



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2026 – 04:48 pm BST

PDB ID : 9HMI / pdb_00009hmi
Title : Crystal structure of the Calf domains of Integrin Alpha5 in complex with angiopoietin2 peptide
Authors : Murthy, A.V.; Sipila, T.J.O.; Ponna, S.K.; Leppanen, V.M.L.; Saharinen, P.I.
Deposited on : 2024-12-09
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

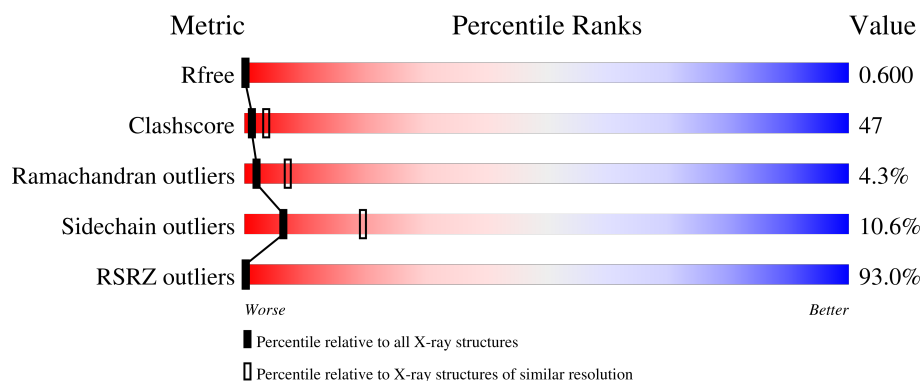
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	346	93% 33% 52% 13% .
2	P	9	89% 33% 67%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2903 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2721	1707	487	515	12			

- Molecule 2 is a protein called Angiopoietin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	0	0	0
			74	46	12	16			

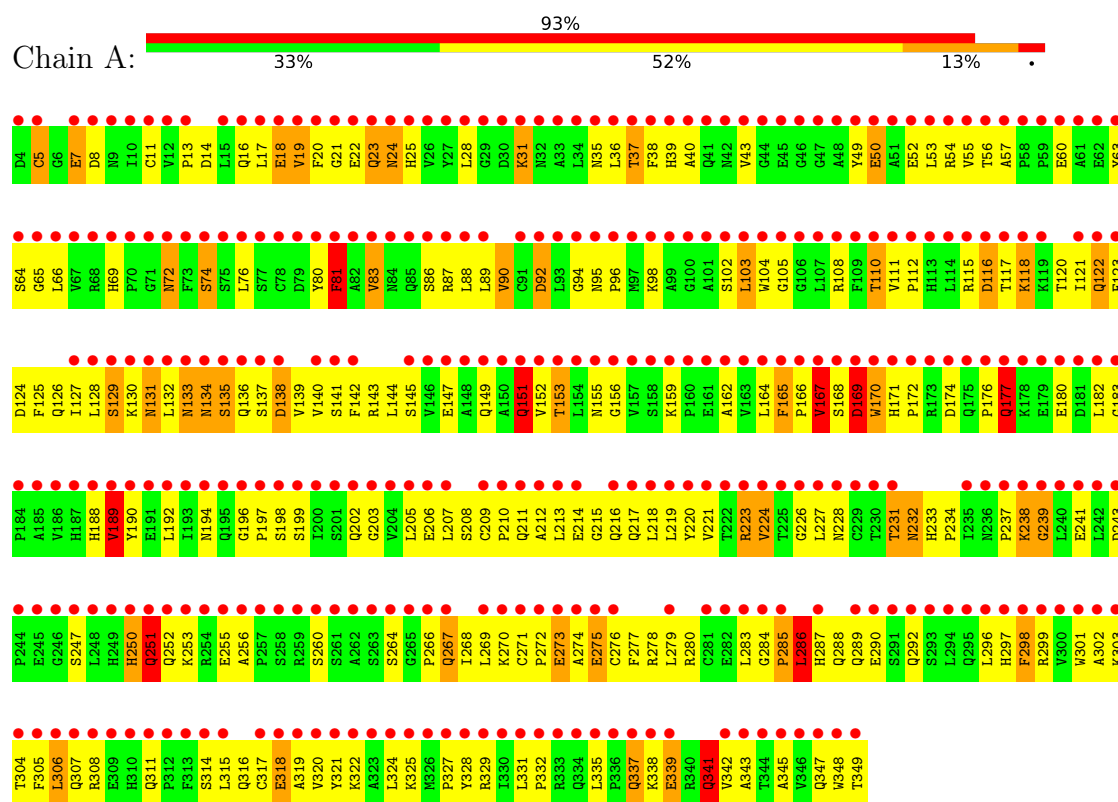
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	P	4	Total	O	0	0
			4	4		

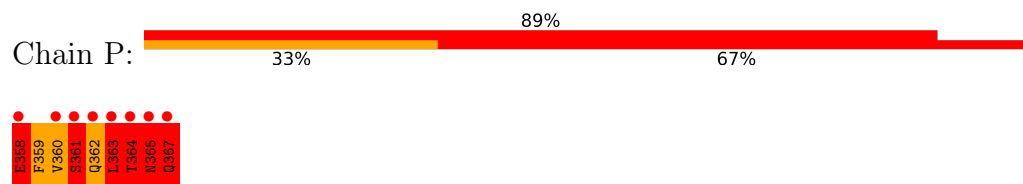
3 Residue-property plots

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

• Molecule 1: Integrin alpha-5



• Molecule 2: Angiopoietin-2



4 Data and refinement statistics

Property	Value
Space group	P 21 21 21
Cell constants a, b, c, α , β , γ	49.98Å 69.23Å 137.83Å 90.00° 90.00° 90.00°
Resolution (Å)	50.34 – 2.87 50.34 – 2.87
% Data completeness (in resolution range)	98.1 (50.34-2.87) 99.9 (50.34-2.87)
R_{merge}	0.20
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.77Å)
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.128), REFMAC 5.8.0431 (refmacat 0.4.128)
R, R_{free}	0.233 , 0.281 0.566 , 0.600
R_{free} test set	610 reflections (4.97%)
Wilson B-factor (Å ²)	90.2
Anisotropy	0.365
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 999.0
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$
Estimated twinning fraction	No twinning to report.
F_o, F_c correlation	0.55
Total number of atoms	2903
Average B, all atoms (Å ²)	100.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/2786	1.47	41/3786 (1.1%)
2	P	3.20	5/74 (6.8%)	15.24	24/99 (24.2%)
All	All	0.78	5/2860 (0.2%)	2.83	65/3885 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	P	4	8
All	All	4	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	361	SER	CA-C	15.89	1.75	1.52
2	P	367	GLN	CG-CD	14.14	1.87	1.52
2	P	367	GLN	CB-CG	-12.10	1.16	1.52
2	P	364	THR	C-N	7.30	1.39	1.33
2	P	363	LEU	N-CA	6.45	1.54	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	365	ASN	O-C-N	-94.48	50.61	121.47
2	P	363	LEU	O-C-N	-57.38	46.27	122.59
2	P	367	GLN	OE1-CD-NE2	-40.40	82.20	122.60
2	P	363	LEU	N-CA-CB	38.88	176.19	110.49
2	P	359	PHE	N-CA-CB	32.69	163.69	110.40
2	P	363	LEU	CA-C-O	-32.51	74.02	120.51
2	P	362	GLN	CB-CA-C	-32.24	46.27	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	362	GLN	OE1-CD-NE2	-30.73	91.88	122.60
2	P	367	GLN	CA-C-O	-25.12	78.09	120.80
2	P	364	THR	N-CA-CB	22.48	148.48	110.49
2	P	364	THR	CB-CA-C	-18.98	72.65	110.42
2	P	358	GLU	CA-C-O	-18.21	89.84	120.80
2	P	367	GLN	CG-CD-NE2	15.68	139.92	116.40
2	P	362	GLN	CG-CD-NE2	14.23	137.74	116.40
2	P	363	LEU	N-CA-C	-14.11	80.74	110.80
2	P	365	ASN	N-CA-CB	-13.05	88.44	110.49
2	P	365	ASN	N-CA-C	12.21	118.79	108.78
1	A	81	PHE	CA-CB-CG	12.06	125.86	113.80
1	A	341	GLN	CB-CA-C	-11.90	89.96	109.72
1	A	131	ASN	CB-CA-C	-11.81	87.03	112.78
1	A	189	VAL	N-CA-CB	10.87	124.03	110.99
2	P	364	THR	N-CA-C	10.15	132.42	110.80
1	A	153	THR	CA-CB-OG1	-9.05	96.02	109.60
2	P	359	PHE	N-CA-C	-8.53	102.31	112.89
1	A	37	THR	CA-CB-OG1	-8.21	97.29	109.60
2	P	359	PHE	CB-CA-C	-8.13	92.99	109.99
1	A	202	GLN	CB-CA-C	-8.12	95.30	110.16
2	P	358	GLU	N-CA-CB	7.87	123.88	110.50
1	A	151	GLN	CB-CA-C	7.77	124.21	109.37
1	A	167	VAL	N-CA-CB	7.47	120.49	110.26
2	P	363	LEU	CB-CA-C	-7.43	95.63	110.42
2	P	360	VAL	N-CA-CB	7.42	123.48	111.23
1	A	69	HIS	CB-CA-C	7.08	120.95	109.97
1	A	18	GLU	CB-CA-C	6.69	123.35	109.38
1	A	69	HIS	CA-CB-CG	6.61	120.41	113.80
1	A	92	ASP	CB-CA-C	-6.45	99.58	109.89
2	P	360	VAL	N-CA-C	6.42	122.68	109.34
1	A	190	TYR	N-CA-CB	6.12	120.97	110.68
1	A	286	LEU	N-CA-CB	-6.12	101.36	110.90
1	A	7	GLU	N-CA-C	-6.09	105.97	113.41
1	A	164	LEU	N-CA-CB	-6.06	101.04	110.55
1	A	337	GLN	N-CA-CB	-5.96	100.81	110.71
1	A	241	GLU	CB-CG-CD	-5.75	102.82	112.60
1	A	11	CYS	CB-CA-C	5.70	118.94	109.53
1	A	339	GLU	CB-CG-CD	5.68	122.26	112.60
1	A	325	LYS	N-CA-CB	-5.65	100.77	111.00
1	A	83	VAL	N-CA-CB	5.60	119.27	110.31
1	A	169	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	118	LYS	CB-CG-CD	5.53	124.03	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	23	GLN	N-CA-CB	-5.46	101.51	110.52
1	A	188	HIS	CA-CB-CG	5.45	119.25	113.80
1	A	50	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	122	GLN	N-CA-CB	-5.43	101.70	110.71
1	A	331	LEU	N-CA-CB	5.41	117.77	110.14
1	A	238	LYS	N-CA-CB	-5.40	102.38	110.91
1	A	138	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	116	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	232	ASN	CB-CA-C	5.20	118.78	110.09
1	A	60	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	298	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	243	ASP	CB-CA-C	5.08	117.59	109.62
1	A	138	ASP	CB-CA-C	-5.03	99.36	109.68
1	A	177	GLN	CB-CA-C	-5.03	100.41	110.42
1	A	320	VAL	N-CA-CB	5.00	118.82	111.52

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	359	PHE	CA
2	P	363	LEU	CA
2	P	364	THR	CA
2	P	365	ASN	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain
2	P	358	GLU	Peptide,Mainchain
2	P	361	SER	Peptide,Mainchain
2	P	363	LEU	Mainchain
2	P	365	ASN	Peptide,Mainchain
2	P	367	GLN	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	A	2721	0	2646	221	744
2	P	74	0	62	85	65
3	A	104	0	0	79	3
3	P	4	0	0	8	0
All	All	2903	0	2708	260	745

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 47.

