



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:10 AM UTC

PDB ID : 1LL0 / pdb_00001ll0
Title : Crystal Structure of Rabbit Muscle Glycogenin
Authors : Gibbons, B.J.; Roach, P.J.; Hurley, T.D.
Deposited on : 2002-04-26
Resolution : 3.43 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

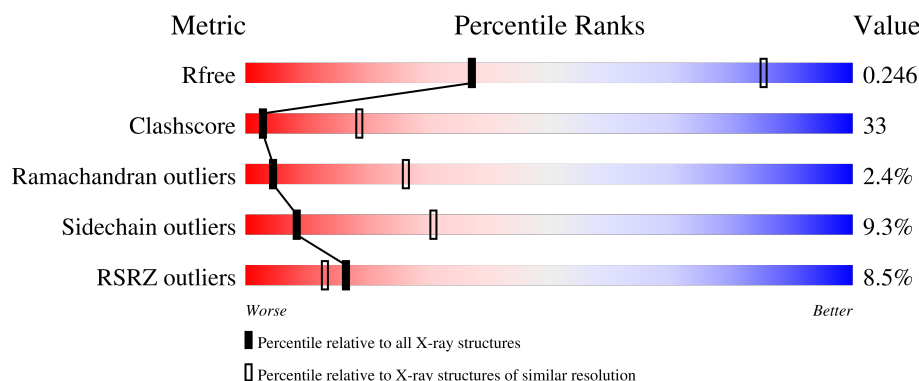
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	339	6% 39% 33% 6% 22%
1	B	339	7% 39% 32% 7% 21%
1	C	339	5% 40% 32% 6% 23%
1	D	339	4% 41% 29% 7% 23%
1	E	339	4% 40% 31% 6% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	339	7% 39% 32% 6% 23%
1	G	339	6% 38% 33% 6% 23%
1	H	339	8% 39% 30% 7% 23%
1	I	339	6% 38% 33% 6% 22%
1	J	339	13% 40% 29% 5% 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20736 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 GLYCOGENIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2092	1346	342	396	8			
1	B	267	Total	C	N	O	S	0	0	0
			2115	1360	350	397	8			
1	C	262	Total	C	N	O	S	0	0	0
			2077	1337	340	392	8			
1	D	261	Total	C	N	O	S	0	0	0
			2071	1333	339	392	7			
1	E	262	Total	C	N	O	S	0	0	0
			2081	1339	342	393	7			
1	F	261	Total	C	N	O	S	0	0	0
			2071	1333	339	392	7			
1	G	262	Total	C	N	O	S	0	0	0
			2079	1338	340	393	8			
1	H	260	Total	C	N	O	S	0	0	0
			2064	1327	338	391	8			
1	I	264	Total	C	N	O	S	0	0	0
			2095	1346	347	395	7			
1	J	251	Total	C	N	O	S	0	0	0
			1991	1281	327	377	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	VAL	-	expression tag	UNP P13280
A	-6	PRO	-	expression tag	UNP P13280
A	-5	ARG	-	expression tag	UNP P13280
A	-4	GLY	-	expression tag	UNP P13280
A	-3	SER	-	expression tag	UNP P13280
A	-2	HIS	-	expression tag	UNP P13280
B	-7	VAL	-	expression tag	UNP P13280
B	-6	PRO	-	expression tag	UNP P13280
B	-5	ARG	-	expression tag	UNP P13280

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P13280
B	-3	SER	-	expression tag	UNP P13280
B	-2	HIS	-	expression tag	UNP P13280
C	-7	VAL	-	expression tag	UNP P13280
C	-6	PRO	-	expression tag	UNP P13280
C	-5	ARG	-	expression tag	UNP P13280
C	-4	GLY	-	expression tag	UNP P13280
C	-3	SER	-	expression tag	UNP P13280
C	-2	HIS	-	expression tag	UNP P13280
D	-7	VAL	-	expression tag	UNP P13280
D	-6	PRO	-	expression tag	UNP P13280
D	-5	ARG	-	expression tag	UNP P13280
D	-4	GLY	-	expression tag	UNP P13280
D	-3	SER	-	expression tag	UNP P13280
D	-2	HIS	-	expression tag	UNP P13280
E	-7	VAL	-	expression tag	UNP P13280
E	-6	PRO	-	expression tag	UNP P13280
E	-5	ARG	-	expression tag	UNP P13280
E	-4	GLY	-	expression tag	UNP P13280
E	-3	SER	-	expression tag	UNP P13280
E	-2	HIS	-	expression tag	UNP P13280
F	-7	VAL	-	expression tag	UNP P13280
F	-6	PRO	-	expression tag	UNP P13280
F	-5	ARG	-	expression tag	UNP P13280
F	-4	GLY	-	expression tag	UNP P13280
F	-3	SER	-	expression tag	UNP P13280
F	-2	HIS	-	expression tag	UNP P13280
G	-7	VAL	-	expression tag	UNP P13280
G	-6	PRO	-	expression tag	UNP P13280
G	-5	ARG	-	expression tag	UNP P13280
G	-4	GLY	-	expression tag	UNP P13280
G	-3	SER	-	expression tag	UNP P13280
G	-2	HIS	-	expression tag	UNP P13280
H	-7	VAL	-	expression tag	UNP P13280
H	-6	PRO	-	expression tag	UNP P13280
H	-5	ARG	-	expression tag	UNP P13280
H	-4	GLY	-	expression tag	UNP P13280
H	-3	SER	-	expression tag	UNP P13280
H	-2	HIS	-	expression tag	UNP P13280
I	-7	VAL	-	expression tag	UNP P13280
I	-6	PRO	-	expression tag	UNP P13280
I	-5	ARG	-	expression tag	UNP P13280

Continued on next page...

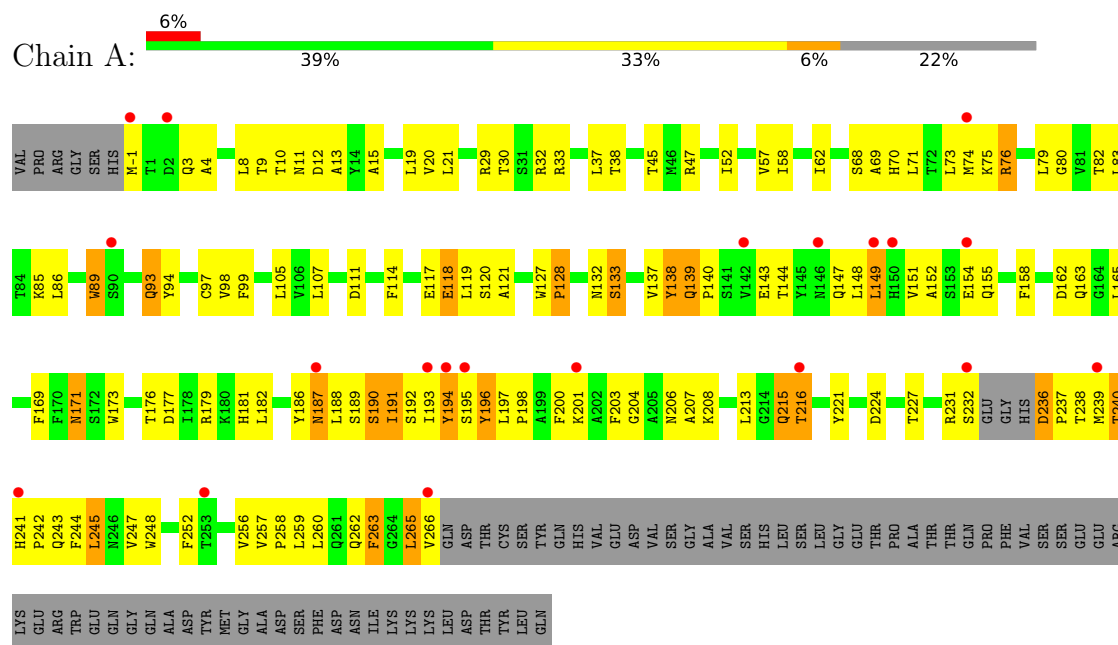
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	GLY	-	expression tag	UNP P13280
I	-3	SER	-	expression tag	UNP P13280
I	-2	HIS	-	expression tag	UNP P13280
J	-7	VAL	-	expression tag	UNP P13280
J	-6	PRO	-	expression tag	UNP P13280
J	-5	ARG	-	expression tag	UNP P13280
J	-4	GLY	-	expression tag	UNP P13280
J	-3	SER	-	expression tag	UNP P13280
J	-2	HIS	-	expression tag	UNP P13280

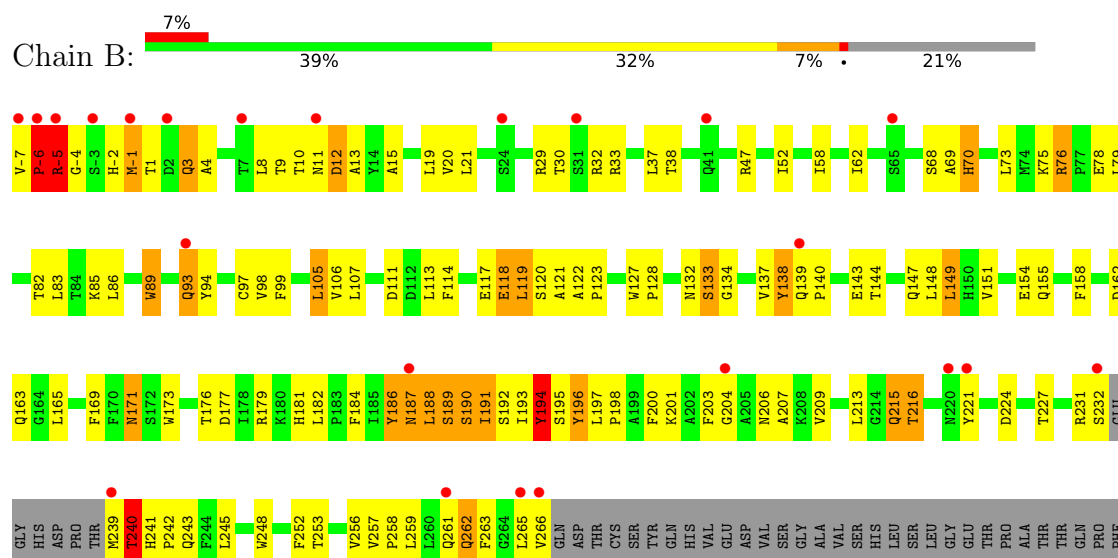
3 Residue-property plots

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.

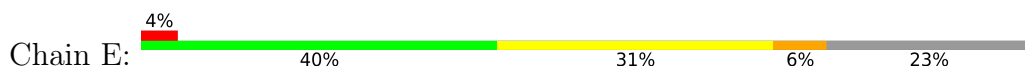
• Molecule 1: GLYCOGENIN-1

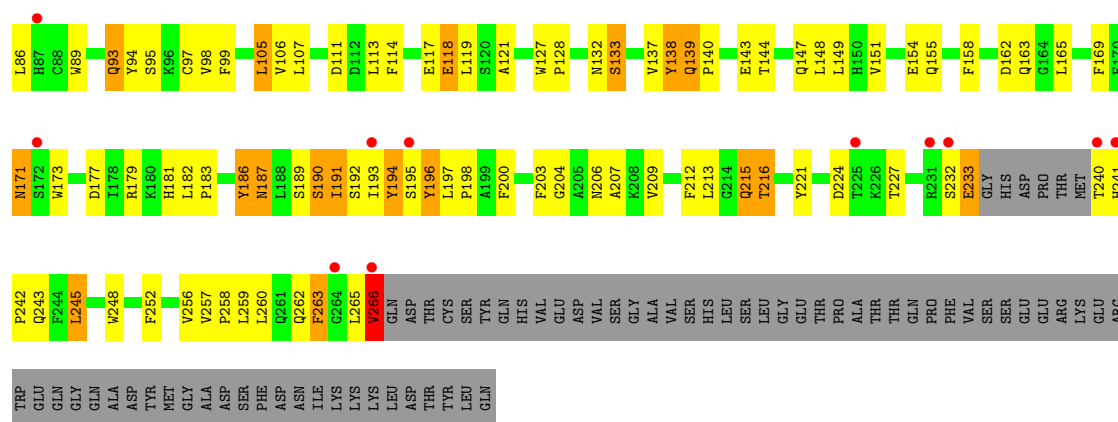


• Molecule 1: GLYCOGENIN-1

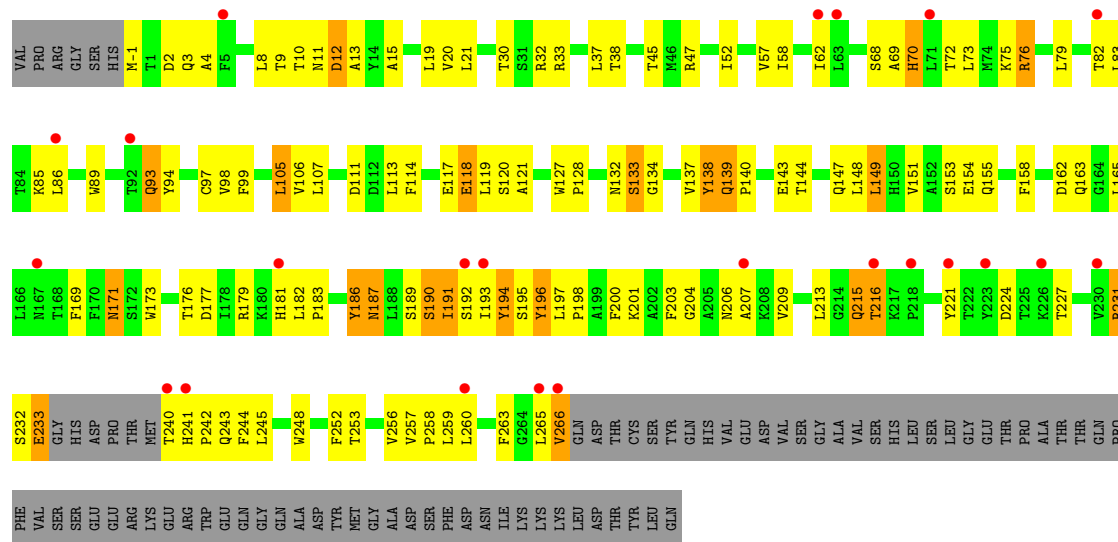


Chain C: 5% 40% 32% 6% 23%

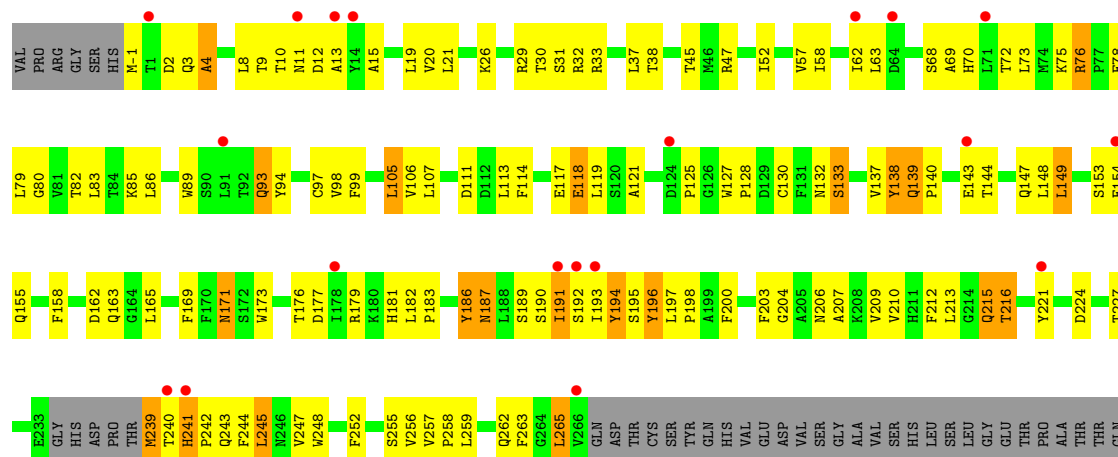




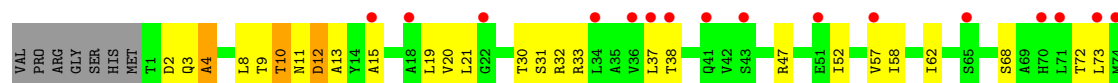
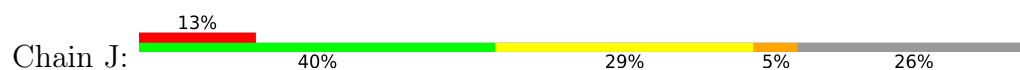
• Molecule 1: GLYCOGENIN-1

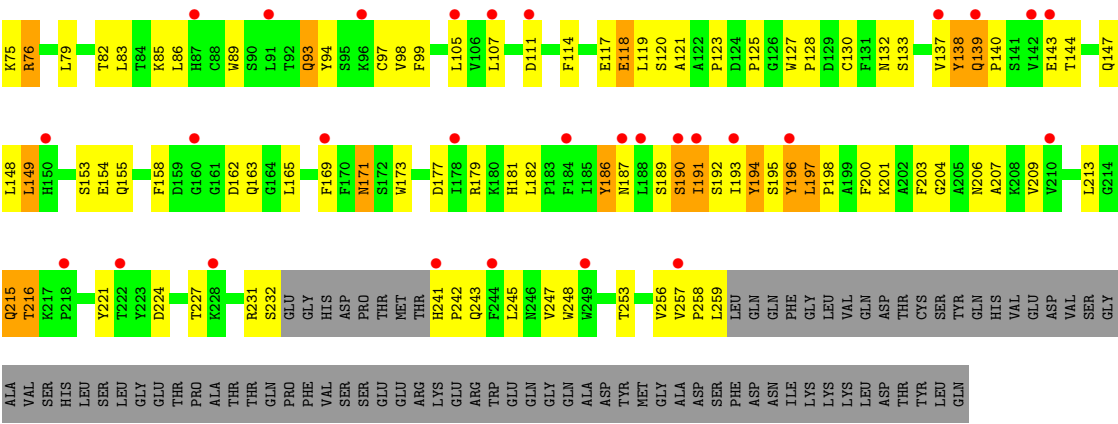


• Molecule 1: GLYCOGENIN-1



Chain H:





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.46Å 139.46Å 416.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.43 25.00 – 3.43	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-3.43) 95.4 (25.00-3.43)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 3.47Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287 0.245 , 0.246	Depositor DCC
R_{free} test set	2837 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	90.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.6	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	0.87	EDS
Total number of atoms	20736	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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	0.70	1/2146 (0.0%)	1.11	20/2927 (0.7%)
1	B	0.88	6/2170 (0.3%)	1.18	28/2958 (0.9%)
1	C	0.65	1/2130 (0.0%)	1.04	8/2904 (0.3%)
1	D	0.65	1/2123 (0.0%)	1.14	18/2893 (0.6%)
1	E	0.63	0/2135	1.06	11/2911 (0.4%)
1	F	0.59	1/2124 (0.0%)	1.08	14/2896 (0.5%)
1	G	0.61	0/2132	1.08	18/2906 (0.6%)
1	H	0.86	6/2117 (0.3%)	1.15	20/2885 (0.7%)
1	I	0.68	2/2149 (0.1%)	1.15	26/2928 (0.9%)
1	J	0.52	0/2043	1.04	12/2787 (0.4%)
All	All	0.69	18/21269 (0.1%)	1.10	175/28995 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	241	HIS	C-N	19.02	1.50	1.33
1	B	188	LEU	N-CA	17.02	1.68	1.46
1	H	241	HIS	CA-C	14.27	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	LEU	N-CA	12.65	1.62	1.46
1	B	-4	GLY	C-N	9.97	1.47	1.33
1	B	120	SER	N-CA	9.74	1.57	1.46
1	I	-1	MET	N-CA	8.40	1.56	1.46
1	H	120	SER	N-CA	-8.04	1.36	1.46
1	B	-5	ARG	N-CA	7.24	1.55	1.46
1	H	241	HIS	CA-CB	6.91	1.64	1.53
1	F	187	ASN	C-N	-6.74	1.24	1.33
1	I	-3	SER	C-O	6.44	1.32	1.23
1	B	188	LEU	C-N	6.42	1.42	1.33
1	H	241	HIS	C-O	-5.77	1.16	1.24
1	C	187	ASN	C-N	-5.55	1.25	1.33
1	H	242	PRO	N-CA	5.48	1.54	1.47
1	D	-1	MET	SD-CE	5.17	1.92	1.79
1	B	187	ASN	C-N	-5.00	1.26	1.33

