



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:19 AM UTC

PDB ID : 1GFF / pdb_00001gff
Title : THE ATOMIC STRUCTURE OF THE DEGRADED PROCAPSID PARTICLE OF THE BACTERIOPHAGE G4: INDUCED STRUCTURAL CHANGES IN THE PRESENCE OF CALCIUM IONS AND FUNCTIONAL IMPLICATIONS
Authors : Rossmann, M.G.
Deposited on : 1995-11-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

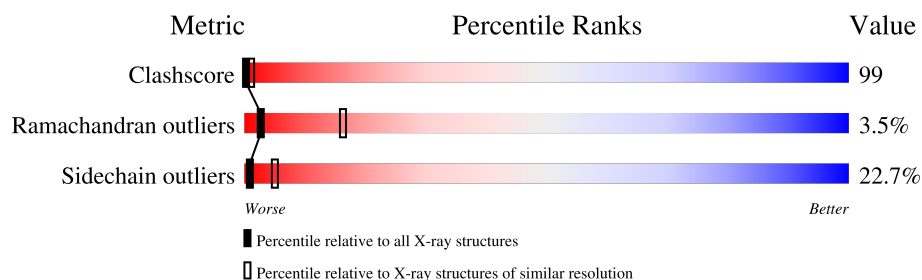
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	426	29% 47% 20% • •
2	2	177	19% 51% 27% •
3	3	25	20% 16% 8% • 52%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4779 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 BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	417	Total	C	N	O	S	0	0	0
			3357	2144	571	623	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	378	ASP	GLU	conflict	UNP P03642

- Molecule 2 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	177	Total	C	N	O	S	0	0	0
			1325	840	229	252	4			

- Molecule 3 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

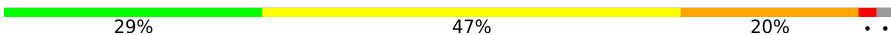
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	3	12	Total	C	N	O	0	0	0
			97	64	17	16			

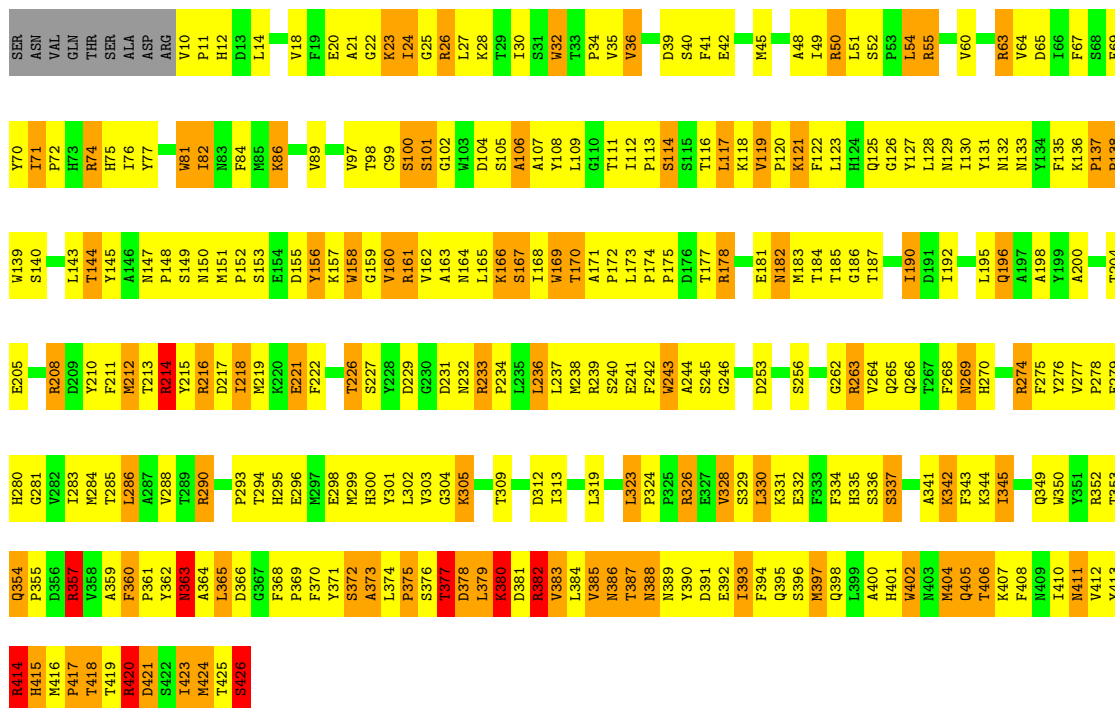
3 Residue-property plots

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

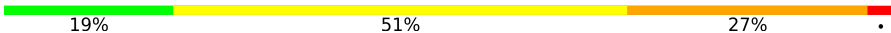
Note EDS was not executed.

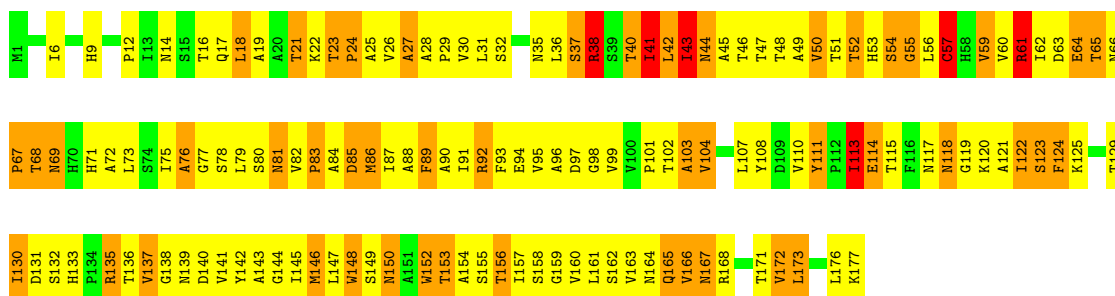
• Molecule 1: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ

Chain 1: 

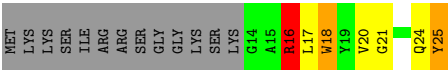
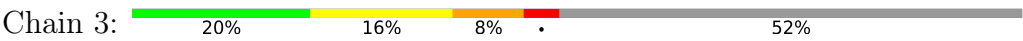


• Molecule 2: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ

Chain 2: 



● Molecule 3: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	414.20Å 414.20Å 263.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.352 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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	1.05	8/3461 (0.2%)	1.40	31/4713 (0.7%)
2	2	1.15	2/1354 (0.1%)	1.59	21/1859 (1.1%)
3	3	1.32	1/100 (1.0%)	1.37	1/135 (0.7%)
All	All	1.08	11/4915 (0.2%)	1.46	53/6707 (0.8%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	139	TRP	NE1-CE2	-5.56	1.31	1.37
1	1	32	TRP	NE1-CE2	-5.53	1.31	1.37
1	1	169	TRP	NE1-CE2	-5.47	1.31	1.37
2	2	148	TRP	NE1-CE2	-5.46	1.31	1.37
1	1	402	TRP	NE1-CE2	-5.42	1.31	1.37
1	1	243	TRP	NE1-CE2	-5.41	1.31	1.37
2	2	152	TRP	NE1-CE2	-5.39	1.31	1.37
1	1	350	TRP	NE1-CE2	-5.37	1.31	1.37
1	1	81	TRP	NE1-CE2	-5.36	1.31	1.37
3	3	18	TRP	NE1-CE2	-5.27	1.31	1.37
1	1	158	TRP	NE1-CE2	-5.07	1.31	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	64	GLU	CB-CA-C	-9.38	99.58	111.22
2	2	41	ILE	CB-CG1-CD1	-8.87	95.17	113.80
2	2	43	ILE	CB-CA-C	-8.76	103.41	113.22
2	2	47	THR	CB-CA-C	-7.61	99.46	111.17
1	1	426	SER	CA-C-O	-7.43	108.16	120.80
1	1	39	ASP	CA-CB-CG	7.21	119.81	112.60
1	1	232	ASN	CB-CA-C	-7.02	101.92	111.89
2	2	43	ILE	N-CA-C	6.91	113.60	106.21
2	2	55	GLY	N-CA-C	6.41	120.17	110.18
1	1	138	PRO	CB-CA-C	-6.36	101.84	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	336	SER	O-C-N	6.28	128.76	122.10
2	2	124	PHE	O-C-N	6.09	129.49	123.46
2	2	167	ASN	N-CA-C	-5.85	105.81	113.12
2	2	177	LYS	CA-C-O	-5.65	111.19	120.80
1	1	214	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	1	357	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	1	55	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	2	61	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	1	208	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	2	83	PRO	CB-CA-C	5.47	118.51	111.56
1	1	137	PRO	CA-C-N	5.45	125.53	119.87
1	1	137	PRO	C-N-CA	5.45	125.53	119.87
2	2	168	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	1	216	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	1	414	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	2	146	MET	O-C-N	5.38	129.92	123.36
1	1	326	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	1	74	ARG	NE-CZ-NH2	5.37	124.04	119.20
2	2	24	PRO	CB-CA-C	-5.37	102.70	111.56
1	1	50	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	1	139	TRP	N-CA-C	-5.36	106.75	113.72
1	1	290	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	1	382	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	2	38	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	1	161	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	1	420	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	2	171	THR	O-C-N	5.32	129.55	123.27
2	2	135	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	1	139	TRP	O-C-N	5.32	128.89	122.35
3	3	16	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	1	26	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	2	57	CYS	O-C-N	5.28	130.37	122.76
1	1	274	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	2	92	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	1	233	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	2	104	VAL	CB-CA-C	-5.22	105.25	110.89
1	1	63	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	1	365	LEU	N-CA-C	5.20	116.89	108.26
2	2	89	PHE	N-CA-C	-5.20	103.06	110.59
1	1	106	ALA	O-C-N	5.17	127.73	122.09
1	1	137	PRO	O-C-N	5.07	127.45	121.46
1	1	178	ARG	NE-CZ-NH2	5.04	123.73	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	263	ARG	NE-CZ-NH2	5.03	123.73	119.20

There are no chirality outliers.

There are no planarity outliers.

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	3357	0	3220	577	0
2	2	1325	0	1334	357	0
3	3	97	0	89	41	0
All	All	4779	0	4643	931	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 99.