All (260) 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:P:361:SER:C	2:P:361:SER:CA	1.74	1.55
2:P:367:GLN:CD	2:P:367:GLN:CG	1.87	1.48
1:A:308:ARG:HB3	3:A:413:HOH:O	1.22	1.35
1:A:54:ARG:HD3	2:P:367:GLN:O	1.27	1.34
2:P:358:GLU:HG3	3:P:402:HOH:O	1.26	1.26
1:A:221:VAL:HG22	3:A:485:HOH:O	1.08	1.22
1:A:54:ARG:NH1	2:P:365:ASN:H	1.37	1.19
2:P:360:VAL:HG13	2:P:362:GLN:O	1.40	1.16
1:A:90:VAL:CG1	2:P:367:GLN:HG2	1.52	1.16
1:A:23:GLN:HG3	3:A:411:HOH:O	1.41	1.15
1:A:24:ASN:N	3:A:411:HOH:O	1.73	1.15
2:P:362:GLN:CG	3:P:403:HOH:O	1.93	1.14
1:A:54:ARG:NE	2:P:365:ASN:HA	1.62	1.14
1:A:138:ASP:N	3:A:412:HOH:O	1.80	1.13
1:A:171:HIS:C	3:A:410:HOH:O	1.87	1.12
1:A:40:ALA:O	1:A:102:SER:O	1.69	1.10
1:A:221:VAL:CG2	3:A:485:HOH:O	1.66	1.10
1:A:308:ARG:CB	3:A:413:HOH:O	1.80	1.09
1:A:54:ARG:CZ	2:P:365:ASN:CA	2.30	1.08
1:A:219:LEU:O	3:A:409:HOH:O	1.70	1.08
1:A:305:PHE:CZ	3:A:499:HOH:O	2.06	1.08
1:A:308:ARG:CG	3:A:413:HOH:O	1.91	1.08
2:P:364:THR:O	2:P:365:ASN:HB2	1.54	1.07
1:A:54:ARG:CD	2:P:367:GLN:O	2.03	1.06
1:A:90:VAL:HG12	2:P:367:GLN:CG	1.36	1.06
1:A:52:GLU:HA	2:P:367:GLN:OE1	1.56	1.03
1:A:54:ARG:CZ	2:P:365:ASN:HA	1.89	1.02
1:A:171:HIS:O	3:A:410:HOH:O	1.71	1.02
2:P:364:THR:O	2:P:365:ASN:CB	2.07	1.02
1:A:54:ARG:NH1	2:P:365:ASN:N	2.07	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:CD	3:A:422:HOH:O	2.02	1.00
1:A:305:PHE:CE2	3:A:499:HOH:O	2.13	0.99
1:A:95:ASN:ND2	3:A:417:HOH:O	1.93	0.98
1:A:311:GLN:OE1	3:A:413:HOH:O	1.80	0.98
1:A:25:HIS:N	3:A:411:HOH:O	1.88	0.98
2:P:362:GLN:CB	3:P:403:HOH:O	2.05	0.98
1:A:212:ALA:HB3	1:A:275:GLU:HB2	1.45	0.97
2:P:365:ASN:HA	2:P:367:GLN:C	1.91	0.96
2:P:362:GLN:HG2	3:P:403:HOH:O	1.56	0.95
1:A:90:VAL:HG11	2:P:365:ASN:O	1.58	0.94
1:A:322:LYS:HE2	1:A:337:GLN:NE2	1.82	0.93
1:A:90:VAL:HG12	2:P:367:GLN:HG3	1.47	0.92
2:P:364:THR:HG23	2:P:365:ASN:HB2	1.39	0.92
1:A:177:GLN:NE2	3:A:419:HOH:O	2.04	0.91
1:A:287:HIS:O	3:A:415:HOH:O	1.87	0.91
1:A:221:VAL:HG13	3:A:485:HOH:O	1.65	0.91
2:P:358:GLU:HG3	2:P:361:SER:HB3	1.50	0.90
2:P:358:GLU:N	2:P:360:VAL:H	1.68	0.90
1:A:52:GLU:HG2	2:P:367:GLN:CD	1.96	0.90
1:A:87:ARG:NE	3:A:408:HOH:O	1.73	0.90
1:A:169:ASP:O	1:A:170:TRP:HB2	1.73	0.89
1:A:288:GLN:HA	3:A:415:HOH:O	1.71	0.89
1:A:212:ALA:HB3	1:A:275:GLU:CB	2.03	0.89
1:A:159:LYS:HG3	3:A:464:HOH:O	1.74	0.88
1:A:194:ASN:CG	3:A:415:HOH:O	2.16	0.87
2:P:365:ASN:CA	2:P:367:GLN:C	2.45	0.86
1:A:177:GLN:CD	3:A:419:HOH:O	2.19	0.86
2:P:360:VAL:HG12	2:P:360:VAL:O	1.73	0.86
1:A:305:PHE:HA	3:A:432:HOH:O	1.76	0.85
1:A:5:CYS:HB2	3:A:496:HOH:O	1.76	0.84
1:A:194:ASN:HB3	3:A:415:HOH:O	1.78	0.82
1:A:23:GLN:C	3:A:411:HOH:O	2.06	0.82
1:A:13:PRO:HD2	1:A:135:SER:OG	1.80	0.82
1:A:54:ARG:HE	2:P:367:GLN:CA	1.92	0.81
1:A:199:SER:OG	3:A:418:HOH:O	1.96	0.81
1:A:221:VAL:CG1	3:A:485:HOH:O	2.07	0.80
1:A:54:ARG:HH12	2:P:365:ASN:H	1.28	0.80
1:A:54:ARG:CD	2:P:365:ASN:HA	2.12	0.80
1:A:221:VAL:CB	3:A:485:HOH:O	1.96	0.79
1:A:90:VAL:CG1	2:P:367:GLN:HG3	2.07	0.78
1:A:182:LEU:HD22	1:A:301:TRP:CZ3	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PHE:O	1:A:306:LEU:HB2	1.81	0.78
1:A:194:ASN:CB	3:A:415:HOH:O	2.31	0.78
1:A:308:ARG:CD	3:A:413:HOH:O	2.25	0.78
1:A:118:LYS:HB3	3:A:472:HOH:O	1.85	0.76
2:P:367:GLN:CD	2:P:367:GLN:CB	2.54	0.76
1:A:54:ARG:CZ	2:P:365:ASN:N	2.47	0.76
2:P:360:VAL:O	2:P:360:VAL:CG1	2.32	0.76
1:A:24:ASN:O	1:A:144:LEU:HA	1.86	0.74
2:P:358:GLU:OE2	2:P:361:SER:HB2	1.86	0.74
1:A:306:LEU:HD12	1:A:348:TRP:HH2	1.51	0.74
2:P:358:GLU:CG	2:P:361:SER:HB3	2.09	0.74
1:A:307:GLN:HG3	3:A:442:HOH:O	1.86	0.74
1:A:110:THR:OG1	3:A:407:HOH:O	1.67	0.73
1:A:14:ASP:HB3	1:A:43:VAL:HG23	1.70	0.73
1:A:54:ARG:HD3	2:P:367:GLN:C	2.13	0.73
1:A:194:ASN:ND2	3:A:415:HOH:O	2.18	0.73
1:A:54:ARG:CD	2:P:367:GLN:C	2.61	0.72
1:A:203:GLY:HA2	1:A:324:LEU:HG	1.72	0.72
1:A:54:ARG:HE	2:P:367:GLN:HA	1.55	0.71
1:A:64:SER:C	3:A:444:HOH:O	2.32	0.71
1:A:220:TYR:CZ	1:A:237:PRO:HD2	2.26	0.71
2:P:358:GLU:N	2:P:360:VAL:N	2.39	0.71
2:P:361:SER:C	2:P:361:SER:CB	2.62	0.71
2:P:367:GLN:O	2:P:367:GLN:HG3	1.88	0.70
1:A:180:GLU:OE1	3:A:423:HOH:O	2.09	0.70
1:A:308:ARG:HD3	3:A:413:HOH:O	1.90	0.70
1:A:155:ASN:OD1	3:A:421:HOH:O	2.10	0.70
1:A:92:ASP:HA	2:P:367:GLN:OE1	1.83	0.69
2:P:358:GLU:CG	3:P:402:HOH:O	2.05	0.69
2:P:360:VAL:HG21	2:P:363:LEU:CD1	2.22	0.69
1:A:14:ASP:HB3	1:A:43:VAL:CG2	2.23	0.69
1:A:76:LEU:HB2	3:A:469:HOH:O	1.93	0.69
1:A:54:ARG:CZ	2:P:365:ASN:H	1.99	0.69
1:A:341:GLN:NE2	3:A:427:HOH:O	2.25	0.69
1:A:54:ARG:CZ	2:P:365:ASN:C	2.66	0.69
1:A:288:GLN:CA	3:A:415:HOH:O	2.35	0.68
1:A:54:ARG:NE	2:P:367:GLN:CA	2.57	0.68
1:A:217:GLN:NE2	3:A:426:HOH:O	2.27	0.68
1:A:90:VAL:HG12	2:P:367:GLN:HG2	0.73	0.67
1:A:151:GLN:H	1:A:196:GLY:HA3	1.58	0.67
2:P:361:SER:CA	2:P:362:GLN:N	2.54	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:NE	2:P:367:GLN:C	2.53	0.67
1:A:224:VAL:HG11	1:A:279:LEU:HD21	1.76	0.66
1:A:306:LEU:HD12	1:A:348:TRP:CH2	2.30	0.66
1:A:130:LYS:HA	1:A:134:ASN:ND2	2.10	0.66
1:A:94:GLY:HA2	3:A:449:HOH:O	1.95	0.65
1:A:272:PRO:C	1:A:274:ALA:H	2.05	0.65
2:P:364:THR:CG2	2:P:365:ASN:HB2	2.20	0.64
2:P:364:THR:O	2:P:365:ASN:HB3	1.90	0.64
1:A:54:ARG:NE	2:P:367:GLN:O	2.30	0.64
1:A:277:PHE:HE2	1:A:279:LEU:HD11	1.63	0.64
1:A:54:ARG:NH2	2:P:365:ASN:C	2.57	0.63
1:A:169:ASP:O	1:A:170:TRP:CB	2.46	0.63
1:A:19:VAL:HG11	1:A:125:PHE:CZ	2.35	0.62
1:A:54:ARG:NH1	2:P:365:ASN:CA	2.58	0.62
2:P:358:GLU:CG	2:P:358:GLU:O	2.48	0.62
1:A:149:GLN:O	1:A:197:PRO:HD2	2.00	0.62
1:A:223:ARG:O	1:A:224:VAL:HG23	1.99	0.62
1:A:18:GLU:CD	3:A:428:HOH:O	2.43	0.61
1:A:90:VAL:CG1	2:P:367:GLN:CG	2.12	0.60
1:A:131:ASN:HB2	1:A:134:ASN:H	1.65	0.60
1:A:183:GLY:O	1:A:299:ARG:HD2	2.01	0.60
1:A:72:ASN:OD1	1:A:104:TRP:HB2	2.01	0.59
1:A:52:GLU:HB3	2:P:367:GLN:O	2.02	0.59
1:A:35:ASN:ND2	1:A:108:ARG:HG2	2.17	0.59
1:A:134:ASN:O	1:A:135:SER:C	2.44	0.59
1:A:314:SER:OG	3:A:424:HOH:O	2.16	0.59
1:A:28:LEU:HD22	1:A:328:TYR:CD1	2.38	0.58
1:A:49:TYR:CE1	1:A:96:PRO:HG3	2.39	0.58
1:A:226:GLY:O	1:A:227:LEU:HG	2.04	0.58
1:A:277:PHE:HE2	1:A:279:LEU:CD1	2.17	0.57
1:A:130:LYS:HA	1:A:134:ASN:HD22	1.67	0.57
1:A:162:ALA:HB2	1:A:345:ALA:HB3	1.87	0.56
1:A:86:SER:OG	1:A:87:ARG:N	2.38	0.56
1:A:287:HIS:C	3:A:415:HOH:O	2.37	0.56
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.71	0.56
2:P:363:LEU:N	3:P:403:HOH:O	2.06	0.56
1:A:116:ASP:OD2	1:A:329:ARG:HD3	2.06	0.55
1:A:264:SER:HA	1:A:347:GLN:NE2	2.22	0.55
2:P:358:GLU:CD	2:P:361:SER:HB3	2.31	0.55
2:P:360:VAL:HG21	2:P:363:LEU:HD12	1.88	0.55
2:P:358:GLU:CD	2:P:361:SER:CB	2.80	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:OE1	3:A:422:HOH:O	2.11	0.54
1:A:43:VAL:C	3:A:438:HOH:O	2.49	0.54
1:A:5:CYS:CB	3:A:496:HOH:O	2.44	0.54
1:A:129:SER:HB3	1:A:135:SER:O	2.09	0.53
1:A:72:ASN:CG	1:A:104:TRP:HB2	2.33	0.53
2:P:360:VAL:HG21	2:P:363:LEU:HD13	1.91	0.53
1:A:303:LYS:O	1:A:305:PHE:O	2.26	0.53
1:A:35:ASN:HD22	1:A:108:ARG:HG2	1.73	0.53
1:A:53:LEU:HD12	1:A:126:GLN:O	2.09	0.53
2:P:358:GLU:CD	3:P:402:HOH:O	2.44	0.53
1:A:28:LEU:HD12	1:A:28:LEU:H	1.74	0.53
1:A:308:ARG:HB3	1:A:311:GLN:OE1	2.09	0.52
1:A:31:LYS:HA	1:A:31:LYS:HE3	1.92	0.52
1:A:301:TRP:HD1	1:A:304:THR:OG1	1.93	0.52
1:A:198:SER:HB3	1:A:328:TYR:HE2	1.74	0.52
1:A:56:THR:HG21	2:P:361:SER:HA	1.92	0.52
2:P:358:GLU:OE2	2:P:361:SER:CB	2.56	0.51
1:A:198:SER:HB3	1:A:328:TYR:CE2	2.45	0.51
1:A:307:GLN:N	3:A:442:HOH:O	2.43	0.51
1:A:112:PRO:HG3	3:A:407:HOH:O	2.10	0.51
2:P:358:GLU:CA	2:P:360:VAL:N	2.74	0.50
1:A:213:LEU:O	1:A:216:GLN:HB2	2.12	0.50
1:A:22:GLU:HG2	3:A:497:HOH:O	2.11	0.50
1:A:88:LEU:HD22	2:P:363:LEU:C	2.36	0.50
1:A:138:ASP:CA	3:A:412:HOH:O	2.45	0.50
1:A:297:HIS:O	1:A:298:PHE:HB3	2.10	0.50
1:A:170:TRP:CH2	1:A:183:GLY:HA2	2.47	0.50
1:A:252:GLN:O	1:A:253:LYS:HD2	2.12	0.49
1:A:307:GLN:CG	3:A:442:HOH:O	2.55	0.49
2:P:360:VAL:CG2	2:P:363:LEU:HD12	2.42	0.49
2:P:361:SER:C	2:P:361:SER:N	2.63	0.49
1:A:264:SER:HA	1:A:347:GLN:HE21	1.76	0.49
1:A:205:LEU:HD11	1:A:319:ALA:HB1	1.94	0.49
1:A:308:ARG:HD3	3:A:447:HOH:O	2.12	0.49
1:A:98:LYS:HG3	3:A:501:HOH:O	2.13	0.48
1:A:120:THR:HG22	1:A:145:SER:HA	1.95	0.48
1:A:54:ARG:NE	2:P:365:ASN:CA	2.47	0.48
1:A:174:ASP:N	3:A:430:HOH:O	2.27	0.48
1:A:272:PRO:C	1:A:274:ALA:N	2.69	0.48
1:A:65:GLY:N	3:A:444:HOH:O	2.46	0.48
1:A:63:TYR:HB3	1:A:80:TYR:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:C	1:A:66:LEU:HG	2.38	0.47
1:A:301:TRP:CD1	1:A:304:THR:HG1	2.33	0.47
1:A:133:ASN:O	1:A:134:ASN:HB2	2.15	0.47
1:A:250:HIS:O	1:A:251:GLN:CB	2.63	0.47
1:A:94:GLY:CA	3:A:449:HOH:O	2.59	0.46
1:A:207:LEU:HB3	1:A:279:LEU:HB2	1.96	0.46
1:A:277:PHE:CE2	1:A:279:LEU:CD1	2.97	0.46
1:A:219:LEU:HD23	1:A:315:LEU:HD13	1.98	0.46
1:A:120:THR:HG21	1:A:143:ARG:HD3	1.97	0.46
1:A:308:ARG:CD	3:A:447:HOH:O	2.64	0.45
1:A:115:ARG:HB2	3:A:453:HOH:O	2.16	0.45
1:A:54:ARG:HD2	2:P:365:ASN:HA	1.98	0.45
1:A:90:VAL:HG11	2:P:367:GLN:HG2	1.75	0.45
1:A:81:PHE:CZ	2:P:365:ASN:HB2	2.50	0.45
1:A:88:LEU:CD2	2:P:364:THR:CA	2.95	0.45
1:A:131:ASN:HB3	1:A:132:LEU:H	1.58	0.45
1:A:349:THR:HA	3:A:441:HOH:O	2.17	0.44
1:A:54:ARG:NH1	3:P:403:HOH:O	2.50	0.44
1:A:306:LEU:N	3:A:432:HOH:O	2.48	0.44
1:A:136:GLN:NE2	3:A:422:HOH:O	2.38	0.44
1:A:308:ARG:N	3:A:432:HOH:O	2.33	0.44
1:A:19:VAL:HG11	1:A:125:PHE:CE2	2.52	0.44
1:A:238:LYS:O	1:A:239:GLY:C	2.60	0.44
1:A:338:LYS:NZ	3:A:429:HOH:O	2.50	0.44
1:A:88:LEU:HD23	2:P:364:THR:CA	2.48	0.44
1:A:182:LEU:CD2	1:A:301:TRP:CZ3	2.96	0.44
1:A:54:ARG:NE	2:P:365:ASN:C	2.75	0.44
1:A:212:ALA:CB	1:A:275:GLU:HB2	2.32	0.44
2:P:358:GLU:CD	2:P:361:SER:HB2	2.43	0.44
1:A:14:ASP:HB3	1:A:43:VAL:HG22	2.00	0.43
1:A:118:LYS:HA	3:A:495:HOH:O	2.18	0.43
1:A:174:ASP:C	1:A:176:PRO:HD3	2.43	0.43
1:A:280:ARG:HG2	1:A:280:ARG:HH11	1.81	0.43
1:A:165:PHE:HB3	1:A:348:TRP:CZ3	2.53	0.43
1:A:332:PRO:HG2	1:A:335:LEU:HD23	2.00	0.43
1:A:54:ARG:N	3:A:445:HOH:O	2.49	0.43
1:A:137:SER:C	3:A:412:HOH:O	2.45	0.43
1:A:115:ARG:CB	3:A:453:HOH:O	2.67	0.43
1:A:301:TRP:CD1	1:A:304:THR:OG1	2.72	0.43
1:A:52:GLU:HA	2:P:367:GLN:CD	2.40	0.42
1:A:301:TRP:CE2	3:A:468:HOH:O	2.69	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:C	2:P:365:ASN:ND2	2.77	0.42
1:A:39:HIS:ND1	1:A:104:TRP:NE1	2.67	0.42
1:A:55:VAL:O	1:A:88:LEU:HA	2.18	0.42
1:A:231:THR:HG21	1:A:277:PHE:CZ	2.55	0.42
1:A:23:GLN:CG	3:A:411:HOH:O	2.26	0.42
1:A:116:ASP:CG	1:A:329:ARG:HD3	2.44	0.42
1:A:153:THR:HG23	3:A:421:HOH:O	2.19	0.42
1:A:165:PHE:HA	1:A:166:PRO:C	2.43	0.42
1:A:210:PRO:HG3	1:A:269:LEU:O	2.20	0.42
1:A:277:PHE:CE2	1:A:279:LEU:HD12	2.55	0.42
1:A:28:LEU:HD12	1:A:147:GLU:O	2.19	0.41
1:A:221:VAL:HA	3:A:485:HOH:O	2.20	0.41
1:A:199:SER:O	1:A:327:PRO:HD2	2.20	0.41
1:A:237:PRO:HB3	3:A:406:HOH:O	2.20	0.41
1:A:88:LEU:HD23	2:P:364:THR:C	2.46	0.41
1:A:117:THR:C	1:A:118:LYS:HG3	2.45	0.41
1:A:49:TYR:O	1:A:50:GLU:HB2	2.19	0.41
1:A:39:HIS:ND1	1:A:104:TRP:CE2	2.88	0.41
1:A:54:ARG:NH2	2:P:367:GLN:N	2.69	0.41
1:A:194:ASN:OD1	1:A:194:ASN:C	2.62	0.41
1:A:52:GLU:OE1	1:A:54:ARG:NE	2.36	0.40
1:A:124:ASP:OD2	2:P:358:GLU:OE2	2.39	0.40
1:A:156:GLY:HA2	1:A:189:VAL:O	2.21	0.40
1:A:165:PHE:O	1:A:348:TRP:HA	2.20	0.40
1:A:302:ALA:O	1:A:305:PHE:O	2.39	0.40

