



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 3BG0 / pdb_00003bg0
Title : Architecture of a Coat for the Nuclear Pore Membrane
Authors : Hoelz, A.
Deposited on : 2007-11-23
Resolution : 3.15 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

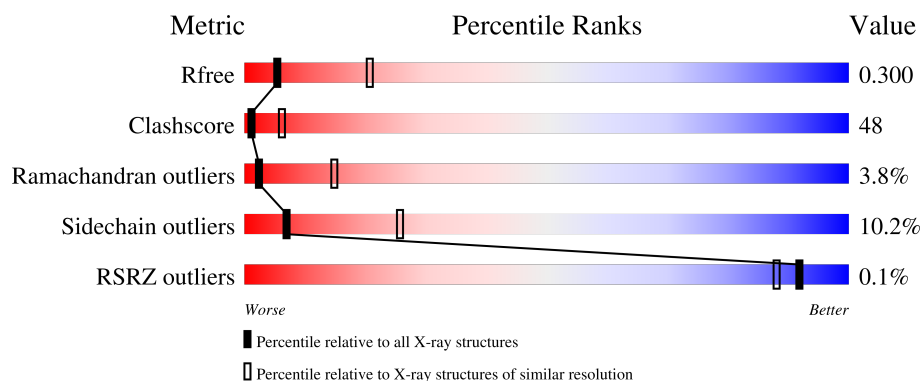
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



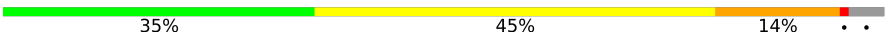
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	316	
1	D	316	
1	E	316	
1	H	316	
2	B	442	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	442	 35% 47% 12% • 5%
2	F	442	 35% 45% 14% • •
2	G	442	 33% 48% 12% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22562 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 Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2220	1399	387	422	12			
1	D	281	Total	C	N	O	S	0	0	0
			2205	1390	384	419	12			
1	E	283	Total	C	N	O	S	0	0	0
			2220	1399	387	422	12			
1	H	281	Total	C	N	O	S	0	0	0
			2205	1390	384	419	12			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	19	0	0
			3438	2201	570	656	11			
2	C	420	Total	C	N	O	S	19	0	0
			3418	2188	566	653	11			
2	F	423	Total	C	N	O	S	19	0	0
			3438	2201	570	656	11			
2	G	420	Total	C	N	O	S	19	0	0
			3418	2188	566	653	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	expression tag	UNP P49687
B	112	GLY	-	expression tag	UNP P49687
B	113	SER	-	expression tag	UNP P49687
B	114	SER	-	expression tag	UNP P49687
B	115	HIS	-	expression tag	UNP P49687
B	116	HIS	-	expression tag	UNP P49687
B	117	HIS	-	expression tag	UNP P49687
B	118	HIS	-	expression tag	UNP P49687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	HIS	-	expression tag	UNP P49687
B	120	HIS	-	expression tag	UNP P49687
B	121	SER	-	expression tag	UNP P49687
B	122	GLY	-	expression tag	UNP P49687
B	123	ASP	-	expression tag	UNP P49687
B	124	PRO	-	expression tag	UNP P49687
C	111	MET	-	expression tag	UNP P49687
C	112	GLY	-	expression tag	UNP P49687
C	113	SER	-	expression tag	UNP P49687
C	114	SER	-	expression tag	UNP P49687
C	115	HIS	-	expression tag	UNP P49687
C	116	HIS	-	expression tag	UNP P49687
C	117	HIS	-	expression tag	UNP P49687
C	118	HIS	-	expression tag	UNP P49687
C	119	HIS	-	expression tag	UNP P49687
C	120	HIS	-	expression tag	UNP P49687
C	121	SER	-	expression tag	UNP P49687
C	122	GLY	-	expression tag	UNP P49687
C	123	ASP	-	expression tag	UNP P49687
C	124	PRO	-	expression tag	UNP P49687
F	111	MET	-	expression tag	UNP P49687
F	112	GLY	-	expression tag	UNP P49687
F	113	SER	-	expression tag	UNP P49687
F	114	SER	-	expression tag	UNP P49687
F	115	HIS	-	expression tag	UNP P49687
F	116	HIS	-	expression tag	UNP P49687
F	117	HIS	-	expression tag	UNP P49687
F	118	HIS	-	expression tag	UNP P49687
F	119	HIS	-	expression tag	UNP P49687
F	120	HIS	-	expression tag	UNP P49687
F	121	SER	-	expression tag	UNP P49687
F	122	GLY	-	expression tag	UNP P49687
F	123	ASP	-	expression tag	UNP P49687
F	124	PRO	-	expression tag	UNP P49687
G	111	MET	-	expression tag	UNP P49687
G	112	GLY	-	expression tag	UNP P49687
G	113	SER	-	expression tag	UNP P49687
G	114	SER	-	expression tag	UNP P49687
G	115	HIS	-	expression tag	UNP P49687
G	116	HIS	-	expression tag	UNP P49687
G	117	HIS	-	expression tag	UNP P49687
G	118	HIS	-	expression tag	UNP P49687

Continued on next page...

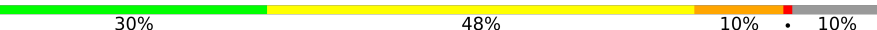
Continued from previous page...

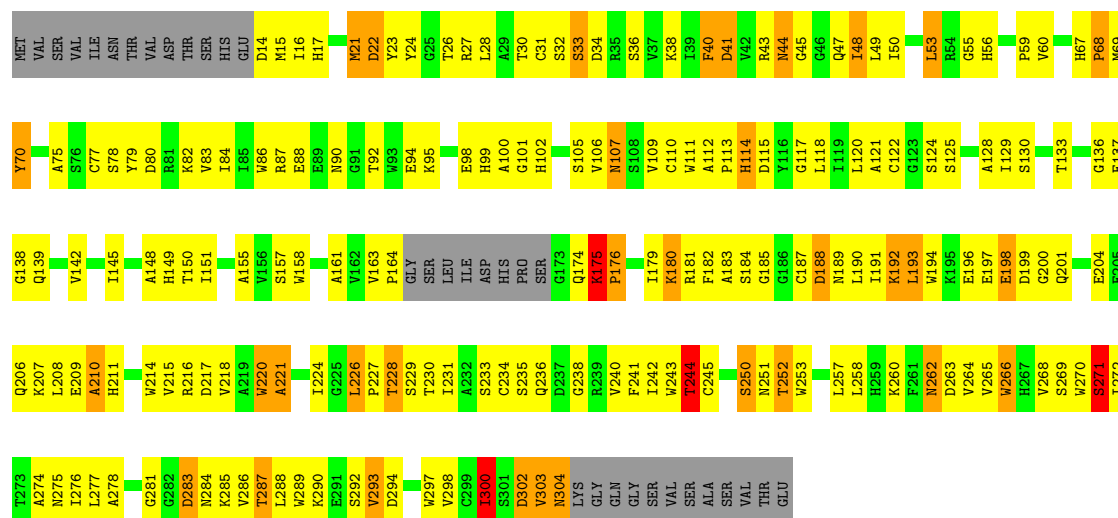
Chain	Residue	Modelled	Actual	Comment	Reference
G	119	HIS	-	expression tag	UNP P49687
G	120	HIS	-	expression tag	UNP P49687
G	121	SER	-	expression tag	UNP P49687
G	122	GLY	-	expression tag	UNP P49687
G	123	ASP	-	expression tag	UNP P49687
G	124	PRO	-	expression tag	UNP P49687

3 Residue-property plots

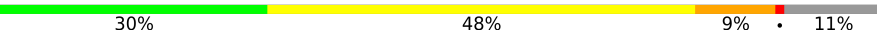
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

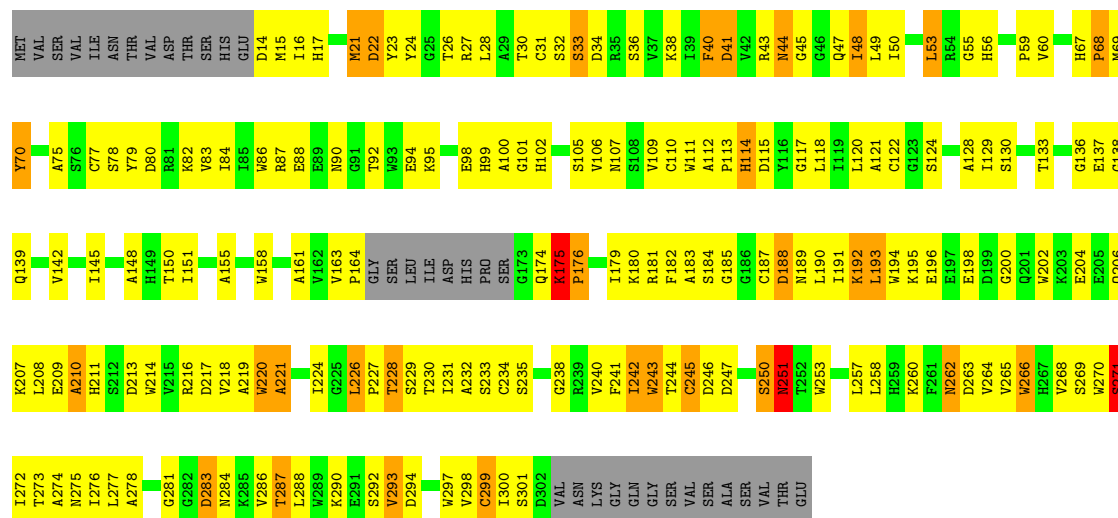
• Molecule 1: Protein SEC13 homolog

Chain A: 

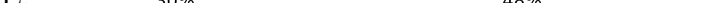


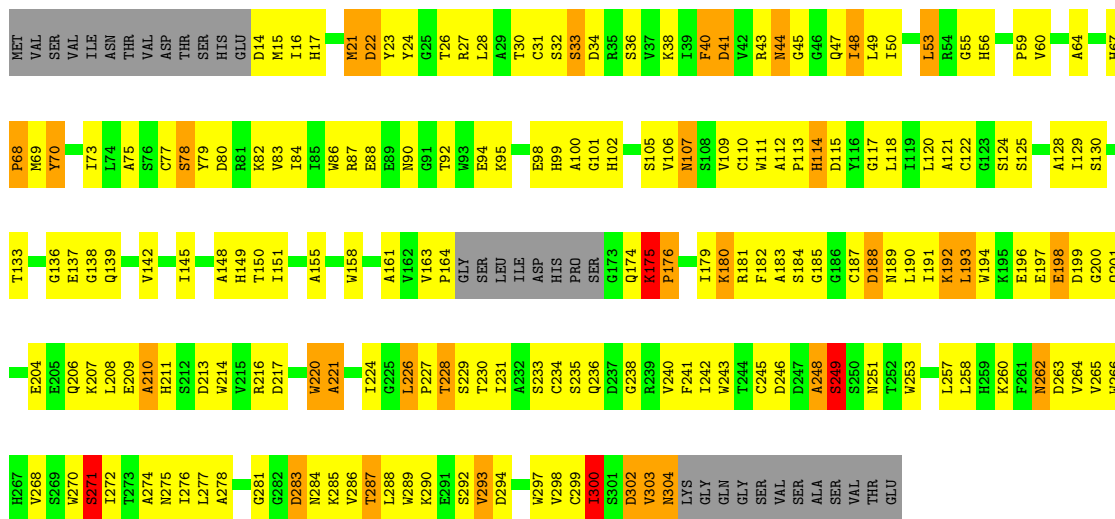
• Molecule 1: Protein SEC13 homolog

Chain D: 

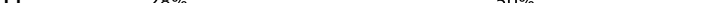


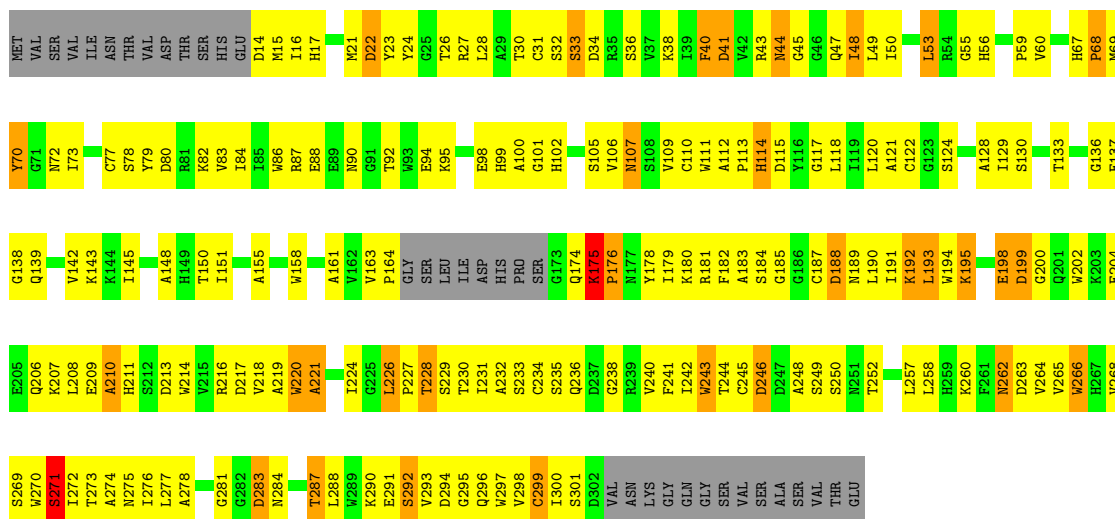
- Molecule 1: Protein SEC13 homolog

Chain E:  30% 48% 10% • 10%



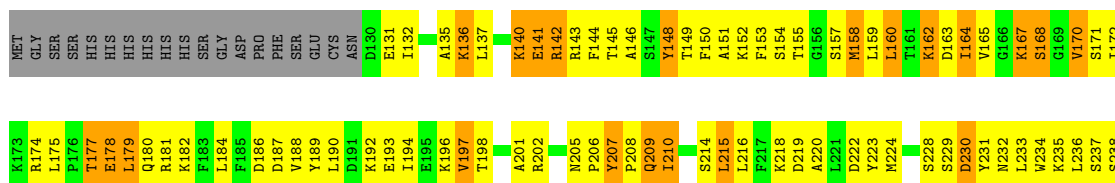
- Molecule 1: Protein SEC13 homolog

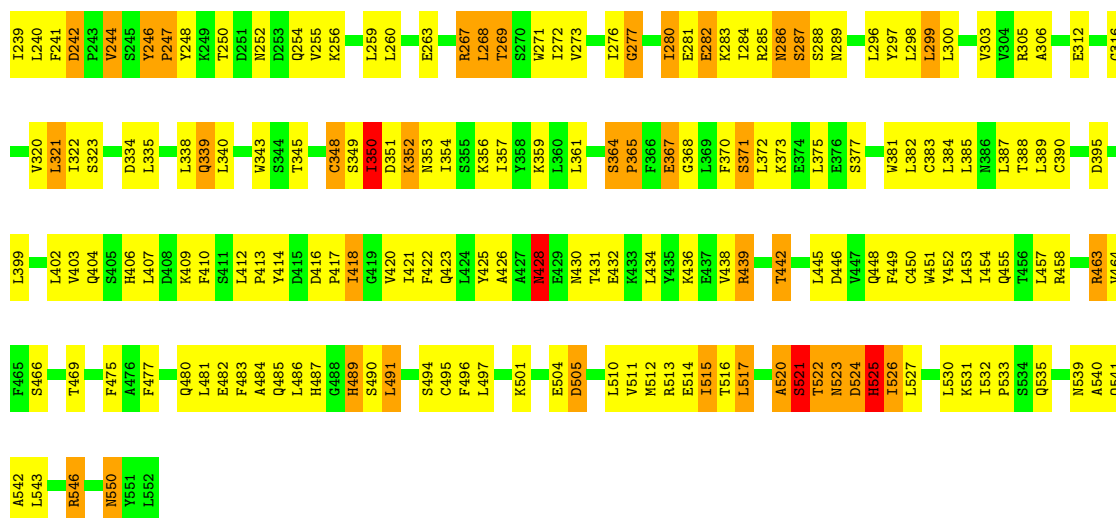
Chain H:  28% 50% 10% • 11%



- Molecule 2: Nucleoporin NUP145

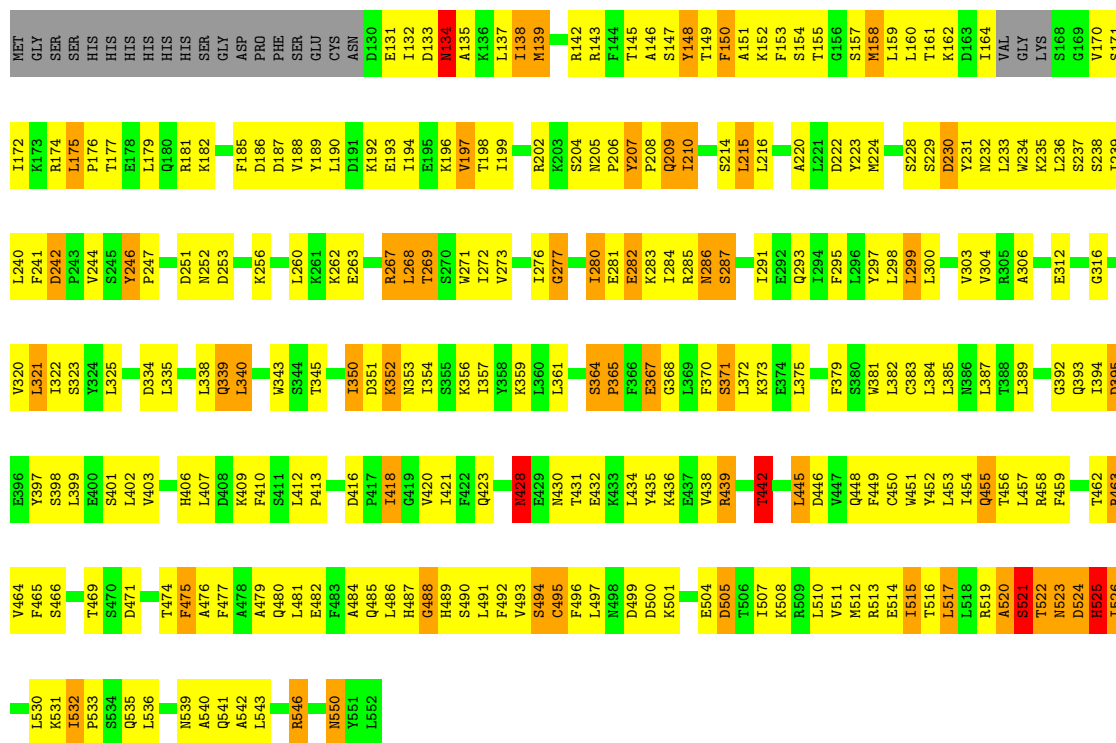
Chain B: 37% 45% 13% 5%





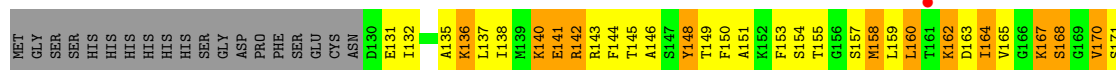
• Molecule 2: Nucleoporin NUP145

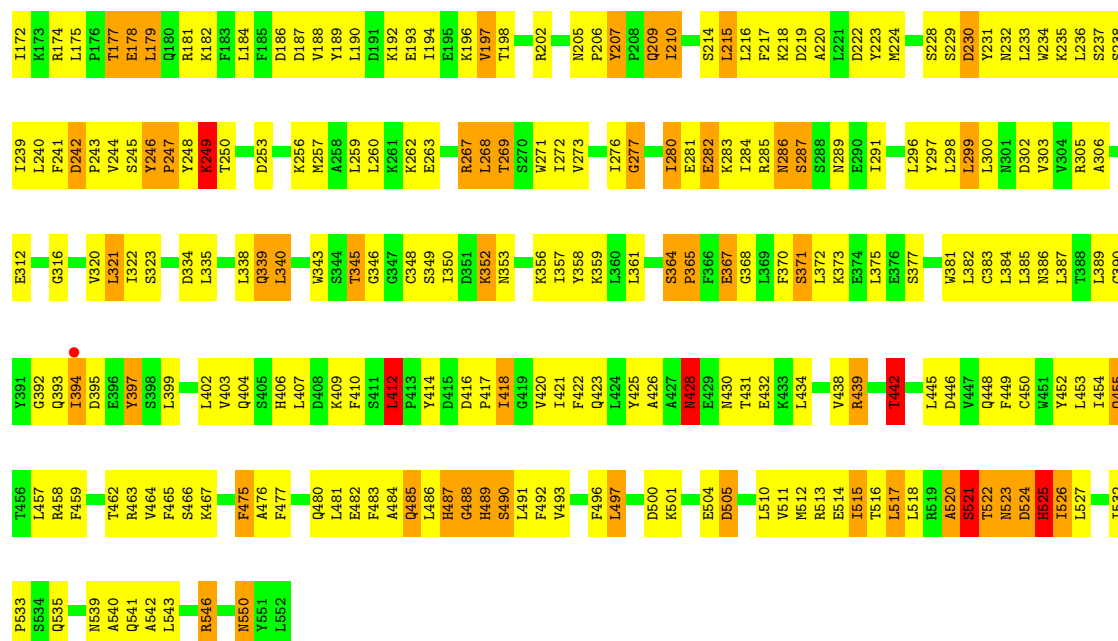
Chain C: 35% 47% 12% 5%



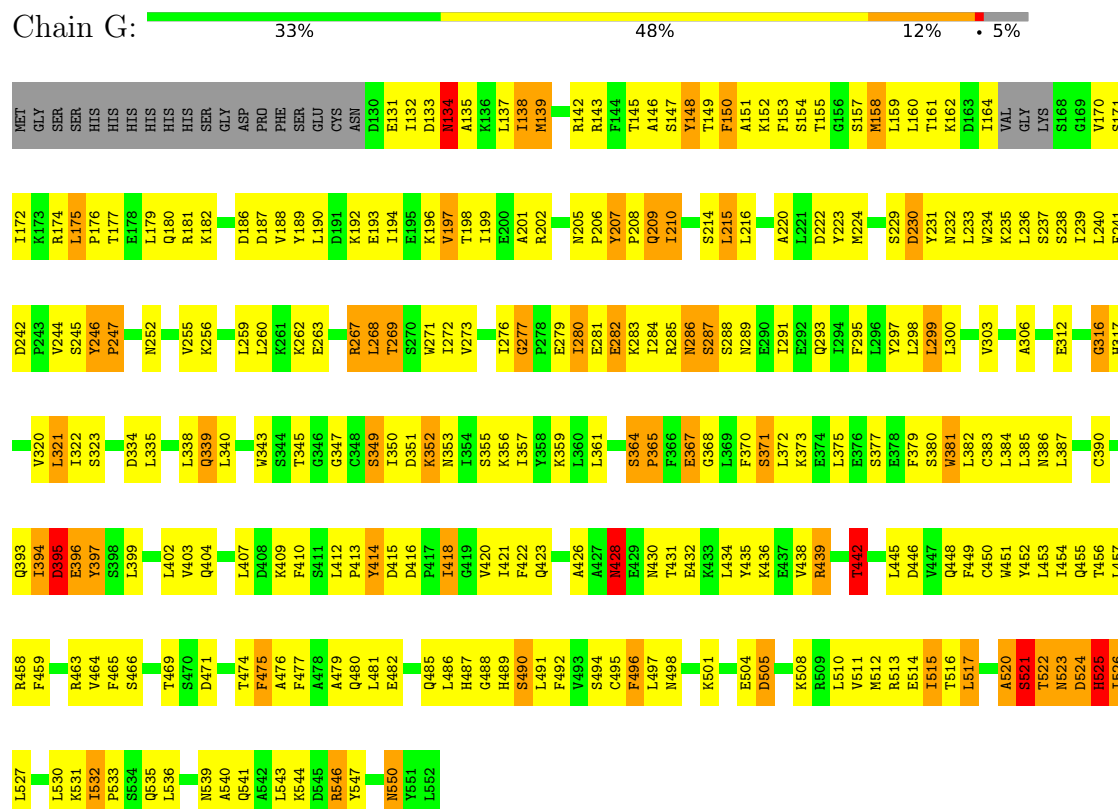
• Molecule 2: Nucleoporin NUP145

Chain F: 35% 45% 14% . .





- Molecule 2: Nucleoporin NUP145



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.82Å 216.57Å 100.96Å 90.00° 108.11° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.15) 87.4 (20.00-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.294 0.264 , 0.300	Depositor DCC
R_{free} test set	3096 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 87.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22562	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	1/2283 (0.0%)	1.11	14/3112 (0.4%)
1	D	0.63	2/2268 (0.1%)	1.10	16/3091 (0.5%)
1	E	0.66	2/2283 (0.1%)	1.09	16/3112 (0.5%)
1	H	0.62	2/2268 (0.1%)	1.08	19/3091 (0.6%)
2	B	0.64	0/3504	1.20	41/4728 (0.9%)
2	C	0.63	1/3483 (0.0%)	1.16	39/4699 (0.8%)
2	F	0.65	1/3504 (0.0%)	1.22	42/4728 (0.9%)
2	G	0.61	0/3483	1.17	39/4699 (0.8%)
All	All	0.64	9/23076 (0.0%)	1.15	226/31260 (0.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	394	ILE	CA-CB	6.36	1.62	1.54
1	D	262	ASN	CG-OD1	5.83	1.34	1.23
2	C	350	ILE	CA-CB	5.75	1.62	1.54
1	E	262	ASN	CG-OD1	5.50	1.33	1.23
1	H	262	ASN	CG-OD1	5.42	1.33	1.23
1	D	262	ASN	CA-C	5.19	1.62	1.52
1	E	262	ASN	CA-C	5.14	1.62	1.52
1	H	262	ASN	CA-C	5.08	1.61	1.52
1	A	262	ASN	CA-C	5.03	1.61	1.52