All (931) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:LEU:HD23	2:2:41:ILE:CD1	1.26	1.60
1:1:138:PRO:HG2	3:3:20:VAL:CG1	1.20	1.57
2:2:18:LEU:CB	2:2:43:ILE:HG22	1.19	1.57
1:1:138:PRO:CG	3:3:20:VAL:HG12	1.13	1.56
2:2:18:LEU:CD2	2:2:41:ILE:HD11	1.32	1.53
2:2:82:VAL:CG1	2:2:86:MET:SD	2.05	1.44
2:2:118:ASN:CG	2:2:119:GLY:H	1.22	1.40
2:2:82:VAL:HG11	2:2:86:MET:SD	1.61	1.39
1:1:328:VAL:HG12	1:1:332:GLU:OE1	1.23	1.38
1:1:138:PRO:CG	3:3:20:VAL:CG1	1.79	1.38
2:2:26:VAL:CA	2:2:54:SER:OG	1.70	1.37
2:2:21:THR:HA	2:2:46:THR:CG2	1.56	1.36
1:1:108:TYR:CE1	1:1:109:LEU:HD21	1.60	1.35
1:1:419:THR:O	1:1:423:ILE:CD1	1.73	1.35
2:2:26:VAL:N	2:2:54:SER:OG	1.58	1.33
1:1:138:PRO:CD	3:3:20:VAL:CG1	2.06	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:ALA:HA	2:2:152:TRP:O	1.21	1.30
1:1:138:PRO:CD	3:3:20:VAL:HG11	1.59	1.30
1:1:419:THR:O	1:1:423:ILE:HD12	1.19	1.29
2:2:40:THR:HG23	2:2:162:SER:OG	1.11	1.29
2:2:18:LEU:CB	2:2:43:ILE:CG2	2.10	1.28
2:2:21:THR:CA	2:2:46:THR:HG22	1.63	1.28
1:1:296:GLU:OE1	1:1:363:ASN:HA	1.33	1.22
2:2:43:ILE:O	2:2:45:ALA:N	1.72	1.21
2:2:164:ASN:OD1	2:2:165:GLN:N	1.73	1.20
2:2:94:GLU:OE2	2:2:135:ARG:N	1.76	1.18
1:1:295:HIS:NE2	1:1:373:ALA:O	1.76	1.18
1:1:357:ARG:HH11	1:1:357:ARG:CG	1.57	1.18
1:1:420:ARG:CA	1:1:423:ILE:HD11	1.73	1.18
2:2:40:THR:CG2	2:2:162:SER:OG	1.90	1.18
1:1:18:VAL:CG1	1:1:406:THR:HG23	1.74	1.15
2:2:82:VAL:HG13	2:2:86:MET:SD	1.85	1.15
1:1:175:PRO:HG3	1:1:379:LEU:HD23	1.23	1.15
1:1:390:TYR:O	1:1:393:ILE:HG23	1.44	1.15
1:1:10:VAL:O	1:1:12:HIS:HD2	1.28	1.15
2:2:49:ALA:CA	2:2:152:TRP:O	1.93	1.15
2:2:21:THR:CA	2:2:46:THR:CG2	2.23	1.15
2:2:21:THR:HB	2:2:46:THR:CG2	1.77	1.15
1:1:145:TYR:CD2	1:1:151:MET:HG2	1.82	1.14
1:1:138:PRO:HD2	3:3:20:VAL:CG1	1.75	1.14
2:2:43:ILE:O	2:2:43:ILE:HG12	1.42	1.13
2:2:18:LEU:HB3	2:2:43:ILE:CG2	1.71	1.13
1:1:108:TYR:CE1	1:1:109:LEU:CD2	2.32	1.12
1:1:424:MET:O	1:1:426:SER:OG	1.68	1.11
2:2:40:THR:CG2	2:2:162:SER:CB	2.28	1.11
2:2:12:PRO:HG3	2:2:38:ARG:HB2	1.31	1.11
1:1:213:THR:HG22	3:3:21:GLY:O	1.49	1.11
2:2:42:LEU:O	2:2:42:LEU:HG	1.42	1.11
2:2:118:ASN:ND2	2:2:119:GLY:H	1.49	1.10
1:1:359:ALA:C	1:1:361:PRO:HD2	1.77	1.10
1:1:63:ARG:NE	1:1:241:GLU:OE2	1.83	1.10
2:2:18:LEU:CD2	2:2:32:SER:HB2	1.82	1.10
1:1:269:ASN:HD22	1:1:270:HIS:N	1.49	1.09
1:1:238:MET:HE3	1:1:239:ARG:H	1.16	1.09
2:2:32:SER:HB2	2:2:41:ILE:HD11	1.24	1.09
1:1:368:PHE:HB3	1:1:370:PHE:CD2	1.87	1.09
2:2:18:LEU:CG	2:2:43:ILE:HG22	1.83	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:LEU:HB3	2:2:43:ILE:HG22	1.14	1.08
2:2:21:THR:CB	2:2:46:THR:CG2	2.31	1.08
1:1:418:THR:HG22	1:1:421:ASP:HB2	1.32	1.08
1:1:418:THR:CG2	1:1:421:ASP:HB2	1.82	1.08
2:2:26:VAL:N	2:2:54:SER:CB	2.17	1.08
2:2:118:ASN:CG	2:2:119:GLY:N	1.99	1.08
2:2:18:LEU:HB2	2:2:43:ILE:HG22	1.13	1.07
1:1:386:ASN:ND2	1:1:386:ASN:O	1.87	1.07
1:1:18:VAL:HG13	1:1:406:THR:HG23	1.34	1.06
1:1:10:VAL:CG2	1:1:11:PRO:HD2	1.85	1.06
2:2:18:LEU:HB3	2:2:43:ILE:CB	1.85	1.06
2:2:40:THR:HG23	2:2:162:SER:CB	1.84	1.06
1:1:386:ASN:C	1:1:386:ASN:HD22	1.60	1.05
2:2:94:GLU:HG2	2:2:141:VAL:HG12	1.33	1.05
1:1:420:ARG:HA	1:1:423:ILE:CD1	1.86	1.04
1:1:10:VAL:O	1:1:12:HIS:CD2	2.10	1.04
2:2:21:THR:HB	2:2:46:THR:HG21	1.04	1.04
1:1:10:VAL:HG23	1:1:11:PRO:HD2	1.40	1.03
1:1:63:ARG:CZ	1:1:241:GLU:OE2	2.06	1.03
1:1:300:HIS:O	1:1:303:VAL:HG12	1.57	1.03
2:2:31:LEU:HG	2:2:57:CYS:O	1.59	1.02
1:1:175:PRO:HG3	1:1:379:LEU:CD2	1.89	1.02
2:2:26:VAL:CB	2:2:54:SER:OG	2.07	1.02
1:1:71:ILE:CD1	1:1:126:GLY:HA2	1.88	1.01
1:1:242:PHE:CZ	1:1:268:PHE:HB3	1.94	1.01
2:2:21:THR:CB	2:2:46:THR:HG21	1.87	1.01
1:1:390:TYR:O	1:1:393:ILE:CG2	2.09	1.01
1:1:71:ILE:CD1	1:1:76:ILE:HD11	1.89	1.00
1:1:108:TYR:CZ	1:1:151:MET:HE1	1.96	1.00
1:1:49:ILE:CG2	1:1:266:GLN:HB3	1.92	0.99
2:2:25:ALA:C	2:2:54:SER:HB3	1.86	0.99
1:1:108:TYR:HE1	1:1:109:LEU:HD21	1.22	0.99
1:1:178:ARG:HH22	1:1:205:GLU:CD	1.52	0.99
2:2:50:VAL:HG12	2:2:152:TRP:HB2	1.44	0.99
2:2:18:LEU:HD21	2:2:32:SER:HB2	1.40	0.98
1:1:319:LEU:O	1:1:323:LEU:CD2	2.11	0.98
1:1:357:ARG:NH1	1:1:357:ARG:HG2	1.58	0.98
1:1:70:TYR:HB2	1:1:237:LEU:HD11	1.46	0.97
1:1:133:ASN:O	1:1:214:ARG:NH2	1.98	0.97
2:2:28:ALA:CB	2:2:55:GLY:O	2.12	0.97
1:1:18:VAL:HG12	1:1:406:THR:O	1.65	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:357:ARG:HH11	1:1:357:ARG:HG2	0.79	0.96
2:2:69:ASN:C	2:2:69:ASN:HD22	1.74	0.96
1:1:127:TYR:N	1:1:284:MET:HE1	1.81	0.95
1:1:363:ASN:O	1:1:363:ASN:ND2	1.99	0.95
1:1:363:ASN:HD22	1:1:363:ASN:C	1.72	0.95
2:2:86:MET:HE2	2:2:147:LEU:HD22	1.49	0.95
1:1:269:ASN:HD22	1:1:270:HIS:H	1.06	0.95
1:1:319:LEU:O	1:1:323:LEU:HD22	1.64	0.95
1:1:416:MET:SD	1:1:417:PRO:HD2	2.07	0.95
1:1:98:THR:HG22	1:1:147:ASN:ND2	1.82	0.94
2:2:32:SER:HB2	2:2:41:ILE:CD1	1.96	0.94
2:2:86:MET:CE	2:2:147:LEU:HD22	1.97	0.94
1:1:178:ARG:NH2	1:1:205:GLU:CD	2.21	0.94
2:2:36:LEU:HD13	2:2:61:ARG:HH21	1.32	0.94
1:1:244:ALA:HA	1:1:266:GLN:HG2	1.47	0.93
2:2:9:HIS:CE1	2:2:162:SER:HB3	2.03	0.93
2:2:82:VAL:CG1	2:2:86:MET:CG	2.47	0.93
1:1:268:PHE:HZ	1:1:404:MET:HE3	1.29	0.93
1:1:132:ASN:HD21	1:1:143:LEU:H	0.98	0.92
2:2:94:GLU:OE1	2:2:135:ARG:HB2	1.68	0.92
2:2:18:LEU:HD12	2:2:19:ALA:H	1.35	0.92
2:2:26:VAL:HB	2:2:54:SER:OG	1.68	0.92
2:2:43:ILE:O	2:2:44:ASN:C	2.03	0.92
2:2:59:VAL:HG23	2:2:143:ALA:O	1.69	0.92
1:1:132:ASN:ND2	1:1:143:LEU:H	1.67	0.92
2:2:136:THR:O	2:2:139:ASN:OD1	1.88	0.91
2:2:57:CYS:SG	2:2:91:ILE:HD11	2.09	0.91
1:1:323:LEU:CD2	1:1:323:LEU:H	1.84	0.91
1:1:71:ILE:HD11	1:1:76:ILE:HD11	1.50	0.91
2:2:136:THR:HB	2:2:139:ASN:HD21	1.34	0.91
2:2:95:VAL:O	2:2:139:ASN:HB2	1.70	0.90
1:1:323:LEU:CD2	1:1:323:LEU:N	2.34	0.90
2:2:37:SER:C	2:2:38:ARG:HD3	1.95	0.90
2:2:40:THR:CG2	2:2:162:SER:HB2	2.01	0.90
1:1:239:ARG:NH1	3:3:25:TYR:HE1	1.68	0.90
1:1:268:PHE:CZ	1:1:404:MET:HE3	2.06	0.90
2:2:18:LEU:CG	2:2:43:ILE:CG2	2.46	0.90
2:2:50:VAL:N	2:2:152:TRP:O	2.04	0.90
1:1:242:PHE:CZ	1:1:268:PHE:CB	2.54	0.89
1:1:328:VAL:CG1	1:1:332:GLU:OE1	2.17	0.89
2:2:79:LEU:HD23	2:2:159:GLY:HA3	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:92:ARG:HD2	2:2:130:ILE:HG13	1.54	0.89
1:1:296:GLU:OE1	1:1:363:ASN:CA	2.20	0.89
1:1:323:LEU:HD22	1:1:323:LEU:N	1.86	0.89
2:2:64:GLU:OE2	2:2:140:ASP:OD1	1.90	0.89
2:2:97:ASP:CB	2:2:138:GLY:O	2.21	0.89
2:2:97:ASP:N	2:2:139:ASN:HA	1.87	0.89
2:2:40:THR:HG22	2:2:162:SER:HB2	1.53	0.89
1:1:368:PHE:HB3	1:1:370:PHE:CE2	2.08	0.88
2:2:61:ARG:HG3	2:2:142:TYR:CE1	2.09	0.88
1:1:420:ARG:HA	1:1:423:ILE:HD11	0.92	0.88
2:2:28:ALA:HA	2:2:55:GLY:O	1.72	0.88
2:2:118:ASN:ND2	2:2:121:ALA:H	1.71	0.88
2:2:18:LEU:HB2	2:2:41:ILE:HG12	1.52	0.88
1:1:99:CYS:SG	1:1:148:PRO:HG2	2.12	0.88
1:1:138:PRO:HD2	3:3:20:VAL:HG11	1.41	0.87
1:1:221:GLU:O	1:1:221:GLU:HG3	1.74	0.87
2:2:56:LEU:O	2:2:56:LEU:HD12	1.73	0.87