All (745) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:CZ	1:A:273:GLU:OE2[3_444]	0.19	2.01
1:A:38:PHE:CA	1:A:214:GLU:N[3_444]	0.21	1.99
1:A:168:SER:OG	1:A:283:LEU:CG[3_554]	0.22	1.98
1:A:120:THR:CB	1:A:341:GLN:OE1[3_444]	0.28	1.92
1:A:37:THR:CG2	1:A:214:GLU:OE1[3_444]	0.31	1.89
1:A:170:TRP:CB	1:A:286:LEU:CA[3_554]	0.36	1.84
1:A:124:ASP:N	1:A:271:CYS:CB[3_444]	0.37	1.83
1:A:138:ASP:O	1:A:211:GLN:CD[3_444]	0.45	1.75
1:A:24:ASN:ND2	1:A:266:PRO:C[3_444]	0.51	1.69
1:A:56:THR:OG1	1:A:278:ARG:CZ[3_444]	0.51	1.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:CE	1:A:339:GLU:OE1[3_444]	0.55	1.65
1:A:126:GLN:OE1	1:A:232:ASN:CG[3_444]	0.55	1.65
1:A:39:HIS:CG	1:A:215:GLY:O[3_444]	0.62	1.58
1:A:206:GLU:CD	2:P:359:PHE:CA[3_454]	0.62	1.58
1:A:24:ASN:CG	1:A:267:GLN:N[3_444]	0.63	1.57
1:A:120:THR:OG1	1:A:341:GLN:CD[3_444]	0.63	1.57
1:A:124:ASP:CA	1:A:271:CYS:SG[3_444]	0.64	1.56
1:A:125:PHE:CG	1:A:274:ALA:C[3_444]	0.65	1.55
1:A:167:VAL:C	1:A:292:GLN:OE1[3_554]	0.65	1.55
1:A:22:GLU:C	1:A:267:GLN:NE2[3_444]	0.66	1.54
1:A:171:HIS:NE2	1:A:289:GLN:CB[3_554]	0.66	1.54
1:A:278:ARG:NE	2:P:361:SER:O[3_454]	0.66	1.54
1:A:37:THR:OG1	1:A:214:GLU:OE2[3_444]	0.69	1.51
1:A:280:ARG:NE	2:P:359:PHE:CE2[3_454]	0.71	1.49
1:A:39:HIS:CA	1:A:215:GLY:CA[3_444]	0.72	1.48
1:A:141:SER:N	1:A:210:PRO:N[3_444]	0.73	1.47
1:A:18:GLU:CA	1:A:216:GLN:O[3_444]	0.74	1.46
1:A:141:SER:C	1:A:210:PRO:CG[3_444]	0.75	1.45
1:A:166:PRO:O	1:A:292:GLN:NE2[3_554]	0.75	1.45
1:A:38:PHE:O	1:A:214:GLU:C[3_444]	0.76	1.44
1:A:125:PHE:C	1:A:276:CYS:N[3_444]	0.76	1.44
1:A:24:ASN:OD1	1:A:267:GLN:CA[3_444]	0.77	1.43
1:A:140:VAL:C	1:A:210:PRO:C[3_444]	0.77	1.43
1:A:140:VAL:C	1:A:210:PRO:CA[3_444]	0.79	1.41
1:A:140:VAL:CB	1:A:211:GLN:CA[3_444]	0.82	1.38
1:A:55:VAL:CG1	1:A:272:PRO:O[3_444]	0.84	1.36
1:A:123:PHE:C	1:A:271:CYS:CA[3_444]	0.84	1.36
1:A:169:ASP:C	1:A:286:LEU:CB[3_554]	0.84	1.36
1:A:18:GLU:OE1	1:A:304:THR:OG1[3_444]	0.85	1.35
1:A:141:SER:O	1:A:210:PRO:CG[3_444]	0.85	1.35
1:A:38:PHE:C	1:A:214:GLU:C[3_444]	0.86	1.34
1:A:124:ASP:CB	1:A:276:CYS:SG[3_444]	0.86	1.34
1:A:139:VAL:CB	1:A:277:PHE:CB[3_444]	0.86	1.34
1:A:126:GLN:OE1	1:A:232:ASN:OD1[3_444]	0.87	1.33
1:A:206:GLU:CB	2:P:358:GLU:O[3_454]	0.87	1.33
1:A:125:PHE:CG	1:A:275:GLU:N[3_444]	0.89	1.31
1:A:24:ASN:O	1:A:268:ILE:CG1[3_444]	0.90	1.30
1:A:39:HIS:CB	1:A:215:GLY:C[3_444]	0.90	1.30
1:A:206:GLU:OE1	2:P:359:PHE:N[3_454]	0.90	1.30
1:A:123:PHE:C	1:A:271:CYS:N[3_444]	0.91	1.29
1:A:17:LEU:CG	1:A:212:ALA:CB[3_444]	0.92	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:CE2	1:A:268:ILE:O[3_444]	0.92	1.28
1:A:143:ARG:CB	1:A:316:GLN:CB[3_444]	0.92	1.28
1:A:140:VAL:CG2	1:A:211:GLN:CA[3_444]	0.93	1.27
1:A:142:PHE:CA	1:A:269:LEU:C[3_444]	0.93	1.27
1:A:120:THR:CB	1:A:341:GLN:CD[3_444]	0.95	1.25
1:A:142:PHE:CA	1:A:269:LEU:O[3_444]	0.95	1.25
1:A:125:PHE:CE1	1:A:274:ALA:CA[3_444]	0.96	1.24
1:A:168:SER:N	1:A:292:GLN:OE1[3_554]	0.96	1.24
1:A:171:HIS:CG	1:A:288:GLN:C[3_554]	0.96	1.24
1:A:39:HIS:C	1:A:215:GLY:CA[3_444]	0.97	1.23
1:A:24:ASN:O	1:A:268:ILE:CD1[3_444]	0.98	1.22
1:A:280:ARG:NE	2:P:359:PHE:CD2[3_454]	0.98	1.22
1:A:125:PHE:CA	1:A:275:GLU:C[3_444]	0.99	1.21
1:A:140:VAL:CB	1:A:211:GLN:N[3_444]	0.99	1.21
1:A:125:PHE:CB	1:A:275:GLU:N[3_444]	1.00	1.20
1:A:140:VAL:CA	1:A:211:GLN:N[3_444]	1.00	1.20
1:A:278:ARG:CZ	2:P:361:SER:O[3_454]	1.00	1.20
1:A:123:PHE:O	1:A:271:CYS:N[3_444]	1.01	1.19
1:A:206:GLU:CD	2:P:359:PHE:C[3_454]	1.01	1.19
1:A:123:PHE:CD1	1:A:273:GLU:OE1[3_444]	1.02	1.18
1:A:138:ASP:O	1:A:211:GLN:OE1[3_444]	1.02	1.18
1:A:139:VAL:CG2	1:A:277:PHE:C[3_444]	1.02	1.18
1:A:139:VAL:CB	1:A:277:PHE:CA[3_444]	1.03	1.17
1:A:170:TRP:CA	1:A:286:LEU:C[3_554]	1.03	1.17
1:A:39:HIS:N	1:A:215:GLY:N[3_444]	1.04	1.16
1:A:171:HIS:N	1:A:287:HIS:O[3_554]	1.05	1.15
1:A:39:HIS:CB	1:A:215:GLY:O[3_444]	1.06	1.14
1:A:39:HIS:CA	1:A:215:GLY:C[3_444]	1.06	1.14
1:A:123:PHE:CA	1:A:271:CYS:C[3_444]	1.06	1.14
1:A:171:HIS:CG	1:A:289:GLN:N[3_554]	1.06	1.14
1:A:125:PHE:CA	1:A:276:CYS:N[3_444]	1.07	1.13
1:A:136:GLN:CG	1:A:233:HIS:CA[3_444]	1.07	1.13
1:A:139:VAL:CG2	1:A:277:PHE:CA[3_444]	1.07	1.13
1:A:125:PHE:C	1:A:275:GLU:C[3_444]	1.08	1.12
1:A:56:THR:OG1	1:A:278:ARG:NH1[3_444]	1.09	1.11
1:A:125:PHE:CD1	1:A:274:ALA:CA[3_444]	1.09	1.11
1:A:125:PHE:CB	1:A:275:GLU:CA[3_444]	1.09	1.11
1:A:142:PHE:O	1:A:270:LYS:CB[3_444]	1.09	1.11
1:A:24:ASN:C	1:A:268:ILE:CG1[3_444]	1.11	1.09
1:A:121:ILE:O	1:A:316:GLN:NE2[3_444]	1.11	1.09
1:A:140:VAL:O	1:A:210:PRO:CA[3_444]	1.11	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CA	1:A:210:PRO:C[3_444]	1.11	1.09
1:A:141:SER:CA	1:A:210:PRO:CD[3_444]	1.11	1.09
1:A:142:PHE:CG	1:A:269:LEU:CA[3_444]	1.11	1.09
1:A:38:PHE:O	1:A:214:GLU:CA[3_444]	1.12	1.08
1:A:38:PHE:CA	1:A:213:LEU:C[3_444]	1.12	1.08
1:A:278:ARG:CD	2:P:361:SER:C[3_454]	1.12	1.08
1:A:140:VAL:CG2	1:A:211:GLN:C[3_444]	1.14	1.06
1:A:170:TRP:N	1:A:286:LEU:CB[3_554]	1.14	1.06
1:A:38:PHE:C	1:A:214:GLU:CA[3_444]	1.15	1.05
1:A:170:TRP:CZ2	1:A:287:HIS:CD2[3_554]	1.15	1.05
1:A:206:GLU:OE2	2:P:359:PHE:C[3_454]	1.15	1.05
1:A:24:ASN:CG	1:A:266:PRO:C[3_444]	1.16	1.04
1:A:125:PHE:CE1	1:A:274:ALA:N[3_444]	1.16	1.04
1:A:139:VAL:CA	1:A:277:PHE:CB[3_444]	1.16	1.04
1:A:141:SER:N	1:A:210:PRO:CA[3_444]	1.16	1.04
1:A:206:GLU:CG	2:P:359:PHE:CA[3_454]	1.16	1.04
1:A:123:PHE:CG	1:A:273:GLU:OE1[3_444]	1.17	1.03
1:A:169:ASP:OD1	1:A:192:LEU:CD1[3_554]	1.17	1.03
1:A:142:PHE:CB	1:A:270:LYS:N[3_444]	1.18	1.02
1:A:123:PHE:CA	1:A:271:CYS:CA[3_444]	1.19	1.01
1:A:125:PHE:CD1	1:A:274:ALA:CB[3_444]	1.19	1.01
1:A:142:PHE:CE1	1:A:269:LEU:CD2[3_444]	1.19	1.01
1:A:280:ARG:CD	2:P:359:PHE:CZ[3_454]	1.19	1.01
1:A:18:GLU:O	1:A:213:LEU:N[3_444]	1.20	1.00
1:A:168:SER:CB	1:A:283:LEU:CB[3_554]	1.21	0.99
1:A:169:ASP:O	1:A:286:LEU:CB[3_554]	1.21	0.99
1:A:171:HIS:CG	1:A:288:GLN:O[3_554]	1.21	0.99
1:A:280:ARG:CD	2:P:359:PHE:CE2[3_454]	1.21	0.99
1:A:18:GLU:C	1:A:216:GLN:O[3_444]	1.22	0.98
1:A:37:THR:CB	1:A:214:GLU:OE1[3_444]	1.22	0.98
1:A:138:ASP:CA	1:A:211:GLN:NE2[3_444]	1.22	0.98
1:A:169:ASP:OD2	1:A:321:TYR:CZ[3_554]	1.22	0.98
1:A:171:HIS:CE1	1:A:289:GLN:CB[3_554]	1.22	0.98
1:A:226:GLY:O	1:A:349:THR:CG2[3_544]	1.22	0.98
1:A:24:ASN:ND2	1:A:266:PRO:CA[3_444]	1.23	0.97
1:A:141:SER:CA	1:A:210:PRO:N[3_444]	1.23	0.97
1:A:227:LEU:N	1:A:349:THR:OG1[3_544]	1.23	0.97
1:A:120:THR:CG2	1:A:341:GLN:OE1[3_444]	1.24	0.96
1:A:18:GLU:CG	1:A:216:GLN:C[3_444]	1.25	0.95
1:A:24:ASN:OD1	1:A:267:GLN:N[3_444]	1.25	0.95
1:A:24:ASN:C	1:A:268:ILE:CD1[3_444]	1.25	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TRP:CB	1:A:286:LEU:N[3_554]	1.25	0.95
1:A:171:HIS:CB	1:A:288:GLN:C[3_554]	1.25	0.95
1:A:172:PRO:CD	1:A:290:GLU:CG[3_554]	1.25	0.95
1:A:24:ASN:OD1	1:A:267:GLN:CB[3_444]	1.26	0.94
1:A:143:ARG:CG	1:A:316:GLN:CG[3_444]	1.26	0.94
1:A:171:HIS:CD2	1:A:289:GLN:CA[3_554]	1.26	0.94
1:A:38:PHE:O	1:A:214:GLU:O[3_444]	1.27	0.93
1:A:125:PHE:CE1	1:A:274:ALA:CB[3_444]	1.27	0.93
1:A:126:GLN:CG	1:A:233:HIS:ND1[3_444]	1.27	0.93
1:A:168:SER:OG	1:A:283:LEU:CB[3_554]	1.27	0.93
1:A:37:THR:CB	1:A:214:GLU:CD[3_444]	1.28	0.92
1:A:105:GLY:O	1:A:214:GLU:CG[3_444]	1.28	0.92
1:A:142:PHE:O	1:A:270:LYS:CA[3_444]	1.28	0.92
1:A:123:PHE:CZ	1:A:273:GLU:CD[3_444]	1.29	0.91
1:A:141:SER:CB	1:A:210:PRO:CD[3_444]	1.29	0.91
