



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:03 PM GMT

PDB ID : 1RVF
Title : FAB COMPLEXED WITH INTACT HUMAN RHINOVIRUS
Authors : Smith, T.J.
Deposited on : 1996-09-05
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

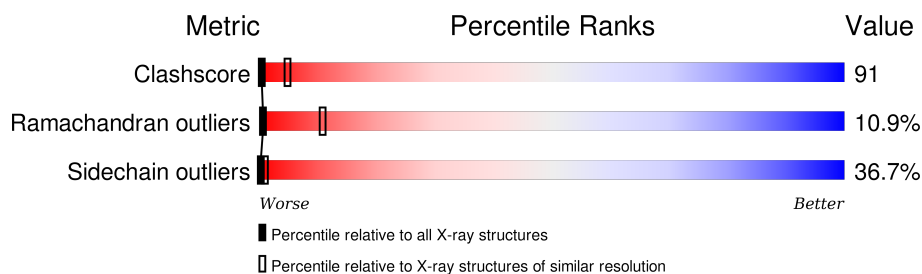
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	
2	2	262	
3	3	236	
4	4	68	
5	L	110	
6	H	119	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8019 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 HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	CONFLICT	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	110	Total	C	N	O	S	0	0	0
			834	524	139	166	5			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	14	PHE	SER	CONFLICT	UNP X79906
L	15	PRO	LEU	CONFLICT	UNP X79906
L	18	LYS	ARG	CONFLICT	UNP X79906
L	21	ILE	MET	CONFLICT	UNP X79906
L	24	SER	THR	CONFLICT	UNP X79906
L	26	THR	SER	CONFLICT	UNP X79906
L	?	-	SER	DELETION	UNP X79906
L	?	-	SER	DELETION	UNP X79906
L	31	ASN	SER	CONFLICT	UNP X79906
L	33	MET	LEU	CONFLICT	UNP X79906
L	36	PHE	TYR	CONFLICT	UNP X79906
L	42	THR	SER	CONFLICT	UNP X79906
L	51	SER	THR	CONFLICT	UNP X79906
L	77	ARG	SER	CONFLICT	UNP X79906
L	89	GLN	HIS	CONFLICT	UNP X79906
L	91	ARG	TYR	CONFLICT	UNP X79906
L	92	SER	HIS	CONFLICT	UNP X79906
L	93	SER	ARG	CONFLICT	UNP X79906
L	94	TYR	PHE	CONFLICT	UNP X79906
L	96	ILE	HIS	CONFLICT	UNP X79906
L	100	SER	GLY	CONFLICT	UNP X79906

- Molecule 6 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	119	Total	C	N	O	S	0	0	0
			917	579	153	181	4			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	2	GLY	ILE	CONFLICT	UNP S38950
H	9	ALA	PRO	CONFLICT	UNP S38950
H	16	SER	ALA	CONFLICT	UNP S38950
H	28	ALA	THR	CONFLICT	UNP S38950
H	30	SER	THR	CONFLICT	UNP S38950
H	31	SER	ASP	CONFLICT	UNP S38950
H	32	PHE	TYR	CONFLICT	UNP S38950
H	33	TRP	TYR	CONFLICT	UNP S38950
H	34	VAL	ILE	CONFLICT	UNP S38950
H	35	ASN	HIS	CONFLICT	UNP S38950

Continued on next page...

Continued from previous page...

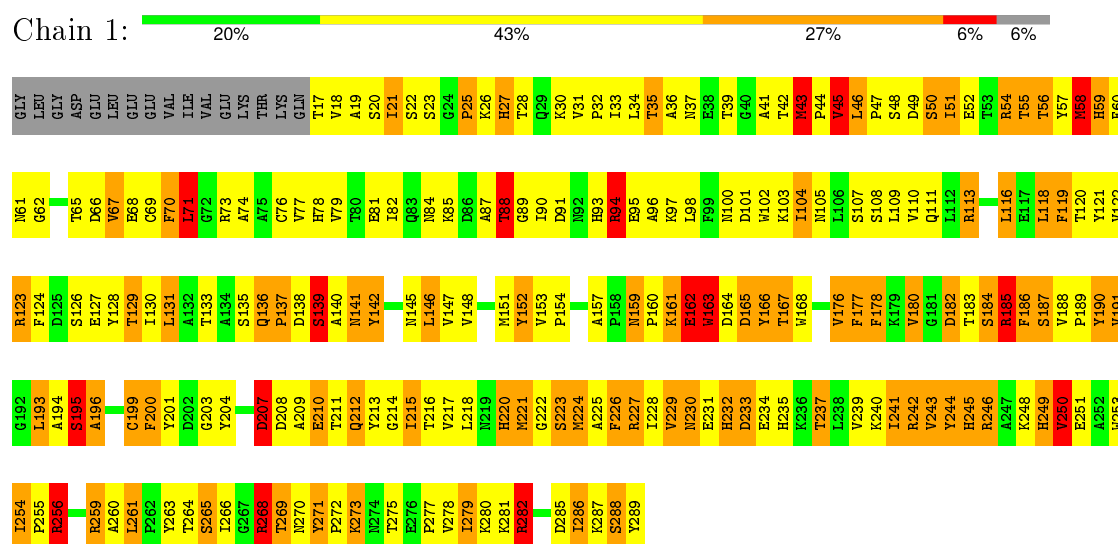
Chain	Residue	Modelled	Actual	Comment	Reference
H	43	GLN	GLU	CONFLICT	UNP S38950
H	50	GLN	TRP	CONFLICT	UNP S38950
H	54	ASP	SER	CONFLICT	UNP S38950
H	56	ASP	ASN	CONFLICT	UNP S38950
H	57	ASN	THR	CONFLICT	UNP S38950
H	61	GLY	GLU	CONFLICT	UNP S38950
H	71	ALA	VAL	CONFLICT	UNP S38950
H	73	LYS	THR	CONFLICT	UNP S38950
H	76	THR	SER	CONFLICT	UNP S38950
H	82A	TYR	SER	CONFLICT	UNP S38950
H	95	SER	GLY	CONFLICT	UNP S38950
H	97	ASN	-	INSERTION	UNP S38950
H	98	TYR	-	INSERTION	UNP S38950
H	99	PRO	LYS	CONFLICT	UNP S38950
H	100I	TYR	PHE	CONFLICT	UNP S38950

3 Residue-property plots

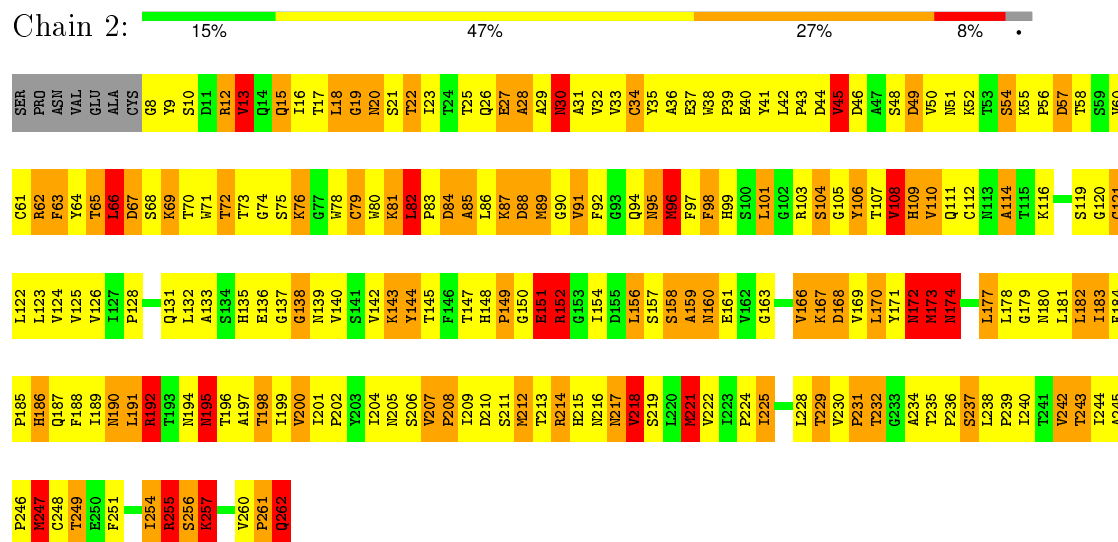
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

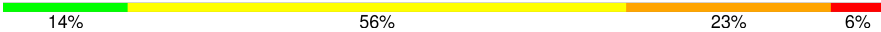
- Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN

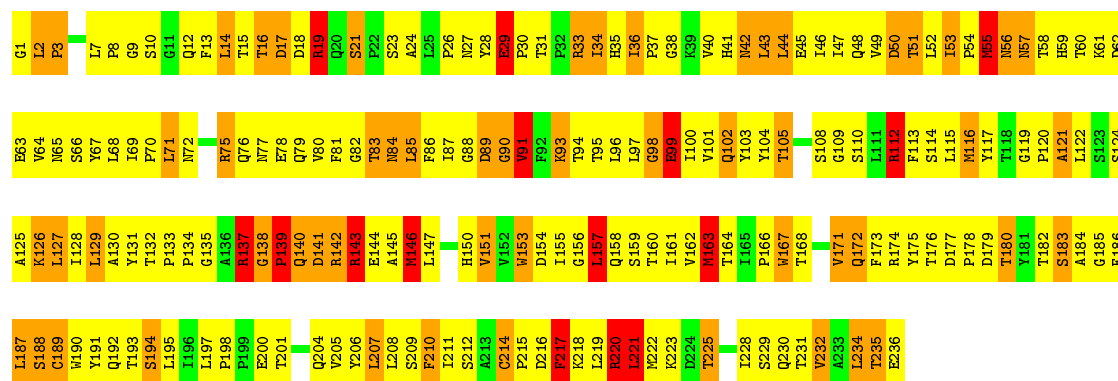


- Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN



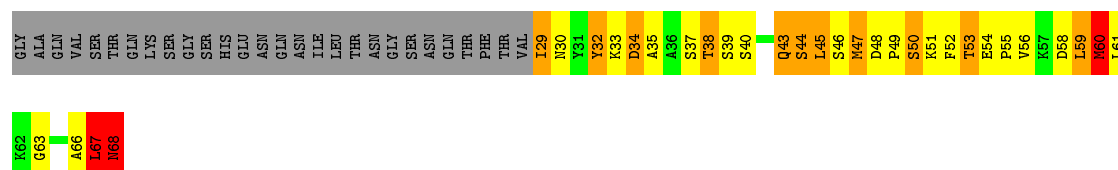
- Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN

Chain 3: 



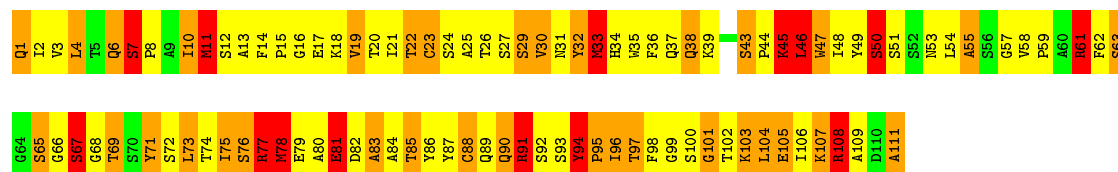
• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN

Chain 4: 




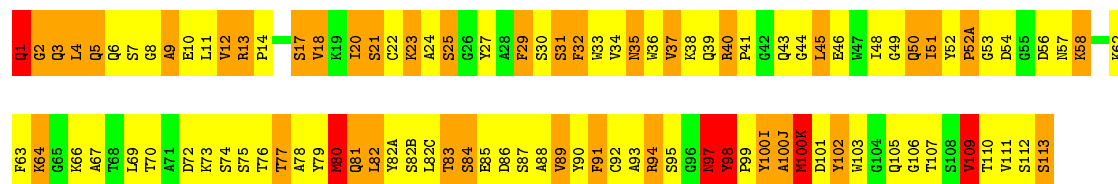
• Molecule 5: FAB 17-IA

Chain L: 



• Molecule 6: FAB 17-IA

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	372.00 Å 372.00 Å 372.00 Å 108.40° 108.40° 108.40°	Depositor
Resolution (Å)	10.00 – 4.00	Depositor
% Data completeness (in resolution range)	64.5 (10.00-4.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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	1	1.03	1/2228 (0.0%)	1.51	32/3031 (1.1%)
2	2	1.04	2/2001 (0.1%)	1.42	20/2735 (0.7%)
3	3	1.09	4/1898 (0.2%)	1.46	22/2597 (0.8%)
4	4	1.12	2/302 (0.7%)	1.70	6/406 (1.5%)
5	L	1.09	3/854 (0.4%)	1.61	16/1157 (1.4%)
6	H	1.15	3/941 (0.3%)	1.58	16/1272 (1.3%)
All	All	1.07	15/8224 (0.2%)	1.50	112/11198 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	H	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	111	ALA	CA-C	9.21	1.76	1.52
6	H	113	SER	C-OXT	7.97	1.38	1.23
2	2	8	GLY	N-CA	7.97	1.58	1.46
4	4	29	ILE	N-CA	7.16	1.60	1.46
5	L	111	ALA	C-OXT	6.86	1.36	1.23
4	4	68	ASN	C-OXT	6.47	1.35	1.23
5	L	111	ALA	C-O	6.47	1.35	1.23
1	1	128	TYR	CB-CG	6.39	1.61	1.51
6	H	113	SER	CA-C	6.18	1.69	1.52
3	3	1	GLY	N-CA	5.84	1.54	1.46
6	H	113	SER	C-O	5.75	1.34	1.23
2	2	262	GLN	C-OXT	5.35	1.33	1.23
3	3	99	GLU	CD-OE2	5.28	1.31	1.25
3	3	135	GLY	N-CA	5.12	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	139	PRO	CA-C	-5.03	1.42	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	261	PRO	O-C-N	9.93	138.59	122.70
1	1	128	TYR	CB-CG-CD1	9.88	126.92	121.00
4	4	67	LEU	O-C-N	9.24	137.49	122.70
5	L	108	ARG	NE-CZ-NH2	8.57	124.59	120.30
6	H	97	ASN	O-C-N	8.50	136.29	122.70
1	1	185	ARG	NE-CZ-NH2	8.36	124.48	120.30
3	3	137	ARG	NE-CZ-NH2	8.17	124.39	120.30
2	2	214	ARG	NE-CZ-NH2	7.98	124.29	120.30
3	3	33	ARG	NE-CZ-NH2	7.87	124.24	120.30
2	2	192	ARG	NE-CZ-NH2	7.76	124.18	120.30
3	3	225	THR	O-C-N	7.71	135.04	122.70
1	1	268	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	1	227	ARG	NE-CZ-NH2	7.60	124.10	120.30
5	L	94	TYR	O-C-N	-7.58	106.69	121.10
5	L	32	TYR	O-C-N	7.57	134.81	122.70
2	2	62	ARG	NE-CZ-NH2	7.56	124.08	120.30
3	3	112	ARG	NE-CZ-NH2	7.56	124.08	120.30
6	H	13	ARG	NE-CZ-NH2	7.51	124.05	120.30
6	H	1	GLN	O-C-N	7.51	135.96	123.20
1	1	282	ARG	NE-CZ-NH2	7.50	124.05	120.30
3	3	220	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	1	242	ARG	NE-CZ-NH2	7.43	124.02	120.30
5	L	61	ARG	NE-CZ-NH2	7.42	124.01	120.30
3	3	75	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	1	54	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	1	246	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	2	12	ARG	NE-CZ-NH2	7.30	123.95	120.30
6	H	40	ARG	NE-CZ-NH2	7.29	123.94	120.30
5	L	91	ARG	NE-CZ-NH2	7.28	123.94	120.30
6	H	94	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	1	113	ARG	NE-CZ-NH2	7.26	123.93	120.30
2	2	152	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	1	94	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	2	255	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	1	259	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	1	123	ARG	NE-CZ-NH2	7.08	123.84	120.30
2	2	103	ARG	NE-CZ-NH2	7.04	123.82	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	256	ARG	NE-CZ-NH2	7.00	123.80	120.30
3	3	174	ARG	NE-CZ-NH2	6.97	123.78	120.30
4	4	67	LEU	CA-C-N	-6.94	101.92	117.20
5	L	77	ARG	NE-CZ-NH2	6.78	123.69	120.30
6	H	1	GLN	CA-C-N	-6.49	103.22	116.20
2	2	261	PRO	CA-C-N	-6.48	102.95	117.20
1	1	73	ARG	NE-CZ-NH2	6.47	123.54	120.30
6	H	97	ASN	CA-C-N	-6.45	103.02	117.20
1	1	223	SER	O-C-N	6.44	133.01	122.70
2	2	247	MET	CG-SD-CE	6.44	110.50	100.20
1	1	43	MET	CG-SD-CE	6.42	110.47	100.20
3	3	235	THR	O-C-N	6.33	132.82	122.70
1	1	58	MET	CG-SD-CE	6.30	110.29	100.20
3	3	143	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	1	151	MET	CG-SD-CE	6.28	110.25	100.20
1	1	221	MET	CG-SD-CE	6.25	110.20	100.20
2	2	212	MET	CG-SD-CE	6.23	110.16	100.20
3	3	19	ARG	NE-CZ-NH2	6.22	123.41	120.30
5	L	11	MET	CG-SD-CE	6.22	110.14	100.20
2	2	96	MET	CG-SD-CE	6.21	110.14	100.20
3	3	163	MET	CG-SD-CE	6.18	110.08	100.20
4	4	32	TYR	CB-CG-CD2	-6.17	117.30	121.00
6	H	80	MET	CG-SD-CE	6.14	110.03	100.20
1	1	128	TYR	CA-CB-CG	6.13	125.06	113.40
4	4	32	TYR	O-C-N	6.13	132.52	122.70
5	L	78	MET	CG-SD-CE	6.12	110.00	100.20
1	1	224	MET	CG-SD-CE	6.11	109.98	100.20
3	3	55	MET	CG-SD-CE	6.09	109.95	100.20
6	H	100(K)	MET	CG-SD-CE	6.09	109.94	100.20
5	L	94	TYR	CB-CG-CD1	-6.07	117.36	121.00
2	2	89	MET	CG-SD-CE	6.07	109.91	100.20
5	L	33	MET	CG-SD-CE	6.04	109.87	100.20
2	2	67	ASP	O-C-N	6.03	132.34	122.70
2	2	221	MET	CG-SD-CE	6.00	109.80	100.20
4	4	47	MET	CG-SD-CE	6.00	109.80	100.20
1	1	162	GLU	O-C-N	6.00	132.30	122.70
2	2	173	MET	CG-SD-CE	5.99	109.79	100.20
6	H	109	VAL	O-C-N	5.99	132.28	122.70
1	1	277	PRO	O-C-N	5.97	132.25	122.70
5	L	45	LYS	O-C-N	5.96	132.24	122.70
5	L	7	SER	O-C-N	-5.96	109.78	121.10
3	3	222	MET	CG-SD-CE	5.94	109.71	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	72	ASP	O-C-N	5.91	132.15	122.70
4	4	60	MET	CG-SD-CE	5.89	109.62	100.20
3	3	146	MET	CG-SD-CE	5.88	109.61	100.20
6	H	89	VAL	O-C-N	5.84	132.05	122.70
1	1	244	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	1	220	HIS	N-CA-CB	5.81	121.05	110.60
5	L	32	TYR	CA-CB-CG	-5.80	102.39	113.40
5	L	32	TYR	CA-C-N	-5.75	104.55	117.20
3	3	225	THR	CA-C-N	-5.66	104.75	117.20
3	3	116	MET	CG-SD-CE	5.62	109.20	100.20
5	L	32	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	1	220	HIS	O-C-N	5.52	131.53	122.70
1	1	128	TYR	CB-CG-CD2	-5.49	117.71	121.00
6	H	98	TYR	CB-CG-CD1	-5.41	117.76	121.00
2	2	106	TYR	CB-CG-CD1	-5.35	117.79	121.00
6	H	91	PHE	CB-CA-C	-5.35	99.70	110.40
3	3	3	PRO	O-C-N	5.34	131.25	122.70
1	1	176	VAL	CB-CA-C	-5.34	101.25	111.40
3	3	72	ASN	O-C-N	5.34	131.25	122.70
2	2	159	ALA	O-C-N	5.27	131.13	122.70
2	2	82	LEU	O-C-N	-5.24	111.14	121.10
5	L	94	TYR	CA-C-N	5.23	131.75	117.10
6	H	98	TYR	O-C-N	-5.20	111.22	121.10
1	1	250	VAL	O-C-N	5.20	131.02	122.70
1	1	139	SER	O-C-N	5.17	130.98	122.70
3	3	235	THR	CA-C-N	-5.14	105.90	117.20
2	2	168	ASP	O-C-N	5.13	130.90	122.70
3	3	29	GLU	O-C-N	5.12	130.83	121.10
1	1	223	SER	CA-C-N	-5.11	105.95	117.20
6	H	52(A)	PRO	O-C-N	5.11	131.88	123.20
3	3	85	LEU	O-C-N	5.10	130.87	122.70
3	3	139	PRO	N-CA-C	-5.06	98.95	112.10
1	1	271	TYR	O-C-N	5.02	130.63	121.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	H	102	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2107	367	0
2	2	1952	0	1927	317	0
3	3	1849	0	1833	337	0
4	4	297	0	294	40	0
5	L	834	0	814	311	0
6	H	917	0	870	241	0
All	All	8019	0	7845	1439	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 91.