2:2:79:LEU:O	2:2:121:ALA:HA	1.74	0.87
1:1:245:SER:H	1:1:266:GLN:HE21	1.20	0.87
1:1:49:ILE:HG22	1:1:266:GLN:HB3	1.55	0.87
1:1:104:ASP:OD2	1:1:157:LYS:HE2	1.73	0.87
1:1:128:LEU:HD22	1:1:143:LEU:O	1.75	0.87
2:2:18:LEU:HD23	2:2:41:ILE:CG1	2.04	0.87
2:2:153:THR:HG23	2:2:154:ALA:N	1.87	0.86
1:1:420:ARG:O	1:1:424:MET:HG2	1.75	0.86
2:2:97:ASP:HB3	2:2:138:GLY:O	1.76	0.86
1:1:21:ALA:O	1:1:28:LYS:NZ	2.09	0.86
1:1:30:ILE:CD1	1:1:45:MET:HE1	2.06	0.86
1:1:172:PRO:HG2	1:1:379:LEU:HD11	1.58	0.85
1:1:18:VAL:HG11	1:1:406:THR:HG23	1.56	0.85
2:2:9:HIS:HE1	2:2:162:SER:HB3	1.39	0.85
1:1:161:ARG:O	1:1:384:LEU:HD22	1.75	0.85
1:1:167:SER:H	1:1:170:THR:HG22	1.41	0.85
2:2:28:ALA:CA	2:2:55:GLY:O	2.24	0.85
1:1:377:THR:O	1:1:382:ARG:NH1	2.09	0.85
2:2:52:THR:CG2	2:2:52:THR:O	2.23	0.85
1:1:138:PRO:HD2	3:3:20:VAL:HG13	1.59	0.85
2:2:26:VAL:HA	2:2:54:SER:OG	1.72	0.85
1:1:363:ASN:ND2	1:1:363:ASN:C	2.31	0.84
1:1:138:PRO:CG	3:3:20:VAL:HG11	1.83	0.84
2:2:41:ILE:HG23	2:2:43:ILE:HG23	1.56	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:ASN:HD21	2:2:131:ASP:HB2	1.40	0.84
2:2:40:THR:HG23	2:2:162:SER:HG	0.88	0.84
1:1:423:ILE:HD13	1:1:423:ILE:H	1.43	0.84
1:1:162:VAL:C	1:1:384:LEU:HD23	2.03	0.84
2:2:95:VAL:O	2:2:139:ASN:CB	2.27	0.83
1:1:145:TYR:CG	1:1:151:MET:HG2	2.13	0.83
1:1:18:VAL:HG22	1:1:20:GLU:CG	2.07	0.83
1:1:120:PRO:HG2	1:1:123:LEU:HD12	1.58	0.83
1:1:368:PHE:HB3	1:1:370:PHE:HD2	1.42	0.83
2:2:44:ASN:HD22	2:2:158:SER:HB2	1.42	0.83
1:1:133:ASN:C	1:1:214:ARG:NH2	2.36	0.83
2:2:82:VAL:HG12	2:2:86:MET:HG3	1.59	0.83
1:1:353:THR:HG22	1:1:354:GLN:N	1.93	0.83
2:2:73:LEU:HD12	2:2:164:ASN:O	1.78	0.83
2:2:153:THR:CG2	2:2:154:ALA:N	2.42	0.82
1:1:71:ILE:HD13	1:1:126:GLY:HA2	1.62	0.82
1:1:52:SER:HB2	1:1:394:PHE:CD2	2.15	0.82
1:1:269:ASN:ND2	1:1:270:HIS:N	2.28	0.82
1:1:144:THR:O	1:1:144:THR:HG23	1.78	0.82
1:1:360:PHE:N	1:1:361:PRO:CD	2.42	0.82
2:2:23:THR:HA	2:2:48:THR:CG2	2.10	0.82
1:1:238:MET:HE3	1:1:239:ARG:N	1.95	0.81
2:2:36:LEU:O	2:2:61:ARG:O	1.98	0.81
1:1:108:TYR:CD1	1:1:109:LEU:CD2	2.64	0.81
1:1:163:ALA:O	1:1:290:ARG:NH1	2.12	0.81
1:1:210:TYR:O	3:3:21:GLY:HA2	1.82	0.80
1:1:372:SER:H	1:1:389:ASN:HD21	1.28	0.80
1:1:360:PHE:N	1:1:361:PRO:HD2	1.95	0.80
1:1:387:THR:HG22	1:1:388:ASN:N	1.96	0.80
2:2:26:VAL:C	2:2:28:ALA:H	1.88	0.80
1:1:120:PRO:HG2	1:1:123:LEU:CD1	2.11	0.80
1:1:239:ARG:NH1	3:3:25:TYR:CE1	2.50	0.80
2:2:52:THR:O	2:2:52:THR:HG23	1.81	0.80
2:2:95:VAL:CG1	2:2:142:TYR:HE2	1.94	0.79
2:2:9:HIS:HB3	2:2:125:LYS:HE2	1.63	0.79
2:2:157:ILE:HG13	2:2:157:ILE:O	1.83	0.79
1:1:164:ASN:ND2	1:1:385:VAL:HB	1.98	0.79
2:2:118:ASN:ND2	2:2:119:GLY:N	2.23	0.79
2:2:23:THR:HA	2:2:48:THR:HG22	1.64	0.79
2:2:37:SER:HB3	2:2:38:ARG:CD	2.12	0.79
2:2:130:ILE:HG12	2:2:131:ASP:N	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:372:SER:N	1:1:389:ASN:HD21	1.79	0.79
1:1:216:ARG:HA	1:1:226:THR:HG21	1.65	0.78
1:1:420:ARG:CA	1:1:423:ILE:CD1	2.55	0.78
1:1:231:ASP:CG	1:1:233:ARG:HH11	1.91	0.78
1:1:387:THR:CG2	1:1:388:ASN:N	2.46	0.78
1:1:417:PRO:O	1:1:418:THR:HB	1.84	0.78
1:1:238:MET:CE	1:1:239:ARG:H	1.96	0.78
2:2:77:GLY:O	2:2:123:SER:HA	1.83	0.78
2:2:37:SER:HB3	2:2:38:ARG:NH1	1.99	0.78
2:2:101:PRO:HD3	2:2:142:TYR:CZ	2.19	0.78
2:2:82:VAL:HG12	2:2:86:MET:CG	2.14	0.78
2:2:165:GLN:OE1	2:2:167:ASN:OD1	2.02	0.78
1:1:156:TYR:CD1	1:1:156:TYR:C	2.62	0.78
2:2:63:ASP:OD1	2:2:65:THR:HG23	1.82	0.78
2:2:36:LEU:HD13	2:2:61:ARG:NH2	2.00	0.77
1:1:71:ILE:HD13	1:1:126:GLY:CA	2.15	0.77
2:2:101:PRO:CD	2:2:142:TYR:CZ	2.67	0.77
1:1:345:ILE:HD11	1:1:349:GLN:HB3	1.67	0.77
1:1:416:MET:SD	1:1:417:PRO:CD	2.72	0.77
2:2:94:GLU:CD	2:2:135:ARG:HB2	2.10	0.77
1:1:97:VAL:CG2	1:1:121:LYS:HA	2.14	0.77
1:1:63:ARG:NH2	1:1:241:GLU:CD	2.43	0.77
2:2:44:ASN:HD22	2:2:158:SER:CB	1.98	0.77
1:1:30:ILE:HD11	1:1:45:MET:HE1	1.67	0.76
1:1:319:LEU:O	1:1:323:LEU:HD21	1.84	0.76
2:2:18:LEU:HB3	2:2:43:ILE:CA	2.15	0.76
2:2:165:GLN:CD	2:2:167:ASN:OD1	2.28	0.76
2:2:18:LEU:HD21	2:2:32:SER:CB	2.15	0.76
1:1:125:GLN:OE1	1:1:129:ASN:ND2	2.17	0.76
1:1:10:VAL:HG22	1:1:11:PRO:HD2	1.67	0.76
1:1:145:TYR:CD2	1:1:151:MET:CG	2.68	0.76
1:1:136:LYS:O	1:1:136:LYS:HG3	1.85	0.76
1:1:63:ARG:HH21	1:1:241:GLU:CD	1.94	0.76
2:2:49:ALA:CB	2:2:153:THR:HA	2.15	0.76
2:2:153:THR:HG23	2:2:154:ALA:H	1.49	0.75
1:1:170:THR:HG23	1:1:170:THR:O	1.85	0.75
1:1:329:SER:C	1:1:331:LYS:H	1.94	0.75
2:2:94:GLU:OE2	2:2:135:ARG:CB	2.34	0.75
1:1:63:ARG:HE	1:1:241:GLU:CD	1.95	0.75
2:2:43:ILE:O	2:2:43:ILE:CG1	2.21	0.75
1:1:166:LYS:CD	3:3:18:TRP:CD1	2.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:ASN:HD21	1:1:143:LEU:N	1.81	0.75
2:2:38:ARG:HD3	2:2:38:ARG:N	2.02	0.74
2:2:18:LEU:HG	2:2:43:ILE:CG2	2.15	0.74
2:2:82:VAL:CG1	2:2:86:MET:HG3	2.16	0.74
1:1:323:LEU:HD22	1:1:323:LEU:H	1.50	0.74
2:2:37:SER:C	2:2:38:ARG:CD	2.60	0.74
2:2:137:VAL:HG13	2:2:138:GLY:N	2.01	0.74
1:1:63:ARG:NE	1:1:241:GLU:CD	2.44	0.73
1:1:166:LYS:HD3	3:3:18:TRP:CD1	2.23	0.73
2:2:69:ASN:HA	2:2:133:HIS:CE1	2.22	0.73
1:1:268:PHE:CZ	1:1:404:MET:CE	2.71	0.73
1:1:18:VAL:HG21	1:1:20:GLU:OE2	1.89	0.73
1:1:162:VAL:CG1	1:1:290:ARG:HD3	2.17	0.73
1:1:387:THR:HG22	1:1:388:ASN:HD22	1.53	0.73
1:1:213:THR:CG2	3:3:21:GLY:O	2.34	0.73
2:2:118:ASN:HD21	2:2:121:ALA:H	1.34	0.73
1:1:323:LEU:H	1:1:323:LEU:HD23	1.54	0.73
2:2:40:THR:HG22	2:2:162:SER:CB	2.09	0.72
2:2:21:THR:HA	2:2:46:THR:HG22	0.77	0.72
1:1:133:ASN:C	1:1:214:ARG:HH21	1.95	0.72
1:1:299:MET:SD	1:1:304:GLY:HA3	2.30	0.72
2:2:18:LEU:HD21	2:2:41:ILE:HD11	1.61	0.72
1:1:30:ILE:HD12	1:1:45:MET:CE	2.19	0.72
2:2:26:VAL:N	2:2:54:SER:HB3	1.94	0.72
1:1:379:LEU:O	1:1:383:VAL:HG13	1.89	0.72
1:1:18:VAL:CG1	1:1:406:THR:CG2	2.64	0.72
1:1:71:ILE:CD1	1:1:126:GLY:CA	2.65	0.71
1:1:300:HIS:O	1:1:303:VAL:CG1	2.38	0.71
1:1:359:ALA:CB	1:1:361:PRO:HD2	2.20	0.71
1:1:72:PRO:O	1:1:75:HIS:HB2	1.90	0.71
2:2:95:VAL:HG11	2:2:142:TYR:HE2	1.53	0.71
1:1:55:ARG:NH1	1:1:392:GLU:O	2.23	0.71
2:2:9:HIS:HE1	2:2:162:SER:CB	2.03	0.71
2:2:29:PRO:HA	2:2:103:ALA:HB2	1.72	0.71
2:2:28:ALA:HB1	2:2:55:GLY:O	1.89	0.71
2:2:90:ALA:O	2:2:91:ILE:CG2	2.39	0.71
1:1:108:TYR:CZ	1:1:151:MET:CE	2.71	0.71
2:2:36:LEU:CD1	2:2:61:ARG:HH21	2.03	0.71
2:2:115:THR:OG1	2:2:122:ILE:HD11	1.90	0.71
1:1:386:ASN:ND2	1:1:386:ASN:C	2.31	0.70
1:1:138:PRO:HD3	3:3:20:VAL:HG11	1.70	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:81:ASN:O	2:2:157:ILE:HG22	1.91	0.70
2:2:137:VAL:HG13	2:2:138:GLY:H	1.56	0.70
1:1:12:HIS:CE1	1:1:416:MET:HG3	2.27	0.70
2:2:49:ALA:HA	2:2:152:TRP:C	2.13	0.70
2:2:49:ALA:C	2:2:152:TRP:O	2.34	0.70
1:1:49:ILE:HG23	1:1:266:GLN:HB3	1.72	0.70
1:1:295:HIS:CE1	1:1:373:ALA:O	2.45	0.70
2:2:18:LEU:CD2	2:2:41:ILE:CD1	2.17	0.70
2:2:59:VAL:HA	2:2:144:GLY:HA3	1.74	0.70
2:2:65:THR:O	2:2:65:THR:OG1	2.09	0.70
