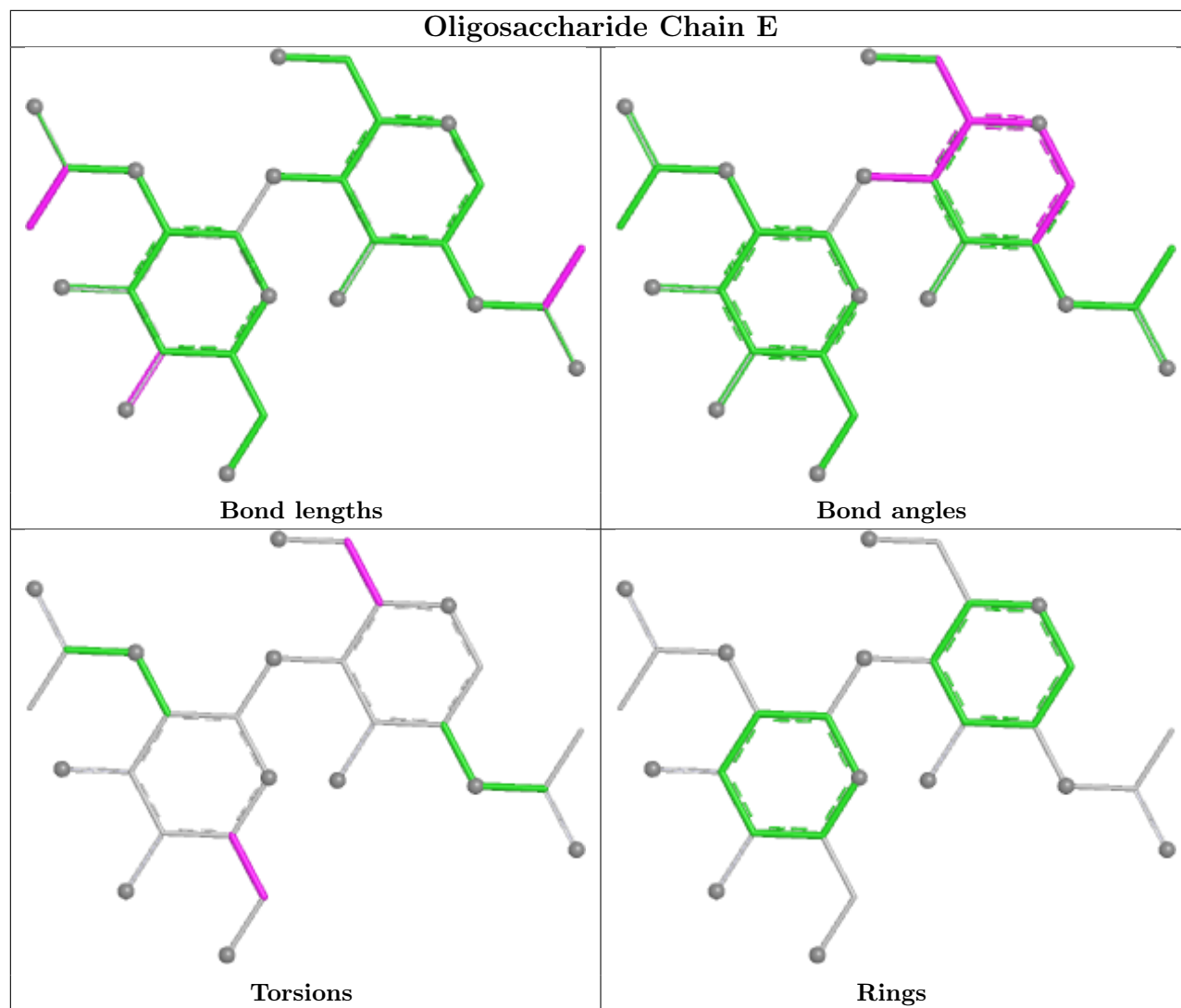
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