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ASN	O-C-N	-18.36	99.45	122.21
1	D	241	HIS	CA-C-N	-15.70	101.73	118.85
1	D	241	HIS	C-N-CA	-15.70	101.73	118.85
1	A	208	LYS	N-CA-CB	14.25	131.07	110.40
1	D	187	ASN	O-C-N	-13.74	104.95	121.99
1	H	187	ASN	O-C-N	-13.70	105.00	121.99
1	G	187	ASN	O-C-N	-13.65	105.07	121.99
1	J	187	ASN	O-C-N	-13.41	105.36	121.99
1	I	187	ASN	O-C-N	-13.35	105.44	121.99
1	E	187	ASN	O-C-N	-12.99	105.88	121.99
1	C	187	ASN	O-C-N	-12.42	106.59	121.99
1	B	3	GLN	OE1-CD-NE2	-10.09	112.51	122.60
1	H	241	HIS	CA-C-O	-9.77	106.78	120.16
1	B	262	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	B	-6	PRO	CB-CA-C	9.62	127.43	111.56
1	I	3	GLN	OE1-CD-NE2	-9.38	113.22	122.60
1	B	119	LEU	CA-C-N	-9.08	110.18	122.99
1	B	119	LEU	C-N-CA	-9.08	110.18	122.99
1	H	243	GLN	N-CA-C	-8.92	103.23	114.56
1	I	-1	MET	N-CA-C	8.72	123.98	110.20
1	D	196	TYR	N-CA-C	-8.68	99.66	111.55
1	E	196	TYR	N-CA-C	-8.67	99.67	111.55
1	A	196	TYR	N-CA-C	-8.58	99.79	111.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	-5	ARG	N-CA-CB	8.56	125.06	110.50
1	B	196	TYR	N-CA-C	-8.55	99.84	111.55
1	I	196	TYR	N-CA-C	-8.44	99.98	111.55
1	G	196	TYR	N-CA-C	-8.43	100.01	111.55
1	J	196	TYR	N-CA-C	-8.31	100.16	111.55
1	C	196	TYR	N-CA-C	-8.25	100.25	111.55
1	H	196	TYR	N-CA-C	-8.25	100.25	111.55
1	A	188	LEU	N-CA-C	8.11	128.08	110.80
1	B	188	LEU	N-CA-CB	-8.10	96.81	110.49
1	I	76	ARG	CA-C-N	8.04	128.12	119.28
1	I	76	ARG	C-N-CA	8.04	128.12	119.28
1	E	191	ILE	N-CA-C	-8.01	105.39	112.12
1	F	196	TYR	N-CA-C	-7.88	100.76	111.55
1	B	188	LEU	N-CA-C	7.67	127.15	110.80
1	G	76	ARG	CA-C-N	7.49	128.16	119.47
1	G	76	ARG	C-N-CA	7.49	128.16	119.47
1	C	191	ILE	N-CA-C	-7.47	105.84	112.12
1	G	191	ILE	N-CA-C	-7.42	105.89	111.90
1	B	191	ILE	N-CA-C	-7.41	105.89	112.12
1	D	191	ILE	N-CA-C	-7.41	105.90	112.12
1	F	191	ILE	N-CA-C	-7.34	105.96	111.90
1	I	191	ILE	N-CA-C	-7.28	106.01	112.12
1	A	191	ILE	N-CA-C	-7.27	106.01	111.90
1	H	191	ILE	N-CA-C	-7.11	106.15	112.12
1	H	76	ARG	CA-C-N	7.05	127.03	119.28
1	H	76	ARG	C-N-CA	7.05	127.03	119.28
1	H	241	HIS	C-N-CD	-6.97	96.41	125.00
1	I	3	GLN	CG-CD-NE2	6.97	126.86	116.40
1	E	266	VAL	CA-C-O	-6.96	108.97	120.80
1	B	187	ASN	CA-C-N	-6.92	108.31	121.54
1	B	187	ASN	C-N-CA	-6.92	108.31	121.54
1	C	76	ARG	CA-C-N	6.88	127.44	119.47
1	C	76	ARG	C-N-CA	6.88	127.44	119.47
1	E	76	ARG	CA-C-N	6.87	127.44	119.47
1	E	76	ARG	C-N-CA	6.87	127.44	119.47
1	A	76	ARG	CA-C-N	6.85	127.42	119.47
1	A	76	ARG	C-N-CA	6.85	127.42	119.47
1	I	-4	GLY	CA-C-N	6.83	132.41	120.87
1	I	-4	GLY	C-N-CA	6.83	132.41	120.87
1	A	187	ASN	CA-C-N	-6.82	108.51	121.54
1	A	187	ASN	C-N-CA	-6.82	108.51	121.54
1	H	241	HIS	N-CA-C	6.79	124.81	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	76	ARG	CA-C-N	6.75	127.31	119.47
1	J	76	ARG	C-N-CA	6.75	127.31	119.47
1	D	76	ARG	CA-C-N	6.73	127.28	119.47
1	D	76	ARG	C-N-CA	6.73	127.28	119.47
1	B	262	GLN	CG-CD-NE2	6.72	126.49	116.40
1	F	76	ARG	CA-C-N	6.68	127.22	119.47
1	F	76	ARG	C-N-CA	6.68	127.22	119.47
1	J	191	ILE	N-CA-C	-6.65	106.51	111.90
1	B	119	LEU	N-CA-C	6.63	118.66	110.91
1	G	239	MET	CA-C-N	6.61	131.58	120.81
1	G	239	MET	C-N-CA	6.61	131.58	120.81
1	A	208	LYS	N-CA-C	-6.43	105.45	113.55
1	B	76	ARG	CA-C-N	6.38	126.88	119.47
1	B	76	ARG	C-N-CA	6.38	126.88	119.47
1	I	-1	MET	N-CA-CB	6.37	119.67	110.06
1	B	3	GLN	CG-CD-NE2	6.32	125.89	116.40
1	A	186	TYR	CA-C-N	-6.26	109.58	121.54
1	A	186	TYR	C-N-CA	-6.26	109.58	121.54
1	D	4	ALA	N-CA-C	6.22	118.23	108.96
1	F	187	ASN	CA-C-N	6.18	133.35	121.54
1	F	187	ASN	C-N-CA	6.18	133.35	121.54
1	H	186	TYR	N-CA-C	-6.11	105.98	113.50
1	G	187	ASN	CA-C-N	6.10	131.18	121.66
1	G	187	ASN	C-N-CA	6.10	131.18	121.66
1	E	186	TYR	N-CA-C	-6.04	106.08	113.50
1	H	263	PHE	N-CA-C	-6.01	105.26	112.59
1	D	241	HIS	CB-CA-C	-6.01	98.69	110.10
1	H	242	PRO	CA-N-CD	-6.00	103.60	112.00
1	B	188	LEU	O-C-N	6.00	130.56	122.59
1	A	188	LEU	N-CA-CB	-5.99	100.36	110.49
1	B	188	LEU	CA-C-N	-5.94	113.80	122.65
1	B	188	LEU	C-N-CA	-5.94	113.80	122.65
1	C	186	TYR	N-CA-C	-5.92	106.10	113.38
1	F	127	TRP	CA-C-N	5.92	127.24	119.84
1	F	127	TRP	C-N-CA	5.92	127.24	119.84
1	G	186	TYR	N-CA-C	-5.92	106.22	113.50
1	J	127	TRP	CA-C-N	5.88	127.19	119.84
1	J	127	TRP	C-N-CA	5.88	127.19	119.84
1	A	186	TYR	O-C-N	5.87	129.68	122.34
1	I	-2	HIS	CA-C-N	-5.86	113.04	121.42
1	I	-2	HIS	C-N-CA	-5.86	113.04	121.42
1	G	127	TRP	CA-C-N	5.82	127.11	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	127	TRP	C-N-CA	5.82	127.11	119.84
1	B	186	TYR	N-CA-C	-5.80	106.37	113.50
1	A	127	TRP	CA-C-N	5.78	127.07	119.84
1	A	127	TRP	C-N-CA	5.78	127.07	119.84
1	E	263	PHE	N-CA-C	-5.75	105.85	112.92
1	D	242	PRO	N-CA-C	-5.74	105.72	113.40
1	I	263	PHE	N-CA-C	-5.73	105.87	112.92
1	H	242	PRO	CA-C-N	5.69	130.78	122.08
1	H	242	PRO	C-N-CA	5.69	130.78	122.08
1	A	263	PHE	N-CA-C	-5.67	105.94	112.92
1	E	127	TRP	CA-C-N	5.67	126.93	119.84
1	E	127	TRP	C-N-CA	5.67	126.93	119.84
1	J	186	TYR	N-CA-C	-5.67	106.41	113.38
1	G	265	LEU	N-CA-C	5.66	118.18	111.33
1	H	242	PRO	CA-C-O	5.66	127.86	120.85
1	B	127	TRP	CA-C-N	5.63	126.88	119.84
1	B	127	TRP	C-N-CA	5.63	126.88	119.84
1	D	186	TYR	N-CA-C	-5.57	106.53	113.38
1	I	127	TRP	CA-C-N	5.57	126.80	119.84
1	I	127	TRP	C-N-CA	5.57	126.80	119.84
1	I	186	TYR	N-CA-C	-5.57	106.65	113.50
1	G	255	SER	N-CA-C	5.55	120.19	113.41
1	I	-2	HIS	CB-CA-C	5.54	121.75	109.94
1	F	12	ASP	N-CA-C	5.53	118.07	111.71
1	H	119	LEU	N-CA-C	5.50	118.71	111.28
1	B	176	THR	N-CA-C	5.50	118.40	109.06
1	A	186	TYR	N-CA-C	-5.47	106.27	113.17
1	H	127	TRP	CA-C-N	5.46	126.67	119.84
1	H	127	TRP	C-N-CA	5.46	126.67	119.84
1	I	-4	GLY	N-CA-C	-5.46	106.33	112.33
1	B	12	ASP	N-CA-C	5.42	117.95	111.71
1	H	4	ALA	N-CA-C	5.41	117.03	108.96
1	A	29	ARG	N-CA-C	5.41	118.70	111.24
1	G	130	CYS	N-CA-C	-5.37	101.12	109.72
1	D	127	TRP	CA-C-N	5.37	126.55	119.84
1	D	127	TRP	C-N-CA	5.37	126.55	119.84
1	F	186	TYR	N-CA-C	-5.36	106.79	113.38
1	I	-3	SER	CA-C-N	-5.36	112.37	121.85
1	I	-3	SER	C-N-CA	-5.36	112.37	121.85
1	E	12	ASP	N-CA-C	5.31	117.82	111.71
1	I	255	SER	N-CA-C	5.30	120.40	113.88
1	G	4	ALA	N-CA-C	5.30	116.86	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	SER	N-CA-C	-5.30	99.77	108.41
1	B	-5	ARG	N-CA-CB	5.30	119.44	110.49
1	D	120	SER	N-CA-C	-5.27	99.70	108.34
1	F	120	SER	N-CA-C	-5.27	99.83	108.41
1	D	12	ASP	N-CA-C	5.23	117.72	111.71
1	B	29	ARG	N-CA-C	5.20	118.42	111.24
1	D	187	ASN	CA-C-N	5.16	131.39	121.54
1	D	187	ASN	C-N-CA	5.16	131.39	121.54
1	H	130	CYS	N-CA-C	-5.15	101.49	109.72
1	F	2	ASP	N-CA-C	-5.13	105.70	112.94
1	B	120	SER	N-CA-CB	-5.13	102.06	110.68
1	I	12	ASP	N-CA-C	5.12	117.60	111.71
1	J	130	CYS	N-CA-C	-5.12	101.53	109.72
1	J	12	ASP	N-CA-C	5.11	117.58	111.71
1	G	2	ASP	N-CA-C	-5.10	105.74	112.94
1	G	176	THR	N-CA-C	5.10	117.73	109.06
1	D	176	THR	N-CA-C	5.09	117.72	109.06
1	F	176	THR	N-CA-C	5.09	117.46	108.75
1	I	130	CYS	N-CA-C	-5.07	101.61	109.72
1	I	29	ARG	N-CA-C	5.06	118.23	111.24
1	J	4	ALA	N-CA-C	5.06	116.50	108.96
1	C	127	TRP	CA-C-N	5.05	126.16	119.84
1	C	127	TRP	C-N-CA	5.05	126.16	119.84
1	B	194	TYR	N-CA-C	-5.04	108.39	114.75
1	A	176	THR	N-CA-C	5.04	117.63	109.06
1	J	120	SER	N-CA-C	-5.03	100.22	108.41

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	ASN	Mainchain
1	D	187	ASN	Mainchain
1	E	187	ASN	Mainchain
1	F	187	ASN	Mainchain
1	G	187	ASN	Mainchain
1	H	187	ASN	Mainchain
1	I	187	ASN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2092	0	2048	159	0
1	B	2115	0	2074	166	0
1	C	2077	0	2037	153	0
1	D	2071	0	2026	115	0
1	E	2081	0	2034	137	0
1	F	2071	0	2027	128	0
1	G	2079	0	2036	145	0
1	H	2064	0	2016	126	0
1	I	2095	0	2048	145	0
1	J	1991	0	1946	103	0
All	All	20736	0	20292	1337	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 33.