1:1:100:SER:O	1:1:105:SER:CB	2.39	0.70
1:1:353:THR:CG2	1:1:354:GLN:N	2.54	0.70
2:2:24:PRO:HB3	2:2:56:LEU:HG	1.72	0.70
1:1:108:TYR:CD1	1:1:109:LEU:HD23	2.25	0.70
2:2:89:PHE:CE1	2:2:110:VAL:HG12	2.27	0.70
1:1:335:HIS:CG	1:1:335:HIS:O	2.45	0.69
1:1:246:GLY:HA3	1:1:263:ARG:O	1.92	0.69
1:1:360:PHE:CD1	1:1:360:PHE:C	2.70	0.69
1:1:65:ASP:HB2	1:1:288:VAL:CG1	2.21	0.69
1:1:144:THR:O	1:1:144:THR:CG2	2.40	0.69
2:2:85:ASP:OD1	2:2:85:ASP:C	2.35	0.69
1:1:71:ILE:CG1	1:1:76:ILE:HD11	2.21	0.69
1:1:359:ALA:C	1:1:361:PRO:CD	2.61	0.69
1:1:98:THR:O	1:1:148:PRO:HD2	1.93	0.69
1:1:116:THR:HB	1:1:118:LYS:NZ	2.08	0.69
2:2:37:SER:HB3	2:2:38:ARG:HD3	1.74	0.69
1:1:97:VAL:HG23	1:1:121:LYS:HA	1.74	0.68
1:1:24:ILE:HG12	1:1:401:HIS:HD2	1.57	0.68
1:1:98:THR:HG22	1:1:147:ASN:HD22	1.55	0.68
1:1:227:SER:C	1:1:229:ASP:H	1.99	0.68
1:1:301:TYR:HE1	1:1:332:GLU:OE1	1.76	0.68
2:2:172:VAL:HG23	2:2:173:LEU:N	2.08	0.68
2:2:32:SER:CB	2:2:41:ILE:CD1	2.69	0.68
1:1:45:MET:HE3	1:1:408:PHE:CZ	2.29	0.68
1:1:30:ILE:CD1	1:1:45:MET:CE	2.70	0.68
1:1:164:ASN:HD21	1:1:385:VAL:HB	1.55	0.68
1:1:196:GLN:NE2	1:1:196:GLN:HA	2.07	0.68
1:1:240:SER:CB	1:1:270:HIS:HD1	2.06	0.68
2:2:26:VAL:HG13	2:2:27:ALA:H	1.57	0.68
1:1:63:ARG:CZ	1:1:241:GLU:CD	2.66	0.68
1:1:183:MET:HE2	1:1:190:ILE:CD1	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:300:HIS:CD2	1:1:302:LEU:HB2	2.29	0.68
1:1:357:ARG:CG	1:1:357:ARG:NH1	2.29	0.68
2:2:86:MET:HE2	2:2:147:LEU:HB3	1.75	0.68
1:1:156:TYR:C	1:1:156:TYR:HD1	2.01	0.68
1:1:387:THR:HG22	1:1:388:ASN:H	1.56	0.68
1:1:10:VAL:CG2	1:1:11:PRO:CD	2.69	0.68
1:1:208:ARG:NH1	1:1:218:ILE:HD12	2.10	0.67
1:1:368:PHE:CD1	1:1:370:PHE:HE2	2.12	0.67
1:1:18:VAL:HG22	1:1:20:GLU:HG2	1.74	0.67
1:1:323:LEU:HB2	1:1:324:PRO:HD2	1.75	0.67
1:1:299:MET:HE3	1:1:335:HIS:HA	1.77	0.67
1:1:349:GLN:HE21	1:1:349:GLN:HA	1.59	0.67
2:2:41:ILE:CG2	2:2:43:ILE:HG23	2.24	0.67
1:1:101:SER:HA	1:1:117:LEU:HD21	1.77	0.67
1:1:419:THR:C	1:1:423:ILE:CD1	2.65	0.67
2:2:86:MET:HB2	2:2:117:ASN:HD22	1.60	0.67
1:1:22:GLY:HA2	1:1:158:TRP:CE3	2.30	0.67
1:1:182:ASN:N	1:1:182:ASN:HD22	1.92	0.67
2:2:32:SER:CB	2:2:41:ILE:HD11	2.15	0.66
1:1:353:THR:CG2	1:1:354:GLN:H	2.09	0.66
1:1:98:THR:H	1:1:147:ASN:HD22	1.44	0.66
1:1:162:VAL:O	1:1:385:VAL:HG13	1.95	0.66
1:1:100:SER:O	1:1:105:SER:OG	2.14	0.66
1:1:97:VAL:HG23	1:1:121:LYS:CA	2.26	0.66
1:1:162:VAL:HG13	1:1:290:ARG:HD3	1.78	0.66
1:1:387:THR:HG22	1:1:388:ASN:ND2	2.10	0.66
1:1:108:TYR:CE2	1:1:151:MET:CE	2.79	0.66
1:1:156:TYR:HD1	1:1:156:TYR:O	1.78	0.66
2:2:12:PRO:CG	2:2:38:ARG:HB2	2.19	0.66
2:2:90:ALA:O	2:2:91:ILE:HG23	1.95	0.65
1:1:24:ILE:HG12	1:1:401:HIS:CD2	2.32	0.65
1:1:268:PHE:CE2	1:1:404:MET:SD	2.89	0.65
2:2:50:VAL:HG12	2:2:152:TRP:CB	2.23	0.65
1:1:70:TYR:CE1	1:1:277:VAL:HG13	2.32	0.65
2:2:86:MET:HE2	2:2:147:LEU:CD2	2.24	0.65
1:1:376:SER:O	1:1:378:ASP:N	2.29	0.65
1:1:242:PHE:HE2	1:1:266:GLN:HG3	1.62	0.65
1:1:329:SER:C	1:1:331:LYS:N	2.55	0.65
1:1:23:LYS:HZ3	1:1:158:TRP:CD1	2.15	0.65
1:1:70:TYR:OH	1:1:277:VAL:HG13	1.97	0.65
1:1:167:SER:HB3	1:1:170:THR:HB	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:26:VAL:C	2:2:28:ALA:N	2.53	0.65
1:1:162:VAL:C	1:1:384:LEU:CD2	2.71	0.64
1:1:167:SER:OG	1:1:168:ILE:N	2.30	0.64
2:2:18:LEU:CD2	2:2:41:ILE:CG1	2.70	0.64
2:2:12:PRO:HG3	2:2:38:ARG:CB	2.20	0.64
1:1:63:ARG:HE	1:1:241:GLU:CG	2.11	0.64
2:2:37:SER:HB3	2:2:38:ARG:HH11	1.60	0.64
1:1:97:VAL:HG21	1:1:121:LYS:HA	1.80	0.64
2:2:78:SER:HA	2:2:122:ILE:O	1.98	0.64
2:2:94:GLU:OE2	2:2:135:ARG:CA	2.46	0.64
2:2:94:GLU:CD	2:2:135:ARG:HG3	2.23	0.64
1:1:70:TYR:CZ	1:1:277:VAL:HG13	2.33	0.63
1:1:116:THR:CB	1:1:118:LYS:NZ	2.62	0.63
2:2:59:VAL:CG2	2:2:60:VAL:N	2.61	0.63
2:2:87:ILE:HG22	2:2:148:TRP:O	1.98	0.63
1:1:183:MET:HE2	1:1:190:ILE:HD11	1.81	0.63
1:1:214:ARG:O	1:1:217:ASP:HB2	1.99	0.63
1:1:153:SER:O	1:1:157:LYS:HG3	1.97	0.63
1:1:389:ASN:OD1	1:1:389:ASN:O	2.17	0.63
2:2:89:PHE:CD1	2:2:110:VAL:HG12	2.33	0.63
1:1:63:ARG:HE	1:1:241:GLU:HG3	1.62	0.63
2:2:90:ALA:C	2:2:91:ILE:HG23	2.23	0.63
1:1:240:SER:OG	1:1:270:HIS:ND1	1.90	0.63
1:1:420:ARG:O	1:1:424:MET:HB2	1.99	0.63
2:2:49:ALA:HB2	2:2:153:THR:HA	1.80	0.63
2:2:18:LEU:CD2	2:2:32:SER:CB	2.69	0.63
1:1:166:LYS:CG	3:3:18:TRP:CD1	2.82	0.62
1:1:238:MET:CE	1:1:239:ARG:O	2.47	0.62
2:2:18:LEU:HD23	2:2:41:ILE:HD11	0.63	0.62
1:1:23:LYS:O	1:1:402:TRP:CD1	2.53	0.62
1:1:82:ILE:O	1:1:86:LYS:HG3	1.98	0.62
1:1:239:ARG:HH11	3:3:25:TYR:HE1	1.43	0.62
1:1:67:PHE:HB3	1:1:69:PHE:CE2	2.34	0.62
1:1:133:ASN:CA	1:1:214:ARG:HH21	2.13	0.62
2:2:59:VAL:HB	2:2:144:GLY:HA3	1.81	0.62
1:1:359:ALA:HB1	1:1:361:PRO:HD2	1.82	0.62
1:1:26:ARG:NE	1:1:159:GLY:O	2.31	0.62
2:2:26:VAL:HG13	2:2:27:ALA:N	2.15	0.62
2:2:94:GLU:OE2	2:2:135:ARG:HB2	1.99	0.62
1:1:294:THR:HG21	1:1:370:PHE:CD1	2.35	0.62
1:1:71:ILE:HG13	1:1:76:ILE:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:294:THR:CG2	1:1:370:PHE:HD1	2.13	0.61
2:2:69:ASN:C	2:2:69:ASN:ND2	2.45	0.61
1:1:226:THR:O	1:1:233:ARG:NH2	2.26	0.61
1:1:414:ARG:CG	1:1:415:HIS:H	2.13	0.61
1:1:102:GLY:O	1:1:105:SER:HB3	2.00	0.61
1:1:295:HIS:HA	1:1:371:TYR:HB2	1.82	0.61
1:1:296:GLU:CD	1:1:363:ASN:HA	2.24	0.61
1:1:300:HIS:HD2	1:1:302:LEU:HB2	1.65	0.61
2:2:37:SER:CB	2:2:38:ARG:HD3	2.30	0.61
1:1:126:GLY:C	1:1:284:MET:HE1	2.25	0.61
1:1:227:SER:C	1:1:229:ASP:N	2.58	0.61
2:2:50:VAL:O	2:2:50:VAL:CG1	2.47	0.61
1:1:116:THR:CB	1:1:118:LYS:HZ3	2.13	0.61
1:1:242:PHE:CE1	1:1:268:PHE:HB2	2.36	0.61
1:1:138:PRO:HG3	3:3:20:VAL:CG1	2.19	0.61
1:1:30:ILE:HD12	1:1:45:MET:HE3	1.81	0.61
1:1:60:VAL:HG13	1:1:369:PRO:HG2	1.83	0.61
1:1:102:GLY:O	1:1:105:SER:CB	2.49	0.61
1:1:240:SER:HG	1:1:270:HIS:CE1	2.07	0.61
1:1:376:SER:O	1:1:377:THR:C	2.44	0.61
2:2:36:LEU:CD1	2:2:61:ARG:NH2	2.63	0.61
1:1:77:TYR:HB2	1:1:81:TRP:HB2	1.81	0.61
2:2:51:THR:HG23	2:2:51:THR:O	2.00	0.61
1:1:305:LYS:O	1:1:305:LYS:HG3	2.01	0.60
2:2:59:VAL:HG23	2:2:143:ALA:C	2.26	0.60
2:2:94:GLU:CD	2:2:135:ARG:CB	2.74	0.60
1:1:137:PRO:O	1:1:140:SER:HB3	2.01	0.60
1:1:397:MET:O	2:2:68:THR:OG1	2.08	0.60
1:1:133:ASN:HA	1:1:214:ARG:HH21	1.66	0.60
1:1:204:THR:O	1:1:208:ARG:HG3	2.02	0.60
1:1:383:VAL:CG2	1:1:384:LEU:N	2.64	0.60
1:1:420:ARG:O	1:1:424:MET:CG	2.47	0.60
1:1:18:VAL:HG22	1:1:20:GLU:HG3	1.83	0.60
1:1:418:THR:HG22	1:1:421:ASP:CB	2.20	0.60
2:2:92:ARG:HG2	2:2:92:ARG:HH11	1.65	0.60
1:1:153:SER:HA	1:1:156:TYR:CE2	2.37	0.59
2:2:95:VAL:HG12	2:2:142:TYR:HE2	1.67	0.59
1:1:108:TYR:CE2	1:1:151:MET:HE1	2.35	0.59
2:2:97:ASP:HB2	2:2:138:GLY:O	2.01	0.59
1:1:69:PHE:CE1	1:1:236:LEU:HG	2.37	0.59
1:1:185:THR:HG23	1:1:186:GLY:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:245:SER:N	1:1:266:GLN:HE21	1.96	0.59
2:2:38:ARG:CD	2:2:38:ARG:N	2.65	0.59
1:1:11:PRO:HG3	1:1:413:TYR:CE1	2.38	0.59
2:2:94:GLU:OE1	2:2:135:ARG:CB	2.45	0.59