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	287	SER	N-CA-C	10.16	126.11	108.02
1	A	303	VAL	N-CA-C	9.99	122.40	107.51
1	E	303	VAL	N-CA-C	9.97	122.37	107.51
2	G	475	PHE	N-CA-C	-9.23	101.30	111.36
2	C	475	PHE	N-CA-C	-9.14	101.40	111.36
2	F	475	PHE	N-CA-C	-9.12	101.41	111.36
2	B	475	PHE	N-CA-C	-9.09	101.45	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	GLN	N-CA-C	-8.98	100.92	112.23
1	D	200	GLY	N-CA-C	-8.94	102.30	115.63
2	F	428	ASN	N-CA-C	8.48	120.14	111.07
1	A	252	THR	N-CA-C	8.47	122.53	108.73
2	B	428	ASN	N-CA-C	8.44	120.10	111.07
2	C	428	ASN	N-CA-C	8.42	120.08	111.07
2	G	428	ASN	N-CA-C	8.42	120.08	111.07
2	B	162	LYS	N-CA-C	8.39	122.05	108.63
1	E	107	ASN	N-CA-C	8.39	121.55	111.82
1	D	107	ASN	N-CA-C	8.39	121.55	111.82
1	H	107	ASN	N-CA-C	8.39	121.55	111.82
2	F	162	LYS	N-CA-C	8.38	122.04	108.63
1	A	107	ASN	N-CA-C	8.37	121.53	111.82
2	F	177	THR	N-CA-C	-8.20	99.71	110.53
2	B	177	THR	N-CA-C	-8.17	99.74	110.53
2	C	364	SER	CA-C-N	8.13	128.82	120.04
2	C	364	SER	C-N-CA	8.13	128.82	120.04
2	F	524	ASP	N-CA-C	8.09	121.13	111.02
2	F	242	ASP	CA-C-N	8.07	128.07	119.76
2	F	242	ASP	C-N-CA	8.07	128.07	119.76
2	G	364	SER	CA-C-N	8.06	128.74	120.04
2	G	364	SER	C-N-CA	8.06	128.74	120.04
2	B	364	SER	CA-C-N	8.05	128.73	120.04
2	B	364	SER	C-N-CA	8.05	128.73	120.04
2	B	524	ASP	N-CA-C	8.05	121.08	111.02
2	G	524	ASP	N-CA-C	8.04	121.08	111.02
2	F	364	SER	CA-C-N	8.03	128.71	120.04
2	F	364	SER	C-N-CA	8.03	128.71	120.04
2	C	524	ASP	N-CA-C	8.00	121.02	111.02
2	C	287	SER	N-CA-C	7.75	122.11	110.64
2	F	178	GLU	N-CA-C	-7.68	101.05	110.88
2	B	178	GLU	N-CA-C	-7.66	101.08	110.88
2	B	246	TYR	CA-C-N	7.52	129.24	119.84
2	B	246	TYR	C-N-CA	7.52	129.24	119.84
2	F	316	GLY	N-CA-C	7.32	121.49	112.64
2	B	316	GLY	N-CA-C	7.29	121.46	112.64
2	G	316	GLY	N-CA-C	7.28	121.45	112.64
2	C	253	ASP	N-CA-C	7.27	121.05	111.75
2	C	316	GLY	N-CA-C	7.26	121.42	112.64
2	B	286	ASN	CA-C-N	-7.25	109.89	122.37
2	B	286	ASN	C-N-CA	-7.25	109.89	122.37
1	D	251	ASN	N-CA-C	7.17	126.08	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	ASP	CA-C-N	6.85	126.82	119.76
2	B	242	ASP	C-N-CA	6.85	126.82	119.76
1	H	248	ALA	N-CA-C	-6.84	104.19	112.54
2	G	131	GLU	N-CA-C	-6.84	104.51	112.92
2	C	131	GLU	N-CA-C	-6.83	104.52	112.92
2	G	349	SER	N-CA-C	6.77	118.09	108.54
2	F	286	ASN	CA-C-N	-6.75	113.28	122.86
2	F	286	ASN	C-N-CA	-6.75	113.28	122.86
2	B	288	SER	N-CA-C	-6.66	105.47	112.93
1	D	41	ASP	CB-CA-C	6.65	121.13	109.89
2	F	245	SER	N-CA-C	6.64	119.31	108.55
1	H	41	ASP	CB-CA-C	6.63	121.10	109.89
2	C	182	LYS	N-CA-C	6.56	124.76	110.80
2	B	414	TYR	N-CA-C	6.54	119.23	111.71
2	F	182	LYS	N-CA-C	6.54	124.72	110.80
2	G	182	LYS	N-CA-C	6.53	124.72	110.80
2	G	397	TYR	N-CA-C	-6.50	98.67	109.46
2	B	182	LYS	N-CA-C	6.50	124.64	110.80
2	G	394	ILE	N-CA-C	-6.49	95.84	109.34
1	H	243	TRP	N-CA-C	6.36	119.94	107.98
2	B	287	SER	N-CA-C	6.35	119.86	109.06
2	G	352	LYS	N-CA-C	-6.35	104.63	112.38
2	C	352	LYS	N-CA-C	-6.35	104.64	112.38
2	F	352	LYS	N-CA-C	-6.33	104.66	112.38
2	B	352	LYS	N-CA-C	-6.32	104.67	112.38
2	B	197	VAL	N-CA-C	6.29	117.89	108.96
2	F	222	ASP	N-CA-C	6.27	118.92	111.33
2	C	532	ILE	CA-C-N	6.22	126.58	119.93
2	C	532	ILE	C-N-CA	6.22	126.58	119.93
2	B	222	ASP	N-CA-C	6.20	118.83	111.33
2	G	393	GLN	N-CA-C	6.18	119.45	110.42
2	C	252	ASN	N-CA-C	6.17	118.47	107.80
2	C	222	ASP	N-CA-C	6.17	118.79	111.33
2	G	222	ASP	N-CA-C	6.17	118.79	111.33
2	C	520	ALA	N-CA-C	6.16	123.91	110.80
2	B	207	TYR	CA-C-N	6.15	126.10	119.76
2	B	207	TYR	C-N-CA	6.15	126.10	119.76
2	F	520	ALA	N-CA-C	6.13	123.86	110.80
2	G	520	ALA	N-CA-C	6.13	123.86	110.80
2	G	247	PRO	N-CA-C	6.12	125.07	112.47
2	B	286	ASN	N-CA-C	6.11	120.74	113.16
2	F	207	TYR	CA-C-N	6.10	126.05	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	207	TYR	C-N-CA	6.10	126.05	119.76
2	B	520	ALA	N-CA-C	6.10	123.79	110.80
2	F	197	VAL	N-CA-C	6.09	117.94	109.29
2	G	532	ILE	N-CA-C	6.08	114.91	108.95
2	C	197	VAL	N-CA-C	6.08	117.92	109.29
2	G	207	TYR	CA-C-N	6.06	126.00	119.76
2	G	207	TYR	C-N-CA	6.06	126.00	119.76
2	C	207	TYR	CA-C-N	6.05	125.99	119.76
2	C	207	TYR	C-N-CA	6.05	125.99	119.76
2	B	367	GLU	N-CA-C	-6.04	106.16	112.93
2	G	197	VAL	N-CA-C	6.03	117.86	109.29
2	F	488	GLY	N-CA-C	-6.03	98.89	113.18
2	F	367	GLU	N-CA-C	-6.02	106.19	112.93
2	C	494	SER	N-CA-C	6.00	117.90	111.36
2	B	180	GLN	N-CA-C	6.00	118.17	107.80
1	E	248	ALA	N-CA-C	-5.99	105.28	112.59
2	C	285	ARG	N-CA-C	-5.99	105.82	113.01
2	C	367	GLU	N-CA-C	-5.98	106.23	112.93
2	G	288	SER	N-CA-C	-5.97	98.07	110.80
2	F	285	ARG	N-CA-C	-5.94	105.88	113.01
2	G	285	ARG	N-CA-C	-5.93	105.89	113.01
2	C	397	TYR	N-CA-C	5.92	119.35	108.58
2	B	285	ARG	N-CA-C	-5.91	105.92	113.01
2	G	367	GLU	N-CA-C	-5.91	106.31	112.93
2	C	134	ASN	N-CA-C	-5.89	105.58	112.89
2	G	134	ASN	N-CA-C	-5.85	105.64	112.89
2	G	246	TYR	CA-C-N	5.85	127.15	119.84
2	G	246	TYR	C-N-CA	5.85	127.15	119.84
2	F	412	LEU	N-CA-C	5.84	113.47	108.22
1	A	244	THR	N-CA-C	5.82	118.25	109.23
1	E	175	LYS	CA-C-N	5.81	127.10	119.84
1	E	175	LYS	C-N-CA	5.81	127.10	119.84
1	H	175	LYS	CA-C-N	5.80	127.09	119.84
1	H	175	LYS	C-N-CA	5.80	127.09	119.84
2	C	246	TYR	CA-C-N	5.79	127.08	119.84
2	C	246	TYR	C-N-CA	5.79	127.08	119.84
1	A	175	LYS	CA-C-N	5.79	127.07	119.84
1	A	175	LYS	C-N-CA	5.79	127.07	119.84
2	F	286	ASN	N-CA-C	5.79	120.34	113.28
2	F	246	TYR	CA-C-N	-5.77	112.62	119.84
2	F	246	TYR	C-N-CA	-5.77	112.62	119.84
1	D	175	LYS	CA-C-N	5.75	127.03	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	175	LYS	C-N-CA	5.75	127.03	119.84
2	G	486	LEU	N-CA-C	-5.73	97.42	107.73
1	D	244	THR	N-CA-C	5.72	117.98	108.20
2	F	242	ASP	N-CA-C	-5.72	102.54	109.57
2	B	136	LYS	N-CA-C	-5.72	107.30	114.56
2	F	136	LYS	N-CA-C	-5.71	107.31	114.56
2	G	480	GLN	N-CA-C	-5.70	105.07	111.28
2	F	394	ILE	N-CA-C	-5.69	105.03	113.39
2	G	396	GLU	N-CA-C	5.68	120.03	113.38
2	C	463	ARG	N-CA-C	5.68	117.91	108.99
2	C	480	GLN	N-CA-C	-5.67	105.11	111.28
2	B	480	GLN	N-CA-C	-5.65	105.12	111.28
2	F	480	GLN	N-CA-C	-5.64	105.13	111.28
2	C	442	THR	N-CA-C	5.61	122.74	110.80
2	F	442	THR	N-CA-C	5.60	122.73	110.80
2	G	442	THR	N-CA-C	5.60	122.73	110.80
2	B	442	THR	N-CA-C	5.57	122.66	110.80
2	G	286	ASN	N-CA-C	5.55	119.67	113.02
2	B	482	GLU	N-CA-C	-5.54	105.15	111.14
2	C	286	ASN	N-CA-C	5.53	119.66	113.02
1	H	292	SER	N-CA-C	-5.51	101.56	110.32
2	B	521	SER	N-CA-C	5.50	121.54	114.56
2	F	521	SER	N-CA-C	5.50	121.54	114.56
1	H	296	GLN	CA-C-N	-5.49	114.46	122.65
1	H	296	GLN	C-N-CA	-5.49	114.46	122.65
2	C	521	SER	N-CA-C	5.48	121.52	114.56
1	D	243	TRP	N-CA-C	5.47	117.67	107.99
2	G	521	SER	N-CA-C	5.47	121.50	114.56
2	C	242	ASP	CA-C-N	5.44	125.38	119.78
2	C	242	ASP	C-N-CA	5.44	125.38	119.78
1	D	271	SER	CA-C-N	-5.42	115.33	122.16
1	D	271	SER	C-N-CA	-5.42	115.33	122.16
1	A	271	SER	CA-C-N	-5.39	115.36	122.16
1	A	271	SER	C-N-CA	-5.39	115.36	122.16
1	H	271	SER	CA-C-N	-5.38	115.38	122.16
1	H	271	SER	C-N-CA	-5.38	115.38	122.16
2	B	210	ILE	N-CA-C	5.38	115.94	108.84
2	G	381	TRP	N-CA-C	-5.38	105.45	112.23
1	A	300	ILE	CB-CA-C	-5.37	104.08	111.65
2	B	350	ILE	CA-C-N	5.37	128.33	120.71
2	B	350	ILE	C-N-CA	5.37	128.33	120.71
2	G	395	ASP	N-CA-C	5.36	122.22	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	482	GLU	N-CA-C	-5.36	105.35	111.14
1	A	192	LYS	N-CA-C	5.35	117.43	109.25
1	E	192	LYS	N-CA-C	5.34	117.43	109.25
2	B	496	PHE	N-CA-C	-5.34	106.63	112.72
2	F	210	ILE	N-CA-C	5.34	115.89	108.84
2	F	243	PRO	N-CA-C	5.33	119.46	111.14
2	G	287	SER	N-CA-C	5.32	117.80	110.35
2	C	210	ILE	N-CA-C	5.31	115.85	108.84
1	E	300	ILE	CB-CA-C	-5.30	104.17	111.65
2	G	210	ILE	N-CA-C	5.30	115.84	108.84
2	C	482	GLU	N-CA-C	-5.29	105.42	111.14
2	F	482	GLU	N-CA-C	-5.29	104.95	111.40
1	E	271	SER	CA-C-N	-5.27	115.52	122.16
1	E	271	SER	C-N-CA	-5.27	115.52	122.16
1	H	133	THR	N-CA-C	-5.24	102.30	110.42
1	A	133	THR	N-CA-C	-5.24	102.30	110.42
1	E	133	THR	N-CA-C	-5.23	102.31	110.42
1	D	133	THR	N-CA-C	-5.23	102.31	110.42
1	E	262	ASN	CA-CB-CG	-5.21	107.39	112.60
2	F	515	ILE	CB-CA-C	-5.21	105.30	111.97
2	G	515	ILE	CB-CA-C	-5.18	105.34	111.97
2	F	249	LYS	N-CA-C	5.17	118.69	111.30
1	H	262	ASN	CA-CB-CG	-5.15	107.45	112.60
2	B	515	ILE	CB-CA-C	-5.13	105.40	111.97
2	C	515	ILE	CB-CA-C	-5.11	105.43	111.97
1	D	192	LYS	N-CA-C	5.09	117.04	109.25
1	A	221	ALA	CA-C-N	5.08	126.20	119.84
1	A	221	ALA	C-N-CA	5.08	126.20	119.84
2	C	445	LEU	N-CA-C	5.08	116.54	108.67
1	E	221	ALA	CA-C-N	5.08	126.18	119.84
1	E	221	ALA	C-N-CA	5.08	126.18	119.84
1	H	192	LYS	N-CA-C	5.08	117.02	109.25
1	D	266	TRP	N-CA-C	5.07	119.42	112.68
1	H	221	ALA	CA-C-N	5.07	126.17	119.84
1	H	221	ALA	C-N-CA	5.07	126.17	119.84
2	F	377	SER	N-CA-C	5.06	116.80	111.28
1	D	299	CYS	N-CA-C	5.05	117.78	109.76
2	G	377	SER	N-CA-C	5.04	116.77	111.28
1	H	73	ILE	N-CA-C	5.04	115.74	108.48
1	D	221	ALA	CA-C-N	5.03	126.13	119.84
1	D	221	ALA	C-N-CA	5.03	126.13	119.84
2	B	377	SER	N-CA-C	5.03	116.76	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	SER	N-CA-C	5.03	115.94	108.60
2	C	304	VAL	N-CA-C	5.02	115.25	110.53
2	C	488	GLY	N-CA-C	-5.02	101.28	113.18
1	H	266	TRP	N-CA-C	5.02	119.36	112.68
1	H	299	CYS	N-CA-C	5.02	117.74	109.76
1	A	266	TRP	N-CA-C	5.01	119.34	112.68
2	F	467	LYS	N-CA-C	-5.01	105.90	111.36
1	E	64	ALA	N-CA-C	5.00	117.48	108.48
1	E	73	ILE	N-CA-C	5.00	115.68	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2220	0	2096	251	0
1	D	2205	0	2081	220	0
1	E	2220	0	2096	250	0
1	H	2205	0	2081	236	0
2	B	3438	0	3452	320	0
2	C	3418	0	3426	315	0
2	F	3438	0	3452	356	0
2	G	3418	0	3426	349	0
All	All	22562	0	22110	2147	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 48.