All (1439) 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)
5:L:111:ALA:C	5:L:111:ALA:CA	1.76	1.53
5:L:7:SER:CB	5:L:22:THR:HG23	1.50	1.40
6:H:99:PRO:HG2	6:H:100(I):TYR:CE1	1.59	1.38
5:L:6:GLN:HG3	5:L:101:GLY:N	1.40	1.34
5:L:94:TYR:O	5:L:96:ILE:N	1.62	1.31
4:4:44:SER:O	4:4:45:LEU:HD23	1.40	1.18
4:4:35:ALA:O	4:4:38:THR:HG23	1.44	1.17
6:H:51:ILE:HG22	6:H:69:LEU:HD13	1.17	1.15
3:3:151:VAL:CG2	3:3:163:MET:HG3	1.76	1.15
3:3:19:ARG:HE	3:3:19:ARG:HA	1.14	1.13
1:1:193:LEU:CD1	1:1:193:LEU:H	1.60	1.12
5:L:67:SER:HA	5:L:71:TYR:CZ	1.85	1.11
5:L:19:VAL:HG23	5:L:75:ILE:HB	1.32	1.10
6:H:27:TYR:CE1	6:H:94:ARG:HD2	1.88	1.09
5:L:54:LEU:HD12	5:L:58:VAL:HG23	1.25	1.09
1:1:107:SER:HB2	1:1:266:ILE:HG23	1.11	1.09
1:1:193:LEU:HD12	1:1:193:LEU:N	1.64	1.09
3:3:214:CYS:SG	3:3:215:PRO:HD2	1.92	1.08
5:L:94:TYR:CE2	6:H:58:LYS:HD3	1.88	1.08
5:L:6:GLN:CG	5:L:101:GLY:H	1.66	1.08
5:L:12:SER:HA	5:L:105:GLU:HB3	1.12	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:33:MET:HG2	5:L:71:TYR:CG	1.90	1.07
1:1:21:ILE:H	1:1:21:ILE:CD1	1.67	1.07
5:L:18:LYS:HD2	5:L:76:SER:HA	1.37	1.06
3:3:151:VAL:HG21	3:3:163:MET:HG3	1.09	1.06
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.32	1.06
5:L:54:LEU:CD1	5:L:58:VAL:HG23	1.85	1.06
1:1:45:VAL:CG2	3:3:162:VAL:HG11	1.85	1.06
6:H:52:TYR:HD1	6:H:52(A):PRO:HD2	1.19	1.06
1:1:70:PHE:CD2	1:1:70:PHE:O	2.07	1.06
2:2:30:ASN:ND2	4:4:58:ASP:HB2	1.68	1.05
2:2:23:ILE:HD12	2:2:63:PHE:CE2	1.90	1.05
3:3:151:VAL:HG21	3:3:163:MET:CG	1.86	1.05
5:L:78:MET:SD	5:L:79:GLU:O	2.15	1.05
5:L:91:ARG:HH11	5:L:91:ARG:HG2	1.14	1.05
1:1:45:VAL:HG21	3:3:162:VAL:CG1	1.87	1.04
2:2:63:PHE:CD1	2:2:245:ALA:HB2	1.92	1.04
6:H:99:PRO:CG	6:H:100(I):TYR:CE1	2.41	1.03
3:3:179:ASP:HB3	3:3:182:THR:CG2	1.88	1.03
5:L:44:PRO:CG	6:H:45:LEU:HD11	1.87	1.03
6:H:69:LEU:HD23	6:H:80:MET:HB2	1.39	1.02
5:L:21:ILE:HD12	5:L:73:LEU:HD22	1.40	1.02
5:L:104:LEU:HD12	5:L:105:GLU:N	1.75	1.02
5:L:7:SER:HB2	5:L:22:THR:HG23	1.36	1.01
5:L:104:LEU:HD12	5:L:105:GLU:H	1.24	1.01
6:H:40:ARG:HB2	6:H:43:GLN:HG3	1.43	1.01
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.43	1.01
3:3:19:ARG:NE	3:3:19:ARG:HA	1.68	1.01
3:3:218:LYS:O	3:3:219:LEU:HD12	1.61	1.00
5:L:18:LYS:CD	5:L:76:SER:HA	1.91	0.99
1:1:68:GLU:O	1:1:68:GLU:HG3	1.60	0.99
1:1:190:TYR:OH	1:1:194:ALA:O	1.79	0.99
5:L:6:GLN:HG3	5:L:101:GLY:H	0.82	0.98
5:L:12:SER:CA	5:L:105:GLU:HB3	1.92	0.98
2:2:123:LEU:HG	2:2:123:LEU:O	1.61	0.98
5:L:7:SER:CB	5:L:22:THR:CG2	2.40	0.98
1:1:21:ILE:HD13	1:1:21:ILE:N	1.78	0.98
4:4:32:TYR:HB2	4:4:37:SER:HB3	1.43	0.98
5:L:43:SER:O	5:L:45:LYS:HD3	1.62	0.98
5:L:11:MET:HE1	5:L:104:LEU:HA	1.46	0.97
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.43	0.97
3:3:126:LYS:O	3:3:192:GLN:HB3	1.63	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21:ILE:H	1:1:21:ILE:HD13	1.26	0.96
6:H:99:PRO:HG2	6:H:100(I):TYR:HE1	1.23	0.96
5:L:62:PHE:CD1	5:L:75:ILE:HG12	2.01	0.96
3:3:68:LEU:O	3:3:70:PRO:HD3	1.65	0.95
3:3:2:LEU:HG	3:3:2:LEU:O	1.67	0.95
3:3:214:CYS:SG	3:3:215:PRO:CD	2.54	0.95
1:1:193:LEU:HD12	1:1:193:LEU:H	0.79	0.94
2:2:27:GLU:O	2:2:28:ALA:O	1.85	0.94
6:H:37:VAL:HB	6:H:46:GLU:O	1.68	0.94
4:4:35:ALA:O	4:4:38:THR:CG2	2.15	0.94
1:1:107:SER:HB2	1:1:266:ILE:CG2	1.97	0.94
3:3:85:LEU:O	3:3:184:ALA:HB3	1.66	0.94
5:L:30:VAL:CG2	5:L:90:GLN:HG3	1.98	0.94
5:L:46:LEU:HD23	6:H:101:ASP:HA	1.49	0.94
2:2:104:SER:OG	2:2:249:THR:HG23	1.67	0.93
2:2:83:PRO:HG2	2:2:216:ASN:HA	1.50	0.93
5:L:7:SER:N	5:L:22:THR:O	2.00	0.93
5:L:33:MET:HG2	5:L:71:TYR:CB	1.98	0.93
3:3:126:LYS:HE2	3:3:154:ASP:HB2	1.50	0.93
3:3:153:TRP:CE3	3:3:161:ILE:HG21	2.03	0.93
1:1:248:LYS:O	1:1:249:HIS:HB2	1.68	0.93
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.49	0.93
5:L:7:SER:OG	5:L:22:THR:OG1	1.87	0.92
6:H:105:GLN:HG2	6:H:106:GLY:N	1.81	0.92
2:2:98:PHE:CE1	2:2:257:LYS:HB2	2.05	0.92
5:L:44:PRO:HG3	6:H:45:LEU:HD11	1.50	0.92
5:L:10:ILE:HG13	5:L:103:LYS:O	1.68	0.92
5:L:14:PHE:CA	5:L:107:LYS:HB2	1.98	0.92
6:H:35:ASN:HD21	6:H:95:SER:HB2	1.35	0.91
6:H:40:ARG:HB2	6:H:43:GLN:CG	2.00	0.91
4:4:44:SER:O	4:4:45:LEU:CD2	2.18	0.91
5:L:2:ILE:HG22	5:L:25:ALA:HB1	1.53	0.91
1:1:124:PHE:O	1:1:190:TYR:HB2	1.71	0.91
2:2:207:VAL:HG12	2:2:208:PRO:HD2	1.53	0.91
1:1:107:SER:CB	1:1:266:ILE:HG23	1.99	0.91
5:L:108:ARG:HG3	5:L:109:ALA:N	1.83	0.91
2:2:29:ALA:HA	4:4:67:LEU:HD23	1.51	0.91
3:3:173:PHE:HE2	3:3:220:ARG:NH1	1.68	0.90
2:2:12:ARG:HA	2:2:27:GLU:O	1.72	0.90
6:H:97:ASN:HD21	6:H:101:ASP:CB	1.85	0.90
6:H:39:GLN:HA	6:H:44:GLY:O	1.70	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:157:LEU:O	3:3:157:LEU:HD23	1.72	0.90
2:2:190:ASN:O	2:2:192:ARG:N	2.04	0.90
6:H:36:TRP:CD1	6:H:69:LEU:HD21	2.07	0.89
5:L:75:ILE:O	5:L:77:ARG:N	2.05	0.89
2:2:183:ILE:CG1	3:3:96:LEU:HD22	2.03	0.89
1:1:46:LEU:HD21	3:3:215:PRO:CG	2.02	0.89
1:1:45:VAL:HG21	3:3:162:VAL:HG11	0.94	0.89
1:1:65:THR:OG1	3:3:42:ASN:ND2	2.04	0.89
1:1:87:ALA:O	1:1:90:ILE:HG12	1.72	0.89
5:L:62:PHE:HA	5:L:74:THR:O	1.71	0.89
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.55	0.89
5:L:7:SER:OG	5:L:22:THR:CG2	2.21	0.88
5:L:7:SER:HB3	5:L:22:THR:HG23	1.55	0.88
3:3:97:LEU:O	3:3:101:VAL:HB	1.72	0.88
5:L:13:ALA:CB	5:L:78:MET:HG2	2.03	0.88
5:L:33:MET:HE2	5:L:88:CYS:HB2	1.56	0.88
2:2:187:GLN:NE2	2:2:198:THR:H	1.71	0.88
5:L:12:SER:HA	5:L:105:GLU:CB	2.03	0.88
3:3:115:LEU:CD2	3:3:129:LEU:HD11	2.04	0.88
2:2:108:VAL:HG12	2:2:244:ILE:HG12	1.55	0.87
5:L:89:GLN:HG3	5:L:98:PHE:CD2	2.09	0.87
1:1:260:ALA:HB1	1:1:278:VAL:HG21	1.55	0.87
1:1:207:ASP:HA	2:2:144:TYR:CE2	2.08	0.87
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.57	0.87
2:2:30:ASN:HD21	4:4:58:ASP:HB2	1.29	0.87
2:2:85:ALA:HA	2:2:150:GLY:HA2	1.55	0.87
1:1:279:ILE:HB	3:3:62:ASP:OD1	1.73	0.87
3:3:173:PHE:CE2	3:3:220:ARG:NH1	2.43	0.86
1:1:160:PRO:HB3	1:1:168:TRP:NE1	1.89	0.86
5:L:91:ARG:NH1	5:L:91:ARG:HG2	1.85	0.86
3:3:173:PHE:HE2	3:3:220:ARG:HH11	1.20	0.86
6:H:52:TYR:CD1	6:H:52(A):PRO:HD2	2.10	0.86
1:1:186:PHE:CD1	3:3:24:ALA:HB2	2.10	0.86
6:H:97:ASN:HD21	6:H:101:ASP:CG	1.79	0.86
3:3:85:LEU:O	3:3:184:ALA:CB	2.23	0.86
4:4:59:LEU:HG	4:4:60:MET:N	1.89	0.86
6:H:2:GLY:HA2	6:H:25:SER:O	1.76	0.85
5:L:15:PRO:HA	5:L:78:MET:O	1.77	0.85
2:2:234:ALA:O	2:2:236:PRO:HD3	1.76	0.85
1:1:70:PHE:CG	3:3:43:LEU:HD11	2.11	0.85
5:L:77:ARG:NE	5:L:79:GLU:OE2	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:18:ASP:OD1	4:4:40:SER:HB3	1.75	0.85
5:L:2:ILE:HD12	5:L:93:SER:HB2	1.59	0.85
5:L:94:TYR:HE2	6:H:58:LYS:HD3	1.38	0.85
1:1:153:VAL:HG13	1:1:157:ALA:HB3	1.57	0.85
5:L:77:ARG:HG2	5:L:77:ARG:HH11	1.42	0.85
5:L:14:PHE:HA	5:L:107:LYS:HB2	1.57	0.84
5:L:7:SER:OG	5:L:22:THR:HG23	1.77	0.84
2:2:84:ASP:OD1	2:2:85:ALA:N	2.10	0.84
1:1:178:PHE:CD2	1:1:184:SER:HB3	2.12	0.84
5:L:30:VAL:O	5:L:71:TYR:OH	1.96	0.84
1:1:289:TYR:OH	3:3:139:PRO:O	1.95	0.84
5:L:67:SER:HA	5:L:71:TYR:CE1	2.13	0.84
1:1:110:VAL:HG22	3:3:230:GLN:OE1	1.76	0.84
5:L:21:ILE:HG12	5:L:102:THR:HG21	1.60	0.84
3:3:146:MET:O	3:3:146:MET:HG2	1.77	0.84
5:L:6:GLN:OE1	5:L:87:TYR:HA	1.77	0.83
3:3:14:LEU:HD12	3:3:15:THR:N	1.92	0.83
6:H:81:GLN:NE2	6:H:82(A):TYR:CE1	2.46	0.83
5:L:29:SER:HA	5:L:68:GLY:O	1.79	0.83
4:4:32:TYR:CB	4:4:37:SER:HB3	2.09	0.83
3:3:18:ASP:O	4:4:39:SER:HB2	1.77	0.83
1:1:282:ARG:HB2	3:3:57:ASN:HB2	1.59	0.83
6:H:12:VAL:CG1	6:H:18:VAL:HG13	2.08	0.83
6:H:23:LYS:HD3	6:H:77:THR:HG22	1.60	0.83
3:3:110:SER:O	3:3:214:CYS:HB2	1.79	0.83
3:3:105:THR:C	3:3:176:THR:HG23	1.98	0.83
2:2:187:GLN:HE21	2:2:198:THR:H	1.24	0.83
1:1:88:THR:CG2	1:1:88:THR:O	2.26	0.83
1:1:70:PHE:CG	1:1:70:PHE:O	2.30	0.82
1:1:201:TYR:H	2:2:131:GLN:HE22	1.28	0.82
3:3:214:CYS:CB	3:3:215:PRO:HD2	2.08	0.82
2:2:71:TRP:CE2	2:2:228:LEU:HB2	2.13	0.82
5:L:54:LEU:HD11	5:L:62:PHE:HB2	1.61	0.82
5:L:4:LEU:HD12	5:L:88:CYS:SG	2.19	0.82
1:1:281:LYS:HG2	1:1:282:ARG:N	1.95	0.82
3:3:14:LEU:HD12	3:3:16:THR:H	1.44	0.81
5:L:48:ILE:HD11	5:L:54:LEU:HD13	1.62	0.81
1:1:166:TYR:CD1	1:1:167:THR:N	2.48	0.81
1:1:178:PHE:HD2	1:1:184:SER:HB3	1.45	0.81
1:1:259:ARG:NH1	2:2:174:ASN:O	2.14	0.81
6:H:18:VAL:HG22	6:H:82(C):LEU:HD11	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:VAL:O	1:1:109:LEU:HD12	1.81	0.81
1:1:253:TRP:NE1	3:3:36:ILE:HG13	1.95	0.81
1:1:77:VAL:C	1:1:109:LEU:HD12	2.01	0.81
2:2:10:SER:O	2:2:13:VAL:HG23	1.80	0.81
2:2:217:ASN:O	2:2:218:VAL:HG12	1.81	0.80
2:2:184:PHE:HB3	2:2:185:PRO:HD2	1.64	0.80
6:H:20:ILE:CG2	6:H:107:THR:HG21	2.11	0.80
2:2:38:TRP:CG	2:2:39:PRO:HD2	2.17	0.80
6:H:37:VAL:HA	6:H:46:GLU:O	1.81	0.80
5:L:30:VAL:CG2	5:L:90:GLN:CG	2.59	0.80
6:H:97:ASN:HD21	6:H:101:ASP:HB3	1.46	0.80
3:3:172:GLN:O	3:3:173:PHE:CD1	2.35	0.79
3:3:141:ASP:HA	3:3:190:TRP:CZ3	2.17	0.79
1:1:30:LYS:HG2	4:4:63:GLY:O	1.81	0.79
3:3:198:PRO:O	3:3:201:THR:HG22	1.81	0.79
5:L:13:ALA:N	5:L:105:GLU:O	2.15	0.79
2:2:255:ARG:O	2:2:257:LYS:N	2.13	0.79
5:L:13:ALA:HB1	5:L:78:MET:HG2	1.63	0.79
1:1:74:ALA:HB3	3:3:15:THR:HB	1.63	0.79
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.63	0.79
1:1:141:ASN:OD1	1:1:141:ASN:N	2.15	0.79
5:L:55:ALA:HB3	5:L:58:VAL:HG11	1.63	0.79
6:H:20:ILE:HG22	6:H:107:THR:HG21	1.63	0.79
5:L:1:GLN:HA	5:L:1:GLN:OE1	1.83	0.79
1:1:148:VAL:HG11	1:1:241:ILE:HD11	1.65	0.79
5:L:43:SER:O	5:L:45:LYS:CD	2.32	0.78
5:L:2:ILE:CG2	5:L:25:ALA:HB1	2.14	0.78
2:2:195:ASN:HD22	2:2:196:THR:N	1.80	0.78
1:1:135:SER:C	1:1:137:PRO:HD3	2.03	0.78
6:H:101:ASP:CG	6:H:102:TYR:H	1.87	0.78
6:H:17:SER:HB3	6:H:82(A):TYR:HA	1.64	0.78
6:H:100(I):TYR:N	6:H:100(I):TYR:CD1	2.51	0.78
1:1:161:LYS:HE2	1:1:161:LYS:HA	1.66	0.78
3:3:126:LYS:HE2	3:3:154:ASP:CB	2.14	0.77
1:1:201:TYR:CE2	1:1:203:GLY:HA3	2.19	0.77
3:3:157:LEU:C	3:3:157:LEU:HD23	2.04	0.77
3:3:157:LEU:HD22	3:3:158:GLN:OE1	1.84	0.77
5:L:30:VAL:HG23	5:L:90:GLN:HG3	1.65	0.77
3:3:46:ILE:O	3:3:49:VAL:HG23	1.85	0.77
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.66	0.77
5:L:77:ARG:CG	5:L:77:ARG:HH11	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:65:ASN:HA	3:3:68:LEU:HD12	1.65	0.77
1:1:186:PHE:HD1	3:3:24:ALA:HB2	1.48	0.77
5:L:33:MET:HE3	5:L:89:GLN:H	1.50	0.77
2:2:166:VAL:HG12	2:2:173:MET:HB3	1.67	0.77
1:1:282:ARG:HD3	1:1:285:ASP:O	1.85	0.77
4:4:68:ASN:OD1	4:4:68:ASN:N	2.18	0.77
2:2:83:PRO:CG	2:2:216:ASN:HA	2.14	0.77
3:3:142:ARG:O	3:3:143:ARG:C	2.22	0.77
2:2:232:THR:HG22	2:2:232:THR:O	1.83	0.77
1:1:46:LEU:HD21	3:3:215:PRO:HG3	1.66	0.77
5:L:36:PHE:HE2	6:H:103:TRP:NE1	1.83	0.76
1:1:204:TYR:HD2	1:1:211:THR:HG23	1.49	0.76
3:3:157:LEU:C	3:3:157:LEU:CD2	2.53	0.76
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.20	0.76
6:H:52:TYR:HD1	6:H:52(A):PRO:CD	1.97	0.76
6:H:40:ARG:HA	6:H:88:ALA:HB1	1.65	0.76
5:L:7:SER:HG	5:L:22:THR:HG1	1.29	0.76
1:1:65:THR:O	3:3:42:ASN:ND2	2.18	0.76
1:1:41:ALA:HB3	4:4:60:MET:HE1	1.67	0.76
1:1:26:LYS:O	1:1:27:HIS:HB2	1.84	0.76
2:2:150:GLY:O	2:2:152:ARG:N	2.19	0.76
5:L:19:VAL:CG2	5:L:75:ILE:HB	2.12	0.75
2:2:116:LYS:HA	3:3:121:ALA:HB3	1.68	0.75
2:2:254:ILE:O	2:2:255:ARG:HB3	1.83	0.75
3:3:105:THR:O	3:3:176:THR:HG23	1.85	0.75
6:H:33:TRP:HZ3	6:H:57:ASN:HA	1.52	0.75
1:1:88:THR:HG22	1:1:88:THR:O	1.85	0.75
2:2:86:LEU:O	2:2:88:ASP:N	2.20	0.74
1:1:45:VAL:O	1:1:46:LEU:HD23	1.88	0.74
3:3:18:ASP:CG	4:4:40:SER:HB3	2.07	0.74
6:H:4:LEU:HG	6:H:102:TYR:CD2	2.22	0.74
2:2:195:ASN:ND2	2:2:196:THR:HG23	2.03	0.74
1:1:266:ILE:HD12	3:3:236:GLU:HG2	1.70	0.74
5:L:13:ALA:CA	5:L:107:LYS:HG3	2.18	0.74
5:L:14:PHE:N	5:L:107:LYS:HB2	2.02	0.74
5:L:89:GLN:HG2	5:L:98:PHE:HA	1.68	0.74
3:3:108:SER:O	3:3:218:LYS:N	2.20	0.74
3:3:214:CYS:CB	3:3:215:PRO:CD	2.65	0.73
3:3:128:ILE:HG22	3:3:190:TRP:O	1.88	0.73
6:H:12:VAL:CG1	6:H:18:VAL:CG1	2.65	0.73
1:1:268:ARG:HG3	1:1:268:ARG:HH11	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:97:ASN:ND2	6:H:101:ASP:CG	2.42	0.73
3:3:126:LYS:O	3:3:192:GLN:CB	2.35	0.73
3:3:141:ASP:HA	3:3:190:TRP:CH2	2.24	0.73
2:2:69:LYS:HG2	2:2:78:TRP:NE1	2.04	0.73
5:L:105:GLU:HA	5:L:105:GLU:OE1	1.89	0.73
1:1:191:VAL:HG12	3:3:28:TYR:CZ	2.24	0.73
5:L:83:ALA:HB2	5:L:106:ILE:HB	1.71	0.73
1:1:282:ARG:HG3	3:3:57:ASN:ND2	2.04	0.73
3:3:124:SER:O	3:3:195:LEU:HD12	1.89	0.72
3:3:55:MET:HA	3:3:91:VAL:CG1	2.18	0.72
5:L:33:MET:HG2	5:L:71:TYR:CD2	2.24	0.72
5:L:94:TYR:HE2	6:H:58:LYS:CD	2.02	0.72
2:2:62:ARG:O	2:2:245:ALA:HB1	1.89	0.72
6:H:7:SER:HB2	6:H:21:SER:H	1.54	0.72
5:L:36:PHE:HE2	6:H:103:TRP:HE1	1.37	0.72
6:H:39:GLN:HB2	6:H:45:LEU:HD23	1.71	0.72