C3-C2-N2-C7

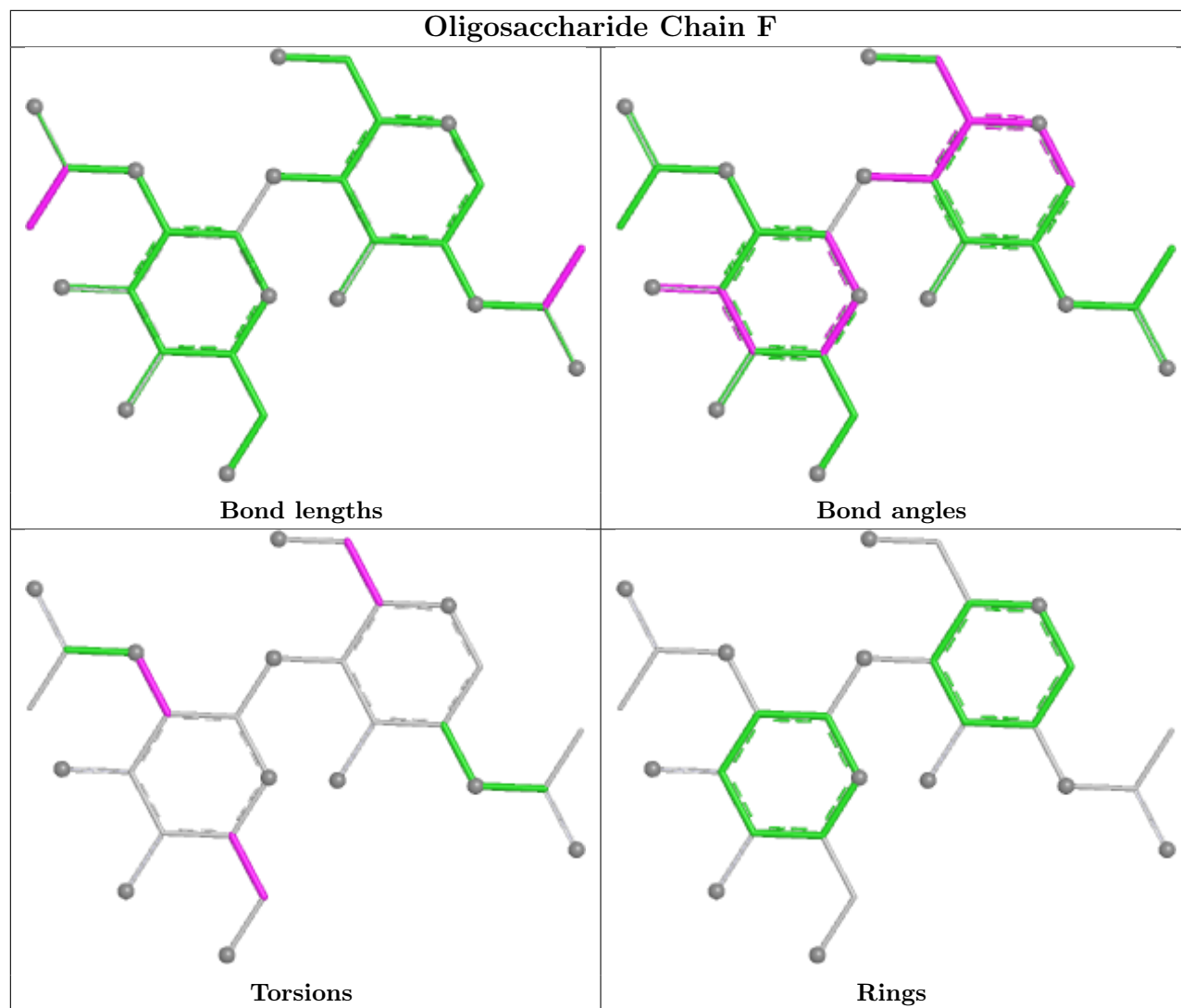
There are no ring outliers.