All (1337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:N	1:B:188:LEU:CA	1.68	1.52
1:A:193:ILE:CB	1:A:240:THR:HG21	1.55	1.37
1:B:200:PHE:CE2	1:B:240:THR:HB	1.58	1.36
1:A:193:ILE:HB	1:A:240:THR:CG2	1.57	1.32
1:C:200:PHE:CE2	1:C:240:THR:HB	1.66	1.30
1:B:200:PHE:CZ	1:B:240:THR:HB	1.72	1.24
1:C:193:ILE:HB	1:C:240:THR:CG2	1.67	1.23
1:B:261:GLN:CA	1:B:266:VAL:HG12	1.69	1.21
1:C:193:ILE:CB	1:C:240:THR:HG21	1.73	1.16
1:A:193:ILE:HD12	1:A:240:THR:HG23	1.25	1.13
1:E:240:THR:HG23	1:E:242:PRO:HD2	1.23	1.13
1:A:231:ARG:HG3	1:A:232:SER:H	1.11	1.12
1:B:261:GLN:HA	1:B:266:VAL:HG12	1.11	1.08
1:G:240:THR:HG22	1:G:241:HIS:H	0.93	1.08
1:J:194:TYR:HA	1:J:197:LEU:HD13	1.36	1.08
1:A:193:ILE:HG22	1:A:200:PHE:CD1	1.89	1.07
1:G:194:TYR:HA	1:G:197:LEU:HD13	1.34	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TYR:HA	1:C:197:LEU:HD13	1.31	1.04
1:E:194:TYR:HA	1:E:197:LEU:HD13	1.35	1.04
1:I:194:TYR:HA	1:I:197:LEU:HD13	1.37	1.04
1:B:194:TYR:HA	1:B:197:LEU:HD13	1.33	1.04
1:H:194:TYR:HA	1:H:197:LEU:HD13	1.37	1.03
1:A:194:TYR:HA	1:A:197:LEU:HD13	1.35	1.03
1:C:193:ILE:HD13	1:C:240:THR:HG23	1.40	1.01
1:B:261:GLN:CB	1:B:266:VAL:HG12	1.90	1.01
1:F:215:GLN:HG2	1:F:216:THR:H	1.25	1.01
1:A:240:THR:HG23	1:A:241:HIS:H	1.24	1.01
1:F:194:TYR:HA	1:F:197:LEU:HD13	1.38	1.00
1:G:240:THR:HG22	1:G:241:HIS:N	1.70	1.00
1:B:231:ARG:HG3	1:B:232:SER:H	1.25	1.00
1:D:194:TYR:HA	1:D:197:LEU:HD13	1.38	0.99
1:B:200:PHE:CE2	1:B:240:THR:CB	2.45	0.99
1:B:261:GLN:HG2	1:B:266:VAL:HB	1.44	0.99
1:B:215:GLN:HG2	1:B:216:THR:H	1.26	0.98
1:A:215:GLN:HG2	1:A:216:THR:H	1.27	0.98
1:J:231:ARG:HG3	1:J:232:SER:H	1.27	0.98
1:C:239:MET:O	1:C:243:GLN:HB2	1.64	0.97
1:G:215:GLN:HG2	1:G:216:THR:H	1.30	0.97
1:B:261:GLN:HA	1:B:266:VAL:CG1	1.95	0.97
1:E:80:GLY:HA3	1:G:262:GLN:NE2	1.80	0.97
1:J:215:GLN:HG2	1:J:216:THR:H	1.27	0.96
1:C:215:GLN:HG2	1:C:216:THR:H	1.29	0.96
1:I:215:GLN:HG2	1:I:216:THR:H	1.27	0.96
1:D:215:GLN:HG2	1:D:216:THR:H	1.31	0.95
1:B:187:ASN:C	1:B:188:LEU:CA	2.39	0.94
1:G:240:THR:CG2	1:G:241:HIS:H	1.77	0.94
1:A:193:ILE:HB	1:A:240:THR:CB	1.97	0.94
1:C:240:THR:O	1:C:243:GLN:HB3	1.68	0.94
1:B:240:THR:O	1:B:243:GLN:HB3	1.67	0.94
1:E:190:SER:HB2	1:E:241:HIS:CE1	2.03	0.94
1:B:261:GLN:HG2	1:B:266:VAL:CB	1.98	0.94
1:E:215:GLN:HG2	1:E:216:THR:H	1.30	0.94
1:H:215:GLN:HG2	1:H:216:THR:H	1.31	0.94
1:F:231:ARG:HG3	1:F:233:GLU:H	1.32	0.93
1:F:231:ARG:HG3	1:F:232:SER:H	1.31	0.93
1:C:262:GLN:NE2	1:I:80:GLY:HA3	1.82	0.92
1:C:231:ARG:HG3	1:C:232:SER:H	1.31	0.92
1:C:262:GLN:HE22	1:I:80:GLY:HA3	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:CG1	1:A:240:THR:HG21	1.99	0.92
1:C:239:MET:HB3	1:C:242:PRO:HD2	1.52	0.92
1:A:193:ILE:HB	1:A:240:THR:HG21	0.91	0.91
1:G:212:PHE:CE2	1:G:245:LEU:HD13	2.06	0.91
1:F:190:SER:HB2	1:F:241:HIS:NE2	1.87	0.89
1:C:200:PHE:CE2	1:C:240:THR:CB	2.53	0.89
1:I:93:GLN:H	1:I:93:GLN:HE21	1.20	0.89
1:E:80:GLY:HA3	1:G:262:GLN:HE22	1.38	0.89
1:A:193:ILE:HD12	1:A:240:THR:CG2	2.02	0.88
1:H:93:GLN:H	1:H:93:GLN:HE21	1.21	0.88
1:I:215:GLN:HG2	1:I:216:THR:N	1.89	0.88
1:J:32:ARG:HG3	1:J:114:PHE:CE1	2.10	0.87
1:B:215:GLN:HG2	1:B:216:THR:N	1.88	0.87
1:C:193:ILE:HD13	1:C:240:THR:CG2	2.04	0.86
1:I:48:LYS:HA	1:I:51:GLU:HG3	1.57	0.86
1:B:240:THR:O	1:B:243:GLN:CB	2.22	0.86
1:I:32:ARG:HG3	1:I:114:PHE:CE1	2.10	0.86
1:C:200:PHE:CZ	1:C:240:THR:CB	2.59	0.86
1:A:260:LEU:HB3	1:A:266:VAL:CG2	2.05	0.86
1:C:200:PHE:CZ	1:C:240:THR:OG1	2.29	0.85
1:J:93:GLN:H	1:J:93:GLN:HE21	1.21	0.85
1:A:93:GLN:HE21	1:A:93:GLN:H	1.24	0.85
1:B:188:LEU:N	1:B:188:LEU:CB	2.40	0.85
1:F:32:ARG:HG3	1:F:114:PHE:CE1	2.11	0.85
1:F:215:GLN:HG2	1:F:216:THR:N	1.87	0.85
1:G:241:HIS:ND1	1:G:241:HIS:C	2.35	0.85
1:E:190:SER:CB	1:E:241:HIS:CE1	2.60	0.85
1:B:241:HIS:HB3	1:B:242:PRO:HD3	1.59	0.84
1:B:32:ARG:HG3	1:B:114:PHE:CE1	2.13	0.84
1:D:3:GLN:HB2	1:D:32:ARG:HD2	1.59	0.84
1:F:93:GLN:HE21	1:F:93:GLN:H	1.21	0.84
1:D:215:GLN:HG2	1:D:216:THR:N	1.93	0.83
1:A:215:GLN:HG2	1:A:216:THR:N	1.91	0.83
1:C:32:ARG:HG3	1:C:114:PHE:CE1	2.12	0.83
1:G:193:ILE:HD13	1:G:241:HIS:HB3	1.60	0.83
1:J:215:GLN:HG2	1:J:216:THR:N	1.92	0.83
1:A:231:ARG:CG	1:A:232:SER:H	1.90	0.83
1:D:93:GLN:H	1:D:93:GLN:HE21	1.23	0.82
1:H:32:ARG:HG3	1:H:114:PHE:CE1	2.14	0.82
1:G:93:GLN:H	1:G:93:GLN:HE21	1.25	0.82
1:A:80:GLY:HA3	1:I:262:GLN:NE2	1.94	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:PHE:CZ	1:C:240:THR:HB	2.14	0.82
1:E:32:ARG:HG3	1:E:114:PHE:CE1	2.14	0.82
1:B:93:GLN:H	1:B:93:GLN:HE21	1.25	0.82
1:A:32:ARG:HG3	1:A:114:PHE:CE1	2.14	0.82
1:C:52:ILE:HA	1:I:74:MET:HE1	1.60	0.82
1:H:3:GLN:HB2	1:H:32:ARG:HD2	1.62	0.82
1:H:119:LEU:HG	1:H:170:PHE:CG	2.15	0.82
1:C:215:GLN:HG2	1:C:216:THR:N	1.94	0.81
1:E:215:GLN:HG2	1:E:216:THR:N	1.94	0.81
1:G:32:ARG:HG3	1:G:114:PHE:CE1	2.14	0.81
1:E:93:GLN:H	1:E:93:GLN:HE21	1.28	0.81
1:A:47:ARG:HH11	1:A:47:ARG:HG2	1.44	0.81
1:B:231:ARG:HG3	1:B:232:SER:N	1.95	0.81
1:J:241:HIS:HB3	1:J:242:PRO:HD3	1.62	0.81
1:A:240:THR:OG1	1:A:244:PHE:HE1	1.62	0.81
1:C:241:HIS:HB3	1:C:242:PRO:HD3	1.61	0.81
1:D:32:ARG:HG3	1:D:114:PHE:CE1	2.16	0.81
1:H:215:GLN:HG2	1:H:216:THR:N	1.91	0.81
1:D:190:SER:HB2	1:D:241:HIS:CD2	2.14	0.81
1:D:47:ARG:HH11	1:D:47:ARG:HG2	1.46	0.81
1:D:98:VAL:HG22	1:D:137:VAL:HG22	1.63	0.81
1:A:236:ASP:OD1	1:A:237:PRO:HD2	1.82	0.80
1:B:200:PHE:CZ	1:B:240:THR:CB	2.63	0.80
1:C:240:THR:OG1	1:C:244:PHE:CE1	2.34	0.80
1:G:215:GLN:HG2	1:G:216:THR:N	1.93	0.80
1:G:240:THR:HB	1:G:242:PRO:HD2	1.63	0.80
1:G:241:HIS:C	1:G:241:HIS:HD1	1.89	0.80
1:H:47:ARG:HG2	1:H:47:ARG:HH11	1.43	0.80
1:A:231:ARG:HG3	1:A:232:SER:N	1.94	0.80
1:B:-5:ARG:HG3	1:B:-5:ARG:O	1.79	0.80
1:B:3:GLN:HB2	1:B:32:ARG:HD2	1.61	0.80
1:E:97:CYS:HB2	1:E:138:TYR:CE2	2.16	0.80
1:G:212:PHE:CE2	1:G:245:LEU:CD1	2.64	0.79
1:H:243:GLN:O	1:H:247:VAL:HG23	1.83	0.79
1:A:240:THR:HG23	1:A:241:HIS:N	1.96	0.79
1:A:240:THR:OG1	1:A:244:PHE:CE1	2.35	0.79
1:F:98:VAL:HG22	1:F:137:VAL:HG22	1.64	0.79
1:G:47:ARG:HG2	1:G:47:ARG:HH11	1.47	0.79
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.46	0.79
1:C:193:ILE:HB	1:C:240:THR:HG21	0.85	0.79
1:C:93:GLN:H	1:C:93:GLN:HE21	1.26	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:CG2	1:A:241:HIS:H	1.95	0.79
1:I:3:GLN:HB2	1:I:32:ARG:HD2	1.65	0.79
1:E:3:GLN:HB2	1:E:32:ARG:HD2	1.62	0.78
1:F:97:CYS:HB2	1:F:138:TYR:CE2	2.18	0.78
1:G:97:CYS:HB2	1:G:138:TYR:CE2	2.18	0.78
1:E:233:GLU:HA	1:E:233:GLU:OE1	1.82	0.78
1:G:3:GLN:HB2	1:G:32:ARG:HD2	1.64	0.78
1:H:231:ARG:HD2	1:H:233:GLU:OE2	1.84	0.78
1:J:47:ARG:HG2	1:J:47:ARG:HH11	1.46	0.78
1:E:190:SER:HB2	1:E:241:HIS:ND1	1.98	0.78
1:C:47:ARG:HG2	1:C:47:ARG:HH11	1.49	0.78
1:D:132:ASN:HD22	1:D:163:GLN:HE22	1.32	0.78
1:H:97:CYS:HB2	1:H:138:TYR:CE2	2.19	0.78
1:F:216:THR:HB	1:F:221:TYR:HE1	1.49	0.78
1:C:97:CYS:HB2	1:C:138:TYR:CE2	2.19	0.78
1:I:97:CYS:HB2	1:I:138:TYR:CE2	2.19	0.78
1:I:98:VAL:HG22	1:I:137:VAL:HG22	1.64	0.78
1:B:231:ARG:CG	1:B:232:SER:H	1.96	0.78
1:J:97:CYS:HB2	1:J:138:TYR:CE2	2.19	0.78
1:B:-7:VAL:C	1:B:-5:ARG:H	1.91	0.77
1:B:132:ASN:HD22	1:B:163:GLN:HE22	1.31	0.77
1:E:47:ARG:HG2	1:E:47:ARG:HH11	1.49	0.77
1:A:97:CYS:HB2	1:A:138:TYR:CE2	2.18	0.77
1:C:263:PHE:CE2	1:I:63:LEU:HD13	2.18	0.77
1:H:230:VAL:O	1:H:231:ARG:HG2	1.82	0.77
1:A:3:GLN:HB2	1:A:32:ARG:HD2	1.65	0.77
1:C:3:GLN:HB2	1:C:32:ARG:HD2	1.67	0.77
1:B:97:CYS:HB2	1:B:138:TYR:CE2	2.20	0.77
1:F:231:ARG:HG3	1:F:232:SER:N	2.00	0.77
1:J:231:ARG:HG3	1:J:232:SER:N	2.00	0.77
1:E:132:ASN:HD22	1:E:163:GLN:HE22	1.31	0.77
1:I:132:ASN:HD22	1:I:163:GLN:HE22	1.32	0.77
1:B:-1:MET:HB2	1:B:32:ARG:HD3	1.66	0.76
1:F:231:ARG:CG	1:F:232:SER:H	1.98	0.76
1:H:98:VAL:HG22	1:H:137:VAL:HG22	1.67	0.76
1:B:261:GLN:HG2	1:B:266:VAL:CG1	2.15	0.76
1:A:132:ASN:HD22	1:A:163:GLN:HE22	1.31	0.76
1:B:216:THR:HB	1:B:221:TYR:HE1	1.50	0.76
1:D:97:CYS:HB2	1:D:138:TYR:CE2	2.20	0.76
1:J:132:ASN:HD22	1:J:163:GLN:HE22	1.34	0.76
1:F:190:SER:CB	1:F:241:HIS:NE2	2.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:THR:HB	1:E:221:TYR:HE1	1.51	0.75
1:A:193:ILE:CD1	1:A:240:THR:HG23	2.11	0.75
1:A:241:HIS:HB3	1:A:242:PRO:HD3	1.68	0.75
1:A:262:GLN:HE22	1:G:80:GLY:HA3	1.48	0.75
1:C:132:ASN:HD22	1:C:163:GLN:HE22	1.34	0.75
1:D:190:SER:HB2	1:D:241:HIS:NE2	2.02	0.75
1:H:216:THR:HB	1:H:221:TYR:HE1	1.51	0.75
1:B:9:THR:CG2	1:B:38:THR:HG22	2.17	0.75
1:G:193:ILE:CD1	1:G:241:HIS:HB3	2.17	0.75
1:A:9:THR:CG2	1:A:38:THR:HG22	2.17	0.75
1:A:240:THR:O	1:A:243:GLN:HB3	1.86	0.75
1:D:9:THR:CG2	1:D:38:THR:HG22	2.17	0.75
1:J:216:THR:HB	1:J:221:TYR:HE1	1.52	0.75
1:J:231:ARG:CG	1:J:232:SER:H	1.99	0.75
1:A:98:VAL:HG22	1:A:137:VAL:HG22	1.70	0.74
1:B:98:VAL:HG22	1:B:137:VAL:HG22	1.69	0.74
1:F:47:ARG:HH11	1:F:47:ARG:HG2	1.51	0.74
1:G:193:ILE:HD13	1:G:241:HIS:CB	2.17	0.74
1:A:200:PHE:CE2	1:A:240:THR:HB	2.22	0.74
1:F:132:ASN:HD22	1:F:163:GLN:HE22	1.34	0.74
1:G:9:THR:CG2	1:G:38:THR:HG22	2.17	0.74
1:G:186:TYR:O	1:G:209:VAL:HB	1.87	0.74
1:I:121:ALA:HA	1:I:182:LEU:HD12	1.69	0.74
1:J:9:THR:CG2	1:J:38:THR:HG22	2.17	0.74
1:B:132:ASN:HA	1:B:163:GLN:NE2	2.03	0.74
1:J:257:VAL:HB	1:J:258:PRO:HD3	1.69	0.73
1:F:9:THR:CG2	1:F:38:THR:HG22	2.17	0.73
1:F:93:GLN:HE21	1:F:93:GLN:N	1.86	0.73
1:C:231:ARG:CG	1:C:232:SER:H	2.01	0.73
1:F:93:GLN:H	1:F:93:GLN:NE2	1.86	0.73
1:B:257:VAL:HB	1:B:258:PRO:HD3	1.69	0.73
1:F:132:ASN:HA	1:F:163:GLN:NE2	2.03	0.73
1:B:193:ILE:O	1:B:240:THR:HG21	1.88	0.73
1:G:132:ASN:HD22	1:G:163:GLN:HE22	1.35	0.73
1:H:132:ASN:HD22	1:H:163:GLN:HE22	1.36	0.73
1:I:93:GLN:H	1:I:93:GLN:NE2	1.87	0.73
1:I:216:THR:HB	1:I:221:TYR:HE1	1.54	0.73
1:C:216:THR:HB	1:C:221:TYR:HE1	1.54	0.73
1:I:9:THR:CG2	1:I:38:THR:HG22	2.19	0.73
1:D:132:ASN:HA	1:D:163:GLN:NE2	2.04	0.73
1:D:216:THR:HB	1:D:221:TYR:HE1	1.52	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:GLN:H	1:J:93:GLN:NE2	1.87	0.73
1:B:261:GLN:CB	1:B:266:VAL:CG1	2.67	0.72
1:H:9:THR:CG2	1:H:38:THR:HG22	2.19	0.72
1:C:80:GLY:HA3	1:E:262:GLN:NE2	2.04	0.72
1:A:241:HIS:NE2	1:A:245:LEU:HD11	2.04	0.72
1:A:260:LEU:HB3	1:A:266:VAL:HG23	1.70	0.72
1:A:193:ILE:CG1	1:A:240:THR:CG2	2.67	0.72
1:F:193:ILE:HG22	1:F:200:PHE:CD1	2.25	0.72
1:G:98:VAL:HG22	1:G:137:VAL:HG22	1.70	0.72
1:I:257:VAL:HB	1:I:258:PRO:HD3	1.72	0.72
1:H:47:ARG:HG2	1:H:47:ARG:NH1	2.02	0.72
1:C:132:ASN:HA	1:C:163:GLN:NE2	2.04	0.72
1:J:47:ARG:HG2	1:J:47:ARG:NH1	2.05	0.72
1:B:47:ARG:HG2	1:B:47:ARG:NH1	2.05	0.71
1:C:121:ALA:HA	1:C:182:LEU:HD12	1.72	0.71
1:C:231:ARG:HG3	1:C:232:SER:N	2.04	0.71
1:J:98:VAL:HG22	1:J:137:VAL:HG22	1.70	0.71
1:C:193:ILE:HG22	1:C:200:PHE:CD1	2.26	0.71
1:I:93:GLN:HE21	1:I:93:GLN:N	1.87	0.71
1:A:260:LEU:CB	1:A:266:VAL:CG2	2.68	0.71
1:I:231:ARG:HG3	1:I:232:SER:H	1.54	0.71
1:B:85:LYS:HE3	1:B:99:PHE:CE2	2.25	0.71
1:I:132:ASN:HA	1:I:163:GLN:NE2	2.05	0.71
1:C:9:THR:CG2	1:C:38:THR:HG22	2.20	0.71
1:H:257:VAL:HB	1:H:258:PRO:HD3	1.71	0.71
1:G:216:THR:HB	1:G:221:TYR:HE1	1.53	0.71
1:J:121:ALA:HA	1:J:182:LEU:HD12	1.71	0.71
1:J:132:ASN:HA	1:J:163:GLN:NE2	2.06	0.71
1:C:98:VAL:HG22	1:C:137:VAL:HG22	1.72	0.71
1:D:47:ARG:HG2	1:D:47:ARG:NH1	2.05	0.71
1:D:93:GLN:H	1:D:93:GLN:NE2	1.89	0.71
1:E:85:LYS:HE3	1:E:99:PHE:CE2	2.26	0.71
1:G:257:VAL:HB	1:G:258:PRO:HD3	1.72	0.71
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.04	0.71
1:D:257:VAL:HB	1:D:258:PRO:HD3	1.73	0.71
1:E:98:VAL:HG22	1:E:137:VAL:HG22	1.71	0.70
1:H:93:GLN:H	1:H:93:GLN:NE2	1.89	0.70
1:B:261:GLN:CG	1:B:266:VAL:HG12	2.21	0.70
1:G:85:LYS:HE3	1:G:99:PHE:CE2	2.27	0.70
1:G:121:ALA:HA	1:G:182:LEU:HD12	1.73	0.70
1:H:93:GLN:HE21	1:H:93:GLN:N	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HA	1:A:163:GLN:NE2	2.06	0.70
1:A:85:LYS:HE3	1:A:99:PHE:CE2	2.27	0.70
1:I:186:TYR:O	1:I:209:VAL:HB	1.91	0.70
1:D:93:GLN:HE21	1:D:93:GLN:N	1.90	0.70
1:J:93:GLN:HE21	1:J:93:GLN:N	1.89	0.70
1:B:261:GLN:CA	1:B:266:VAL:CG1	2.60	0.70
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.06	0.70
1:D:121:ALA:HA	1:D:182:LEU:HD12	1.74	0.70
1:G:47:ARG:HG2	1:G:47:ARG:NH1	2.04	0.70
1:I:2:ASP:O	1:I:94:TYR:HA	1.92	0.70
1:A:216:THR:HB	1:A:221:TYR:HE1	1.54	0.70
1:B:93:GLN:HE21	1:B:93:GLN:N	1.90	0.70
1:E:121:ALA:HA	1:E:182:LEU:HD12	1.74	0.69
1:F:3:GLN:HB2	1:F:32:ARG:HD2	1.72	0.69
1:H:85:LYS:HE3	1:H:99:PHE:CE2	2.27	0.69
1:B:93:GLN:H	1:B:93:GLN:NE2	1.90	0.69
1:F:190:SER:CB	1:F:241:HIS:CE1	2.76	0.69
1:B:193:ILE:HG22	1:B:200:PHE:CD1	2.27	0.69
1:E:132:ASN:HA	1:E:163:GLN:NE2	2.07	0.69
1:E:233:GLU:OE1	1:E:233:GLU:CA	2.40	0.69
1:F:257:VAL:HB	1:F:258:PRO:HD3	1.73	0.69
1:E:193:ILE:HG22	1:E:200:PHE:CD1	2.28	0.69
1:H:62:ILE:HD12	1:H:73:LEU:HD22	1.75	0.69
1:B:121:ALA:HA	1:B:182:LEU:HD12	1.74	0.69
1:J:193:ILE:HG22	1:J:200:PHE:CD1	2.27	0.69
1:A:93:GLN:H	1:A:93:GLN:NE2	1.89	0.69
1:D:85:LYS:HE3	1:D:99:PHE:CE2	2.28	0.69
1:E:47:ARG:HG2	1:E:47:ARG:NH1	2.06	0.69
1:F:121:ALA:HA	1:F:182:LEU:HD12	1.74	0.69
1:H:186:TYR:O	1:H:209:VAL:HB	1.91	0.69
1:C:85:LYS:HE3	1:C:99:PHE:CE2	2.28	0.69
1:E:186:TYR:O	1:E:209:VAL:HB	1.93	0.69
1:A:262:GLN:NE2	1:G:80:GLY:HA3	2.07	0.69
1:A:193:ILE:CD1	1:A:240:THR:CG2	2.69	0.69
1:C:240:THR:HG23	1:C:241:HIS:N	2.08	0.69
1:E:240:THR:CG2	1:E:242:PRO:HD2	2.15	0.69
1:E:257:VAL:HB	1:E:258:PRO:HD3	1.74	0.68
1:E:9:THR:CG2	1:E:38:THR:HG22	2.22	0.68
1:F:241:HIS:CE1	1:F:244:PHE:HD1	2.11	0.68
1:A:93:GLN:HE21	1:A:93:GLN:N	1.90	0.68
1:I:85:LYS:HE3	1:I:99:PHE:CE2	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HB	1:A:258:PRO:HD3	1.74	0.68
1:H:132:ASN:HA	1:H:163:GLN:NE2	2.09	0.68
1:J:85:LYS:HE3	1:J:99:PHE:CE2	2.28	0.68
1:A:121:ALA:HA	1:A:182:LEU:HD12	1.76	0.68
1:F:62:ILE:HD12	1:F:73:LEU:HD22	1.73	0.68
1:G:193:ILE:HG22	1:G:200:PHE:CD1	2.30	0.67
1:C:257:VAL:HB	1:C:258:PRO:HD3	1.74	0.67
1:E:194:TYR:C	1:E:194:TYR:CD2	2.72	0.67
1:F:47:ARG:HG2	1:F:47:ARG:NH1	2.08	0.67
1:F:186:TYR:O	1:F:209:VAL:HB	1.95	0.67
1:F:194:TYR:C	1:F:194:TYR:CD2	2.72	0.67
1:G:93:GLN:H	1:G:93:GLN:NE2	1.92	0.67
1:I:62:ILE:HD12	1:I:73:LEU:HD22	1.76	0.67
1:I:194:TYR:C	1:I:194:TYR:CD2	2.72	0.67
1:A:194:TYR:CD2	1:A:194:TYR:C	2.73	0.67
1:C:93:GLN:H	1:C:93:GLN:NE2	1.92	0.67
1:C:240:THR:O	1:C:243:GLN:CB	2.41	0.67
1:D:62:ILE:HD12	1:D:73:LEU:HD22	1.76	0.67
1:I:1:THR:HA	1:I:33:ARG:HD2	1.76	0.67
1:D:241:HIS:ND1	1:D:245:LEU:CD1	2.58	0.67
1:I:193:ILE:HG22	1:I:200:PHE:CD1	2.30	0.67
1:C:93:GLN:HE21	1:C:93:GLN:N	1.92	0.67
1:F:194:TYR:C	1:F:194:TYR:HD2	2.03	0.67
1:J:62:ILE:HD12	1:J:73:LEU:HD22	1.76	0.67
1:C:193:ILE:CD1	1:C:240:THR:CG2	2.73	0.67
1:G:132:ASN:HA	1:G:163:GLN:NE2	2.10	0.67
1:G:194:TYR:C	1:G:194:TYR:CD2	2.73	0.67
1:C:52:ILE:HG23	1:I:74:MET:HE2	1.77	0.66
1:A:194:TYR:C	1:A:194:TYR:HD2	2.04	0.66
1:H:193:ILE:HG22	1:H:200:PHE:CD1	2.30	0.66
1:H:194:TYR:HD2	1:H:194:TYR:C	2.03	0.66
1:A:193:ILE:HG22	1:A:200:PHE:CE1	2.30	0.66
1:B:216:THR:HB	1:B:221:TYR:CE1	2.31	0.66
1:F:193:ILE:HD13	1:F:241:HIS:HB2	1.76	0.66
1:H:240:THR:HG23	1:H:242:PRO:HD2	1.78	0.66
1:I:194:TYR:C	1:I:194:TYR:HD2	2.03	0.66
1:H:194:TYR:C	1:H:194:TYR:CD2	2.72	0.66
1:E:93:GLN:H	1:E:93:GLN:NE2	1.93	0.66
1:E:194:TYR:C	1:E:194:TYR:HD2	2.03	0.66
1:J:194:TYR:HD2	1:J:194:TYR:C	2.04	0.66
1:G:221:TYR:CD2	1:G:245:LEU:HD23	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLN:HE21	1:E:93:GLN:N	1.94	0.66
1:G:93:GLN:HE21	1:G:93:GLN:N	1.94	0.66
1:C:263:PHE:CZ	1:I:63:LEU:HD22	2.31	0.66
1:F:216:THR:HB	1:F:221:TYR:CE1	2.30	0.66
1:C:200:PHE:CD2	1:C:240:THR:HB	2.28	0.65
1:H:216:THR:HB	1:H:221:TYR:CE1	2.31	0.65
1:C:186:TYR:O	1:C:209:VAL:HB	1.95	0.65
1:D:193:ILE:HG22	1:D:200:PHE:CD1	2.31	0.65
1:E:74:MET:HE1	1:G:52:ILE:HD13	1.78	0.65
1:J:194:TYR:C	1:J:194:TYR:CD2	2.73	0.65
1:A:193:ILE:CB	1:A:240:THR:CG2	2.39	0.65
1:B:200:PHE:CE2	1:B:240:THR:CG2	2.79	0.65
1:C:240:THR:HG23	1:C:241:HIS:H	1.59	0.65
1:E:132:ASN:HD22	1:E:163:GLN:NE2	1.94	0.65
1:F:190:SER:HB2	1:F:241:HIS:CE1	2.31	0.65
1:G:52:ILE:HG21	1:G:259:LEU:HD11	1.78	0.65
1:J:216:THR:HB	1:J:221:TYR:CE1	2.31	0.65
1:C:194:TYR:HD2	1:C:194:TYR:C	2.05	0.65
1:E:-2:HIS:ND1	1:E:-2:HIS:N	2.42	0.65
1:C:193:ILE:CD1	1:C:240:THR:HG23	2.21	0.64
1:C:194:TYR:C	1:C:194:TYR:CD2	2.74	0.64
1:G:194:TYR:C	1:G:194:TYR:HD2	2.04	0.64
1:B:194:TYR:C	1:B:194:TYR:CD2	2.75	0.64
1:E:52:ILE:HG21	1:E:259:LEU:HD11	1.80	0.64
1:H:118:GLU:HB2	1:H:139:GLN:NE2	2.12	0.64
1:I:-1:MET:HB3	1:I:2:ASP:OD1	1.96	0.64
1:E:171:ASN:C	1:E:171:ASN:HD22	2.06	0.64
1:G:241:HIS:HE1	1:G:245:LEU:HD22	1.61	0.64
1:A:80:GLY:HA3	1:I:262:GLN:HE22	1.61	0.64
1:D:216:THR:HB	1:D:221:TYR:CE1	2.32	0.64
1:E:260:LEU:HB3	1:E:266:VAL:HG23	1.79	0.64
1:G:193:ILE:CD1	1:G:241:HIS:CB	2.75	0.64
1:B:62:ILE:HD12	1:B:73:LEU:HD22	1.80	0.64
1:D:132:ASN:HD22	1:D:163:GLN:NE2	1.95	0.64
1:D:194:TYR:C	1:D:194:TYR:HD2	2.06	0.64
1:E:240:THR:O	1:E:243:GLN:CB	2.46	0.64
1:J:52:ILE:HG21	1:J:259:LEU:HD11	1.79	0.64
1:A:132:ASN:HD22	1:A:163:GLN:NE2	1.95	0.63
1:C:200:PHE:CE1	1:C:204:GLY:HA3	2.33	0.63
1:J:4:ALA:HB2	1:J:33:ARG:HB2	1.81	0.63
1:B:-7:VAL:O	1:B:-5:ARG:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:GLN:HB2	1:J:32:ARG:HD2	1.79	0.63
1:B:132:ASN:HD22	1:B:163:GLN:NE2	1.96	0.63
1:C:240:THR:OG1	1:C:244:PHE:HE1	1.79	0.63
1:D:186:TYR:O	1:D:209:VAL:HB	1.99	0.63
1:I:216:THR:HB	1:I:221:TYR:CE1	2.33	0.63
1:A:171:ASN:C	1:A:171:ASN:HD22	2.04	0.63
1:E:62:ILE:HD12	1:E:73:LEU:HD22	1.79	0.63
1:F:85:LYS:HE3	1:F:99:PHE:CE2	2.34	0.63
1:A:216:THR:HB	1:A:221:TYR:CE1	2.33	0.63
1:B:-6:PRO:O	1:B:-5:ARG:C	2.42	0.63
1:B:194:TYR:C	1:B:194:TYR:HD2	2.07	0.63
1:H:200:PHE:CD1	1:H:204:GLY:HA3	2.34	0.63
1:A:62:ILE:HD12	1:A:73:LEU:HD22	1.81	0.63
1:E:216:THR:HB	1:E:221:TYR:CE1	2.31	0.63
1:G:216:THR:HB	1:G:221:TYR:CE1	2.34	0.63
1:G:221:TYR:CE2	1:G:245:LEU:HD23	2.34	0.63
1:D:241:HIS:HD1	1:D:245:LEU:CD1	2.11	0.62
1:D:194:TYR:C	1:D:194:TYR:CD2	2.76	0.62
1:I:231:ARG:HG3	1:I:232:SER:N	2.14	0.62
1:B:200:PHE:CD2	1:B:240:THR:CG2	2.81	0.62
1:B:261:GLN:HG2	1:B:266:VAL:HG12	1.79	0.62
1:C:216:THR:HB	1:C:221:TYR:CE1	2.34	0.62
1:B:186:TYR:O	1:B:209:VAL:HB	1.98	0.62
1:C:200:PHE:CD1	1:C:204:GLY:HA3	2.35	0.62
1:I:200:PHE:CE1	1:I:204:GLY:HA3	2.35	0.62
1:H:210:VAL:HG22	1:H:244:PHE:CE1	2.35	0.62
1:C:52:ILE:HG21	1:C:259:LEU:HD11	1.82	0.62
1:J:200:PHE:CD1	1:J:204:GLY:HA3	2.35	0.62
1:E:4:ALA:HB2	1:E:33:ARG:HB2	1.82	0.62
1:I:-1:MET:CB	1:I:2:ASP:OD1	2.47	0.62
1:I:171:ASN:C	1:I:171:ASN:HD22	2.08	0.62
1:I:215:GLN:CG	1:I:216:THR:H	2.09	0.62
1:G:240:THR:HB	1:G:242:PRO:CD	2.30	0.62
1:A:241:HIS:CD2	1:A:245:LEU:CD1	2.82	0.61
1:E:200:PHE:CD1	1:E:204:GLY:HA3	2.35	0.61
1:A:200:PHE:CD1	1:A:204:GLY:HA3	2.35	0.61
1:G:200:PHE:CD1	1:G:204:GLY:HA3	2.35	0.61
1:I:200:PHE:CD1	1:I:204:GLY:HA3	2.35	0.61
1:G:62:ILE:HD12	1:G:73:LEU:HD22	1.82	0.61
1:B:-7:VAL:C	1:B:-5:ARG:N	2.58	0.61
1:G:9:THR:HG23	1:G:9:THR:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:HG21	1:A:240:THR:OG1	2.01	0.61
1:D:171:ASN:C	1:D:171:ASN:HD22	2.09	0.61
1:E:97:CYS:HB2	1:E:138:TYR:HE2	1.64	0.61
1:F:171:ASN:C	1:F:171:ASN:HD22	2.08	0.61
1:G:243:GLN:O	1:G:247:VAL:HG23	2.01	0.61
1:C:9:THR:O	1:C:9:THR:HG23	2.00	0.61
1:E:232:SER:O	1:E:233:GLU:C	2.42	0.61
1:E:58:ILE:HD12	1:E:58:ILE:H	1.66	0.60
1:F:52:ILE:HG21	1:F:259:LEU:HD11	1.82	0.60
1:A:9:THR:HG23	1:A:9:THR:O	2.02	0.60
1:B:4:ALA:HB2	1:B:33:ARG:HB2	1.83	0.60
1:A:200:PHE:CE1	1:A:204:GLY:HA3	2.36	0.60
1:B:187:ASN:O	1:B:188:LEU:CA	2.48	0.60
1:G:171:ASN:C	1:G:171:ASN:HD22	2.09	0.60
1:H:200:PHE:CE1	1:H:204:GLY:HA3	2.37	0.60
1:A:177:ASP:OD1	1:A:179:ARG:HB2	2.01	0.60
1:H:97:CYS:HB2	1:H:138:TYR:HE2	1.65	0.60
1:A:215:GLN:CG	1:A:216:THR:H	2.11	0.60
1:D:200:PHE:CD1	1:D:204:GLY:HA3	2.36	0.60