1:1:201:TYR:H	2:2:131:GLN:NE2	1.87	0.72
1:1:287:LYS:HE3	3:3:79:GLN:HB3	1.71	0.72
6:H:75:SER:OG	6:H:77:THR:OG1	2.08	0.72
5:L:21:ILE:HD12	5:L:73:LEU:CD2	2.19	0.72
5:L:4:LEU:HD12	5:L:99:GLY:HA2	1.71	0.72
2:2:111:GLN:HG2	2:2:196:THR:CG2	2.19	0.72
1:1:210:GLU:OE1	1:1:210:GLU:HA	1.84	0.72
2:2:217:ASN:C	2:2:218:VAL:HG12	2.10	0.72
3:3:102:GLN:HG2	3:3:225:THR:OG1	1.88	0.72
6:H:82:LEU:HB2	6:H:82(C):LEU:HD21	1.72	0.72
6:H:38:LYS:CG	6:H:90:TYR:HE1	2.03	0.72
4:4:43:GLN:HG3	4:4:45:LEU:HB3	1.71	0.72
1:1:67:VAL:HG22	3:3:41:HIS:O	1.90	0.72
2:2:183:ILE:HG12	3:3:96:LEU:HD22	1.70	0.72
3:3:115:LEU:HD23	3:3:129:LEU:HD11	1.72	0.72
1:1:161:LYS:HE2	1:1:161:LYS:CA	2.16	0.72
2:2:42:LEU:HD12	2:2:43:PRO:HD2	1.70	0.72
1:1:118:LEU:HD12	1:1:118:LEU:O	1.89	0.72
1:1:110:VAL:HG22	3:3:230:GLN:CD	2.10	0.72
6:H:3:GLN:O	6:H:24:ALA:HA	1.88	0.71
1:1:130:ILE:HD13	1:1:243:VAL:HG13	1.71	0.71
5:L:78:MET:CE	5:L:82:ASP:HB2	2.20	0.71
5:L:62:PHE:HD1	5:L:75:ILE:HG12	1.50	0.71
4:4:45:LEU:O	4:4:45:LEU:HG	1.90	0.71
2:2:180:ASN:HA	3:3:51:THR:HG22	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:152:TYR:O	1:1:154:PRO:HD3	1.91	0.71
6:H:41:PRO:HD3	6:H:88:ALA:HA	1.71	0.71
1:1:67:VAL:CG2	3:3:41:HIS:O	2.38	0.71
6:H:35:ASN:ND2	6:H:95:SER:HB2	2.06	0.71
6:H:4:LEU:HG	6:H:102:TYR:HD2	1.56	0.71
1:1:285:ASP:O	1:1:288:SER:HB2	1.90	0.71
1:1:102:TRP:HB3	1:1:224:MET:HB3	1.72	0.71
4:4:49:PRO:HB2	4:4:53:THR:OG1	1.89	0.71
1:1:77:VAL:HG11	1:1:245:HIS:HB3	1.73	0.71
2:2:29:ALA:HA	4:4:67:LEU:CD2	2.21	0.70
2:2:229:THR:HG22	2:2:229:THR:O	1.90	0.70
2:2:81:LYS:HA	2:2:219:SER:HB3	1.72	0.70
6:H:40:ARG:HB2	6:H:43:GLN:CB	2.21	0.70
2:2:183:ILE:HG13	3:3:96:LEU:HD22	1.73	0.70
6:H:101:ASP:CG	6:H:102:TYR:N	2.45	0.70
6:H:27:TYR:HD1	6:H:32:PHE:CE1	2.09	0.70
5:L:4:LEU:CD1	5:L:88:CYS:SG	2.79	0.70
3:3:65:ASN:C	3:3:67:TYR:H	1.94	0.70
2:2:84:ASP:O	2:2:86:LEU:N	2.24	0.70
3:3:115:LEU:HD22	3:3:129:LEU:HD11	1.71	0.70
2:2:158:SER:OG	2:2:159:ALA:N	2.21	0.70
6:H:51:ILE:CG2	6:H:69:LEU:HD13	2.09	0.70
5:L:33:MET:HG2	5:L:71:TYR:HB2	1.73	0.70
2:2:94:GLN:O	2:2:97:PHE:N	2.23	0.70
6:H:37:VAL:CA	6:H:46:GLU:O	2.39	0.70
5:L:2:ILE:HG12	5:L:27:SER:HB2	1.73	0.70
1:1:58:MET:CE	3:3:216:ASP:HA	2.21	0.70
5:L:94:TYR:CE2	6:H:58:LYS:CD	2.72	0.70
3:3:16:THR:O	3:3:16:THR:CG2	2.40	0.70
5:L:54:LEU:HD11	5:L:62:PHE:CB	2.22	0.70
3:3:193:THR:O	3:3:194:SER:HB3	1.92	0.70
1:1:46:LEU:HD22	1:1:47:PRO:HD3	1.74	0.70
5:L:62:PHE:O	5:L:63:SER:HB3	1.92	0.69
2:2:111:GLN:HG2	2:2:196:THR:HG22	1.73	0.69
5:L:86:TYR:O	5:L:101:GLY:HA2	1.92	0.69
5:L:44:PRO:CB	6:H:45:LEU:HD11	2.22	0.69
1:1:259:ARG:NH2	1:1:270:ASN:O	2.25	0.69
1:1:37:ASN:HB3	3:3:116:MET:HE3	1.73	0.69
1:1:161:LYS:N	1:1:165:ASP:OD2	2.22	0.69
6:H:97:ASN:OD1	6:H:97:ASN:N	2.25	0.69
3:3:19:ARG:CA	3:3:19:ARG:HE	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:151:VAL:CG2	3:3:163:MET:CG	2.58	0.69
1:1:43:MET:CE	1:1:44:PRO:HD2	2.23	0.69
3:3:214:CYS:SG	3:3:215:PRO:HD3	2.32	0.69
3:3:179:ASP:CB	3:3:182:THR:HG22	2.21	0.69
2:2:126:VAL:HG23	2:2:199:ILE:HD12	1.75	0.69
1:1:41:ALA:HB3	4:4:60:MET:CE	2.22	0.69
2:2:69:LYS:HG2	2:2:78:TRP:CD1	2.28	0.69
6:H:5:GLN:O	6:H:23:LYS:HE3	1.92	0.69
6:H:99:PRO:HG2	6:H:100(I):TYR:CZ	2.25	0.69
3:3:153:TRP:CD2	3:3:161:ILE:HG21	2.28	0.69
3:3:140:GLN:O	3:3:141:ASP:HB3	1.91	0.69
3:3:117:TYR:CZ	3:3:119:GLY:HA3	2.27	0.69
1:1:46:LEU:HD22	1:1:47:PRO:CD	2.23	0.68
6:H:62:LYS:HG3	6:H:63:PHE:CD1	2.28	0.68
2:2:182:LEU:HD12	2:2:182:LEU:H	1.57	0.68
2:2:137:GLY:O	2:2:140:VAL:HG23	1.92	0.68
6:H:6:GLN:HE22	6:H:91:PHE:HA	1.55	0.68
2:2:10:SER:OG	2:2:12:ARG:HB2	1.93	0.68
5:L:77:ARG:O	5:L:77:ARG:HD3	1.94	0.68
3:3:71:LEU:HD22	3:3:207:LEU:HD21	1.75	0.68
5:L:94:TYR:C	5:L:96:ILE:N	2.46	0.68
1:1:147:VAL:O	1:1:229:VAL:HG22	1.94	0.68
1:1:254:ILE:HD11	2:2:204:ILE:CG2	2.24	0.68
1:1:25:PRO:HD3	1:1:52:GLU:OE2	1.94	0.68
5:L:14:PHE:CD2	5:L:107:LYS:HD3	2.28	0.68
3:3:231:THR:OG1	3:3:232:VAL:HG22	1.94	0.68
6:H:40:ARG:C	6:H:43:GLN:HB2	2.14	0.68
5:L:26:THR:OG1	5:L:27:SER:N	2.25	0.68
4:4:34:ASP:HB2	4:4:37:SER:OG	1.94	0.68
3:3:14:LEU:HD11	3:3:16:THR:HB	1.75	0.68
1:1:208:ASP:CA	2:2:261:PRO:HG3	2.24	0.68
3:3:142:ARG:O	3:3:145:ALA:N	2.27	0.68
2:2:232:THR:CG2	2:2:232:THR:O	2.41	0.68
6:H:105:GLN:HG2	6:H:106:GLY:H	1.58	0.68
6:H:3:GLN:HG2	6:H:5:GLN:NE2	2.09	0.68
5:L:23:CYS:HB2	5:L:88:CYS:SG	2.34	0.68
5:L:37:GLN:HG2	5:L:38:GLN:N	2.07	0.68
2:2:122:LEU:HD11	2:2:240:ILE:HD11	1.76	0.67
5:L:91:ARG:HD2	5:L:96:ILE:HD13	1.75	0.67
1:1:78:HIS:HA	1:1:109:LEU:HD11	1.74	0.67
5:L:31:ASN:O	5:L:32:TYR:CD1	2.46	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:37:VAL:CB	6:H:46:GLU:O	2.41	0.67
3:3:19:ARG:N	3:3:19:ARG:HD2	2.09	0.67
3:3:42:ASN:O	3:3:44:LEU:N	2.27	0.67
3:3:117:TYR:CE1	3:3:119:GLY:HA3	2.29	0.67
2:2:79:CYS:HB2	2:2:221:MET:HG3	1.75	0.67
1:1:136:GLN:HB3	1:1:140:ALA:HB2	1.75	0.67
5:L:31:ASN:O	5:L:32:TYR:CG	2.48	0.67
5:L:76:SER:C	5:L:77:ARG:HG3	2.14	0.67
1:1:76:CYS:HB2	1:1:244:TYR:CE1	2.30	0.67
1:1:131:LEU:HB2	1:1:183:THR:HG22	1.76	0.67
5:L:13:ALA:O	5:L:78:MET:SD	2.53	0.67
1:1:245:HIS:ND1	1:1:245:HIS:C	2.48	0.67
1:1:121:TYR:OH	2:2:205:ASN:HA	1.95	0.67
1:1:110:VAL:HG22	3:3:230:GLN:CG	2.25	0.67
1:1:282:ARG:NH1	1:1:288:SER:O	2.28	0.67
5:L:13:ALA:C	5:L:107:LYS:HG3	2.14	0.66
5:L:78:MET:HA	5:L:82:ASP:OD2	1.95	0.66
6:H:35:ASN:HD22	6:H:35:ASN:N	1.93	0.66
1:1:207:ASP:HA	2:2:144:TYR:HE2	1.57	0.66
2:2:195:ASN:C	2:2:195:ASN:HD22	1.98	0.66
5:L:54:LEU:CD1	5:L:58:VAL:CG2	2.70	0.66
5:L:90:GLN:NE2	5:L:97:THR:HG23	2.09	0.66
2:2:65:THR:O	2:2:65:THR:HG22	1.96	0.66
1:1:209:ALA:H	2:2:261:PRO:HB3	1.59	0.66
1:1:160:PRO:HB3	1:1:168:TRP:HE1	1.60	0.66
3:3:83:THR:HG23	3:3:187:LEU:CD2	2.26	0.66
6:H:62:LYS:HG2	6:H:63:PHE:CE1	2.31	0.66
5:L:66:GLY:O	5:L:67:SER:HB3	1.96	0.66
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.30	0.66
2:2:21:SER:OG	2:2:63:PHE:HB2	1.95	0.66
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.09	0.66
2:2:109:HIS:HA	2:2:197:ALA:O	1.95	0.66
1:1:282:ARG:NH2	3:3:82:GLY:O	2.26	0.66
6:H:22:CYS:HG	6:H:92:CYS:HG	1.33	0.66
1:1:129:THR:HG21	3:3:13:PHE:CZ	2.31	0.66
2:2:230:VAL:HB	2:2:231:PRO:CD	2.24	0.66
5:L:94:TYR:O	5:L:94:TYR:CD1	2.49	0.66
3:3:71:LEU:HD22	3:3:207:LEU:CD2	2.24	0.66
1:1:282:ARG:HH22	3:3:83:THR:HB	1.61	0.66
1:1:120:THR:O	1:1:199:CYS:HB2	1.95	0.66
3:3:42:ASN:O	3:3:45:GLU:N	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:ALA:HB2	1:1:57:TYR:O	1.95	0.66
1:1:81:GLU:HB3	1:1:240:LYS:HG2	1.76	0.66
2:2:205:ASN:OD1	2:2:207:VAL:HG23	1.96	0.66
5:L:3:VAL:H	5:L:26:THR:HG23	1.60	0.65
5:L:75:ILE:C	5:L:77:ARG:H	1.99	0.65
1:1:201:TYR:H	1:1:215:ILE:HG22	1.61	0.65
6:H:7:SER:CB	6:H:21:SER:H	2.08	0.65
5:L:31:ASN:HB3	5:L:32:TYR:CD2	2.31	0.65
5:L:55:ALA:HB3	5:L:58:VAL:CG1	2.25	0.65
2:2:68:SER:HA	2:2:240:ILE:O	1.96	0.65
2:2:86:LEU:C	2:2:88:ASP:H	1.99	0.65
3:3:18:ASP:OD2	4:4:40:SER:HB3	1.96	0.65
6:H:48:ILE:HA	6:H:63:PHE:CD2	2.30	0.65
5:L:18:LYS:HA	5:L:77:ARG:HA	1.78	0.65
5:L:54:LEU:O	5:L:55:ALA:O	2.14	0.65
3:3:47:ILE:O	3:3:47:ILE:HG13	1.95	0.65
2:2:198:THR:O	2:2:199:ILE:HG12	1.96	0.65
5:L:10:ILE:HD11	5:L:105:GLU:HG2	1.78	0.65
5:L:78:MET:HE1	5:L:82:ASP:HB2	1.78	0.65
2:2:171:TYR:O	2:2:173:MET:N	2.30	0.65
2:2:37:GLU:CG	3:3:37:PRO:HB3	2.26	0.65
6:H:87:SER:HA	6:H:109:VAL:O	1.97	0.65
1:1:68:GLU:O	1:1:68:GLU:CG	2.42	0.65
2:2:123:LEU:HD12	2:2:188:PHE:CE1	2.32	0.65
2:2:166:VAL:HG12	2:2:173:MET:CB	2.27	0.65
2:2:18:LEU:O	2:2:19:GLY:C	2.35	0.65
6:H:12:VAL:HG13	6:H:18:VAL:HG11	1.78	0.65
6:H:57:ASN:C	6:H:58:LYS:HG2	2.17	0.65
1:1:44:PRO:HD3	4:4:54:GLU:OE2	1.96	0.65
2:2:95:ASN:HB3	2:2:251:PHE:CD2	2.32	0.65
1:1:208:ASP:N	2:2:261:PRO:HG3	2.10	0.65
3:3:57:ASN:O	3:3:59:HIS:N	2.29	0.65
1:1:84:ASN:ND2	1:1:232:HIS:HA	2.12	0.65
6:H:17:SER:HB3	6:H:82:LEU:O	1.97	0.65
5:L:16:GLY:HA2	5:L:77:ARG:NH1	2.12	0.64
1:1:78:HIS:HA	1:1:109:LEU:CD1	2.27	0.64
5:L:62:PHE:HE1	5:L:75:ILE:CD1	2.09	0.64
1:1:46:LEU:HD21	3:3:215:PRO:HG2	1.75	0.64
1:1:261:LEU:HG	2:2:171:TYR:CE2	2.33	0.64
1:1:97:LYS:HD2	6:H:52:TYR:HE2	1.62	0.64
3:3:137:ARG:O	3:3:138:GLY:C	2.35	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG21	6:H:82(C):LEU:HD13	1.78	0.64
5:L:2:ILE:CD1	5:L:93:SER:HB2	2.26	0.64
2:2:67:ASP:CG	2:2:68:SER:N	2.50	0.64
2:2:94:GLN:C	2:2:96:MET:N	2.46	0.64
5:L:65:SER:OG	5:L:66:GLY:N	2.28	0.64
5:L:77:ARG:CZ	5:L:77:ARG:HB2	2.27	0.64
3:3:89:ASP:HA	3:3:93:LYS:CD	2.19	0.64
1:1:166:TYR:HD1	1:1:167:THR:H	1.45	0.64
4:4:48:ASP:OD2	4:4:50:SER:HB2	1.98	0.64
4:4:49:PRO:O	4:4:51:LYS:N	2.30	0.64
3:3:218:LYS:C	3:3:219:LEU:HD12	2.18	0.64
2:2:123:LEU:O	2:2:123:LEU:CG	2.41	0.64
2:2:27:GLU:HA	2:2:27:GLU:OE1	1.96	0.64
2:2:18:LEU:O	2:2:20:ASN:N	2.31	0.64
6:H:22:CYS:C	6:H:23:LYS:HD3	2.18	0.63
2:2:108:VAL:CG2	2:2:199:ILE:HB	2.28	0.63
1:1:153:VAL:HG12	1:1:153:VAL:O	1.99	0.63
3:3:14:LEU:CD1	3:3:16:THR:H	2.11	0.63
1:1:110:VAL:N	3:3:230:GLN:OE1	2.30	0.63
3:3:195:LEU:HD21	3:3:205:VAL:CG2	2.28	0.63
6:H:63:PHE:O	6:H:64:LYS:C	2.37	0.63
5:L:14:PHE:N	5:L:107:LYS:HG3	2.13	0.63
5:L:34:HIS:CD2	5:L:50:SER:H	2.17	0.63
3:3:101:VAL:CG2	3:3:219:LEU:HD21	2.27	0.63
6:H:22:CYS:O	6:H:77:THR:HG22	1.99	0.63
5:L:84:ALA:O	5:L:104:LEU:N	2.32	0.63
3:3:127:LEU:HA	3:3:192:GLN:H	1.63	0.63
5:L:33:MET:CE	5:L:89:GLN:H	2.10	0.63
5:L:7:SER:HB2	5:L:22:THR:CG2	2.15	0.63
2:2:230:VAL:HG11	2:2:236:PRO:HA	1.80	0.63
3:3:86:PHE:C	3:3:88:GLY:H	2.00	0.63
5:L:6:GLN:HB2	5:L:100:SER:OG	1.98	0.63
5:L:14:PHE:CD2	5:L:107:LYS:HB3	2.34	0.63
1:1:102:TRP:O	1:1:223:SER:HA	1.99	0.63
6:H:3:GLN:HA	6:H:102:TYR:CZ	2.34	0.63
6:H:27:TYR:CD1	6:H:32:PHE:CE1	2.87	0.63
6:H:69:LEU:HA	6:H:80:MET:HB2	1.81	0.63
1:1:190:TYR:CD1	1:1:190:TYR:C	2.71	0.63
6:H:6:GLN:H	6:H:105:GLN:HE22	1.47	0.62
1:1:161:LYS:HB2	1:1:162:GLU:OE1	1.98	0.62
6:H:38:LYS:HG3	6:H:90:TYR:CE1	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:80:MET:HG2	6:H:81:GLN:N	2.12	0.62
2:2:170:LEU:HD13	2:2:170:LEU:O	1.98	0.62
5:L:18:LYS:HD2	5:L:76:SER:CA	2.21	0.62
1:1:109:LEU:HA	3:3:230:GLN:OE1	1.98	0.62
6:H:100(J):ALA:HB1	6:H:100(K):MET:CE	2.29	0.62
5:L:44:PRO:HG2	6:H:103:TRP:CH2	2.34	0.62
3:3:98:GLY:O	3:3:100:ILE:N	2.32	0.62
3:3:21:SER:O	4:4:37:SER:HA	2.00	0.62
2:2:95:ASN:O	2:2:99:HIS:ND1	2.32	0.62
2:2:34:CYS:HB3	2:2:185:PRO:HG3	1.81	0.62
1:1:281:LYS:HG2	1:1:282:ARG:H	1.63	0.62
6:H:50:GLN:H	6:H:69:LEU:HD12	1.65	0.62
5:L:48:ILE:HA	5:L:53:ASN:O	1.99	0.62
2:2:30:ASN:OD1	4:4:58:ASP:O	2.18	0.62
3:3:124:SER:OG	3:3:125:ALA:N	2.32	0.62
1:1:254:ILE:CD1	2:2:204:ILE:HG21	2.30	0.62
5:L:7:SER:HB3	5:L:8:PRO:HD3	1.81	0.62
3:3:153:TRP:CE3	3:3:161:ILE:CG2	2.81	0.62
1:1:289:TYR:CE1	3:3:139:PRO:HD2	2.35	0.62
6:H:22:CYS:O	6:H:77:THR:HA	1.99	0.62
2:2:110:VAL:HG11	2:2:124:VAL:CG2	2.30	0.62
6:H:12:VAL:HG11	6:H:18:VAL:HG13	1.80	0.62
1:1:194:ALA:O	1:1:196:ALA:N	2.31	0.61
3:3:54:PRO:O	3:3:56:ASN:N	2.33	0.61
1:1:163:TRP:NE1	1:1:164:ASP:HB2	2.13	0.61
5:L:47:TRP:O	5:L:55:ALA:CB	2.48	0.61
3:3:217:PHE:CE2	3:3:219:LEU:HD11	2.35	0.61
5:L:73:LEU:HG	5:L:74:THR:N	2.14	0.61
1:1:107:SER:HB3	1:1:113:ARG:NH1	2.14	0.61
1:1:194:ALA:C	1:1:196:ALA:H	2.02	0.61
2:2:230:VAL:CG1	2:2:236:PRO:HA	2.31	0.61
1:1:44:PRO:O	1:1:45:VAL:O	2.17	0.61
1:1:20:SER:O	1:1:55:THR:HA	2.00	0.61
2:2:10:SER:C	2:2:12:ARG:H	2.02	0.61
2:2:229:THR:O	2:2:229:THR:CG2	2.47	0.61
2:2:41:TYR:O	2:2:43:PRO:HD3	2.00	0.61
1:1:19:ALA:HB3	1:1:56:THR:OG1	2.00	0.61
5:L:79:GLU:O	5:L:106:ILE:HD13	2.00	0.61
5:L:7:SER:OG	5:L:22:THR:CB	2.47	0.61
2:2:94:GLN:C	2:2:96:MET:H	2.02	0.61
6:H:80:MET:HE2	6:H:82:LEU:HG	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:100:ILE:HG22	3:3:101:VAL:N	2.14	0.61
3:3:214:CYS:HB3	3:3:216:ASP:OD1	2.00	0.61
1:1:195:SER:O	1:1:196:ALA:HB2	2.01	0.61
5:L:62:PHE:CE1	5:L:75:ILE:HG12	2.35	0.61
1:1:42:THR:HG23	3:3:50:ASP:OD2	2.00	0.61
6:H:62:LYS:HG2	6:H:63:PHE:CZ	2.35	0.61
5:L:33:MET:HB2	5:L:71:TYR:CD2	2.36	0.61
6:H:69:LEU:HD23	6:H:80:MET:CB	2.24	0.60
5:L:13:ALA:HA	5:L:17:GLU:OE1	2.00	0.60
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.82	0.60
3:3:117:TYR:CE1	3:3:119:GLY:CA	2.84	0.60
6:H:38:LYS:HG3	6:H:90:TYR:HE1	1.65	0.60
5:L:30:VAL:HG21	5:L:90:GLN:CG	2.31	0.60
1:1:254:ILE:HD11	2:2:204:ILE:HG23	1.82	0.60
3:3:141:ASP:CA	3:3:190:TRP:CH2	2.85	0.60
3:3:167:TRP:CD1	3:3:167:TRP:O	2.54	0.60
5:L:111:ALA:C	5:L:111:ALA:CB	2.64	0.60
6:H:40:ARG:HA	6:H:88:ALA:CB	2.32	0.60
6:H:38:LYS:O	6:H:46:GLU:HB2	2.00	0.60
6:H:40:ARG:CA	6:H:88:ALA:HB1	2.31	0.60
2:2:30:ASN:HD21	4:4:58:ASP:CB	2.08	0.60