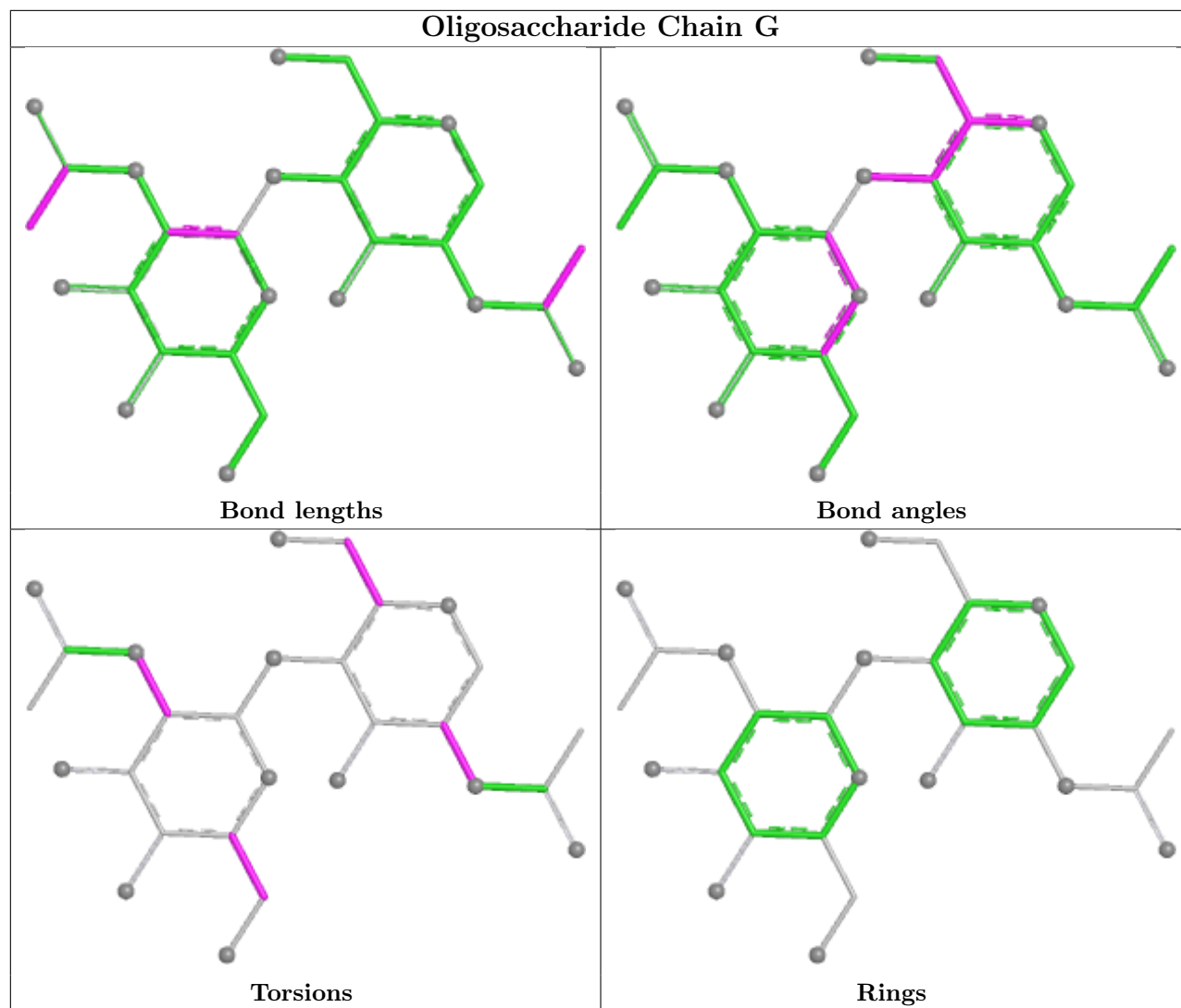
11 monomers are involved in 23 short contacts:

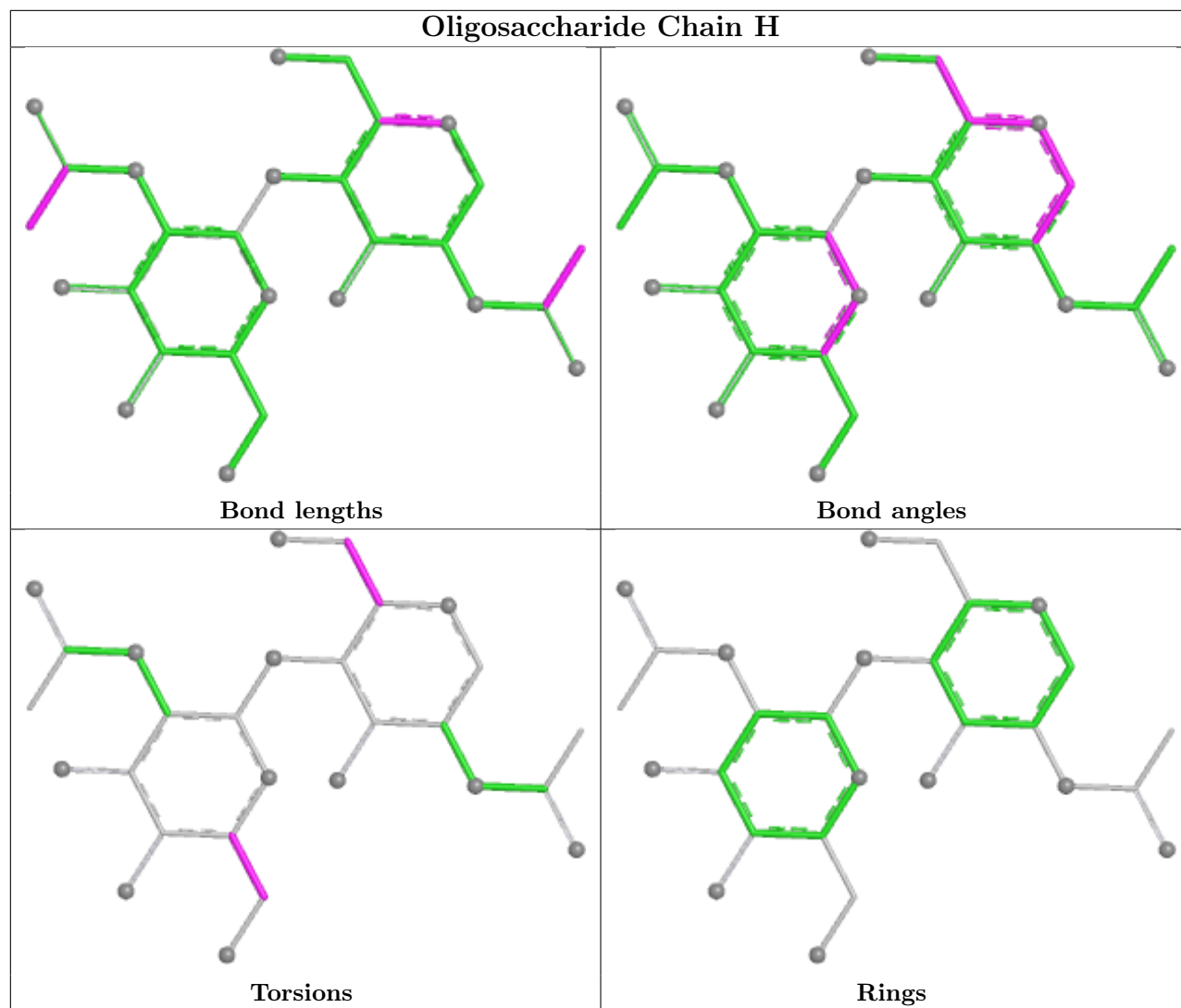
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	3	0
3	F	1	NAG	1	0
3	G	1	NAG	3	0
3	E	1	NAG	1	0
3	J	1	NAG	7	0
3	I	1	NAG	5	0
3	F	2	NAG	1	0
3	H	2	NAG	1	0
3	I	2	NAG	4	0
3	J	2	NAG	2	0
3	E	2	NAG	2	0

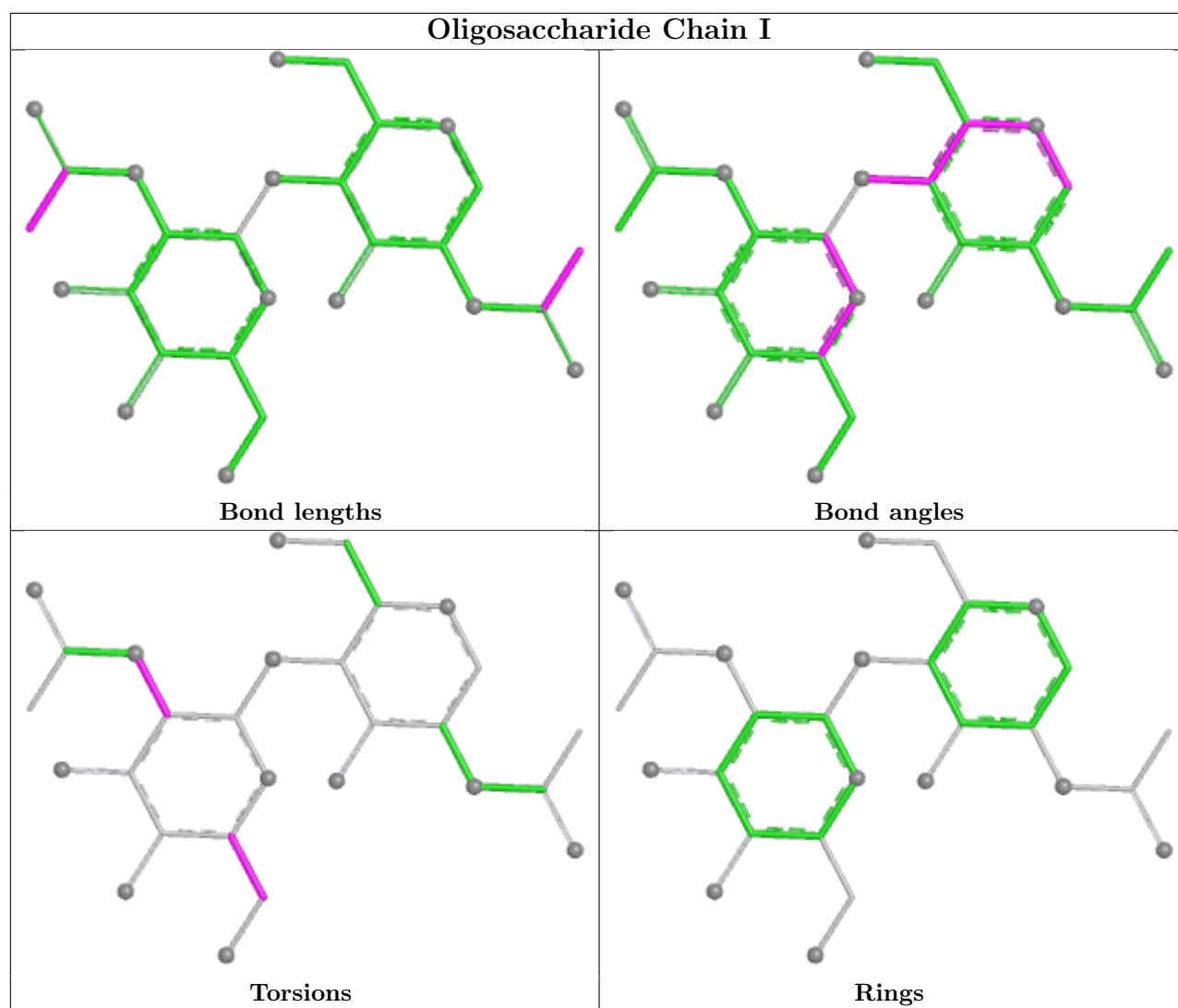
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

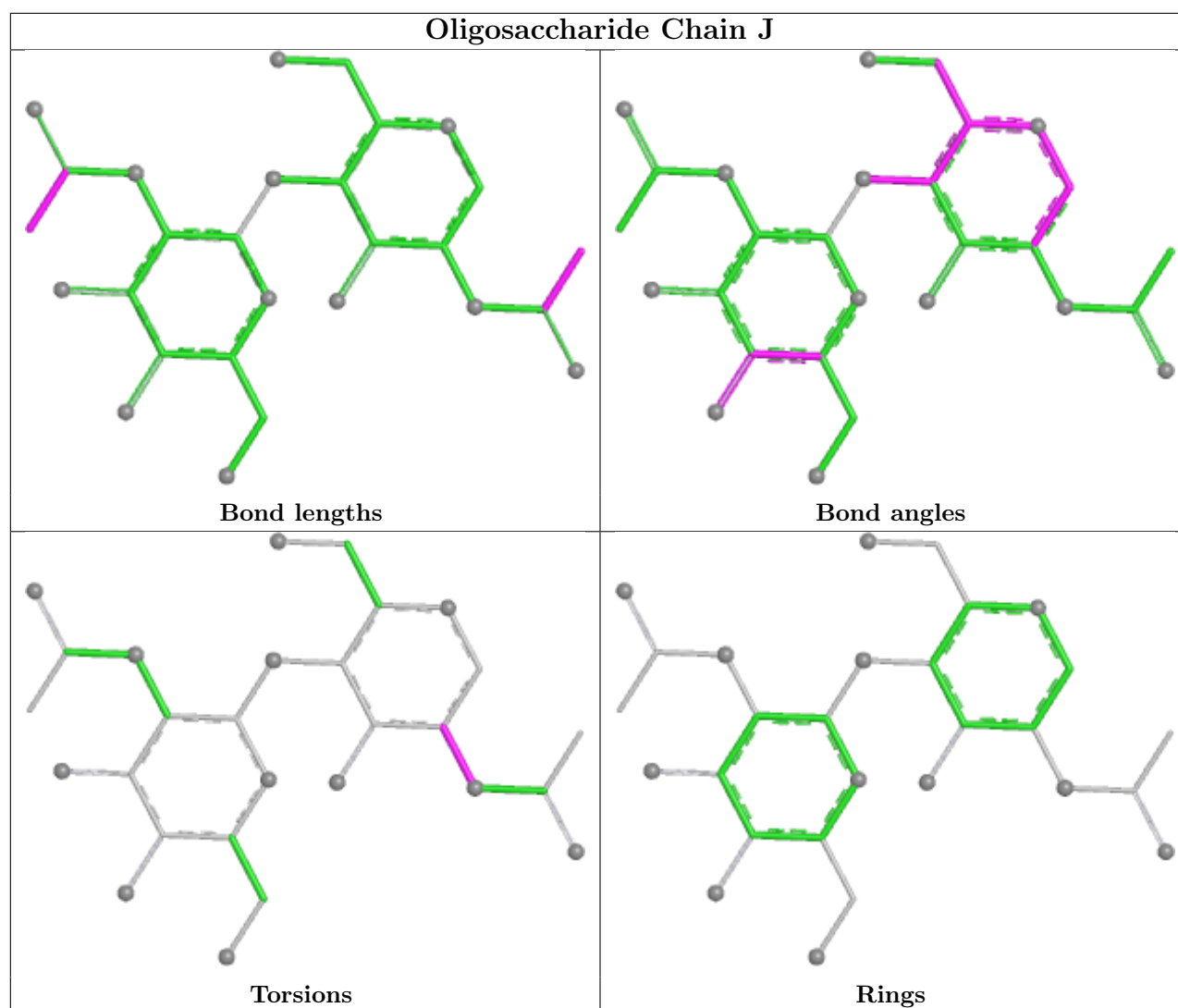