1:I:132:ASN:HD22	1:I:163:GLN:NE2	1.97	0.60
1:J:171:ASN:C	1:J:171:ASN:HD22	2.08	0.60
1:A:187:ASN:OD1	1:A:187:ASN:O	2.19	0.60
1:B:-1:MET:CB	1:B:32:ARG:HD3	2.32	0.60
1:F:58:ILE:HD12	1:F:58:ILE:H	1.67	0.60
1:J:58:ILE:HD12	1:J:58:ILE:H	1.67	0.60
1:J:186:TYR:O	1:J:209:VAL:HB	2.01	0.60
1:C:80:GLY:HA3	1:E:262:GLN:HE22	1.65	0.60
1:D:241:HIS:ND1	1:D:245:LEU:HD12	2.17	0.60
1:I:-5:ARG:HH12	1:I:-2:HIS:CE1	2.20	0.60
1:I:58:ILE:HD12	1:I:58:ILE:H	1.66	0.60
1:H:132:ASN:HD22	1:H:163:GLN:NE2	2.00	0.59
1:H:4:ALA:HB2	1:H:33:ARG:HB2	1.83	0.59
1:A:231:ARG:O	1:A:232:SER:CB	2.51	0.59
1:A:193:ILE:CG2	1:A:240:THR:OG1	2.50	0.59
1:B:171:ASN:HD22	1:B:171:ASN:C	2.09	0.59
1:D:143:GLU:O	1:D:147:GLN:HG2	2.03	0.59
1:G:240:THR:CG2	1:G:242:PRO:HD3	2.33	0.59
1:D:200:PHE:CE1	1:D:204:GLY:HA3	2.37	0.59
1:G:132:ASN:HD22	1:G:163:GLN:NE2	2.00	0.59
1:D:9:THR:HG23	1:D:9:THR:O	2.03	0.59
1:J:177:ASP:OD1	1:J:179:ARG:HB2	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HG23	1:B:9:THR:O	2.03	0.59
1:G:200:PHE:CE1	1:G:204:GLY:HA3	2.37	0.59
1:D:224:ASP:OD1	1:D:227:THR:HG23	2.02	0.59
1:D:241:HIS:ND1	1:D:245:LEU:HD11	2.17	0.59
1:B:215:GLN:CG	1:B:216:THR:H	2.08	0.58
1:E:240:THR:O	1:E:243:GLN:HB3	2.01	0.58
1:B:200:PHE:CD1	1:B:204:GLY:HA3	2.37	0.58
1:C:58:ILE:H	1:C:58:ILE:HD12	1.66	0.58
1:F:9:THR:HG23	1:F:9:THR:O	2.03	0.58
1:I:-5:ARG:NH1	1:I:-2:HIS:CE1	2.71	0.58
1:B:261:GLN:CG	1:B:266:VAL:CG1	2.79	0.58
1:F:97:CYS:HB2	1:F:138:TYR:HE2	1.66	0.58
1:B:193:ILE:O	1:B:240:THR:CG2	2.52	0.58
1:G:58:ILE:HD12	1:G:58:ILE:H	1.68	0.58
1:I:9:THR:HG23	1:I:9:THR:O	2.02	0.58
1:J:132:ASN:HD22	1:J:163:GLN:NE2	1.99	0.58
1:B:262:GLN:HG2	1:B:263:PHE:CD1	2.39	0.58
1:E:9:THR:HG23	1:E:9:THR:O	2.04	0.58
1:G:221:TYR:CE2	1:G:245:LEU:CD2	2.86	0.58
1:J:200:PHE:CE1	1:J:204:GLY:HA3	2.38	0.58
1:B:200:PHE:CD2	1:B:240:THR:HG21	2.39	0.58
1:D:241:HIS:N	1:D:242:PRO:CD	2.66	0.58
1:E:63:LEU:HD13	1:G:263:PHE:CE2	2.39	0.58
1:E:200:PHE:CE1	1:E:204:GLY:HA3	2.38	0.58
1:H:75:LYS:HG3	1:H:76:ARG:HG3	1.84	0.58
1:B:189:SER:HB2	1:B:213:LEU:HD21	1.84	0.58
1:C:82:THR:HG23	1:C:162:ASP:HA	1.86	0.58
1:C:171:ASN:C	1:C:171:ASN:HD22	2.12	0.58
1:H:171:ASN:C	1:H:171:ASN:HD22	2.10	0.58
1:A:82:THR:HG23	1:A:162:ASP:HA	1.86	0.57
1:G:215:GLN:CG	1:G:216:THR:H	2.12	0.57
1:H:52:ILE:HG21	1:H:259:LEU:HD11	1.84	0.57
1:A:231:ARG:O	1:A:232:SER:HB2	2.03	0.57
1:I:52:ILE:HG21	1:I:259:LEU:HD11	1.85	0.57
1:B:52:ILE:HG21	1:B:259:LEU:HD11	1.87	0.57
1:H:230:VAL:O	1:H:231:ARG:CG	2.50	0.57
1:C:132:ASN:HD22	1:C:163:GLN:NE2	2.00	0.57
1:F:200:PHE:CD1	1:F:204:GLY:HA3	2.39	0.57
1:I:231:ARG:CG	1:I:232:SER:H	2.17	0.57
1:A:58:ILE:HD12	1:A:58:ILE:H	1.70	0.57
1:C:193:ILE:CB	1:C:240:THR:CG2	2.55	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:MET:HE1	1:G:52:ILE:CD1	2.34	0.57
1:J:215:GLN:CG	1:J:216:THR:H	2.08	0.57
1:D:52:ILE:HG21	1:D:259:LEU:HD11	1.87	0.57
1:H:3:GLN:CB	1:H:32:ARG:HD2	2.35	0.57
1:F:32:ARG:HH11	1:F:32:ARG:HG2	1.70	0.57
1:G:177:ASP:OD1	1:G:179:ARG:HB2	2.05	0.57
1:G:240:THR:HG22	1:G:242:PRO:HD3	1.87	0.57
1:B:177:ASP:OD1	1:B:179:ARG:HB2	2.05	0.57
1:D:215:GLN:CG	1:D:216:THR:H	2.12	0.57
1:E:86:LEU:HD11	1:E:165:LEU:HD23	1.87	0.57
1:H:210:VAL:HG21	1:H:244:PHE:CD1	2.40	0.57
1:J:20:VAL:HG21	1:J:248:TRP:CZ2	2.40	0.57
1:C:62:ILE:HD12	1:C:73:LEU:HD22	1.87	0.56
1:F:143:GLU:O	1:F:147:GLN:HG2	2.05	0.56
1:B:200:PHE:CE1	1:B:204:GLY:HA3	2.40	0.56
1:E:-2:HIS:HA	1:E:31:SER:O	2.05	0.56
1:H:82:THR:HG23	1:H:162:ASP:HA	1.87	0.56
1:I:125:PRO:O	1:J:125:PRO:O	2.22	0.56
1:A:241:HIS:CD2	1:A:245:LEU:HD11	2.40	0.56
1:F:132:ASN:HD22	1:F:163:GLN:NE2	2.00	0.56
1:J:82:THR:HG23	1:J:162:ASP:HA	1.86	0.56
1:F:86:LEU:HD11	1:F:165:LEU:HD23	1.87	0.56
1:I:177:ASP:OD1	1:I:179:ARG:HB2	2.06	0.56
1:I:183:PRO:HD2	1:I:186:TYR:CD2	2.41	0.56
1:B:75:LYS:HG3	1:B:76:ARG:HG3	1.85	0.56
1:G:75:LYS:HG3	1:G:76:ARG:HG3	1.88	0.56
1:A:190:SER:HA	1:A:193:ILE:HG12	1.88	0.56
1:C:97:CYS:HB2	1:C:138:TYR:HE2	1.69	0.56
1:C:263:PHE:CZ	1:I:63:LEU:HD13	2.40	0.56
1:D:58:ILE:HD12	1:D:58:ILE:H	1.71	0.56
1:B:257:VAL:HG12	1:B:261:GLN:CD	2.30	0.56
1:D:82:THR:HG23	1:D:162:ASP:HA	1.88	0.56
1:D:148:LEU:HD23	1:D:169:PHE:CD2	2.41	0.56
1:F:193:ILE:CD1	1:F:241:HIS:HB2	2.36	0.56
1:I:97:CYS:HB2	1:I:138:TYR:HE2	1.70	0.56
1:A:240:THR:O	1:A:243:GLN:CB	2.54	0.56
1:B:144:THR:HA	1:B:147:GLN:HG3	1.87	0.56
1:F:241:HIS:ND1	1:F:244:PHE:HD1	2.04	0.56
1:I:4:ALA:HB2	1:I:33:ARG:HB2	1.88	0.56
1:B:86:LEU:HD11	1:B:165:LEU:HD23	1.87	0.56
1:C:52:ILE:HD13	1:I:74:MET:HE1	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:MET:HE1	1:E:52:ILE:CD1	2.35	0.55
1:C:74:MET:HE1	1:E:52:ILE:HD13	1.86	0.55
1:E:143:GLU:O	1:E:147:GLN:HG2	2.06	0.55
1:F:113:LEU:HD21	1:F:186:TYR:CD1	2.40	0.55
1:H:177:ASP:OD1	1:H:179:ARG:HB2	2.05	0.55
1:C:240:THR:CG2	1:C:241:HIS:H	2.20	0.55
1:E:183:PRO:HD2	1:E:186:TYR:CD2	2.41	0.55
1:B:82:THR:HG23	1:B:162:ASP:HA	1.89	0.55
1:F:200:PHE:CE1	1:F:204:GLY:HA3	2.40	0.55
1:I:48:LYS:CA	1:I:51:GLU:HG3	2.33	0.55
1:A:52:ILE:HG21	1:A:259:LEU:HD11	1.88	0.55
1:B:97:CYS:HB2	1:B:138:TYR:HE2	1.69	0.55
1:C:148:LEU:HD23	1:C:169:PHE:CD2	2.41	0.55
1:C:143:GLU:O	1:C:147:GLN:HG2	2.06	0.55
1:D:86:LEU:HD11	1:D:165:LEU:HD23	1.89	0.55
1:D:97:CYS:HB2	1:D:138:TYR:HE2	1.70	0.55
1:E:215:GLN:CG	1:E:216:THR:H	2.12	0.55
1:F:75:LYS:HG3	1:F:76:ARG:HG3	1.88	0.55
1:H:119:LEU:HG	1:H:170:PHE:CB	2.37	0.55
1:B:-7:VAL:O	1:B:-7:VAL:HG13	2.07	0.55
1:B:193:ILE:HB	1:B:240:THR:OG1	2.07	0.55
1:B:224:ASP:OD1	1:B:227:THR:HG23	2.07	0.55
1:B:266:VAL:HG23	1:B:266:VAL:O	2.07	0.55
1:F:82:THR:HG23	1:F:162:ASP:HA	1.88	0.55
1:H:20:VAL:HG21	1:H:248:TRP:CZ2	2.41	0.55
1:I:82:THR:HG23	1:I:162:ASP:HA	1.88	0.55
1:C:200:PHE:CE1	1:C:240:THR:OG1	2.51	0.54
1:F:215:GLN:CG	1:F:216:THR:H	2.07	0.54
1:G:143:GLU:O	1:G:147:GLN:HG2	2.08	0.54
1:H:32:ARG:HG2	1:H:32:ARG:HH11	1.71	0.54
1:H:215:GLN:CG	1:H:216:THR:H	2.12	0.54
1:D:241:HIS:CB	1:D:242:PRO:HD3	2.38	0.54
1:F:177:ASP:OD1	1:F:179:ARG:HB2	2.06	0.54
1:I:20:VAL:HG21	1:I:248:TRP:CZ2	2.42	0.54
1:A:75:LYS:HG3	1:A:76:ARG:HG3	1.89	0.54
1:B:76:ARG:HG2	1:B:76:ARG:HH11	1.73	0.54
1:C:75:LYS:HG3	1:C:76:ARG:HG3	1.89	0.54
1:E:82:THR:HG23	1:E:162:ASP:HA	1.89	0.54
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.72	0.54
1:F:224:ASP:OD1	1:F:227:THR:HG23	2.08	0.54
1:B:58:ILE:HD12	1:B:58:ILE:H	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ASP:O	1:C:15:ALA:HB3	2.08	0.54
1:E:32:ARG:HG2	1:E:32:ARG:HH11	1.73	0.54
1:G:76:ARG:HG2	1:G:76:ARG:HH11	1.72	0.54
1:J:52:ILE:HG21	1:J:259:LEU:CD1	2.37	0.54
1:G:86:LEU:HD11	1:G:165:LEU:HD23	1.89	0.54
1:G:82:THR:HG23	1:G:162:ASP:HA	1.90	0.54
1:G:148:LEU:HD23	1:G:169:PHE:CD2	2.43	0.54
1:H:243:GLN:O	1:H:243:GLN:OE1	2.25	0.54
1:I:128:PRO:CG	1:J:123:PRO:HG2	2.38	0.54
1:G:76:ARG:HG2	1:G:76:ARG:NH1	2.23	0.53
1:G:183:PRO:HD2	1:G:186:TYR:CD2	2.42	0.53
1:I:32:ARG:HH11	1:I:32:ARG:HG2	1.73	0.53
1:I:86:LEU:HD11	1:I:165:LEU:HD23	1.90	0.53
1:J:86:LEU:HD11	1:J:165:LEU:HD23	1.89	0.53
1:J:148:LEU:HD23	1:J:169:PHE:CD2	2.43	0.53
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.73	0.53
1:D:241:HIS:CE1	1:D:245:LEU:HD11	2.43	0.53
1:J:75:LYS:HG3	1:J:76:ARG:HG3	1.90	0.53
1:E:75:LYS:HG3	1:E:76:ARG:HG3	1.89	0.53
1:I:2:ASP:OD1	1:I:3:GLN:N	2.42	0.53
1:A:20:VAL:HG21	1:A:248:TRP:CZ2	2.43	0.53
1:H:58:ILE:H	1:H:58:ILE:HD12	1.73	0.53
1:I:113:LEU:HD21	1:I:186:TYR:CD1	2.44	0.53
1:J:213:LEU:HD23	1:J:213:LEU:H	1.74	0.53
1:A:8:LEU:HD12	1:A:37:LEU:O	2.09	0.53
1:A:86:LEU:HD11	1:A:165:LEU:HD23	1.91	0.53
1:C:74:MET:HE2	1:E:52:ILE:HG23	1.90	0.53
1:H:239:MET:C	1:H:240:THR:O	2.51	0.53
1:I:143:GLU:O	1:I:147:GLN:HG2	2.08	0.53
1:C:86:LEU:HD11	1:C:165:LEU:HD23	1.90	0.53
1:D:177:ASP:OD1	1:D:179:ARG:HB2	2.09	0.53
1:E:-2:HIS:N	1:E:31:SER:HB2	2.24	0.53
1:H:9:THR:O	1:H:9:THR:HG23	2.08	0.53
1:C:213:LEU:H	1:C:213:LEU:HD23	1.73	0.53
1:I:148:LEU:HD23	1:I:169:PHE:CD2	2.43	0.53
1:J:215:GLN:HG2	1:J:216:THR:OG1	2.09	0.53
1:F:190:SER:HB3	1:F:241:HIS:CE1	2.42	0.53
1:I:215:GLN:HG2	1:I:216:THR:OG1	2.09	0.53
1:I:241:HIS:HB3	1:I:242:PRO:HD3	1.91	0.53
1:A:4:ALA:HB2	1:A:33:ARG:HB2	1.89	0.53
1:G:97:CYS:HB2	1:G:138:TYR:HE2	1.68	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:LEU:HD23	1:H:169:PHE:CD2	2.43	0.53
1:G:113:LEU:HD21	1:G:186:TYR:CD1	2.44	0.52
1:J:12:ASP:O	1:J:15:ALA:HB3	2.09	0.52
1:D:113:LEU:HD21	1:D:186:TYR:CD1	2.44	0.52
1:H:86:LEU:HD11	1:H:165:LEU:HD23	1.90	0.52
1:H:118:GLU:HB2	1:H:139:GLN:HE21	1.73	0.52
1:J:143:GLU:O	1:J:147:GLN:HG2	2.08	0.52
1:E:183:PRO:HD2	1:E:186:TYR:CE2	2.45	0.52
1:F:183:PRO:HD2	1:F:186:TYR:CD2	2.44	0.52
1:H:94:TYR:O	1:H:140:PRO:HG2	2.10	0.52
1:H:240:THR:HG23	1:H:242:PRO:CD	2.39	0.52
1:J:8:LEU:HD12	1:J:9:THR:H	1.74	0.52
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.74	0.52
1:A:94:TYR:O	1:A:140:PRO:HG2	2.09	0.52
1:C:8:LEU:HD12	1:C:9:THR:H	1.75	0.52
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.75	0.52
1:C:76:ARG:HG2	1:C:76:ARG:NH1	2.24	0.52
1:C:260:LEU:HB3	1:C:266:VAL:HG23	1.91	0.52
1:D:94:TYR:O	1:D:140:PRO:HG2	2.10	0.52
1:F:8:LEU:HD12	1:F:9:THR:H	1.73	0.52
1:G:215:GLN:HG2	1:G:216:THR:OG1	2.09	0.52
1:B:20:VAL:HG21	1:B:248:TRP:CZ2	2.43	0.52
1:H:8:LEU:HD12	1:H:9:THR:H	1.74	0.52
1:H:213:LEU:H	1:H:213:LEU:HD23	1.75	0.52
1:I:12:ASP:O	1:I:15:ALA:HB3	2.10	0.52
1:C:63:LEU:HD13	1:E:263:PHE:CE2	2.44	0.52
1:H:183:PRO:HD2	1:H:186:TYR:CD2	2.44	0.52
1:A:97:CYS:HB2	1:A:138:TYR:HE2	1.69	0.52
1:B:-5:ARG:HD2	1:B:-2:HIS:HD2	1.74	0.52
1:D:241:HIS:O	1:D:242:PRO:C	2.47	0.52
1:C:177:ASP:OD1	1:C:179:ARG:HB2	2.10	0.52
1:E:76:ARG:HG2	1:E:76:ARG:HH11	1.74	0.52
1:F:193:ILE:HG12	1:F:241:HIS:ND1	2.25	0.52
1:H:113:LEU:HD21	1:H:186:TYR:CD1	2.44	0.52
1:H:119:LEU:HG	1:H:170:PHE:CD2	2.44	0.52
1:J:8:LEU:HD12	1:J:37:LEU:O	2.10	0.52
1:A:173:TRP:O	1:A:181:HIS:HE1	1.93	0.52
1:D:32:ARG:HH11	1:D:32:ARG:HG2	1.74	0.52
1:F:4:ALA:HB2	1:F:33:ARG:HB2	1.92	0.52
1:I:8:LEU:HD12	1:I:9:THR:H	1.75	0.52
1:I:75:LYS:HG3	1:I:76:ARG:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HB2	1:A:266:VAL:HG21	1.90	0.52
1:B:76:ARG:HG2	1:B:76:ARG:NH1	2.25	0.52
1:G:8:LEU:HD12	1:G:37:LEU:O	2.10	0.52
1:G:224:ASP:OD1	1:G:227:THR:HG23	2.10	0.52
1:G:242:PRO:O	1:G:245:LEU:N	2.42	0.52
1:I:76:ARG:HH11	1:I:76:ARG:HG2	1.74	0.52
1:J:3:GLN:HB3	1:J:114:PHE:CE2	2.45	0.52
1:E:177:ASP:OD1	1:E:179:ARG:HB2	2.10	0.51
1:F:20:VAL:HG21	1:F:248:TRP:CZ2	2.45	0.51
1:G:4:ALA:HB2	1:G:33:ARG:HB2	1.91	0.51
1:I:183:PRO:HD2	1:I:186:TYR:CE2	2.45	0.51
1:J:9:THR:HG23	1:J:9:THR:O	2.10	0.51
1:B:215:GLN:HG2	1:B:216:THR:OG1	2.11	0.51
1:D:241:HIS:HB3	1:D:242:PRO:CD	2.40	0.51
1:J:32:ARG:HG2	1:J:32:ARG:HH11	1.75	0.51
1:A:11:ASN:OD1	1:A:13:ALA:N	2.42	0.51
1:C:215:GLN:HG2	1:C:216:THR:OG1	2.10	0.51
1:A:8:LEU:HD12	1:A:9:THR:H	1.76	0.51
1:A:206:ASN:O	1:A:207:ALA:C	2.54	0.51
1:G:8:LEU:HD12	1:G:9:THR:H	1.74	0.51
1:G:125:PRO:O	1:H:125:PRO:O	2.29	0.51
1:I:213:LEU:HD23	1:I:213:LEU:H	1.75	0.51
1:B:206:ASN:O	1:B:207:ALA:C	2.54	0.51
1:C:4:ALA:HB2	1:C:33:ARG:HB2	1.93	0.51
1:C:240:THR:CG2	1:C:241:HIS:N	2.73	0.51
1:F:148:LEU:HD23	1:F:169:PHE:CD2	2.45	0.51
1:F:215:GLN:HG2	1:F:216:THR:OG1	2.10	0.51
1:H:183:PRO:HD2	1:H:186:TYR:CE2	2.46	0.51
1:I:2:ASP:O	1:I:94:TYR:CA	2.58	0.51
1:I:76:ARG:HG2	1:I:76:ARG:NH1	2.25	0.51
1:E:76:ARG:HG2	1:E:76:ARG:NH1	2.26	0.51
1:B:187:ASN:O	1:B:187:ASN:OD1	2.27	0.51
1:D:12:ASP:O	1:D:15:ALA:HB3	2.11	0.51
1:E:189:SER:HB2	1:E:213:LEU:HD21	1.92	0.51
1:F:241:HIS:O	1:F:242:PRO:C	2.53	0.51
1:I:11:ASN:OD1	1:I:13:ALA:N	2.43	0.51
1:I:94:TYR:O	1:I:140:PRO:HG2	2.10	0.51
1:A:76:ARG:HG2	1:A:76:ARG:NH1	2.25	0.51
1:C:20:VAL:HG21	1:C:248:TRP:CZ2	2.45	0.51
1:D:241:HIS:HB3	1:D:242:PRO:HD3	1.92	0.51
1:E:58:ILE:HD12	1:E:58:ILE:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LEU:HD23	1:E:169:PHE:CD2	2.46	0.51
1:B:241:HIS:HB3	1:B:242:PRO:CD	2.36	0.51
1:H:37:LEU:HD23	1:H:58:ILE:HB	1.93	0.51
1:H:121:ALA:HA	1:H:182:LEU:HD12	1.92	0.51
1:J:19:LEU:HD13	1:J:256:VAL:HG13	1.93	0.51
1:J:97:CYS:HB2	1:J:138:TYR:HE2	1.71	0.51
1:E:12:ASP:O	1:E:15:ALA:HB3	2.11	0.50
1:H:76:ARG:HG2	1:H:76:ARG:HH11	1.76	0.50
1:H:215:GLN:HG2	1:H:216:THR:OG1	2.10	0.50
1:J:11:ASN:OD1	1:J:13:ALA:N	2.41	0.50
1:A:238:THR:O	1:A:238:THR:HG22	2.10	0.50
1:C:11:ASN:OD1	1:C:13:ALA:N	2.43	0.50
1:E:113:LEU:HD21	1:E:186:TYR:CD1	2.45	0.50
1:E:260:LEU:HB3	1:E:266:VAL:CG2	2.40	0.50
1:F:94:TYR:O	1:F:140:PRO:HG2	2.11	0.50
1:G:20:VAL:HG21	1:G:248:TRP:CZ2	2.46	0.50
1:I:-5:ARG:O	1:I:-5:ARG:CD	2.60	0.50
1:I:-3:SER:O	1:I:-2:HIS:HB3	2.12	0.50
1:A:193:ILE:C	1:A:240:THR:HG21	2.36	0.50
1:C:190:SER:HB2	1:C:241:HIS:ND1	2.26	0.50
1:E:213:LEU:HD23	1:E:213:LEU:H	1.76	0.50
1:J:58:ILE:HD12	1:J:58:ILE:N	2.26	0.50
1:D:20:VAL:HG21	1:D:248:TRP:CZ2	2.47	0.50
1:D:260:LEU:HB3	1:D:266:VAL:HG23	1.94	0.50
1:E:8:LEU:HD12	1:E:9:THR:H	1.76	0.50
1:G:183:PRO:HD2	1:G:186:TYR:CE2	2.46	0.50
1:B:8:LEU:HD12	1:B:9:THR:H	1.76	0.50
1:B:192:SER:HA	1:B:195:SER:HB3	1.93	0.50
1:D:76:ARG:HH11	1:D:76:ARG:HG2	1.76	0.50
1:H:143:GLU:O	1:H:147:GLN:HG2	2.10	0.50
1:A:224:ASP:OD1	1:A:227:THR:HG23	2.12	0.50
1:C:58:ILE:HD12	1:C:58:ILE:N	2.27	0.50
1:D:75:LYS:HG3	1:D:76:ARG:HG3	1.93	0.50
1:D:189:SER:HB2	1:D:213:LEU:HD21	1.94	0.50
1:F:183:PRO:HD2	1:F:186:TYR:CE2	2.46	0.50
1:F:213:LEU:H	1:F:213:LEU:HD23	1.76	0.50
1:F:242:PRO:O	1:F:243:GLN:C	2.55	0.50
1:H:11:ASN:OD1	1:H:13:ALA:N	2.44	0.50
1:F:12:ASP:O	1:F:15:ALA:HB3	2.12	0.50
1:B:187:ASN:O	1:B:188:LEU:C	2.54	0.50
1:B:242:PRO:O	1:B:243:GLN:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HA	1:I:74:MET:CE	2.38	0.50
1:F:58:ILE:HD12	1:F:58:ILE:N	2.27	0.50
1:G:12:ASP:O	1:G:15:ALA:HB3	2.12	0.50
1:G:173:TRP:O	1:G:181:HIS:HE1	1.95	0.50
1:I:133:SER:H	1:I:163:GLN:HE21	1.60	0.50
1:A:37:LEU:HD23	1:A:58:ILE:HB	1.94	0.49
1:B:184:PHE:O	1:B:188:LEU:N	2.45	0.49
1:E:215:GLN:HG2	1:E:216:THR:OG1	2.12	0.49
1:I:128:PRO:HG2	1:J:123:PRO:HG2	1.94	0.49
1:J:224:ASP:OD1	1:J:227:THR:HG23	2.12	0.49
1:C:63:LEU:HD22	1:E:263:PHE:CZ	2.46	0.49
1:C:215:GLN:CG	1:C:216:THR:H	2.11	0.49
1:I:52:ILE:HG21	1:I:259:LEU:CD1	2.42	0.49
1:I:193:ILE:HA	1:I:200:PHE:HB2	1.94	0.49
1:A:171:ASN:C	1:A:171:ASN:ND2	2.70	0.49
1:B:94:TYR:O	1:B:140:PRO:HG2	2.12	0.49
1:F:37:LEU:HD23	1:F:58:ILE:HB	1.94	0.49
1:G:52:ILE:HG21	1:G:259:LEU:CD1	2.42	0.49
1:H:210:VAL:CG2	1:H:244:PHE:CD1	2.96	0.49
1:H:224:ASP:OD1	1:H:227:THR:HG23	2.12	0.49
1:D:8:LEU:HD12	1:D:9:THR:H	1.76	0.49
1:E:256:VAL:O	1:E:257:VAL:C	2.56	0.49
1:A:45:THR:CG2	1:A:265:LEU:HD23	2.43	0.49
1:A:242:PRO:O	1:A:243:GLN:C	2.55	0.49
1:B:144:THR:O	1:B:147:GLN:HB2	2.13	0.49
1:E:206:ASN:O	1:E:207:ALA:C	2.55	0.49
1:B:213:LEU:HD23	1:B:213:LEU:H	1.77	0.49
1:B:231:ARG:CG	1:B:232:SER:N	2.63	0.49
1:E:52:ILE:HG21	1:E:259:LEU:CD1	2.42	0.49
1:F:76:ARG:HG2	1:F:76:ARG:HH11	1.78	0.49
1:G:11:ASN:OD1	1:G:13:ALA:N	2.42	0.49
1:H:12:ASP:O	1:H:15:ALA:HB3	2.13	0.49
1:C:52:ILE:CD1	1:I:74:MET:HE1	2.43	0.49
1:D:76:ARG:HG2	1:D:76:ARG:NH1	2.28	0.49
1:D:190:SER:CB	1:D:241:HIS:NE2	2.75	0.49
1:F:189:SER:HB2	1:F:213:LEU:HD21	1.95	0.49
1:G:58:ILE:HD12	1:G:58:ILE:N	2.28	0.49
1:G:206:ASN:O	1:G:207:ALA:C	2.56	0.49
1:J:37:LEU:HD23	1:J:58:ILE:HB	1.93	0.49
1:A:148:LEU:HD23	1:A:169:PHE:CD2	2.47	0.49
1:A:200:PHE:CD2	1:A:240:THR:HB	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:LEU:HD23	1:D:58:ILE:HB	1.93	0.49
1:D:206:ASN:O	1:D:207:ALA:C	2.55	0.49
1:E:8:LEU:HD12	1:E:37:LEU:O	2.11	0.49
1:H:206:ASN:O	1:H:207:ALA:C	2.55	0.49
1:F:241:HIS:CE1	1:F:244:PHE:CD1	2.97	0.49
1:F:260:LEU:HB3	1:F:266:VAL:HG23	1.93	0.49
1:H:76:ARG:HG2	1:H:76:ARG:NH1	2.28	0.49
1:J:76:ARG:NH1	1:J:76:ARG:HG2	2.28	0.49
1:J:94:TYR:O	1:J:140:PRO:HG2	2.12	0.49
1:D:213:LEU:HD23	1:D:213:LEU:H	1.78	0.49
1:F:52:ILE:HG21	1:F:259:LEU:CD1	2.43	0.49
1:G:94:TYR:O	1:G:140:PRO:HG2	2.12	0.49
1:A:58:ILE:HD12	1:A:58:ILE:N	2.28	0.48
1:A:143:GLU:O	1:A:147:GLN:HG2	2.13	0.48
1:A:213:LEU:H	1:A:213:LEU:HD23	1.78	0.48
1:A:239:MET:O	1:A:243:GLN:HB2	2.12	0.48
1:E:241:HIS:CD2	1:E:245:LEU:CD1	2.96	0.48
1:H:210:VAL:CG2	1:H:244:PHE:CE1	2.95	0.48
1:G:31:SER:OG	1:G:32:ARG:NH1	2.47	0.48
1:C:3:GLN:CB	1:C:32:ARG:HD2	2.40	0.48
1:C:242:PRO:O	1:C:243:GLN:C	2.56	0.48
1:F:133:SER:H	1:F:163:GLN:HE21	1.61	0.48
1:J:76:ARG:HG2	1:J:76:ARG:HH11	1.77	0.48
1:J:173:TRP:O	1:J:181:HIS:HE1	1.95	0.48
1:A:9:THR:HG21	1:A:38:THR:HG22	1.95	0.48
1:A:190:SER:HA	1:A:193:ILE:CD1	2.43	0.48
1:A:256:VAL:O	1:A:257:VAL:C	2.56	0.48
1:B:1:THR:HA	1:B:33:ARG:HD2	1.95	0.48
1:F:190:SER:HB2	1:F:241:HIS:CD2	2.49	0.48
1:F:192:SER:HA	1:F:195:SER:HB3	1.95	0.48
1:I:58:ILE:HD12	1:I:58:ILE:N	2.28	0.48
1:C:19:LEU:HD13	1:C:256:VAL:HG13	1.96	0.48
1:D:11:ASN:OD1	1:D:13:ALA:N	2.44	0.48
1:E:86:LEU:HD11	1:E:165:LEU:CD2	2.43	0.48
1:E:240:THR:O	1:E:243:GLN:HB2	2.13	0.48
1:I:1:MET:O	1:I:33:ARG:HG2	2.14	0.48
1:I:260:LEU:HB3	1:I:266:VAL:HG23	1.94	0.48
1:F:232:SER:O	1:F:233:GLU:C	2.57	0.48
1:F:252:PHE:O	1:F:257:VAL:HG23	2.13	0.48
1:F:256:VAL:O	1:F:257:VAL:C	2.56	0.48
1:G:32:ARG:HG2	1:G:32:ARG:HH11	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:LEU:HD13	1:I:256:VAL:HG13	1.96	0.48
1:C:52:ILE:HG23	1:I:74:MET:CE	2.43	0.48
1:C:191:ILE:HG13	1:C:192:SER:N	2.29	0.48
1:D:78:GLU:OE2	1:D:78:GLU:N	2.32	0.48
1:D:193:ILE:HA	1:D:200:PHE:HB2	1.96	0.48
1:E:47:ARG:HH11	1:E:47:ARG:CG	2.23	0.48
1:E:94:TYR:O	1:E:140:PRO:HG2	2.12	0.48
1:F:173:TRP:O	1:F:181:HIS:HE1	1.97	0.48
1:G:241:HIS:ND1	1:G:241:HIS:O	2.33	0.48
1:I:173:TRP:O	1:I:181:HIS:HE1	1.97	0.48
1:A:191:ILE:HG13	1:A:192:SER:N	2.28	0.48
1:B:133:SER:H	1:B:163:GLN:HE21	1.62	0.48
1:C:183:PRO:HD2	1:C:186:TYR:CE2	2.48	0.48
1:E:224:ASP:OD1	1:E:227:THR:HG23	2.13	0.48
1:G:193:ILE:HA	1:G:200:PHE:HB2	1.96	0.48
1:I:-5:ARG:NH2	1:I:-2:HIS:CE1	2.82	0.48
1:C:262:GLN:HE22	1:I:80:GLY:CA	2.15	0.48
1:D:133:SER:H	1:D:163:GLN:HE21	1.60	0.48
1:D:183:PRO:HD2	1:D:186:TYR:CD2	2.49	0.48
1:G:47:ARG:HH11	1:G:47:ARG:CG	2.22	0.48
1:B:19:LEU:HD13	1:B:256:VAL:HG13	1.95	0.47
1:C:32:ARG:HG2	1:C:32:ARG:HH11	1.79	0.47
1:E:242:PRO:O	1:E:243:GLN:C	2.56	0.47
1:F:8:LEU:HD12	1:F:37:LEU:O	2.14	0.47
1:F:76:ARG:HG2	1:F:76:ARG:NH1	2.29	0.47
1:I:242:PRO:O	1:I:243:GLN:C	2.56	0.47
1:A:215:GLN:HG2	1:A:216:THR:OG1	2.13	0.47
1:C:94:TYR:O	1:C:140:PRO:HG2	2.13	0.47
1:C:193:ILE:HA	1:C:200:PHE:HB2	1.95	0.47
1:G:45:THR:HG22	1:G:263:PHE:HB3	1.96	0.47
1:I:45:THR:HG22	1:I:263:PHE:HB3	1.96	0.47
1:B:86:LEU:HD11	1:B:165:LEU:CD2	2.45	0.47
1:B:191:ILE:O	1:B:195:SER:N	2.47	0.47
1:G:37:LEU:HD23	1:G:58:ILE:HB	1.95	0.47
1:H:52:ILE:HG21	1:H:259:LEU:CD1	2.44	0.47
1:H:192:SER:HA	1:H:195:SER:HB3	1.96	0.47
1:I:224:ASP:OD1	1:I:227:THR:HG23	2.13	0.47
1:J:256:VAL:O	1:J:257:VAL:C	2.57	0.47
1:A:241:HIS:HB3	1:A:242:PRO:CD	2.43	0.47
1:D:192:SER:HA	1:D:195:SER:HB3	1.95	0.47
1:D:215:GLN:HG2	1:D:216:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LEU:HD11	1:F:165:LEU:CD2	2.44	0.47
1:F:191:ILE:HG13	1:F:192:SER:N	2.29	0.47
1:F:206:ASN:O	1:F:207:ALA:C	2.56	0.47
1:I:37:LEU:HD23	1:I:58:ILE:HB	1.95	0.47
1:A:45:THR:HG22	1:A:263:PHE:HB3	1.97	0.47
1:A:139:GLN:HE21	1:A:139:GLN:HB2	1.53	0.47
1:C:173:TRP:O	1:C:181:HIS:HE1	1.96	0.47
1:C:183:PRO:HD2	1:C:186:TYR:CD2	2.50	0.47
1:E:2:ASP:O	1:E:95:SER:N	2.40	0.47
1:E:191:ILE:HG13	1:E:192:SER:N	2.29	0.47
1:E:193:ILE:HA	1:E:200:PHE:HB2	1.96	0.47
1:F:45:THR:HG22	1:F:263:PHE:HB3	1.94	0.47
1:J:193:ILE:HD12	1:J:193:ILE:C	2.40	0.47
1:A:193:ILE:HD12	1:A:241:HIS:N	2.30	0.47
1:B:-7:VAL:HA	1:B:-6:PRO:HD2	1.66	0.47
1:G:133:SER:H	1:G:163:GLN:HE21	1.63	0.47
1:I:2:ASP:OD1	1:I:3:GLN:HG3	2.13	0.47
1:I:256:VAL:O	1:I:257:VAL:C	2.56	0.47
1:A:12:ASP:O	1:A:15:ALA:HB3	2.14	0.47