All (2147) 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:F:174:ARG:HH22	2:F:485:GLN:HB2	0.96	1.12
2:B:174:ARG:HH22	2:B:485:GLN:HG2	0.96	1.11
2:C:481:LEU:HD13	2:C:489:HIS:HB3	1.31	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:481:LEU:HD13	2:F:489:HIS:HB3	1.16	1.11
2:B:174:ARG:HH22	2:B:485:GLN:CG	1.64	1.09
2:C:364:SER:HB3	2:C:394:ILE:HG13	1.32	1.09
2:G:481:LEU:HD13	2:G:489:HIS:HB3	1.24	1.08
2:F:343:TRP:HZ3	2:F:350:ILE:HG21	1.17	1.06
2:B:177:THR:CG2	2:B:179:LEU:HB3	1.85	1.06
2:F:177:THR:CG2	2:F:179:LEU:HB3	1.85	1.05
2:B:174:ARG:NH2	2:B:485:GLN:HG2	1.72	1.03
2:B:250:THR:HG22	2:B:252:ASN:H	1.24	1.02
2:F:233:LEU:HD13	2:F:417:PRO:HB2	1.41	1.01
2:G:532:ILE:HG23	2:G:533:PRO:HD2	1.43	1.01
1:A:28:LEU:CD1	2:B:172:ILE:HD11	1.90	1.01
2:F:343:TRP:CZ3	2:F:350:ILE:HG21	1.97	1.00
2:G:134:ASN:O	2:G:138:ILE:HB	1.62	0.99
2:C:134:ASN:O	2:C:138:ILE:HB	1.61	0.98
1:A:15:MET:HE2	2:B:162:LYS:NZ	1.78	0.97
2:G:238:SER:HA	2:G:242:ASP:OD2	1.63	0.97
1:H:79:TYR:HD1	1:H:105:SER:HB2	1.30	0.97
1:A:79:TYR:HD1	1:A:105:SER:HB2	1.30	0.97
1:D:79:TYR:HD1	1:D:105:SER:HB2	1.30	0.97
1:E:79:TYR:HD1	1:E:105:SER:HB2	1.30	0.96
2:C:375:LEU:HB3	2:C:379:PHE:HD2	1.28	0.96
1:E:28:LEU:CD1	2:F:172:ILE:HD11	1.95	0.95
2:F:174:ARG:NH2	2:F:485:GLN:HB2	1.81	0.95
2:G:380:SER:HB3	2:G:383:CYS:HB2	1.47	0.95
1:D:151:ILE:HB	1:D:187:CYS:HB2	1.49	0.94
2:G:442:THR:HG23	2:G:445:LEU:HB2	1.49	0.93
2:G:155:THR:HG22	2:G:513:ARG:HD2	1.47	0.92
1:E:278:ALA:HB2	2:F:153:PHE:HE1	1.32	0.92
2:B:404:GLN:HG2	2:B:426:ALA:HB1	1.51	0.92
1:E:226:LEU:HD13	1:E:227:PRO:HD2	1.51	0.92
1:A:226:LEU:HD13	1:A:227:PRO:HD2	1.51	0.91
1:H:226:LEU:HD13	1:H:227:PRO:HD2	1.51	0.91
1:A:278:ALA:HB2	2:B:153:PHE:HE1	1.35	0.91
1:D:226:LEU:HD13	1:D:227:PRO:HD2	1.51	0.91
1:E:15:MET:HE2	2:F:162:LYS:NZ	1.85	0.91
2:G:442:THR:HG22	2:G:442:THR:O	1.71	0.90
2:B:442:THR:HG22	2:B:442:THR:O	1.71	0.90
2:B:491:LEU:HD21	2:B:532:ILE:HD11	1.51	0.90
2:G:155:THR:CG2	2:G:513:ARG:HD2	2.01	0.90
2:G:532:ILE:CG2	2:G:533:PRO:HD2	2.01	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:343:TRP:HZ3	2:F:350:ILE:CG2	1.85	0.89
2:C:442:THR:O	2:C:442:THR:HG22	1.71	0.89
2:B:159:LEU:C	2:B:160:LEU:HD23	1.98	0.89
2:B:359:LYS:HD2	2:B:365:PRO:HA	1.55	0.89
2:F:359:LYS:HD2	2:F:365:PRO:HA	1.55	0.89
2:B:515:ILE:HD11	2:B:540:ALA:HB1	1.55	0.88
1:E:40:PHE:CE2	2:F:168:SER:HB2	2.09	0.88
2:F:159:LEU:C	2:F:160:LEU:HD23	1.98	0.88
2:G:359:LYS:HD2	2:G:365:PRO:HA	1.55	0.88
2:F:442:THR:O	2:F:442:THR:HG22	1.71	0.88
2:C:359:LYS:HD2	2:C:365:PRO:HA	1.55	0.87
2:B:172:ILE:O	2:B:172:ILE:HG22	1.75	0.86
2:F:439:ARG:HA	2:F:442:THR:OG1	1.74	0.86
2:C:439:ARG:HG2	2:C:439:ARG:HH11	1.41	0.86
2:B:177:THR:HG22	2:B:179:LEU:H	1.41	0.86
2:B:439:ARG:HA	2:B:442:THR:OG1	1.74	0.86
2:G:439:ARG:HA	2:G:442:THR:OG1	1.74	0.86
1:E:278:ALA:HB2	2:F:153:PHE:CE1	2.11	0.86
1:D:95:LYS:HE3	1:D:98:GLU:HB2	1.58	0.85
2:B:439:ARG:HG2	2:B:439:ARG:HH11	1.41	0.85
2:C:439:ARG:HA	2:C:442:THR:OG1	1.74	0.85
1:A:220:TRP:CZ3	1:A:229:SER:HB2	2.12	0.85
2:C:532:ILE:HG23	2:C:533:PRO:HD2	1.56	0.85
1:D:220:TRP:CZ3	1:D:229:SER:HB2	2.11	0.85
2:B:490:SER:OG	2:B:510:LEU:HD21	1.76	0.85
1:E:220:TRP:CZ3	1:E:229:SER:HB2	2.11	0.85
2:G:439:ARG:HH11	2:G:439:ARG:HG2	1.41	0.85
2:C:210:ILE:CD1	2:C:495:CYS:HB2	2.05	0.85
2:F:484:ALA:O	2:F:486:LEU:HG	1.76	0.85
1:A:40:PHE:CZ	2:B:168:SER:HB2	2.12	0.85
2:C:151:ALA:HA	2:C:160:LEU:O	1.77	0.85
1:E:95:LYS:HE3	1:E:98:GLU:HB2	1.59	0.85
2:G:490:SER:HB3	2:G:510:LEU:HD21	1.55	0.85
1:H:95:LYS:HE3	1:H:98:GLU:HB2	1.58	0.85
1:H:220:TRP:CZ3	1:H:229:SER:HB2	2.11	0.84
2:G:291:ILE:HG22	2:G:353:ASN:HB2	1.58	0.84
2:G:522:THR:HG22	2:G:526:ILE:HD11	1.59	0.84
2:F:172:ILE:HG22	2:F:172:ILE:O	1.75	0.84
2:F:439:ARG:HG2	2:F:439:ARG:HH11	1.41	0.84
2:C:522:THR:HG22	2:C:526:ILE:HD11	1.59	0.84
1:A:278:ALA:HB2	2:B:153:PHE:CE1	2.13	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:365:PRO:HB2	2:C:372:LEU:HD12	1.59	0.84
2:F:522:THR:HG22	2:F:526:ILE:HD11	1.59	0.84
2:B:321:LEU:HB3	2:B:361:LEU:HD11	1.60	0.84
2:B:365:PRO:HB2	2:B:372:LEU:HD12	1.59	0.84
1:E:221:ALA:HB2	1:E:270:TRP:CE2	2.12	0.84
2:G:151:ALA:HA	2:G:160:LEU:O	1.77	0.83
2:G:365:PRO:HB2	2:G:372:LEU:HD12	1.59	0.83
2:F:442:THR:O	2:F:442:THR:CG2	2.26	0.83
2:F:177:THR:HG22	2:F:179:LEU:H	1.41	0.83
1:A:40:PHE:CE2	2:B:168:SER:HB2	2.14	0.83
1:E:40:PHE:CZ	2:F:168:SER:HB2	2.13	0.83
2:B:151:ALA:HB1	2:B:159:LEU:HD11	1.61	0.83
2:C:149:THR:HG22	2:C:150:PHE:H	1.44	0.83
1:A:82:LYS:HG2	1:A:100:ALA:HB2	1.60	0.83
1:A:95:LYS:HE3	1:A:98:GLU:HB2	1.59	0.83
2:B:522:THR:HG22	2:B:526:ILE:HD11	1.59	0.82
2:F:365:PRO:HB2	2:F:372:LEU:HD12	1.59	0.82
2:B:487:HIS:H	2:B:487:HIS:CD2	1.95	0.82
2:C:515:ILE:HD11	2:C:540:ALA:HB1	1.59	0.82
2:G:481:LEU:HD13	2:G:489:HIS:CB	2.09	0.82
1:H:82:LYS:HG2	1:H:100:ALA:HB2	1.60	0.82
1:D:82:LYS:HG2	1:D:100:ALA:HB2	1.60	0.82
1:H:79:TYR:CD1	1:H:105:SER:HB2	2.14	0.82
2:B:442:THR:O	2:B:442:THR:CG2	2.27	0.82
2:C:238:SER:HA	2:C:242:ASP:OD2	1.79	0.82
2:G:442:THR:O	2:G:442:THR:CG2	2.26	0.82
1:D:79:TYR:CD1	1:D:105:SER:HB2	2.13	0.82
1:E:82:LYS:HG2	1:E:100:ALA:HB2	1.60	0.81
1:E:107:ASN:CG	2:F:142:ARG:HH12	1.88	0.81
2:G:284:ILE:HD13	2:G:297:TYR:CE1	2.15	0.81
1:A:79:TYR:CD1	1:A:105:SER:HB2	2.13	0.81
1:A:190:LEU:HD13	1:A:207:LYS:HD3	1.61	0.81
2:C:515:ILE:HD11	2:C:540:ALA:CB	2.10	0.81
1:D:290:LYS:HB2	1:D:300:ILE:CD1	2.09	0.81
2:B:343:TRP:HZ3	2:B:350:ILE:HG21	1.45	0.81
1:E:16:ILE:HA	1:E:32:SER:HB3	1.63	0.81
1:D:16:ILE:HA	1:D:32:SER:HB3	1.63	0.81
1:E:151:ILE:HB	1:E:187:CYS:HB2	1.62	0.81
2:F:151:ALA:HB1	2:F:159:LEU:HD11	1.61	0.81
1:E:79:TYR:CD1	1:E:105:SER:HB2	2.14	0.80
1:E:190:LEU:HD13	1:E:207:LYS:HD3	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:455:GLN:HG2	2:F:496:PHE:CE2	2.16	0.80
2:C:532:ILE:CG2	2:C:533:PRO:HD2	2.11	0.80
2:G:149:THR:HG22	2:G:150:PHE:H	1.44	0.80
2:C:284:ILE:HD13	2:C:297:TYR:CE1	2.16	0.80
1:E:180:LYS:HD2	1:E:196:GLU:OE1	1.82	0.80
1:E:263:ASP:OD1	1:E:264:VAL:N	2.15	0.80
1:D:263:ASP:OD1	1:D:264:VAL:N	2.15	0.79
2:B:515:ILE:HD11	2:B:540:ALA:CB	2.12	0.79
2:B:481:LEU:HD13	2:B:489:HIS:HB3	1.65	0.79
1:A:15:MET:HE2	2:B:162:LYS:HZ1	1.43	0.79
1:A:16:ILE:HA	1:A:32:SER:HB3	1.63	0.79
2:F:491:LEU:CD1	2:F:510:LEU:HD23	2.13	0.79
2:C:442:THR:O	2:C:442:THR:CG2	2.26	0.79
1:H:151:ILE:HB	1:H:187:CYS:HB2	1.64	0.79
2:F:490:SER:HB3	2:F:510:LEU:HD21	1.62	0.79
2:B:233:LEU:HD13	2:B:417:PRO:HB2	1.64	0.79
1:H:16:ILE:HA	1:H:32:SER:HB3	1.63	0.79
1:H:263:ASP:OD1	1:H:264:VAL:N	2.15	0.79
2:C:155:THR:HG22	2:C:513:ARG:HD2	1.65	0.79
2:C:375:LEU:HB3	2:C:379:PHE:CD2	2.17	0.79
2:G:432:GLU:OE2	2:G:466:SER:HB2	1.83	0.79
1:A:263:ASP:OD1	1:A:264:VAL:N	2.15	0.79
2:F:491:LEU:HD12	2:F:510:LEU:HD23	1.65	0.79
2:F:162:LYS:HG3	2:F:162:LYS:O	1.81	0.78
2:G:343:TRP:CZ3	2:G:350:ILE:HD12	2.18	0.78
1:A:70:TYR:CE2	1:A:118:LEU:HB2	2.18	0.78
1:D:70:TYR:CE2	1:D:118:LEU:HB2	2.19	0.78
1:E:226:LEU:HD12	1:E:228:THR:OG1	1.84	0.78
1:A:102:HIS:HD1	1:A:124:SER:HB3	1.48	0.78
2:C:181:ARG:HH12	2:C:234:TRP:HE1	1.32	0.78
2:C:246:TYR:CD1	2:C:247:PRO:HD2	2.18	0.78
2:F:248:TYR:CE2	2:G:343:TRP:CZ2	2.71	0.78
2:B:162:LYS:HG3	2:B:162:LYS:O	1.81	0.78
2:C:177:THR:HG22	2:C:179:LEU:H	1.49	0.78
1:E:70:TYR:CE2	1:E:118:LEU:HB2	2.18	0.78
1:H:70:TYR:CE2	1:H:118:LEU:HB2	2.18	0.78
1:D:190:LEU:HD13	1:D:207:LYS:HD3	1.64	0.78
1:D:226:LEU:HD12	1:D:228:THR:OG1	1.84	0.78
1:E:102:HIS:HD1	1:E:124:SER:HB3	1.48	0.78
2:F:339:GLN:O	2:F:343:TRP:HD1	1.68	0.77
2:C:287:SER:HB3	2:C:293:GLN:NE2	1.99	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:GLN:O	2:C:343:TRP:HD1	1.68	0.77
1:D:102:HIS:HD1	1:D:124:SER:HB3	1.48	0.77
1:A:145:ILE:HG22	1:A:148:ALA:HB2	1.67	0.77
2:G:339:GLN:O	2:G:343:TRP:HD1	1.68	0.77
1:A:226:LEU:HD12	1:A:228:THR:OG1	1.84	0.77
2:G:531:LYS:O	2:G:531:LYS:HG3	1.83	0.77
2:B:339:GLN:O	2:B:343:TRP:HD1	1.68	0.77
1:D:145:ILE:HG22	1:D:148:ALA:HB2	1.67	0.77
2:F:159:LEU:O	2:F:160:LEU:HD23	1.85	0.77
2:G:215:LEU:HD12	2:G:452:TYR:OH	1.84	0.77
1:H:226:LEU:HD12	1:H:228:THR:OG1	1.85	0.77
2:F:404:GLN:HG2	2:F:426:ALA:HB1	1.65	0.76
2:G:177:THR:HG22	2:G:179:LEU:H	1.49	0.76
2:F:177:THR:HG21	2:F:179:LEU:HB3	1.67	0.76
2:B:238:SER:HA	2:B:242:ASP:OD2	1.85	0.76
2:B:177:THR:HG21	2:B:179:LEU:HB3	1.68	0.76
2:G:527:LEU:HA	2:G:532:ILE:HD12	1.66	0.76
1:H:102:HIS:HD1	1:H:124:SER:HB3	1.48	0.76
1:E:248:ALA:O	1:E:249:SER:HB2	1.85	0.76
2:F:276:ILE:CD1	2:F:383:CYS:HA	2.14	0.76
1:E:220:TRP:HZ3	1:E:229:SER:HB2	1.51	0.76
1:H:145:ILE:HG22	1:H:148:ALA:HB2	1.67	0.76
1:A:40:PHE:N	1:A:40:PHE:HD1	1.84	0.75
2:B:276:ILE:CD1	2:B:383:CYS:HA	2.15	0.75
1:E:294:ASP:OD1	1:E:294:ASP:O	2.04	0.75
2:B:197:VAL:HG12	2:B:198:THR:N	2.02	0.75
1:E:40:PHE:HD1	1:E:40:PHE:N	1.84	0.75
1:E:145:ILE:HG22	1:E:148:ALA:HB2	1.66	0.75
2:F:276:ILE:HD13	2:F:383:CYS:HA	1.67	0.75
2:G:267:ARG:HH11	2:G:267:ARG:HG3	1.52	0.75
2:C:197:VAL:HG12	2:C:198:THR:N	2.02	0.75
1:E:245:CYS:HB2	1:E:253:TRP:CE3	2.22	0.75
2:G:320:VAL:O	2:G:323:SER:HB3	1.86	0.75
2:B:159:LEU:O	2:B:160:LEU:HD23	1.84	0.75
1:D:155:ALA:HB2	1:D:217:ASP:HA	1.68	0.75
1:D:257:LEU:HD12	1:D:258:LEU:N	2.01	0.75
1:H:257:LEU:HD12	1:H:258:LEU:N	2.01	0.75
1:E:257:LEU:HD12	1:E:258:LEU:N	2.01	0.75
1:D:220:TRP:HZ3	1:D:229:SER:HB2	1.51	0.75
1:E:16:ILE:HD11	2:F:168:SER:O	1.87	0.75
2:G:531:LYS:O	2:G:531:LYS:CG	2.34	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:197:VAL:HG12	2:G:198:THR:N	2.02	0.74
1:A:257:LEU:HD12	1:A:258:LEU:N	2.00	0.74
2:B:159:LEU:HD12	2:B:160:LEU:H	1.53	0.74
1:H:143:LYS:HD2	1:H:200:GLY:O	1.87	0.74
1:A:221:ALA:HB2	1:A:270:TRP:CE2	2.22	0.74
1:E:230:THR:HG22	1:E:231:ILE:N	2.02	0.74
2:G:256:LYS:O	2:G:260:LEU:HG	1.87	0.74
1:H:220:TRP:HZ3	1:H:229:SER:HB2	1.51	0.74
1:A:294:ASP:OD1	1:A:294:ASP:O	2.04	0.74
2:B:527:LEU:HD22	2:B:532:ILE:HD12	1.69	0.74
2:B:320:VAL:O	2:B:323:SER:HB3	1.86	0.74
1:E:150:THR:HB	1:E:188:ASP:HB3	1.69	0.74
2:F:159:LEU:HD12	2:F:160:LEU:H	1.53	0.74
1:A:230:THR:HG22	1:A:231:ILE:N	2.03	0.74
2:C:267:ARG:HH11	2:C:267:ARG:HG3	1.52	0.74
2:C:320:VAL:O	2:C:323:SER:HB3	1.87	0.74
2:F:174:ARG:HH22	2:F:485:GLN:CB	1.90	0.74
2:G:276:ILE:CD1	2:G:383:CYS:HA	2.18	0.74
1:D:294:ASP:OD1	1:D:294:ASP:O	2.04	0.74
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.52	0.74
2:F:428:ASN:C	2:F:428:ASN:OD1	2.31	0.74
2:G:280:ILE:HB	2:G:300:LEU:HD21	1.69	0.74
1:H:40:PHE:N	1:H:40:PHE:HD1	1.85	0.74
1:H:230:THR:HG22	1:H:231:ILE:N	2.03	0.74
2:F:320:VAL:O	2:F:323:SER:HB3	1.86	0.74
2:G:436:LYS:HE3	2:G:469:THR:OG1	1.88	0.74
1:A:220:TRP:HZ3	1:A:229:SER:HB2	1.51	0.73
2:B:256:LYS:O	2:B:260:LEU:HG	1.87	0.73
2:F:256:LYS:O	2:F:260:LEU:HG	1.87	0.73
2:B:484:ALA:HB3	2:B:486:LEU:HD12	1.69	0.73
2:G:527:LEU:CA	2:G:532:ILE:HD12	2.18	0.73
2:G:289:ASN:OD1	2:G:291:ILE:HB	1.89	0.73
2:G:421:ILE:HD11	2:G:449:PHE:HE2	1.54	0.73
2:B:381:TRP:CE3	2:B:412:LEU:HD22	2.24	0.73
2:G:428:ASN:C	2:G:428:ASN:OD1	2.31	0.73
1:D:40:PHE:N	1:D:40:PHE:HD1	1.85	0.73
1:E:40:PHE:N	1:E:40:PHE:CD1	2.56	0.73
2:F:197:VAL:HG12	2:F:198:THR:N	2.02	0.73
2:C:321:LEU:HB3	2:C:361:LEU:HD11	1.71	0.73
2:C:215:LEU:HD12	2:C:452:TYR:OH	1.89	0.73
1:A:40:PHE:N	1:A:40:PHE:CD1	2.56	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:256:LYS:O	2:C:260:LEU:HG	1.88	0.72
2:B:201:ALA:H	2:B:531:LYS:HZ2	1.35	0.72
2:F:267:ARG:HH11	2:F:267:ARG:HG3	1.52	0.72
2:F:481:LEU:HD13	2:F:489:HIS:CB	2.08	0.72
2:G:145:THR:HG22	2:G:147:SER:H	1.55	0.72
2:B:428:ASN:C	2:B:428:ASN:OD1	2.32	0.72
2:B:276:ILE:HD13	2:B:383:CYS:HA	1.71	0.72
1:H:95:LYS:CE	1:H:98:GLU:HB2	2.19	0.72
1:E:245:CYS:HB2	1:E:253:TRP:CD2	2.25	0.72
2:F:462:THR:O	2:F:463:ARG:HD3	1.87	0.72
2:G:190:LEU:HB2	2:G:489:HIS:CE1	2.24	0.72
2:F:321:LEU:HB3	2:F:361:LEU:HD11	1.69	0.72
2:C:394:ILE:O	2:C:395:ASP:HB2	1.89	0.72
2:C:428:ASN:C	2:C:428:ASN:OD1	2.32	0.72
1:D:95:LYS:CE	1:D:98:GLU:HB2	2.19	0.72
2:G:279:GLU:OE2	2:G:380:SER:HB2	1.89	0.72
2:G:284:ILE:HD13	2:G:297:TYR:CD1	2.24	0.72
1:D:150:THR:HB	1:D:188:ASP:HB3	1.72	0.72
2:F:359:LYS:NZ	2:F:368:GLY:HA3	2.05	0.72
2:G:149:THR:HG22	2:G:150:PHE:N	2.04	0.72
1:D:230:THR:HG22	1:D:231:ILE:N	2.03	0.71
1:H:26:THR:HG22	1:H:27:ARG:HD2	1.72	0.71
1:A:107:ASN:ND2	2:B:142:ARG:HH22	1.89	0.71
1:E:15:MET:HE2	2:F:162:LYS:HZ2	1.55	0.71
2:B:491:LEU:CD2	2:B:532:ILE:HD11	2.20	0.71
2:C:145:THR:HG22	2:C:147:SER:H	1.55	0.71
1:A:155:ALA:HB2	1:A:217:ASP:HA	1.71	0.71
2:B:494:SER:O	2:B:497:LEU:HD13	1.90	0.71
1:D:26:THR:HG22	1:D:27:ARG:HD2	1.72	0.71
1:E:28:LEU:HD12	2:F:172:ILE:HD11	1.72	0.71
2:B:215:LEU:HD12	2:B:452:TYR:OH	1.91	0.71
2:B:359:LYS:NZ	2:B:368:GLY:HA3	2.06	0.71
1:E:15:MET:HE2	2:F:162:LYS:HZ1	1.56	0.71
1:E:95:LYS:CE	1:E:98:GLU:HB2	2.20	0.71
1:E:107:ASN:OD1	2:F:142:ARG:NH1	2.24	0.71
2:G:359:LYS:NZ	2:G:368:GLY:HA3	2.05	0.71
1:E:56:HIS:CE1	1:E:84:ILE:HD12	2.26	0.71
1:A:26:THR:HG22	1:A:27:ARG:HD2	1.72	0.71
2:F:233:LEU:CD1	2:F:417:PRO:HB2	2.20	0.71
1:H:190:LEU:HD13	1:H:207:LYS:HD3	1.71	0.71
1:A:95:LYS:CE	1:A:98:GLU:HB2	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:THR:HG22	2:F:179:LEU:N	2.06	0.70
1:D:40:PHE:N	1:D:40:PHE:CD1	2.57	0.70
1:D:102:HIS:NE2	1:D:130:SER:HB3	2.06	0.70
1:E:107:ASN:ND2	2:F:142:ARG:HH22	1.88	0.70
2:C:170:VAL:HG12	2:C:171:SER:N	2.06	0.70
1:E:26:THR:HG22	1:E:27:ARG:HD2	1.72	0.70
1:H:56:HIS:CE1	1:H:84:ILE:HD12	2.27	0.70
2:C:448:GLN:HG3	2:C:477:PHE:CE1	2.26	0.70
1:H:102:HIS:NE2	1:H:130:SER:HB3	2.06	0.70
1:A:16:ILE:HD11	2:B:168:SER:O	1.92	0.70
1:D:290:LYS:HB2	1:D:300:ILE:HD11	1.72	0.70
1:E:208:LEU:HB3	1:E:243:TRP:CZ3	2.26	0.70
2:B:384:LEU:HD13	2:B:410:PHE:CE1	2.27	0.70
2:C:149:THR:HG22	2:C:150:PHE:N	2.04	0.70
1:E:125:SER:HB2	2:F:142:ARG:NH2	2.07	0.70
2:C:481:LEU:HD13	2:C:489:HIS:CB	2.17	0.70
2:B:177:THR:HG22	2:B:179:LEU:N	2.06	0.70
2:B:174:ARG:HH22	2:B:485:GLN:CD	2.00	0.69
2:C:210:ILE:HD12	2:C:495:CYS:HB2	1.73	0.69
2:G:170:VAL:HG12	2:G:171:SER:N	2.06	0.69
1:E:102:HIS:NE2	1:E:130:SER:HB3	2.07	0.69
1:E:214:TRP:O	1:E:235:SER:HB2	1.92	0.69
1:A:56:HIS:CE1	1:A:84:ILE:HD12	2.26	0.69
1:D:30:THR:HG22	1:D:31:CYS:N	2.08	0.69
1:E:137:GLU:O	1:E:139:GLN:N	2.24	0.69
2:G:515:ILE:HD11	2:G:540:ALA:CB	2.22	0.69
1:H:137:GLU:O	1:H:139:GLN:N	2.25	0.69
1:A:102:HIS:NE2	1:A:130:SER:HB3	2.06	0.69
1:D:56:HIS:CE1	1:D:84:ILE:HD12	2.27	0.69
2:G:150:PHE:H	2:G:150:PHE:HD2	1.40	0.69
2:G:421:ILE:HD11	2:G:449:PHE:CE2	2.27	0.69
1:H:288:LEU:N	1:H:301:SER:HB3	2.08	0.69
2:C:359:LYS:NZ	2:C:368:GLY:HA3	2.05	0.69
1:E:230:THR:HG22	1:E:231:ILE:H	1.57	0.69
1:A:230:THR:HG22	1:A:231:ILE:H	1.57	0.69
1:D:137:GLU:O	1:D:139:GLN:N	2.25	0.69
1:E:17:HIS:ND1	2:F:148:TYR:HE2	1.91	0.69
1:D:214:TRP:O	1:D:235:SER:HB2	1.93	0.69
2:G:521:SER:C	2:G:523:ASN:H	2.01	0.69
1:H:40:PHE:N	1:H:40:PHE:CD1	2.57	0.69
2:F:521:SER:C	2:F:523:ASN:H	2.01	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:481:LEU:CD1	2:C:489:HIS:HB3	2.18	0.68
1:E:30:THR:HG22	1:E:31:CYS:N	2.07	0.68
2:F:515:ILE:HD11	2:F:540:ALA:HB1	1.75	0.68
1:A:30:THR:HG22	1:A:31:CYS:N	2.07	0.68
1:A:137:GLU:O	1:A:139:GLN:N	2.25	0.68
2:G:181:ARG:HH12	2:G:234:TRP:HE1	1.39	0.68
2:C:150:PHE:H	2:C:150:PHE:HD2	1.40	0.68
1:A:28:LEU:HD12	2:B:172:ILE:HD11	1.72	0.68
1:A:214:TRP:O	1:A:235:SER:HB2	1.93	0.68
2:F:170:VAL:O	2:F:172:ILE:HG13	1.93	0.68
1:A:15:MET:HE2	2:B:162:LYS:HZ2	1.57	0.68
1:E:216:ARG:NH2	2:F:142:ARG:O	2.26	0.68
2:G:515:ILE:HD11	2:G:540:ALA:HB1	1.74	0.68
2:G:527:LEU:HD22	2:G:532:ILE:CD1	2.24	0.68
1:H:30:THR:HG22	1:H:31:CYS:N	2.08	0.68
1:H:150:THR:HB	1:H:188:ASP:HB3	1.76	0.68
1:A:107:ASN:HD21	2:B:142:ARG:HH22	1.37	0.68
2:C:439:ARG:HD2	2:C:442:THR:HG21	1.76	0.68
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.23	0.68
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.76	0.68
1:D:290:LYS:CB	1:D:300:ILE:HD11	2.24	0.68
2:B:197:VAL:HG12	2:B:198:THR:H	1.59	0.67
2:C:521:SER:C	2:C:523:ASN:H	2.01	0.67
2:G:515:ILE:HD13	2:G:541:GLN:HA	1.76	0.67
2:B:439:ARG:HD2	2:B:442:THR:HG21	1.76	0.67
2:G:291:ILE:HG22	2:G:353:ASN:CB	2.24	0.67
2:G:527:LEU:CB	2:G:532:ILE:HD12	2.24	0.67
1:A:151:ILE:HB	1:A:187:CYS:HB2	1.76	0.67
2:C:135:ALA:O	2:C:139:MET:HG3	1.94	0.67
1:H:288:LEU:H	1:H:301:SER:HB3	1.59	0.67
2:G:205:ASN:HB2	2:G:206:PRO:HD2	1.77	0.67
1:H:214:TRP:O	1:H:235:SER:HB2	1.93	0.67
1:A:163:VAL:HG13	1:A:164:PRO:HD2	1.77	0.67
1:H:230:THR:HG22	1:H:231:ILE:H	1.58	0.67
2:C:277:GLY:O	2:C:281:GLU:HB2	1.95	0.67
1:D:195:LYS:CG	1:D:196:GLU:N	2.57	0.67
1:E:163:VAL:HG13	1:E:164:PRO:HD2	1.77	0.67
1:H:287:THR:HG22	1:H:301:SER:OG	1.95	0.67
2:F:197:VAL:HG12	2:F:198:THR:H	1.60	0.67
2:G:135:ALA:O	2:G:139:MET:HG3	1.94	0.67
1:A:180:LYS:HD2	1:A:196:GLU:OE1	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:ASN:HB2	2:C:206:PRO:HD2	1.77	0.67
2:F:277:GLY:O	2:F:281:GLU:HB2	1.95	0.67
2:G:481:LEU:CD1	2:G:489:HIS:HB3	2.14	0.67
2:G:142:ARG:NH2	1:H:107:ASN:HD21	1.93	0.67
2:B:170:VAL:O	2:B:172:ILE:HG13	1.95	0.67
2:B:521:SER:C	2:B:523:ASN:H	2.01	0.67
1:D:230:THR:HG22	1:D:231:ILE:H	1.58	0.67
2:C:381:TRP:CE3	2:C:412:LEU:HD21	2.30	0.66
1:E:257:LEU:HD12	1:E:258:LEU:H	1.60	0.66
2:G:277:GLY:O	2:G:281:GLU:HB2	1.95	0.66
2:F:205:ASN:HB2	2:F:206:PRO:HD2	1.77	0.66
2:F:238:SER:O	2:F:242:ASP:HB2	1.96	0.66
2:G:159:LEU:O	2:G:160:LEU:HD23	1.95	0.66
2:G:161:THR:O	2:G:170:VAL:HG13	1.95	0.66
1:H:163:VAL:HG13	1:H:164:PRO:HD2	1.77	0.66
1:H:234:CYS:SG	1:H:268:VAL:HG23	2.36	0.66
1:H:290:LYS:HB3	1:H:300:ILE:HD11	1.77	0.66
1:D:287:THR:HG22	1:D:301:SER:OG	1.96	0.66
2:F:487:HIS:HB2	2:F:518:LEU:HD21	1.75	0.66
2:C:159:LEU:O	2:C:160:LEU:HD23	1.96	0.66
1:E:145:ILE:HG22	1:E:145:ILE:O	1.95	0.66
2:G:439:ARG:HD2	2:G:442:THR:HG21	1.76	0.66
2:B:205:ASN:HB2	2:B:206:PRO:HD2	1.77	0.66
1:D:163:VAL:HG13	1:D:164:PRO:HD2	1.77	0.66
2:F:246:TYR:HD1	2:F:248:TYR:O	1.79	0.66
2:B:136:LYS:O	2:B:140:LYS:HB2	1.96	0.66
2:C:276:ILE:CD1	2:C:383:CYS:HA	2.26	0.66
2:C:494:SER:O	2:C:497:LEU:HG	1.96	0.66
2:F:532:ILE:HG23	2:F:533:PRO:HD2	1.76	0.66
1:H:257:LEU:HD12	1:H:258:LEU:H	1.60	0.66
1:D:221:ALA:HB2	1:D:270:TRP:CE2	2.30	0.66
1:D:257:LEU:HD12	1:D:258:LEU:H	1.60	0.66
1:D:290:LYS:HB2	1:D:300:ILE:HD12	1.76	0.66
2:G:246:TYR:CE1	2:G:259:LEU:HD13	2.30	0.66
2:C:197:VAL:HG12	2:C:198:THR:H	1.60	0.65
2:G:152:LYS:O	2:G:159:LEU:HD12	1.96	0.65
2:B:277:GLY:O	2:B:281:GLU:HB2	1.95	0.65
2:C:161:THR:O	2:C:170:VAL:HG13	1.95	0.65
2:F:439:ARG:HD2	2:F:442:THR:HG21	1.76	0.65
2:F:172:ILE:O	2:F:172:ILE:CG2	2.45	0.65
1:A:145:ILE:HG22	1:A:145:ILE:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HB	1:D:187:CYS:CB	2.23	0.65
1:D:195:LYS:HG2	1:D:196:GLU:N	2.11	0.65
2:G:197:VAL:HG12	2:G:198:THR:H	1.60	0.65
1:A:109:VAL:CG1	1:A:120:LEU:HD11	2.26	0.65
2:F:177:THR:HG22	2:F:179:LEU:HB3	1.77	0.65
2:F:249:LYS:HG3	2:F:249:LYS:O	1.95	0.65
2:F:490:SER:CB	2:F:510:LEU:HD21	2.27	0.65
2:G:142:ARG:HH22	1:H:107:ASN:HD21	1.44	0.65
1:D:145:ILE:HG22	1:D:145:ILE:O	1.96	0.65
2:F:165:VAL:O	2:F:165:VAL:HG12	1.95	0.65
2:C:238:SER:O	2:C:242:ASP:HB2	1.95	0.65
1:D:109:VAL:CG1	1:D:120:LEU:HD11	2.26	0.65
2:F:136:LYS:O	2:F:140:LYS:HB2	1.96	0.65
2:G:152:LYS:HG2	1:H:269:SER:HB2	1.77	0.65
2:G:448:GLN:HG3	2:G:477:PHE:CE1	2.31	0.65
2:C:133:ASP:O	2:C:137:LEU:HG	1.97	0.65
2:C:241:PHE:CD2	2:C:457:LEU:HD21	2.31	0.65
1:E:109:VAL:CG1	1:E:120:LEU:HD11	2.27	0.65
1:H:145:ILE:HG22	1:H:145:ILE:O	1.96	0.65
2:B:241:PHE:CD2	2:B:457:LEU:HD21	2.32	0.65
1:E:107:ASN:HD21	2:F:142:ARG:NH2	1.94	0.65
1:E:274:ALA:HB1	1:E:290:LYS:HE3	1.79	0.65
2:F:353:ASN:O	2:F:357:ILE:HG13	1.97	0.65
2:G:142:ARG:O	1:H:216:ARG:NH2	2.28	0.65
2:G:353:ASN:O	2:G:357:ILE:HG13	1.97	0.65
1:H:291:GLU:HB3	1:H:297:TRP:CE3	2.32	0.65
1:A:257:LEU:HD12	1:A:258:LEU:H	1.60	0.64
2:B:515:ILE:CD1	2:B:540:ALA:C	2.70	0.64
1:E:155:ALA:HB2	1:E:217:ASP:HA	1.79	0.64
2:B:172:ILE:O	2:B:172:ILE:CG2	2.45	0.64
1:E:47:GLN:OE1	2:F:167:LYS:N	2.29	0.64
1:E:107:ASN:HD21	2:F:142:ARG:HH22	1.45	0.64
2:G:133:ASP:O	2:G:137:LEU:HG	1.97	0.64
2:G:547:TYR:HE1	1:H:72:ASN:HD21	1.45	0.64
2:G:287:SER:HB3	2:G:293:GLN:NE2	2.12	0.64
2:B:165:VAL:HG12	2:B:165:VAL:O	1.96	0.64
2:C:392:GLY:O	2:C:394:ILE:N	2.31	0.64
2:C:421:ILE:HD11	2:C:449:PHE:HE2	1.62	0.64
2:C:515:ILE:CD1	2:C:540:ALA:C	2.70	0.64
2:F:399:LEU:HD23	2:F:425:TYR:OH	1.98	0.64
2:C:280:ILE:HB	2:C:300:LEU:HD21	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:TYR:CD2	2:F:504:GLU:HA	2.33	0.64
1:H:206:GLN:HG3	1:H:207:LYS:N	2.12	0.64
1:A:206:GLN:HG3	1:A:207:LYS:N	2.13	0.64
1:E:17:HIS:CE1	2:F:148:TYR:CE2	2.86	0.64
2:F:455:GLN:HG2	2:F:496:PHE:HE2	1.63	0.64
2:G:241:PHE:CD2	2:G:457:LEU:HD21	2.33	0.64
1:H:109:VAL:CG1	1:H:120:LEU:HD11	2.27	0.64
1:A:268:VAL:CG1	1:A:277:LEU:HD11	2.28	0.64
1:E:49:LEU:HD12	1:E:50:ILE:N	2.13	0.64
1:E:268:VAL:CG1	1:E:277:LEU:HD11	2.28	0.64
1:H:268:VAL:CG1	1:H:277:LEU:HD11	2.28	0.64
1:A:107:ASN:HD21	2:B:142:ARG:NH2	1.96	0.64
2:C:158:MET:HE1	2:C:174:ARG:HG3	1.80	0.64
1:D:193:LEU:HD21	1:D:208:LEU:HD11	1.80	0.64
1:D:206:GLN:HG3	1:D:207:LYS:N	2.13	0.64
1:D:268:VAL:CG1	1:D:277:LEU:HD11	2.28	0.64
1:E:238:GLY:O	1:E:260:LYS:HA	1.97	0.64
2:G:158:MET:HE1	2:G:174:ARG:HG3	1.80	0.64
1:A:49:LEU:HD12	1:A:50:ILE:N	2.13	0.63
2:C:276:ILE:HG22	2:C:280:ILE:HG13	1.80	0.63
1:D:262:ASN:C	1:D:262:ASN:OD1	2.41	0.63
2:B:353:ASN:O	2:B:357:ILE:HG13	1.97	0.63
1:A:174:GLN:O	1:A:175:LYS:HB2	1.99	0.63
2:C:353:ASN:O	2:C:357:ILE:HG13	1.97	0.63
2:F:455:GLN:HG2	2:F:496:PHE:CD2	2.32	0.63
1:H:221:ALA:HB2	1:H:270:TRP:CE2	2.34	0.63
1:H:226:LEU:HD13	1:H:227:PRO:CD	2.28	0.63
1:E:283:ASP:O	1:E:284:ASN:HB2	1.98	0.63
2:C:152:LYS:O	2:C:159:LEU:HD12	1.96	0.63
2:C:190:LEU:HD21	2:C:488:GLY:HA3	1.81	0.63
2:C:487:HIS:HA	2:C:490:SER:CB	2.28	0.63
2:G:512:MET:SD	2:G:540:ALA:HB2	2.38	0.63
1:E:206:GLN:HG3	1:E:207:LYS:N	2.13	0.63
2:F:246:TYR:CD1	2:F:248:TYR:O	2.52	0.63
2:G:439:ARG:HG2	2:G:439:ARG:NH1	2.12	0.63
1:H:262:ASN:C	1:H:262:ASN:OD1	2.42	0.63
1:E:49:LEU:HD12	1:E:50:ILE:H	1.64	0.63
2:F:439:ARG:HG2	2:F:439:ARG:NH1	2.12	0.63
2:G:276:ILE:HD13	2:G:383:CYS:HA	1.79	0.63
1:A:49:LEU:HD12	1:A:50:ILE:H	1.64	0.63
1:A:262:ASN:C	1:A:262:ASN:OD1	2.41	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:HD12	1:D:242:ILE:N	2.14	0.63
1:E:174:GLN:O	1:E:175:LYS:HB2	1.99	0.63
1:H:155:ALA:HB2	1:H:217:ASP:HA	1.81	0.63
1:D:49:LEU:HD12	1:D:50:ILE:N	2.14	0.62
1:D:208:LEU:HD22	1:D:243:TRP:CE3	2.34	0.62
1:E:28:LEU:C	1:E:28:LEU:HD23	2.24	0.62
2:F:276:ILE:HG22	2:F:280:ILE:HG13	1.81	0.62
1:H:49:LEU:HD12	1:H:50:ILE:N	2.14	0.62
1:H:246:ASP:HB2	1:H:252:THR:O	1.99	0.62
2:C:181:ARG:NH1	2:C:234:TRP:HE1	1.98	0.62
2:C:515:ILE:HD13	2:C:541:GLN:HA	1.81	0.62
1:H:82:LYS:HG2	1:H:100:ALA:CB	2.28	0.62
1:A:283:ASP:O	1:A:284:ASN:HB2	1.98	0.62
2:B:188:VAL:O	2:B:192:LYS:HB2	2.00	0.62
2:C:188:VAL:O	2:C:192:LYS:HB2	2.00	0.62
2:C:487:HIS:HA	2:C:490:SER:HB2	1.81	0.62
1:D:82:LYS:HG2	1:D:100:ALA:CB	2.29	0.62
1:D:174:GLN:O	1:D:175:LYS:HB2	1.99	0.62
2:F:392:GLY:O	2:F:394:ILE:HG13	1.99	0.62
1:A:285:LYS:HG2	1:A:304:ASN:HD21	1.65	0.62
2:F:432:GLU:OE2	2:F:466:SER:HB2	2.00	0.62
2:F:515:ILE:HD11	2:F:540:ALA:CB	2.28	0.62
1:D:28:LEU:HD23	1:D:28:LEU:C	2.25	0.62
2:G:276:ILE:HG22	2:G:280:ILE:HG13	1.80	0.62
1:E:38:LYS:HB3	1:E:40:PHE:HE1	1.65	0.62
1:H:49:LEU:HD12	1:H:50:ILE:H	1.65	0.62
1:H:174:GLN:O	1:H:175:LYS:HB2	1.99	0.62
2:C:339:GLN:O	2:C:343:TRP:CD1	2.52	0.62
1:E:226:LEU:HD13	1:E:227:PRO:CD	2.28	0.62
2:B:174:ARG:NH2	2:B:485:GLN:CD	2.58	0.62
1:D:60:VAL:HG13	1:D:77:CYS:O	2.00	0.62
2:F:188:VAL:O	2:F:192:LYS:HB2	2.00	0.62
2:G:172:ILE:O	2:G:172:ILE:HG22	2.00	0.62
2:G:188:VAL:O	2:G:192:LYS:HB2	2.00	0.62
1:A:82:LYS:HG2	1:A:100:ALA:CB	2.29	0.61
1:A:226:LEU:HD13	1:A:227:PRO:CD	2.27	0.61