2:2:260:VAL:HB	2:2:261:PRO:HD2	1.82	0.60
6:H:39:GLN:HG2	6:H:43:GLN:O	2.01	0.60
5:L:82:ASP:O	5:L:104:LEU:HB3	2.01	0.60
1:1:66:ASP:OD2	4:4:43:GLN:HA	2.01	0.60
5:L:6:GLN:NE2	5:L:102:THR:H	1.99	0.60
1:1:282:ARG:CG	3:3:57:ASN:ND2	2.64	0.60
5:L:6:GLN:OE1	5:L:87:TYR:CA	2.48	0.60
3:3:65:ASN:C	3:3:67:TYR:N	2.53	0.60
1:1:159:ASN:C	1:1:167:THR:HG21	2.21	0.60
1:1:21:ILE:H	1:1:21:ILE:HD12	1.63	0.60
2:2:110:VAL:HG23	2:2:242:VAL:HG22	1.83	0.60
5:L:13:ALA:N	5:L:107:LYS:HG3	2.17	0.60
3:3:177:ASP:CG	3:3:178:PRO:HD2	2.23	0.60
5:L:31:ASN:C	5:L:32:TYR:CG	2.76	0.60
5:L:82:ASP:O	5:L:84:ALA:N	2.34	0.59
1:1:37:ASN:HB2	3:3:160:THR:OG1	2.01	0.59
1:1:37:ASN:CB	3:3:116:MET:HE3	2.31	0.59
2:2:171:TYR:O	2:2:172:ASN:C	2.41	0.59
6:H:33:TRP:CZ3	6:H:57:ASN:HA	2.36	0.59
5:L:100:SER:OG	5:L:101:GLY:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:VAL:C	1:1:109:LEU:CD1	2.70	0.59
1:1:113:ARG:HD3	1:1:263:TYR:CE2	2.37	0.59
2:2:123:LEU:CD1	2:2:188:PHE:HE1	2.15	0.59
2:2:99:HIS:HD2	2:2:254:ILE:HA	1.66	0.59
1:1:201:TYR:N	1:1:215:ILE:HG22	2.17	0.59
1:1:201:TYR:N	2:2:131:GLN:NE2	2.50	0.59
1:1:160:PRO:HB3	1:1:168:TRP:CE2	2.36	0.59
2:2:116:LYS:CA	3:3:121:ALA:HB3	2.33	0.59
5:L:31:ASN:HB3	5:L:32:TYR:CE2	2.37	0.59
5:L:14:PHE:HB2	5:L:17:GLU:HG3	1.84	0.59
5:L:21:ILE:HG22	5:L:22:THR:N	2.16	0.59
3:3:47:ILE:HG22	3:3:100:ILE:CD1	2.32	0.59
1:1:286:ILE:HD11	3:3:81:PHE:HB3	1.84	0.59
2:2:76:LYS:HG3	2:2:169:VAL:HG11	1.83	0.59
6:H:36:TRP:CD1	6:H:69:LEU:CD2	2.85	0.59
5:L:11:MET:CE	5:L:104:LEU:HD13	2.32	0.59
2:2:23:ILE:HD12	2:2:63:PHE:CZ	2.37	0.59
5:L:21:ILE:HG12	5:L:102:THR:CG2	2.31	0.59
1:1:261:LEU:HD12	1:1:271:TYR:CD1	2.37	0.59
1:1:84:ASN:HD21	1:1:232:HIS:HA	1.66	0.59
6:H:27:TYR:CD1	6:H:94:ARG:HD2	2.37	0.59
1:1:265:SER:N	3:3:234:LEU:HD13	2.17	0.59
2:2:84:ASP:O	2:2:87:LYS:N	2.23	0.59
2:2:71:TRP:HB3	2:2:238:LEU:O	2.03	0.59
5:L:77:ARG:CG	5:L:77:ARG:NH1	2.62	0.59
5:L:11:MET:N	5:L:11:MET:SD	2.75	0.59
2:2:255:ARG:C	2:2:257:LYS:H	2.06	0.59
1:1:281:LYS:HE3	1:1:282:ARG:O	2.03	0.59
6:H:12:VAL:HG13	6:H:18:VAL:CG1	2.33	0.59
3:3:140:GLN:O	3:3:141:ASP:CB	2.50	0.59
3:3:153:TRP:CD1	3:3:153:TRP:C	2.76	0.59
2:2:228:LEU:HD12	2:2:229:THR:N	2.18	0.58
1:1:30:LYS:O	1:1:32:PRO:HD3	2.02	0.58
2:2:44:ASP:O	2:2:45:VAL:C	2.40	0.58
2:2:122:LEU:HD22	2:2:222:VAL:HG12	1.84	0.58
6:H:41:PRO:O	6:H:43:GLN:HG2	2.03	0.58
3:3:164:THR:O	3:3:166:PRO:HD3	2.04	0.58
3:3:43:LEU:O	3:3:46:ILE:HG12	2.03	0.58
1:1:228:ILE:CD1	1:1:239:VAL:HG21	2.29	0.58
6:H:27:TYR:CE1	6:H:32:PHE:CD1	2.91	0.58
5:L:94:TYR:O	5:L:94:TYR:HD1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:129:THR:HG22	1:1:244:TYR:HB2	1.86	0.58
1:1:207:ASP:OD1	2:2:213:THR:HB	2.04	0.58
1:1:200:PHE:N	1:1:200:PHE:HD1	2.01	0.58
6:H:100(J):ALA:O	6:H:101:ASP:N	2.36	0.58
1:1:44:PRO:HG3	4:4:54:GLU:OE2	2.03	0.58
1:1:204:TYR:CD2	1:1:211:THR:HG23	2.35	0.58
4:4:49:PRO:O	4:4:50:SER:C	2.41	0.58
1:1:138:ASP:OD1	1:1:138:ASP:N	2.37	0.58
6:H:48:ILE:CG2	6:H:67:ALA:CB	2.82	0.58
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.85	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.03	0.58
6:H:27:TYR:HE1	6:H:32:PHE:CD1	2.22	0.58
5:L:6:GLN:HB3	5:L:102:THR:OG1	2.04	0.58
5:L:54:LEU:HD13	5:L:58:VAL:HG23	1.82	0.58
2:2:123:LEU:CD1	2:2:188:PHE:CE1	2.86	0.58
6:H:94:ARG:O	6:H:100(K):MET:HA	2.04	0.58
3:3:41:HIS:HB2	3:3:45:GLU:OE2	2.04	0.58
5:L:16:GLY:O	5:L:77:ARG:HB3	2.03	0.57
5:L:38:GLN:CG	5:L:44:PRO:HA	2.34	0.57
1:1:31:VAL:HG12	1:1:34:LEU:HB2	1.83	0.57
2:2:116:LYS:HA	3:3:121:ALA:CB	2.34	0.57
3:3:75:ARG:HB3	3:3:78:GLU:OE2	2.03	0.57
5:L:73:LEU:HG	5:L:74:THR:H	1.69	0.57
5:L:7:SER:HB2	5:L:22:THR:N	2.18	0.57
1:1:289:TYR:CZ	3:3:139:PRO:O	2.57	0.57
2:2:94:GLN:O	2:2:96:MET:N	2.38	0.57
2:2:182:LEU:N	2:2:182:LEU:HD12	2.19	0.57
6:H:6:GLN:HB2	6:H:105:GLN:NE2	2.19	0.57
5:L:38:GLN:HG3	5:L:44:PRO:HA	1.86	0.57
1:1:123:ARG:NH1	3:3:33:ARG:HB3	2.19	0.57
2:2:110:VAL:HG11	2:2:124:VAL:HG21	1.87	0.57
3:3:14:LEU:HD12	3:3:14:LEU:C	2.24	0.57
1:1:286:ILE:HD11	3:3:81:PHE:CB	2.35	0.57
1:1:200:PHE:CD1	1:1:200:PHE:N	2.71	0.57
5:L:3:VAL:N	5:L:26:THR:HG23	2.19	0.57
5:L:62:PHE:CE1	5:L:75:ILE:CD1	2.87	0.57
5:L:77:ARG:NH1	5:L:77:ARG:CB	2.67	0.57
6:H:54:ASP:OD1	6:H:56:ASP:HB2	2.05	0.57
2:2:49:ASP:OD1	2:2:51:ASN:HB2	2.03	0.57
5:L:33:MET:CG	5:L:71:TYR:HB2	2.35	0.57
1:1:245:HIS:HD1	1:1:245:HIS:C	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:36:ALA:O	1:1:39:THR:HG23	2.05	0.57
5:L:57:GLY:O	5:L:59:PRO:HD3	2.05	0.57
1:1:60:PHE:CD2	3:3:218:LYS:HG2	2.40	0.57
6:H:86:ASP:HA	6:H:90:TYR:OH	2.05	0.57
6:H:3:GLN:C	6:H:4:LEU:HD23	2.25	0.57
1:1:67:VAL:HG22	3:3:41:HIS:C	2.24	0.57
1:1:185:ARG:HH22	3:3:17:ASP:HB3	1.70	0.56
6:H:62:LYS:CG	6:H:63:PHE:CE1	2.88	0.56
1:1:180:VAL:C	1:1:182:ASP:H	2.08	0.56
6:H:39:GLN:HB2	6:H:45:LEU:CD2	2.35	0.56
6:H:6:GLN:NE2	6:H:91:PHE:HA	2.18	0.56
5:L:79:GLU:H	5:L:82:ASP:CG	2.08	0.56
1:1:71:LEU:HD11	1:1:116:LEU:HD22	1.86	0.56
2:2:135:HIS:HE1	2:2:163:GLY:H	1.53	0.56
5:L:82:ASP:HB3	5:L:104:LEU:CD2	2.36	0.56
5:L:95:PRO:O	5:L:96:ILE:C	2.43	0.56
3:3:104:TYR:CD2	3:3:219:LEU:HD23	2.40	0.56
6:H:50:GLN:N	6:H:69:LEU:HD12	2.20	0.56
2:2:63:PHE:CD1	2:2:245:ALA:CB	2.79	0.56
3:3:188:SER:O	3:3:189:CYS:HB2	2.05	0.56
2:2:76:LYS:CG	2:2:169:VAL:HG11	2.35	0.56
1:1:113:ARG:HG2	1:1:113:ARG:O	2.03	0.56
2:2:66:LEU:HD21	2:2:85:ALA:HB1	1.88	0.56
3:3:55:MET:HA	3:3:91:VAL:HG12	1.86	0.56
3:3:51:THR:O	3:3:210:PHE:HA	2.05	0.56
1:1:104:ILE:HG13	1:1:222:GLY:O	2.06	0.56
5:L:33:MET:CG	5:L:71:TYR:CB	2.79	0.56
2:2:214:ARG:O	2:2:215:HIS:HB2	2.04	0.56
1:1:94:ARG:C	1:1:96:ALA:H	2.09	0.56
3:3:200:GLU:HA	3:3:200:GLU:OE1	2.05	0.56
2:2:101:LEU:HD12	2:2:209:ILE:HG12	1.88	0.56
6:H:35:ASN:ND2	6:H:35:ASN:N	2.54	0.56
1:1:282:ARG:HB2	3:3:57:ASN:CB	2.34	0.56
1:1:177:PHE:HD1	1:1:177:PHE:H	1.51	0.56
2:2:172:ASN:ND2	2:2:181:LEU:HD13	2.21	0.56
5:L:14:PHE:O	5:L:15:PRO:C	2.42	0.56
5:L:4:LEU:CD2	5:L:25:ALA:HB2	2.35	0.56
3:3:41:HIS:CD2	4:4:46:SER:HB2	2.40	0.56
2:2:121:CYS:HB2	2:2:190:ASN:HA	1.87	0.55
1:1:248:LYS:O	1:1:249:HIS:CB	2.48	0.55
2:2:156:LEU:HD21	2:2:173:MET:SD	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:146:LEU:H	1:1:180:VAL:HG21	1.70	0.55
6:H:3:GLN:HG2	6:H:5:GLN:HE22	1.69	0.55
2:2:128:PRO:HA	2:2:218:VAL:HB	1.88	0.55
2:2:182:LEU:CD1	2:2:182:LEU:H	2.19	0.55
2:2:160:ASN:HA	2:2:167:LYS:NZ	2.20	0.55
2:2:72:THR:C	2:2:74:GLY:H	2.08	0.55
5:L:47:TRP:O	5:L:58:VAL:HG11	2.07	0.55
3:3:128:ILE:O	3:3:189:CYS:HA	2.07	0.55
2:2:44:ASP:O	2:2:46:ASP:N	2.39	0.55
5:L:44:PRO:C	5:L:45:LYS:HD3	2.27	0.55
1:1:110:VAL:HG22	3:3:230:GLN:HG2	1.87	0.55
1:1:260:ALA:HB2	2:2:177:LEU:HD11	1.88	0.55
2:2:179:GLY:O	3:3:51:THR:HG22	2.07	0.55
5:L:2:ILE:HB	5:L:90:GLN:HE21	1.70	0.55
1:1:31:VAL:CG1	1:1:34:LEU:HB2	2.36	0.55
2:2:178:LEU:O	2:2:181:LEU:HB2	2.06	0.55
2:2:187:GLN:HE21	2:2:198:THR:N	2.01	0.55
3:3:83:THR:CG2	3:3:187:LEU:HD21	2.35	0.55
1:1:146:LEU:HA	1:1:230:ASN:HD21	1.70	0.55
6:H:10:GLU:OE1	6:H:10:GLU:HA	2.06	0.55
3:3:129:LEU:O	3:3:130:ALA:HB2	2.07	0.55
3:3:141:ASP:N	3:3:190:TRP:CH2	2.74	0.55
3:3:55:MET:HA	3:3:91:VAL:HG11	1.88	0.55
3:3:133:PRO:CB	3:3:134:PRO:HD2	2.37	0.55
3:3:9:GLY:O	3:3:12:GLN:HG2	2.07	0.55
5:L:77:ARG:HB2	5:L:77:ARG:NH1	2.21	0.55
1:1:70:PHE:CZ	1:1:118:LEU:HD23	2.41	0.55
2:2:110:VAL:CG2	2:2:242:VAL:HG22	2.37	0.55
6:H:50:GLN:N	6:H:69:LEU:CD1	2.69	0.55
1:1:217:VAL:HG23	1:1:218:LEU:N	2.22	0.55
1:1:39:THR:HG22	2:2:29:ALA:HB1	1.89	0.55
2:2:34:CYS:HB3	2:2:185:PRO:CG	2.37	0.55
1:1:146:LEU:O	1:1:180:VAL:HG22	2.06	0.55
3:3:41:HIS:NE2	4:4:46:SER:HB2	2.22	0.55
3:3:63:GLU:O	3:3:66:SER:OG	2.24	0.55
3:3:195:LEU:HD21	3:3:205:VAL:HG21	1.89	0.55
3:3:16:THR:O	3:3:16:THR:HG22	2.07	0.55
2:2:37:GLU:HG2	3:3:37:PRO:HB3	1.88	0.55
1:1:177:PHE:CD1	1:1:177:PHE:N	2.75	0.55
5:L:35:TRP:CH2	5:L:88:CYS:HB3	2.42	0.54
5:L:6:GLN:OE1	5:L:88:CYS:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:40:ARG:HB2	6:H:43:GLN:HB2	1.89	0.54
5:L:13:ALA:HB3	5:L:78:MET:HG2	1.86	0.54
1:1:166:TYR:CE1	1:1:167:THR:HG23	2.43	0.54
1:1:146:LEU:O	1:1:180:VAL:CG2	2.55	0.54
2:2:63:PHE:HA	2:2:245:ALA:HB2	1.90	0.54
2:2:144:TYR:CE1	2:2:148:HIS:CD2	2.95	0.54
1:1:147:VAL:O	1:1:229:VAL:CG2	2.55	0.54
2:2:105:GLY:O	2:2:247:MET:N	2.40	0.54
6:H:99:PRO:CD	6:H:100(I):TYR:CE1	2.90	0.54
2:2:217:ASN:C	2:2:218:VAL:CG1	2.75	0.54
6:H:62:LYS:HG3	6:H:63:PHE:N	2.22	0.54
6:H:5:GLN:O	6:H:22:CYS:HA	2.08	0.54
6:H:51:ILE:HD12	6:H:52:TYR:H	1.72	0.54
1:1:65:THR:C	3:3:42:ASN:ND2	2.60	0.54
6:H:27:TYR:HE1	6:H:32:PHE:HD1	1.54	0.54
5:L:10:ILE:HD12	5:L:103:LYS:HB3	1.89	0.54
1:1:228:ILE:HD11	1:1:239:VAL:CG2	2.29	0.54
2:2:255:ARG:HD3	2:2:255:ARG:N	2.22	0.54
1:1:271:TYR:HB2	1:1:272:PRO:CD	2.34	0.54
1:1:141:ASN:O	1:1:142:TYR:HB3	2.07	0.54
6:H:40:ARG:CA	6:H:43:GLN:HB2	2.38	0.54
5:L:11:MET:HE2	5:L:104:LEU:HD13	1.88	0.54
1:1:265:SER:OG	1:1:268:ARG:HG3	2.08	0.54
3:3:109:GLY:HA3	3:3:217:PHE:HA	1.89	0.54
1:1:123:ARG:O	1:1:250:VAL:HA	2.07	0.54
3:3:63:GLU:C	3:3:65:ASN:N	2.61	0.54
1:1:207:ASP:C	2:2:261:PRO:HG3	2.28	0.54
1:1:254:ILE:CD1	2:2:204:ILE:CG2	2.85	0.54
5:L:58:VAL:O	5:L:58:VAL:HG23	2.08	0.54
2:2:99:HIS:ND1	2:2:251:PHE:HB3	2.23	0.54
1:1:74:ALA:HB3	3:3:15:THR:CB	2.35	0.54
5:L:18:LYS:HD3	5:L:76:SER:HA	1.88	0.53
1:1:47:PRO:HA	3:3:164:THR:HG21	1.90	0.53
3:3:42:ASN:N	3:3:45:GLU:OE2	2.37	0.53
2:2:62:ARG:HG3	2:2:63:PHE:N	2.22	0.53
2:2:215:HIS:CD2	2:2:216:ASN:N	2.76	0.53
2:2:34:CYS:SG	2:2:202:PRO:HD2	2.48	0.53
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.72	0.53
3:3:86:PHE:C	3:3:88:GLY:N	2.62	0.53
2:2:126:VAL:HG21	2:2:199:ILE:HG21	1.89	0.53
2:2:76:LYS:HG2	2:2:169:VAL:CG1	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:99:PRO:CG	6:H:100(I):TYR:HE1	2.03	0.53
5:L:25:ALA:O	5:L:69:THR:HG22	2.08	0.53
2:2:225:ILE:CG2	3:3:208:LEU:HD21	2.39	0.53
2:2:180:ASN:HA	3:3:51:THR:CG2	2.37	0.53
5:L:6:GLN:HG2	5:L:100:SER:H	1.72	0.53
1:1:67:VAL:HG23	3:3:41:HIS:O	2.09	0.53
2:2:110:VAL:HG12	2:2:189:ILE:HD11	1.91	0.53
6:H:35:ASN:HD22	6:H:35:ASN:H	1.56	0.53
5:L:4:LEU:HD22	5:L:25:ALA:HB2	1.90	0.53
3:3:173:PHE:CE2	3:3:220:ARG:HD3	2.44	0.53
2:2:71:TRP:O	2:2:237:SER:HA	2.08	0.53
5:L:6:GLN:CG	5:L:101:GLY:N	2.35	0.53
5:L:54:LEU:HD21	5:L:63:SER:HA	1.91	0.53
2:2:10:SER:C	2:2:12:ARG:N	2.61	0.53
2:2:181:LEU:O	2:2:183:ILE:N	2.42	0.53
2:2:37:GLU:HG3	3:3:37:PRO:HB3	1.89	0.53
5:L:30:VAL:HG21	5:L:90:GLN:HG3	1.83	0.53
1:1:129:THR:OG1	1:1:185:ARG:CD	2.56	0.53
1:1:263:TYR:HB3	3:3:234:LEU:HD11	1.91	0.53
1:1:188:VAL:CG1	1:1:189:PRO:HD2	2.38	0.53
5:L:13:ALA:C	5:L:78:MET:HG2	2.30	0.52
1:1:201:TYR:CE2	1:1:203:GLY:CA	2.91	0.52
5:L:16:GLY:HA2	5:L:77:ARG:CZ	2.38	0.52
3:3:2:LEU:HD12	3:3:3:PRO:N	2.24	0.52
3:3:115:LEU:HD23	3:3:129:LEU:CD1	2.39	0.52
1:1:254:ILE:HG23	2:2:35:TYR:CZ	2.45	0.52
6:H:32:PHE:HB3	6:H:95:SER:O	2.09	0.52
5:L:94:TYR:CE1	5:L:96:ILE:HG13	2.45	0.52
1:1:193:LEU:CD1	1:1:193:LEU:N	2.39	0.52
3:3:126:LYS:HG2	3:3:154:ASP:HA	1.91	0.52
1:1:41:ALA:CB	4:4:60:MET:CE	2.87	0.52
1:1:102:TRP:CZ3	1:1:104:ILE:HG23	2.44	0.52
3:3:185:GLY:C	3:3:186:PHE:CD1	2.82	0.52
6:H:40:ARG:HB3	6:H:41:PRO:HD2	1.91	0.52
6:H:27:TYR:CZ	6:H:94:ARG:HD2	2.41	0.52
2:2:85:ALA:HA	2:2:150:GLY:CA	2.36	0.52
1:1:163:TRP:CD1	1:1:164:ASP:N	2.78	0.52
1:1:253:TRP:CD1	3:3:36:ILE:HG13	2.43	0.52
6:H:32:PHE:CD1	6:H:32:PHE:N	2.76	0.52
6:H:6:GLN:NE2	6:H:106:GLY:HA2	2.25	0.52
6:H:70:THR:HG23	6:H:79:TYR:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:29:PHE:CE2	6:H:76:THR:HA	2.45	0.52
1:1:69:CYS:C	1:1:71:LEU:H	2.10	0.52
3:3:101:VAL:HG23	3:3:219:LEU:HD21	1.91	0.52
5:L:82:ASP:HB3	5:L:104:LEU:HD21	1.91	0.52
2:2:111:GLN:HG2	2:2:196:THR:HG21	1.91	0.52
3:3:51:THR:O	3:3:210:PHE:HB3	2.09	0.52
3:3:216:ASP:O	3:3:217:PHE:C	2.48	0.52
2:2:61:CYS:SG	2:2:249:THR:OG1	2.67	0.52
1:1:178:PHE:C	1:1:178:PHE:HD1	2.13	0.52
2:2:116:LYS:O	3:3:122:LEU:HB2	2.10	0.52
1:1:248:LYS:HG3	1:1:248:LYS:O	2.10	0.52
2:2:89:MET:HE1	2:2:151:GLU:OE2	2.10	0.52
2:2:225:ILE:HG21	3:3:208:LEU:HD21	1.91	0.52
5:L:59:PRO:O	5:L:62:PHE:HB2	2.10	0.52
3:3:175:TYR:CD2	3:3:182:THR:HG21	2.44	0.52
1:1:256:ARG:NH2	2:2:128:PRO:O	2.43	0.52
2:2:64:TYR:O	2:2:243:THR:HG22	2.10	0.52
3:3:113:PHE:CE2	3:3:129:LEU:HD21	2.45	0.52
1:1:199:CYS:HB3	1:1:200:PHE:CD1	2.45	0.52
5:L:13:ALA:CB	5:L:78:MET:CG	2.83	0.51
5:L:22:THR:HA	5:L:72:SER:HA	1.92	0.51
3:3:83:THR:HG23	3:3:187:LEU:HD21	1.90	0.51
1:1:199:CYS:C	1:1:200:PHE:HD1	2.14	0.51
3:3:126:LYS:CE	3:3:154:ASP:HB2	2.31	0.51