1:A:170:TRP:CA	1:A:286:LEU:CA[3_554]	1.29	0.91
1:A:170:TRP:N	1:A:286:LEU:CG[3_554]	1.29	0.91
1:A:170:TRP:CE2	1:A:287:HIS:CD2[3_554]	1.29	0.91
1:A:120:THR:OG1	1:A:341:GLN:NE2[3_444]	1.30	0.90
1:A:126:GLN:CB	1:A:276:CYS:O[3_444]	1.30	0.90
1:A:171:HIS:ND1	1:A:288:GLN:C[3_554]	1.30	0.90
1:A:56:THR:CB	1:A:278:ARG:NH1[3_444]	1.31	0.89
1:A:123:PHE:CE2	1:A:273:GLU:OE2[3_444]	1.31	0.89
1:A:125:PHE:CZ	1:A:274:ALA:N[3_444]	1.31	0.89
1:A:143:ARG:CA	1:A:316:GLN:CB[3_444]	1.31	0.89
1:A:170:TRP:CZ2	1:A:287:HIS:NE2[3_554]	1.31	0.89
1:A:19:VAL:CA	1:A:213:LEU:CB[3_444]	1.32	0.88
1:A:38:PHE:N	1:A:214:GLU:N[3_444]	1.32	0.88
1:A:123:PHE:CA	1:A:271:CYS:O[3_444]	1.32	0.88
1:A:125:PHE:CZ	1:A:274:ALA:CA[3_444]	1.32	0.88
1:A:126:GLN:CD	1:A:232:ASN:OD1[3_444]	1.32	0.88
1:A:126:GLN:O	1:A:275:GLU:OE2[3_444]	1.32	0.88
1:A:138:ASP:C	1:A:211:GLN:NE2[3_444]	1.32	0.88
1:A:208:SER:OG	2:P:358:GLU:OE2[3_454]	1.32	0.88
1:A:23:GLN:N	1:A:267:GLN:NE2[3_444]	1.33	0.87
1:A:142:PHE:CD2	1:A:268:ILE:O[3_444]	1.33	0.87
1:A:141:SER:OG	1:A:209:CYS:CA[3_444]	1.34	0.86
1:A:7:GLU:O	1:A:74:SER:CB[4_435]	1.35	0.85
1:A:38:PHE:CB	1:A:214:GLU:N[3_444]	1.35	0.85
1:A:126:GLN:OE1	1:A:232:ASN:ND2[3_444]	1.36	0.84
1:A:136:GLN:NE2	1:A:233:HIS:N[3_444]	1.36	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TRP:CE3	1:A:290:GLU:OE1[3_554]	1.36	0.84
1:A:120:THR:OG1	1:A:341:GLN:CG[3_444]	1.37	0.83
1:A:123:PHE:CE2	1:A:273:GLU:CD[3_444]	1.37	0.83
1:A:124:ASP:N	1:A:271:CYS:CA[3_444]	1.37	0.83
1:A:125:PHE:CB	1:A:275:GLU:C[3_444]	1.37	0.83
1:A:136:GLN:CD	1:A:233:HIS:N[3_444]	1.37	0.83
1:A:56:THR:OG1	1:A:278:ARG:NH2[3_444]	1.38	0.82
1:A:123:PHE:CA	1:A:271:CYS:N[3_444]	1.38	0.82
1:A:125:PHE:CD1	1:A:274:ALA:C[3_444]	1.38	0.82
1:A:141:SER:C	1:A:210:PRO:CB[3_444]	1.38	0.82
1:A:142:PHE:CB	1:A:269:LEU:C[3_444]	1.38	0.82
1:A:55:VAL:CG1	1:A:272:PRO:C[3_444]	1.39	0.81
1:A:127:ILE:O	1:A:233:HIS:NE2[3_444]	1.39	0.81
1:A:142:PHE:CE2	1:A:268:ILE:C[3_444]	1.39	0.81
1:A:278:ARG:NE	2:P:361:SER:C[3_454]	1.39	0.81
1:A:22:GLU:O	1:A:267:GLN:NE2[3_444]	1.41	0.79
1:A:24:ASN:ND2	1:A:267:GLN:N[3_444]	1.41	0.79
1:A:37:THR:CG2	1:A:214:GLU:CD[3_444]	1.41	0.79
1:A:138:ASP:C	1:A:211:GLN:CD[3_444]	1.41	0.79
1:A:206:GLU:CD	2:P:359:PHE:N[3_454]	1.41	0.79
1:A:39:HIS:CA	1:A:215:GLY:N[3_444]	1.42	0.78
1:A:126:GLN:CG	1:A:233:HIS:CE1[3_444]	1.42	0.78
1:A:143:ARG:O	1:A:268:ILE:CG2[3_444]	1.42	0.78
1:A:144:LEU:CA	1:A:268:ILE:CG2[3_444]	1.42	0.78
1:A:169:ASP:C	1:A:286:LEU:CG[3_554]	1.42	0.78
1:A:169:ASP:CA	1:A:286:LEU:CD1[3_554]	1.42	0.78
1:A:171:HIS:N	1:A:287:HIS:C[3_554]	1.42	0.78
1:A:37:THR:OG1	1:A:214:GLU:CD[3_444]	1.43	0.77
1:A:123:PHE:CE1	1:A:273:GLU:OE2[3_444]	1.43	0.77
1:A:125:PHE:CZ	1:A:273:GLU:C[3_444]	1.43	0.77
1:A:140:VAL:CB	1:A:211:GLN:C[3_444]	1.43	0.77
1:A:56:THR:N	1:A:278:ARG:NH2[3_444]	1.44	0.76
1:A:144:LEU:N	1:A:268:ILE:CG2[3_444]	1.44	0.76
1:A:168:SER:CB	1:A:283:LEU:CG[3_554]	1.44	0.76
1:A:7:GLU:O	1:A:74:SER:OG[4_435]	1.45	0.75
1:A:18:GLU:CG	1:A:217:GLN:N[3_444]	1.45	0.75
1:A:38:PHE:C	1:A:215:GLY:N[3_444]	1.45	0.75
1:A:118:LYS:CE	1:A:339:GLU:CD[3_444]	1.45	0.75
1:A:127:ILE:O	1:A:233:HIS:CD2[3_444]	1.45	0.75
1:A:141:SER:CA	1:A:210:PRO:CG[3_444]	1.45	0.75
1:A:169:ASP:OD2	1:A:321:TYR:CE2[3_554]	1.45	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:HIS:CA	1:A:287:HIS:O[3_554]	1.45	0.75
1:A:226:GLY:CA	1:A:349:THR:C[3_544]	1.45	0.75
1:A:14:ASP:OD2	1:A:238:LYS:CD[3_444]	1.46	0.74
1:A:124:ASP:O	1:A:276:CYS:CB[3_444]	1.46	0.74
1:A:125:PHE:CZ	1:A:273:GLU:O[3_444]	1.46	0.74
1:A:167:VAL:C	1:A:292:GLN:CD[3_554]	1.46	0.74
1:A:170:TRP:CB	1:A:286:LEU:C[3_554]	1.46	0.74
1:A:171:HIS:O	1:A:287:HIS:CB[3_554]	1.46	0.74
1:A:171:HIS:CD2	1:A:289:GLN:C[3_554]	1.46	0.74
1:A:19:VAL:CB	1:A:213:LEU:CB[3_444]	1.47	0.73
1:A:19:VAL:CG1	1:A:213:LEU:CB[3_444]	1.47	0.73
1:A:141:SER:N	1:A:210:PRO:CD[3_444]	1.47	0.73
1:A:206:GLU:OE2	2:P:359:PHE:CA[3_454]	1.47	0.73
1:A:37:THR:O	1:A:213:LEU:CG[3_444]	1.48	0.72
1:A:38:PHE:CA	1:A:214:GLU:CA[3_444]	1.48	0.72
1:A:123:PHE:C	1:A:271:CYS:CB[3_444]	1.48	0.72
1:A:125:PHE:O	1:A:276:CYS:C[3_444]	1.48	0.72
1:A:143:ARG:NH2	1:A:342:VAL:O[3_444]	1.48	0.72
1:A:167:VAL:CG2	1:A:285:PRO:O[3_554]	1.48	0.72
1:A:226:GLY:C	1:A:349:THR:OG1[3_544]	1.48	0.72
1:A:280:ARG:CD	2:P:359:PHE:CE1[3_454]	1.48	0.72
1:A:125:PHE:CD2	1:A:275:GLU:N[3_444]	1.49	0.71
1:A:142:PHE:CA	1:A:270:LYS:N[3_444]	1.49	0.71
1:A:125:PHE:CD2	1:A:274:ALA:C[3_444]	1.50	0.70
1:A:139:VAL:CG1	1:A:277:PHE:N[3_444]	1.50	0.70
1:A:18:GLU:CB	1:A:216:GLN:O[3_444]	1.51	0.69
1:A:21:GLY:C	1:A:267:GLN:OE1[3_444]	1.51	0.69
1:A:125:PHE:CG	1:A:274:ALA:CA[3_444]	1.51	0.69
1:A:142:PHE:C	1:A:269:LEU:O[3_444]	1.51	0.69
1:A:143:ARG:C	1:A:268:ILE:CG2[3_444]	1.51	0.69
1:A:166:PRO:C	1:A:292:GLN:NE2[3_554]	1.51	0.69
1:A:168:SER:OG	1:A:283:LEU:CD2[3_554]	1.51	0.69
1:A:18:GLU:CB	1:A:216:GLN:C[3_444]	1.52	0.68
1:A:20:PHE:CD2	1:A:308:ARG:NH2[3_444]	1.52	0.68
1:A:39:HIS:N	1:A:214:GLU:C[3_444]	1.52	0.68
1:A:137:SER:O	1:A:233:HIS:CB[3_444]	1.52	0.68
1:A:138:ASP:O	1:A:211:GLN:NE2[3_444]	1.52	0.68
1:A:24:ASN:ND2	1:A:266:PRO:O[3_444]	1.53	0.67
1:A:136:GLN:CD	1:A:233:HIS:CA[3_444]	1.53	0.67
1:A:120:THR:CA	1:A:341:GLN:OE1[3_444]	1.54	0.66
1:A:123:PHE:N	1:A:271:CYS:O[3_444]	1.54	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:CD2	1:A:232:ASN:O[3_444]	1.54	0.66
1:A:140:VAL:CG2	1:A:211:GLN:O[3_444]	1.54	0.66
1:A:142:PHE:CD1	1:A:269:LEU:CA[3_444]	1.54	0.66
1:A:171:HIS:ND1	1:A:289:GLN:N[3_554]	1.54	0.66
1:A:138:ASP:N	1:A:211:GLN:NE2[3_444]	1.55	0.65
1:A:139:VAL:CG2	1:A:278:ARG:N[3_444]	1.55	0.65
1:A:170:TRP:CE2	1:A:287:HIS:NE2[3_554]	1.55	0.65
1:A:18:GLU:C	1:A:213:LEU:N[3_444]	1.56	0.64
1:A:39:HIS:CD2	1:A:215:GLY:O[3_444]	1.56	0.64
1:A:124:ASP:N	1:A:271:CYS:SG[3_444]	1.56	0.64
1:A:126:GLN:C	1:A:275:GLU:OE2[3_444]	1.56	0.64
1:A:127:ILE:C	1:A:233:HIS:NE2[3_444]	1.56	0.64
1:A:140:VAL:O	1:A:210:PRO:C[3_444]	1.56	0.64
1:A:141:SER:CA	1:A:210:PRO:CB[3_444]	1.56	0.64
1:A:142:PHE:C	1:A:269:LEU:C[3_444]	1.56	0.64
1:A:168:SER:OG	1:A:283:LEU:CD1[3_554]	1.56	0.64
1:A:280:ARG:CD	2:P:359:PHE:CD2[3_454]	1.56	0.64
1:A:24:ASN:CG	1:A:267:GLN:CA[3_444]	1.57	0.63
1:A:38:PHE:C	1:A:214:GLU:N[3_444]	1.57	0.63
1:A:171:HIS:CG	1:A:289:GLN:CA[3_554]	1.57	0.63
1:A:57:ALA:CB	1:A:272:PRO:CG[3_444]	1.58	0.62
1:A:206:GLU:OE1	2:P:359:PHE:CA[3_454]	1.58	0.62
1:A:228:ASN:ND2	1:A:253:LYS:CE[3_544]	1.58	0.62
1:A:17:LEU:O	1:A:211:GLN:O[3_444]	1.59	0.61
1:A:18:GLU:CA	1:A:216:GLN:C[3_444]	1.59	0.61
1:A:208:SER:OG	2:P:358:GLU:CD[3_454]	1.59	0.61
1:A:118:LYS:NZ	1:A:339:GLU:OE1[3_444]	1.60	0.60
1:A:122:GLN:NE2	1:A:208:SER:O[3_444]	1.60	0.60
1:A:124:ASP:CA	1:A:271:CYS:CB[3_444]	1.60	0.60
1:A:142:PHE:CD1	1:A:269:LEU:CB[3_444]	1.60	0.60
1:A:143:ARG:NH2	1:A:317:CYS:N[3_444]	1.60	0.60
1:A:170:TRP:CZ3	1:A:290:GLU:OE1[3_554]	1.60	0.60
1:A:208:SER:N	2:P:358:GLU:OE1[3_454]	1.60	0.60
1:A:39:HIS:CB	1:A:216:GLN:N[3_444]	1.61	0.59
1:A:120:THR:OG1	1:A:341:GLN:OE1[3_444]	1.61	0.59
1:A:123:PHE:CE1	1:A:273:GLU:CD[3_444]	1.61	0.59
1:A:123:PHE:CE1	1:A:273:GLU:OE1[3_444]	1.61	0.59
1:A:124:ASP:CB	1:A:271:CYS:SG[3_444]	1.61	0.59
1:A:125:PHE:O	1:A:276:CYS:CA[3_444]	1.61	0.59
1:A:138:ASP:O	1:A:211:GLN:CG[3_444]	1.61	0.59