2:B:276:ILE:HG22	2:B:280:ILE:HG13	1.80	0.61
2:B:339:GLN:O	2:B:343:TRP:CD1	2.52	0.61
2:C:155:THR:HG21	1:D:23:TYR:O	2.00	0.61
2:C:515:ILE:HD13	2:C:541:GLN:N	2.15	0.61
2:F:339:GLN:O	2:F:343:TRP:CD1	2.52	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:GLU:OE2	2:B:466:SER:HB2	1.99	0.61
2:C:287:SER:CB	2:C:293:GLN:NE2	2.63	0.61
1:A:60:VAL:HG13	1:A:77:CYS:O	2.00	0.61
2:C:524:ASP:O	2:C:525:HIS:HB3	2.01	0.61
1:D:234:CYS:SG	1:D:268:VAL:HG23	2.41	0.61
1:E:145:ILE:CG2	1:E:148:ALA:HB2	2.30	0.61
1:D:220:TRP:CH2	1:D:229:SER:HB2	2.36	0.61
1:E:38:LYS:CB	1:E:40:PHE:HE1	2.14	0.61
1:A:38:LYS:CB	1:A:40:PHE:HE1	2.14	0.61
2:C:299:LEU:HD22	2:C:383:CYS:SG	2.40	0.61
1:D:49:LEU:HD12	1:D:50:ILE:H	1.65	0.61
1:H:145:ILE:CG2	1:H:148:ALA:HB2	2.31	0.61
2:C:162:LYS:HG3	2:C:162:LYS:O	2.00	0.61
2:C:172:ILE:HG22	2:C:172:ILE:O	2.00	0.61
2:C:210:ILE:HG22	2:C:459:PHE:CE2	2.35	0.61
2:F:421:ILE:HD11	2:F:449:PHE:CE2	2.36	0.61
2:G:210:ILE:HG22	2:G:459:PHE:CE2	2.36	0.61
1:A:145:ILE:CG2	1:A:148:ALA:HB2	2.30	0.61
1:A:238:GLY:O	1:A:260:LYS:HA	2.01	0.61
2:B:524:ASP:O	2:B:525:HIS:HB3	2.01	0.61
1:D:292:SER:C	1:D:294:ASP:H	2.09	0.61
2:G:162:LYS:HG3	2:G:162:LYS:O	2.01	0.61
1:A:28:LEU:HD23	1:A:28:LEU:C	2.25	0.61
1:A:48:ILE:HG22	1:A:48:ILE:O	2.00	0.61
1:A:150:THR:HB	1:A:188:ASP:HB3	1.83	0.61
1:A:220:TRP:CH2	1:A:229:SER:HB2	2.36	0.61
2:B:177:THR:HG22	2:B:179:LEU:HB3	1.77	0.61
1:D:226:LEU:HD13	1:D:227:PRO:CD	2.28	0.61
2:G:527:LEU:CD2	2:G:532:ILE:CD1	2.79	0.61
1:D:38:LYS:CB	1:D:40:PHE:HE1	2.14	0.61
1:E:78:SER:HB3	1:E:80:ASP:OD1	2.01	0.61
2:G:149:THR:CG2	2:G:150:PHE:H	2.13	0.61
2:G:246:TYR:HB2	2:G:260:LEU:HD21	1.82	0.61
2:G:515:ILE:HD13	2:G:541:GLN:CA	2.29	0.61
1:H:38:LYS:HB3	1:H:40:PHE:HE1	1.65	0.61
2:B:421:ILE:HD11	2:B:449:PHE:CE2	2.36	0.60
2:C:151:ALA:HB2	1:D:286:VAL:HG21	1.83	0.60
2:G:524:ASP:O	2:G:525:HIS:HB3	2.01	0.60
1:A:292:SER:C	1:A:294:ASP:H	2.09	0.60
2:C:439:ARG:HG2	2:C:439:ARG:NH1	2.12	0.60
1:E:48:ILE:O	1:E:48:ILE:HG22	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:SER:C	1:E:294:ASP:H	2.09	0.60
2:G:435:TYR:CE2	2:G:454:ILE:HD11	2.36	0.60
2:C:523:ASN:HB3	2:C:525:HIS:CE1	2.37	0.60
1:D:78:SER:HB3	1:D:80:ASP:OD1	2.01	0.60
2:G:180:GLN:HG2	2:G:180:GLN:O	1.99	0.60
1:H:28:LEU:C	1:H:28:LEU:HD23	2.25	0.60
1:H:60:VAL:HG13	1:H:77:CYS:O	2.00	0.60
1:H:87:ARG:HG3	1:H:88:GLU:H	1.66	0.60
1:A:87:ARG:HG3	1:A:88:GLU:H	1.66	0.60
2:B:153:PHE:HE2	2:B:175:LEU:HD22	1.66	0.60
1:E:220:TRP:CH2	1:E:229:SER:HB2	2.36	0.60
2:C:435:TYR:CE2	2:C:454:ILE:HD11	2.36	0.60
1:E:87:ARG:HG3	1:E:88:GLU:H	1.66	0.60
2:F:532:ILE:HG23	2:F:533:PRO:CD	2.31	0.60
2:B:491:LEU:HD12	2:B:510:LEU:HD23	1.84	0.60
2:F:218:LYS:HG3	2:F:242:ASP:OD2	2.01	0.60
2:G:170:VAL:H	1:H:47:GLN:HE22	1.49	0.60
2:G:512:MET:HA	2:G:540:ALA:HB1	1.83	0.60
1:H:48:ILE:O	1:H:48:ILE:HG22	2.01	0.60
1:A:70:TYR:N	1:A:70:TYR:CD1	2.70	0.60
1:A:191:ILE:HD11	1:A:211:HIS:CD2	2.37	0.60
2:B:343:TRP:CZ3	2:B:350:ILE:HG21	2.33	0.60
1:E:262:ASN:C	1:E:262:ASN:OD1	2.42	0.60
1:H:38:LYS:CB	1:H:40:PHE:HE1	2.14	0.60
1:A:265:VAL:HA	1:A:281:GLY:HA3	1.84	0.60
2:B:439:ARG:HG2	2:B:439:ARG:NH1	2.12	0.60
1:D:87:ARG:HG3	1:D:88:GLU:H	1.67	0.60
2:G:216:LEU:HB3	2:G:242:ASP:OD1	2.01	0.60
2:G:527:LEU:HA	2:G:532:ILE:CD1	2.32	0.60
1:A:78:SER:HB3	1:A:80:ASP:OD1	2.01	0.60
2:B:148:TYR:C	2:B:148:TYR:CD1	2.80	0.60
2:B:523:ASN:HB3	2:B:525:HIS:CE1	2.37	0.60
1:A:288:LEU:HB3	1:A:300:ILE:HD11	1.83	0.60
2:C:435:TYR:CZ	2:C:454:ILE:HD11	2.36	0.60
2:C:448:GLN:HG3	2:C:477:PHE:CZ	2.36	0.60
2:C:487:HIS:HA	2:C:490:SER:OG	2.02	0.60
1:E:82:LYS:HG2	1:E:100:ALA:CB	2.29	0.60
1:E:234:CYS:HB2	1:E:265:VAL:HB	1.83	0.60
1:E:265:VAL:HA	1:E:281:GLY:HA3	1.84	0.60
2:F:269:THR:HG21	2:F:390:CYS:SG	2.42	0.60
2:G:201:ALA:HB2	2:G:531:LYS:NZ	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:TYR:CD1	1:H:70:TYR:N	2.70	0.60
1:H:220:TRP:CH2	1:H:229:SER:HB2	2.36	0.60
2:B:215:LEU:HD12	2:B:452:TYR:CZ	2.37	0.59
2:C:170:VAL:HG12	2:C:171:SER:H	1.67	0.59
2:C:276:ILE:HD13	2:C:383:CYS:HA	1.84	0.59
1:D:48:ILE:HG22	1:D:48:ILE:O	2.01	0.59
1:E:60:VAL:HG13	1:E:77:CYS:O	2.01	0.59
2:F:155:THR:HG22	2:F:513:ARG:HD2	1.84	0.59
2:B:348:CYS:O	2:B:348:CYS:SG	2.60	0.59
2:G:381:TRP:CE3	2:G:412:LEU:HD23	2.37	0.59
1:H:78:SER:HB3	1:H:80:ASP:OD1	2.01	0.59
2:B:184:LEU:HD21	2:B:448:GLN:NE2	2.17	0.59
2:F:153:PHE:HE2	2:F:175:LEU:HD22	1.66	0.59
2:C:515:ILE:HD13	2:C:541:GLN:CA	2.33	0.59
1:D:265:VAL:HA	1:D:281:GLY:HA3	1.84	0.59
1:E:243:TRP:N	1:E:243:TRP:CD1	2.70	0.59
2:F:263:GLU:HA	2:G:320:VAL:HG22	1.84	0.59
2:C:181:ARG:HH12	2:C:234:TRP:NE1	1.99	0.59
1:D:70:TYR:N	1:D:70:TYR:CD1	2.70	0.59
1:E:242:ILE:HD11	1:E:258:LEU:HD22	1.84	0.59
1:A:111:TRP:CE2	1:A:120:LEU:HD13	2.38	0.59
2:B:352:LYS:O	2:B:356:LYS:HG3	2.02	0.59
2:C:240:LEU:HD21	2:C:268:LEU:CD1	2.32	0.59
1:A:38:LYS:HB3	1:A:40:PHE:HE1	1.65	0.59
2:C:153:PHE:CE2	1:D:278:ALA:HB2	2.38	0.59
1:E:111:TRP:CE2	1:E:120:LEU:HD13	2.37	0.59
2:G:240:LEU:HD21	2:G:268:LEU:CD1	2.33	0.59
2:G:523:ASN:HB3	2:G:525:HIS:CE1	2.37	0.59
2:C:381:TRP:CE3	2:C:412:LEU:CD2	2.85	0.59
2:G:148:TYR:HB2	1:H:266:TRP:CD2	2.38	0.59
2:G:199:ILE:CD1	2:G:530:LEU:HA	2.32	0.59
2:G:339:GLN:O	2:G:343:TRP:CD1	2.52	0.59
1:H:111:TRP:CE2	1:H:120:LEU:HD13	2.38	0.59
1:A:16:ILE:HD13	1:A:30:THR:HG21	1.85	0.59
2:F:524:ASP:O	2:F:525:HIS:HB3	2.01	0.59
2:G:487:HIS:HA	2:G:490:SER:HB2	1.85	0.59
2:C:352:LYS:O	2:C:356:LYS:HG3	2.03	0.58
1:D:111:TRP:CE2	1:D:120:LEU:HD13	2.38	0.58
1:E:21:MET:CE	2:F:160:LEU:HD11	2.32	0.58
1:E:242:ILE:HD13	1:E:297:TRP:CE2	2.37	0.58
2:G:162:LYS:NZ	1:H:15:MET:HE2	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:279:GLU:CD	2:G:380:SER:HB2	2.27	0.58
2:G:352:LYS:O	2:G:356:LYS:HG3	2.02	0.58
1:H:193:LEU:HD21	1:H:208:LEU:HD11	1.85	0.58
2:C:421:ILE:HD11	2:C:449:PHE:CE2	2.37	0.58
1:E:70:TYR:N	1:E:70:TYR:CD1	2.70	0.58
2:F:523:ASN:HB3	2:F:525:HIS:CE1	2.37	0.58
2:G:335:LEU:O	2:G:339:GLN:HG3	2.03	0.58
2:G:527:LEU:HB3	2:G:532:ILE:HD12	1.85	0.58
1:A:293:VAL:O	1:A:293:VAL:HG12	2.02	0.58
2:B:335:LEU:O	2:B:339:GLN:HG3	2.04	0.58
2:B:487:HIS:ND1	2:B:514:GLU:HG3	2.18	0.58
2:F:287:SER:C	2:F:289:ASN:H	2.11	0.58
2:C:194:ILE:HG12	2:C:492:PHE:CE2	2.39	0.58
2:C:284:ILE:HD13	2:C:297:TYR:CD1	2.38	0.58
1:A:191:ILE:HD11	1:A:211:HIS:HD2	1.69	0.58
1:D:38:LYS:HB3	1:D:40:PHE:HE1	1.65	0.58
1:D:208:LEU:HD22	1:D:243:TRP:CZ3	2.38	0.58
1:E:293:VAL:O	1:E:293:VAL:HG12	2.02	0.58
1:E:258:LEU:CD1	1:E:297:TRP:CB	2.81	0.58
1:A:17:HIS:ND1	2:B:148:TYR:HE2	2.01	0.58
2:B:284:ILE:HG12	2:B:296:LEU:HD12	1.86	0.58
2:B:432:GLU:OE1	2:B:466:SER:N	2.35	0.58
1:D:293:VAL:O	1:D:293:VAL:HG12	2.02	0.58
2:F:532:ILE:CG2	2:F:533:PRO:CD	2.82	0.58
1:H:265:VAL:HA	1:H:281:GLY:HA3	1.84	0.58
1:A:107:ASN:CG	2:B:142:ARG:HH12	2.11	0.58
1:A:192:LYS:HE2	1:A:207:LYS:HE2	1.86	0.58
2:C:335:LEU:O	2:C:339:GLN:HG3	2.03	0.58
1:D:242:ILE:HD11	1:D:258:LEU:HB2	1.85	0.58
2:F:532:ILE:CG2	2:F:533:PRO:HD2	2.33	0.58
1:A:187:CYS:HB3	1:A:214:TRP:NE1	2.19	0.58
1:A:208:LEU:HB3	1:A:243:TRP:CZ3	2.38	0.58
2:B:269:THR:HG21	2:B:390:CYS:SG	2.44	0.58
2:C:162:LYS:NZ	1:D:15:MET:HE2	2.19	0.58
1:D:145:ILE:CG2	1:D:148:ALA:HB2	2.31	0.58
2:F:299:LEU:HD22	2:F:383:CYS:SG	2.43	0.58
2:G:291:ILE:CG2	2:G:353:ASN:HB2	2.31	0.58
2:G:432:GLU:OE1	2:G:466:SER:N	2.35	0.58
2:C:499:ASP:O	2:C:501:LYS:N	2.37	0.57
2:F:148:TYR:CD1	2:F:148:TYR:C	2.80	0.57
2:G:515:ILE:CD1	2:G:540:ALA:C	2.76	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:SER:HB3	1:H:276:ILE:HB	1.86	0.57
2:B:515:ILE:HD13	2:B:541:GLN:N	2.19	0.57
1:E:113:PRO:HB3	1:E:161:ALA:HB2	1.85	0.57
2:F:352:LYS:O	2:F:356:LYS:HG3	2.02	0.57
2:G:196:LYS:HD2	2:G:214:SER:O	2.04	0.57
2:C:297:TYR:HB3	2:C:306:ALA:HB2	1.85	0.57
1:E:191:ILE:HD11	1:E:211:HIS:CD2	2.40	0.57
1:E:271:SER:HB3	1:E:276:ILE:HB	1.86	0.57
1:H:191:ILE:HD11	1:H:211:HIS:CD2	2.39	0.57
1:D:185:GLY:N	1:D:218:VAL:HG21	2.19	0.57
1:D:247:ASP:HA	1:D:251:ASN:HB3	1.87	0.57
2:F:543:LEU:O	2:F:543:LEU:HD12	2.04	0.57
1:A:41:ASP:OD1	1:A:41:ASP:O	2.22	0.57
2:B:142:ARG:HB3	2:B:144:PHE:CD1	2.40	0.57
1:D:179:ILE:CG2	1:D:181:ARG:HE	2.18	0.57
1:D:195:LYS:CG	1:D:196:GLU:H	2.16	0.57
2:F:142:ARG:HB3	2:F:144:PHE:CD1	2.39	0.57
2:F:207:TYR:CE1	2:F:504:GLU:HG3	2.40	0.57
2:F:335:LEU:O	2:F:339:GLN:HG3	2.04	0.57
2:G:349:SER:O	2:G:350:ILE:HG12	2.05	0.57
2:G:527:LEU:HD22	2:G:532:ILE:HD13	1.85	0.57
1:A:271:SER:HB3	1:A:276:ILE:HB	1.86	0.57
1:A:274:ALA:HB1	1:A:290:LYS:HE3	1.85	0.57
2:B:543:LEU:HD12	2:B:543:LEU:O	2.04	0.57
2:B:174:ARG:NH2	2:B:485:GLN:CG	2.46	0.57
2:B:527:LEU:CD2	2:B:532:ILE:HD12	2.33	0.57
2:C:145:THR:HG22	2:C:146:ALA:N	2.20	0.57
1:D:192:LYS:NZ	1:D:207:LYS:HE2	2.19	0.57
1:E:41:ASP:O	1:E:41:ASP:OD1	2.23	0.57
2:F:215:LEU:HD12	2:F:452:TYR:OH	2.05	0.57
1:A:21:MET:CE	2:B:160:LEU:HD11	2.35	0.57
1:D:16:ILE:HD13	1:D:30:THR:HG21	1.85	0.57
1:E:16:ILE:HD13	1:E:30:THR:HG21	1.86	0.57
2:G:170:VAL:HG12	2:G:171:SER:H	1.67	0.57
2:G:543:LEU:HD12	2:G:543:LEU:O	2.04	0.57
1:H:92:THR:HG22	1:H:94:GLU:HG3	1.87	0.57
2:C:522:THR:HG22	2:C:522:THR:O	2.05	0.57
1:E:179:ILE:CG2	1:E:181:ARG:HE	2.18	0.57
1:E:192:LYS:HE2	1:E:207:LYS:HE2	1.85	0.57
1:H:16:ILE:HD13	1:H:30:THR:HG21	1.85	0.57
1:A:92:THR:HG22	1:A:94:GLU:HG3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:LYS:HD2	2:C:214:SER:O	2.05	0.57
2:C:210:ILE:HG22	2:C:459:PHE:HE2	1.70	0.57
1:D:181:ARG:NH2	1:D:247:ASP:OD2	2.36	0.57
2:F:434:LEU:O	2:F:438:VAL:HG23	2.05	0.57
2:F:491:LEU:HD13	2:F:510:LEU:HD23	1.87	0.57
2:C:436:LYS:HE3	2:C:469:THR:OG1	2.05	0.56
2:F:395:ASP:HB2	2:F:397:TYR:CE2	2.39	0.56
1:A:113:PRO:HB3	1:A:161:ALA:HB2	1.87	0.56
1:A:224:ILE:C	1:A:226:LEU:H	2.13	0.56
2:B:434:LEU:O	2:B:438:VAL:HG23	2.05	0.56
2:B:522:THR:HG22	2:B:522:THR:O	2.04	0.56
2:C:149:THR:CG2	2:C:150:PHE:H	2.13	0.56
1:E:206:GLN:OE1	1:E:251:ASN:HB3	2.05	0.56
2:F:240:LEU:HD21	2:F:268:LEU:CD1	2.36	0.56
2:G:515:ILE:HD13	2:G:541:GLN:N	2.20	0.56
1:A:193:LEU:HD21	1:A:208:LEU:HD11	1.87	0.56
2:C:148:TYR:HB2	1:D:266:TRP:CE2	2.41	0.56
2:C:432:GLU:OE2	2:C:466:SER:HB2	2.05	0.56
2:C:434:LEU:O	2:C:438:VAL:HG23	2.05	0.56
2:C:543:LEU:HD12	2:C:543:LEU:O	2.04	0.56
1:E:107:ASN:ND2	2:F:142:ARG:HH12	2.02	0.56
1:E:109:VAL:HG22	1:E:122:CYS:SG	2.45	0.56
2:F:196:LYS:HD2	2:F:214:SER:O	2.05	0.56
2:F:241:PHE:CD2	2:F:457:LEU:HD21	2.41	0.56
2:G:210:ILE:CD1	2:G:495:CYS:HB3	2.35	0.56
2:G:252:ASN:ND2	2:G:255:VAL:HG23	2.20	0.56
1:H:148:ALA:HB1	1:H:194:TRP:CH2	2.40	0.56
1:D:92:THR:HG22	1:D:94:GLU:HG3	1.87	0.56
2:F:409:LYS:C	2:F:410:PHE:HD2	2.13	0.56
2:F:445:LEU:HD22	2:F:449:PHE:HD2	1.71	0.56
2:F:522:THR:HG22	2:F:522:THR:O	2.05	0.56
2:G:284:ILE:HG21	2:G:297:TYR:HE1	1.70	0.56
2:C:490:SER:HB3	2:C:510:LEU:HD21	1.87	0.56
1:D:271:SER:HB3	1:D:276:ILE:HB	1.86	0.56
1:A:179:ILE:CG2	1:A:181:ARG:HE	2.18	0.56
1:A:250:SER:O	1:A:252:THR:HG23	2.06	0.56
2:B:196:LYS:HD2	2:B:214:SER:O	2.05	0.56
2:C:291:ILE:HG22	2:C:353:ASN:HB2	1.88	0.56
1:D:109:VAL:HG22	1:D:122:CYS:SG	2.45	0.56
2:G:409:LYS:C	2:G:410:PHE:HD2	2.13	0.56
2:G:434:LEU:O	2:G:438:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:190:LEU:HB2	2:C:489:HIS:CE1	2.41	0.56
1:D:288:LEU:H	1:D:301:SER:HB3	1.71	0.56
1:E:92:THR:HG22	1:E:94:GLU:HG3	1.87	0.56
2:F:348:CYS:O	2:F:349:SER:HB2	2.05	0.56
2:C:409:LYS:C	2:C:410:PHE:HD2	2.13	0.56
2:F:154:SER:O	2:F:157:SER:N	2.39	0.56
2:G:190:LEU:HD22	2:G:489:HIS:ND1	2.21	0.56
2:G:436:LYS:CE	2:G:469:THR:OG1	2.53	0.56
2:G:514:GLU:OE1	2:G:517:LEU:HD23	2.06	0.56
1:H:109:VAL:HG22	1:H:122:CYS:SG	2.46	0.56
1:H:243:TRP:N	1:H:243:TRP:CD1	2.73	0.56
2:B:155:THR:HG22	2:B:513:ARG:HD2	1.88	0.56
2:B:515:ILE:HD13	2:B:541:GLN:HA	1.87	0.56
2:C:514:GLU:OE1	2:C:517:LEU:HD23	2.06	0.56
1:D:198:GLU:HG3	1:D:198:GLU:O	2.06	0.56
1:E:193:LEU:CD2	1:E:193:LEU:N	2.69	0.56
2:G:269:THR:O	2:G:273:VAL:HG23	2.06	0.56
1:H:258:LEU:CD1	1:H:297:TRP:HB2	2.36	0.56
1:A:182:PHE:CD1	1:A:182:PHE:O	2.59	0.56
2:C:210:ILE:HD11	2:C:495:CYS:HB2	1.87	0.56
1:D:232:ALA:HB2	1:D:270:TRP:CZ2	2.41	0.56
2:F:248:TYR:CE2	2:G:343:TRP:CH2	2.94	0.56
2:F:515:ILE:HD13	2:F:541:GLN:HA	1.88	0.56
2:G:190:LEU:HB2	2:G:489:HIS:HE1	1.70	0.56
2:F:420:VAL:HA	2:F:423:GLN:OE1	2.06	0.55
2:G:371:SER:OG	2:G:373:LYS:HG3	2.06	0.55
1:A:24:TYR:OH	2:B:543:LEU:HG	2.06	0.55
2:B:350:ILE:HD12	2:B:354:ILE:HD12	1.88	0.55
2:B:359:LYS:HZ2	2:B:368:GLY:HA3	1.70	0.55
2:B:514:GLU:OE1	2:B:517:LEU:HD23	2.06	0.55
1:D:224:ILE:C	1:D:226:LEU:H	2.13	0.55
1:D:274:ALA:HB1	1:D:290:LYS:HE3	1.88	0.55
2:F:269:THR:O	2:F:273:VAL:HG23	2.06	0.55
2:G:276:ILE:HD11	2:G:383:CYS:HA	1.88	0.55
1:A:216:ARG:NH2	2:B:142:ARG:O	2.39	0.55
2:B:409:LYS:C	2:B:410:PHE:HD2	2.14	0.55
1:D:23:TYR:CD2	1:D:68:PRO:HG3	2.41	0.55
2:F:179:LEU:HD11	2:F:184:LEU:CD1	2.36	0.55
1:H:179:ILE:CG2	1:H:181:ARG:HE	2.18	0.55
1:H:224:ILE:C	1:H:226:LEU:H	2.14	0.55
1:A:109:VAL:HG22	1:A:122:CYS:SG	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LEU:CD2	2:B:389:LEU:HD13	2.36	0.55
2:C:175:LEU:HD13	2:C:176:PRO:HD2	1.89	0.55
1:D:208:LEU:HB3	1:D:243:TRP:CZ3	2.41	0.55
1:E:21:MET:HE3	2:F:160:LEU:HD11	1.89	0.55
1:E:258:LEU:HD13	1:E:297:TRP:CB	2.36	0.55
2:F:432:GLU:OE1	2:F:466:SER:N	2.39	0.55
2:F:445:LEU:HD22	2:F:449:PHE:CD2	2.42	0.55
2:G:522:THR:HG22	2:G:522:THR:O	2.05	0.55
2:B:267:ARG:HH11	2:B:267:ARG:CG	2.20	0.55
2:B:269:THR:O	2:B:273:VAL:HG23	2.07	0.55
2:C:269:THR:O	2:C:273:VAL:HG23	2.06	0.55
1:E:243:TRP:CD1	1:E:243:TRP:H	2.23	0.55
2:G:145:THR:HG22	2:G:146:ALA:N	2.20	0.55
2:B:420:VAL:HA	2:B:423:GLN:OE1	2.07	0.55
2:G:280:ILE:CB	2:G:300:LEU:HD21	2.35	0.55
1:A:193:LEU:N	1:A:193:LEU:CD2	2.69	0.55
2:B:197:VAL:CG1	2:B:198:THR:N	2.69	0.55
2:C:172:ILE:HD11	1:D:28:LEU:CD1	2.37	0.55
2:C:491:LEU:O	2:C:494:SER:HB2	2.06	0.55
2:C:515:ILE:HD11	2:C:540:ALA:C	2.32	0.55
1:E:148:ALA:HB1	1:E:194:TRP:CH2	2.42	0.55
2:F:487:HIS:NE2	2:F:514:GLU:HG3	2.22	0.55
2:F:514:GLU:OE1	2:F:517:LEU:HD23	2.07	0.55
2:G:494:SER:O	2:G:497:LEU:HG	2.07	0.55
1:H:113:PRO:CB	1:H:161:ALA:HB2	2.37	0.55
1:A:23:TYR:CD2	1:A:68:PRO:HG3	2.42	0.55
2:B:230:ASP:O	2:B:231:TYR:C	2.49	0.55
2:C:420:VAL:HA	2:C:423:GLN:OE1	2.07	0.55
1:E:43:ARG:O	1:E:44:ASN:HB2	2.07	0.55
1:E:113:PRO:CB	1:E:161:ALA:HB2	2.36	0.55
1:E:224:ILE:C	1:E:226:LEU:H	2.13	0.55
2:F:434:LEU:O	2:F:438:VAL:N	2.39	0.55
2:B:155:THR:C	2:B:157:SER:H	2.15	0.55
2:C:202:ARG:HG2	2:C:209:GLN:OE1	2.07	0.55
2:C:471:ASP:OD2	2:C:497:LEU:HA	2.07	0.55
1:D:193:LEU:CD2	1:D:193:LEU:N	2.70	0.55
2:G:384:LEU:HD13	2:G:410:PHE:CE1	2.41	0.55
1:H:290:LYS:CB	1:H:300:ILE:HD11	2.37	0.55
1:D:206:GLN:HG3	1:D:207:LYS:H	1.72	0.55
1:D:292:SER:O	1:D:294:ASP:N	2.40	0.55
1:E:30:THR:CG2	1:E:31:CYS:N	2.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:TYR:CD2	1:H:68:PRO:HG3	2.41	0.55
1:H:220:TRP:CE2	1:H:231:ILE:HD11	2.42	0.55
2:B:421:ILE:HD11	2:B:449:PHE:HE2	1.71	0.54
2:C:375:LEU:HD22	2:C:379:PHE:HE2	1.73	0.54
2:C:512:MET:SD	2:C:540:ALA:HB2	2.48	0.54
1:E:88:GLU:HA	1:E:92:THR:O	2.08	0.54
1:E:107:ASN:CG	2:F:142:ARG:HH22	2.14	0.54
2:F:230:ASP:O	2:F:231:TYR:C	2.50	0.54
2:F:253:ASP:O	2:F:257:MET:HB2	2.07	0.54
2:F:280:ILE:HB	2:F:300:LEU:HD21	1.89	0.54
1:H:230:THR:CG2	1:H:242:ILE:HG23	2.37	0.54
1:A:43:ARG:O	1:A:44:ASN:HB2	2.07	0.54
1:A:302:ASP:C	1:A:302:ASP:OD1	2.50	0.54
2:B:487:HIS:CE1	2:B:514:GLU:HG3	2.42	0.54
2:C:158:MET:HE2	2:C:174:ARG:HA	1.89	0.54
2:C:412:LEU:CD2	2:C:413:PRO:HD2	2.37	0.54
2:G:150:PHE:N	2:G:150:PHE:HD2	2.06	0.54
1:A:125:SER:HB2	2:B:142:ARG:NH2	2.22	0.54
2:C:334:ASP:O	2:C:338:LEU:HB2	2.08	0.54
2:F:381:TRP:CG	2:F:382:LEU:N	2.74	0.54
2:G:143:ARG:HD3	1:H:214:TRP:CZ3	2.42	0.54
2:G:210:ILE:HD12	2:G:495:CYS:HB3	1.89	0.54
2:G:420:VAL:HA	2:G:423:GLN:OE1	2.07	0.54
1:H:148:ALA:HB1	1:H:194:TRP:CZ2	2.43	0.54
1:A:90:ASN:C	1:A:92:THR:H	2.16	0.54
1:A:234:CYS:HB2	1:A:265:VAL:HB	1.90	0.54
2:B:434:LEU:O	2:B:438:VAL:N	2.39	0.54
1:D:16:ILE:HA	1:D:32:SER:CB	2.36	0.54
1:D:30:THR:CG2	1:D:31:CYS:N	2.71	0.54
1:E:292:SER:O	1:E:294:ASP:N	2.41	0.54
2:G:380:SER:HB3	2:G:383:CYS:CB	2.31	0.54
2:G:479:ALA:HB1	1:H:273:THR:CG2	2.37	0.54
1:A:292:SER:O	1:A:294:ASP:N	2.40	0.54
2:B:515:ILE:HD11	2:B:540:ALA:C	2.33	0.54
2:F:167:LYS:O	2:F:167:LYS:HD3	2.08	0.54
2:F:267:ARG:HH11	2:F:267:ARG:CG	2.20	0.54
1:H:193:LEU:N	1:H:193:LEU:CD2	2.70	0.54
1:H:291:GLU:HB3	1:H:297:TRP:CD2	2.42	0.54
1:A:30:THR:CG2	1:A:31:CYS:N	2.70	0.54
1:A:220:TRP:CE2	1:A:231:ILE:HD11	2.43	0.54
2:B:371:SER:OG	2:B:373:LYS:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:371:SER:OG	2:C:373:LYS:HG3	2.07	0.54
2:C:454:ILE:O	2:C:458:ARG:HB2	2.08	0.54
1:E:258:LEU:CD1	1:E:297:TRP:HB3	2.38	0.54
2:G:148:TYR:HB2	1:H:266:TRP:CE2	2.43	0.54
2:G:479:ALA:CB	1:H:273:THR:CG2	2.86	0.54
1:A:199:ASP:OD1	1:A:200:GLY:N	2.40	0.54
2:B:202:ARG:HG2	2:B:209:GLN:OE1	2.07	0.54
2:C:155:THR:CG2	2:C:513:ARG:HD2	2.37	0.54
1:D:182:PHE:CD1	1:D:182:PHE:O	2.61	0.54
1:E:302:ASP:C	1:E:302:ASP:OD1	2.50	0.54
2:F:145:THR:HG22	2:F:146:ALA:N	2.22	0.54
2:G:454:ILE:O	2:G:458:ARG:HB2	2.08	0.54
1:H:43:ARG:O	1:H:44:ASN:HB2	2.07	0.54
1:A:47:GLN:OE1	2:B:167:LYS:N	2.41	0.54
1:A:88:GLU:HA	1:A:92:THR:O	2.08	0.54
1:A:288:LEU:HB2	1:A:300:ILE:HG13	1.90	0.54
2:B:491:LEU:HD21	2:B:532:ILE:CD1	2.33	0.54
1:D:90:ASN:C	1:D:92:THR:H	2.16	0.54
1:E:16:ILE:HA	1:E:32:SER:CB	2.36	0.54
1:E:199:ASP:OD1	1:E:200:GLY:N	2.40	0.54
2:F:137:LEU:O	2:F:141:GLU:HB3	2.08	0.54
2:G:175:LEU:HD13	2:G:176:PRO:HD2	1.89	0.54
2:G:230:ASP:O	2:G:231:TYR:C	2.51	0.54
2:G:334:ASP:O	2:G:338:LEU:HB2	2.08	0.54
2:G:547:TYR:HE1	1:H:72:ASN:ND2	2.04	0.54
1:H:238:GLY:O	1:H:260:LYS:HA	2.07	0.54
2:B:154:SER:O	2:B:157:SER:N	2.38	0.54
1:D:88:GLU:HA	1:D:92:THR:O	2.08	0.54
1:D:220:TRP:CE2	1:D:231:ILE:HD11	2.42	0.54
2:F:155:THR:C	2:F:157:SER:H	2.14	0.54
2:G:229:SER:O	2:G:232:ASN:HB2	2.08	0.54
1:H:30:THR:CG2	1:H:31:CYS:N	2.71	0.54
1:A:250:SER:C	1:A:252:THR:H	2.14	0.54
2:B:334:ASP:O	2:B:338:LEU:HB2	2.08	0.54
2:C:350:ILE:HB	2:C:354:ILE:HD12	1.90	0.54
1:E:23:TYR:CD2	1:E:68:PRO:HG3	2.42	0.54
1:E:182:PHE:O	1:E:182:PHE:CD1	2.60	0.54
2:F:202:ARG:HG2	2:F:209:GLN:OE1	2.07	0.54
2:F:268:LEU:CD2	2:F:389:LEU:HD13	2.37	0.54
2:F:371:SER:OG	2:F:373:LYS:HG3	2.07	0.54
2:G:158:MET:HE2	2:G:174:ARG:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HA	1:A:41:ASP:HA	1.91	0.53
2:B:145:THR:HG22	2:B:146:ALA:N	2.22	0.53
2:B:240:LEU:HD21	2:B:268:LEU:CD1	2.39	0.53
2:C:150:PHE:N	2:C:150:PHE:HD2	2.06	0.53
2:C:181:ARG:NH1	2:C:234:TRP:NE1	2.56	0.53
1:D:43:ARG:O	1:D:44:ASN:HB2	2.07	0.53
1:E:47:GLN:HE22	2:F:170:VAL:HG23	1.73	0.53
2:F:280:ILE:HD11	2:F:383:CYS:SG	2.48	0.53
2:G:170:VAL:CG1	2:G:171:SER:N	2.70	0.53
2:G:347:GLY:C	2:G:349:SER:H	2.16	0.53
2:B:137:LEU:O	2:B:141:GLU:HB3	2.08	0.53
2:B:238:SER:O	2:B:242:ASP:HB2	2.08	0.53
1:E:206:GLN:HG3	1:E:207:LYS:H	1.72	0.53
1:H:88:GLU:HA	1:H:92:THR:O	2.08	0.53
1:H:182:PHE:O	1:H:182:PHE:CD1	2.61	0.53
1:H:192:LYS:NZ	1:H:207:LYS:HE2	2.24	0.53
2:C:150:PHE:N	2:C:150:PHE:CD2	2.76	0.53
2:C:170:VAL:CG1	2:C:171:SER:N	2.71	0.53
2:C:208:PRO:HG3	2:C:532:ILE:HD13	1.90	0.53
2:C:229:SER:O	2:C:232:ASN:HB2	2.08	0.53
2:C:230:ASP:O	2:C:231:TYR:C	2.51	0.53
1:E:90:ASN:C	1:E:92:THR:H	2.16	0.53
2:F:334:ASP:O	2:F:338:LEU:HB2	2.08	0.53
2:F:381:TRP:CD1	2:F:382:LEU:N	2.77	0.53
1:H:189:ASN:ND2	1:H:213:ASP:C	2.66	0.53
2:B:210:ILE:HD12	2:B:210:ILE:N	2.24	0.53
2:C:364:SER:HB3	2:C:394:ILE:CG1	2.22	0.53
1:E:67:HIS:O	1:E:69:MET:N	2.42	0.53
2:F:229:SER:O	2:F:232:ASN:HB2	2.08	0.53
1:H:206:GLN:HG3	1:H:207:LYS:H	1.72	0.53
2:B:454:ILE:O	2:B:458:ARG:HB2	2.09	0.53
1:E:145:ILE:HD13	1:E:194:TRP:CE3	2.44	0.53
2:G:197:VAL:CG1	2:G:198:THR:H	2.22	0.53
1:D:241:PHE:C	1:D:242:ILE:HD12	2.33	0.53
1:E:230:THR:CG2	1:E:231:ILE:H	2.21	0.53
2:G:299:LEU:HD22	2:G:383:CYS:SG	2.49	0.53
1:H:16:ILE:HA	1:H:32:SER:CB	2.36	0.53
2:B:197:VAL:CG1	2:B:198:THR:H	2.21	0.53
2:C:197:VAL:CG1	2:C:198:THR:N	2.70	0.53
2:C:546:ARG:HH11	2:C:546:ARG:HG3	1.74	0.53
1:E:148:ALA:HB1	1:E:194:TRP:CZ2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:TRP:CE2	1:E:231:ILE:HD11	2.42	0.53
2:F:210:ILE:N	2:F:210:ILE:HD12	2.24	0.53
1:H:252:THR:O	1:H:252:THR:HG22	2.08	0.53
1:A:21:MET:HB3	2:B:154:SER:OG	2.09	0.53
2:B:167:LYS:O	2:B:167:LYS:HD3	2.08	0.53
1:D:99:HIS:CE1	1:D:142:VAL:HG11	2.44	0.53
2:F:202:ARG:HG2	2:F:209:GLN:HB2	1.91	0.53
1:H:241:PHE:C	1:H:242:ILE:HD12	2.34	0.53
1:A:67:HIS:O	1:A:69:MET:N	2.42	0.53
2:C:202:ARG:HG2	2:C:209:GLN:HB2	1.91	0.53
2:C:210:ILE:HD12	2:C:210:ILE:N	2.24	0.53
1:E:27:ARG:HA	1:E:41:ASP:HA	1.90	0.53
1:E:193:LEU:HD21	1:E:208:LEU:HD11	1.90	0.53
2:G:197:VAL:CG1	2:G:198:THR:N	2.70	0.53
2:G:382:LEU:HD12	2:G:385:LEU:HD23	1.90	0.53
2:G:434:LEU:O	2:G:438:VAL:N	2.39	0.53
1:H:90:ASN:C	1:H:92:THR:H	2.16	0.53
1:H:99:HIS:CE1	1:H:142:VAL:HG11	2.44	0.53
1:A:16:ILE:HA	1:A:32:SER:CB	2.36	0.53
1:A:230:THR:CG2	1:A:231:ILE:H	2.22	0.53
2:B:248:TYR:HB2	2:C:339:GLN:HE22	1.74	0.53
1:E:191:ILE:HD11	1:E:211:HIS:HD2	1.73	0.53
2:G:432:GLU:OE2	2:G:466:SER:CB	2.55	0.53
1:A:99:HIS:CE1	1:A:142:VAL:HG11	2.44	0.52
2:C:382:LEU:HD12	2:C:385:LEU:HD23	1.90	0.52
2:C:523:ASN:HB3	2:C:525:HIS:HE1	1.75	0.52
1:E:107:ASN:CG	2:F:142:ARG:NH1	2.64	0.52
2:G:149:THR:CG2	2:G:150:PHE:N	2.72	0.52
2:G:202:ARG:HG2	2:G:209:GLN:OE1	2.08	0.52
2:G:202:ARG:HG2	2:G:209:GLN:HB2	1.91	0.52
2:G:343:TRP:CH2	2:G:350:ILE:HD12	2.44	0.52
2:G:384:LEU:O	2:G:387:LEU:HB2	2.10	0.52
2:G:515:ILE:HD11	2:G:540:ALA:C	2.33	0.52
1:A:17:HIS:CE1	2:B:148:TYR:CE2	2.97	0.52
1:A:69:MET:CE	1:A:114:HIS:HB2	2.40	0.52
2:B:174:ARG:CZ	2:B:485:GLN:HG2	2.39	0.52
2:F:181:ARG:HH12	2:F:234:TRP:HE1	1.58	0.52
2:G:394:ILE:O	2:G:397:TYR:HD1	1.91	0.52
2:C:359:LYS:HZ2	2:C:368:GLY:HA3	1.71	0.52
2:G:414:TYR:HD2	2:G:415:ASP:H	1.56	0.52
1:A:230:THR:CG2	1:A:231:ILE:N	2.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:CD1	1:A:243:TRP:H	2.26	0.52
2:C:251:ASP:OD1	2:C:251:ASP:O	2.27	0.52
1:E:287:THR:O	1:E:288:LEU:HD23	2.10	0.52
2:F:359:LYS:HZ2	2:F:368:GLY:HA3	1.72	0.52
1:H:270:TRP:C	1:H:271:SER:O	2.52	0.52
2:B:229:SER:O	2:B:232:ASN:HB2	2.08	0.52
2:B:515:ILE:HD13	2:B:541:GLN:CA	2.39	0.52
2:C:224:MET:HE1	2:C:230:ASP:OD1	2.10	0.52
2:C:384:LEU:O	2:C:387:LEU:HB2	2.10	0.52
1:D:69:MET:CE	1:D:114:HIS:HB2	2.40	0.52
1:E:99:HIS:CE1	1:E:142:VAL:HG11	2.44	0.52
1:E:192:LYS:CE	1:E:207:LYS:HE2	2.40	0.52
2:F:382:LEU:HD12	2:F:385:LEU:HD23	1.91	0.52
2:G:150:PHE:N	2:G:150:PHE:CD2	2.76	0.52
2:G:210:ILE:HD12	2:G:210:ILE:N	2.24	0.52
2:G:409:LYS:C	2:G:410:PHE:CD2	2.88	0.52
1:H:33:SER:HA	1:H:59:PRO:HB3	1.92	0.52
1:A:33:SER:HA	1:A:59:PRO:HB3	1.92	0.52
2:B:399:LEU:O	2:B:402:LEU:HB3	2.09	0.52
2:C:399:LEU:O	2:C:402:LEU:HB3	2.10	0.52
1:D:195:LYS:HG3	1:D:196:GLU:H	1.75	0.52
1:D:221:ALA:HB2	1:D:270:TRP:CD2	2.45	0.52
1:E:33:SER:HA	1:E:59:PRO:HB3	1.92	0.52
1:E:125:SER:HB2	2:F:142:ARG:HH21	1.75	0.52
2:F:359:LYS:HZ1	2:F:368:GLY:HA3	1.74	0.52
2:F:546:ARG:HH11	2:F:546:ARG:HG3	1.74	0.52
2:G:142:ARG:NH2	1:H:107:ASN:ND2	2.56	0.52
2:G:172:ILE:HD11	1:H:28:LEU:CD1	2.40	0.52
2:G:267:ARG:HH11	2:G:267:ARG:CG	2.20	0.52
2:G:544:LYS:HD2	1:H:24:TYR:CE2	2.45	0.52
2:G:546:ARG:HH11	2:G:546:ARG:HG3	1.74	0.52
1:H:67:HIS:O	1:H:69:MET:N	2.42	0.52
1:A:258:LEU:CD1	1:A:297:TRP:CB	2.88	0.52
2:B:149:THR:HG22	2:B:150:PHE:N	2.25	0.52
2:B:202:ARG:HG2	2:B:209:GLN:HB2	1.91	0.52
2:B:215:LEU:CD1	2:B:452:TYR:OH	2.58	0.52
2:B:276:ILE:HD11	2:B:383:CYS:HA	1.91	0.52
2:B:297:TYR:HB3	2:B:306:ALA:HB2	1.91	0.52
2:C:409:LYS:C	2:C:410:PHE:CD2	2.88	0.52
2:F:399:LEU:O	2:F:402:LEU:HB3	2.09	0.52
2:F:454:ILE:O	2:F:458:ARG:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:149:THR:HG23	2:G:162:LYS:HG2	1.92	0.52
2:G:359:LYS:HZ2	2:G:368:GLY:HA3	1.73	0.52