2:2:207:VAL:HG12	2:2:208:PRO:CD	2.35	0.51
3:3:141:ASP:O	3:3:142:ARG:C	2.49	0.51
3:3:76:GLN:O	3:3:77:ASN:HB2	2.09	0.51
2:2:210:ASP:CG	2:2:211:SER:H	2.12	0.51
1:1:199:CYS:HB3	1:1:200:PHE:HD1	1.76	0.51
3:3:175:TYR:HD2	3:3:182:THR:HG21	1.76	0.51
1:1:214:GLY:O	1:1:217:VAL:HG22	2.09	0.51
5:L:15:PRO:HA	5:L:78:MET:HG3	1.91	0.51
5:L:38:GLN:HE21	5:L:44:PRO:CD	2.22	0.51
5:L:7:SER:HB3	5:L:8:PRO:CD	2.40	0.51
1:1:190:TYR:O	1:1:190:TYR:HD1	1.94	0.51
2:2:150:GLY:C	2:2:152:ARG:N	2.62	0.51
3:3:53:ILE:CD1	3:3:113:PHE:HE1	2.22	0.51
6:H:29:PHE:CD2	6:H:76:THR:HG22	2.46	0.51
2:2:181:LEU:C	2:2:183:ILE:H	2.14	0.51
3:3:128:ILE:CG2	3:3:190:TRP:O	2.57	0.51
3:3:28:TYR:CD1	3:3:28:TYR:C	2.83	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:152:TYR:C	1:1:152:TYR:CD1	2.84	0.51
5:L:86:TYR:CE2	5:L:104:LEU:HB2	2.45	0.51
1:1:46:LEU:HD22	1:1:47:PRO:HD2	1.92	0.51
3:3:2:LEU:C	3:3:2:LEU:HD12	2.31	0.51
3:3:113:PHE:HE2	3:3:129:LEU:HD21	1.75	0.51
1:1:208:ASP:HA	2:2:261:PRO:HG3	1.92	0.51
1:1:166:TYR:HD1	1:1:166:TYR:H	1.59	0.51
2:2:76:LYS:HG2	2:2:169:VAL:HG13	1.92	0.51
6:H:12:VAL:O	6:H:111:VAL:HA	2.11	0.51
6:H:3:GLN:HG3	6:H:102:TYR:OH	2.10	0.51
5:L:6:GLN:CB	5:L:100:SER:OG	2.58	0.51
5:L:54:LEU:HD12	5:L:58:VAL:O	2.11	0.51
2:2:190:ASN:C	2:2:192:ARG:H	2.13	0.51
1:1:178:PHE:C	1:1:178:PHE:CD1	2.83	0.51
2:2:62:ARG:O	2:2:245:ALA:CB	2.56	0.51
5:L:30:VAL:HG21	5:L:90:GLN:CB	2.41	0.50
2:2:185:PRO:O	2:2:186:HIS:HB3	2.11	0.50
3:3:35:HIS:ND1	3:3:36:ILE:N	2.59	0.50
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.93	0.50
2:2:33:VAL:HG22	2:2:200:VAL:HG21	1.92	0.50
6:H:79:TYR:O	6:H:80:MET:CB	2.59	0.50
5:L:3:VAL:HB	5:L:26:THR:CG2	2.41	0.50
5:L:80:ALA:C	5:L:82:ASP:H	2.14	0.50
1:1:67:VAL:C	1:1:69:CYS:H	2.14	0.50
1:1:188:VAL:HG12	1:1:189:PRO:HD2	1.92	0.50
6:H:22:CYS:O	6:H:23:LYS:HD3	2.11	0.50
5:L:21:ILE:CG2	5:L:22:THR:N	2.74	0.50
5:L:30:VAL:HG21	5:L:90:GLN:HB2	1.92	0.50
2:2:15:GLN:C	2:2:16:ILE:HG13	2.32	0.50
1:1:176:VAL:O	1:1:176:VAL:HG23	2.12	0.50
6:H:22:CYS:O	6:H:77:THR:CA	2.59	0.50
1:1:70:PHE:HZ	1:1:118:LEU:HD23	1.75	0.50
2:2:99:HIS:HD2	2:2:254:ILE:CA	2.25	0.50
5:L:108:ARG:CG	5:L:109:ALA:N	2.65	0.50
3:3:101:VAL:HG22	3:3:219:LEU:HD21	1.91	0.50
3:3:50:ASP:HB2	3:3:210:PHE:HB3	1.93	0.50
3:3:117:TYR:CE1	3:3:119:GLY:N	2.79	0.50
2:2:79:CYS:SG	2:2:80:TRP:N	2.84	0.50
1:1:50:SER:O	1:1:51:ILE:CG2	2.60	0.50
6:H:2:GLY:HA2	6:H:25:SER:C	2.30	0.50
6:H:3:GLN:O	6:H:4:LEU:HD23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:14:PHE:CD2	5:L:107:LYS:CB	2.95	0.50
5:L:34:HIS:HD2	5:L:49:TYR:HA	1.76	0.50
3:3:82:GLY:O	3:3:83:THR:HB	2.11	0.50
5:L:14:PHE:CG	5:L:107:LYS:HB2	2.47	0.50
5:L:71:TYR:N	5:L:71:TYR:CD1	2.80	0.50
2:2:108:VAL:HG22	2:2:199:ILE:O	2.11	0.50
5:L:6:GLN:CB	5:L:101:GLY:H	2.23	0.50
5:L:7:SER:O	5:L:8:PRO:C	2.45	0.50
3:3:195:LEU:HD21	3:3:205:VAL:HG22	1.93	0.50
1:1:165:ASP:HB3	1:1:167:THR:OG1	2.12	0.50
1:1:136:GLN:HG2	1:1:235:HIS:CD2	2.47	0.50
3:3:210:PHE:N	3:3:210:PHE:CD1	2.79	0.50
5:L:36:PHE:CE2	6:H:103:TRP:NE1	2.69	0.50
5:L:89:GLN:OE1	6:H:100(K):MET:HE1	2.11	0.50
2:2:23:ILE:O	2:2:23:ILE:HG22	2.11	0.50
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.50
5:L:18:LYS:HG3	5:L:75:ILE:O	2.12	0.49
5:L:38:GLN:HE21	5:L:44:PRO:HD3	1.77	0.49
1:1:77:VAL:HG23	1:1:77:VAL:O	2.11	0.49
3:3:47:ILE:HG22	3:3:100:ILE:HD12	1.94	0.49
1:1:88:THR:HG23	1:1:88:THR:O	2.10	0.49
1:1:136:GLN:N	1:1:137:PRO:HD3	2.27	0.49
2:2:135:HIS:CB	2:2:160:ASN:ND2	2.75	0.49
5:L:58:VAL:O	5:L:58:VAL:CG2	2.60	0.49
1:1:46:LEU:CB	1:1:47:PRO:HD2	2.42	0.49
3:3:192:GLN:NE2	3:3:192:GLN:HA	2.26	0.49
3:3:54:PRO:HA	3:3:67:TYR:CD1	2.48	0.49
6:H:82(C):LEU:HB3	6:H:111:VAL:CG2	2.42	0.49
6:H:14:PRO:HD3	6:H:112:SER:C	2.32	0.49
1:1:21:ILE:HA	1:1:55:THR:HG23	1.95	0.49
1:1:94:ARG:NH1	6:H:56:ASP:OD2	2.45	0.49
3:3:52:LEU:HA	3:3:209:SER:O	2.13	0.49
6:H:33:TRP:CE3	6:H:50:GLN:NE2	2.80	0.49
5:L:21:ILE:HB	5:L:73:LEU:HB3	1.95	0.49
5:L:21:ILE:HG23	5:L:102:THR:OG1	2.12	0.49
1:1:81:GLU:HB3	1:1:240:LYS:CG	2.40	0.49
6:H:100(J):ALA:HB1	6:H:100(K):MET:HE3	1.94	0.49
6:H:24:ALA:HB1	6:H:27:TYR:CE2	2.47	0.49
6:H:4:LEU:HD12	6:H:93:ALA:HA	1.94	0.49
1:1:186:PHE:CD1	3:3:24:ALA:CB	2.92	0.49
1:1:230:ASN:OD1	1:1:230:ASN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:47:TRP:CZ2	5:L:62:PHE:CE2	3.00	0.49
1:1:119:PHE:HA	1:1:255:PRO:HA	1.94	0.49
1:1:47:PRO:C	1:1:49:ASP:H	2.16	0.49
2:2:166:VAL:O	2:2:173:MET:HG2	2.11	0.49
6:H:82(C):LEU:HB3	6:H:111:VAL:HG21	1.94	0.49
6:H:98:TYR:O	6:H:99:PRO:C	2.50	0.49
5:L:47:TRP:HZ2	5:L:62:PHE:CE2	2.31	0.49
2:2:126:VAL:CG2	2:2:199:ILE:HD12	2.43	0.49
3:3:26:PRO:C	3:3:28:TYR:H	2.16	0.49
1:1:102:TRP:O	1:1:223:SER:CA	2.60	0.49
1:1:94:ARG:C	1:1:96:ALA:N	2.64	0.49
3:3:131:TYR:HD1	3:3:186:PHE:O	1.96	0.49
6:H:12:VAL:HG11	6:H:18:VAL:CG1	2.41	0.49
6:H:36:TRP:HA	6:H:91:PHE:O	2.12	0.49
5:L:83:ALA:HA	5:L:104:LEU:O	2.12	0.49
2:2:120:GLY:O	2:2:191:LEU:HB2	2.13	0.49
6:H:95:SER:HA	6:H:100(K):MET:HA	1.94	0.49
5:L:30:VAL:O	5:L:71:TYR:CZ	2.66	0.49
3:3:104:TYR:O	3:3:176:THR:HG21	2.12	0.49
6:H:39:GLN:CB	6:H:45:LEU:HD23	2.39	0.48
6:H:81:GLN:HG2	6:H:82:LEU:N	2.25	0.48
1:1:82:ILE:HD12	1:1:228:ILE:HG13	1.95	0.48
5:L:47:TRP:O	5:L:55:ALA:HB3	2.12	0.48
5:L:54:LEU:C	5:L:55:ALA:O	2.50	0.48
1:1:122:VAL:CG1	1:1:124:PHE:CE2	2.95	0.48
3:3:54:PRO:C	3:3:56:ASN:H	2.17	0.48
2:2:150:GLY:O	2:2:151:GLU:C	2.52	0.48
1:1:41:ALA:CB	4:4:60:MET:HE2	2.43	0.48
5:L:49:TYR:CE1	5:L:55:ALA:HA	2.48	0.48
5:L:15:PRO:HB3	5:L:79:GLU:HA	1.95	0.48
2:2:184:PHE:HB3	2:2:185:PRO:CD	2.39	0.48
2:2:261:PRO:O	2:2:262:GLN:HB3	2.13	0.48
3:3:90:GLY:O	3:3:91:VAL:C	2.52	0.48
6:H:51:ILE:HD12	6:H:52:TYR:N	2.29	0.48
6:H:38:LYS:HE3	6:H:85:GLU:O	2.13	0.48
5:L:65:SER:O	5:L:71:TYR:HB3	2.12	0.48
3:3:47:ILE:HG21	3:3:100:ILE:HG21	1.95	0.48
1:1:201:TYR:CD2	1:1:201:TYR:O	2.66	0.48
6:H:40:ARG:CB	6:H:43:GLN:HB2	2.42	0.48
6:H:37:VAL:HG22	6:H:91:PHE:HD2	1.78	0.48
5:L:48:ILE:CD1	5:L:54:LEU:HD13	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:76:CYS:SG	1:1:77:VAL:N	2.87	0.48
2:2:65:THR:HA	2:2:243:THR:HG23	1.94	0.48
2:2:67:ASP:CG	2:2:68:SER:H	2.17	0.48
5:L:50:SER:OG	6:H:99:PRO:O	2.30	0.48
5:L:48:ILE:HD11	5:L:54:LEU:CD1	2.41	0.48
1:1:264:THR:O	1:1:265:SER:HB3	2.13	0.48
1:1:264:THR:OG1	1:1:270:ASN:HB2	2.13	0.48
3:3:104:TYR:HD2	3:3:219:LEU:HD23	1.79	0.48
1:1:124:PHE:CD1	1:1:124:PHE:C	2.87	0.48
1:1:261:LEU:HD12	1:1:271:TYR:CG	2.49	0.48
3:3:16:THR:O	3:3:16:THR:HG23	2.14	0.48
6:H:11:LEU:HD12	6:H:110:THR:O	2.13	0.48
6:H:3:GLN:O	6:H:23:LYS:O	2.31	0.48
5:L:78:MET:SD	5:L:106:ILE:HD13	2.53	0.48
5:L:74:THR:CG2	5:L:75:ILE:N	2.75	0.48
2:2:30:ASN:ND2	2:2:31:ALA:H	2.11	0.48
2:2:183:ILE:O	2:2:183:ILE:CG2	2.61	0.48
6:H:38:LYS:O	6:H:38:LYS:HG2	2.14	0.48
5:L:19:VAL:HG23	5:L:75:ILE:O	2.14	0.48
3:3:42:ASN:O	3:3:43:LEU:C	2.52	0.48
3:3:153:TRP:CD2	3:3:161:ILE:CG2	2.96	0.48
6:H:23:LYS:HA	6:H:76:THR:O	2.14	0.48
1:1:78:HIS:ND1	1:1:79:VAL:N	2.62	0.48
1:1:122:VAL:HG11	1:1:124:PHE:HE2	1.78	0.48
1:1:271:TYR:CB	1:1:272:PRO:CD	2.85	0.48
3:3:53:ILE:HD11	3:3:113:PHE:CE1	2.49	0.48
2:2:135:HIS:CG	2:2:160:ASN:HD22	2.32	0.48
1:1:87:ALA:O	1:1:89:GLY:N	2.47	0.48
1:1:285:ASP:HB3	1:1:288:SER:H	1.79	0.48
1:1:94:ARG:O	1:1:96:ALA:N	2.47	0.48
6:H:1:GLN:O	6:H:2:GLY:O	2.31	0.47
6:H:22:CYS:N	6:H:23:LYS:HE2	2.29	0.47
5:L:6:GLN:CG	5:L:100:SER:H	2.27	0.47
5:L:62:PHE:CE1	5:L:75:ILE:HD13	2.49	0.47
2:2:256:SER:O	2:2:257:LYS:O	2.31	0.47
1:1:163:TRP:C	1:1:163:TRP:CD1	2.83	0.47
5:L:44:PRO:CG	6:H:45:LEU:CD1	2.77	0.47
1:1:110:VAL:CG2	3:3:230:GLN:HG2	2.44	0.47
3:3:177:ASP:OD1	3:3:178:PRO:HD2	2.13	0.47
3:3:175:TYR:CB	3:3:182:THR:HG21	2.29	0.47
3:3:65:ASN:O	3:3:67:TYR:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:82:LEU:O	2:2:83:PRO:C	2.50	0.47
2:2:34:CYS:C	2:2:36:ALA:H	2.17	0.47
3:3:143:ARG:O	3:3:144:GLU:C	2.53	0.47
5:L:14:PHE:CG	5:L:107:LYS:CB	2.98	0.47
2:2:104:SER:OG	2:2:249:THR:CG2	2.51	0.47
3:3:36:ILE:HG22	3:3:37:PRO:HD2	1.96	0.47
5:L:85:THR:HA	5:L:103:LYS:HA	1.96	0.47
5:L:14:PHE:N	5:L:107:LYS:CB	2.75	0.47
1:1:121:TYR:CD2	2:2:206:SER:HB3	2.49	0.47
2:2:207:VAL:CG1	2:2:208:PRO:HD2	2.36	0.47
2:2:108:VAL:HG23	2:2:199:ILE:HB	1.95	0.47
6:H:4:LEU:H	6:H:102:TYR:HE2	1.62	0.47
2:2:123:LEU:HD13	2:2:188:PHE:HE1	1.80	0.47
3:3:63:GLU:C	3:3:65:ASN:H	2.18	0.47
2:2:122:LEU:HD22	2:2:222:VAL:CG1	2.44	0.47
6:H:100(J):ALA:HB1	6:H:100(K):MET:HE1	1.97	0.47
6:H:12:VAL:HG21	6:H:82(C):LEU:CD1	2.44	0.47
3:3:47:ILE:HG22	3:3:100:ILE:HD13	1.95	0.47
1:1:20:SER:O	1:1:54:ARG:O	2.31	0.47
3:3:26:PRO:O	3:3:28:TYR:N	2.47	0.47
1:1:93:HIS:CD2	1:1:93:HIS:N	2.82	0.47
6:H:4:LEU:N	6:H:102:TYR:CE2	2.82	0.47
5:L:107:LYS:HB3	5:L:107:LYS:HZ2	1.78	0.47
5:L:13:ALA:O	5:L:78:MET:HG2	2.15	0.47
6:H:39:GLN:HG3	6:H:45:LEU:HD23	1.95	0.47
5:L:78:MET:SD	5:L:106:ILE:CD1	3.02	0.47
1:1:46:LEU:HB3	1:1:47:PRO:HD2	1.96	0.47
2:2:30:ASN:HD21	4:4:58:ASP:H	1.63	0.47
1:1:123:ARG:O	1:1:124:PHE:HB3	2.15	0.47
3:3:126:LYS:HE2	3:3:154:ASP:CG	2.34	0.47
2:2:12:ARG:C	2:2:13:VAL:HG22	2.35	0.47
1:1:37:ASN:HB3	3:3:116:MET:CE	2.44	0.47
2:2:107:THR:O	2:2:244:ILE:HG23	2.15	0.47
1:1:285:ASP:HB3	1:1:287:LYS:H	1.80	0.47
1:1:232:HIS:C	1:1:233:ASP:O	2.53	0.47
2:2:33:VAL:HA	2:2:200:VAL:HG23	1.97	0.47
5:L:81:GLU:HG2	5:L:81:GLU:H	1.36	0.47
2:2:54:SER:C	2:2:55:LYS:HG3	2.34	0.47
3:3:7:LEU:HB3	3:3:8:PRO:HD2	1.97	0.47
1:1:127:GLU:HB3	1:1:246:ARG:HB3	1.97	0.47
6:H:6:GLN:H	6:H:105:GLN:NE2	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:49:TYR:HE1	5:L:55:ALA:HA	1.80	0.47
3:3:171:VAL:HG22	3:3:173:PHE:H	1.80	0.47
1:1:136:GLN:C	1:1:138:ASP:H	2.17	0.47
2:2:69:LYS:HG2	2:2:78:TRP:CE2	2.50	0.47
2:2:33:VAL:O	4:4:55:PRO:HB3	2.15	0.47
6:H:35:ASN:O	6:H:92:CYS:HA	2.15	0.47
5:L:7:SER:HB2	5:L:22:THR:H	1.80	0.47
5:L:43:SER:O	5:L:45:LYS:CE	2.63	0.47
5:L:54:LEU:HD13	5:L:58:VAL:CG2	2.41	0.47
1:1:268:ARG:CG	1:1:268:ARG:HH11	2.25	0.47
3:3:42:ASN:C	3:3:44:LEU:N	2.68	0.47
1:1:251:GLU:HB3	1:1:253:TRP:CH2	2.50	0.47
2:2:135:HIS:CB	2:2:160:ASN:HD22	2.28	0.47
6:H:34:VAL:HG21	6:H:78:ALA:HB2	1.97	0.47
1:1:78:HIS:N	1:1:109:LEU:CD1	2.78	0.47
2:2:171:TYR:C	2:2:173:MET:N	2.65	0.47
1:1:147:VAL:HG13	1:1:178:PHE:O	2.15	0.47
2:2:71:TRP:NE1	2:2:228:LEU:HB2	2.30	0.47
3:3:141:ASP:O	3:3:142:ARG:O	2.33	0.47
6:H:40:ARG:CB	6:H:43:GLN:CB	2.92	0.46
6:H:40:ARG:CB	6:H:43:GLN:HG3	2.31	0.46
6:H:39:GLN:CG	6:H:45:LEU:HD23	2.45	0.46
5:L:94:TYR:C	5:L:94:TYR:CD1	2.78	0.46
1:1:204:TYR:CZ	1:1:213:TYR:HB2	2.50	0.46
3:3:142:ARG:O	3:3:143:ARG:O	2.32	0.46
2:2:42:LEU:HD12	2:2:43:PRO:CD	2.43	0.46
1:1:231:GLU:O	1:1:232:HIS:C	2.54	0.46
6:H:29:PHE:O	6:H:52(A):PRO:HG2	2.15	0.46
2:2:17:THR:OG1	2:2:22:THR:HG23	2.16	0.46
5:L:44:PRO:HD3	6:H:91:PHE:CZ	2.50	0.46
5:L:14:PHE:CE2	5:L:107:LYS:HB3	2.51	0.46
1:1:35:THR:OG1	1:1:36:ALA:N	2.48	0.46
3:3:53:ILE:HD11	3:3:113:PHE:HE1	1.80	0.46
1:1:260:ALA:HB2	2:2:177:LEU:CD1	2.44	0.46
1:1:166:TYR:HE1	1:1:167:THR:HG23	1.79	0.46
2:2:25:THR:O	2:2:25:THR:HG23	2.14	0.46
6:H:4:LEU:HB2	6:H:102:TYR:HE2	1.81	0.46
5:L:18:LYS:HA	5:L:77:ARG:CA	2.45	0.46
3:3:76:GLN:C	3:3:78:GLU:H	2.16	0.46
2:2:92:PHE:C	2:2:92:PHE:CD1	2.89	0.46
6:H:38:LYS:HD2	6:H:90:TYR:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:50:GLN:O	6:H:50:GLN:HG3	2.16	0.46
6:H:23:LYS:CD	6:H:77:THR:HG22	2.40	0.46
5:L:17:GLU:O	5:L:77:ARG:HA	2.16	0.46
2:2:181:LEU:HD12	2:2:181:LEU:HA	1.80	0.46
2:2:125:VAL:HG22	2:2:126:VAL:N	2.31	0.46
2:2:86:LEU:C	2:2:88:ASP:N	2.66	0.46
5:L:47:TRP:CE3	5:L:47:TRP:HA	2.50	0.46
1:1:19:ALA:HB3	1:1:56:THR:CB	2.45	0.46
3:3:186:PHE:CD1	3:3:186:PHE:N	2.83	0.46
6:H:97:ASN:C	6:H:99:PRO:HD2	2.37	0.46
1:1:168:TRP:CZ3	1:1:227:ARG:HG2	2.51	0.46
2:2:114:ALA:HB2	2:2:238:LEU:CD2	2.46	0.46
6:H:62:LYS:CG	6:H:63:PHE:CD1	2.99	0.46
6:H:34:VAL:O	6:H:50:GLN:HA	2.15	0.46
5:L:33:MET:CE	5:L:89:GLN:N	2.78	0.46
3:3:40:VAL:HG12	3:3:41:HIS:N	2.31	0.46
1:1:102:TRP:CE3	1:1:104:ILE:HG23	2.51	0.46
3:3:75:ARG:HB2	3:3:191:TYR:HE2	1.81	0.46
2:2:246:PRO:O	2:2:247:MET:HB3	2.15	0.46
6:H:40:ARG:O	6:H:43:GLN:HB2	2.15	0.45
5:L:13:ALA:HB3	5:L:78:MET:CG	2.45	0.45
1:1:264:THR:O	1:1:265:SER:CB	2.63	0.45
1:1:69:CYS:O	1:1:71:LEU:N	2.34	0.45
1:1:70:PHE:CD2	3:3:43:LEU:HD11	2.49	0.45
3:3:130:ALA:HA	3:3:150:HIS:HA	1.97	0.45
6:H:29:PHE:C	6:H:31:SER:H	2.19	0.45
6:H:33:TRP:CD2	6:H:52:TYR:HB2	2.51	0.45
1:1:67:VAL:CG2	3:3:41:HIS:C	2.84	0.45
3:3:19:ARG:NE	3:3:19:ARG:CA	2.42	0.45
1:1:204:TYR:CZ	2:2:144:TYR:HA	2.52	0.45