1:1:26:ARG:HB3	1:1:159:GLY:O	2.03	0.58
1:1:120:PRO:CG	1:1:123:LEU:HD12	2.31	0.58
1:1:163:ALA:N	1:1:384:LEU:HD23	2.17	0.58
2:2:95:VAL:HG12	2:2:142:TYR:CE2	2.39	0.58
2:2:118:ASN:HD21	2:2:120:LYS:H	1.50	0.58
1:1:231:ASP:OD1	1:1:233:ARG:NH1	2.35	0.58
1:1:349:GLN:HA	1:1:349:GLN:NE2	2.19	0.58
2:2:96:ALA:C	2:2:139:ASN:HA	2.29	0.58
1:1:164:ASN:ND2	1:1:385:VAL:CB	2.67	0.58
1:1:300:HIS:C	1:1:303:VAL:HG12	2.29	0.58
1:1:166:LYS:CD	3:3:18:TRP:HD1	2.15	0.58
1:1:397:MET:HG2	2:2:68:THR:OG1	2.03	0.58
1:1:155:ASP:O	1:1:159:GLY:HA2	2.04	0.58
2:2:57:CYS:HG	2:2:91:ILE:HD11	1.69	0.58
1:1:166:LYS:HD3	3:3:18:TRP:HD1	1.69	0.58
1:1:173:LEU:HB2	1:1:344:LYS:O	2.04	0.58
2:2:30:VAL:HG23	2:2:103:ALA:HA	1.86	0.58
2:2:156:THR:HG22	2:2:156:THR:O	2.04	0.58
1:1:63:ARG:NH2	1:1:241:GLU:OE1	2.37	0.57
1:1:128:LEU:CD2	1:1:143:LEU:O	2.51	0.57
2:2:79:LEU:HD23	2:2:159:GLY:CA	2.29	0.57
1:1:165:LEU:HB2	1:1:293:PRO:HD3	1.85	0.57
1:1:383:VAL:CG2	1:1:384:LEU:H	2.17	0.57
2:2:94:GLU:OE1	2:2:135:ARG:HG3	2.05	0.57
2:2:95:VAL:CG1	2:2:142:TYR:CE2	2.82	0.57
2:2:137:VAL:CG1	2:2:138:GLY:H	2.17	0.57
1:1:362:TYR:C	1:1:364:ALA:H	2.13	0.57
2:2:165:GLN:O	2:2:167:ASN:N	2.37	0.57
1:1:18:VAL:HG11	1:1:406:THR:CG2	2.31	0.57
1:1:70:TYR:OH	1:1:279:GLU:O	2.21	0.57
1:1:166:LYS:HB3	3:3:18:TRP:NE1	2.19	0.57
1:1:166:LYS:HG2	3:3:18:TRP:CG	2.39	0.57
1:1:167:SER:O	3:3:18:TRP:CH2	2.57	0.57
2:2:137:VAL:CG1	2:2:138:GLY:N	2.68	0.57
1:1:27:LEU:O	1:1:159:GLY:HA3	2.04	0.57
1:1:277:VAL:HG12	1:1:279:GLU:O	2.05	0.57
1:1:14:LEU:HD12	1:1:412:VAL:HG21	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:106:ALA:O	1:1:109:LEU:N	2.29	0.56
2:2:18:LEU:HB2	2:2:43:ILE:CG2	2.04	0.56
2:2:156:THR:O	2:2:156:THR:CG2	2.53	0.56
1:1:335:HIS:O	1:1:335:HIS:CD2	2.57	0.56
1:1:40:SER:OG	1:1:413:TYR:HB2	2.06	0.56
1:1:135:PHE:CE1	3:3:25:TYR:HB3	2.40	0.56
1:1:268:PHE:CZ	1:1:404:MET:SD	2.98	0.56
1:1:378:ASP:O	1:1:382:ARG:HD2	2.05	0.56
2:2:37:SER:HB3	2:2:38:ARG:CZ	2.36	0.56
2:2:94:GLU:CD	2:2:135:ARG:CG	2.78	0.56
2:2:101:PRO:HD3	2:2:142:TYR:OH	2.03	0.56
2:2:101:PRO:HG3	2:2:142:TYR:CE2	2.40	0.56
1:1:362:TYR:O	1:1:364:ALA:N	2.39	0.56
2:2:18:LEU:HB3	2:2:43:ILE:HB	1.85	0.56
1:1:242:PHE:CE1	1:1:268:PHE:CB	2.89	0.56
1:1:300:HIS:HB3	1:1:303:VAL:HG12	1.87	0.56
1:1:276:TYR:O	1:1:278:PRO:HD3	2.06	0.56
1:1:178:ARG:HD3	1:1:181:GLU:OE1	2.06	0.56
2:2:98:GLY:N	2:2:140:ASP:OD2	2.27	0.56
1:1:210:TYR:C	3:3:21:GLY:HA2	2.31	0.56
1:1:12:HIS:CE1	1:1:416:MET:HB2	2.41	0.55
2:2:108:TYR:CD1	2:2:108:TYR:C	2.84	0.55
1:1:71:ILE:HD11	1:1:76:ILE:CD1	2.31	0.55
1:1:167:SER:O	3:3:18:TRP:CZ3	2.59	0.55
2:2:92:ARG:HH22	2:2:141:VAL:HG11	1.70	0.55
1:1:11:PRO:HG3	1:1:413:TYR:HE1	1.71	0.55
1:1:45:MET:SD	1:1:408:PHE:CE1	3.00	0.55
1:1:69:PHE:CD1	1:1:236:LEU:HA	2.41	0.55
1:1:161:ARG:C	1:1:384:LEU:HD22	2.31	0.55
2:2:101:PRO:HD3	2:2:142:TYR:CE2	2.42	0.55
2:2:59:VAL:CG2	2:2:143:ALA:C	2.80	0.55
2:2:50:VAL:O	2:2:50:VAL:HG13	2.05	0.55
1:1:14:LEU:HD12	1:1:412:VAL:CG2	2.36	0.55
1:1:382:ARG:O	1:1:382:ARG:HG2	2.02	0.55
2:2:97:ASP:OD1	2:2:140:ASP:OD1	2.23	0.55
1:1:135:PHE:CE1	3:3:25:TYR:CB	2.90	0.55
1:1:171:ALA:N	1:1:172:PRO:HD3	2.22	0.55
2:2:18:LEU:HG	2:2:43:ILE:HG21	1.87	0.55
1:1:70:TYR:OH	1:1:277:VAL:CG1	2.55	0.55
1:1:119:VAL:HG13	1:1:120:PRO:HD2	1.89	0.55
2:2:18:LEU:CG	2:2:43:ILE:HG21	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:166:LYS:HB3	3:3:18:TRP:CD1	2.41	0.54
2:2:59:VAL:HG23	2:2:60:VAL:N	2.21	0.54
2:2:110:VAL:C	2:2:111:TYR:CD1	2.85	0.54
2:2:26:VAL:CA	2:2:54:SER:CB	2.76	0.54
1:1:383:VAL:HG22	1:1:384:LEU:H	1.72	0.54
1:1:386:ASN:O	1:1:386:ASN:CG	2.46	0.54
2:2:40:THR:HA	2:2:161:LEU:O	2.06	0.54
1:1:50:ARG:NH1	1:1:265:GLN:OE1	2.35	0.54
1:1:387:THR:CG2	1:1:388:ASN:HD22	2.19	0.54
2:2:18:LEU:HB3	2:2:43:ILE:HA	1.89	0.54
2:2:23:THR:O	2:2:23:THR:OG1	2.21	0.54
2:2:117:ASN:OD1	2:2:118:ASN:N	2.40	0.54
1:1:299:MET:SD	1:1:304:GLY:CA	2.96	0.54
1:1:35:VAL:HG22	1:1:281:GLY:O	2.07	0.54
1:1:97:VAL:HG12	1:1:148:PRO:HD2	1.89	0.54
2:2:41:ILE:HG12	2:2:43:ILE:CG2	2.37	0.54
2:2:84:ALA:HB2	2:2:119:GLY:O	2.08	0.54
1:1:18:VAL:CG2	1:1:20:GLU:HG2	2.38	0.54
1:1:25:GLY:HA3	1:1:385:VAL:HG21	1.90	0.53
1:1:108:TYR:CE1	1:1:109:LEU:CG	2.91	0.53
1:1:98:THR:HG22	1:1:147:ASN:CG	2.34	0.53
1:1:242:PHE:CE2	1:1:266:GLN:HG3	2.41	0.53
1:1:331:LYS:HG3	1:1:337:SER:O	2.08	0.53
2:2:59:VAL:CG2	2:2:143:ALA:O	2.51	0.53
1:1:60:VAL:CG1	1:1:369:PRO:HG2	2.38	0.53
1:1:326:ARG:O	1:1:345:ILE:HG22	2.08	0.53
1:1:18:VAL:CG2	1:1:20:GLU:OE2	2.56	0.53
2:2:80:SER:HA	2:2:120:LYS:O	2.09	0.53
1:1:152:PRO:HG2	1:1:155:ASP:OD2	2.08	0.53
1:1:372:SER:H	1:1:389:ASN:ND2	2.02	0.53
1:1:216:ARG:HD3	1:1:231:ASP:OD2	2.08	0.53
1:1:238:MET:HG3	1:1:270:HIS:CE1	2.43	0.53
1:1:420:ARG:O	1:1:424:MET:CB	2.57	0.53
1:1:418:THR:HG23	1:1:421:ASP:H	1.74	0.53
1:1:101:SER:HA	1:1:117:LEU:CD2	2.40	0.52
2:2:52:THR:O	2:2:52:THR:HG22	2.07	0.52
2:2:111:TYR:CD1	2:2:111:TYR:N	2.77	0.52
1:1:55:ARG:HH11	1:1:366:ASP:HB3	1.73	0.52
1:1:398:GLN:HB2	2:2:66:ASN:HD21	1.74	0.52
2:2:26:VAL:O	2:2:28:ALA:N	2.25	0.52
2:2:59:VAL:HB	2:2:144:GLY:CA	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:ASN:HD21	2:2:131:ASP:CB	2.17	0.52
1:1:67:PHE:O	1:1:285:THR:HA	2.10	0.52
2:2:44:ASN:HA	2:2:158:SER:HA	1.91	0.52
2:2:59:VAL:CG2	2:2:60:VAL:O	2.57	0.52
1:1:120:PRO:HD2	1:1:123:LEU:HD12	1.92	0.52
1:1:163:ALA:HA	1:1:384:LEU:HA	1.92	0.52
2:2:160:VAL:HG22	2:2:161:LEU:N	2.22	0.52
1:1:65:ASP:HB2	1:1:288:VAL:HG12	1.90	0.52
1:1:379:LEU:O	1:1:380:LYS:C	2.52	0.52
1:1:294:THR:CG2	1:1:370:PHE:CD1	2.91	0.51
2:2:44:ASN:ND2	2:2:158:SER:OG	2.42	0.51
2:2:63:ASP:H	2:2:165:GLN:HE22	1.56	0.51
2:2:97:ASP:N	2:2:138:GLY:O	2.40	0.51
1:1:208:ARG:HG2	1:1:212:MET:CE	2.41	0.51
1:1:244:ALA:HA	1:1:266:GLN:CG	2.32	0.51
1:1:21:ALA:HA	1:1:402:TRP:O	2.11	0.51
1:1:63:ARG:HB2	1:1:243:TRP:CZ3	2.45	0.51
1:1:182:ASN:N	1:1:182:ASN:ND2	2.55	0.51
2:2:160:VAL:CG2	2:2:161:LEU:N	2.73	0.51
1:1:10:VAL:HG23	1:1:11:PRO:CD	2.27	0.51
1:1:359:ALA:HB1	1:1:361:PRO:CD	2.40	0.51
2:2:37:SER:CA	2:2:38:ARG:HD3	2.41	0.51
1:1:238:MET:HE3	1:1:239:ARG:O	2.10	0.51
1:1:345:ILE:CD1	1:1:349:GLN:HB3	2.38	0.51
1:1:231:ASP:OD1	1:1:233:ARG:HG2	2.09	0.51
1:1:48:ALA:HA	1:1:266:GLN:O	2.11	0.51
2:2:66:ASN:C	2:2:68:THR:H	2.18	0.51
1:1:50:ARG:HA	1:1:264:VAL:O	2.11	0.51
1:1:131:TYR:CE2	1:1:136:LYS:HB3	2.46	0.51
2:2:37:SER:CB	2:2:38:ARG:NH1	2.74	0.51
1:1:404:MET:HG2	1:1:406:THR:HG22	1.93	0.51
2:2:59:VAL:HG23	2:2:60:VAL:O	2.11	0.51
1:1:353:THR:HG22	1:1:354:GLN:H	1.64	0.50
2:2:92:ARG:CD	2:2:130:ILE:HG13	2.33	0.50
1:1:67:PHE:CE2	3:3:25:TYR:CE2	2.99	0.50
1:1:71:ILE:HG13	1:1:76:ILE:CD1	2.40	0.50
1:1:166:LYS:HD3	3:3:18:TRP:HB2	1.93	0.50
1:1:380:LYS:O	1:1:383:VAL:HG22	2.11	0.50
1:1:390:TYR:O	1:1:393:ILE:HG22	2.07	0.50