2:G:471:ASP:CG	2:G:498:ASN:H	2.18	0.52
2:G:525:HIS:O	2:G:526:ILE:C	2.53	0.52
1:H:244:THR:HG22	1:H:245:CYS:N	2.24	0.52
2:B:181:ARG:HH12	2:B:234:TRP:HE1	1.58	0.52
2:G:170:VAL:CG1	2:G:171:SER:H	2.23	0.52
2:G:194:ILE:HG12	2:G:492:PHE:CE2	2.45	0.52
2:G:215:LEU:CD1	2:G:452:TYR:OH	2.58	0.52
2:B:523:ASN:HB3	2:B:525:HIS:HE1	1.75	0.52
2:C:508:LYS:HA	2:C:536:LEU:HD21	1.92	0.52
1:D:67:HIS:O	1:D:69:MET:N	2.43	0.52
1:D:287:THR:O	1:D:288:LEU:HD23	2.10	0.52
1:E:230:THR:CG2	1:E:231:ILE:N	2.71	0.52
2:F:149:THR:HG22	2:F:150:PHE:N	2.24	0.52
2:G:399:LEU:O	2:G:402:LEU:HB3	2.10	0.52
1:H:69:MET:CE	1:H:114:HIS:HB2	2.40	0.52
1:H:287:THR:O	1:H:288:LEU:HD23	2.10	0.52
2:C:199:ILE:CD1	2:C:530:LEU:HA	2.40	0.52
1:D:33:SER:HA	1:D:59:PRO:HB3	1.92	0.52
2:F:196:LYS:HE3	2:F:219:ASP:OD1	2.10	0.52
2:F:525:HIS:O	2:F:526:ILE:C	2.53	0.52
2:G:359:LYS:HZ1	2:G:368:GLY:HA3	1.74	0.52
1:H:230:THR:CG2	1:H:231:ILE:N	2.72	0.52
1:H:293:VAL:O	1:H:293:VAL:HG12	2.09	0.52
1:D:69:MET:HE2	1:D:114:HIS:HB2	1.93	0.51
1:D:292:SER:C	1:D:294:ASP:N	2.68	0.51
1:E:270:TRP:C	1:E:271:SER:O	2.53	0.51
2:F:384:LEU:O	2:F:387:LEU:HB2	2.09	0.51
2:F:523:ASN:HB3	2:F:525:HIS:HE1	1.75	0.51
2:G:435:TYR:CZ	2:G:454:ILE:HD11	2.46	0.51
1:H:288:LEU:H	1:H:301:SER:CB	2.23	0.51
1:A:107:ASN:CG	2:B:142:ARG:HH22	2.17	0.51
2:F:177:THR:HG22	2:F:178:GLU:N	2.25	0.51
2:F:409:LYS:C	2:F:410:PHE:CD2	2.88	0.51
1:H:208:LEU:HB3	1:H:243:TRP:CZ3	2.45	0.51
1:A:292:SER:C	1:A:294:ASP:N	2.68	0.51
2:B:409:LYS:C	2:B:410:PHE:CD2	2.88	0.51
2:C:512:MET:HA	2:C:540:ALA:HB1	1.92	0.51
1:E:17:HIS:CE1	2:F:148:TYR:HE2	2.28	0.51
1:E:107:ASN:OD1	2:F:142:ARG:CZ	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LYS:HG2	1:E:304:ASN:HD21	1.75	0.51
2:F:475:PHE:CE2	2:F:497:LEU:HD11	2.45	0.51
1:H:53:LEU:N	1:H:53:LEU:HD23	2.26	0.51
1:D:113:PRO:CB	1:D:161:ALA:HB2	2.40	0.51
2:F:197:VAL:CG1	2:F:198:THR:H	2.22	0.51
1:H:102:HIS:HD1	1:H:124:SER:CB	2.22	0.51
1:A:287:THR:O	1:A:288:LEU:HD23	2.10	0.51
2:B:335:LEU:O	2:B:335:LEU:HD12	2.11	0.51
2:C:170:VAL:CG1	2:C:171:SER:H	2.23	0.51
1:D:155:ALA:CB	1:D:218:VAL:H	2.23	0.51
1:H:69:MET:HE2	1:H:114:HIS:HB2	1.93	0.51
1:A:206:GLN:HG3	1:A:207:LYS:H	1.72	0.51
2:B:164:ILE:HG23	2:B:164:ILE:O	2.11	0.51
2:C:154:SER:OG	2:C:158:MET:HB2	2.11	0.51
2:C:335:LEU:O	2:C:335:LEU:HD12	2.11	0.51
1:D:27:ARG:HA	1:D:41:ASP:HA	1.91	0.51
1:D:53:LEU:N	1:D:53:LEU:HD23	2.26	0.51
1:D:230:THR:CG2	1:D:231:ILE:N	2.72	0.51
2:F:224:MET:HE1	2:F:230:ASP:OD1	2.11	0.51
2:F:297:TYR:HB3	2:F:306:ALA:HB2	1.91	0.51
2:G:224:MET:HE1	2:G:230:ASP:OD1	2.10	0.51
2:B:384:LEU:O	2:B:387:LEU:HB2	2.09	0.51
2:B:413:PRO:HB2	2:B:416:ASP:HB2	1.93	0.51
2:C:525:HIS:O	2:C:526:ILE:C	2.53	0.51
1:E:69:MET:HE2	1:E:114:HIS:HB2	1.93	0.51
2:F:250:THR:HG21	2:G:335:LEU:HD13	1.92	0.51
2:F:302:ASP:OD1	2:F:305:ARG:HB2	2.11	0.51
1:H:27:ARG:HA	1:H:41:ASP:HA	1.91	0.51
1:A:53:LEU:N	1:A:53:LEU:HD23	2.26	0.51
2:B:163:ASP:C	2:B:165:VAL:H	2.19	0.51
2:B:224:MET:HE1	2:B:230:ASP:OD1	2.10	0.51
2:C:148:TYR:HD1	1:D:266:TRP:CG	2.29	0.51
2:C:484:ALA:O	2:C:485:GLN:HB2	2.11	0.51
1:E:69:MET:CE	1:E:114:HIS:HB2	2.40	0.51
1:E:292:SER:C	1:E:294:ASP:N	2.68	0.51
2:F:392:GLY:O	2:F:394:ILE:N	2.43	0.51
2:G:154:SER:OG	2:G:158:MET:HB2	2.10	0.51
2:G:215:LEU:HD12	2:G:452:TYR:CZ	2.45	0.51
2:B:232:ASN:O	2:B:233:LEU:C	2.53	0.51
2:B:280:ILE:HB	2:B:300:LEU:HD21	1.93	0.51
1:D:208:LEU:HB3	1:D:243:TRP:CH2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ARG:HG2	1:E:27:ARG:NH1	2.26	0.51
2:F:335:LEU:O	2:F:335:LEU:HD12	2.11	0.51
2:G:297:TYR:HB3	2:G:306:ALA:HB2	1.91	0.51
2:B:177:THR:HG22	2:B:178:GLU:N	2.25	0.51
2:B:525:HIS:O	2:B:526:ILE:C	2.53	0.51
2:C:175:LEU:HD13	2:C:176:PRO:CD	2.41	0.51
1:H:27:ARG:HG2	1:H:27:ARG:NH1	2.26	0.51
1:A:14:ASP:CG	1:A:15:MET:H	2.19	0.50
2:B:382:LEU:HD12	2:B:385:LEU:HD23	1.91	0.50
2:B:546:ARG:HH11	2:B:546:ARG:HG3	1.74	0.50
1:D:270:TRP:C	1:D:271:SER:O	2.52	0.50
2:F:550:ASN:OD1	2:F:550:ASN:N	2.44	0.50
1:A:15:MET:O	1:A:32:SER:HB2	2.12	0.50
2:C:530:LEU:HB2	2:C:532:ILE:HG12	1.92	0.50
1:D:14:ASP:CG	1:D:15:MET:H	2.20	0.50
2:G:181:ARG:NH1	2:G:234:TRP:HE1	2.07	0.50
2:F:232:ASN:O	2:F:233:LEU:C	2.54	0.50
2:G:210:ILE:HG22	2:G:459:PHE:HE2	1.76	0.50
1:H:185:GLY:N	1:H:218:VAL:HG21	2.26	0.50
1:A:109:VAL:HG12	1:A:110:CYS:N	2.27	0.50
1:A:193:LEU:C	1:A:194:TRP:CD1	2.90	0.50
2:B:403:VAL:O	2:B:407:LEU:HD13	2.11	0.50
2:C:149:THR:HG23	2:C:162:LYS:HG2	1.92	0.50
2:F:155:THR:HG22	2:F:513:ARG:CD	2.41	0.50
2:F:163:ASP:C	2:F:165:VAL:H	2.19	0.50
2:F:412:LEU:HD12	2:F:412:LEU:N	2.27	0.50
2:G:276:ILE:HD13	2:G:383:CYS:SG	2.51	0.50
2:G:523:ASN:HB3	2:G:525:HIS:HE1	1.75	0.50
1:A:113:PRO:CB	1:A:161:ALA:HB2	2.41	0.50
2:C:143:ARG:HD3	1:D:214:TRP:CZ3	2.47	0.50
2:C:434:LEU:O	2:C:438:VAL:N	2.39	0.50
1:D:193:LEU:C	1:D:194:TRP:CD1	2.90	0.50
1:E:53:LEU:N	1:E:53:LEU:HD23	2.26	0.50
1:E:182:PHE:CD1	1:E:182:PHE:C	2.90	0.50
2:F:197:VAL:CG1	2:F:198:THR:N	2.70	0.50
2:G:279:GLU:OE1	2:G:380:SER:HB2	2.12	0.50
1:H:109:VAL:HG12	1:H:110:CYS:N	2.27	0.50
1:H:195:LYS:HD2	1:H:195:LYS:O	2.12	0.50
1:A:145:ILE:HD13	1:A:194:TRP:CE3	2.46	0.50
2:B:237:SER:C	2:B:239:ILE:N	2.68	0.50
1:E:14:ASP:CG	1:E:15:MET:H	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:PHE:CZ	2:F:168:SER:CB	2.91	0.50
2:G:335:LEU:O	2:G:335:LEU:HD12	2.11	0.50
1:H:15:MET:O	1:H:32:SER:HB2	2.12	0.50
2:C:197:VAL:CG1	2:C:198:THR:H	2.22	0.50
2:C:280:ILE:CB	2:C:300:LEU:HD21	2.41	0.50
2:C:451:TRP:CE2	2:C:493:VAL:HG13	2.46	0.50
1:D:15:MET:O	1:D:32:SER:HB2	2.12	0.50
1:E:149:HIS:HB3	1:E:188:ASP:OD1	2.12	0.50
1:E:193:LEU:C	1:E:194:TRP:CD1	2.90	0.50
2:F:164:ILE:HG23	2:F:164:ILE:O	2.11	0.50
1:H:290:LYS:HG2	1:H:291:GLU:N	2.27	0.50
2:C:403:VAL:O	2:C:407:LEU:HD13	2.12	0.50
1:E:288:LEU:HB2	1:E:300:ILE:HG13	1.94	0.50
2:G:148:TYR:HD1	1:H:266:TRP:CG	2.30	0.50
2:G:381:TRP:CD1	2:G:381:TRP:H	2.29	0.50
1:A:27:ARG:NH1	1:A:27:ARG:HG2	2.26	0.50
2:C:216:LEU:HB3	2:C:242:ASP:OD1	2.12	0.50
2:C:384:LEU:HD13	2:C:410:PHE:CE1	2.47	0.50
1:E:109:VAL:HG12	1:E:110:CYS:N	2.26	0.50
2:F:132:ILE:HG22	2:F:135:ALA:HB3	1.94	0.50
2:F:412:LEU:HD12	2:F:412:LEU:H	1.76	0.50
1:H:193:LEU:C	1:H:194:TRP:CD1	2.90	0.50
1:A:182:PHE:CD1	1:A:182:PHE:C	2.89	0.49
2:C:185:PHE:HA	2:C:486:LEU:CD1	2.42	0.49
1:E:79:TYR:CD2	2:F:138:ILE:HD13	2.46	0.49
2:F:284:ILE:HD13	2:F:297:TYR:CE1	2.47	0.49
2:G:138:ILE:O	2:G:142:ARG:HG2	2.12	0.49
2:G:439:ARG:HA	2:G:442:THR:CB	2.42	0.49
2:C:451:TRP:CZ2	2:C:493:VAL:HG13	2.46	0.49
1:A:69:MET:HE2	1:A:114:HIS:HB2	1.93	0.49
1:A:191:ILE:HB	1:A:208:LEU:HB2	1.93	0.49
2:C:442:THR:HG23	2:C:445:LEU:HB2	1.94	0.49
1:E:236:GLN:HA	1:E:264:VAL:HG22	1.94	0.49
2:F:210:ILE:HG12	2:F:496:PHE:CE1	2.47	0.49
1:H:219:ALA:O	1:H:270:TRP:NE1	2.44	0.49
2:C:521:SER:C	2:C:523:ASN:N	2.70	0.49
1:D:191:ILE:HD11	1:D:211:HIS:CD2	2.47	0.49
1:D:230:THR:CG2	1:D:231:ILE:H	2.23	0.49
2:F:524:ASP:O	2:F:525:HIS:CB	2.60	0.49
2:G:403:VAL:O	2:G:407:LEU:HD13	2.12	0.49
2:G:479:ALA:HB1	1:H:273:THR:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:489:HIS:O	2:G:490:SER:C	2.54	0.49
2:G:508:LYS:HA	2:G:536:LEU:HD21	1.94	0.49
1:H:182:PHE:CD1	1:H:182:PHE:C	2.90	0.49
1:A:107:ASN:OD1	2:B:142:ARG:NH1	2.45	0.49
1:A:198:GLU:HG2	1:A:198:GLU:O	2.13	0.49
1:A:204:GLU:HG3	1:A:204:GLU:O	2.13	0.49
2:B:237:SER:C	2:B:239:ILE:H	2.21	0.49
2:B:399:LEU:HD23	2:B:425:TYR:OH	2.11	0.49
2:C:359:LYS:HZ1	2:C:368:GLY:HA3	1.75	0.49
2:C:550:ASN:OD1	2:C:550:ASN:N	2.44	0.49
1:D:189:ASN:ND2	1:D:213:ASP:C	2.70	0.49
2:F:155:THR:O	2:F:513:ARG:NH1	2.45	0.49
2:G:550:ASN:N	2:G:550:ASN:OD1	2.44	0.49
1:A:47:GLN:HE22	2:B:170:VAL:HG23	1.77	0.49
1:A:112:ALA:HB2	1:A:158:TRP:CZ2	2.48	0.49
1:E:15:MET:O	1:E:32:SER:HB2	2.12	0.49
2:F:403:VAL:O	2:F:407:LEU:HD13	2.12	0.49
2:G:175:LEU:HD13	2:G:176:PRO:CD	2.41	0.49
1:H:14:ASP:CG	1:H:15:MET:H	2.20	0.49
1:H:258:LEU:HD13	1:H:297:TRP:CB	2.43	0.49
2:B:276:ILE:CG2	2:B:280:ILE:HG13	2.42	0.49
2:B:524:ASP:O	2:B:525:HIS:CB	2.61	0.49
2:C:138:ILE:O	2:C:142:ARG:HG2	2.12	0.49
2:C:162:LYS:NZ	1:D:15:MET:CE	2.76	0.49
2:C:179:LEU:HD11	2:C:448:GLN:HB2	1.94	0.49
2:C:412:LEU:HD22	2:C:413:PRO:HD2	1.94	0.49
2:F:210:ILE:HD13	2:F:496:PHE:CD1	2.48	0.49
2:F:485:GLN:HE21	2:F:517:LEU:HD21	1.77	0.49
2:G:245:SER:O	2:G:247:PRO:HD3	2.11	0.49
1:H:195:LYS:HD2	1:H:195:LYS:C	2.37	0.49
2:C:237:SER:C	2:C:239:ILE:H	2.21	0.49
2:C:237:SER:C	2:C:239:ILE:N	2.69	0.49
1:E:102:HIS:HD1	1:E:124:SER:CB	2.22	0.49
2:F:237:SER:C	2:F:239:ILE:H	2.21	0.49
2:G:414:TYR:HD2	2:G:415:ASP:N	2.11	0.49
2:G:479:ALA:CB	1:H:273:THR:HG21	2.42	0.49
2:G:487:HIS:O	2:G:488:GLY:C	2.55	0.49
2:G:512:MET:SD	2:G:540:ALA:CB	3.01	0.49
1:H:230:THR:CG2	1:H:231:ILE:H	2.23	0.49
1:D:109:VAL:HG12	1:D:110:CYS:N	2.27	0.49
2:F:457:LEU:HD12	2:F:465:PHE:HE1	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:O	1:A:253:TRP:HA	2.13	0.49
2:B:550:ASN:N	2:B:550:ASN:OD1	2.45	0.49
2:C:194:ILE:HG12	2:C:492:PHE:HE2	1.78	0.49
2:C:232:ASN:O	2:C:233:LEU:C	2.54	0.49
1:D:182:PHE:CD1	1:D:182:PHE:C	2.90	0.49
1:E:28:LEU:HD11	2:F:172:ILE:HD11	1.92	0.49
1:E:288:LEU:HB3	1:E:300:ILE:HD11	1.94	0.49
2:F:179:LEU:HD11	2:F:184:LEU:HD11	1.95	0.49
2:F:244:VAL:HG11	2:F:263:GLU:HB3	1.95	0.49
2:F:439:ARG:HA	2:F:442:THR:CB	2.42	0.49
1:A:243:TRP:CD1	1:A:243:TRP:N	2.80	0.48
1:D:204:GLU:O	1:D:204:GLU:HG3	2.13	0.48
2:G:181:ARG:HH12	2:G:234:TRP:NE1	2.08	0.48
2:B:223:TYR:N	2:B:223:TYR:CD1	2.81	0.48
2:C:267:ARG:HH11	2:C:267:ARG:CG	2.20	0.48
2:C:439:ARG:HA	2:C:442:THR:CB	2.42	0.48
1:D:113:PRO:HB3	1:D:161:ALA:HB2	1.95	0.48
2:F:217:PHE:HA	2:F:452:TYR:HE2	1.76	0.48
2:F:276:ILE:CG2	2:F:280:ILE:HG13	2.43	0.48
2:F:320:VAL:HG22	2:G:263:GLU:HA	1.94	0.48
2:G:269:THR:HG21	2:G:390:CYS:SG	2.52	0.48
2:G:524:ASP:O	2:G:525:HIS:CB	2.61	0.48
1:A:26:THR:CG2	1:A:27:ARG:HD2	2.42	0.48
1:A:192:LYS:CE	1:A:207:LYS:HE2	2.43	0.48
2:B:132:ILE:HG22	2:B:135:ALA:HB3	1.94	0.48
2:B:439:ARG:HA	2:B:442:THR:CB	2.42	0.48
2:B:521:SER:O	2:B:523:ASN:N	2.42	0.48
1:D:192:LYS:HE2	1:D:207:LYS:HE2	1.94	0.48
1:D:192:LYS:CE	1:D:207:LYS:HE2	2.42	0.48
1:D:238:GLY:O	1:D:260:LYS:HA	2.13	0.48
1:E:107:ASN:OD1	2:F:142:ARG:NH2	2.46	0.48
1:E:109:VAL:CG1	1:E:110:CYS:N	2.77	0.48
1:E:198:GLU:O	1:E:198:GLU:HG2	2.13	0.48
2:F:521:SER:C	2:F:523:ASN:N	2.70	0.48
2:G:223:TYR:N	2:G:223:TYR:CD1	2.81	0.48
1:A:102:HIS:HD1	1:A:124:SER:CB	2.22	0.48
1:A:185:GLY:HA3	1:A:215:VAL:HG11	1.96	0.48
2:B:403:VAL:O	2:B:407:LEU:CD1	2.62	0.48
2:C:524:ASP:O	2:C:525:HIS:CB	2.60	0.48
1:E:183:ALA:O	1:E:184:SER:HB3	2.13	0.48
2:F:512:MET:SD	2:F:540:ALA:HB2	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:ALA:O	1:H:184:SER:HB3	2.14	0.48
2:B:196:LYS:HE3	2:B:219:ASP:OD1	2.14	0.48
2:B:215:LEU:C	2:B:216:LEU:HD23	2.38	0.48
2:C:215:LEU:C	2:C:216:LEU:HD23	2.39	0.48
2:C:489:HIS:O	2:C:490:SER:C	2.56	0.48
2:F:248:TYR:OH	2:G:343:TRP:HH2	1.96	0.48
2:F:403:VAL:O	2:F:407:LEU:CD1	2.62	0.48
2:G:232:ASN:O	2:G:233:LEU:C	2.54	0.48
2:G:395:ASP:OD1	2:G:396:GLU:HG3	2.14	0.48
1:H:113:PRO:HB3	1:H:161:ALA:HB2	1.94	0.48
1:A:148:ALA:HB1	1:A:194:TRP:CH2	2.48	0.48
1:A:274:ALA:O	1:A:275:ASN:C	2.57	0.48
2:B:207:TYR:CD2	2:B:504:GLU:HA	2.48	0.48
1:D:27:ARG:NH1	1:D:27:ARG:HG2	2.27	0.48
2:F:247:PRO:HG3	2:G:317:HIS:CD2	2.48	0.48
2:G:155:THR:HG21	1:H:23:TYR:O	2.13	0.48
1:H:204:GLU:HG3	1:H:204:GLU:O	2.14	0.48
1:A:115:ASP:C	1:A:117:GLY:H	2.22	0.48
2:B:385:LEU:HA	2:B:406:HIS:CE1	2.48	0.48
1:D:288:LEU:N	1:D:301:SER:HB3	2.28	0.48
1:E:274:ALA:O	1:E:275:ASN:C	2.57	0.48
2:F:215:LEU:HD12	2:F:452:TYR:CZ	2.48	0.48
2:F:223:TYR:CD1	2:F:223:TYR:N	2.81	0.48
2:F:515:ILE:HD13	2:F:541:GLN:CA	2.44	0.48
2:G:521:SER:O	2:G:523:ASN:N	2.41	0.48
1:H:164:PRO:CG	1:H:176:PRO:HB2	2.44	0.48
1:A:185:GLY:N	1:A:218:VAL:HG21	2.28	0.48
1:D:164:PRO:CG	1:D:176:PRO:HB2	2.44	0.48
1:E:115:ASP:C	1:E:117:GLY:H	2.22	0.48
2:F:522:THR:HG22	2:F:526:ILE:CD1	2.37	0.48
2:G:276:ILE:CG2	2:G:280:ILE:HG13	2.42	0.48
2:G:347:GLY:C	2:G:349:SER:N	2.71	0.48
1:A:164:PRO:CG	1:A:176:PRO:HB2	2.44	0.48
1:A:21:MET:HE3	2:B:160:LEU:HD11	1.96	0.48
2:B:215:LEU:HD12	2:B:452:TYR:CE1	2.49	0.48
1:D:115:ASP:C	1:D:117:GLY:H	2.22	0.48
1:D:274:ALA:O	1:D:275:ASN:C	2.57	0.48
1:E:204:GLU:HG3	1:E:204:GLU:O	2.13	0.48
2:G:403:VAL:O	2:G:407:LEU:CD1	2.62	0.48
1:H:109:VAL:CG1	1:H:110:CYS:N	2.77	0.48
1:H:112:ALA:HB2	1:H:158:TRP:CZ2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ARG:O	2:B:143:ARG:HB2	2.14	0.47
2:C:491:LEU:HD11	2:C:507:ILE:HG23	1.96	0.47
2:G:138:ILE:HD13	1:H:59:PRO:CD	2.43	0.47
1:A:193:LEU:HD21	1:A:208:LEU:CD1	2.45	0.47
1:A:236:GLN:NE2	1:A:264:VAL:HG21	2.29	0.47
2:C:150:PHE:HE2	2:C:162:LYS:N	2.12	0.47
1:D:112:ALA:HB2	1:D:158:TRP:CZ2	2.49	0.47
2:G:237:SER:C	2:G:239:ILE:N	2.69	0.47
1:H:106:VAL:HA	1:H:124:SER:HA	1.96	0.47
1:H:192:LYS:CE	1:H:207:LYS:HE2	2.44	0.47
1:A:109:VAL:CG1	1:A:110:CYS:N	2.77	0.47
2:C:474:THR:HG23	2:C:493:VAL:HG12	1.97	0.47
1:E:128:ALA:C	1:E:129:ILE:HG13	2.40	0.47
2:G:385:LEU:HD21	2:G:422:PHE:CE2	2.49	0.47
1:A:183:ALA:O	1:A:184:SER:HB3	2.14	0.47
1:A:270:TRP:C	1:A:271:SER:O	2.52	0.47
2:B:184:LEU:HD21	2:B:448:GLN:HE22	1.78	0.47
2:B:297:TYR:CE2	2:B:305:ARG:HB3	2.49	0.47
2:C:148:TYR:HB2	1:D:266:TRP:CD2	2.49	0.47
2:C:276:ILE:CG2	2:C:280:ILE:HG13	2.42	0.47
2:C:298:LEU:HD22	2:C:325:LEU:CD2	2.44	0.47
2:C:449:PHE:O	2:C:450:CYS:C	2.58	0.47
1:D:102:HIS:HD1	1:D:124:SER:CB	2.22	0.47
2:F:215:LEU:C	2:F:216:LEU:HD23	2.39	0.47
2:G:291:ILE:HD12	2:G:351:ASP:OD2	2.13	0.47
1:H:258:LEU:CD1	1:H:297:TRP:CB	2.92	0.47
1:H:274:ALA:O	1:H:275:ASN:C	2.57	0.47
1:A:16:ILE:HG21	1:A:30:THR:HG23	1.97	0.47
2:C:381:TRP:HE3	2:C:412:LEU:HD21	1.78	0.47
2:C:403:VAL:O	2:C:407:LEU:CD1	2.62	0.47
1:D:195:LYS:O	1:D:202:TRP:CD1	2.68	0.47
1:E:56:HIS:NE2	1:E:84:ILE:HD12	2.29	0.47
1:E:164:PRO:CG	1:E:176:PRO:HB2	2.44	0.47
1:E:236:GLN:NE2	1:E:264:VAL:HG21	2.30	0.47
1:E:289:TRP:HA	1:E:298:VAL:O	2.15	0.47
2:F:237:SER:C	2:F:239:ILE:N	2.69	0.47
2:F:384:LEU:HD13	2:F:410:PHE:CE1	2.50	0.47
2:F:449:PHE:O	2:F:450:CYS:C	2.58	0.47
2:G:547:TYR:CE1	1:H:72:ASN:ND2	2.76	0.47
1:H:26:THR:O	1:H:41:ASP:OD1	2.33	0.47
1:A:106:VAL:HA	1:A:124:SER:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:GLN:CG	2:B:426:ALA:HB1	2.32	0.47
2:C:149:THR:CG2	2:C:150:PHE:N	2.72	0.47
1:D:56:HIS:NE2	1:D:84:ILE:HD12	2.30	0.47
1:D:183:ALA:O	1:D:184:SER:HB3	2.14	0.47
1:A:16:ILE:HD11	2:B:168:SER:C	2.39	0.47
1:A:234:CYS:SG	1:A:268:VAL:HG23	2.54	0.47
2:B:205:ASN:HB2	2:B:206:PRO:CD	2.45	0.47
2:C:142:ARG:O	1:D:216:ARG:NH2	2.47	0.47
2:C:148:TYR:OH	1:D:17:HIS:CE1	2.67	0.47
2:C:175:LEU:HD22	2:C:176:PRO:HD2	1.96	0.47
2:C:223:TYR:CD1	2:C:223:TYR:N	2.82	0.47
1:D:106:VAL:HA	1:D:124:SER:HA	1.97	0.47
1:D:268:VAL:HG13	1:D:277:LEU:HD11	1.96	0.47
1:E:26:THR:CG2	1:E:27:ARG:HD2	2.42	0.47
1:E:220:TRP:NE1	1:E:231:ILE:HD11	2.30	0.47
1:E:268:VAL:HG13	1:E:277:LEU:HD11	1.97	0.47
2:F:175:LEU:HD23	2:F:483:PHE:CZ	2.50	0.47
2:G:150:PHE:HE2	2:G:162:LYS:N	2.13	0.47
1:H:258:LEU:HD13	1:H:297:TRP:HB2	1.97	0.47
1:A:56:HIS:NE2	1:A:84:ILE:HD12	2.29	0.47
1:A:128:ALA:C	1:A:129:ILE:HG13	2.40	0.47
1:A:236:GLN:HA	1:A:264:VAL:HG22	1.97	0.47
2:B:208:PRO:HB3	2:B:531:LYS:HB3	1.95	0.47
2:B:323:SER:OG	2:C:262:LYS:HE2	2.14	0.47
1:E:106:VAL:HA	1:E:124:SER:HA	1.96	0.47
2:F:164:ILE:O	2:F:164:ILE:CG2	2.62	0.47
2:F:210:ILE:HG22	2:F:459:PHE:CE2	2.50	0.47
1:H:192:LYS:HE2	1:H:207:LYS:HE2	1.97	0.47
1:H:193:LEU:HD21	1:H:208:LEU:CD1	2.45	0.47
1:H:198:GLU:O	1:H:199:ASP:CB	2.63	0.47
2:B:321:LEU:N	2:B:321:LEU:HD23	2.30	0.47
2:B:439:ARG:NH1	2:B:439:ARG:CG	2.78	0.47
1:D:26:THR:O	1:D:41:ASP:OD1	2.32	0.47
2:G:175:LEU:HD22	2:G:176:PRO:HD2	1.97	0.47
2:G:237:SER:C	2:G:239:ILE:H	2.21	0.47
2:G:449:PHE:O	2:G:450:CYS:C	2.57	0.47
2:B:244:VAL:HG12	2:B:260:LEU:HD22	1.97	0.47
2:B:343:TRP:HZ3	2:B:350:ILE:CG2	2.23	0.47
2:B:375:LEU:HB2	2:B:384:LEU:HD21	1.96	0.47
2:B:522:THR:HG22	2:B:526:ILE:CD1	2.37	0.47
1:D:16:ILE:HG21	1:D:30:THR:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:VAL:CG1	1:D:110:CYS:N	2.77	0.47
2:F:202:ARG:HG3	2:F:500:ASP:OD1	2.14	0.47
2:G:246:TYR:HE1	2:G:259:LEU:HD13	1.76	0.47
2:G:404:GLN:HG2	2:G:426:ALA:HB1	1.97	0.47
1:H:292:SER:C	1:H:294:ASP:H	2.23	0.47
2:C:432:GLU:OE1	2:C:466:SER:N	2.47	0.46
2:C:487:HIS:O	2:C:488:GLY:C	2.56	0.46
1:D:128:ALA:C	1:D:129:ILE:HG13	2.40	0.46
1:D:179:ILE:HG21	1:D:181:ARG:HE	1.80	0.46
1:E:112:ALA:HB2	1:E:158:TRP:CZ2	2.49	0.46
1:E:179:ILE:HG21	1:E:181:ARG:HE	1.80	0.46
2:F:142:ARG:O	2:F:143:ARG:HB2	2.14	0.46
2:G:448:GLN:HG3	2:G:477:PHE:CZ	2.50	0.46
2:G:527:LEU:CD2	2:G:532:ILE:HD12	2.45	0.46
1:H:56:HIS:NE2	1:H:84:ILE:HD12	2.30	0.46
2:B:535:GLN:O	2:B:539:ASN:HB2	2.15	0.46
2:C:499:ASP:C	2:C:499:ASP:OD2	2.58	0.46
2:F:475:PHE:HE2	2:F:497:LEU:HD21	1.80	0.46
2:G:380:SER:CB	2:G:383:CYS:HB2	2.32	0.46
2:G:432:GLU:OE1	2:G:465:PHE:HA	2.15	0.46
2:G:491:LEU:O	2:G:492:PHE:C	2.58	0.46
2:B:175:LEU:HD23	2:B:483:PHE:CZ	2.51	0.46
2:C:370:PHE:O	2:C:371:SER:O	2.34	0.46
1:D:242:ILE:CD1	1:D:258:LEU:HB2	2.44	0.46
1:E:221:ALA:HB2	1:E:270:TRP:NE1	2.28	0.46
2:F:291:ILE:HG22	2:F:353:ASN:HB2	1.97	0.46
2:G:267:ARG:CG	2:G:267:ARG:NH1	2.78	0.46
2:G:479:ALA:CB	1:H:273:THR:HG22	2.45	0.46
1:A:250:SER:O	1:A:252:THR:N	2.48	0.46
1:D:188:ASP:O	1:D:189:ASN:HB2	2.15	0.46
1:E:107:ASN:ND2	2:F:142:ARG:NH2	2.56	0.46
2:G:215:LEU:C	2:G:216:LEU:HD23	2.39	0.46
1:H:26:THR:CG2	1:H:27:ARG:HD2	2.43	0.46
1:A:258:LEU:CD1	1:A:297:TRP:HB3	2.45	0.46
2:B:425:TYR:O	2:B:463:ARG:NH2	2.48	0.46
2:B:491:LEU:HD23	2:B:530:LEU:HD12	1.97	0.46
2:C:364:SER:HB2	2:C:367:GLU:HG2	1.98	0.46
2:C:535:GLN:O	2:C:539:ASN:HB2	2.15	0.46
1:E:16:ILE:HG21	1:E:30:THR:HG23	1.97	0.46
2:F:321:LEU:HD23	2:F:321:LEU:N	2.30	0.46
2:F:416:ASP:OD1	2:F:418:ILE:HG13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:492:PHE:CD1	2:F:492:PHE:C	2.94	0.46
2:G:244:VAL:HG11	2:G:260:LEU:HA	1.97	0.46
2:G:522:THR:HG22	2:G:526:ILE:CD1	2.36	0.46
2:B:202:ARG:NE	2:B:209:GLN:HB3	2.31	0.46
2:B:501:LYS:O	2:B:505:ASP:HB2	2.16	0.46
1:D:232:ALA:HB2	1:D:270:TRP:HZ2	1.78	0.46
2:F:421:ILE:HD11	2:F:449:PHE:CZ	2.51	0.46
2:F:521:SER:O	2:F:523:ASN:N	2.42	0.46
1:H:115:ASP:C	1:H:117:GLY:H	2.22	0.46
1:H:188:ASP:O	1:H:189:ASN:HB2	2.15	0.46
2:B:267:ARG:CG	2:B:267:ARG:NH1	2.78	0.46
2:B:449:PHE:O	2:B:450:CYS:C	2.58	0.46
2:C:205:ASN:HB2	2:C:206:PRO:CD	2.45	0.46
2:F:370:PHE:O	2:F:371:SER:O	2.33	0.46
1:H:290:LYS:HB2	1:H:300:ILE:HD12	1.97	0.46
1:A:179:ILE:HG21	1:A:181:ARG:HE	1.80	0.46
2:B:164:ILE:O	2:B:164:ILE:CG2	2.62	0.46
1:D:26:THR:CG2	1:D:27:ARG:HD2	2.43	0.46
1:D:220:TRP:NE1	1:D:231:ILE:HD11	2.31	0.46
2:F:527:LEU:HD22	2:F:532:ILE:HD12	1.98	0.46
2:G:202:ARG:NE	2:G:209:GLN:HB3	2.31	0.46
2:G:298:LEU:HD23	2:G:298:LEU:HA	1.76	0.46
2:G:409:LYS:O	2:G:410:PHE:HD2	1.99	0.46
1:H:191:ILE:HG23	1:H:218:VAL:HG21	1.97	0.46
1:H:242:ILE:HD12	1:H:242:ILE:N	2.30	0.46
1:H:290:LYS:CB	1:H:300:ILE:CD1	2.94	0.46
2:B:177:THR:CG2	2:B:178:GLU:N	2.79	0.46
2:B:409:LYS:O	2:B:410:PHE:HD2	1.99	0.46
2:B:416:ASP:OD1	2:B:418:ILE:HG13	2.16	0.46
2:C:199:ILE:HD12	2:C:530:LEU:HA	1.97	0.46
1:E:145:ILE:HG21	1:E:194:TRP:CZ3	2.51	0.46
2:F:177:THR:HG23	2:F:179:LEU:HB3	1.90	0.46
2:F:267:ARG:HH22	2:G:316:GLY:HA3	1.81	0.46
2:F:409:LYS:O	2:F:410:PHE:HD2	1.99	0.46
2:F:535:GLN:O	2:F:539:ASN:HB2	2.15	0.46
2:G:416:ASP:OD1	2:G:418:ILE:HG13	2.16	0.46
2:G:532:ILE:CG2	2:G:533:PRO:CD	2.86	0.46
1:A:67:HIS:C	1:A:69:MET:H	2.24	0.46
2:C:152:LYS:HG2	1:D:269:SER:HB2	1.98	0.46
2:C:154:SER:HB3	1:D:21:MET:HE3	1.98	0.46
2:C:501:LYS:O	2:C:505:ASP:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ALA:O	1:D:270:TRP:NE1	2.48	0.46
1:D:245:CYS:SG	1:D:253:TRP:CE2	3.04	0.46
1:E:67:HIS:ND1	1:E:69:MET:HB2	2.31	0.46
1:E:188:ASP:O	1:E:189:ASN:HB2	2.16	0.46
2:G:321:LEU:HB3	2:G:361:LEU:HD11	1.97	0.46
1:H:16:ILE:HG21	1:H:30:THR:HG23	1.97	0.46
1:H:128:ALA:C	1:H:129:ILE:HG13	2.40	0.46
1:A:56:HIS:CE1	1:A:84:ILE:CD1	2.97	0.45
1:A:157:SER:HB2	1:A:218:VAL:O	2.16	0.45
2:C:224:MET:CE	2:C:230:ASP:HB3	2.46	0.45
2:C:321:LEU:N	2:C:321:LEU:HD23	2.30	0.45
2:C:416:ASP:OD1	2:C:418:ILE:HG13	2.16	0.45
1:D:258:LEU:CD1	1:D:297:TRP:HB2	2.46	0.45
2:F:248:TYR:CZ	2:G:343:TRP:CZ2	3.04	0.45
2:G:153:PHE:CE2	1:H:278:ALA:HB2	2.50	0.45
2:G:224:MET:CE	2:G:230:ASP:HB3	2.46	0.45
2:G:364:SER:HB2	2:G:367:GLU:HG2	1.98	0.45
1:H:67:HIS:ND1	1:H:69:MET:HB2	2.31	0.45
1:H:287:THR:HA	1:H:301:SER:CB	2.46	0.45
2:B:252:ASN:HB3	2:B:255:VAL:HB	1.98	0.45
2:B:370:PHE:O	2:B:371:SER:O	2.33	0.45
2:C:351:ASP:C	2:C:353:ASN:N	2.74	0.45
2:C:462:THR:C	2:C:463:ARG:HG2	2.40	0.45
1:D:67:HIS:C	1:D:69:MET:H	2.25	0.45
2:F:155:THR:C	2:F:157:SER:N	2.74	0.45
2:F:501:LYS:O	2:F:505:ASP:HB2	2.16	0.45
2:G:521:SER:C	2:G:523:ASN:N	2.70	0.45
1:H:268:VAL:HG13	1:H:277:LEU:HD11	1.96	0.45
1:A:193:LEU:N	1:A:193:LEU:HD23	2.32	0.45
1:A:220:TRP:NE1	1:A:231:ILE:HD11	2.30	0.45
2:B:155:THR:C	2:B:157:SER:N	2.74	0.45
1:D:67:HIS:ND1	1:D:69:MET:HB2	2.32	0.45
1:E:16:ILE:HD11	2:F:168:SER:C	2.39	0.45
1:E:41:ASP:OD1	1:E:41:ASP:C	2.60	0.45
2:F:224:MET:CE	2:F:230:ASP:HB3	2.47	0.45
2:F:297:TYR:CE2	2:F:305:ARG:HB3	2.51	0.45
2:G:370:PHE:O	2:G:371:SER:O	2.34	0.45
2:G:535:GLN:O	2:G:539:ASN:HB2	2.15	0.45
1:A:22:ASP:OD1	1:A:22:ASP:C	2.60	0.45
1:A:87:ARG:CG	1:A:88:GLU:H	2.30	0.45
2:C:410:PHE:CD2	2:C:410:PHE:N	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ASP:OD2	1:D:36:SER:HB2	2.17	0.45
1:E:34:ASP:OD2	1:E:36:SER:HB2	2.17	0.45
1:E:69:MET:HE2	1:E:70:TYR:HE1	1.80	0.45
2:G:190:LEU:O	2:G:194:ILE:HG13	2.17	0.45
2:G:430:ASN:O	2:G:431:THR:C	2.60	0.45
1:H:220:TRP:NE1	1:H:231:ILE:HD11	2.31	0.45
2:B:155:THR:HG22	2:B:513:ARG:CD	2.46	0.45
2:B:430:ASN:O	2:B:431:THR:C	2.60	0.45
2:C:202:ARG:NE	2:C:209:GLN:HB3	2.31	0.45
1:E:101:GLY:C	1:E:102:HIS:HD2	2.25	0.45
2:F:493:VAL:O	2:F:496:PHE:HB2	2.17	0.45
2:F:525:HIS:ND1	2:F:526:ILE:N	2.65	0.45
2:G:321:LEU:N	2:G:321:LEU:HD23	2.31	0.45
1:H:34:ASP:OD2	1:H:36:SER:HB2	2.17	0.45
1:A:155:ALA:O	1:A:184:SER:HB2	2.17	0.45
1:D:69:MET:HE2	1:D:70:TYR:HE1	1.81	0.45
2:F:177:THR:CG2	2:F:178:GLU:N	2.79	0.45
2:F:190:LEU:HD12	2:F:190:LEU:O	2.16	0.45
2:F:190:LEU:O	2:F:194:ILE:HG13	2.17	0.45
1:H:67:HIS:C	1:H:69:MET:H	2.24	0.45
1:H:236:GLN:HA	1:H:264:VAL:HG13	1.97	0.45
1:A:188:ASP:O	1:A:189:ASN:HB2	2.16	0.45
1:A:197:GLU:O	1:A:199:ASP:N	2.50	0.45
2:B:190:LEU:HD12	2:B:190:LEU:O	2.17	0.45
2:B:525:HIS:ND1	2:B:526:ILE:N	2.65	0.45
2:C:190:LEU:O	2:C:194:ILE:HG13	2.17	0.45
1:A:224:ILE:O	1:A:226:LEU:N	2.46	0.45
2:B:190:LEU:O	2:B:194:ILE:HG13	2.17	0.45
2:B:224:MET:CE	2:B:230:ASP:HB3	2.46	0.45
2:C:267:ARG:CG	2:C:267:ARG:NH1	2.79	0.45
1:E:197:GLU:O	1:E:199:ASP:N	2.50	0.45
2:F:276:ILE:HD13	2:F:383:CYS:CA	2.43	0.45
2:F:343:TRP:CZ3	2:F:350:ILE:CG2	2.75	0.45
2:G:205:ASN:HB2	2:G:206:PRO:CD	2.45	0.45
2:G:215:LEU:O	2:G:456:THR:HG23	2.17	0.45
2:B:155:THR:O	2:B:513:ARG:NH1	2.50	0.45
2:B:359:LYS:HZ1	2:B:368:GLY:HA3	1.77	0.45
2:B:484:ALA:CB	2:B:486:LEU:HD12	2.42	0.45
2:C:190:LEU:CD2	2:C:488:GLY:HA3	2.47	0.45
2:C:409:LYS:O	2:C:410:PHE:HD2	1.99	0.45
2:C:522:THR:HG22	2:C:526:ILE:CD1	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:N	1:D:242:ILE:CD1	2.79	0.45
2:F:269:THR:HG22	2:F:386:ASN:OD1	2.16	0.45
2:F:515:ILE:CD1	2:F:540:ALA:C	2.90	0.45
1:A:40:PHE:CZ	2:B:168:SER:CB	2.93	0.45
1:A:67:HIS:ND1	1:A:69:MET:HB2	2.31	0.45
2:B:527:LEU:HD22	2:B:532:ILE:CD1	2.42	0.45
1:D:87:ARG:CG	1:D:88:GLU:H	2.30	0.45
1:D:101:GLY:C	1:D:102:HIS:HD2	2.25	0.45
1:D:283:ASP:O	1:D:284:ASN:HB3	2.17	0.45
2:F:202:ARG:NE	2:F:209:GLN:HB3	2.31	0.45
2:F:430:ASN:O	2:F:431:THR:C	2.60	0.45
2:G:162:LYS:HZ2	1:H:15:MET:HE2	1.81	0.45
2:G:501:LYS:O	2:G:505:ASP:HB2	2.16	0.45
1:A:28:LEU:HD13	2:B:172:ILE:HD11	1.87	0.44