1:A:19:LEU:HD13	1:A:256:VAL:HG13	1.97	0.47
1:B:11:ASN:OD1	1:B:13:ALA:N	2.45	0.47
1:C:158:PHE:CD1	1:C:158:PHE:C	2.92	0.47
1:D:8:LEU:HD12	1:D:37:LEU:O	2.15	0.47
1:D:191:ILE:HG13	1:D:192:SER:N	2.28	0.47
1:G:212:PHE:CD2	1:G:245:LEU:CD1	2.98	0.47
1:H:19:LEU:HD13	1:H:256:VAL:HG13	1.95	0.47
1:H:119:LEU:HD11	1:H:131:PHE:CZ	2.50	0.47
1:H:191:ILE:O	1:H:195:SER:N	2.47	0.47
1:H:256:VAL:O	1:H:257:VAL:C	2.58	0.47
1:I:47:ARG:O	1:I:51:GLU:HG2	2.14	0.47
1:J:171:ASN:C	1:J:171:ASN:ND2	2.73	0.47
1:J:191:ILE:O	1:J:195:SER:N	2.47	0.47
1:D:31:SER:OG	1:D:32:ARG:NH1	2.48	0.47
1:D:173:TRP:O	1:D:181:HIS:HE1	1.98	0.47
1:E:20:VAL:HG21	1:E:248:TRP:CZ2	2.48	0.47
1:G:213:LEU:HD23	1:G:213:LEU:H	1.79	0.47
1:A:252:PHE:O	1:A:257:VAL:HG23	2.14	0.47
1:B:191:ILE:HG13	1:B:192:SER:N	2.28	0.47
1:C:192:SER:HA	1:C:195:SER:HB3	1.97	0.47
1:D:252:PHE:O	1:D:257:VAL:HG23	2.15	0.47
1:G:72:THR:HG23	1:G:153:SER:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:LEU:HD11	1:G:165:LEU:CD2	2.45	0.47
1:J:62:ILE:CD1	1:J:73:LEU:HD22	2.43	0.47
1:A:76:ARG:HD2	1:A:152:ALA:O	2.15	0.47
1:B:-5:ARG:HD2	1:B:-2:HIS:CD2	2.50	0.47
1:B:148:LEU:HD23	1:B:169:PHE:CD2	2.50	0.47
1:C:9:THR:HG21	1:C:38:THR:HG22	1.97	0.47
1:E:63:LEU:HD22	1:G:263:PHE:CZ	2.49	0.47
1:E:173:TRP:O	1:E:181:HIS:HE1	1.98	0.47
1:I:158:PHE:CD1	1:I:158:PHE:C	2.93	0.47
1:B:261:GLN:HB3	1:B:266:VAL:CG1	2.44	0.46
1:C:113:LEU:HD21	1:C:186:TYR:CD1	2.51	0.46
1:D:30:THR:HA	1:D:111:ASP:OD2	2.14	0.46
1:H:193:ILE:C	1:H:193:ILE:HD12	2.40	0.46
1:J:241:HIS:HB3	1:J:242:PRO:CD	2.40	0.46
1:A:241:HIS:CD2	1:A:245:LEU:HD12	2.50	0.46
1:B:37:LEU:HD23	1:B:58:ILE:HB	1.98	0.46
1:E:11:ASN:OD1	1:E:13:ALA:N	2.44	0.46
1:E:80:GLY:CA	1:G:262:GLN:HE22	2.18	0.46
1:F:19:LEU:HD13	1:F:256:VAL:HG13	1.98	0.46
1:F:149:LEU:HD12	1:F:149:LEU:HA	1.78	0.46
1:G:245:LEU:HD12	1:G:245:LEU:HA	1.74	0.46
1:J:206:ASN:O	1:J:207:ALA:C	2.59	0.46
1:A:69:ALA:O	1:A:70:HIS:C	2.59	0.46
1:A:94:TYR:O	1:A:140:PRO:CG	2.63	0.46
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.78	0.46
1:B:189:SER:HB2	1:B:213:LEU:CD2	2.44	0.46
1:C:256:VAL:O	1:C:257:VAL:C	2.57	0.46
1:D:183:PRO:HD2	1:D:186:TYR:CE2	2.50	0.46
1:F:62:ILE:CD1	1:F:73:LEU:HD22	2.43	0.46
1:B:173:TRP:O	1:B:181:HIS:HE1	1.97	0.46
1:D:9:THR:HG21	1:D:38:THR:HG22	1.97	0.46
1:D:19:LEU:HD13	1:D:256:VAL:HG13	1.98	0.46
1:D:193:ILE:HD12	1:D:194:TYR:HB3	1.97	0.46
1:F:193:ILE:HA	1:F:200:PHE:HB2	1.96	0.46
1:F:231:ARG:CG	1:F:232:SER:N	2.64	0.46
1:H:31:SER:OG	1:H:32:ARG:NH1	2.49	0.46
1:J:30:THR:HA	1:J:111:ASP:OD2	2.16	0.46
1:A:240:THR:CG2	1:A:241:HIS:N	2.64	0.46
1:B:190:SER:HB2	1:B:241:HIS:ND1	2.30	0.46
1:E:37:LEU:HD23	1:E:58:ILE:HB	1.97	0.46
1:E:45:THR:HG22	1:E:263:PHE:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:PHE:CD2	1:G:245:LEU:HD13	2.47	0.46
1:A:74:MET:HE1	1:I:52:ILE:CD1	2.46	0.46
1:A:193:ILE:HB	1:A:240:THR:OG1	2.15	0.46
1:B:-5:ARG:NH1	1:B:-2:HIS:HD2	2.14	0.46
1:C:74:MET:HE1	1:E:52:ILE:HA	1.97	0.46
1:C:241:HIS:HB3	1:C:242:PRO:CD	2.36	0.46
1:D:158:PHE:CD1	1:D:158:PHE:C	2.93	0.46
1:D:241:HIS:CB	1:D:242:PRO:CD	2.93	0.46
1:G:256:VAL:O	1:G:257:VAL:C	2.57	0.46
1:H:144:THR:O	1:H:147:GLN:HB2	2.15	0.46
1:B:69:ALA:O	1:B:70:HIS:C	2.59	0.46
1:B:122:ALA:HB3	1:B:187:ASN:HB3	1.98	0.46
1:D:58:ILE:HD12	1:D:58:ILE:N	2.30	0.46
1:F:224:ASP:HB3	1:F:227:THR:OG1	2.16	0.46
1:H:173:TRP:O	1:H:181:HIS:HE1	1.99	0.46
1:J:144:THR:O	1:J:147:GLN:HB2	2.16	0.46
1:A:192:SER:HA	1:A:195:SER:HB3	1.98	0.46
1:B:9:THR:HG21	1:B:38:THR:HG22	1.96	0.46
1:I:191:ILE:HG13	1:I:192:SER:N	2.29	0.46
1:A:260:LEU:CB	1:A:266:VAL:HG23	2.40	0.46
1:B:259:LEU:O	1:B:263:PHE:HD1	1.99	0.46
1:F:139:GLN:HE21	1:F:139:GLN:HB2	1.60	0.46
1:G:193:ILE:CD1	1:G:241:HIS:HB2	2.46	0.46
1:J:79:LEU:O	1:J:83:LEU:HG	2.16	0.46
1:J:191:ILE:HG13	1:J:192:SER:N	2.30	0.46
1:B:262:GLN:HG2	1:B:263:PHE:CE1	2.50	0.46
1:C:191:ILE:O	1:C:195:SER:N	2.49	0.46
1:E:69:ALA:O	1:E:70:HIS:C	2.59	0.46
1:G:196:TYR:C	1:G:198:PRO:HD2	2.42	0.46
1:I:30:THR:HA	1:I:111:ASP:OD2	2.16	0.46
1:A:79:LEU:O	1:A:83:LEU:HG	2.15	0.45
1:A:193:ILE:HA	1:A:200:PHE:HB2	1.97	0.45
1:B:193:ILE:HA	1:B:200:PHE:HB2	1.98	0.45
1:C:189:SER:HB2	1:C:213:LEU:HD21	1.97	0.45
1:D:191:ILE:O	1:D:195:SER:N	2.49	0.45
1:G:158:PHE:CD1	1:G:158:PHE:C	2.94	0.45
1:G:212:PHE:HE2	1:G:245:LEU:HD13	1.74	0.45
1:H:191:ILE:HG13	1:H:192:SER:N	2.30	0.45
1:I:192:SER:HA	1:I:195:SER:HB3	1.98	0.45
1:I:193:ILE:HD12	1:I:194:TYR:HB3	1.97	0.45
1:J:193:ILE:HA	1:J:200:PHE:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ALA:HB2	1:D:33:ARG:HB2	1.98	0.45
1:E:133:SER:H	1:E:163:GLN:HE21	1.63	0.45
1:F:193:ILE:HD12	1:F:194:TYR:HB3	1.98	0.45
1:H:193:ILE:HD12	1:H:194:TYR:HB3	1.98	0.45
1:J:158:PHE:CD1	1:J:158:PHE:C	2.95	0.45
1:J:242:PRO:O	1:J:243:GLN:C	2.59	0.45
1:B:240:THR:O	1:B:243:GLN:HB2	2.12	0.45
1:C:133:SER:H	1:C:163:GLN:HE21	1.64	0.45
1:E:144:THR:O	1:E:147:GLN:HB2	2.17	0.45
1:E:192:SER:HA	1:E:195:SER:HB3	1.98	0.45
1:E:257:VAL:O	1:E:258:PRO:C	2.59	0.45
1:F:9:THR:HG21	1:F:38:THR:HG22	1.98	0.45
1:G:224:ASP:HB3	1:G:227:THR:OG1	2.16	0.45
1:H:158:PHE:CD1	1:H:158:PHE:C	2.95	0.45
1:I:117:GLU:O	1:I:118:GLU:C	2.59	0.45
1:I:231:ARG:CG	1:I:232:SER:N	2.77	0.45
1:B:193:ILE:HD12	1:B:194:TYR:HB3	1.97	0.45
1:B:257:VAL:HG12	1:B:261:GLN:HG3	1.97	0.45
1:F:11:ASN:OD1	1:F:13:ALA:N	2.48	0.45
1:H:171:ASN:C	1:H:171:ASN:ND2	2.74	0.45
1:J:192:SER:HA	1:J:195:SER:HB3	1.97	0.45
1:E:241:HIS:CD2	1:E:245:LEU:HD12	2.52	0.45
1:H:58:ILE:HD12	1:H:58:ILE:N	2.31	0.45
1:H:86:LEU:HD11	1:H:165:LEU:CD2	2.46	0.45
1:H:121:ALA:HB3	1:H:131:PHE:HB2	1.98	0.45
1:H:133:SER:H	1:H:163:GLN:HE21	1.65	0.45
1:H:193:ILE:HA	1:H:200:PHE:HB2	1.98	0.45
1:I:206:ASN:O	1:I:207:ALA:C	2.59	0.45
1:J:133:SER:H	1:J:163:GLN:HE21	1.63	0.45
1:J:224:ASP:HB3	1:J:227:THR:OG1	2.17	0.45
1:A:3:GLN:CB	1:A:32:ARG:HD2	2.41	0.45
1:A:133:SER:H	1:A:163:GLN:HE21	1.65	0.45
1:C:11:ASN:OD1	1:C:11:ASN:C	2.60	0.45
1:D:241:HIS:HD1	1:D:245:LEU:HD11	1.76	0.45
1:H:8:LEU:HD12	1:H:37:LEU:O	2.16	0.45
1:I:57:VAL:HG12	1:I:57:VAL:O	2.15	0.45
1:J:20:VAL:HG21	1:J:248:TRP:CE2	2.51	0.45
1:A:62:ILE:CD1	1:A:73:LEU:HD22	2.46	0.45
1:D:132:ASN:ND2	1:D:163:GLN:NE2	2.65	0.45
1:F:144:THR:O	1:F:147:GLN:HB2	2.15	0.45
1:H:189:SER:HB2	1:H:213:LEU:HD21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ARG:O	1:I:51:GLU:CG	2.65	0.45
1:A:260:LEU:CB	1:A:266:VAL:HG21	2.46	0.45
1:C:52:ILE:HG21	1:C:259:LEU:CD1	2.46	0.45
1:C:86:LEU:HD11	1:C:165:LEU:CD2	2.47	0.45
1:D:86:LEU:HD11	1:D:165:LEU:CD2	2.47	0.45
1:H:79:LEU:O	1:H:83:LEU:HG	2.17	0.45
1:H:119:LEU:HD23	1:H:170:PHE:CE2	2.51	0.45
1:D:3:GLN:CB	1:D:32:ARG:HD2	2.39	0.45
1:D:62:ILE:CD1	1:D:73:LEU:HD22	2.46	0.45
1:D:105:LEU:HD23	1:D:106:VAL:N	2.32	0.45
1:D:232:SER:O	1:D:233:GLU:C	2.60	0.45
1:E:132:ASN:ND2	1:E:163:GLN:NE2	2.63	0.45
1:G:241:HIS:O	1:G:242:PRO:C	2.59	0.45
1:G:241:HIS:CE1	1:G:245:LEU:HD22	2.46	0.45
1:I:-5:ARG:HH22	1:I:-2:HIS:CE1	2.34	0.45
1:D:149:LEU:HA	1:D:149:LEU:HD12	1.74	0.44
1:D:171:ASN:C	1:D:171:ASN:ND2	2.73	0.44
1:G:257:VAL:O	1:G:258:PRO:C	2.60	0.44
1:I:8:LEU:HD12	1:I:37:LEU:O	2.17	0.44
1:A:200:PHE:CE2	1:A:240:THR:CB	2.97	0.44
1:B:12:ASP:O	1:B:15:ALA:HB3	2.18	0.44
1:B:78:GLU:OE2	1:B:78:GLU:N	2.34	0.44
1:B:259:LEU:O	1:B:263:PHE:CD1	2.70	0.44
1:D:45:THR:HG22	1:D:263:PHE:HB3	1.98	0.44
1:F:194:TYR:HD2	1:F:194:TYR:O	1.99	0.44
1:G:193:ILE:HD12	1:G:193:ILE:C	2.42	0.44
1:G:252:PHE:O	1:G:257:VAL:HG23	2.17	0.44
1:I:79:LEU:O	1:I:83:LEU:HG	2.18	0.44
1:D:79:LEU:O	1:D:83:LEU:HG	2.17	0.44
1:E:158:PHE:CD1	1:E:158:PHE:C	2.95	0.44
1:F:158:PHE:C	1:F:158:PHE:CD1	2.96	0.44
1:G:149:LEU:HD12	1:G:149:LEU:HA	1.74	0.44
1:J:86:LEU:HD11	1:J:165:LEU:CD2	2.47	0.44
1:J:193:ILE:HD12	1:J:194:TYR:HB3	1.99	0.44
1:B:193:ILE:HD12	1:B:193:ILE:C	2.43	0.44
1:G:191:ILE:HG13	1:G:192:SER:N	2.31	0.44
1:A:132:ASN:ND2	1:A:163:GLN:NE2	2.63	0.44
1:A:151:VAL:HG21	1:A:169:PHE:HD2	1.82	0.44
1:A:158:PHE:C	1:A:158:PHE:CD1	2.95	0.44
1:B:-5:ARG:NH1	1:B:-2:HIS:CD2	2.85	0.44
1:D:256:VAL:O	1:D:257:VAL:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:ASN:C	1:F:171:ASN:ND2	2.73	0.44
1:I:193:ILE:HD12	1:I:193:ILE:C	2.42	0.44
1:A:257:VAL:O	1:A:258:PRO:C	2.60	0.44
1:E:193:ILE:HD12	1:E:194:TYR:HB3	2.00	0.44
1:F:47:ARG:HH11	1:F:47:ARG:CG	2.25	0.44
1:G:9:THR:HG21	1:G:38:THR:HG22	1.96	0.44
1:B:58:ILE:HD12	1:B:58:ILE:N	2.32	0.44
1:C:186:TYR:C	1:C:209:VAL:HB	2.43	0.44
1:C:193:ILE:HD12	1:C:194:TYR:HB3	1.99	0.44
1:C:224:ASP:OD1	1:C:227:THR:HG23	2.18	0.44
1:G:30:THR:HA	1:G:111:ASP:OD2	2.18	0.44
1:H:194:TYR:HD2	1:H:194:TYR:O	2.01	0.44
1:H:200:PHE:O	1:H:204:GLY:N	2.45	0.44
1:I:86:LEU:HD11	1:I:165:LEU:CD2	2.47	0.44
1:I:252:PHE:O	1:I:257:VAL:HG23	2.18	0.44
1:A:263:PHE:CE2	1:G:63:LEU:HD13	2.52	0.44
1:B:117:GLU:O	1:B:118:GLU:C	2.61	0.44
1:B:188:LEU:HD11	1:B:193:ILE:HG23	1.99	0.44
1:B:224:ASP:HB3	1:B:227:THR:OG1	2.18	0.44
1:C:117:GLU:O	1:C:118:GLU:C	2.60	0.44
1:F:79:LEU:O	1:F:83:LEU:HG	2.18	0.44
1:G:78:GLU:OE2	1:G:78:GLU:N	2.35	0.44
1:G:171:ASN:C	1:G:171:ASN:ND2	2.73	0.44
1:G:192:SER:HA	1:G:195:SER:HB3	1.98	0.44
1:H:30:THR:HA	1:H:111:ASP:OD2	2.18	0.44
1:I:72:THR:HG23	1:I:153:SER:HB2	2.00	0.44
1:C:196:TYR:C	1:C:198:PRO:HD2	2.43	0.44
1:D:224:ASP:HB3	1:D:227:THR:OG1	2.17	0.44
1:F:186:TYR:C	1:F:209:VAL:HB	2.43	0.44
1:F:190:SER:HB3	1:F:241:HIS:NE2	2.28	0.44
1:G:69:ALA:O	1:G:70:HIS:C	2.61	0.44
1:G:242:PRO:O	1:G:243:GLN:C	2.60	0.44
1:B:8:LEU:HD12	1:B:37:LEU:O	2.18	0.43
1:E:31:SER:OG	1:E:32:ARG:NH1	2.51	0.43
1:F:8:LEU:HD12	1:F:9:THR:N	2.32	0.43
1:G:189:SER:HB2	1:G:213:LEU:HD21	2.00	0.43
1:G:193:ILE:HD12	1:G:194:TYR:HB3	1.99	0.43
1:A:86:LEU:HD11	1:A:165:LEU:CD2	2.48	0.43
1:B:52:ILE:HG21	1:B:259:LEU:CD1	2.47	0.43
1:B:265:LEU:O	1:B:265:LEU:HG	2.18	0.43
1:E:196:TYR:C	1:E:198:PRO:HD2	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:ALA:O	1:H:70:HIS:C	2.61	0.43
1:A:200:PHE:CZ	1:A:240:THR:OG1	2.71	0.43
1:B:30:THR:HA	1:B:111:ASP:OD2	2.18	0.43
1:C:8:LEU:HD12	1:C:37:LEU:O	2.18	0.43
1:F:241:HIS:C	1:F:243:GLN:N	2.74	0.43
1:G:210:VAL:HG21	1:G:244:PHE:CD2	2.53	0.43
1:H:72:THR:HG23	1:H:153:SER:HB2	2.00	0.43
1:I:132:ASN:ND2	1:I:163:GLN:NE2	2.66	0.43
1:A:71:LEU:O	1:A:74:MET:HB2	2.18	0.43
1:F:117:GLU:O	1:F:118:GLU:C	2.61	0.43
1:F:143:GLU:O	1:F:144:THR:C	2.61	0.43
1:C:171:ASN:C	1:C:171:ASN:ND2	2.76	0.43
1:E:19:LEU:HD13	1:E:256:VAL:HG13	1.99	0.43
1:H:8:LEU:HD12	1:H:9:THR:N	2.34	0.43
1:I:2:ASP:O	1:I:95:SER:N	2.49	0.43
1:I:196:TYR:C	1:I:198:PRO:HD2	2.44	0.43
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.20	0.43
1:C:37:LEU:HD23	1:C:58:ILE:HB	1.99	0.43
1:C:193:ILE:CG1	1:C:240:THR:CG2	2.96	0.43
1:D:57:VAL:HG12	1:D:57:VAL:O	2.18	0.43
1:E:191:ILE:O	1:E:195:SER:N	2.51	0.43
1:F:69:ALA:O	1:F:70:HIS:C	2.60	0.43
1:F:191:ILE:O	1:F:195:SER:N	2.50	0.43
1:H:89:TRP:CE2	1:H:138:TYR:HD1	2.37	0.43
1:H:239:MET:O	1:H:240:THR:O	2.37	0.43
1:I:8:LEU:HD12	1:I:9:THR:N	2.33	0.43
1:I:191:ILE:O	1:I:195:SER:N	2.50	0.43
1:B:171:ASN:C	1:B:171:ASN:ND2	2.74	0.43
1:C:57:VAL:HG12	1:C:57:VAL:O	2.19	0.43
1:D:117:GLU:O	1:D:118:GLU:C	2.62	0.43
1:E:171:ASN:C	1:E:171:ASN:ND2	2.70	0.43
1:F:32:ARG:HG2	1:F:32:ARG:NH1	2.33	0.43
1:I:194:TYR:HD2	1:I:194:TYR:O	2.02	0.43
1:A:128:PRO:CG	1:B:123:PRO:HG2	2.49	0.43
1:C:63:LEU:HD13	1:E:263:PHE:CZ	2.54	0.43
1:C:224:ASP:HB3	1:C:227:THR:OG1	2.19	0.43
1:E:212:PHE:CD2	1:E:241:HIS:CE1	3.07	0.43
1:G:3:GLN:CB	1:G:32:ARG:HD2	2.40	0.43
1:I:171:ASN:C	1:I:171:ASN:ND2	2.72	0.43
1:A:117:GLU:O	1:A:118:GLU:C	2.61	0.43
1:A:224:ASP:HB3	1:A:227:THR:OG1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLN:O	1:A:247:VAL:HG23	2.18	0.43
1:C:-1:MET:HB3	1:C:2:ASP:OD1	2.18	0.43
1:D:196:TYR:C	1:D:198:PRO:HD2	2.44	0.43
1:H:132:ASN:C	1:H:134:GLY:H	2.27	0.43
1:A:149:LEU:HD12	1:A:149:LEU:HA	1.78	0.43
1:A:196:TYR:C	1:A:198:PRO:HD2	2.44	0.43
1:B:257:VAL:HB	1:B:258:PRO:CD	2.44	0.43
1:C:72:THR:HG23	1:C:153:SER:HB2	2.01	0.43
1:C:79:LEU:O	1:C:83:LEU:HG	2.19	0.43
1:D:197:LEU:O	1:D:201:LYS:HG3	2.19	0.43
1:E:143:GLU:O	1:E:144:THR:C	2.62	0.43
1:E:194:TYR:HD2	1:E:194:TYR:O	2.01	0.43
1:F:94:TYR:O	1:F:140:PRO:CG	2.66	0.43
1:G:117:GLU:O	1:G:118:GLU:C	2.62	0.43
1:A:143:GLU:O	1:A:144:THR:C	2.62	0.42
1:B:196:TYR:C	1:B:198:PRO:HD2	2.44	0.42
1:D:193:ILE:HD12	1:D:193:ILE:C	2.43	0.42
1:E:241:HIS:CD2	1:E:245:LEU:HD11	2.54	0.42
1:F:196:TYR:C	1:F:198:PRO:HD2	2.44	0.42
1:H:197:LEU:O	1:H:201:LYS:HG3	2.19	0.42
1:J:149:LEU:HD12	1:J:149:LEU:HA	1.81	0.42
1:A:200:PHE:CZ	1:A:240:THR:CB	3.02	0.42
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.74	0.42
1:D:69:ALA:O	1:D:70:HIS:C	2.61	0.42
1:H:20:VAL:HG21	1:H:248:TRP:CE2	2.54	0.42
1:H:62:ILE:CD1	1:H:73:LEU:HD22	2.45	0.42
1:E:117:GLU:O	1:E:118:GLU:C	2.62	0.42
1:G:19:LEU:HD13	1:G:256:VAL:HG13	2.01	0.42
1:G:118:GLU:HB2	1:G:139:GLN:NE2	2.34	0.42
1:I:62:ILE:CD1	1:I:73:LEU:HD22	2.44	0.42
1:B:256:VAL:O	1:B:257:VAL:C	2.62	0.42
1:C:31:SER:OG	1:C:32:ARG:NH1	2.52	0.42
1:D:242:PRO:O	1:D:243:GLN:C	2.62	0.42
1:E:57:VAL:O	1:E:57:VAL:HG12	2.19	0.42
1:E:79:LEU:O	1:E:83:LEU:HG	2.19	0.42
1:E:193:ILE:HD12	1:E:193:ILE:C	2.44	0.42
1:F:151:VAL:HG21	1:F:169:PHE:HD2	1.84	0.42
1:H:94:TYR:O	1:H:140:PRO:CG	2.68	0.42
1:A:52:ILE:HG21	1:A:259:LEU:CD1	2.49	0.42
1:B:113:LEU:HD21	1:B:186:TYR:CD1	2.54	0.42
1:C:105:LEU:HD23	1:C:106:VAL:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:SER:HB2	1:C:241:HIS:CE1	2.54	0.42
1:E:-2:HIS:HA	1:E:31:SER:HB2	2.01	0.42
1:F:3:GLN:CB	1:F:32:ARG:HD2	2.45	0.42
1:G:139:GLN:HE21	1:G:139:GLN:HB2	1.59	0.42
1:J:243:GLN:O	1:J:247:VAL:HG23	2.20	0.42
1:B:239:MET:O	1:B:243:GLN:HB2	2.19	0.42
1:E:30:THR:HA	1:E:111:ASP:OD2	2.19	0.42
1:G:8:LEU:HD12	1:G:9:THR:N	2.33	0.42
1:H:25:LEU:CD2	1:H:106:VAL:HG21	2.50	0.42
1:H:196:TYR:C	1:H:198:PRO:HD2	2.44	0.42
1:J:72:THR:HG23	1:J:153:SER:HB2	2.01	0.42
1:D:94:TYR:O	1:D:140:PRO:CG	2.67	0.42
1:G:57:VAL:O	1:G:57:VAL:HG12	2.19	0.42
1:G:94:TYR:O	1:G:140:PRO:CG	2.67	0.42
1:H:32:ARG:HG2	1:H:32:ARG:NH1	2.34	0.42
1:I:20:VAL:HG21	1:I:248:TRP:CE2	2.55	0.42
1:J:31:SER:OG	1:J:32:ARG:NH1	2.53	0.42
1:J:132:ASN:ND2	1:J:163:GLN:NE2	2.66	0.42
1:A:89:TRP:CE2	1:A:138:TYR:HD1	2.38	0.42
1:B:132:ASN:C	1:B:134:GLY:H	2.28	0.42
1:G:105:LEU:HD23	1:G:106:VAL:N	2.34	0.42
1:H:78:GLU:OE2	1:H:78:GLU:N	2.35	0.42
1:I:197:LEU:O	1:I:201:LYS:HG3	2.19	0.42
1:E:94:TYR:O	1:E:140:PRO:CG	2.67	0.42
1:F:72:THR:HG23	1:F:153:SER:HB2	2.01	0.42
1:F:193:ILE:HD12	1:F:193:ILE:C	2.45	0.42
1:F:240:THR:O	1:F:243:GLN:HB2	2.20	0.42
1:G:144:THR:O	1:G:147:GLN:HB2	2.20	0.42
1:G:191:ILE:O	1:G:195:SER:N	2.49	0.42
1:I:189:SER:HB2	1:I:213:LEU:HD21	2.01	0.42
1:J:10:THR:O	1:J:11:ASN:HB3	2.20	0.42
1:J:117:GLU:O	1:J:118:GLU:C	2.62	0.42
1:J:189:SER:HB2	1:J:213:LEU:HD21	2.02	0.42
1:G:212:PHE:CE2	1:G:245:LEU:HD12	2.53	0.42
1:J:139:GLN:HE21	1:J:139:GLN:HB2	1.57	0.42
1:J:190:SER:HB2	1:J:241:HIS:ND1	2.35	0.42
1:C:125:PRO:O	1:D:125:PRO:O	2.38	0.41
1:C:132:ASN:ND2	1:C:163:GLN:NE2	2.66	0.41
1:F:253:THR:HA	1:F:257:VAL:HG23	2.02	0.41
1:I:221:TYR:CD2	1:I:245:LEU:HD22	2.55	0.41
1:F:89:TRP:CE2	1:F:138:TYR:HD1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:LEU:HD23	1:F:106:VAL:N	2.35	0.41
1:G:62:ILE:CD1	1:G:73:LEU:HD22	2.48	0.41
1:A:190:SER:HA	1:A:193:ILE:CG1	2.50	0.41
1:A:194:TYR:HD2	1:A:194:TYR:O	2.02	0.41
1:B:158:PHE:CD1	1:B:158:PHE:C	2.97	0.41
1:E:3:GLN:CB	1:E:32:ARG:HD2	2.43	0.41
1:E:105:LEU:HD23	1:E:106:VAL:N	2.36	0.41
1:G:26:LYS:O	1:G:29:ARG:N	2.49	0.41
1:G:186:TYR:C	1:G:209:VAL:HB	2.44	0.41
1:A:57:VAL:O	1:A:57:VAL:HG12	2.19	0.41
1:C:45:THR:HG22	1:C:263:PHE:HB3	2.01	0.41
1:I:31:SER:OG	1:I:32:ARG:NH1	2.54	0.41
1:B:252:PHE:O	1:B:257:VAL:HG23	2.20	0.41
1:C:10:THR:O	1:C:11:ASN:HB3	2.20	0.41
1:F:57:VAL:O	1:F:57:VAL:HG12	2.21	0.41
1:G:79:LEU:O	1:G:83:LEU:HG	2.20	0.41
1:I:1:MET:HB2	1:I:2:ASP:OD1	2.20	0.41
1:J:257:VAL:HB	1:J:258:PRO:CD	2.45	0.41
1:A:138:TYR:N	1:A:138:TYR:CD2	2.89	0.41
1:B:143:GLU:O	1:B:144:THR:C	2.63	0.41
1:C:30:THR:HA	1:C:111:ASP:OD2	2.20	0.41
1:E:139:GLN:HE21	1:E:139:GLN:HB2	1.55	0.41
1:H:9:THR:HG21	1:H:38:THR:HG22	2.00	0.41
1:I:118:GLU:HB2	1:I:139:GLN:NE2	2.35	0.41
1:B:132:ASN:ND2	1:B:163:GLN:NE2	2.66	0.41
1:C:132:ASN:C	1:C:134:GLY:H	2.29	0.41
1:C:221:TYR:CD2	1:C:245:LEU:HD22	2.56	0.41
1:C:252:PHE:O	1:C:257:VAL:HG23	2.21	0.41
1:I:1:MET:O	1:I:33:ARG:CG	2.69	0.41
1:J:143:GLU:O	1:J:144:THR:C	2.63	0.41
1:A:8:LEU:HD12	1:A:9:THR:N	2.35	0.41
1:B:20:VAL:HG21	1:B:248:TRP:CE2	2.56	0.41
1:B:89:TRP:CE2	1:B:138:TYR:HD1	2.39	0.41
1:B:253:THR:HA	1:B:257:VAL:HG23	2.02	0.41
1:D:138:TYR:H	1:D:138:TYR:HD2	1.69	0.41
1:H:47:ARG:HH11	1:H:47:ARG:CG	2.21	0.41
1:H:119:LEU:CG	1:H:170:PHE:CD2	3.04	0.41
1:H:224:ASP:HB3	1:H:227:THR:OG1	2.20	0.41
1:I:9:THR:HG21	1:I:38:THR:HG22	1.99	0.41
1:I:144:THR:O	1:I:147:GLN:HB2	2.21	0.41
1:I:200:PHE:O	1:I:204:GLY:N	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:VAL:O	1:I:258:PRO:C	2.63	0.41
1:J:196:TYR:C	1:J:198:PRO:HD2	2.45	0.41
1:J:253:THR:HA	1:J:257:VAL:HG23	2.03	0.41
1:A:144:THR:O	1:A:147:GLN:HB2	2.21	0.41
1:B:62:ILE:CD1	1:B:73:LEU:HD22	2.49	0.41
1:F:30:THR:HA	1:F:111:ASP:OD2	2.21	0.41
1:F:132:ASN:C	1:F:134:GLY:H	2.29	0.41
1:I:-5:ARG:CZ	1:I:-2:HIS:CE1	3.04	0.41
1:I:149:LEU:HA	1:I:149:LEU:HD12	1.78	0.41
1:B:11:ASN:OD1	1:B:11:ASN:C	2.63	0.40
1:C:2:ASP:O	1:C:95:SER:N	2.47	0.40
1:D:138:TYR:CD2	1:D:138:TYR:N	2.89	0.40
1:E:233:GLU:OE1	1:E:233:GLU:C	2.64	0.40
1:H:138:TYR:N	1:H:138:TYR:CD2	2.89	0.40
1:J:197:LEU:O	1:J:201:LYS:HG3	2.21	0.40
1:J:257:VAL:O	1:J:258:PRO:C	2.65	0.40
1:A:30:THR:HA	1:A:111:ASP:OD2	2.20	0.40
1:B:79:LEU:O	1:B:83:LEU:HG	2.21	0.40
1:B:105:LEU:HD23	1:B:106:VAL:N	2.36	0.40
1:C:139:GLN:HE21	1:C:139:GLN:HB2	1.55	0.40
1:D:8:LEU:HD12	1:D:9:THR:N	2.37	0.40
1:E:11:ASN:OD1	1:E:11:ASN:C	2.64	0.40
1:H:149:LEU:HD12	1:H:149:LEU:HA	1.80	0.40
1:I:94:TYR:O	1:I:140:PRO:CG	2.69	0.40
1:A:197:LEU:O	1:A:201:LYS:HG3	2.21	0.40
1:B:188:LEU:HD11	1:B:193:ILE:CG2	2.51	0.40
1:B:197:LEU:O	1:B:201:LYS:HG3	2.21	0.40
1:C:69:ALA:O	1:C:70:HIS:C	2.63	0.40
1:H:231:ARG:CD	1:H:233:GLU:OE2	2.61	0.40
1:H:240:THR:OG1	1:H:241:HIS:N	2.54	0.40
1:B:8:LEU:HD12	1:B:9:THR:N	2.37	0.40
1:B:94:TYR:O	1:B:140:PRO:CG	2.68	0.40
1:B:151:VAL:HG21	1:B:169:PHE:HD2	1.86	0.40
1:D:52:ILE:HG21	1:D:259:LEU:CD1	2.49	0.40
1:E:-2:HIS:CA	1:E:31:SER:HB2	2.51	0.40
1:E:224:ASP:HB3	1:E:227:THR:OG1	2.21	0.40
1:F:197:LEU:O	1:F:201:LYS:HG3	2.21	0.40
1:G:193:ILE:HD11	1:G:241:HIS:HB3	2.00	0.40
1:J:57:VAL:O	1:J:57:VAL:HG12	2.20	0.40
1:A:193:ILE:CA	1:A:240:THR:HG21	2.40	0.40
1:E:151:VAL:HG21	1:E:169:PHE:HD2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:PHE:O	1:E:257:VAL:HG23	2.21	0.40
1:F:253:THR:HA	1:F:257:VAL:CG2	2.52	0.40
1:G:132:ASN:ND2	1:G:163:GLN:NE2	2.67	0.40
1:H:143:GLU:O	1:H:144:THR:C	2.64	0.40
1:H:221:TYR:CD2	1:H:245:LEU:HD22	2.57	0.40
1:I:11:ASN:OD1	1:I:11:ASN:C	2.64	0.40
1:I:138:TYR:N	1:I:138:TYR:CD2	2.90	0.40
1:I:243:GLN:O	1:I:247:VAL:HG23	2.21	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	260/339 (77%)	223 (86%)	31 (12%)	6 (2%)	5	27
1	B	263/339 (78%)	223 (85%)	31 (12%)	9 (3%)	3	21
1	C	258/339 (76%)	220 (85%)	33 (13%)	5 (2%)	6	30
1	D	256/339 (76%)	219 (86%)	31 (12%)	6 (2%)	5	27
1	E	258/339 (76%)	224 (87%)	28 (11%)	6 (2%)	5	27
1	F	257/339 (76%)	221 (86%)	29 (11%)	7 (3%)	4	24
1	G	258/339 (76%)	225 (87%)	28 (11%)	5 (2%)	6	30
1	H	256/339 (76%)	221 (86%)	26 (10%)	9 (4%)	3	20
1	I	260/339 (77%)	226 (87%)	30 (12%)	4 (2%)	8	34
1	J	247/339 (73%)	213 (86%)	30 (12%)	4 (2%)	7	33
All	All	2573/3390 (76%)	2215 (86%)	297 (12%)	61 (2%)	4	26