1:A:139:VAL:CA	1:A:277:PHE:CA[3_444]	1.61	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:O	1:A:292:GLN:OE1[3_554]	1.61	0.59
1:A:40:ALA:N	1:A:215:GLY:CA[3_444]	1.62	0.58
1:A:124:ASP:C	1:A:276:CYS:CB[3_444]	1.62	0.58
1:A:138:ASP:CB	1:A:211:GLN:NE2[3_444]	1.63	0.57
1:A:171:HIS:CD2	1:A:289:GLN:CB[3_554]	1.63	0.57
1:A:206:GLU:CG	2:P:359:PHE:CB[3_454]	1.63	0.57
1:A:17:LEU:CD1	1:A:212:ALA:CB[3_444]	1.64	0.56
1:A:171:HIS:N	1:A:287:HIS:N[3_554]	1.64	0.56
1:A:206:GLU:CB	2:P:358:GLU:C[3_454]	1.64	0.56
1:A:126:GLN:N	1:A:276:CYS:N[3_444]	1.65	0.55
1:A:140:VAL:CA	1:A:211:GLN:CA[3_444]	1.65	0.55
1:A:171:HIS:CB	1:A:289:GLN:N[3_554]	1.65	0.55
1:A:37:THR:CA	1:A:214:GLU:CD[3_444]	1.66	0.54
1:A:56:THR:OG1	1:A:278:ARG:NE[3_444]	1.66	0.54
1:A:126:GLN:CD	1:A:232:ASN:CG[3_444]	1.66	0.54
1:A:139:VAL:CB	1:A:277:PHE:C[3_444]	1.66	0.54
1:A:139:VAL:N	1:A:277:PHE:CB[3_444]	1.66	0.54
1:A:171:HIS:ND1	1:A:288:GLN:O[3_554]	1.66	0.54
1:A:171:HIS:CB	1:A:287:HIS:O[3_554]	1.66	0.54
1:A:24:ASN:CA	1:A:268:ILE:CG1[3_444]	1.67	0.53
1:A:37:THR:CB	1:A:214:GLU:OE2[3_444]	1.67	0.53
1:A:123:PHE:CB	1:A:271:CYS:C[3_444]	1.67	0.53
1:A:140:VAL:CG2	1:A:211:GLN:CB[3_444]	1.67	0.53
1:A:206:GLU:OE2	2:P:359:PHE:O[3_454]	1.67	0.53
1:A:22:GLU:CA	1:A:267:GLN:NE2[3_444]	1.68	0.52
1:A:39:HIS:C	1:A:215:GLY:C[3_444]	1.68	0.52
1:A:125:PHE:O	1:A:276:CYS:N[3_444]	1.68	0.52
1:A:140:VAL:C	1:A:211:GLN:N[3_444]	1.68	0.52
1:A:170:TRP:C	1:A:287:HIS:N[3_554]	1.68	0.52
1:A:180:GLU:O	1:A:287:HIS:CE1[3_554]	1.68	0.52
1:A:38:PHE:N	1:A:214:GLU:CA[3_444]	1.69	0.51
1:A:56:THR:CB	1:A:278:ARG:CZ[3_444]	1.69	0.51
1:A:125:PHE:CE2	1:A:274:ALA:CA[3_444]	1.69	0.51
1:A:206:GLU:OE1	2:P:360:VAL:N[3_454]	1.69	0.51
1:A:226:GLY:C	1:A:349:THR:CG2[3_544]	1.69	0.51
1:A:278:ARG:CD	2:P:361:SER:O[3_454]	1.69	0.51
1:A:18:GLU:CB	1:A:217:GLN:N[3_444]	1.70	0.50
1:A:25:HIS:N	1:A:268:ILE:CD1[3_444]	1.70	0.50
1:A:139:VAL:CG1	1:A:277:PHE:O[3_444]	1.70	0.50
1:A:24:ASN:CB	1:A:267:GLN:N[3_444]	1.71	0.49
1:A:57:ALA:CA	1:A:272:PRO:CG[3_444]	1.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:C	1:A:270:LYS:N[3_444]	1.71	0.49
1:A:143:ARG:CB	1:A:316:GLN:CA[3_444]	1.71	0.49
1:A:143:ARG:CG	1:A:316:GLN:CB[3_444]	1.71	0.49
1:A:17:LEU:CD2	1:A:275:GLU:CB[3_444]	1.72	0.48
1:A:21:GLY:O	1:A:267:GLN:OE1[3_444]	1.72	0.48
1:A:142:PHE:CG	1:A:269:LEU:C[3_444]	1.72	0.48
1:A:180:GLU:O	1:A:287:HIS:NE2[3_554]	1.72	0.48
1:A:18:GLU:N	1:A:216:GLN:O[3_444]	1.73	0.47
1:A:104:TRP:CH2	1:A:216:GLN:CD[3_444]	1.73	0.47
1:A:118:LYS:CD	1:A:339:GLU:OE1[3_444]	1.73	0.47
1:A:125:PHE:C	1:A:276:CYS:CA[3_444]	1.73	0.47
1:A:136:GLN:CG	1:A:233:HIS:C[3_444]	1.73	0.47
1:A:167:VAL:CA	1:A:292:GLN:OE1[3_554]	1.73	0.47
1:A:170:TRP:CA	1:A:286:LEU:O[3_554]	1.73	0.47
1:A:18:GLU:CB	1:A:217:GLN:C[3_444]	1.74	0.46
1:A:56:THR:CA	1:A:278:ARG:NH2[3_444]	1.74	0.46
1:A:57:ALA:CA	1:A:272:PRO:CD[3_444]	1.74	0.46
1:A:123:PHE:O	1:A:270:LYS:C[3_444]	1.74	0.46
1:A:124:ASP:CA	1:A:276:CYS:SG[3_444]	1.74	0.46
1:A:140:VAL:CA	1:A:210:PRO:O[3_444]	1.74	0.46
1:A:141:SER:CA	1:A:210:PRO:CA[3_444]	1.74	0.46
1:A:38:PHE:N	1:A:214:GLU:CB[3_444]	1.75	0.45
1:A:56:THR:CB	1:A:278:ARG:NH2[3_444]	1.75	0.45
1:A:57:ALA:N	1:A:272:PRO:CG[3_444]	1.75	0.45
1:A:122:GLN:OE1	1:A:318:GLU:CB[3_444]	1.75	0.45
1:A:125:PHE:CB	1:A:274:ALA:C[3_444]	1.75	0.45
1:A:125:PHE:CD2	1:A:274:ALA:CA[3_444]	1.75	0.45
1:A:127:ILE:CG1	1:A:275:GLU:OE1[3_444]	1.75	0.45
1:A:142:PHE:CD2	1:A:269:LEU:CA[3_444]	1.75	0.45
1:A:143:ARG:NH1	1:A:317:CYS:O[3_444]	1.75	0.45
1:A:170:TRP:CA	1:A:286:LEU:CB[3_554]	1.75	0.45
1:A:171:HIS:NE2	1:A:289:GLN:CA[3_554]	1.75	0.45
1:A:171:HIS:CE1	1:A:289:GLN:CG[3_554]	1.75	0.45
1:A:20:PHE:N	1:A:213:LEU:CD2[3_444]	1.76	0.44
1:A:38:PHE:O	1:A:214:GLU:CB[3_444]	1.76	0.44
1:A:39:HIS:N	1:A:215:GLY:CA[3_444]	1.76	0.44
1:A:122:GLN:N	1:A:270:LYS:CE[3_444]	1.76	0.44
1:A:123:PHE:CD2	1:A:273:GLU:CD[3_444]	1.76	0.44
1:A:126:GLN:N	1:A:275:GLU:OE2[3_444]	1.76	0.44
1:A:140:VAL:C	1:A:210:PRO:N[3_444]	1.76	0.44
1:A:170:TRP:O	1:A:290:GLU:CB[3_554]	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:OE1	3:A:402:HOH:O[3_454]	1.76	0.44
1:A:280:ARG:CD	2:P:359:PHE:CD1[3_454]	1.76	0.44
1:A:122:GLN:NE2	1:A:318:GLU:N[3_444]	1.77	0.43
1:A:124:ASP:OD2	1:A:208:SER:CB[3_444]	1.77	0.43
1:A:140:VAL:N	1:A:211:GLN:N[3_444]	1.77	0.43
1:A:171:HIS:N	1:A:287:HIS:CA[3_554]	1.77	0.43
1:A:206:GLU:OE2	2:P:359:PHE:CB[3_454]	1.77	0.43
1:A:18:GLU:CG	1:A:216:GLN:CA[3_444]	1.78	0.42
1:A:18:GLU:N	1:A:216:GLN:C[3_444]	1.78	0.42
1:A:36:LEU:CD1	1:A:273:GLU:CB[3_444]	1.78	0.42
1:A:39:HIS:CG	1:A:215:GLY:C[3_444]	1.78	0.42
1:A:123:PHE:CD2	1:A:273:GLU:OE1[3_444]	1.78	0.42
1:A:123:PHE:CB	1:A:270:LYS:O[3_444]	1.78	0.42
1:A:125:PHE:CG	1:A:274:ALA:O[3_444]	1.78	0.42
1:A:126:GLN:NE2	1:A:232:ASN:OD1[3_444]	1.78	0.42
1:A:126:GLN:CD	1:A:233:HIS:ND1[3_444]	1.78	0.42
1:A:140:VAL:C	1:A:210:PRO:O[3_444]	1.78	0.42
1:A:170:TRP:CG	1:A:286:LEU:N[3_554]	1.78	0.42
1:A:171:HIS:CA	1:A:287:HIS:C[3_554]	1.78	0.42
1:A:208:SER:CB	2:P:358:GLU:OE1[3_454]	1.78	0.42
1:A:278:ARG:CD	2:P:362:GLN:N[3_454]	1.78	0.42
1:A:280:ARG:CZ	2:P:359:PHE:CE2[3_454]	1.78	0.42
1:A:125:PHE:CA	1:A:275:GLU:CA[3_444]	1.79	0.41
1:A:125:PHE:O	1:A:275:GLU:O[3_444]	1.79	0.41
1:A:139:VAL:N	1:A:277:PHE:CD1[3_444]	1.79	0.41
1:A:141:SER:N	1:A:210:PRO:C[3_444]	1.79	0.41
1:A:142:PHE:CE1	1:A:269:LEU:CG[3_444]	1.79	0.41
1:A:206:GLU:OE1	2:P:358:GLU:C[3_454]	1.79	0.41
1:A:226:GLY:C	1:A:349:THR:CB[3_544]	1.79	0.41
1:A:21:GLY:O	1:A:267:GLN:CD[3_444]	1.80	0.40
1:A:122:GLN:CG	1:A:316:GLN:O[3_444]	1.80	0.40
1:A:139:VAL:CG2	1:A:277:PHE:CB[3_444]	1.80	0.40
1:A:141:SER:OG	1:A:209:CYS:C[3_444]	1.80	0.40
1:A:142:PHE:C	1:A:270:LYS:CA[3_444]	1.80	0.40
1:A:142:PHE:CD2	1:A:268:ILE:C[3_444]	1.80	0.40
1:A:143:ARG:N	1:A:269:LEU:O[3_444]	1.80	0.40
1:A:169:ASP:OD2	1:A:321:TYR:OH[3_554]	1.80	0.40
1:A:170:TRP:O	1:A:286:LEU:CD2[3_554]	1.80	0.40
1:A:170:TRP:CG	1:A:286:LEU:CA[3_554]	1.80	0.40
1:A:17:LEU:CB	1:A:212:ALA:CB[3_444]	1.81	0.39
1:A:24:ASN:CG	1:A:266:PRO:O[3_444]	1.81	0.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:CB	1:A:272:PRO:O[3_444]	1.81	0.39
1:A:122:GLN:O	1:A:271:CYS:O[3_444]	1.81	0.39
1:A:123:PHE:N	1:A:271:CYS:N[3_444]	1.81	0.39
1:A:139:VAL:CB	1:A:277:PHE:N[3_444]	1.81	0.39
1:A:142:PHE:CD1	1:A:269:LEU:CD2[3_444]	1.81	0.39
1:A:167:VAL:CA	1:A:292:GLN:CD[3_554]	1.81	0.39
1:A:170:TRP:CB	1:A:286:LEU:CB[3_554]	1.81	0.39
1:A:206:GLU:OE1	2:P:359:PHE:C[3_454]	1.81	0.39
1:A:206:GLU:CD	2:P:360:VAL:N[3_454]	1.81	0.39
1:A:125:PHE:O	1:A:275:GLU:C[3_444]	1.82	0.38
1:A:169:ASP:C	1:A:286:LEU:CD1[3_554]	1.82	0.38
1:A:170:TRP:N	1:A:286:LEU:CD1[3_554]	1.82	0.38
1:A:24:ASN:OD1	1:A:266:PRO:C[3_444]	1.83	0.37
1:A:56:THR:CG2	1:A:278:ARG:NH1[3_444]	1.83	0.37
1:A:121:ILE:O	1:A:270:LYS:NZ[3_444]	1.83	0.37
1:A:137:SER:O	1:A:233:HIS:CG[3_444]	1.83	0.37
1:A:138:ASP:C	1:A:211:GLN:OE1[3_444]	1.83	0.37
1:A:139:VAL:CG1	1:A:209:CYS:O[3_444]	1.83	0.37
1:A:140:VAL:CG1	1:A:211:GLN:C[3_444]	1.83	0.37
1:A:140:VAL:O	1:A:210:PRO:CB[3_444]	1.83	0.37
1:A:141:SER:C	1:A:210:PRO:CD[3_444]	1.83	0.37
1:A:141:SER:N	1:A:209:CYS:C[3_444]	1.83	0.37
1:A:206:GLU:OE2	2:P:359:PHE:CG[3_454]	1.83	0.37
1:A:207:LEU:C	2:P:358:GLU:OE1[3_454]	1.83	0.37
1:A:122:GLN:C	1:A:271:CYS:O[3_444]	1.84	0.36
1:A:125:PHE:N	1:A:276:CYS:CA[3_444]	1.84	0.36