5:L:91:ARG:CZ	6:H:100(J):ALA:HA	2.47	0.45
1:1:265:SER:HB2	3:3:235:THR:O	2.16	0.45
3:3:71:LEU:HB3	3:3:195:LEU:HD22	1.98	0.45
3:3:57:ASN:H	3:3:57:ASN:ND2	2.13	0.45
3:3:80:VAL:HG12	3:3:81:PHE:HD2	1.81	0.45
2:2:76:LYS:CG	2:2:169:VAL:CG1	2.94	0.45
5:L:39:LYS:HG2	5:L:84:ALA:HB2	1.99	0.45
3:3:100:ILE:O	3:3:103:TYR:HB2	2.17	0.45
3:3:108:SER:HB2	3:3:173:PHE:HD1	1.80	0.45
3:3:71:LEU:HA	3:3:71:LEU:HD12	1.62	0.45
2:2:137:GLY:O	2:2:138:GLY:O	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:169:VAL:HG23	2:2:170:LEU:N	2.32	0.45
1:1:50:SER:O	1:1:51:ILE:HG23	2.17	0.45
1:1:97:LYS:HD2	6:H:52:TYR:CE2	2.47	0.45
5:L:85:THR:HG23	5:L:103:LYS:HG2	1.97	0.45
5:L:89:GLN:HG3	5:L:98:PHE:CE2	2.51	0.45
3:3:70:PRO:HA	3:3:206:TYR:CD1	2.51	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD21	1.80	0.45
1:1:180:VAL:C	1:1:182:ASP:N	2.70	0.45
1:1:195:SER:O	1:1:196:ALA:CB	2.65	0.45
2:2:65:THR:O	2:2:66:LEU:O	2.34	0.45
1:1:213:TYR:OH	2:2:131:GLN:HA	2.17	0.45
3:3:83:THR:CG2	3:3:187:LEU:CD2	2.93	0.45
2:2:111:GLN:CG	2:2:196:THR:HG22	2.45	0.45
5:L:13:ALA:O	5:L:78:MET:CG	2.65	0.45
1:1:129:THR:O	1:1:129:THR:HG22	2.17	0.45
2:2:27:GLU:HG3	2:2:194:ASN:HA	1.99	0.45
2:2:108:VAL:O	2:2:110:VAL:N	2.50	0.45
1:1:130:ILE:HB	1:1:178:PHE:HE2	1.82	0.45
5:L:82:ASP:O	5:L:104:LEU:HG	2.16	0.45
1:1:79:VAL:O	1:1:79:VAL:HG12	2.16	0.45
2:2:63:PHE:HD1	2:2:245:ALA:HB2	1.65	0.45
3:3:175:TYR:HD2	3:3:182:THR:CG2	2.30	0.45
1:1:194:ALA:C	1:1:196:ALA:N	2.71	0.45
1:1:74:ALA:HB3	3:3:15:THR:O	2.17	0.45
1:1:74:ALA:HB3	3:3:15:THR:CA	2.47	0.45
6:H:8:GLY:O	6:H:9:ALA:C	2.55	0.45
1:1:45:VAL:HG23	3:3:112:ARG:HD3	1.99	0.44
3:3:173:PHE:CD2	3:3:220:ARG:NH1	2.84	0.44
3:3:127:LEU:HA	3:3:192:GLN:HB2	1.99	0.44
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.78	0.44
6:H:38:LYS:HD2	6:H:90:TYR:HE1	1.81	0.44
1:1:34:LEU:HD23	3:3:161:ILE:HA	1.99	0.44
3:3:71:LEU:HD22	3:3:207:LEU:HD23	1.98	0.44
2:2:228:LEU:HD22	2:2:238:LEU:HB2	1.98	0.44
2:2:33:VAL:HG22	2:2:200:VAL:CG2	2.47	0.44
6:H:12:VAL:HG11	6:H:18:VAL:HG22	1.99	0.44
6:H:38:LYS:CD	6:H:90:TYR:HE1	2.30	0.44
5:L:44:PRO:HG2	6:H:45:LEU:HD11	1.91	0.44
1:1:129:THR:OG1	1:1:185:ARG:HD2	2.16	0.44
2:2:65:THR:OG1	2:2:243:THR:HG23	2.16	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:136:GLN:HB2	1:1:136:GLN:HE21	1.61	0.44
6:H:105:GLN:CG	6:H:106:GLY:N	2.65	0.44
5:L:77:ARG:O	5:L:77:ARG:CD	2.64	0.44
2:2:148:HIS:N	2:2:149:PRO:HD3	2.32	0.44
1:1:136:GLN:OE1	1:1:237:THR:HG23	2.17	0.44
1:1:232:HIS:CG	1:1:232:HIS:O	2.71	0.44
1:1:232:HIS:O	1:1:233:ASP:O	2.35	0.44
2:2:99:HIS:CD2	2:2:254:ILE:HA	2.51	0.44
2:2:254:ILE:HG12	2:2:255:ARG:H	1.82	0.44
1:1:271:TYR:HA	1:1:272:PRO:HD3	1.58	0.44
6:H:97:ASN:O	6:H:99:PRO:CD	2.65	0.44
6:H:97:ASN:O	6:H:99:PRO:HD2	2.18	0.44
2:2:190:ASN:H	2:2:194:ASN:HB2	1.82	0.44
6:H:7:SER:OG	6:H:8:GLY:N	2.50	0.44
6:H:22:CYS:CA	6:H:23:LYS:HE2	2.48	0.44
6:H:27:TYR:HD1	6:H:32:PHE:HE1	1.63	0.44
6:H:83:THR:C	6:H:85:GLU:H	2.21	0.44
2:2:22:THR:HG22	2:2:23:ILE:H	1.83	0.44
1:1:178:PHE:HD2	1:1:184:SER:CB	2.24	0.44
1:1:152:TYR:C	1:1:152:TYR:HD1	2.21	0.44
5:L:19:VAL:O	5:L:74:THR:HA	2.17	0.44
5:L:67:SER:CA	5:L:71:TYR:CE1	2.92	0.44
3:3:54:PRO:HA	3:3:67:TYR:HD1	1.83	0.44
2:2:57:ASP:HB3	2:2:58:THR:H	1.59	0.44
2:2:122:LEU:HB2	2:2:189:ILE:HB	1.98	0.44
2:2:199:ILE:HG22	2:2:201:ILE:HG13	2.00	0.44
1:1:162:GLU:C	1:1:164:ASP:H	2.20	0.44
1:1:162:GLU:C	1:1:164:ASP:N	2.71	0.44
3:3:120:PRO:O	3:3:121:ALA:C	2.55	0.44
1:1:74:ALA:CB	3:3:15:THR:O	2.66	0.43
5:L:23:CYS:HB2	5:L:88:CYS:CB	2.48	0.43
1:1:69:CYS:C	1:1:71:LEU:N	2.71	0.43
2:2:12:ARG:HH22	3:3:157:LEU:HG	1.83	0.43
5:L:38:GLN:HG2	5:L:44:PRO:HA	2.00	0.43
3:3:41:HIS:N	3:3:45:GLU:OE2	2.44	0.43
2:2:63:PHE:CE1	2:2:245:ALA:HB2	2.48	0.43
1:1:209:ALA:N	2:2:261:PRO:HB3	2.30	0.43
3:3:75:ARG:O	3:3:194:SER:HB3	2.18	0.43
6:H:62:LYS:HG3	6:H:63:PHE:CG	2.53	0.43
1:1:146:LEU:H	1:1:146:LEU:HG	1.43	0.43
1:1:273:LYS:HE2	2:2:136:GLU:C	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:108:ARG:HG3	5:L:109:ALA:O	2.18	0.43
1:1:35:THR:O	3:3:160:THR:HB	2.18	0.43
1:1:271:TYR:CB	1:1:272:PRO:HD2	2.28	0.43
3:3:133:PRO:CB	3:3:134:PRO:CD	2.95	0.43
2:2:34:CYS:SG	2:2:201:ILE:HA	2.57	0.43
3:3:84:ASN:HA	3:3:186:PHE:HA	2.00	0.43
3:3:211:ILE:O	3:3:211:ILE:HG23	2.17	0.43
6:H:22:CYS:C	6:H:23:LYS:CD	2.87	0.43
5:L:35:TRP:HB2	5:L:48:ILE:HB	2.00	0.43
5:L:91:ARG:NE	6:H:100(K):MET:HE3	2.33	0.43
1:1:78:HIS:CA	1:1:109:LEU:CD1	2.95	0.43
1:1:209:ALA:HA	2:2:144:TYR:HB3	1.99	0.43
2:2:195:ASN:ND2	2:2:196:THR:N	2.58	0.43
2:2:106:TYR:HD1	2:2:246:PRO:HA	1.83	0.43
5:L:47:TRP:C	5:L:48:ILE:HD12	2.38	0.43
3:3:153:TRP:CD1	3:3:154:ASP:N	2.87	0.43
1:1:121:TYR:CE2	2:2:206:SER:HB3	2.53	0.43
2:2:181:LEU:C	2:2:183:ILE:N	2.72	0.43
6:H:40:ARG:CB	6:H:41:PRO:HD2	2.49	0.43
5:L:91:ARG:NH1	5:L:91:ARG:CG	2.65	0.43
3:3:217:PHE:CE2	3:3:219:LEU:CD1	3.01	0.43
2:2:124:VAL:O	2:2:186:HIS:HB2	2.19	0.43
2:2:247:MET:O	2:2:248:CYS:HB2	2.19	0.43
6:H:17:SER:CB	6:H:82(A):TYR:HA	2.42	0.43
5:L:62:PHE:CE1	5:L:75:ILE:CG1	3.00	0.43
3:3:176:THR:OG1	3:3:177:ASP:N	2.52	0.43
1:1:168:TRP:CH2	1:1:227:ARG:HB3	2.54	0.43
2:2:71:TRP:CZ2	2:2:228:LEU:HB2	2.54	0.43
1:1:28:THR:HB	1:1:30:LYS:H	1.84	0.43
3:3:55:MET:SD	3:3:81:PHE:CD1	3.12	0.43
6:H:73:LYS:H	6:H:73:LYS:HG2	1.52	0.43
6:H:49:GLY:O	6:H:50:GLN:HB3	2.18	0.43
1:1:212:GLN:HE22	1:1:268:ARG:HE	1.66	0.43
1:1:159:ASN:HA	1:1:160:PRO:HD3	1.93	0.43
1:1:101:ASP:HA	1:1:225:ALA:HA	2.00	0.43
6:H:99:PRO:HD2	6:H:100(I):TYR:CE1	2.54	0.42
6:H:97:ASN:ND2	6:H:101:ASP:OD1	2.51	0.42
1:1:129:THR:OG1	1:1:185:ARG:HD3	2.18	0.42
1:1:77:VAL:O	1:1:78:HIS:HB2	2.19	0.42
1:1:116:LEU:C	1:1:118:LEU:H	2.23	0.42
1:1:70:PHE:CD2	3:3:43:LEU:HD21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:195:LEU:CD2	3:3:205:VAL:CG2	2.95	0.42
2:2:48:SER:O	2:2:49:ASP:C	2.56	0.42
5:L:7:SER:CB	5:L:22:THR:CB	2.96	0.42
5:L:94:TYR:HE1	5:L:96:ILE:HG13	1.84	0.42
1:1:46:LEU:CB	1:1:47:PRO:CD	2.96	0.42
3:3:53:ILE:HG21	3:3:53:ILE:HD13	1.84	0.42
1:1:165:ASP:HB2	1:1:168:TRP:CD1	2.55	0.42
3:3:190:TRP:N	3:3:190:TRP:CD1	2.86	0.42
3:3:75:ARG:HB2	3:3:191:TYR:CE2	2.55	0.42
2:2:143:LYS:H	2:2:143:LYS:HG2	1.62	0.42
6:H:69:LEU:HA	6:H:69:LEU:HD23	1.78	0.42
5:L:66:GLY:HA3	5:L:71:TYR:HA	2.01	0.42
1:1:215:ILE:C	1:1:217:VAL:N	2.70	0.42
5:L:14:PHE:HD2	5:L:107:LYS:HD3	1.80	0.42
2:2:190:ASN:C	2:2:192:ARG:N	2.63	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
2:2:84:ASP:O	2:2:85:ALA:C	2.58	0.42
3:3:195:LEU:CD2	3:3:205:VAL:HG22	2.49	0.42
1:1:208:ASP:O	1:1:211:THR:HG22	2.18	0.42
1:1:153:VAL:CG1	1:1:153:VAL:O	2.67	0.42
1:1:285:ASP:CB	1:1:288:SER:H	2.33	0.42
3:3:145:ALA:O	3:3:147:LEU:N	2.52	0.42
5:L:31:ASN:C	5:L:32:TYR:CD2	2.93	0.42
2:2:20:ASN:O	2:2:20:ASN:CG	2.57	0.42
1:1:269:THR:O	2:2:133:ALA:HB2	2.20	0.42
5:L:10:ILE:HG12	5:L:11:MET:N	2.35	0.42
5:L:47:TRP:O	5:L:58:VAL:HG21	2.20	0.42
3:3:2:LEU:HD12	3:3:3:PRO:O	2.19	0.42
2:2:65:THR:CG2	2:2:65:THR:O	2.65	0.42
6:H:17:SER:CB	6:H:82:LEU:O	2.65	0.42
5:L:14:PHE:N	5:L:107:LYS:CG	2.80	0.42
1:1:185:ARG:NH2	3:3:17:ASP:HB3	2.33	0.42
1:1:58:MET:O	1:1:59:HIS:C	2.58	0.42
2:2:34:CYS:C	2:2:36:ALA:N	2.72	0.42
1:1:135:SER:O	1:1:137:PRO:HD3	2.19	0.42
2:2:160:ASN:HA	2:2:167:LYS:HZ3	1.82	0.42
5:L:78:MET:HE2	5:L:82:ASP:HB2	1.98	0.42
5:L:95:PRO:O	5:L:96:ILE:O	2.38	0.42
2:2:12:ARG:HH22	3:3:157:LEU:CG	2.33	0.42
1:1:281:LYS:CG	1:1:282:ARG:N	2.75	0.42
5:L:36:PHE:HE2	6:H:103:TRP:CE2	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:4:LEU:HD22	5:L:4:LEU:HA	1.80	0.42
5:L:7:SER:C	5:L:8:PRO:O	2.56	0.42
4:4:49:PRO:CB	4:4:53:THR:OG1	2.65	0.42
4:4:33:LYS:HG2	4:4:33:LYS:O	2.20	0.42
3:3:29:GLU:HA	3:3:30:PRO:HD3	1.54	0.42
6:H:91:PHE:CB	6:H:103:TRP:HZ3	2.33	0.42
6:H:66:LYS:NZ	6:H:83:THR:HG22	2.35	0.42
5:L:107:LYS:NZ	5:L:107:LYS:CB	2.82	0.42
5:L:11:MET:HB2	5:L:12:SER:H	1.40	0.42
5:L:86:TYR:HE2	5:L:104:LEU:CB	2.33	0.42
2:2:72:THR:C	2:2:74:GLY:N	2.72	0.42
1:1:58:MET:C	1:1:59:HIS:CD2	2.93	0.42
2:2:190:ASN:O	2:2:191:LEU:C	2.57	0.42
2:2:104:SER:HG	2:2:249:THR:HG23	1.81	0.42
2:2:108:VAL:O	2:2:109:HIS:C	2.56	0.42
1:1:287:LYS:CE	3:3:79:GLN:HB3	2.45	0.42
6:H:91:PHE:CG	6:H:103:TRP:HZ3	2.38	0.41
6:H:70:THR:CG2	6:H:79:TYR:HB2	2.50	0.41
3:3:47:ILE:CG2	3:3:100:ILE:HD13	2.49	0.41
1:1:255:PRO:HG3	3:3:46:ILE:HG21	2.02	0.41
1:1:31:VAL:HG12	1:1:31:VAL:O	2.20	0.41
2:2:256:SER:O	2:2:257:LYS:HB3	2.20	0.41
5:L:30:VAL:O	5:L:30:VAL:HG12	2.19	0.41
2:2:228:LEU:CD2	2:2:238:LEU:HB2	2.51	0.41
1:1:50:SER:C	1:1:51:ILE:HG23	2.41	0.41
6:H:29:PHE:CD2	6:H:76:THR:HA	2.55	0.41
5:L:3:VAL:O	5:L:25:ALA:HA	2.19	0.41
1:1:110:VAL:HG11	3:3:230:GLN:HB3	2.02	0.41
2:2:26:GLN:O	2:2:27:GLU:OE1	2.38	0.41
2:2:168:ASP:H	2:2:173:MET:HG3	1.85	0.41
3:3:71:LEU:CD2	3:3:207:LEU:HD21	2.44	0.41
6:H:80:MET:HE2	6:H:82:LEU:CG	2.50	0.41
1:1:213:TYR:HB3	2:2:142:VAL:O	2.19	0.41
1:1:253:TRP:CD1	3:3:36:ILE:CG1	3.03	0.41
1:1:136:GLN:O	1:1:138:ASP:N	2.53	0.41
6:H:14:PRO:HA	6:H:111:VAL:CG1	2.50	0.41
5:L:86:TYR:HE2	5:L:104:LEU:HB2	1.85	0.41
2:2:63:PHE:CE1	2:2:245:ALA:CB	3.03	0.41
2:2:217:ASN:O	2:2:218:VAL:CG1	2.61	0.41
2:2:150:GLY:C	2:2:152:ARG:H	2.23	0.41
3:3:128:ILE:HG21	3:3:128:ILE:HD13	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:170:LEU:CD1	2:2:170:LEU:O	2.66	0.41
5:L:11:MET:HE1	5:L:104:LEU:HD13	2.02	0.41
3:3:43:LEU:O	3:3:47:ILE:HG23	2.20	0.41
1:1:194:ALA:HA	3:3:31:THR:HG21	2.02	0.41
1:1:165:ASP:HB2	1:1:168:TRP:HD1	1.85	0.41
1:1:254:ILE:HD13	2:2:204:ILE:HG21	2.01	0.41
2:2:41:TYR:CD1	2:2:41:TYR:N	2.89	0.41
2:2:183:ILE:O	2:2:183:ILE:HG22	2.20	0.41
5:L:103:LYS:C	5:L:103:LYS:HD3	2.41	0.41
5:L:47:TRP:O	5:L:48:ILE:HD12	2.20	0.41
1:1:110:VAL:CG2	3:3:230:GLN:CG	2.95	0.41
2:2:125:VAL:CG2	2:2:126:VAL:N	2.84	0.41
3:3:221:LEU:C	3:3:221:LEU:CD2	2.89	0.41
6:H:4:LEU:N	6:H:102:TYR:HE2	2.18	0.41
6:H:2:GLY:HA3	6:H:27:TYR:HD2	1.85	0.41
5:L:61:ARG:NE	5:L:79:GLU:HG2	2.36	0.41
5:L:6:GLN:CG	5:L:100:SER:OG	2.69	0.41
5:L:6:GLN:HE21	5:L:6:GLN:HB3	1.70	0.41
2:2:215:HIS:HD2	2:2:216:ASN:H	1.68	0.41
3:3:115:LEU:HG	3:3:207:LEU:HD12	2.03	0.41
3:3:125:ALA:HB2	3:3:195:LEU:CD1	2.51	0.41
1:1:251:GLU:HB3	1:1:253:TRP:CZ3	2.55	0.41
2:2:81:LYS:HG3	2:2:219:SER:HB3	2.01	0.41
2:2:111:GLN:HA	2:2:196:THR:HG22	2.03	0.41
6:H:7:SER:HB3	6:H:21:SER:H	1.86	0.41
3:3:102:GLN:O	3:3:223:LYS:HE3	2.20	0.41
1:1:226:PHE:CD1	1:1:226:PHE:N	2.88	0.41
1:1:45:VAL:O	1:1:46:LEU:CD2	2.62	0.41
2:2:82:LEU:HB2	2:2:218:VAL:O	2.21	0.41
2:2:114:ALA:HB2	2:2:238:LEU:HD21	2.03	0.41
2:2:76:LYS:HD3	2:2:169:VAL:CG2	2.50	0.41
6:H:4:LEU:HG	6:H:102:TYR:CE2	2.54	0.40
5:L:78:MET:HB2	5:L:78:MET:HE2	1.93	0.40
3:3:46:ILE:HG21	3:3:46:ILE:HD13	1.84	0.40
1:1:34:LEU:HA	1:1:34:LEU:HD23	1.81	0.40
3:3:70:PRO:HA	3:3:206:TYR:HD1	1.87	0.40
6:H:8:GLY:O	6:H:9:ALA:O	2.40	0.40
6:H:48:ILE:CG2	6:H:67:ALA:HB2	2.51	0.40
5:L:91:ARG:HH11	5:L:91:ARG:CG	2.01	0.40
2:2:242:VAL:CG1	2:2:243:THR:N	2.84	0.40
2:2:160:ASN:HA	2:2:167:LYS:HZ2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:38:LYS:CE	6:H:85:GLU:O	2.69	0.40
6:H:52:TYR:CE1	6:H:53:GLY:HA3	2.57	0.40
6:H:57:ASN:O	6:H:58:LYS:HG2	2.20	0.40
6:H:90:TYR:HD2	6:H:109:VAL:HG21	1.85	0.40
5:L:3:VAL:H	5:L:26:THR:CG2	2.30	0.40
3:3:151:VAL:HG21	3:3:163:MET:HG2	1.94	0.40
1:1:195:SER:CB	3:3:34:ILE:HG12	2.51	0.40
2:2:183:ILE:HG13	3:3:96:LEU:CD2	2.48	0.40
2:2:34:CYS:HB3	2:2:185:PRO:CB	2.52	0.40
1:1:285:ASP:HB3	1:1:287:LYS:N	2.35	0.40
3:3:86:PHE:N	3:3:86:PHE:CD1	2.89	0.40
5:L:79:GLU:HB2	5:L:82:ASP:OD1	2.21	0.40
3:3:156:GLY:O	3:3:157:LEU:C	2.60	0.40
2:2:65:THR:OG1	2:2:243:THR:CG2	2.69	0.40
1:1:187:SER:O	3:3:23:SER:HA	2.22	0.40
3:3:197:LEU:HA	3:3:197:LEU:HD23	1.81	0.40
5:L:16:GLY:HA2	5:L:77:ARG:HB2	2.03	0.40
1:1:110:VAL:HA	1:1:113:ARG:HB3	2.02	0.40
1:1:265:SER:HG	1:1:268:ARG:HG3	1.85	0.40
2:2:16:ILE:O	2:2:22:THR:HA	2.21	0.40
2:2:108:VAL:HA	2:2:243:THR:O	2.22	0.40
3:3:14:LEU:HD12	3:3:15:THR:H	1.82	0.40
2:2:96:MET:O	2:2:96:MET:HG3	2.20	0.40
2:2:170:LEU:HA	2:2:170:LEU:HD22	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	271/289 (94%)	205 (76%)	44 (16%)	22 (8%)	1 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	253/262 (97%)	162 (64%)	56 (22%)	35 (14%)	0	6
3	3	234/236 (99%)	172 (74%)	38 (16%)	24 (10%)	1	12
4	4	38/68 (56%)	23 (60%)	11 (29%)	4 (10%)	1	11
5	L	108/110 (98%)	73 (68%)	19 (18%)	16 (15%)	0	5
6	H	117/119 (98%)	84 (72%)	23 (20%)	10 (8%)	1	17
All	All	1021/1084 (94%)	719 (70%)	191 (19%)	111 (11%)	0	11