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	240	THR
1	H	241	HIS
1	A	128	PRO
1	A	190	SER
1	A	215	GLN
1	B	-6	PRO
1	B	128	PRO
1	B	215	GLN
1	C	128	PRO
1	C	215	GLN
1	D	128	PRO
1	D	215	GLN
1	E	128	PRO
1	E	215	GLN
1	F	128	PRO
1	F	215	GLN
1	G	128	PRO
1	G	215	GLN
1	H	128	PRO
1	I	128	PRO
1	I	215	GLN
1	J	215	GLN
1	B	-5	ARG
1	F	231	ARG
1	H	215	GLN
1	J	128	PRO
1	A	118	GLU
1	A	240	THR
1	B	118	GLU
1	B	190	SER
1	B	240	THR
1	C	118	GLU
1	C	190	SER
1	D	118	GLU
1	D	190	SER
1	E	118	GLU
1	E	190	SER
1	F	118	GLU
1	G	118	GLU
1	H	190	SER
1	I	118	GLU
1	I	190	SER
1	J	118	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	190	SER
1	C	133	SER
1	D	70	HIS
1	D	133	SER
1	F	70	HIS
1	F	133	SER
1	F	190	SER
1	G	133	SER
1	G	190	SER
1	H	70	HIS
1	H	133	SER
1	H	230	VAL
1	H	231	ARG
1	A	133	SER
1	B	70	HIS
1	B	133	SER
1	E	70	HIS
1	E	133	SER