1:A:168:SER:CB	1:A:283:LEU:CA[3_554]	1.84	0.36
1:A:171:HIS:CB	1:A:288:GLN:O[3_554]	1.84	0.36
1:A:280:ARG:CD	2:P:359:PHE:CG[3_454]	1.84	0.36
1:A:122:GLN:OE1	1:A:317:CYS:C[3_444]	1.85	0.35
1:A:139:VAL:CG1	1:A:277:PHE:CA[3_444]	1.85	0.35
1:A:170:TRP:NE1	1:A:287:HIS:NE2[3_554]	1.85	0.35
1:A:170:TRP:CG	1:A:286:LEU:C[3_554]	1.85	0.35
1:A:278:ARG:NH1	2:P:361:SER:O[3_454]	1.85	0.35
1:A:39:HIS:ND1	1:A:215:GLY:O[3_444]	1.86	0.34
1:A:56:THR:C	1:A:272:PRO:CB[3_444]	1.86	0.34
1:A:122:GLN:OE1	1:A:318:GLU:N[3_444]	1.86	0.34
1:A:125:PHE:C	1:A:275:GLU:O[3_444]	1.86	0.34
1:A:140:VAL:CB	1:A:210:PRO:C[3_444]	1.86	0.34
1:A:123:PHE:CD2	1:A:273:GLU:N[3_444]	1.87	0.33
1:A:125:PHE:CB	1:A:275:GLU:O[3_444]	1.87	0.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:CD	2:P:359:PHE:CB[3_454]	1.87	0.33
1:A:208:SER:CB	2:P:358:GLU:OE2[3_454]	1.87	0.33
1:A:104:TRP:CH2	1:A:216:GLN:CG[3_444]	1.88	0.32
1:A:142:PHE:O	1:A:270:LYS:N[3_444]	1.88	0.32
1:A:170:TRP:NE1	1:A:287:HIS:CE1[3_554]	1.88	0.32
1:A:172:PRO:CG	1:A:290:GLU:OE2[3_554]	1.88	0.32
1:A:278:ARG:CB	2:P:361:SER:OG[3_454]	1.88	0.32
1:A:278:ARG:CG	2:P:361:SER:OG[3_454]	1.88	0.32
1:A:16:GLN:CB	1:A:217:GLN:OE1[3_444]	1.89	0.31
1:A:38:PHE:N	1:A:214:GLU:CG[3_444]	1.89	0.31
1:A:120:THR:CB	1:A:341:GLN:NE2[3_444]	1.89	0.31
1:A:18:GLU:N	1:A:217:GLN:N[3_444]	1.90	0.30
1:A:38:PHE:C	1:A:214:GLU:O[3_444]	1.90	0.30
1:A:39:HIS:CA	1:A:216:GLN:N[3_444]	1.90	0.30
1:A:57:ALA:CB	1:A:272:PRO:CD[3_444]	1.90	0.30
1:A:121:ILE:C	1:A:270:LYS:CE[3_444]	1.90	0.30
1:A:125:PHE:N	1:A:276:CYS:N[3_444]	1.90	0.30
1:A:139:VAL:N	1:A:277:PHE:CG[3_444]	1.90	0.30
1:A:166:PRO:C	1:A:292:GLN:CD[3_554]	1.90	0.30
1:A:166:PRO:O	1:A:292:GLN:CD[3_554]	1.90	0.30
1:A:125:PHE:CA	1:A:275:GLU:O[3_444]	1.91	0.29
1:A:141:SER:N	1:A:210:PRO:CG[3_444]	1.91	0.29
1:A:142:PHE:CD1	1:A:269:LEU:CG[3_444]	1.91	0.29
1:A:143:ARG:CG	1:A:316:GLN:CD[3_444]	1.91	0.29
1:A:167:VAL:O	1:A:292:GLN:CG[3_554]	1.91	0.29
1:A:169:ASP:CA	1:A:286:LEU:CG[3_554]	1.91	0.29
1:A:22:GLU:C	1:A:267:GLN:CD[3_444]	1.92	0.28
1:A:24:ASN:CA	1:A:268:ILE:N[3_444]	1.92	0.28
1:A:24:ASN:OD1	1:A:267:GLN:C[3_444]	1.92	0.28
1:A:122:GLN:OE1	1:A:318:GLU:CA[3_444]	1.92	0.28
1:A:123:PHE:O	1:A:271:CYS:CA[3_444]	1.92	0.28
1:A:125:PHE:CE1	1:A:273:GLU:C[3_444]	1.92	0.28
1:A:127:ILE:N	1:A:275:GLU:OE1[3_444]	1.92	0.28
1:A:167:VAL:O	1:A:292:GLN:CD[3_554]	1.92	0.28
1:A:169:ASP:OD1	1:A:192:LEU:CG[3_554]	1.92	0.28
1:A:170:TRP:C	1:A:286:LEU:C[3_554]	1.92	0.28
1:A:170:TRP:CA	1:A:287:HIS:N[3_554]	1.92	0.28
1:A:39:HIS:N	1:A:216:GLN:N[3_444]	1.93	0.27
1:A:120:THR:OG1	1:A:341:GLN:CB[3_444]	1.93	0.27
1:A:123:PHE:CB	1:A:271:CYS:CA[3_444]	1.93	0.27
1:A:139:VAL:CA	1:A:277:PHE:N[3_444]	1.93	0.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:CG1	1:A:277:PHE:C[3_444]	1.93	0.27
1:A:142:PHE:CG	1:A:270:LYS:N[3_444]	1.93	0.27
1:A:170:TRP:N	1:A:286:LEU:CD2[3_554]	1.93	0.27
1:A:140:VAL:O	1:A:211:GLN:N[3_444]	1.94	0.26
1:A:141:SER:CB	1:A:210:PRO:N[3_444]	1.94	0.26
1:A:142:PHE:N	1:A:269:LEU:O[3_444]	1.94	0.26
1:A:143:ARG:CB	1:A:316:GLN:CG[3_444]	1.94	0.26
1:A:144:LEU:N	1:A:316:GLN:OE1[3_444]	1.94	0.26
1:A:167:VAL:N	1:A:292:GLN:CD[3_554]	1.94	0.26
1:A:171:HIS:CB	1:A:288:GLN:CA[3_554]	1.94	0.26
1:A:206:GLU:CG	2:P:359:PHE:C[3_454]	1.94	0.26
1:A:226:GLY:CA	1:A:349:THR:OG1[3_544]	1.94	0.26
1:A:17:LEU:C	1:A:217:GLN:CA[3_444]	1.95	0.25
1:A:18:GLU:O	1:A:216:GLN:O[3_444]	1.95	0.25
1:A:18:GLU:CB	1:A:217:GLN:CA[3_444]	1.95	0.25
1:A:19:VAL:O	1:A:218:LEU:CD2[3_444]	1.95	0.25
1:A:20:PHE:CE2	1:A:308:ARG:NH2[3_444]	1.95	0.25
1:A:123:PHE:CD1	1:A:273:GLU:CD[3_444]	1.95	0.25
1:A:126:GLN:OE1	1:A:232:ASN:CB[3_444]	1.95	0.25
1:A:136:GLN:OE1	1:A:232:ASN:C[3_444]	1.95	0.25
1:A:142:PHE:CD2	1:A:269:LEU:N[3_444]	1.95	0.25
1:A:208:SER:OG	2:P:358:GLU:OE1[3_454]	1.95	0.25
1:A:18:GLU:CD	1:A:304:THR:OG1[3_444]	1.96	0.24
1:A:37:THR:CA	1:A:214:GLU:OE2[3_444]	1.96	0.24
1:A:37:THR:OG1	1:A:214:GLU:OE1[3_444]	1.96	0.24
1:A:55:VAL:CG1	1:A:272:PRO:CA[3_444]	1.96	0.24
1:A:127:ILE:N	1:A:233:HIS:NE2[3_444]	1.96	0.24
1:A:171:HIS:CD2	1:A:288:GLN:O[3_554]	1.96	0.24
1:A:206:GLU:CG	2:P:359:PHE:N[3_454]	1.96	0.24
1:A:208:SER:CA	2:P:358:GLU:OE1[3_454]	1.96	0.24
1:A:140:VAL:CB	1:A:212:ALA:N[3_444]	1.97	0.23
1:A:140:VAL:CG1	1:A:212:ALA:N[3_444]	1.97	0.23
1:A:143:ARG:CZ	1:A:342:VAL:O[3_444]	1.97	0.23
1:A:170:TRP:N	1:A:286:LEU:CA[3_554]	1.97	0.23
1:A:280:ARG:NE	2:P:359:PHE:CZ[3_454]	1.97	0.23
1:A:8:ASP:CA	1:A:74:SER:OG[4_435]	1.98	0.22
1:A:14:ASP:OD2	1:A:238:LYS:CG[3_444]	1.98	0.22
1:A:18:GLU:N	1:A:217:GLN:CA[3_444]	1.98	0.22
1:A:122:GLN:CD	1:A:317:CYS:C[3_444]	1.98	0.22
1:A:126:GLN:O	1:A:275:GLU:CD[3_444]	1.98	0.22
1:A:126:GLN:NE2	1:A:233:HIS:ND1[3_444]	1.98	0.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLN:C	1:A:275:GLU:CD[3_444]	1.98	0.22
1:A:136:GLN:NE2	1:A:233:HIS:CA[3_444]	1.98	0.22
1:A:140:VAL:N	1:A:209:CYS:O[3_444]	1.98	0.22
1:A:141:SER:N	1:A:210:PRO:CB[3_444]	1.98	0.22
1:A:171:HIS:CD2	1:A:289:GLN:N[3_554]	1.98	0.22
1:A:226:GLY:N	1:A:349:THR:OG1[3_544]	1.98	0.22
1:A:18:GLU:O	1:A:213:LEU:CA[3_444]	1.99	0.21
1:A:18:GLU:OE1	1:A:304:THR:CB[3_444]	1.99	0.21
1:A:38:PHE:O	1:A:215:GLY:N[3_444]	1.99	0.21
1:A:56:THR:O	1:A:272:PRO:N[3_444]	1.99	0.21
1:A:126:GLN:CA	1:A:275:GLU:OE2[3_444]	1.99	0.21
1:A:136:GLN:NE2	1:A:233:HIS:C[3_444]	1.99	0.21
1:A:139:VAL:CB	1:A:277:PHE:O[3_444]	1.99	0.21
1:A:142:PHE:N	1:A:210:PRO:CB[3_444]	1.99	0.21
1:A:170:TRP:CG	1:A:287:HIS:N[3_554]	1.99	0.21
1:A:228:ASN:ND2	1:A:253:LYS:NZ[3_544]	1.99	0.21
1:A:19:VAL:N	1:A:213:LEU:N[3_444]	2.00	0.20
1:A:38:PHE:CA	1:A:213:LEU:O[3_444]	2.00	0.20
1:A:39:HIS:CA	1:A:215:GLY:O[3_444]	2.00	0.20
1:A:121:ILE:C	1:A:316:GLN:NE2[3_444]	2.00	0.20
1:A:7:GLU:C	1:A:74:SER:OG[4_435]	2.01	0.19
1:A:19:VAL:CG1	1:A:213:LEU:CA[3_444]	2.01	0.19
1:A:105:GLY:O	1:A:214:GLU:CB[3_444]	2.01	0.19
1:A:121:ILE:C	1:A:270:LYS:NZ[3_444]	2.01	0.19
1:A:123:PHE:N	1:A:270:LYS:CB[3_444]	2.01	0.19
1:A:136:GLN:CD	1:A:232:ASN:C[3_444]	2.01	0.19
1:A:16:GLN:OE1	1:A:301:TRP:CH2[3_444]	2.02	0.18
1:A:23:GLN:O	1:A:268:ILE:N[3_444]	2.02	0.18
1:A:37:THR:CA	1:A:214:GLU:CG[3_444]	2.02	0.18
1:A:122:GLN:OE1	1:A:317:CYS:O[3_444]	2.02	0.18
1:A:125:PHE:O	1:A:276:CYS:O[3_444]	2.02	0.18
1:A:136:GLN:CG	1:A:234:PRO:N[3_444]	2.02	0.18
1:A:141:SER:O	1:A:210:PRO:CB[3_444]	2.02	0.18
1:A:142:PHE:CA	1:A:270:LYS:CA[3_444]	2.02	0.18
1:A:142:PHE:CB	1:A:269:LEU:CA[3_444]	2.02	0.18
1:A:21:GLY:C	1:A:267:GLN:CD[3_444]	2.03	0.17
1:A:38:PHE:C	1:A:213:LEU:C[3_444]	2.03	0.17
1:A:122:GLN:CD	1:A:318:GLU:N[3_444]	2.03	0.17
1:A:141:SER:OG	1:A:210:PRO:N[3_444]	2.03	0.17
1:A:168:SER:O	1:A:284:GLY:O[3_554]	2.03	0.17
1:A:206:GLU:OE2	2:P:360:VAL:N[3_454]	2.03	0.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:N	1:A:267:GLN:N[3_444]	2.04	0.16
1:A:38:PHE:N	1:A:213:LEU:C[3_444]	2.04	0.16
1:A:123:PHE:CG	1:A:273:GLU:CD[3_444]	2.04	0.16
1:A:124:ASP:C	1:A:271:CYS:SG[3_444]	2.04	0.16
1:A:125:PHE:CD1	1:A:274:ALA:N[3_444]	2.04	0.16
1:A:125:PHE:CA	1:A:274:ALA:O[3_444]	2.04	0.16
1:A:126:GLN:C	1:A:275:GLU:OE1[3_444]	2.04	0.16
1:A:136:GLN:CG	1:A:234:PRO:CD[3_444]	2.04	0.16
1:A:142:PHE:CE2	1:A:269:LEU:N[3_444]	2.04	0.16
1:A:142:PHE:N	1:A:210:PRO:CG[3_444]	2.04	0.16
1:A:143:ARG:NH2	1:A:317:CYS:O[3_444]	2.04	0.16