2:2:41:ILE:HG12	2:2:43:ILE:HG22	1.93	0.50
1:1:167:SER:N	1:1:170:THR:HG22	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:59:VAL:HB	2:2:144:GLY:N	2.27	0.50
2:2:25:ALA:CA	2:2:54:SER:HB3	2.40	0.50
1:1:414:ARG:HG2	1:1:415:HIS:H	1.77	0.50
2:2:85:ASP:OD1	2:2:85:ASP:O	2.29	0.50
1:1:210:TYR:O	3:3:21:GLY:CA	2.58	0.50
2:2:69:ASN:O	2:2:132:SER:HB3	2.11	0.50
1:1:12:HIS:CE1	1:1:416:MET:CB	2.95	0.50
1:1:397:MET:HG2	2:2:68:THR:HG1	1.77	0.50
2:2:32:SER:CB	2:2:41:ILE:HD12	2.41	0.50
1:1:149:SER:C	1:1:150:ASN:HD22	2.20	0.49
1:1:50:ARG:NH1	1:1:265:GLN:HG2	2.27	0.49
1:1:390:TYR:C	1:1:393:ILE:CG2	2.83	0.49
1:1:55:ARG:NH1	1:1:366:ASP:HB3	2.26	0.49
1:1:76:ILE:CG2	1:1:121:LYS:HG2	2.43	0.49
1:1:148:PRO:HA	1:1:151:MET:HE2	1.93	0.49
1:1:240:SER:OG	1:1:270:HIS:CE1	2.62	0.49
2:2:79:LEU:HB2	2:2:82:VAL:HG21	1.94	0.49
1:1:23:LYS:O	1:1:402:TRP:NE1	2.45	0.49
1:1:127:TYR:OH	1:1:160:VAL:HG12	2.12	0.49
1:1:156:TYR:CD1	1:1:156:TYR:O	2.61	0.49
1:1:237:LEU:HD22	1:1:275:PHE:CD1	2.47	0.49
1:1:359:ALA:CA	1:1:361:PRO:HD2	2.38	0.49
2:2:26:VAL:CG1	2:2:27:ALA:H	2.23	0.49
1:1:63:ARG:NH2	1:1:241:GLU:OE2	2.39	0.49
1:1:208:ARG:HG2	1:1:212:MET:HE2	1.95	0.49
1:1:300:HIS:HB3	1:1:303:VAL:CG1	2.43	0.49
1:1:388:ASN:C	1:1:390:TYR:H	2.20	0.49
1:1:70:TYR:CE2	1:1:278:PRO:HD2	2.47	0.49
1:1:174:PRO:O	1:1:177:THR:OG1	2.21	0.49
1:1:368:PHE:CB	1:1:370:PHE:HD2	2.20	0.49
1:1:329:SER:O	1:1:331:LYS:N	2.46	0.49
2:2:145:ILE:CD1	2:2:163:VAL:HG23	2.43	0.49
1:1:45:MET:SD	1:1:408:PHE:CZ	3.06	0.49
2:2:18:LEU:HD12	2:2:19:ALA:N	2.16	0.49
1:1:45:MET:HE3	1:1:408:PHE:HZ	1.78	0.49
1:1:215:TYR:HA	1:1:218:ILE:HG23	1.94	0.49
1:1:397:MET:O	1:1:397:MET:CG	2.61	0.49
2:2:90:ALA:C	2:2:91:ILE:CG2	2.83	0.49
2:2:96:ALA:HA	2:2:139:ASN:HB3	1.95	0.49
1:1:423:ILE:CD1	1:1:423:ILE:H	2.21	0.48
2:2:30:VAL:HG23	2:2:103:ALA:N	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:LEU:O	2:2:42:LEU:CG	2.33	0.48
2:2:86:MET:SD	2:2:122:ILE:HG21	2.53	0.48
2:2:28:ALA:HB2	2:2:55:GLY:O	2.10	0.48
1:1:420:ARG:C	1:1:423:ILE:CD1	2.86	0.48
1:1:172:PRO:HG2	1:1:379:LEU:CD1	2.37	0.48
2:2:59:VAL:CA	2:2:144:GLY:HA3	2.41	0.48
2:2:76:ALA:HA	2:2:124:PHE:O	2.13	0.48
1:1:126:GLY:C	1:1:284:MET:CE	2.86	0.48
2:2:157:ILE:O	2:2:157:ILE:CG1	2.58	0.48
2:2:21:THR:CB	2:2:46:THR:HG23	2.37	0.48
2:2:85:ASP:OD2	2:2:150:ASN:N	2.45	0.48
1:1:120:PRO:HG2	1:1:123:LEU:CG	2.43	0.48
1:1:382:ARG:O	1:1:382:ARG:CG	2.62	0.48
2:2:57:CYS:SG	2:2:91:ILE:CD1	2.92	0.48
2:2:86:MET:CE	2:2:147:LEU:HD13	2.43	0.48
1:1:130:ILE:O	1:1:130:ILE:HG22	2.14	0.48
2:2:102:THR:O	2:2:103:ALA:HB2	2.14	0.48
1:1:168:ILE:HG23	1:1:169:TRP:N	2.28	0.48
1:1:383:VAL:HG23	1:1:384:LEU:N	2.28	0.48
2:2:118:ASN:HD21	2:2:120:LYS:N	2.12	0.48
1:1:40:SER:HA	1:1:275:PHE:O	2.14	0.48
1:1:237:LEU:HD21	1:1:275:PHE:CE1	2.49	0.48
1:1:299:MET:CE	1:1:335:HIS:HA	2.44	0.48
1:1:360:PHE:CD1	1:1:360:PHE:O	2.66	0.48
2:2:83:PRO:C	2:2:85:ASP:H	2.21	0.48
2:2:86:MET:HE1	2:2:147:LEU:HD22	1.91	0.48
1:1:133:ASN:C	1:1:214:ARG:HH22	2.20	0.47
1:1:69:PHE:CE1	1:1:236:LEU:CG	2.97	0.47
1:1:410:ILE:HG22	1:1:411:ASN:N	2.28	0.47
2:2:61:ARG:HG3	2:2:142:TYR:CD1	2.50	0.47
2:2:89:PHE:HD1	2:2:90:ALA:O	1.97	0.47
2:2:118:ASN:HD21	2:2:121:ALA:N	2.06	0.47
1:1:41:PHE:CD1	1:1:41:PHE:C	2.93	0.47
2:2:94:GLU:OE2	2:2:135:ARG:CG	2.62	0.47
2:2:97:ASP:HA	2:2:140:ASP:OD2	2.14	0.47
2:2:30:VAL:HG23	2:2:103:ALA:CA	2.43	0.47
2:2:45:ALA:HB3	2:2:157:ILE:HG13	1.97	0.47
1:1:12:HIS:CE1	1:1:416:MET:CG	2.98	0.47
1:1:171:ALA:N	1:1:172:PRO:CD	2.77	0.47
1:1:175:PRO:O	1:1:344:LYS:NZ	2.40	0.47
1:1:183:MET:HE2	1:1:190:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:195:LEU:O	1:1:198:ALA:HB3	2.14	0.47
1:1:208:ARG:HH12	1:1:218:ILE:HD12	1.78	0.47
2:2:25:ALA:C	2:2:54:SER:CB	2.61	0.47
1:1:219:MET:O	1:1:222:PHE:HB2	2.14	0.47
2:2:68:THR:O	2:2:71:HIS:CE1	2.67	0.47
1:1:71:ILE:HD13	1:1:126:GLY:HA3	1.95	0.47
1:1:130:ILE:HA	1:1:234:PRO:HG2	1.97	0.47
1:1:218:ILE:O	1:1:222:PHE:HD2	1.97	0.47
1:1:379:LEU:HA	1:1:382:ARG:HD3	1.96	0.47
1:1:419:THR:O	1:1:423:ILE:HD13	1.96	0.47
1:1:301:TYR:CE1	1:1:332:GLU:OE1	2.63	0.47
1:1:309:THR:OG1	1:1:312:ASP:OD2	2.25	0.47
2:2:95:VAL:HG11	2:2:142:TYR:CE2	2.41	0.47
1:1:162:VAL:HG11	1:1:290:ARG:HD3	1.95	0.47
1:1:269:ASN:HD22	1:1:269:ASN:C	2.14	0.47
1:1:330:LEU:HB3	1:1:337:SER:OG	2.15	0.47
1:1:394:PHE:HE1	1:1:401:HIS:CD2	2.33	0.47
1:1:113:PRO:O	1:1:114:SER:O	2.32	0.47
1:1:135:PHE:CD1	3:3:25:TYR:HB2	2.50	0.47
1:1:137:PRO:HA	1:1:138:PRO:HD3	1.78	0.47
2:2:75:ILE:HG22	2:2:163:VAL:HG22	1.96	0.47
2:2:85:ASP:OD1	2:2:149:SER:HA	2.09	0.47
1:1:323:LEU:N	1:1:323:LEU:HD23	2.22	0.46
1:1:71:ILE:HD12	1:1:126:GLY:HA2	1.87	0.46
1:1:377:THR:CG2	1:1:378:ASP:N	2.78	0.46
1:1:419:THR:O	1:1:423:ILE:HD11	1.89	0.46
2:2:73:LEU:CD2	2:2:143:ALA:HB1	2.45	0.46
1:1:18:VAL:HG12	1:1:406:THR:C	2.37	0.46
1:1:416:MET:SD	1:1:417:PRO:HD3	2.54	0.46
1:1:133:ASN:CA	1:1:214:ARG:NH2	2.77	0.46
1:1:391:ASP:OD1	1:1:401:HIS:HE1	1.98	0.46
1:1:23:LYS:HZ3	1:1:158:TRP:NE1	2.14	0.46
1:1:120:PRO:O	1:1:123:LEU:HB2	2.16	0.46
1:1:330:LEU:HD13	1:1:341:ALA:CB	2.46	0.46
2:2:104:VAL:HG23	2:2:104:VAL:O	2.16	0.46
1:1:163:ALA:HB1	3:3:24:GLN:NE2	2.31	0.46
1:1:242:PHE:CE2	1:1:268:PHE:HB3	2.47	0.46
1:1:362:TYR:C	1:1:364:ALA:N	2.74	0.46
1:1:106:ALA:HB3	1:1:111:THR:O	2.16	0.46
1:1:200:ALA:O	1:1:204:THR:HG23	2.16	0.46
1:1:133:ASN:HA	1:1:214:ARG:NH2	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:323:LEU:HB2	1:1:324:PRO:CD	2.43	0.46
3:3:16:ARG:O	3:3:17:LEU:HD23	2.16	0.46
1:1:50:ARG:HH12	1:1:265:GLN:CD	2.23	0.45
1:1:155:ASP:O	1:1:159:GLY:CA	2.64	0.45
2:2:16:THR:O	2:2:16:THR:HG23	2.16	0.45
1:1:165:LEU:O	1:1:170:THR:HG21	2.15	0.45
1:1:242:PHE:CZ	1:1:268:PHE:CG	3.04	0.45
1:1:329:SER:OG	1:1:331:LYS:CB	2.64	0.45
2:2:96:ALA:HB3	2:2:99:VAL:HG21	1.98	0.45
1:1:150:ASN:HD22	1:1:150:ASN:N	2.14	0.45
1:1:354:GLN:HE21	1:1:354:GLN:HB2	1.61	0.45
2:2:59:VAL:HB	2:2:143:ALA:C	2.41	0.45
2:2:72:ALA:O	2:2:166:VAL:HG23	2.17	0.45
1:1:120:PRO:CD	1:1:123:LEU:HD12	2.47	0.45
1:1:231:ASP:CG	1:1:233:ARG:NH1	2.68	0.45
1:1:67:PHE:HE2	3:3:25:TYR:CZ	2.35	0.45
1:1:268:PHE:HZ	1:1:404:MET:CE	2.09	0.45
2:2:94:GLU:OE1	2:2:135:ARG:CG	2.64	0.45
2:2:26:VAL:CG1	2:2:27:ALA:N	2.80	0.45
2:2:28:ALA:CB	2:2:146:MET:HE2	2.47	0.45
2:2:63:ASP:H	2:2:165:GLN:NE2	2.14	0.45
2:2:90:ALA:O	2:2:91:ILE:HG22	2.17	0.45
2:2:136:THR:CB	2:2:139:ASN:HD21	2.17	0.45
1:1:166:LYS:CB	3:3:18:TRP:CD1	2.99	0.45
2:2:49:ALA:HB1	2:2:153:THR:HA	1.97	0.45
1:1:24:ILE:HG22	1:1:25:GLY:N	2.31	0.45
1:1:216:ARG:CA	1:1:226:THR:HG21	2.43	0.45
1:1:392:GLU:H	1:1:392:GLU:HG2	1.56	0.45
2:2:41:ILE:CD1	2:2:43:ILE:CG2	2.95	0.45
2:2:56:LEU:O	2:2:56:LEU:CD1	2.56	0.45
1:1:97:VAL:CG2	1:1:121:LYS:HB2	2.47	0.44
1:1:100:SER:O	1:1:105:SER:HB2	2.17	0.44
1:1:170:THR:O	1:1:170:THR:CG2	2.52	0.44