5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	HEM	C	601	2	50,50,50	1.87	6 (12%)	67,82,82	1.29	6 (8%)
5	HEM	D	602	2	50,50,50	1.46	8 (16%)	67,82,82	1.13	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	C	601	2	-	5/14/54/54	-
5	HEM	D	602	2	-	5/14/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	HEM	FE-NC	7.26	2.19	1.95
5	C	601	HEM	FE-ND	6.97	2.16	1.94
5	D	602	HEM	FE-NB	4.01	2.07	1.94
5	D	602	HEM	CHD-C1D	-3.68	1.30	1.39
5	D	602	HEM	FE-ND	3.16	2.04	1.94
5	D	602	HEM	O2D-CGD	-3.15	1.20	1.30
5	C	601	HEM	O2A-CGA	-3.14	1.20	1.30
5	C	601	HEM	O2D-CGD	-3.11	1.20	1.30
5	D	602	HEM	O2A-CGA	-3.11	1.20	1.30
5	D	602	HEM	C1D-ND	-2.56	1.33	1.38
5	C	601	HEM	C1B-NB	-2.30	1.36	1.40
5	C	601	HEM	C1C-NC	-2.29	1.35	1.39
5	D	602	HEM	C1B-NB	-2.25	1.36	1.40
5	D	602	HEM	CHD-C4C	-2.05	1.34	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	HEM	C2A-C1A-NA	-4.38	105.29	110.15
5	C	601	HEM	CHC-C4B-NB	3.09	127.75	124.42
5	D	602	HEM	CHD-C4C-NC	2.42	127.09	124.45
5	C	601	HEM	CHD-C4C-NC	2.24	126.89	124.45