1:A:171:HIS:NE2	1:A:289:GLN:CG[3_554]	2.04	0.16
3:A:406:HOH:O	3:A:412:HOH:O[3_454]	2.04	0.16
1:A:19:VAL:CG2	1:A:218:LEU:CD1[3_444]	2.05	0.15
1:A:39:HIS:N	1:A:215:GLY:C[3_444]	2.05	0.15
1:A:123:PHE:CA	1:A:270:LYS:C[3_444]	2.05	0.15
1:A:126:GLN:N	1:A:275:GLU:C[3_444]	2.05	0.15
1:A:143:ARG:O	1:A:268:ILE:CA[3_444]	2.05	0.15
1:A:143:ARG:O	1:A:268:ILE:CB[3_444]	2.05	0.15
1:A:170:TRP:CH2	1:A:287:HIS:CD2[3_554]	2.05	0.15
1:A:171:HIS:ND1	1:A:289:GLN:CB[3_554]	2.05	0.15
1:A:172:PRO:N	1:A:290:GLU:CG[3_554]	2.05	0.15
1:A:206:GLU:CA	2:P:358:GLU:O[3_454]	2.05	0.15
1:A:206:GLU:CD	2:P:359:PHE:O[3_454]	2.05	0.15
1:A:208:SER:CB	2:P:358:GLU:CD[3_454]	2.05	0.15
1:A:278:ARG:NH2	2:P:361:SER:O[3_454]	2.05	0.15
1:A:16:GLN:OE1	1:A:217:GLN:OE1[3_444]	2.06	0.14
1:A:17:LEU:O	1:A:217:GLN:CA[3_444]	2.06	0.14
1:A:139:VAL:CB	1:A:277:PHE:CG[3_444]	2.06	0.14
1:A:139:VAL:CG2	1:A:277:PHE:O[3_444]	2.06	0.14
1:A:139:VAL:CG2	1:A:277:PHE:CG[3_444]	2.06	0.14
1:A:140:VAL:CG1	1:A:211:GLN:N[3_444]	2.06	0.14
1:A:168:SER:CA	1:A:292:GLN:OE1[3_554]	2.06	0.14
1:A:25:HIS:CA	1:A:268:ILE:CD1[3_444]	2.07	0.13
1:A:104:TRP:CZ3	1:A:216:GLN:CG[3_444]	2.07	0.13
1:A:121:ILE:CG1	1:A:270:LYS:NZ[3_444]	2.07	0.13
1:A:122:GLN:NE2	1:A:317:CYS:C[3_444]	2.07	0.13
1:A:125:PHE:N	1:A:275:GLU:C[3_444]	2.07	0.13
1:A:125:PHE:CD1	1:A:274:ALA:O[3_444]	2.07	0.13
1:A:126:GLN:CD	1:A:232:ASN:ND2[3_444]	2.07	0.13
1:A:143:ARG:CD	1:A:343:ALA:CB[3_444]	2.07	0.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:CG	1:A:316:GLN:OE1[3_444]	2.07	0.13
1:A:278:ARG:CZ	2:P:361:SER:C[3_454]	2.07	0.13
1:A:8:ASP:C	1:A:74:SER:OG[4_435]	2.08	0.12
1:A:16:GLN:CD	1:A:217:GLN:OE1[3_444]	2.08	0.12
1:A:18:GLU:CB	1:A:217:GLN:O[3_444]	2.08	0.12
1:A:18:GLU:OE1	1:A:217:GLN:O[3_444]	2.08	0.12
1:A:39:HIS:CB	1:A:215:GLY:CA[3_444]	2.08	0.12
1:A:39:HIS:O	1:A:215:GLY:CA[3_444]	2.08	0.12
1:A:39:HIS:O	1:A:215:GLY:C[3_444]	2.08	0.12
1:A:120:THR:CG2	1:A:341:GLN:CD[3_444]	2.08	0.12
1:A:123:PHE:CB	1:A:270:LYS:C[3_444]	2.08	0.12
1:A:124:ASP:OD1	1:A:208:SER:O[3_444]	2.08	0.12
1:A:136:GLN:CB	1:A:233:HIS:CA[3_444]	2.08	0.12
1:A:169:ASP:CG	1:A:321:TYR:CZ[3_554]	2.08	0.12
1:A:170:TRP:C	1:A:287:HIS:O[3_554]	2.08	0.12
1:A:206:GLU:OE1	2:P:358:GLU:N[3_454]	2.08	0.12
1:A:280:ARG:CZ	2:P:359:PHE:CD2[3_454]	2.08	0.12
1:A:39:HIS:CA	1:A:214:GLU:C[3_444]	2.09	0.11
1:A:123:PHE:CE2	1:A:273:GLU:CG[3_444]	2.09	0.11
1:A:124:ASP:C	1:A:276:CYS:CA[3_444]	2.09	0.11
1:A:125:PHE:CA	1:A:276:CYS:CA[3_444]	2.09	0.11
1:A:127:ILE:N	1:A:233:HIS:CE1[3_444]	2.09	0.11
1:A:140:VAL:C	1:A:210:PRO:CB[3_444]	2.09	0.11
1:A:140:VAL:CG2	1:A:211:GLN:CG[3_444]	2.09	0.11
1:A:166:PRO:C	1:A:292:GLN:CG[3_554]	2.09	0.11
1:A:168:SER:N	1:A:292:GLN:CD[3_554]	2.09	0.11
1:A:171:HIS:ND1	1:A:289:GLN:CA[3_554]	2.09	0.11
1:A:171:HIS:CB	1:A:287:HIS:C[3_554]	2.09	0.11
1:A:21:GLY:CA	1:A:267:GLN:OE1[3_444]	2.10	0.10
1:A:24:ASN:CB	1:A:267:GLN:C[3_444]	2.10	0.10
1:A:127:ILE:CA	1:A:233:HIS:NE2[3_444]	2.10	0.10
1:A:136:GLN:OE1	1:A:233:HIS:N[3_444]	2.10	0.10
1:A:140:VAL:CG1	1:A:210:PRO:O[3_444]	2.10	0.10
1:A:278:ARG:CD	2:P:361:SER:OG[3_454]	2.10	0.10
1:A:24:ASN:OD1	1:A:266:PRO:O[3_444]	2.11	0.09
1:A:122:GLN:NE2	1:A:317:CYS:CA[3_444]	2.11	0.09
1:A:123:PHE:C	1:A:270:LYS:C[3_444]	2.11	0.09
1:A:124:ASP:CG	1:A:208:SER:CB[3_444]	2.11	0.09
1:A:139:VAL:C	1:A:277:PHE:CB[3_444]	2.11	0.09
1:A:144:LEU:CG	1:A:268:ILE:CB[3_444]	2.11	0.09
1:A:172:PRO:CD	1:A:290:GLU:CD[3_554]	2.11	0.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:CG1	1:A:213:LEU:CG[3_444]	2.12	0.08
1:A:37:THR:C	1:A:213:LEU:CG[3_444]	2.12	0.08
1:A:39:HIS:C	1:A:215:GLY:N[3_444]	2.12	0.08
1:A:120:THR:CA	1:A:341:GLN:CD[3_444]	2.12	0.08
1:A:123:PHE:CZ	1:A:273:GLU:OE1[3_444]	2.12	0.08
1:A:124:ASP:OD1	1:A:208:SER:C[3_444]	2.12	0.08
1:A:140:VAL:N	1:A:211:GLN:CA[3_444]	2.12	0.08
1:A:141:SER:OG	1:A:209:CYS:N[3_444]	2.12	0.08
1:A:141:SER:N	1:A:210:PRO:O[3_444]	2.12	0.08
1:A:142:PHE:N	1:A:270:LYS:CA[3_444]	2.12	0.08
1:A:169:ASP:O	1:A:286:LEU:N[3_554]	2.12	0.08
1:A:170:TRP:CE2	1:A:287:HIS:CG[3_554]	2.12	0.08
1:A:20:PHE:CZ	1:A:304:THR:CG2[3_444]	2.13	0.07
1:A:123:PHE:CB	1:A:271:CYS:O[3_444]	2.13	0.07
1:A:137:SER:OG	1:A:211:GLN:OE1[3_444]	2.13	0.07
1:A:138:ASP:OD1	1:A:221:VAL:N[3_444]	2.13	0.07
1:A:143:ARG:CZ	1:A:317:CYS:O[3_444]	2.13	0.07
1:A:144:LEU:N	1:A:316:GLN:CD[3_444]	2.13	0.07
1:A:169:ASP:OD2	1:A:321:TYR:CE1[3_554]	2.13	0.07
1:A:170:TRP:NE1	1:A:287:HIS:CD2[3_554]	2.13	0.07
1:A:171:HIS:ND1	1:A:288:GLN:CG[3_554]	2.13	0.07
1:A:206:GLU:CG	2:P:358:GLU:O[3_454]	2.13	0.07
1:A:280:ARG:CB	2:P:359:PHE:CD1[3_454]	2.13	0.07
1:A:280:ARG:CG	2:P:359:PHE:CD1[3_454]	2.13	0.07
1:A:18:GLU:CG	1:A:216:GLN:O[3_444]	2.14	0.06
1:A:20:PHE:O	1:A:213:LEU:CD2[3_444]	2.14	0.06
1:A:123:PHE:C	1:A:271:CYS:C[3_444]	2.14	0.06
1:A:123:PHE:N	1:A:270:LYS:C[3_444]	2.14	0.06
1:A:143:ARG:CZ	1:A:317:CYS:N[3_444]	2.14	0.06
1:A:167:VAL:N	1:A:292:GLN:NE2[3_554]	2.14	0.06
1:A:208:SER:OG	2:P:361:SER:CB[3_454]	2.14	0.06
1:A:216:GLN:CD	3:A:402:HOH:O[3_454]	2.14	0.06
1:A:226:GLY:CA	1:A:349:THR:CA[3_544]	2.14	0.06
1:A:123:PHE:CD1	1:A:270:LYS:CD[3_444]	2.15	0.05
1:A:123:PHE:CD2	1:A:272:PRO:CD[3_444]	2.15	0.05
1:A:136:GLN:N	1:A:234:PRO:CD[3_444]	2.15	0.05
1:A:136:GLN:CG	1:A:233:HIS:N[3_444]	2.15	0.05
1:A:143:ARG:NE	1:A:342:VAL:O[3_444]	2.15	0.05
1:A:56:THR:O	1:A:272:PRO:CB[3_444]	2.16	0.04
1:A:124:ASP:C	1:A:276:CYS:SG[3_444]	2.16	0.04
1:A:136:GLN:OE1	1:A:232:ASN:O[3_444]	2.16	0.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CG1	1:A:210:PRO:C[3_444]	2.16	0.04
1:A:144:LEU:CB	1:A:268:ILE:CG2[3_444]	2.16	0.04
1:A:170:TRP:NE1	1:A:287:HIS:ND1[3_554]	2.16	0.04
1:A:206:GLU:OE1	2:P:358:GLU:CA[3_454]	2.16	0.04
1:A:18:GLU:O	1:A:213:LEU:O[3_444]	2.17	0.03
1:A:18:GLU:CA	1:A:217:GLN:N[3_444]	2.17	0.03
1:A:38:PHE:C	1:A:213:LEU:O[3_444]	2.17	0.03
1:A:136:GLN:NE2	1:A:233:HIS:O[3_444]	2.17	0.03
1:A:140:VAL:CG1	1:A:211:GLN:CA[3_444]	2.17	0.03
1:A:141:SER:OG	1:A:210:PRO:CD[3_444]	2.17	0.03
1:A:141:SER:O	1:A:210:PRO:CD[3_444]	2.17	0.03
1:A:143:ARG:NH2	1:A:317:CYS:CA[3_444]	2.17	0.03
1:A:170:TRP:CD2	1:A:290:GLU:OE1[3_554]	2.17	0.03
1:A:171:HIS:O	1:A:287:HIS:CA[3_554]	2.17	0.03
1:A:171:HIS:O	1:A:287:HIS:C[3_554]	2.17	0.03
1:A:171:HIS:C	1:A:287:HIS:CB[3_554]	2.17	0.03
1:A:206:GLU:CB	2:P:359:PHE:N[3_454]	2.17	0.03
1:A:280:ARG:CG	2:P:359:PHE:CG[3_454]	2.17	0.03
1:A:38:PHE:CB	1:A:213:LEU:C[3_444]	2.18	0.02
1:A:123:PHE:CE2	1:A:273:GLU:OE1[3_444]	2.18	0.02
1:A:125:PHE:O	1:A:277:PHE:N[3_444]	2.18	0.02
1:A:136:GLN:CD	1:A:233:HIS:C[3_444]	2.18	0.02
1:A:140:VAL:N	1:A:211:GLN:CB[3_444]	2.18	0.02
1:A:142:PHE:CG	1:A:269:LEU:CB[3_444]	2.18	0.02
1:A:169:ASP:O	1:A:286:LEU:CA[3_554]	2.18	0.02
1:A:169:ASP:CB	1:A:321:TYR:OH[3_554]	2.18	0.02
1:A:227:LEU:N	1:A:349:THR:CB[3_544]	2.18	0.02
1:A:21:GLY:O	1:A:267:GLN:CG[3_444]	2.19	0.01
1:A:24:ASN:O	1:A:268:ILE:CB[3_444]	2.19	0.01
1:A:120:THR:CB	1:A:341:GLN:CG[3_444]	2.19	0.01
1:A:125:PHE:CG	1:A:275:GLU:CA[3_444]	2.19	0.01
1:A:125:PHE:CG	1:A:274:ALA:CB[3_444]	2.19	0.01
1:A:126:GLN:CA	1:A:276:CYS:O[3_444]	2.19	0.01
1:A:140:VAL:CB	1:A:211:GLN:CB[3_444]	2.19	0.01
1:A:144:LEU:C	1:A:316:GLN:OE1[3_444]	2.19	0.01
1:A:170:TRP:CZ3	1:A:290:GLU:CD[3_554]	2.19	0.01
1:A:171:HIS:CE1	1:A:289:GLN:CA[3_554]	2.19	0.01