2:B:364:SER:HB2	2:B:367:GLU:HG2	1.99	0.44
2:B:484:ALA:O	2:B:486:LEU:HG	2.17	0.44
2:C:282:GLU:OE1	2:C:283:LYS:N	2.50	0.44
1:E:67:HIS:C	1:E:69:MET:H	2.24	0.44
2:F:385:LEU:HA	2:F:406:HIS:CE1	2.51	0.44
2:F:385:LEU:HD21	2:F:422:PHE:CE2	2.51	0.44
2:F:420:VAL:HG11	2:F:445:LEU:HD11	1.98	0.44
2:B:410:PHE:CD2	2:B:410:PHE:N	2.84	0.44
2:C:215:LEU:HD12	2:C:452:TYR:CZ	2.52	0.44
2:C:398:SER:HG	2:C:401:SER:HG	1.64	0.44
2:C:525:HIS:ND1	2:C:526:ILE:N	2.65	0.44
1:D:293:VAL:O	1:D:293:VAL:CG1	2.65	0.44
2:F:284:ILE:HG12	2:F:296:LEU:HD12	1.99	0.44
1:H:56:HIS:CE1	1:H:84:ILE:CD1	2.98	0.44
1:A:41:ASP:OD1	1:A:41:ASP:C	2.59	0.44
1:A:69:MET:HE2	1:A:70:TYR:HE1	1.81	0.44
1:A:268:VAL:HG13	1:A:277:LEU:HD11	1.97	0.44
2:B:282:GLU:OE1	2:B:283:LYS:N	2.50	0.44
2:B:320:VAL:HG22	2:C:263:GLU:HA	1.99	0.44
2:C:190:LEU:O	2:C:190:LEU:HD12	2.17	0.44
1:D:209:GLU:HG2	1:D:210:ALA:N	2.33	0.44
1:E:187:CYS:HB3	1:E:214:TRP:NE1	2.32	0.44
2:G:282:GLU:OE1	2:G:283:LYS:N	2.50	0.44
1:A:101:GLY:C	1:A:102:HIS:HD2	2.25	0.44
2:B:210:ILE:HD13	2:B:495:CYS:C	2.42	0.44
2:C:189:TYR:CZ	2:C:193:GLU:OE1	2.70	0.44
1:D:56:HIS:CE1	1:D:84:ILE:CD1	2.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:GLU:O	1:D:210:ALA:HB2	2.18	0.44
1:E:22:ASP:OD1	1:E:22:ASP:C	2.60	0.44
2:F:238:SER:HA	2:F:242:ASP:OD2	2.17	0.44
2:F:364:SER:HB2	2:F:367:GLU:HG2	1.98	0.44
2:F:515:ILE:HD13	2:F:541:GLN:N	2.32	0.44
2:G:181:ARG:NH1	2:G:234:TRP:NE1	2.66	0.44
1:H:22:ASP:OD1	1:H:22:ASP:C	2.60	0.44
1:H:101:GLY:C	1:H:102:HIS:HD2	2.25	0.44
1:A:34:ASP:OD2	1:A:36:SER:HB2	2.17	0.44
1:A:69:MET:CE	1:A:70:TYR:CE1	3.01	0.44
1:A:250:SER:C	1:A:252:THR:N	2.75	0.44
2:B:259:LEU:HD22	2:C:320:VAL:HG11	2.00	0.44
2:B:532:ILE:HG23	2:B:533:PRO:HD2	2.00	0.44
2:C:150:PHE:CD2	2:C:150:PHE:O	2.71	0.44
2:C:287:SER:HB3	2:C:293:GLN:HE21	1.80	0.44
2:C:430:ASN:O	2:C:431:THR:C	2.59	0.44
1:E:241:PHE:HB2	1:E:243:TRP:HE1	1.82	0.44
2:F:189:TYR:CZ	2:F:193:GLU:OE1	2.71	0.44
2:F:269:THR:C	2:F:271:TRP:N	2.75	0.44
2:F:282:GLU:OE1	2:F:283:LYS:N	2.50	0.44
2:F:323:SER:OG	2:G:262:LYS:HE2	2.16	0.44
2:G:439:ARG:NH1	2:G:439:ARG:CG	2.78	0.44
1:H:69:MET:HE2	1:H:70:TYR:HE1	1.81	0.44
1:A:145:ILE:HD13	1:A:194:TRP:CZ3	2.53	0.44
2:B:280:ILE:HD11	2:B:383:CYS:SG	2.58	0.44
2:B:299:LEU:HD22	2:B:383:CYS:SG	2.57	0.44
2:C:295:PHE:CE2	2:C:356:LYS:HD3	2.53	0.44
2:C:298:LEU:HD22	2:C:325:LEU:HD21	2.00	0.44
1:D:112:ALA:HB2	1:D:158:TRP:CH2	2.53	0.44
1:E:87:ARG:CG	1:E:88:GLU:H	2.30	0.44
1:E:258:LEU:CD1	1:E:297:TRP:HB2	2.47	0.44
2:F:381:TRP:CD1	2:F:382:LEU:H	2.36	0.44
2:G:189:TYR:CZ	2:G:193:GLU:OE1	2.70	0.44
2:G:190:LEU:O	2:G:190:LEU:HD12	2.16	0.44
2:G:201:ALA:CB	2:G:531:LYS:NZ	2.81	0.44
2:G:236:LEU:HD21	2:G:422:PHE:CE1	2.52	0.44
2:G:540:ALA:O	2:G:543:LEU:HB3	2.18	0.44
1:H:70:TYR:N	1:H:70:TYR:HD1	2.15	0.44
1:H:179:ILE:HG21	1:H:181:ARG:HE	1.80	0.44
2:B:312:GLU:HG3	2:B:312:GLU:O	2.18	0.44
2:B:385:LEU:HD21	2:B:422:PHE:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ILE:O	1:D:226:LEU:N	2.47	0.44
1:E:27:ARG:HG2	1:E:27:ARG:HH11	1.83	0.44
1:E:112:ALA:HB2	1:E:158:TRP:CH2	2.53	0.44
2:F:259:LEU:HD11	2:G:335:LEU:HD21	1.99	0.44
2:F:268:LEU:HD23	2:F:389:LEU:HD13	1.99	0.44
1:A:209:GLU:HG2	1:A:210:ALA:N	2.33	0.44
1:A:258:LEU:HD13	1:A:297:TRP:CB	2.48	0.44
2:B:453:LEU:HD23	2:B:453:LEU:C	2.43	0.44
2:C:162:LYS:HZ3	1:D:15:MET:HE2	1.82	0.44
1:D:193:LEU:N	1:D:193:LEU:HD23	2.32	0.44
1:E:193:LEU:N	1:E:193:LEU:HD23	2.31	0.44
1:E:193:LEU:HD21	1:E:208:LEU:CD1	2.47	0.44
2:F:284:ILE:HD13	2:F:297:TYR:CD1	2.52	0.44
2:F:284:ILE:C	2:F:286:ASN:N	2.76	0.44
2:G:312:GLU:HG3	2:G:312:GLU:O	2.18	0.44
1:H:193:LEU:N	1:H:193:LEU:HD23	2.32	0.44
1:H:242:ILE:HD11	1:H:258:LEU:HD22	2.00	0.44
2:B:189:TYR:CZ	2:B:193:GLU:OE1	2.70	0.44
2:B:486:LEU:O	2:B:489:HIS:N	2.51	0.44
2:C:267:ARG:HG3	2:C:267:ARG:NH1	2.28	0.44
2:F:446:ASP:OD2	2:F:448:GLN:HB3	2.18	0.44
1:H:23:TYR:HD2	1:H:24:TYR:CE1	2.36	0.44
1:H:179:ILE:HG22	1:H:181:ARG:HE	1.83	0.44
2:B:177:THR:HG23	2:B:179:LEU:HB3	1.90	0.43
2:B:540:ALA:O	2:B:543:LEU:HB3	2.18	0.43
1:E:197:GLU:C	1:E:199:ASP:H	2.26	0.43
2:F:190:LEU:HD21	2:F:488:GLY:HA3	1.99	0.43
2:F:267:ARG:CG	2:F:267:ARG:NH1	2.79	0.43
2:F:267:ARG:NH2	2:G:316:GLY:HA3	2.33	0.43
2:G:208:PRO:HB3	2:G:531:LYS:HG2	2.00	0.43
2:G:238:SER:O	2:G:242:ASP:HB2	2.17	0.43
2:G:446:ASP:OD2	2:G:448:GLN:HB3	2.18	0.43
1:A:107:ASN:OD1	2:B:142:ARG:NH2	2.51	0.43
1:A:148:ALA:HB1	1:A:194:TRP:CZ2	2.53	0.43
1:A:179:ILE:HG22	1:A:181:ARG:HE	1.83	0.43
2:B:381:TRP:CG	2:B:382:LEU:N	2.84	0.43
2:C:210:ILE:CG2	2:C:459:PHE:CE2	3.01	0.43
1:E:69:MET:CE	1:E:70:TYR:CE1	3.01	0.43
1:H:112:ALA:HB2	1:H:158:TRP:CH2	2.53	0.43
1:H:209:GLU:HG2	1:H:210:ALA:N	2.33	0.43
1:A:241:PHE:HB2	1:A:243:TRP:HE1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ASP:OD1	2:B:187:ASP:N	2.51	0.43
2:B:446:ASP:OD2	2:B:448:GLN:HB3	2.18	0.43
2:C:432:GLU:OE1	2:C:465:PHE:HA	2.19	0.43
2:C:453:LEU:HD23	2:C:453:LEU:C	2.43	0.43
1:D:22:ASP:OD1	1:D:22:ASP:C	2.61	0.43
1:D:155:ALA:HB1	1:D:218:VAL:H	1.82	0.43
1:E:107:ASN:ND2	2:F:142:ARG:NH1	2.66	0.43
1:E:293:VAL:O	1:E:293:VAL:CG1	2.65	0.43
2:F:284:ILE:C	2:F:286:ASN:H	2.26	0.43
2:F:410:PHE:CD2	2:F:410:PHE:N	2.84	0.43
2:F:540:ALA:O	2:F:543:LEU:HB3	2.18	0.43
2:G:150:PHE:CD2	2:G:150:PHE:O	2.71	0.43
2:G:410:PHE:CD2	2:G:410:PHE:N	2.84	0.43
2:G:525:HIS:ND1	2:G:526:ILE:N	2.65	0.43
1:A:187:CYS:HB3	1:A:214:TRP:CE2	2.54	0.43
1:A:258:LEU:HD13	1:A:297:TRP:CG	2.53	0.43
2:B:181:ARG:NH1	2:B:234:TRP:HE1	2.16	0.43
2:B:263:GLU:HA	2:C:320:VAL:HG22	2.00	0.43
2:C:246:TYR:CG	2:C:247:PRO:HD2	2.53	0.43
2:C:276:ILE:HD11	2:C:383:CYS:HA	1.98	0.43
2:C:446:ASP:OD2	2:C:448:GLN:HB3	2.18	0.43
1:D:69:MET:CE	1:D:70:TYR:CE1	3.01	0.43
1:D:193:LEU:HD21	1:D:208:LEU:CD1	2.45	0.43
1:E:209:GLU:O	1:E:210:ALA:HB2	2.18	0.43
2:F:205:ASN:HB2	2:F:206:PRO:CD	2.46	0.43
2:G:280:ILE:CG2	2:G:300:LEU:HD21	2.49	0.43
1:A:69:MET:HE3	1:A:70:TYR:CE1	2.54	0.43
1:A:293:VAL:O	1:A:293:VAL:CG1	2.65	0.43
2:C:186:ASP:OD1	2:C:187:ASP:N	2.51	0.43
1:E:209:GLU:HG2	1:E:210:ALA:N	2.33	0.43
1:E:302:ASP:OD1	1:E:302:ASP:O	2.36	0.43
2:F:235:LYS:O	2:F:239:ILE:HG13	2.19	0.43
2:F:247:PRO:HG3	2:G:317:HIS:CG	2.53	0.43
2:G:269:THR:C	2:G:271:TRP:N	2.75	0.43
2:G:453:LEU:C	2:G:453:LEU:HD23	2.43	0.43
1:H:230:THR:HG21	1:H:242:ILE:HG23	2.00	0.43
1:A:209:GLU:O	1:A:210:ALA:HB2	2.18	0.43
1:A:230:THR:CG2	1:A:242:ILE:HG23	2.48	0.43
1:A:302:ASP:OD1	1:A:302:ASP:O	2.36	0.43
2:C:491:LEU:O	2:C:492:PHE:C	2.62	0.43
1:D:23:TYR:HD2	1:D:24:TYR:CE1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:298:LEU:HD23	2:F:298:LEU:HA	1.77	0.43
2:F:453:LEU:HD23	2:F:453:LEU:C	2.43	0.43
2:G:284:ILE:C	2:G:286:ASN:H	2.26	0.43
2:G:399:LEU:HD12	2:G:402:LEU:HD23	2.01	0.43
2:G:491:LEU:HD12	2:G:491:LEU:HA	1.85	0.43
1:H:69:MET:CE	1:H:70:TYR:CE1	3.01	0.43
1:H:87:ARG:CG	1:H:88:GLU:H	2.30	0.43
1:A:197:GLU:C	1:A:199:ASP:H	2.27	0.43
2:B:235:LYS:O	2:B:239:ILE:HG13	2.19	0.43
2:B:431:THR:OG1	2:B:463:ARG:HG2	2.19	0.43
2:B:487:HIS:CD2	2:B:487:HIS:N	2.73	0.43
2:C:207:TYR:CD2	2:C:504:GLU:HA	2.52	0.43
1:E:286:VAL:HG21	2:F:151:ALA:HB2	1.99	0.43
1:E:288:LEU:O	1:E:299:CYS:HA	2.18	0.43
2:G:186:ASP:OD1	2:G:187:ASP:N	2.51	0.43
2:G:284:ILE:C	2:G:286:ASN:N	2.76	0.43
1:H:283:ASP:O	1:H:284:ASN:HB3	2.18	0.43
1:H:290:LYS:HB2	1:H:300:ILE:CD1	2.48	0.43
1:A:264:VAL:HG12	1:A:265:VAL:N	2.33	0.43
2:B:269:THR:C	2:B:271:TRP:N	2.75	0.43
2:B:448:GLN:HG3	2:B:477:PHE:CZ	2.54	0.43
2:C:235:LYS:O	2:C:239:ILE:HG13	2.18	0.43
2:C:312:GLU:HG3	2:C:312:GLU:O	2.18	0.43
1:E:23:TYR:HD2	1:E:24:TYR:CE1	2.37	0.43
1:E:28:LEU:C	1:E:28:LEU:CD2	2.92	0.43
2:F:132:ILE:HG22	2:F:132:ILE:O	2.19	0.43
2:F:263:GLU:HA	2:G:320:VAL:CG2	2.47	0.43
2:F:455:GLN:CG	2:F:496:PHE:CD2	3.01	0.43
2:G:375:LEU:HB3	2:G:379:PHE:HD1	1.83	0.43
2:B:132:ILE:HG22	2:B:132:ILE:O	2.19	0.43
2:B:420:VAL:HG11	2:B:445:LEU:HD11	2.00	0.43
1:E:16:ILE:HG22	1:E:17:HIS:N	2.33	0.43
2:F:131:GLU:O	2:F:131:GLU:HG3	2.19	0.43
2:F:215:LEU:HD12	2:F:452:TYR:CE1	2.54	0.43
2:F:297:TYR:HE2	2:F:305:ARG:HB3	1.84	0.43
2:F:484:ALA:O	2:F:486:LEU:N	2.52	0.43
2:G:153:PHE:CD2	1:H:271:SER:HA	2.54	0.43
1:H:16:ILE:HG22	1:H:17:HIS:N	2.34	0.43
1:H:27:ARG:HG2	1:H:27:ARG:HH11	1.83	0.43
1:A:216:ARG:HA	1:A:216:ARG:HD3	1.88	0.43
2:C:159:LEU:HD12	2:C:160:LEU:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:MET:HE3	1:E:70:TYR:CE1	2.54	0.43
1:E:234:CYS:HB2	1:E:265:VAL:CG1	2.49	0.43
2:F:186:ASP:OD1	2:F:187:ASP:N	2.51	0.43
2:F:263:GLU:HB2	2:G:320:VAL:HG21	2.00	0.43
2:F:312:GLU:O	2:F:312:GLU:HG3	2.18	0.43
1:H:84:ILE:HG21	1:H:86:TRP:CZ2	2.54	0.43
1:A:271:SER:HA	2:B:153:PHE:CG	2.54	0.42
2:B:142:ARG:O	2:B:143:ARG:CB	2.67	0.42
2:B:228:SER:C	2:B:230:ASP:N	2.77	0.42
2:B:404:GLN:HG2	2:B:426:ALA:CB	2.36	0.42
2:C:161:THR:HG22	2:C:162:LYS:N	2.34	0.42
2:C:280:ILE:CG2	2:C:300:LEU:HD21	2.49	0.42
1:D:69:MET:HE3	1:D:70:TYR:CE1	2.53	0.42
1:E:234:CYS:SG	1:E:268:VAL:HG23	2.59	0.42
2:G:268:LEU:O	2:G:272:ILE:HG13	2.19	0.42
1:H:145:ILE:HD11	1:H:202:TRP:CB	2.49	0.42
1:H:232:ALA:HB2	1:H:270:TRP:HZ2	1.84	0.42
1:A:70:TYR:N	1:A:70:TYR:HD1	2.15	0.42
2:C:268:LEU:O	2:C:272:ILE:HG13	2.19	0.42
2:C:284:ILE:HG21	2:C:297:TYR:HE1	1.83	0.42
2:C:451:TRP:CD1	2:C:474:THR:HA	2.55	0.42
1:D:84:ILE:HG21	1:D:86:TRP:CZ2	2.54	0.42
1:E:155:ALA:O	1:E:184:SER:HB2	2.18	0.42
1:E:197:GLU:HB3	1:E:199:ASP:OD1	2.19	0.42
1:E:233:SER:O	1:E:240:VAL:HA	2.19	0.42
2:F:372:LEU:HD22	2:F:375:LEU:HD11	2.01	0.42
2:F:392:GLY:O	2:F:393:GLN:C	2.61	0.42
2:G:199:ILE:HD12	2:G:530:LEU:HA	2.00	0.42
1:H:69:MET:HE3	1:H:70:TYR:CE1	2.54	0.42
1:H:209:GLU:O	1:H:210:ALA:HB2	2.18	0.42
1:A:16:ILE:HG22	1:A:17:HIS:N	2.34	0.42
2:B:150:PHE:CE2	2:B:162:LYS:HB3	2.54	0.42
2:B:522:THR:CG2	2:B:526:ILE:HD11	2.40	0.42
2:F:150:PHE:CE2	2:F:162:LYS:HB3	2.54	0.42
2:G:172:ILE:HD11	1:H:28:LEU:HD12	2.02	0.42
2:G:372:LEU:HD22	2:G:375:LEU:HD11	2.01	0.42
1:A:28:LEU:HD11	2:B:172:ILE:HD11	1.88	0.42
1:A:112:ALA:HB2	1:A:158:TRP:CH2	2.54	0.42
1:A:197:GLU:HB3	1:A:199:ASP:OD1	2.19	0.42
2:B:131:GLU:HG3	2:B:131:GLU:O	2.19	0.42
2:B:436:LYS:HE3	2:B:469:THR:OG1	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:VAL:H	1:D:47:GLN:HE22	1.67	0.42
2:C:540:ALA:O	2:C:543:LEU:HB3	2.19	0.42
1:D:179:ILE:HG22	1:D:181:ARG:HE	1.83	0.42
1:D:214:TRP:O	1:D:235:SER:CB	2.66	0.42
1:D:233:SER:O	1:D:240:VAL:HA	2.20	0.42
1:E:56:HIS:CE1	1:E:84:ILE:CD1	2.98	0.42
1:E:258:LEU:HD13	1:E:297:TRP:CG	2.54	0.42
2:F:179:LEU:HD11	2:F:184:LEU:HD12	2.01	0.42
2:F:345:THR:HG22	2:F:346:GLY:N	2.35	0.42
2:F:487:HIS:CB	2:F:518:LEU:HD21	2.46	0.42
2:F:490:SER:O	2:F:491:LEU:C	2.63	0.42
2:G:145:THR:CG2	2:G:146:ALA:N	2.83	0.42
2:G:515:ILE:CD1	2:G:541:GLN:N	2.82	0.42
1:H:264:VAL:HG12	1:H:265:VAL:N	2.34	0.42
1:D:16:ILE:HG22	1:D:17:HIS:N	2.34	0.42
2:F:259:LEU:HD11	2:G:335:LEU:CD2	2.50	0.42
2:F:262:LYS:HE2	2:G:323:SER:OG	2.19	0.42
2:F:268:LEU:O	2:F:272:ILE:HG13	2.20	0.42
2:F:321:LEU:C	2:F:323:SER:N	2.77	0.42
2:F:399:LEU:HD12	2:F:402:LEU:HD23	2.01	0.42
2:G:321:LEU:C	2:G:323:SER:N	2.77	0.42
1:H:224:ILE:O	1:H:226:LEU:N	2.47	0.42
1:A:23:TYR:HD2	1:A:24:TYR:CE1	2.37	0.42
2:B:142:ARG:HD3	2:B:142:ARG:HA	1.17	0.42
2:C:269:THR:C	2:C:271:TRP:N	2.75	0.42
2:C:455:GLN:HG2	2:C:496:PHE:CD2	2.54	0.42
2:C:511:VAL:O	2:C:515:ILE:HG13	2.19	0.42
1:D:298:VAL:HG12	1:D:299:CYS:N	2.35	0.42
2:F:246:TYR:CD2	2:F:256:LYS:HE2	2.55	0.42
2:F:425:TYR:HA	2:F:463:ARG:HH22	1.84	0.42
2:G:492:PHE:CE1	2:G:496:PHE:CE1	3.08	0.42
2:B:521:SER:C	2:B:523:ASN:N	2.70	0.42
2:C:215:LEU:CD1	2:C:452:TYR:OH	2.63	0.42
2:C:284:ILE:C	2:C:286:ASN:H	2.26	0.42
1:D:185:GLY:HA2	1:D:191:ILE:HA	2.02	0.42
1:E:214:TRP:O	1:E:235:SER:CB	2.65	0.42
2:F:300:LEU:C	2:F:302:ASP:N	2.76	0.42
2:G:194:ILE:HG12	2:G:492:PHE:CD2	2.54	0.42
1:H:155:ALA:O	1:H:184:SER:HB2	2.20	0.42
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.84	0.42
1:A:77:CYS:HB3	1:A:109:VAL:CG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LEU:O	2:B:272:ILE:HG13	2.20	0.42
1:D:264:VAL:HG12	1:D:265:VAL:N	2.34	0.42
1:E:84:ILE:HG21	1:E:86:TRP:CZ2	2.55	0.42
2:F:181:ARG:NH1	2:F:234:TRP:HE1	2.16	0.42
2:F:184:LEU:HD21	2:F:448:GLN:NE2	2.34	0.42
2:G:148:TYR:HD1	1:H:266:TRP:CB	2.32	0.42
2:G:235:LYS:O	2:G:239:ILE:HG13	2.19	0.42
2:G:381:TRP:HE3	2:G:412:LEU:HD23	1.84	0.42
2:G:511:VAL:O	2:G:515:ILE:HG13	2.20	0.42
1:H:164:PRO:HG3	1:H:176:PRO:HB2	2.02	0.42
1:A:145:ILE:HG21	1:A:194:TRP:CZ3	2.55	0.42
2:B:149:THR:CG2	2:B:150:PHE:N	2.83	0.42
2:B:207:TYR:CE1	2:B:504:GLU:HG3	2.55	0.42
2:B:351:ASP:C	2:B:353:ASN:N	2.74	0.42
2:C:499:ASP:C	2:C:501:LYS:N	2.78	0.42
1:D:67:HIS:C	1:D:69:MET:N	2.78	0.42
2:F:158:MET:CE	2:F:174:ARG:HG3	2.50	0.42
2:F:477:PHE:CD2	2:F:493:VAL:HG21	2.55	0.42
1:H:92:THR:CG2	1:H:94:GLU:HG3	2.50	0.42
1:H:234:CYS:SG	1:H:268:VAL:CG2	3.07	0.42
1:H:292:SER:C	1:H:294:ASP:N	2.78	0.42
1:A:67:HIS:C	1:A:69:MET:N	2.78	0.42
1:A:185:GLY:H	1:A:218:VAL:HG21	1.85	0.42
2:B:137:LEU:O	2:B:141:GLU:N	2.52	0.42
2:B:210:ILE:CD1	2:B:495:CYS:CB	2.96	0.42
2:B:297:TYR:HE2	2:B:305:ARG:HB3	1.84	0.42
2:B:511:VAL:O	2:B:515:ILE:HG13	2.20	0.42
2:C:220:ALA:HB3	2:C:234:TRP:CE3	2.55	0.42
2:C:228:SER:C	2:C:230:ASP:N	2.77	0.42
2:C:439:ARG:O	1:D:293:VAL:HG11	2.20	0.42
1:E:107:ASN:HD21	2:F:142:ARG:CZ	2.33	0.42
1:E:128:ALA:O	1:E:129:ILE:HG13	2.20	0.42
2:F:137:LEU:O	2:F:141:GLU:N	2.52	0.42
2:F:142:ARG:O	2:F:143:ARG:CB	2.67	0.42
2:F:170:VAL:O	2:F:172:ILE:N	2.53	0.42
2:G:161:THR:HG22	2:G:162:LYS:N	2.34	0.42
2:G:492:PHE:CE1	2:G:496:PHE:HE1	2.38	0.42
1:H:290:LYS:HG2	1:H:291:GLU:H	1.85	0.42
1:A:28:LEU:HD12	2:B:172:ILE:CD1	2.47	0.41
2:B:158:MET:CE	2:B:174:ARG:HG3	2.50	0.41
2:C:521:SER:O	2:C:523:ASN:N	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:CYS:HB3	1:D:109:VAL:CG2	2.50	0.41
1:E:208:LEU:HD22	1:E:243:TRP:CE3	2.55	0.41
1:E:264:VAL:HG12	1:E:265:VAL:N	2.34	0.41
2:F:202:ARG:NE	2:F:209:GLN:CB	2.83	0.41
2:G:159:LEU:HD12	2:G:160:LEU:H	1.84	0.41
2:G:351:ASP:C	2:G:353:ASN:N	2.74	0.41
1:H:77:CYS:HB3	1:H:109:VAL:CG2	2.50	0.41
1:A:233:SER:O	1:A:240:VAL:HA	2.20	0.41
2:B:284:ILE:C	2:B:286:ASN:H	2.26	0.41
2:B:372:LEU:HD22	2:B:375:LEU:HD11	2.02	0.41
2:C:190:LEU:HD21	2:C:488:GLY:CA	2.48	0.41
2:C:208:PRO:HB3	2:C:531:LYS:HB3	2.02	0.41
2:C:399:LEU:HD12	2:C:402:LEU:HD23	2.01	0.41
2:C:490:SER:CB	2:C:510:LEU:HD21	2.48	0.41
1:D:40:PHE:HA	1:D:49:LEU:HA	2.02	0.41
1:E:111:TRP:CD2	1:E:120:LEU:HD13	2.55	0.41
2:G:207:TYR:CD2	2:G:504:GLU:HA	2.55	0.41
1:H:233:SER:O	1:H:240:VAL:HA	2.20	0.41
1:A:38:LYS:HB3	1:A:40:PHE:CE1	2.52	0.41
1:A:128:ALA:O	1:A:129:ILE:HG13	2.21	0.41
1:A:289:TRP:HA	1:A:298:VAL:O	2.20	0.41
2:B:145:THR:CG2	2:B:146:ALA:N	2.84	0.41
2:B:165:VAL:O	2:B:165:VAL:CG1	2.65	0.41
2:B:170:VAL:O	2:B:172:ILE:N	2.53	0.41
2:B:220:ALA:HB3	2:B:234:TRP:CE3	2.55	0.41
2:B:246:TYR:HA	2:B:247:PRO:HD2	1.75	0.41
2:C:230:ASP:C	2:C:232:ASN:N	2.78	0.41
2:C:321:LEU:C	2:C:323:SER:N	2.77	0.41
2:C:372:LEU:HD22	2:C:375:LEU:HD11	2.02	0.41
1:D:92:THR:CG2	1:D:94:GLU:HG3	2.50	0.41
1:D:121:ALA:CB	1:D:158:TRP:HE1	2.34	0.41
2:F:149:THR:CG2	2:F:150:PHE:N	2.82	0.41
2:G:158:MET:HE3	2:G:485:GLN:NE2	2.35	0.41
1:H:232:ALA:HB2	1:H:270:TRP:CZ2	2.55	0.41
1:A:84:ILE:HG21	1:A:86:TRP:CZ2	2.55	0.41
1:A:271:SER:CB	1:A:276:ILE:HB	2.50	0.41
2:B:481:LEU:HD13	2:B:489:HIS:CB	2.44	0.41
2:B:522:THR:CG2	2:B:526:ILE:CD1	2.99	0.41
2:C:142:ARG:O	2:C:143:ARG:HB2	2.20	0.41
2:C:208:PRO:CB	2:C:530:LEU:O	2.68	0.41
2:C:340:LEU:HD13	2:C:340:LEU:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:522:THR:CG2	2:C:526:ILE:CD1	2.98	0.41
1:D:27:ARG:HG2	1:D:27:ARG:HH11	1.84	0.41
1:D:243:TRP:HE3	1:D:253:TRP:HB3	1.84	0.41
1:E:21:MET:HB3	2:F:154:SER:OG	2.19	0.41
1:E:67:HIS:C	1:E:69:MET:N	2.78	0.41
1:E:151:ILE:HB	1:E:187:CYS:CB	2.43	0.41
1:E:179:ILE:HG22	1:E:181:ARG:HE	1.83	0.41
2:F:236:LEU:O	2:F:239:ILE:HB	2.20	0.41
2:F:367:GLU:OE2	2:F:394:ILE:HD13	2.20	0.41
1:A:234:CYS:HB2	1:A:265:VAL:CG1	2.49	0.41
1:A:286:VAL:HG21	2:B:151:ALA:HB2	2.03	0.41
2:B:399:LEU:HD12	2:B:402:LEU:HD23	2.01	0.41
2:C:145:THR:CG2	2:C:146:ALA:N	2.83	0.41
2:C:298:LEU:HA	2:C:298:LEU:HD23	1.76	0.41
1:E:121:ALA:CB	1:E:158:TRP:HE1	2.34	0.41
2:G:223:TYR:H	2:G:223:TYR:HD1	1.69	0.41
1:A:266:TRP:HD1	1:A:281:GLY:HA2	1.86	0.41
2:B:246:TYR:CE2	2:B:248:TYR:O	2.73	0.41
2:B:321:LEU:C	2:B:323:SER:N	2.77	0.41
2:C:479:ALA:CB	1:D:273:THR:CG2	2.99	0.41
2:C:519:ARG:HE	2:C:541:GLN:NE2	2.18	0.41
1:E:164:PRO:HG3	1:E:176:PRO:HB2	2.02	0.41
1:E:189:ASN:ND2	1:E:213:ASP:C	2.79	0.41
1:E:224:ILE:O	1:E:226:LEU:N	2.46	0.41
2:F:511:VAL:O	2:F:515:ILE:HG13	2.21	0.41
2:F:522:THR:CG2	2:F:526:ILE:CD1	2.98	0.41
2:G:143:ARG:HD3	1:H:214:TRP:CH2	2.56	0.41
2:G:475:PHE:O	2:G:476:ALA:C	2.64	0.41
1:A:269:SER:HB2	2:B:152:LYS:HG2	2.03	0.41
1:A:283:ASP:C	1:A:285:LYS:H	2.29	0.41
2:B:284:ILE:C	2:B:286:ASN:N	2.76	0.41
2:C:202:ARG:NE	2:C:209:GLN:CB	2.83	0.41
1:D:121:ALA:HB3	1:D:158:TRP:HE1	1.86	0.41
1:E:145:ILE:HD13	1:E:194:TRP:CZ3	2.56	0.41
2:F:136:LYS:HE2	2:F:136:LYS:HA	2.02	0.41
2:F:207:TYR:CD1	2:F:504:GLU:HG3	2.56	0.41
2:F:439:ARG:NH1	2:F:439:ARG:CG	2.78	0.41
2:F:487:HIS:CD2	2:F:514:GLU:HG3	2.55	0.41
2:G:142:ARG:NH2	1:H:107:ASN:OD1	2.52	0.41
2:G:162:LYS:NZ	1:H:15:MET:CE	2.83	0.41
2:G:276:ILE:HG21	2:G:383:CYS:SG	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ALA:CB	1:H:158:TRP:HE1	2.34	0.41
1:H:266:TRP:HD1	1:H:281:GLY:HA2	1.86	0.41
1:H:298:VAL:HG12	1:H:299:CYS:N	2.35	0.41
1:A:149:HIS:HB3	1:A:188:ASP:OD1	2.20	0.41
1:A:151:ILE:HD13	2:F:414:TYR:OH	2.21	0.41
1:A:185:GLY:HA2	1:A:191:ILE:HA	2.02	0.41
2:B:287:SER:C	2:B:289:ASN:H	2.27	0.41
2:B:388:THR:O	2:B:388:THR:HG22	2.21	0.41
2:C:287:SER:HB2	2:C:293:GLN:CD	2.46	0.41
2:C:475:PHE:O	2:C:476:ALA:C	2.64	0.41
1:D:111:TRP:CD2	1:D:120:LEU:HD13	2.56	0.41
1:D:179:ILE:O	1:D:181:ARG:HG3	2.21	0.41
1:E:75:ALA:HB2	1:E:111:TRP:HZ2	1.85	0.41
1:E:112:ALA:O	1:E:113:PRO:C	2.64	0.41
1:E:191:ILE:HB	1:E:208:LEU:HB2	2.02	0.41
2:F:220:ALA:HB3	2:F:234:TRP:CE3	2.55	0.41
2:F:248:TYR:CZ	2:G:343:TRP:CH2	3.09	0.41
2:F:455:GLN:CG	2:F:496:PHE:CE2	2.99	0.41
2:G:153:PHE:HD1	2:G:158:MET:O	2.04	0.41
2:G:162:LYS:HZ3	1:H:15:MET:HE2	1.86	0.41
2:G:181:ARG:CZ	2:G:230:ASP:OD1	2.69	0.41
2:G:295:PHE:CE2	2:G:356:LYS:HD3	2.55	0.41
1:H:33:SER:HA	1:H:59:PRO:CB	2.50	0.41
1:H:121:ALA:HB3	1:H:158:TRP:HE1	1.86	0.41
1:A:40:PHE:HA	1:A:49:LEU:HA	2.03	0.41
1:A:111:TRP:CD2	1:A:120:LEU:HD13	2.56	0.41
1:A:164:PRO:HG3	1:A:176:PRO:HB2	2.02	0.41
1:A:230:THR:CG2	1:A:242:ILE:CG2	2.98	0.41
2:B:350:ILE:HD13	2:B:350:ILE:HA	1.89	0.41
2:B:445:LEU:CD2	2:B:449:PHE:CD2	3.03	0.41
2:B:512:MET:HA	2:B:540:ALA:HB1	2.03	0.41
2:B:542:ALA:O	2:B:543:LEU:C	2.64	0.41
2:C:181:ARG:HD3	2:C:224:MET:HE3	2.02	0.41
2:C:189:TYR:O	2:C:190:LEU:C	2.64	0.41
2:C:236:LEU:O	2:C:239:ILE:HB	2.21	0.41
2:C:268:LEU:CD2	2:C:389:LEU:HD13	2.50	0.41
2:C:284:ILE:C	2:C:286:ASN:N	2.76	0.41
1:E:70:TYR:N	1:E:70:TYR:HD1	2.15	0.41
2:F:475:PHE:O	2:F:476:ALA:C	2.64	0.41
2:F:484:ALA:O	2:F:485:GLN:C	2.63	0.41
2:F:542:ALA:O	2:F:543:LEU:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:ILE:O	2:G:281:GLU:C	2.64	0.41
1:H:112:ALA:O	1:H:113:PRO:C	2.64	0.41
1:H:185:GLY:HA2	1:H:191:ILE:HA	2.02	0.41
1:A:121:ALA:HB3	1:A:158:TRP:HE1	1.86	0.41
1:A:234:CYS:HB3	1:A:240:VAL:HG22	2.03	0.41
2:B:136:LYS:HE2	2:B:136:LYS:HA	2.02	0.41
2:B:218:LYS:HG2	2:B:238:SER:OG	2.21	0.41
2:B:423:GLN:HB3	2:B:434:LEU:HD21	2.03	0.41
2:C:436:LYS:CE	2:C:469:THR:OG1	2.69	0.41
1:D:75:ALA:HB2	1:D:111:TRP:HZ2	1.86	0.41
1:E:77:CYS:HB3	1:E:109:VAL:CG2	2.50	0.41
1:E:266:TRP:HD1	1:E:281:GLY:HA2	1.86	0.41
1:E:303:VAL:C	1:E:304:ASN:CG	2.89	0.41
2:G:148:TYR:HD1	1:H:266:TRP:HB3	1.86	0.41
2:G:202:ARG:NE	2:G:209:GLN:CB	2.84	0.41
2:G:269:THR:HG22	2:G:386:ASN:OD1	2.20	0.41
1:H:179:ILE:O	1:H:181:ARG:HG3	2.21	0.41
1:A:33:SER:HA	1:A:59:PRO:CB	2.51	0.40
1:A:121:ALA:CB	1:A:158:TRP:HE1	2.34	0.40
1:A:163:VAL:CG1	1:A:164:PRO:HD2	2.49	0.40
2:B:350:ILE:CG2	2:B:351:ASP:N	2.84	0.40
2:B:381:TRP:CD2	2:B:381:TRP:C	2.99	0.40
2:C:186:ASP:OD1	2:C:186:ASP:C	2.65	0.40
2:C:284:ILE:HD13	2:C:297:TYR:HE1	1.75	0.40
2:C:457:LEU:HD23	2:C:457:LEU:HA	1.89	0.40
1:D:112:ALA:O	1:D:113:PRO:C	2.64	0.40
1:D:271:SER:CB	1:D:276:ILE:HB	2.51	0.40
1:E:17:HIS:O	2:F:150:PHE:CD2	2.74	0.40
1:E:40:PHE:HA	1:E:49:LEU:HA	2.03	0.40
1:E:185:GLY:HA2	1:E:191:ILE:HA	2.02	0.40
1:E:226:LEU:CD1	1:E:228:THR:OG1	2.63	0.40
2:F:223:TYR:H	2:F:223:TYR:HD1	1.69	0.40
2:F:228:SER:C	2:F:230:ASP:N	2.77	0.40
2:F:280:ILE:O	2:F:281:GLU:C	2.64	0.40
2:F:340:LEU:HD12	2:F:370:PHE:HD1	1.86	0.40
2:G:181:ARG:HD3	2:G:224:MET:HE3	2.03	0.40
2:G:220:ALA:HB3	2:G:234:TRP:CE3	2.55	0.40
2:G:283:LYS:HD2	2:G:379:PHE:HE2	1.85	0.40
1:A:75:ALA:HB2	1:A:111:TRP:HZ2	1.86	0.40
2:B:236:LEU:HD21	2:B:422:PHE:CE1	2.56	0.40
2:B:280:ILE:O	2:B:281:GLU:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:HD23	2:B:298:LEU:HA	1.76	0.40
2:B:546:ARG:HG3	2:B:546:ARG:NH1	2.36	0.40
2:C:153:PHE:HD1	2:C:158:MET:O	2.04	0.40
2:C:519:ARG:HH21	2:C:541:GLN:HE21	1.69	0.40
1:D:38:LYS:HB3	1:D:40:PHE:CE1	2.52	0.40
1:E:179:ILE:O	1:E:181:ARG:HG3	2.22	0.40
2:F:375:LEU:HB2	2:F:384:LEU:HD21	2.03	0.40
2:G:207:TYR:CE1	2:G:504:GLU:HG3	2.56	0.40
1:H:128:ALA:O	1:H:129:ILE:HG13	2.21	0.40
1:H:214:TRP:O	1:H:235:SER:CB	2.66	0.40
1:A:112:ALA:O	1:A:113:PRO:C	2.64	0.40
1:A:303:VAL:C	1:A:304:ASN:CG	2.89	0.40
2:B:268:LEU:HD23	2:B:389:LEU:HD13	2.02	0.40
2:B:445:LEU:CD2	2:B:449:PHE:HD2	2.34	0.40
2:B:450:CYS:O	2:B:451:TRP:C	2.65	0.40
2:C:158:MET:CE	2:C:174:ARG:HG3	2.50	0.40
1:D:28:LEU:C	1:D:28:LEU:CD2	2.93	0.40
1:D:128:ALA:O	1:D:129:ILE:HG13	2.21	0.40
2:F:142:ARG:HA	2:F:142:ARG:HD3	1.17	0.40
2:F:532:ILE:HG22	2:F:533:PRO:N	2.37	0.40
2:G:450:CYS:O	2:G:451:TRP:C	2.65	0.40
2:G:533:PRO:HG2	2:G:536:LEU:HB3	2.04	0.40
1:H:163:VAL:HG22	1:H:178:TYR:HE2	1.87	0.40
1:H:224:ILE:C	1:H:226:LEU:N	2.79	0.40
2:B:202:ARG:NE	2:B:209:GLN:CB	2.83	0.40
2:B:491:LEU:HD11	2:B:511:VAL:HG23	2.04	0.40
1:D:164:PRO:HG3	1:D:176:PRO:HB2	2.02	0.40
1:E:271:SER:CB	1:E:276:ILE:HB	2.50	0.40
2:F:218:LYS:HG2	2:F:238:SER:OG	2.22	0.40
2:G:210:ILE:CG2	2:G:459:PHE:CE2	3.04	0.40
2:G:451:TRP:CD1	2:G:474:THR:HA	2.56	0.40
2:G:457:LEU:HD13	2:G:463:ARG:HG3	2.02	0.40
1:H:145:ILE:HD13	1:H:194:TRP:CE3	2.57	0.40
1:A:214:TRP:O	1:A:235:SER:CB	2.66	0.40
1:A:241:PHE:HB2	1:A:243:TRP:NE1	2.37	0.40
1:A:245:CYS:HA	1:A:252:THR:O	2.21	0.40
2:C:159:LEU:HD12	2:C:159:LEU:HA	1.82	0.40
2:C:204:SER:O	2:C:205:ASN:HB3	2.22	0.40
2:C:215:LEU:O	2:C:456:THR:HG23	2.21	0.40
2:C:375:LEU:HD22	2:C:379:PHE:CE2	2.52	0.40
2:C:385:LEU:HA	2:C:406:HIS:CE1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:542:ALA:O	2:C:543:LEU:C	2.64	0.40
1:D:33:SER:HA	1:D:59:PRO:CB	2.51	0.40
1:D:206:GLN:CG	1:D:207:LYS:N	2.84	0.40
1:D:266:TRP:HD1	1:D:281:GLY:HA2	1.86	0.40
1:E:243:TRP:H	1:E:243:TRP:HD1	1.69	0.40
2:F:165:VAL:O	2:F:165:VAL:CG1	2.65	0.40
2:F:230:ASP:C	2:F:232:ASN:N	2.78	0.40
2:F:321:LEU:CD1	2:F:358:TYR:CE2	3.05	0.40
2:F:420:VAL:HG11	2:F:445:LEU:CD1	2.51	0.40
2:G:355:SER:O	2:G:356:LYS:C	2.65	0.40
2:G:413:PRO:O	2:G:413:PRO:HG2	2.20	0.40
1:H:240:VAL:HG11	1:H:258:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/316 (88%)	217 (78%)	46 (16%)	16 (6%)	1	9
1	D	277/316 (88%)	216 (78%)	45 (16%)	16 (6%)	1	8
1	E	279/316 (88%)	218 (78%)	45 (16%)	16 (6%)	1	9
1	H	277/316 (88%)	215 (78%)	46 (17%)	16 (6%)	1	8
2	B	421/442 (95%)	351 (83%)	61 (14%)	9 (2%)	5	26
2	C	416/442 (94%)	353 (85%)	52 (12%)	11 (3%)	4	21
2	F	421/442 (95%)	342 (81%)	66 (16%)	13 (3%)	3	18
2	G	416/442 (94%)	344 (83%)	62 (15%)	10 (2%)	4	23
All	All	2786/3032 (92%)	2256 (81%)	423 (15%)	107 (4%)	2	15