1:1:323:LEU:CB	1:1:324:PRO:HD2	2.45	0.44
2:2:117:ASN:HB2	2:2:122:ILE:HG13	1.98	0.44
1:1:394:PHE:CE1	1:1:401:HIS:CD2	3.05	0.44
2:2:101:PRO:HG3	2:2:142:TYR:CD2	2.53	0.44
1:1:253:ASP:OD1	1:1:256:SER:OG	2.24	0.44
2:2:56:LEU:HD12	2:2:56:LEU:C	2.39	0.44
2:2:77:GLY:N	2:2:124:PHE:CE1	2.85	0.44
1:1:45:MET:CE	1:1:408:PHE:CZ	2.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:288:VAL:O	1:1:288:VAL:HG13	2.18	0.44
1:1:18:VAL:HG13	1:1:18:VAL:O	2.18	0.44
1:1:113:PRO:C	1:1:114:SER:O	2.60	0.44
1:1:286:LEU:N	1:1:286:LEU:HD12	2.33	0.44
2:2:73:LEU:CD2	2:2:143:ALA:CB	2.95	0.44
2:2:86:MET:HE2	2:2:147:LEU:CB	2.45	0.44
1:1:18:VAL:CG2	1:1:20:GLU:CG	2.86	0.44
1:1:50:ARG:NH2	1:1:265:GLN:OE1	2.49	0.44
1:1:360:PHE:C	1:1:360:PHE:HD1	2.24	0.44
2:2:18:LEU:CD2	2:2:43:ILE:CG2	2.95	0.44
2:2:95:VAL:O	2:2:139:ASN:HB3	2.13	0.44
1:1:116:THR:O	1:1:117:LEU:HB2	2.18	0.44
2:2:41:ILE:HG21	2:2:41:ILE:HD13	1.35	0.44
1:1:104:ASP:CG	1:1:157:LYS:HE2	2.42	0.43
1:1:238:MET:HE2	1:1:239:ARG:O	2.16	0.43
1:1:334:PHE:CD2	1:1:375:PRO:HG3	2.53	0.43
2:2:9:HIS:CE1	2:2:162:SER:CB	2.84	0.43
2:2:23:THR:HA	2:2:48:THR:HG21	1.97	0.43
1:1:64:VAL:O	1:1:241:GLU:HA	2.18	0.43
1:1:165:LEU:O	1:1:293:PRO:CG	2.66	0.43
1:1:368:PHE:O	1:1:370:PHE:N	2.49	0.43
1:1:376:SER:C	1:1:378:ASP:N	2.77	0.43
1:1:70:TYR:HB2	1:1:237:LEU:CD1	2.33	0.43
1:1:269:ASN:ND2	1:1:269:ASN:C	2.73	0.43
2:2:41:ILE:HD13	2:2:43:ILE:HG21	2.01	0.43
1:1:76:ILE:HD12	1:1:76:ILE:N	2.33	0.43
1:1:420:ARG:C	1:1:423:ILE:HD13	2.44	0.43
1:1:298:GLU:HB2	1:1:334:PHE:CE1	2.53	0.43
1:1:97:VAL:CG2	1:1:121:LYS:CA	2.88	0.43
2:2:18:LEU:HD13	2:2:18:LEU:HA	1.78	0.43
2:2:89:PHE:CE1	2:2:110:VAL:CG1	3.00	0.43
1:1:97:VAL:HG11	1:1:148:PRO:HD3	2.01	0.43
1:1:405:GLN:N	1:1:405:GLN:CD	2.77	0.43
1:1:416:MET:CB	1:1:417:PRO:HD2	2.47	0.43
2:2:164:ASN:OD1	2:2:164:ASN:C	2.46	0.43
1:1:328:VAL:HG23	1:1:343:PHE:O	2.19	0.43
2:2:66:ASN:C	2:2:68:THR:N	2.77	0.43
2:2:113:ILE:HB	2:2:114:GLU:H	1.67	0.43
1:1:390:TYR:C	1:1:393:ILE:HG22	2.44	0.43
1:1:97:VAL:HG13	1:1:147:ASN:ND2	2.33	0.42
1:1:107:ALA:CB	1:1:157:LYS:O	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:330:LEU:HD22	1:1:341:ALA:CB	2.49	0.42
2:2:32:SER:HB3	2:2:41:ILE:HD12	2.01	0.42
2:2:69:ASN:O	2:2:132:SER:N	2.36	0.42
2:2:91:ILE:HD13	2:2:146:MET:HB2	2.01	0.42
1:1:54:LEU:HD11	1:1:262:GLY:HA3	2.01	0.42
1:1:97:VAL:HG12	1:1:98:THR:N	2.35	0.42
1:1:135:PHE:CZ	3:3:25:TYR:CD2	3.08	0.42
1:1:145:TYR:CG	1:1:151:MET:CG	2.96	0.42
2:2:22:LYS:HD2	2:2:29:PRO:HB2	2.00	0.42
1:1:45:MET:CG	1:1:408:PHE:CE1	3.03	0.42
1:1:330:LEU:HD13	1:1:341:ALA:O	2.17	0.42
1:1:36:VAL:HG13	1:1:414:ARG:HH11	1.84	0.42
1:1:162:VAL:HG11	1:1:288:VAL:CG2	2.49	0.42
1:1:12:HIS:HE1	1:1:416:MET:CB	2.33	0.42
1:1:102:GLY:C	1:1:104:ASP:N	2.75	0.42
2:2:145:ILE:CD1	2:2:163:VAL:CG2	2.98	0.42
1:1:30:ILE:HD11	1:1:45:MET:CE	2.43	0.42
1:1:130:ILE:O	1:1:130:ILE:CG2	2.67	0.42
1:1:242:PHE:HE2	1:1:266:GLN:CG	2.30	0.42
1:1:63:ARG:NH2	1:1:239:ARG:NH2	2.67	0.42
1:1:71:ILE:CG1	1:1:71:ILE:O	2.67	0.42
1:1:374:LEU:O	1:1:375:PRO:O	2.37	0.42
1:1:65:ASP:HB2	1:1:288:VAL:HG13	2.01	0.42
1:1:122:PHE:O	1:1:126:GLY:HA3	2.20	0.42
1:1:242:PHE:CZ	1:1:268:PHE:HB2	2.48	0.42
1:1:298:GLU:OE2	1:1:355:PRO:HB3	2.20	0.42
2:2:18:LEU:CD2	2:2:43:ILE:HG22	2.46	0.42
1:1:32:TRP:CE3	1:1:34:PRO:HD3	2.55	0.41
1:1:71:ILE:O	1:1:71:ILE:HG12	2.20	0.41
1:1:11:PRO:CG	1:1:413:TYR:CE1	3.01	0.41
1:1:12:HIS:NE2	1:1:416:MET:HB2	2.35	0.41
1:1:67:PHE:HE2	3:3:25:TYR:CE2	2.38	0.41
2:2:41:ILE:CG1	2:2:43:ILE:CG2	2.98	0.41
2:2:88:ALA:O	2:2:113:ILE:HD11	2.20	0.41
1:1:165:LEU:O	1:1:293:PRO:HG3	2.21	0.41
1:1:397:MET:O	1:1:397:MET:HG2	2.19	0.41
2:2:66:ASN:O	2:2:68:THR:N	2.53	0.41
2:2:101:PRO:CD	2:2:142:TYR:OH	2.65	0.41
2:2:93:PHE:CZ	2:2:142:TYR:HB2	2.55	0.41
2:2:94:GLU:HA	2:2:140:ASP:O	2.21	0.41
2:2:101:PRO:HD2	2:2:142:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:164:ASN:OD1	2:2:165:GLN:C	2.62	0.41
2:2:18:LEU:HD23	2:2:43:ILE:CG2	2.50	0.41
2:2:41:ILE:HD13	2:2:43:ILE:CG2	2.51	0.41
2:2:101:PRO:CG	2:2:142:TYR:CE2	3.03	0.41
1:1:42:GLU:HB3	1:1:274:ARG:HA	2.02	0.41
1:1:126:GLY:HA3	1:1:284:MET:HE3	2.02	0.41
1:1:128:LEU:HD21	1:1:143:LEU:HB3	2.02	0.41
2:2:92:ARG:HH12	2:2:94:GLU:CG	2.33	0.41
2:2:123:SER:OG	2:2:124:PHE:N	2.53	0.41
1:1:183:MET:SD	1:1:195:LEU:HA	2.61	0.41
1:1:328:VAL:O	1:1:342:LYS:HA	2.20	0.41
2:2:25:ALA:O	2:2:28:ALA:HA	2.21	0.41
2:2:82:VAL:HG13	2:2:86:MET:CE	2.49	0.41
1:1:120:PRO:HG2	1:1:123:LEU:HG	2.03	0.41
1:1:237:LEU:CD2	1:1:275:PHE:CE1	3.04	0.41
1:1:323:LEU:CB	1:1:324:PRO:CD	2.98	0.41
2:2:164:ASN:OD1	2:2:165:GLN:CA	2.63	0.41
1:1:12:HIS:N	1:1:412:VAL:O	2.42	0.41
1:1:22:GLY:HA2	1:1:158:TRP:CZ3	2.55	0.41
1:1:36:VAL:HB	1:1:280:HIS:CD2	2.56	0.41
1:1:52:SER:OG	1:1:400:ALA:O	2.37	0.41
1:1:74:ARG:CZ	1:1:74:ARG:HB3	2.51	0.41
1:1:135:PHE:CD1	3:3:25:TYR:CB	3.04	0.41
1:1:174:PRO:O	1:1:177:THR:CB	2.69	0.41
1:1:377:THR:HG22	1:1:378:ASP:N	2.36	0.41
1:1:410:ILE:CG2	1:1:411:ASN:N	2.84	0.41
1:1:420:ARG:HE	1:1:420:ARG:HB3	1.53	0.41
2:2:26:VAL:HA	2:2:54:SER:CB	2.49	0.41
2:2:43:ILE:O	2:2:45:ALA:CA	2.61	0.41
2:2:50:VAL:HG12	2:2:152:TRP:CG	2.56	0.41
2:2:92:ARG:NE	2:2:131:ASP:OD1	2.54	0.41
1:1:10:VAL:HG22	1:1:11:PRO:CD	2.42	0.41
2:2:78:SER:O	2:2:79:LEU:HD23	2.21	0.41
1:1:137:PRO:O	1:1:140:SER:CB	2.66	0.40
1:1:215:TYR:C	1:1:217:ASP:N	2.77	0.40
1:1:330:LEU:HD12	1:1:343:PHE:CE1	2.56	0.40
1:1:410:ILE:HD13	1:1:410:ILE:HG21	1.83	0.40
2:2:86:MET:HB2	2:2:117:ASN:ND2	2.31	0.40
2:2:118:ASN:OD1	2:2:119:GLY:N	2.42	0.40
1:1:32:TRP:HA	1:1:283:ILE:O	2.22	0.40
1:1:45:MET:HG3	1:1:408:PHE:CE1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:109:LEU:HD22	1:1:123:LEU:O	2.20	0.40
1:1:374:LEU:C	1:1:375:PRO:O	2.63	0.40
1:1:419:THR:C	1:1:423:ILE:HD11	2.40	0.40
2:2:31:LEU:HD23	2:2:31:LEU:HA	1.91	0.40
2:2:66:ASN:ND2	2:2:67:PRO:HD2	2.36	0.40
2:2:145:ILE:HD12	2:2:163:VAL:HG23	2.03	0.40
2:2:80:SER:C	2:2:82:VAL:N	2.73	0.40
2:2:89:PHE:HE1	2:2:91:ILE:CG2	2.34	0.40
2:2:92:ARG:NH2	2:2:141:VAL:HG11	2.35	0.40
1:1:81:TRP:O	1:1:84:PHE:HB3	2.22	0.40
2:2:86:MET:HE2	2:2:147:LEU:CG	2.51	0.40
1:1:97:VAL:HG23	1:1:121:LYS:CB	2.52	0.40
1:1:380:LYS:HB3	1:1:381:ASP:H	1.75	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	415/426 (97%)	362 (87%)	40 (10%)	13 (3%)	3	19
2	2	175/177 (99%)	137 (78%)	30 (17%)	8 (5%)	2	11
3	3	10/25 (40%)	7 (70%)	3 (30%)	0	100	100
All	All	600/628 (96%)	506 (84%)	73 (12%)	21 (4%)	3	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	114	SER
1	1	377	THR
1	1	417	PRO
2	2	44	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	166	VAL
1	1	101	SER
1	1	363	ASN
1	1	380	LYS
1	1	418	THR
2	2	27	ALA
2	2	103	ALA
1	1	373	ALA
1	1	379	LEU
2	2	76	ALA
1	1	330	LEU
1	1	395	GLN
1	1	375	PRO
1	1	388	ASN
2	2	67	PRO
2	2	113	ILE
2	2	137	VAL