1:A:280:ARG:NE	2:P:359:PHE:CG[3_454]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/346 (99%)	299 (87%)	32 (9%)	13 (4%)	2	9
2	P	7/9 (78%)	3 (43%)	2 (29%)	2 (29%)	0	0
All	All	351/355 (99%)	302 (86%)	34 (10%)	15 (4%)	2	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	TRP
1	A	251	GLN
1	A	267	GLN
2	P	363	LEU
1	A	72	ASN
1	A	134	ASN
1	A	135	SER
1	A	169	ASP
1	A	273	GLU
1	A	224	VAL
1	A	103	LEU
1	A	306	LEU
2	P	364	THR
1	A	239	GLY
1	A	256	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/302 (100%)	272 (90%)	30 (10%)	7	22
2	P	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	311/311 (100%)	278 (89%)	33 (11%)	6	19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	CYS
1	A	19	VAL
1	A	24	ASN
1	A	31	LYS
1	A	74	SER
1	A	81	PHE
1	A	83	VAL
1	A	90	VAL
1	A	103	LEU
1	A	110	THR
1	A	111	VAL
1	A	129	SER
1	A	133	ASN
1	A	151	GLN
1	A	152	VAL
1	A	167	VAL
1	A	177	GLN
1	A	189	VAL
1	A	231	THR
1	A	247	SER
1	A	250	HIS
1	A	251	GLN
1	A	255	GLU
1	A	260	SER
1	A	275	GLU
1	A	285	PRO
1	A	286	LEU
1	A	296	LEU
1	A	318	GLU
1	A	341	GLN
2	P	363	LEU
2	P	365	ASN
2	P	367	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	ASN
1	A	41	GLN
1	A	134	ASN
1	A	177	GLN
1	A	249	HIS
1	A	250	HIS
1	A	287	HIS
1	A	295	GLN
1	A	316	GLN
1	A	341	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/346 (100%)	6.44	322 (93%)  	53, 86, 197, 278	0
2	P	9/9 (100%)	5.95	8 (88%)  	91, 114, 149, 158	0
All	All	355/355 (100%)	6.43	330 (92%)  	53, 87, 197, 278	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ASN	33.6
1	A	220	TYR	32.4
1	A	230	THR	23.9
1	A	203	GLY	22.7
1	A	149	GLN	21.6
1	A	250	HIS	21.0
1	A	257	PRO	20.3
1	A	328	TYR	20.1
1	A	242	LEU	18.7
1	A	34	LEU	18.7
1	A	114	LEU	17.9
1	A	182	LEU	17.6
1	A	28	LEU	16.8
1	A	231	THR	16.6
1	A	164	LEU	16.6
2	P	362	GLN	16.3
1	A	148	ALA	15.8
1	A	17	LEU	15.2
1	A	330	ILE	15.2
1	A	298	PHE	14.5
1	A	258	SER	14.3
1	A	75	SER	13.2
1	A	89	LEU	13.0
1	A	210	PRO	13.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	74	SER	12.9
1	A	301	TRP	12.8
1	A	69	HIS	12.6
1	A	327	PRO	12.5
1	A	104	TRP	12.3
1	A	338	LYS	12.2
1	A	256	ALA	12.2
1	A	346	VAL	12.2
1	A	249	HIS	12.1
1	A	262	ALA	11.9
2	P	360	VAL	11.9
1	A	41	GLN	11.5
1	A	300	VAL	11.5
1	A	129	SER	11.4
1	A	111	VAL	11.3
1	A	283	LEU	11.3
1	A	107	LEU	11.1
1	A	32	ASN	11.0
1	A	103	LEU	11.0
1	A	16	GLN	10.9
1	A	255	GLU	10.7
1	A	19	VAL	10.7
1	A	83	VAL	10.6
1	A	219	LEU	10.4
1	A	26	VAL	10.3
1	A	43	VAL	10.3
1	A	117	THR	10.2
1	A	59	PRO	10.0
1	A	344	THR	9.9
1	A	72	ASN	9.7
1	A	223	ARG	9.6
1	A	270	LYS	9.6
1	A	259	ARG	9.6
1	A	161	GLU	9.4
1	A	106	GLY	9.4
1	A	296	LEU	9.3
1	A	80	TYR	9.3
1	A	204	VAL	9.1
1	A	178	LYS	9.0
1	A	275	GLU	9.0
1	A	154	LEU	8.9
1	A	76	LEU	8.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	53	LEU	8.8
1	A	174	ASP	8.8
1	A	313	PHE	8.8
1	A	305	PHE	8.8
1	A	36	LEU	8.7
1	A	186	VAL	8.6
1	A	299	ARG	8.6
1	A	222	THR	8.6
1	A	40	ALA	8.5
1	A	73	PHE	8.5
1	A	5	CYS	8.5
1	A	163	VAL	8.4
1	A	179	GLU	8.4
1	A	324	LEU	8.3
1	A	96	PRO	8.3
1	A	315	LEU	8.2
1	A	225	THR	8.2
1	A	201	SER	8.1
1	A	285	PRO	8.1
1	A	185	ALA	8.1
1	A	295	GLN	8.0
1	A	165	PHE	7.9
1	A	68	ARG	7.9
1	A	191	GLU	7.8
1	A	110	THR	7.7
1	A	177	GLN	7.7
1	A	105	GLY	7.7
1	A	70	PRO	7.6
1	A	15	LEU	7.6
1	A	115	ARG	7.6
1	A	251	GLN	7.5
1	A	102	SER	7.5
1	A	119	LYS	7.4
1	A	180	GLU	7.4
1	A	336	PRO	7.4
1	A	345	ALA	7.3
1	A	58	PRO	7.3
1	A	141	SER	7.3
1	A	217	GLN	7.2
1	A	152	VAL	7.2
1	A	199	SER	7.2
1	A	168	SER	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	SER	7.1
1	A	241	GLU	7.1
1	A	337	GLN	7.0
1	A	78	CYS	7.0
1	A	116	ASP	7.0
1	A	218	LEU	6.9
1	A	189	VAL	6.9
1	A	97	MET	6.8
1	A	212	ALA	6.8
1	A	319	ALA	6.8
1	A	71	GLY	6.8
1	A	273	GLU	6.8
1	A	188	HIS	6.7
1	A	12	VAL	6.7
1	A	84	ASN	6.6
1	A	310	HIS	6.5
1	A	20	PHE	6.5
1	A	87	ARG	6.4
1	A	264	SER	6.4
1	A	302	ALA	6.4
1	A	184	PRO	6.3
1	A	236	ASN	6.3
1	A	198	SER	6.3
1	A	38	PHE	6.3
1	A	294	LEU	6.2
1	A	147	GLU	6.2
1	A	309	GLU	6.2
1	A	85	GLN	6.2
1	A	211	GLN	6.2
1	A	66	LEU	6.1
1	A	101	ALA	6.1
1	A	308	ARG	6.1
1	A	86	SER	6.1
1	A	113	HIS	6.1
1	A	227	LEU	6.1
1	A	77	SER	6.0
1	A	94	GLY	6.0
1	A	200	ILE	6.0
1	A	127	ILE	5.9
1	A	224	VAL	5.9
1	A	169	ASP	5.9
1	A	292	GLN	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	5.8
1	A	157	VAL	5.8
1	A	243	ASP	5.8
1	A	151	GLN	5.8
1	A	173	ARG	5.8
2	P	363	LEU	5.7
1	A	93	LEU	5.7
1	A	291	SER	5.7
1	A	33	ALA	5.7
1	A	10	ILE	5.6
1	A	57	ALA	5.6
1	A	202	GLN	5.6
1	A	284	GLY	5.6
1	A	323	ALA	5.6
1	A	140	VAL	5.5
1	A	48	ALA	5.5
1	A	21	GLY	5.5
1	A	146	VAL	5.4
1	A	159	LYS	5.4
1	A	100	GLY	5.4
1	A	307	GLN	5.4
1	A	326	MET	5.4
1	A	60	GLU	5.3
1	A	318	GLU	5.3
1	A	8	ASP	5.3
1	A	181	ASP	5.3
1	A	348	TRP	5.3
1	A	166	PRO	5.3
1	A	206	GLU	5.3
1	A	128	LEU	5.2
1	A	130	LYS	5.2
1	A	81	PHE	5.2
1	A	51	ALA	5.2
1	A	192	LEU	5.2
1	A	205	LEU	5.2
1	A	254	ARG	5.2
1	A	52	GLU	5.2
1	A	31	LYS	5.2
1	A	172	PRO	5.2
1	A	98	LYS	5.2
1	A	150	ALA	5.2
1	A	176	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	5.1
1	A	132	LEU	5.1
1	A	266	PRO	5.1
1	A	142	PHE	5.1
1	A	167	VAL	5.0
1	A	183	GLY	5.0
1	A	265	GLY	5.0
1	A	55	VAL	5.0
1	A	252	GLN	5.0
1	A	347	GLN	5.0
1	A	306	LEU	5.0
1	A	325	LYS	5.0
1	A	23	GLN	4.9
1	A	260	SER	4.9
1	A	335	LEU	4.9
1	A	193	ILE	4.9
1	A	332	PRO	4.8
1	A	88	LEU	4.8
2	P	365	ASN	4.8
1	A	246	GLY	4.8
1	A	91	CYS	4.7
1	A	61	ALA	4.7
1	A	30	ASP	4.7
1	A	121	ILE	4.7
1	A	29	GLY	4.7
1	A	237	PRO	4.6
1	A	279	LEU	4.6
1	A	216	GLN	4.6
1	A	261	SER	4.6
1	A	272	PRO	4.6
1	A	247	SER	4.6
1	A	27	TYR	4.5
1	A	334	GLN	4.5
1	A	118	LYS	4.5
1	A	63	TYR	4.5
1	A	333	ARG	4.5
1	A	11	CYS	4.5
1	A	162	ALA	4.5
1	A	79	ASP	4.5
1	A	349	THR	4.5
1	A	4	ASP	4.5
1	A	47	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	99	ALA	4.4
1	A	156	GLY	4.4
1	A	190	TYR	4.3
1	A	131	ASN	4.3
1	A	25	HIS	4.3
1	A	13	PRO	4.3
1	A	320	VAL	4.3
1	A	49	TYR	4.3
1	A	331	LEU	4.3
1	A	145	SER	4.3
1	A	108	ARG	4.3
1	A	134	ASN	4.2
1	A	42	ASN	4.2
1	A	214	GLU	4.1
1	A	303	LYS	4.1
1	A	158	SER	4.1
1	A	281	CYS	4.1
1	A	282	GLU	4.1
1	A	339	GLU	4.1
1	A	65	GLY	4.0
1	A	235	ILE	4.0
1	A	39	HIS	4.0
1	A	138	ASP	3.9
1	A	207	LEU	3.9
1	A	187	HIS	3.9
1	A	263	SER	3.9
1	A	153	THR	3.8
1	A	64	SER	3.8
1	A	269	LEU	3.7
2	P	361	SER	3.7
1	A	175	GLN	3.7
2	P	358	GLU	3.7
1	A	314	SER	3.6
1	A	228	ASN	3.6
1	A	24	ASN	3.5
1	A	253	LYS	3.5
1	A	133	ASN	3.5
1	A	197	PRO	3.5
1	A	329	ARG	3.5
1	A	343	ALA	3.5
1	A	54	ARG	3.5
1	A	311	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	364	THR	3.5
1	A	321	TYR	3.4
1	A	248	LEU	3.4
1	A	45	GLU	3.4
1	A	109	PHE	3.3
1	A	312	PRO	3.3
1	A	7	GLU	3.3
1	A	194	ASN	3.3
1	A	62	GLU	3.2
1	A	137	SER	3.1
1	A	46	GLY	3.1
1	A	322	LYS	3.1
1	A	37	THR	3.1
1	A	304	THR	3.1
1	A	245	GLU	3.1
1	A	226	GLY	3.0
1	A	289	GLN	3.0
1	A	82	ALA	3.0
1	A	135	SER	3.0
1	A	196	GLY	3.0
1	A	240	LEU	3.0
1	A	171	HIS	3.0
2	P	367	GLN	3.0
1	A	271	CYS	2.9
1	A	92	ASP	2.9
1	A	274	ALA	2.9
1	A	267	GLN	2.8
1	A	317	CYS	2.8
1	A	213	LEU	2.8
1	A	297	HIS	2.8
1	A	238	LYS	2.7
1	A	209	CYS	2.7
1	A	195	GLN	2.7
1	A	44	GLY	2.6
1	A	229	CYS	2.6
1	A	123	PHE	2.6
1	A	287	HIS	2.6
1	A	221	VAL	2.6
1	A	9	ASN	2.6
1	A	22	GLU	2.6
1	A	56	THR	2.5
1	A	18	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	244	PRO	2.5
1	A	239	GLY	2.4
1	A	290	GLU	2.4
1	A	50	GLU	2.4
1	A	122	GLN	2.4
1	A	170	TRP	2.4
1	A	342	VAL	2.3
1	A	136	GLN	2.3
1	A	95	ASN	2.2
1	A	155	ASN	2.1
1	A	160	PRO	2.0
1	A	276	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.