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	234/299 (78%)	212 (91%)	22 (9%)	8	30
1	B	236/299 (79%)	215 (91%)	21 (9%)	9	32
1	C	232/299 (78%)	212 (91%)	20 (9%)	10	33
1	D	231/299 (77%)	209 (90%)	22 (10%)	8	30
1	E	232/299 (78%)	210 (90%)	22 (10%)	8	30
1	F	231/299 (77%)	210 (91%)	21 (9%)	9	31
1	G	232/299 (78%)	210 (90%)	22 (10%)	8	30
1	H	230/299 (77%)	206 (90%)	24 (10%)	7	26
1	I	233/299 (78%)	212 (91%)	21 (9%)	9	32
1	J	222/299 (74%)	202 (91%)	20 (9%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2313/2990 (77%)	2098 (91%)	215 (9%)	8 31

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	10	THR
1	A	21	LEU
1	A	68	SER
1	A	89	TRP
1	A	93	GLN
1	A	105	LEU
1	A	107	LEU
1	A	119	LEU
1	A	138	TYR
1	A	139	GLN
1	A	149	LEU
1	A	154	GLU
1	A	155	GLN
1	A	171	ASN
1	A	189	SER
1	A	194	TYR
1	A	203	PHE
1	A	216	THR
1	A	236	ASP
1	A	245	LEU
1	A	265	LEU
1	B	-1	MET
1	B	10	THR
1	B	21	LEU
1	B	68	SER
1	B	89	TRP
1	B	93	GLN
1	B	105	LEU
1	B	107	LEU
1	B	119	LEU
1	B	138	TYR
1	B	139	GLN
1	B	149	LEU
1	B	154	GLU
1	B	155	GLN
1	B	171	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	189	SER
1	B	194	TYR
1	B	203	PHE
1	B	216	THR
1	B	240	THR
1	B	245	LEU
1	C	-1	MET
1	C	10	THR
1	C	21	LEU
1	C	89	TRP
1	C	93	GLN
1	C	105	LEU
1	C	107	LEU
1	C	119	LEU
1	C	138	TYR
1	C	139	GLN
1	C	149	LEU
1	C	154	GLU
1	C	155	GLN
1	C	171	ASN
1	C	194	TYR
1	C	203	PHE
1	C	216	THR
1	C	239	MET
1	C	245	LEU
1	C	265	LEU
1	D	-1	MET
1	D	10	THR
1	D	21	LEU
1	D	68	SER
1	D	93	GLN
1	D	105	LEU
1	D	107	LEU
1	D	119	LEU
1	D	138	TYR
1	D	139	GLN
1	D	149	LEU
1	D	154	GLU
1	D	155	GLN
1	D	171	ASN
1	D	194	TYR
1	D	203	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	216	THR
1	D	233	GLU
1	D	238	THR
1	D	245	LEU
1	D	265	LEU
1	D	266	VAL
1	E	-2	HIS
1	E	10	THR
1	E	21	LEU
1	E	68	SER
1	E	89	TRP
1	E	93	GLN
1	E	105	LEU
1	E	107	LEU
1	E	119	LEU
1	E	138	TYR
1	E	139	GLN
1	E	149	LEU
1	E	154	GLU
1	E	155	GLN
1	E	171	ASN
1	E	194	TYR
1	E	203	PHE
1	E	216	THR
1	E	233	GLU
1	E	245	LEU
1	E	265	LEU
1	E	266	VAL
1	F	-1	MET
1	F	10	THR
1	F	21	LEU
1	F	68	SER
1	F	93	GLN
1	F	105	LEU
1	F	107	LEU
1	F	119	LEU
1	F	138	TYR
1	F	139	GLN
1	F	149	LEU
1	F	154	GLU
1	F	155	GLN
1	F	171	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	194	TYR
1	F	203	PHE
1	F	216	THR
1	F	233	GLU
1	F	245	LEU
1	F	265	LEU
1	F	266	VAL
1	G	-1	MET
1	G	10	THR
1	G	21	LEU
1	G	68	SER
1	G	89	TRP
1	G	93	GLN
1	G	105	LEU
1	G	107	LEU
1	G	119	LEU
1	G	138	TYR
1	G	139	GLN
1	G	149	LEU
1	G	154	GLU
1	G	155	GLN
1	G	171	ASN
1	G	194	TYR
1	G	203	PHE
1	G	216	THR
1	G	239	MET
1	G	241	HIS
1	G	245	LEU
1	G	265	LEU
1	H	-1	MET
1	H	10	THR
1	H	21	LEU
1	H	68	SER
1	H	93	GLN
1	H	105	LEU
1	H	107	LEU
1	H	119	LEU
1	H	138	TYR
1	H	139	GLN
1	H	143	GLU
1	H	149	LEU
1	H	154	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	155	GLN
1	H	171	ASN
1	H	194	TYR
1	H	197	LEU
1	H	203	PHE
1	H	216	THR
1	H	233	GLU
1	H	241	HIS
1	H	242	PRO
1	H	243	GLN
1	H	245	LEU
1	I	-5	ARG
1	I	-3	SER
1	I	-2	HIS
1	I	10	THR
1	I	21	LEU
1	I	51	GLU
1	I	93	GLN
1	I	105	LEU
1	I	107	LEU
1	I	119	LEU
1	I	138	TYR
1	I	139	GLN
1	I	149	LEU
1	I	154	GLU
1	I	155	GLN
1	I	171	ASN
1	I	194	TYR
1	I	203	PHE
1	I	216	THR
1	I	245	LEU
1	I	265	LEU
1	J	2	ASP
1	J	10	THR
1	J	21	LEU
1	J	68	SER
1	J	89	TRP
1	J	93	GLN
1	J	105	LEU
1	J	107	LEU
1	J	119	LEU
1	J	138	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	139	GLN
1	J	149	LEU
1	J	154	GLU
1	J	155	GLN
1	J	171	ASN
1	J	194	TYR
1	J	197	LEU
1	J	203	PHE
1	J	216	THR
1	J	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	93	GLN
1	A	109	ASN
1	A	139	GLN
1	A	147	GLN
1	A	155	GLN
1	A	163	GLN
1	A	171	ASN
1	A	181	HIS
1	A	187	ASN
1	A	261	GLN
1	A	262	GLN
1	B	-2	HIS
1	B	27	GLN
1	B	93	GLN
1	B	109	ASN
1	B	139	GLN
1	B	155	GLN
1	B	163	GLN
1	B	171	ASN
1	B	181	HIS
1	B	187	ASN
1	B	261	GLN
1	C	27	GLN
1	C	41	GLN
1	C	93	GLN
1	C	109	ASN
1	C	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	147	GLN
1	C	155	GLN
1	C	163	GLN
1	C	171	ASN
1	C	181	HIS
1	C	261	GLN
1	D	27	GLN
1	D	93	GLN
1	D	109	ASN
1	D	139	GLN
1	D	147	GLN
1	D	155	GLN
1	D	163	GLN
1	D	171	ASN
1	D	181	HIS
1	D	261	GLN
1	E	27	GLN
1	E	93	GLN
1	E	109	ASN
1	E	139	GLN
1	E	146	ASN
1	E	147	GLN
1	E	155	GLN
1	E	163	GLN
1	E	171	ASN
1	E	181	HIS
1	E	241	HIS
1	E	261	GLN
1	F	27	GLN
1	F	93	GLN
1	F	109	ASN
1	F	139	GLN
1	F	146	ASN
1	F	147	GLN
1	F	155	GLN
1	F	163	GLN
1	F	171	ASN
1	F	181	HIS
1	F	187	ASN
1	G	27	GLN
1	G	93	GLN
1	G	109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	139	GLN
1	G	147	GLN
1	G	155	GLN
1	G	163	GLN
1	G	171	ASN
1	G	181	HIS
1	G	261	GLN
1	H	27	GLN
1	H	93	GLN
1	H	109	ASN
1	H	139	GLN
1	H	146	ASN
1	H	147	GLN
1	H	155	GLN
1	H	163	GLN
1	H	171	ASN
1	H	181	HIS
1	I	-2	HIS
1	I	27	GLN
1	I	93	GLN
1	I	109	ASN
1	I	139	GLN
1	I	147	GLN
1	I	155	GLN
1	I	163	GLN
1	I	171	ASN
1	I	181	HIS
1	I	261	GLN
1	J	27	GLN
1	J	93	GLN
1	J	109	ASN
1	J	139	GLN
1	J	147	GLN
1	J	155	GLN
1	J	163	GLN
1	J	171	ASN
1	J	181	HIS