5	D	602	HEM	CHD-C4C-C3C	-2.17	121.55	125.21
5	D	602	HEM	CAD-CBD-CGD	-2.15	107.96	113.67
5	C	601	HEM	CAD-CBD-CGD	-2.13	108.02	113.67
5	D	602	HEM	C2A-C1A-NA	-2.11	107.81	110.15
5	D	602	HEM	CAA-CBA-CGA	-2.10	108.10	113.67
5	C	601	HEM	CAA-CBA-CGA	-2.09	108.12	113.67
5	C	601	HEM	C3A-C4A-NA	-2.07	106.83	110.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

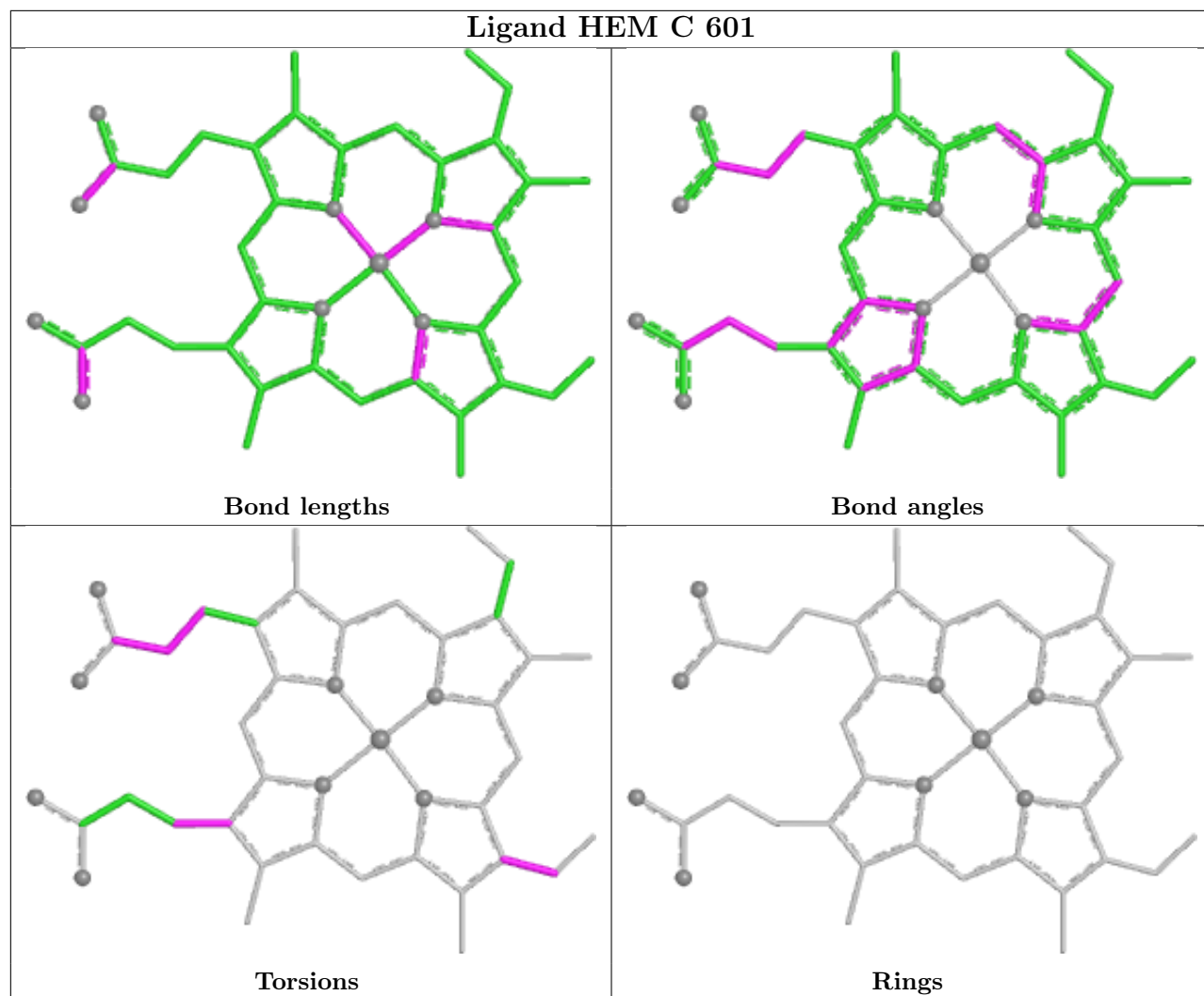
Mol	Chain	Res	Type	Atoms
5	C	601	HEM	C3D-CAD-CBD-CGD
5	C	601	HEM	C4B-C3B-CAB-CBB
5	D	602	HEM	C4B-C3B-CAB-CBB