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLY
1	A	180	LYS
1	A	210	ALA
2	B	371	SER
2	B	520	ALA
2	B	525	HIS
2	C	371	SER
2	C	393	GLN
2	C	500	ASP
2	C	520	ALA
2	C	525	HIS
1	D	138	GLY
1	D	180	LYS
1	D	210	ALA
1	E	138	GLY
1	E	180	LYS
1	E	210	ALA
2	F	371	SER
2	F	520	ALA
2	F	525	HIS
2	G	371	SER
2	G	520	ALA
2	G	525	HIS
1	H	138	GLY
1	H	180	LYS
1	H	210	ALA
1	A	136	GLY
1	A	198	GLU
1	A	293	VAL
2	B	247	PRO
2	B	345	THR
2	B	526	ILE
2	C	345	THR
2	C	395	ASP
2	C	526	ILE
1	D	136	GLY
1	D	293	VAL
1	E	136	GLY
1	E	198	GLU
1	E	249	SER
1	E	271	SER
1	E	293	VAL
2	F	345	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	485	GLN
2	F	526	ILE
2	G	345	THR
2	G	395	ASP
2	G	526	ILE
1	H	136	GLY
1	A	44	ASN
1	A	45	GLY
1	A	176	PRO
1	A	251	ASN
1	A	271	SER
1	D	44	ASN
1	D	45	GLY
1	D	176	PRO
1	D	250	SER
1	D	251	ASN
1	D	271	SER
1	E	44	ASN
1	E	45	GLY
1	E	176	PRO
1	H	44	ASN
1	H	45	GLY
1	H	176	PRO
1	H	198	GLU
1	H	271	SER
1	A	55	GLY
1	A	68	PRO
2	B	171	SER
2	B	522	THR
2	C	522	THR
1	D	55	GLY
1	D	68	PRO
1	E	55	GLY
1	E	68	PRO
2	F	171	SER
2	F	490	SER
2	F	522	THR
2	G	522	THR
1	H	55	GLY
1	H	68	PRO
1	A	114	HIS
1	A	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	HIS
1	D	175	LYS
1	E	114	HIS
1	E	175	LYS
2	F	487	HIS
1	H	114	HIS
1	H	175	LYS
1	H	199	ASP
1	A	48	ILE
2	C	442	THR
1	D	48	ILE
1	E	48	ILE
2	F	442	THR
2	G	442	THR
2	G	496	PHE
1	H	48	ILE
1	H	295	GLY
2	F	247	PRO
2	B	277	GLY
2	C	277	GLY
2	F	277	GLY
2	G	277	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	238/267 (89%)	216 (91%)	22 (9%)	8	30
1	D	236/267 (88%)	217 (92%)	19 (8%)	11	35
1	E	238/267 (89%)	216 (91%)	22 (9%)	8	30
1	H	236/267 (88%)	217 (92%)	19 (8%)	11	35
2	B	386/403 (96%)	339 (88%)	47 (12%)	5	19
2	C	384/403 (95%)	344 (90%)	40 (10%)	7	24
2	F	386/403 (96%)	342 (89%)	44 (11%)	5	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	384/403 (95%)	344 (90%)	40 (10%)	7	24
All	All	2488/2680 (93%)	2235 (90%)	253 (10%)	7	26