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	238:THR	C	241:HIS	N	5.99

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	264/339 (77%)	0.44	20 (7%)	20 15	12, 58, 138, 194	0
1	B	267/339 (78%)	0.51	23 (8%)	16 13	16, 49, 129, 200	0
1	C	262/339 (77%)	0.49	18 (6%)	23 17	18, 49, 119, 189	0
1	D	261/339 (76%)	0.58	14 (5%)	31 21	25, 61, 143, 200	0
1	E	262/339 (77%)	0.35	13 (4%)	34 22	23, 56, 122, 200	0
1	F	261/339 (76%)	0.70	23 (8%)	15 12	27, 73, 151, 189	0
1	G	262/339 (77%)	0.50	19 (7%)	21 16	21, 56, 130, 199	0
1	H	260/339 (76%)	0.62	27 (10%)	11 10	30, 75, 154, 200	0
1	I	264/339 (77%)	0.61	21 (7%)	18 14	19, 59, 134, 187	0
1	J	251/339 (74%)	1.14	45 (17%)	3 4	48, 99, 160, 200	0
All	All	2614/3390 (77%)	0.59	223 (8%)	16 13	12, 63, 145, 200	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	207	ALA	6.7
1	G	240	THR	6.0
1	F	241	HIS	5.6
1	I	-1	MET	5.6
1	B	-7	VAL	5.4
1	H	139	GLN	5.4
1	I	241	HIS	5.3
1	J	218	PRO	5.2
1	D	238	THR	5.2
1	F	63	LEU	4.9
1	H	260	LEU	4.9
1	C	193	ILE	4.9
1	I	266	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	193	ILE	4.7
1	B	204	GLY	4.3
1	J	142	VAL	4.3
1	F	266	VAL	4.3
1	E	172	SER	4.2
1	H	261	GLN	4.2
1	G	193	ILE	4.2
1	D	193	ILE	4.1
1	C	196	TYR	4.1
1	H	193	ILE	4.1
1	J	65	SER	4.0
1	A	195	SER	4.0
1	B	265	LEU	4.0
1	G	71	LEU	3.9
1	H	242	PRO	3.9
1	B	266	VAL	3.9
1	H	53	VAL	3.8
1	I	2	ASP	3.8
1	D	266	VAL	3.7
1	B	220	ASN	3.7
1	G	154	GLU	3.6
1	C	238	THR	3.6
1	C	75	LYS	3.6
1	A	142	VAL	3.6
1	J	105	LEU	3.6
1	A	187	ASN	3.5
1	I	194	TYR	3.5
1	J	184	PHE	3.5
1	D	-1	MET	3.5
1	B	11	ASN	3.5
1	J	38	THR	3.5
1	J	210	VAL	3.4
1	I	-4	GLY	3.4
1	B	-3	SER	3.4
1	C	192	SER	3.4
1	G	178	ILE	3.4
1	H	243	GLN	3.4
1	H	230	VAL	3.4
1	H	1	THR	3.4
1	J	15	ALA	3.4
1	J	244	PHE	3.3
1	B	232	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	172	SER	3.3
1	B	-5	ARG	3.2
1	C	228	LYS	3.2
1	J	191	ILE	3.2
1	J	257	VAL	3.2
1	A	241	HIS	3.2
1	G	64	ASP	3.1
1	D	49	ALA	3.1
1	F	86	LEU	3.1
1	E	74	MET	3.1
1	D	241	HIS	3.1
1	C	71	LEU	3.1
1	E	195	SER	3.1
1	I	192	SER	3.1
1	B	93	GLN	3.0
1	J	57	VAL	3.0
1	H	18	ALA	3.0
1	E	240	THR	3.0
1	G	11	ASN	3.0
1	I	230	VAL	3.0
1	D	263	PHE	3.0
1	I	-3	SER	3.0
1	A	239	MET	3.0
1	E	-2	HIS	3.0
1	A	154	GLU	2.9
1	A	150	HIS	2.9
1	J	73	LEU	2.9
1	J	96	LYS	2.9
1	E	241	HIS	2.9
1	A	193	ILE	2.9
1	J	74	MET	2.9
1	E	232	SER	2.9
1	J	34	LEU	2.9
1	G	241	HIS	2.9
1	C	194	TYR	2.9
1	J	196	TYR	2.9
1	B	261	GLN	2.8
1	H	44	ASP	2.8
1	I	128	PRO	2.8
1	J	169	PHE	2.8
1	C	155	GLN	2.8
1	G	13	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	221	TYR	2.8
1	J	70	HIS	2.8
1	A	216	THR	2.8
1	C	143	GLU	2.8
1	J	193	ILE	2.8
1	A	194	TYR	2.8
1	F	218	PRO	2.8
1	F	265	LEU	2.8
1	F	92	THR	2.8
1	F	193	ILE	2.7
1	A	74	MET	2.7
1	J	190	SER	2.7
1	J	87	HIS	2.7
1	D	253	THR	2.7
1	B	31	SER	2.7
1	F	167	ASN	2.7
1	H	195	SER	2.7
1	J	107	LEU	2.7
1	B	187	ASN	2.7
1	B	-6	PRO	2.6
1	D	143	GLU	2.6
1	C	197	LEU	2.6
1	I	255	SER	2.6
1	F	221	TYR	2.6
1	H	48	LYS	2.6
1	F	192	SER	2.5
1	J	41	GLN	2.5
1	A	2	ASP	2.5
1	B	65	SER	2.5
1	E	225	THR	2.5
1	H	92	THR	2.5
1	H	116	ARG	2.5
1	H	264	GLY	2.5
1	A	90	SER	2.5
1	B	139	GLN	2.5
1	J	137	VAL	2.5
1	B	2	ASP	2.5
1	G	1	THR	2.5
1	H	240	THR	2.5
1	H	221	TYR	2.5
1	G	266	VAL	2.5
1	C	-1	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	231	ARG	2.5
1	B	239	MET	2.4
1	J	22	GLY	2.4
1	A	232	SER	2.4
1	C	232	SER	2.4
1	I	-5	ARG	2.4
1	C	240	THR	2.4
1	C	266	VAL	2.4
1	D	196	TYR	2.4
1	A	-1	MET	2.4
1	J	249	TRP	2.4
1	A	146	ASN	2.4
1	J	36	VAL	2.4
1	G	14	TYR	2.4
1	H	118	GLU	2.4
1	J	71	LEU	2.4
1	H	81	VAL	2.4
1	I	61	ASP	2.4
1	G	221	TYR	2.3
1	C	239	MET	2.3
1	F	216	THR	2.3
1	F	240	THR	2.3
1	J	18	ALA	2.3
1	J	241	HIS	2.3
1	J	111	ASP	2.3
1	I	126	GLY	2.3
1	F	82	THR	2.3
1	F	181	HIS	2.3
1	J	150	HIS	2.3
1	C	142	VAL	2.3
1	E	266	VAL	2.3
1	J	160	GLY	2.3
1	I	213	LEU	2.3
1	J	139	GLN	2.3
1	F	230	VAL	2.3
1	F	62	ILE	2.3
1	B	-1	MET	2.3
1	J	188	LEU	2.2
1	I	127	TRP	2.2
1	I	244	PHE	2.2
1	H	117	GLU	2.2
1	D	160	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	5	PHE	2.2
1	J	228	LYS	2.2
1	B	24	SER	2.2
1	I	31	SER	2.2
1	I	142	VAL	2.2
1	F	226	LYS	2.2
1	D	118	GLU	2.2
1	J	37	LEU	2.2
1	G	192	SER	2.2
1	J	43	SER	2.2
1	H	245	LEU	2.2
1	J	187	ASN	2.2
1	E	264	GLY	2.2
1	D	55	ASP	2.2
1	E	87	HIS	2.2
1	G	91	LEU	2.1
1	A	149	LEU	2.1
1	J	143	GLU	2.1
1	A	253	THR	2.1
1	B	7	THR	2.1
1	F	260	LEU	2.1
1	H	263	PHE	2.1
1	H	249	TRP	2.1
1	G	191	ILE	2.1
1	J	91	LEU	2.1
1	I	223	TYR	2.1
1	C	27	GLN	2.1
1	E	193	ILE	2.1
1	H	62	ILE	2.1
1	G	124	ASP	2.1
1	B	41	GLN	2.1
1	J	178	ILE	2.0
1	H	219	TRP	2.0
1	F	223	TYR	2.0
1	J	51	GLU	2.0
1	G	62	ILE	2.0
1	J	222	THR	2.0
1	A	201	LYS	2.0
1	D	93	GLN	2.0
1	A	266	VAL	2.0
1	G	143	GLU	2.0
1	F	71	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.