5	D	602	HEM	C2A-CAA-CBA-CGA
5	C	601	HEM	C3A-C2A-CAA-CBA
5	C	601	HEM	CAD-CBD-CGD-O1D
5	C	601	HEM	CAD-CBD-CGD-O2D
5	D	602	HEM	CAA-CBA-CGA-O2A
5	D	602	HEM	CAA-CBA-CGA-O1A
5	D	602	HEM	CAD-CBD-CGD-O1D

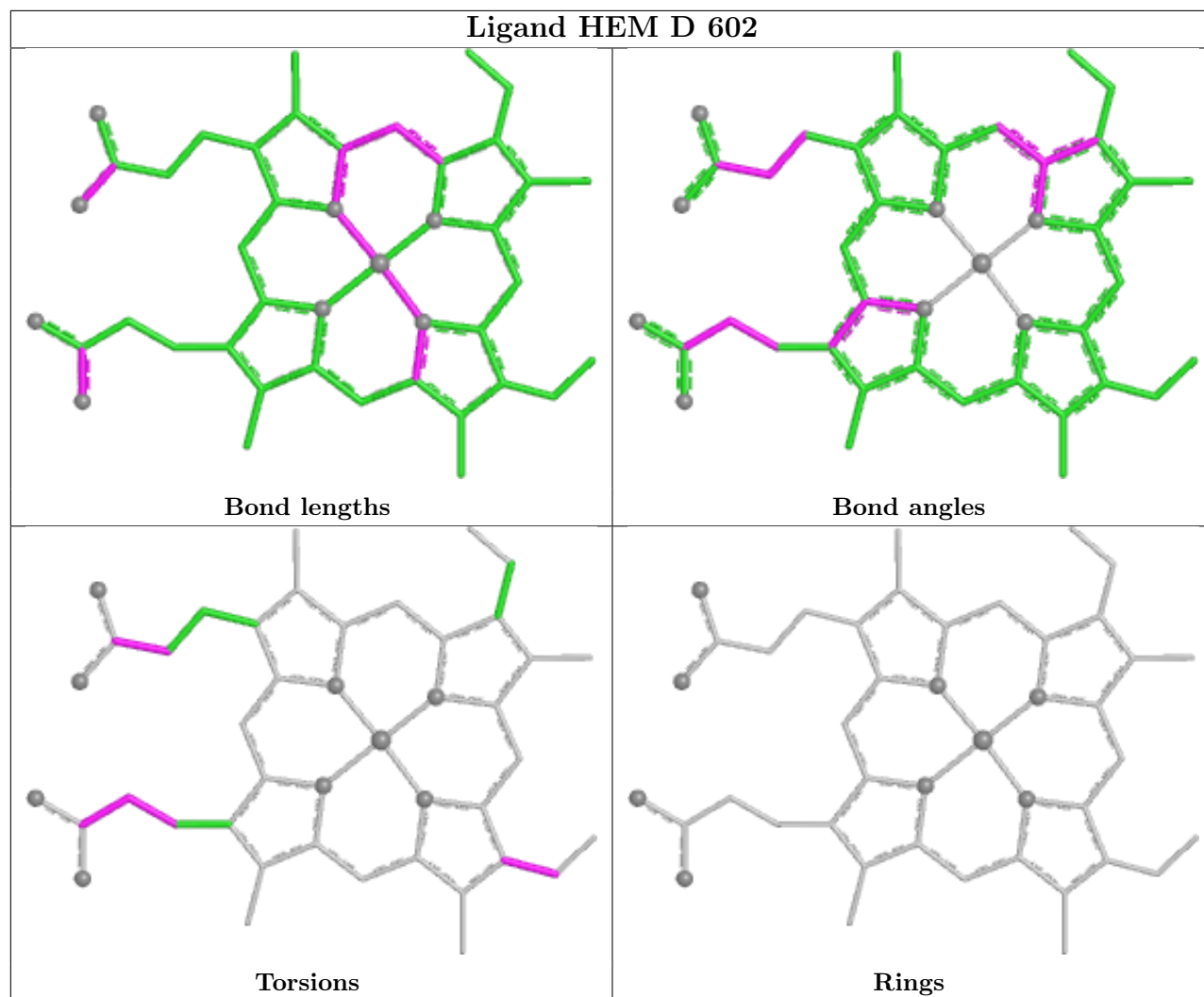
There are no ring outliers.

2 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	HEM	35	0
5	D	602	HEM	33	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	11
2	C	5
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3:GLU	C	4:GLN	N	2.32
1	C	560:ASP	C	561:PHE	N	1.95
1	D	179:SER	C	180:GLU	N	1.81
1	D	560:ASP	C	561:PHE	N	1.78
1	D	203:PHE	C	204:GLN	N	1.74
1	D	557:TYR	C	558:PRO	N	1.73
1	C	516:ASN	C	517:GLU	N	1.72
1	D	556:SER	C	557:TYR	N	1.67
1	C	228:ALA	C	229:ARG	N	1.66
1	D	184:ALA	C	185:ARG	N	1.65
1	C	347:ASP	C	348:ASN	N	1.63
1	D	347:ASP	C	348:ASN	N	1.60
1	C	458:LEU	C	459:LYS	N	1.19
1	D	275:ARG	C	276:LEU	N	1.19
1	D	199:VAL	C	200:ASN	N	1.18
1	D	132:PRO	C	133:ASN	N	1.17
1	D	574:SER	C	575:TRP	N	1.04

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.