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	27	HIS
1	1	45	VAL
1	1	88	THR
1	1	142	TYR
1	1	195	SER
1	1	207	ASP
1	1	233	ASP
1	1	249	HIS
2	2	28	ALA
2	2	66	LEU
2	2	85	ALA
2	2	87	LYS
2	2	151	GLU
2	2	191	LEU
2	2	256	SER
3	3	27	ASN
3	3	43	LEU
3	3	58	THR
3	3	99	GLU
3	3	141	ASP
3	3	142	ARG
3	3	143	ARG
3	3	189	CYS
4	4	47	MET
4	4	50	SER
5	L	7	SER
5	L	10	ILE
5	L	55	ALA
5	L	63	SER
5	L	76	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	96	ILE
6	H	2	GLY
6	H	80	MET
6	H	98	TYR
1	1	48	SER
1	1	196	ALA
2	2	13	VAL
2	2	19	GLY
2	2	57	ASP
2	2	90	GLY
2	2	95	ASN
2	2	138	GLY
2	2	160	ASN
2	2	172	ASN
2	2	174	ASN
2	2	182	LEU
2	2	195	ASN
2	2	218	VAL
2	2	255	ARG
2	2	257	LYS
3	3	38	GLY
3	3	55	MET
3	3	90	GLY
3	3	91	VAL
3	3	146	MET
3	3	221	LEU
5	L	65	SER
5	L	77	ARG
5	L	83	ALA
6	H	9	ALA
6	H	29	PHE
6	H	30	SER
6	H	100(J)	ALA
1	1	62	GLY
1	1	70	PHE
1	1	71	LEU
2	2	45	VAL
2	2	109	HIS
2	2	112	CYS
2	2	149	PRO
2	2	231	PRO
3	3	83	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	138	GLY
3	3	157	LEU
3	3	194	SER
3	3	217	PHE
4	4	43	GLN
5	L	46	LEU
5	L	67	SER
5	L	81	GLU
6	H	100(K)	MET
1	1	95	GLU
1	1	163	TRP
1	1	232	HIS
2	2	30	ASN
2	2	108	VAL
2	2	186	HIS
3	3	121	ALA
4	4	66	ALA
5	L	50	SER
5	L	95	PRO
6	H	50	GLN
6	H	84	SER
1	1	139	SER
2	2	144	TYR
2	2	208	PRO
3	3	98	GLY
1	1	51	ILE
2	2	56	PRO
2	2	114	ALA
2	2	224	PRO
3	3	69	ILE
3	3	87	ILE
1	1	25	PRO
1	1	137	PRO
1	1	33	ILE
1	1	254	ILE
5	L	75	ILE
5	L	101	GLY
2	2	60	VAL
3	3	34	ILE