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	22	ASP
1	A	33	SER
1	A	40	PHE
1	A	41	ASP
1	A	53	LEU
1	A	70	TYR
1	A	83	VAL
1	A	188	ASP
1	A	193	LEU
1	A	201	GLN
1	A	220	TRP
1	A	226	LEU
1	A	228	THR
1	A	244	THR
1	A	250	SER
1	A	272	ILE
1	A	283	ASP
1	A	287	THR
1	A	300	ILE
1	A	302	ASP
1	A	304	ASN
2	B	140	LYS
2	B	141	GLU
2	B	142	ARG
2	B	148	TYR
2	B	158	MET
2	B	160	LEU
2	B	164	ILE
2	B	167	LYS
2	B	168	SER
2	B	170	VAL
2	B	179	LEU
2	B	209	GLN
2	B	215	LEU
2	B	230	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	244	VAL
2	B	267	ARG
2	B	268	LEU
2	B	269	THR
2	B	280	ILE
2	B	282	GLU
2	B	299	LEU
2	B	303	VAL
2	B	321	LEU
2	B	322	ILE
2	B	339	GLN
2	B	340	LEU
2	B	348	CYS
2	B	349	SER
2	B	350	ILE
2	B	365	PRO
2	B	395	ASP
2	B	418	ILE
2	B	428	ASN
2	B	439	ARG
2	B	455	GLN
2	B	463	ARG
2	B	464	VAL
2	B	489	HIS
2	B	491	LEU
2	B	505	ASP
2	B	516	THR
2	B	517	LEU
2	B	521	SER
2	B	523	ASN
2	B	525	HIS
2	B	546	ARG
2	B	550	ASN
2	C	132	ILE
2	C	134	ASN
2	C	138	ILE
2	C	139	MET
2	C	148	TYR
2	C	150	PHE
2	C	157	SER
2	C	158	MET
2	C	164	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	175	LEU
2	C	209	GLN
2	C	215	LEU
2	C	230	ASP
2	C	244	VAL
2	C	267	ARG
2	C	268	LEU
2	C	269	THR
2	C	280	ILE
2	C	282	GLU
2	C	299	LEU
2	C	303	VAL
2	C	321	LEU
2	C	322	ILE
2	C	339	GLN
2	C	340	LEU
2	C	365	PRO
2	C	418	ILE
2	C	428	ASN
2	C	439	ARG
2	C	455	GLN
2	C	464	VAL
2	C	495	CYS
2	C	505	ASP
2	C	516	THR
2	C	517	LEU
2	C	521	SER
2	C	523	ASN
2	C	525	HIS
2	C	546	ARG
2	C	550	ASN
1	D	21	MET
1	D	22	ASP
1	D	33	SER
1	D	40	PHE
1	D	53	LEU
1	D	70	TYR
1	D	83	VAL
1	D	188	ASP
1	D	193	LEU
1	D	220	TRP
1	D	226	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	228	THR
1	D	242	ILE
1	D	245	CYS
1	D	246	ASP
1	D	250	SER
1	D	272	ILE
1	D	283	ASP
1	D	287	THR
1	E	21	MET
1	E	22	ASP
1	E	33	SER
1	E	40	PHE
1	E	41	ASP
1	E	53	LEU
1	E	70	TYR
1	E	83	VAL
1	E	188	ASP
1	E	193	LEU
1	E	201	GLN
1	E	220	TRP
1	E	226	LEU
1	E	228	THR
1	E	246	ASP
1	E	249	SER
1	E	272	ILE
1	E	283	ASP
1	E	287	THR
1	E	300	ILE
1	E	302	ASP
1	E	304	ASN
2	F	140	LYS
2	F	141	GLU
2	F	142	ARG
2	F	148	TYR
2	F	158	MET
2	F	160	LEU
2	F	164	ILE
2	F	167	LYS
2	F	168	SER
2	F	170	VAL
2	F	179	LEU
2	F	209	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	215	LEU
2	F	230	ASP
2	F	249	LYS
2	F	267	ARG
2	F	268	LEU
2	F	269	THR
2	F	280	ILE
2	F	282	GLU
2	F	299	LEU
2	F	303	VAL
2	F	321	LEU
2	F	322	ILE
2	F	339	GLN
2	F	340	LEU
2	F	365	PRO
2	F	397	TYR
2	F	412	LEU
2	F	418	ILE
2	F	428	ASN
2	F	439	ARG
2	F	455	GLN
2	F	464	VAL
2	F	489	HIS
2	F	497	LEU
2	F	505	ASP
2	F	516	THR
2	F	517	LEU
2	F	521	SER
2	F	523	ASN
2	F	525	HIS
2	F	546	ARG
2	F	550	ASN
2	G	132	ILE
2	G	134	ASN
2	G	138	ILE
2	G	139	MET
2	G	148	TYR
2	G	150	PHE
2	G	157	SER
2	G	158	MET
2	G	164	ILE
2	G	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	209	GLN
2	G	215	LEU
2	G	230	ASP
2	G	267	ARG
2	G	268	LEU
2	G	269	THR
2	G	280	ILE
2	G	282	GLU
2	G	299	LEU
2	G	303	VAL
2	G	321	LEU
2	G	322	ILE
2	G	339	GLN
2	G	340	LEU
2	G	365	PRO
2	G	414	TYR
2	G	418	ILE
2	G	428	ASN
2	G	439	ARG
2	G	455	GLN
2	G	464	VAL
2	G	490	SER
2	G	505	ASP
2	G	516	THR
2	G	517	LEU
2	G	521	SER
2	G	523	ASN
2	G	525	HIS
2	G	546	ARG
2	G	550	ASN
1	H	21	MET
1	H	22	ASP
1	H	33	SER
1	H	40	PHE
1	H	53	LEU
1	H	70	TYR
1	H	83	VAL
1	H	188	ASP
1	H	193	LEU
1	H	195	LYS
1	H	220	TRP
1	H	226	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	228	THR
1	H	246	ASP
1	H	249	SER
1	H	250	SER
1	H	272	ILE
1	H	283	ASP
1	H	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	189	ASN
1	A	236	GLN
1	A	304	ASN
2	B	275	GLN
2	B	341	GLN
2	B	353	ASN
2	B	489	HIS
2	B	541	GLN
2	C	341	GLN
2	C	448	GLN
2	C	480	GLN
2	C	541	GLN
1	D	47	GLN
1	D	72	ASN
1	D	189	ASN
1	E	17	HIS
1	E	72	ASN
1	E	189	ASN
1	E	236	GLN
1	E	304	ASN
2	F	341	GLN
2	F	353	ASN
2	G	275	GLN
2	G	341	GLN
2	G	448	GLN
2	G	485	GLN
2	G	489	HIS
2	G	523	ASN
2	G	541	GLN
1	H	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	189	ASN
1	H	284	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	283/316 (89%)	-0.76	0	100	100	78, 133, 192, 202	0
1	D	281/316 (88%)	-0.75	0	100	100	117, 186, 202, 202	0
1	E	283/316 (89%)	-0.75	0	100	100	69, 127, 193, 202	0
1	H	281/316 (88%)	-0.75	0	100	100	121, 186, 202, 202	0
2	B	423/442 (95%)	-0.85	0	100	100	58, 141, 196, 202	4 (0%)
2	C	420/442 (95%)	-0.87	0	100	100	74, 154, 199, 202	4 (0%)
2	F	423/442 (95%)	-0.87	2 (0%)	87	75	34, 144, 194, 202	4 (0%)
2	G	420/442 (95%)	-0.88	0	100	100	68, 160, 202, 202	4 (0%)
All	All	2814/3032 (92%)	-0.82	2 (0%)	92	88	34, 155, 202, 202	16 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	394	ILE	2.1
2	F	161	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.