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	369/377 (98%)	296 (80%)	73 (20%)	1	8
2	2	148/148 (100%)	104 (70%)	44 (30%)	0	2
3	3	8/19 (42%)	6 (75%)	2 (25%)	0	3
All	All	525/544 (96%)	406 (77%)	119 (23%)	1	5

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	23	LYS
1	1	24	ILE
1	1	36	VAL
1	1	51	LEU
1	1	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	71	ILE
1	1	82	ILE
1	1	86	LYS
1	1	89	VAL
1	1	100	SER
1	1	112	ILE
1	1	117	LEU
1	1	119	VAL
1	1	121	LYS
1	1	144	THR
1	1	156	TYR
1	1	160	VAL
1	1	166	LYS
1	1	167	SER
1	1	170	THR
1	1	182	ASN
1	1	184	THR
1	1	187	THR
1	1	190	ILE
1	1	192	ILE
1	1	196	GLN
1	1	211	PHE
1	1	212	MET
1	1	214	ARG
1	1	218	ILE
1	1	221	GLU
1	1	226	THR
1	1	236	LEU
1	1	269	ASN
1	1	286	LEU
1	1	305	LYS
1	1	313	ILE
1	1	323	LEU
1	1	328	VAL
1	1	337	SER
1	1	342	LYS
1	1	345	ILE
1	1	352	ARG
1	1	354	GLN
1	1	357	ARG
1	1	360	PHE
1	1	363	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	365	LEU
1	1	372	SER
1	1	377	THR
1	1	378	ASP
1	1	380	LYS
1	1	382	ARG
1	1	383	VAL
1	1	385	VAL
1	1	386	ASN
1	1	387	THR
1	1	393	ILE
1	1	396	SER
1	1	397	MET
1	1	404	MET
1	1	405	GLN
1	1	406	THR
1	1	407	LYS
1	1	411	ASN
1	1	414	ARG
1	1	415	HIS
1	1	420	ARG
1	1	421	ASP
1	1	423	ILE
1	1	424	MET
1	1	425	THR
1	1	426	SER
2	2	6	ILE
2	2	14	ASN
2	2	17	GLN
2	2	18	LEU
2	2	21	THR
2	2	23	THR
2	2	35	ASN
2	2	37	SER
2	2	38	ARG
2	2	40	THR
2	2	41	ILE
2	2	42	LEU
2	2	43	ILE
2	2	50	VAL
2	2	52	THR
2	2	53	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	54	SER
2	2	57	CYS
2	2	59	VAL
2	2	61	ARG
2	2	62	ILE
2	2	65	THR
2	2	68	THR
2	2	69	ASN
2	2	81	ASN
2	2	85	ASP
2	2	86	MET
2	2	107	LEU
2	2	111	TYR
2	2	113	ILE
2	2	114	GLU
2	2	118	ASN
2	2	122	ILE
2	2	123	SER
2	2	129	THR
2	2	130	ILE
2	2	150	ASN
2	2	153	THR
2	2	155	SER
2	2	156	THR
2	2	165	GLN
2	2	172	VAL
2	2	173	LEU
2	2	176	LEU
3	3	16	ARG
3	3	25	TYR

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

Mol	Chain	Res	Type
1	1	12	HIS
1	1	16	HIS
1	1	79	GLN
1	1	83	ASN
1	1	125	GLN
1	1	129	ASN
1	1	132	ASN
1	1	147	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	150	ASN
1	1	164	ASN
1	1	182	ASN
1	1	196	GLN
1	1	266	GLN
1	1	269	ASN
1	1	300	HIS
1	1	335	HIS
1	1	349	GLN
1	1	354	GLN
1	1	386	ASN
1	1	388	ASN
1	1	389	ASN
1	1	401	HIS
1	1	411	ASN
2	2	9	HIS
2	2	35	ASN
2	2	44	ASN
2	2	66	ASN
2	2	69	ASN
2	2	71	HIS
2	2	81	ASN
2	2	118	ASN
2	2	139	ASN
2	2	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.