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	1	239/253 (94%)	149 (62%)	90 (38%)	0	1
2	2	223/229 (97%)	141 (63%)	82 (37%)	0	1
3	3	209/209 (100%)	142 (68%)	67 (32%)	0	3
4	4	33/57 (58%)	19 (58%)	14 (42%)	0	0
5	L	92/92 (100%)	52 (56%)	40 (44%)	0	0
6	H	96/96 (100%)	62 (65%)	34 (35%)	0	1
All	All	892/936 (95%)	565 (63%)	327 (37%)	0	1

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	THR
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	35	THR
1	1	43	MET
1	1	45	VAL
1	1	46	LEU
1	1	50	SER
1	1	55	THR
1	1	56	THR
1	1	58	MET
1	1	59	HIS
1	1	61	ASN
1	1	67	VAL
1	1	71	LEU
1	1	85	LYS
1	1	88	THR
1	1	91	ASP
1	1	94	ARG
1	1	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	103	LYS
1	1	104	ILE
1	1	105	ASN
1	1	108	SER
1	1	111	GLN
1	1	116	LEU
1	1	118	LEU
1	1	119	PHE
1	1	126	SER
1	1	129	THR
1	1	131	LEU
1	1	133	THR
1	1	136	GLN
1	1	139	SER
1	1	141	ASN
1	1	145	ASN
1	1	146	LEU
1	1	152	TYR
1	1	159	ASN
1	1	161	LYS
1	1	162	GLU
1	1	163	TRP
1	1	165	ASP
1	1	166	TYR
1	1	167	THR
1	1	177	PHE
1	1	178	PHE
1	1	180	VAL
1	1	182	ASP
1	1	184	SER
1	1	185	ARG
1	1	186	PHE
1	1	187	SER
1	1	190	TYR
1	1	191	VAL
1	1	193	LEU
1	1	195	SER
1	1	199	CYS
1	1	200	PHE
1	1	207	ASP
1	1	210	GLU
1	1	212	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	215	ILE
1	1	216	THR
1	1	220	HIS
1	1	221	MET
1	1	226	PHE
1	1	229	VAL
1	1	230	ASN
1	1	234	GLU
1	1	237	THR
1	1	241	ILE
1	1	242	ARG
1	1	243	VAL
1	1	245	HIS
1	1	250	VAL
1	1	256	ARG
1	1	261	LEU
1	1	265	SER
1	1	268	ARG
1	1	269	THR
1	1	273	LYS
1	1	275	THR
1	1	279	ILE
1	1	280	LYS
1	1	282	ARG
1	1	286	ILE
1	1	288	SER
2	2	9	TYR
2	2	13	VAL
2	2	15	GLN
2	2	18	LEU
2	2	20	ASN
2	2	22	THR
2	2	27	GLU
2	2	30	ASN
2	2	32	VAL
2	2	34	CYS
2	2	40	GLU
2	2	45	VAL
2	2	49	ASP
2	2	50	VAL
2	2	52	LYS
2	2	54	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	63	PHE
2	2	65	THR
2	2	66	LEU
2	2	69	LYS
2	2	70	THR
2	2	72	THR
2	2	73	THR
2	2	75	SER
2	2	76	LYS
2	2	79	CYS
2	2	81	LYS
2	2	82	LEU
2	2	84	ASP
2	2	88	ASP
2	2	91	VAL
2	2	96	MET
2	2	98	PHE
2	2	101	LEU
2	2	104	SER
2	2	108	VAL
2	2	110	VAL
2	2	119	SER
2	2	121	CYS
2	2	139	ASN
2	2	143	LYS
2	2	145	THR
2	2	147	THR
2	2	151	GLU
2	2	152	ARG
2	2	154	ILE
2	2	156	LEU
2	2	157	SER
2	2	158	SER
2	2	161	GLU
2	2	166	VAL
2	2	167	LYS
2	2	170	LEU
2	2	172	ASN
2	2	173	MET
2	2	174	ASN
2	2	177	LEU
2	2	183	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	190	ASN
2	2	192	ARG
2	2	195	ASN
2	2	198	THR
2	2	200	VAL
2	2	207	VAL
2	2	212	MET
2	2	217	ASN
2	2	218	VAL
2	2	221	MET
2	2	225	ILE
2	2	229	THR
2	2	232	THR
2	2	235	THR
2	2	237	SER
2	2	239	PRO
2	2	242	VAL
2	2	243	THR
2	2	247	MET
2	2	249	THR
2	2	254	ILE
2	2	255	ARG
2	2	257	LYS
2	2	262	GLN
3	3	2	LEU
3	3	10	SER
3	3	14	LEU
3	3	16	THR
3	3	17	ASP
3	3	19	ARG
3	3	21	SER
3	3	29	GLU
3	3	36	ILE
3	3	42	ASN
3	3	44	LEU
3	3	48	GLN
3	3	50	ASP
3	3	51	THR
3	3	53	ILE
3	3	55	MET
3	3	56	ASN
3	3	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	60	THR
3	3	61	LYS
3	3	64	VAL
3	3	71	LEU
3	3	84	ASN
3	3	89	ASP
3	3	91	VAL
3	3	93	LYS
3	3	94	THR
3	3	95	THR
3	3	99	GLU
3	3	102	GLN
3	3	105	THR
3	3	112	ARG
3	3	114	SER
3	3	126	LYS
3	3	127	LEU
3	3	129	LEU
3	3	132	THR
3	3	137	ARG
3	3	139	PRO
3	3	140	GLN
3	3	143	ARG
3	3	146	MET
3	3	151	VAL
3	3	153	TRP
3	3	157	LEU
3	3	159	SER
3	3	163	MET
3	3	167	TRP
3	3	168	THR
3	3	171	VAL
3	3	172	GLN
3	3	180	THR
3	3	183	SER
3	3	187	LEU
3	3	188	SER
3	3	204	GLN
3	3	207	LEU
3	3	210	PHE
3	3	212	SER
3	3	214	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	217	PHE
3	3	220	ARG
3	3	221	LEU
3	3	228	ILE
3	3	229	SER
3	3	232	VAL
3	3	234	LEU
4	4	29	ILE
4	4	30	ASN
4	4	34	ASP
4	4	38	THR
4	4	44	SER
4	4	45	LEU
4	4	52	PHE
4	4	53	THR
4	4	56	VAL
4	4	59	LEU
4	4	60	MET
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN
5	L	1	GLN
5	L	4	LEU
5	L	6	GLN
5	L	7	SER
5	L	11	MET
5	L	19	VAL
5	L	20	THR
5	L	22	THR
5	L	23	CYS
5	L	24	SER
5	L	29	SER
5	L	30	VAL
5	L	33	MET
5	L	38	GLN
5	L	43	SER
5	L	45	LYS
5	L	46	LEU
5	L	47	TRP
5	L	50	SER
5	L	51	SER
5	L	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	67	SER
5	L	69	THR
5	L	71	TYR
5	L	73	LEU
5	L	77	ARG
5	L	78	MET
5	L	81	GLU
5	L	85	THR
5	L	88	CYS
5	L	90	GLN
5	L	91	ARG
5	L	92	SER
5	L	94	TYR
5	L	97	THR
5	L	103	LYS
5	L	104	LEU
5	L	105	GLU
5	L	107	LYS
5	L	108	ARG
6	H	1	GLN
6	H	3	GLN
6	H	4	LEU
6	H	5	GLN
6	H	12	VAL
6	H	13	ARG
6	H	17	SER
6	H	18	VAL
6	H	20	ILE
6	H	21	SER
6	H	23	LYS
6	H	25	SER
6	H	31	SER
6	H	32	PHE
6	H	35	ASN
6	H	37	VAL
6	H	45	LEU
6	H	51	ILE
6	H	58	LYS
6	H	64	LYS
6	H	74	SER
6	H	77	THR
6	H	80	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	81	GLN
6	H	82	LEU
6	H	82(B)	SER
6	H	83	THR
6	H	84	SER
6	H	89	VAL
6	H	97	ASN
6	H	100(I)	TYR
6	H	100(K)	MET
6	H	109	VAL
6	H	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	29	GLN
1	1	59	HIS
1	1	84	ASN
1	1	100	ASN
1	1	145	ASN
1	1	212	GLN
1	1	235	HIS
1	1	274	ASN
2	2	14	GLN
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	111	GLN
2	2	131	GLN
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	262	GLN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	65	ASN
3	3	77	ASN
3	3	84	ASN
3	3	102	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	106	HIS
3	3	192	GLN
5	L	34	HIS
5	L	38	GLN
5	L	90	GLN
6	H	5	GLN
6	H	6	GLN
6	H	35	ASN
6	H	97	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.