



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:50 AM UTC

PDB ID : 3V89 / pdb_00003v89
Title : The crystal structure of transferrin binding protein A (TbpA) from *Neisseria meningitidis* serogroup B in complex with the C-lobe of human transferrin
Authors : Noinaj, N.; Oke, M.; Easley, N.; Zak, O.; Aisen, P.; Buchanan, S.K.
Deposited on : 2011-12-22
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

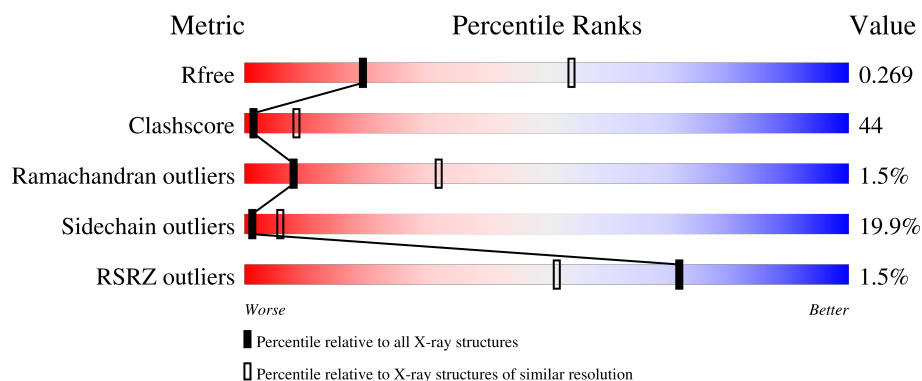
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	904	
2	B	343	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9110 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 Transferrin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	0	0
			6558	4091	1182	1274	11			

There are 13 discrepancies between the modelled and reference sequences:

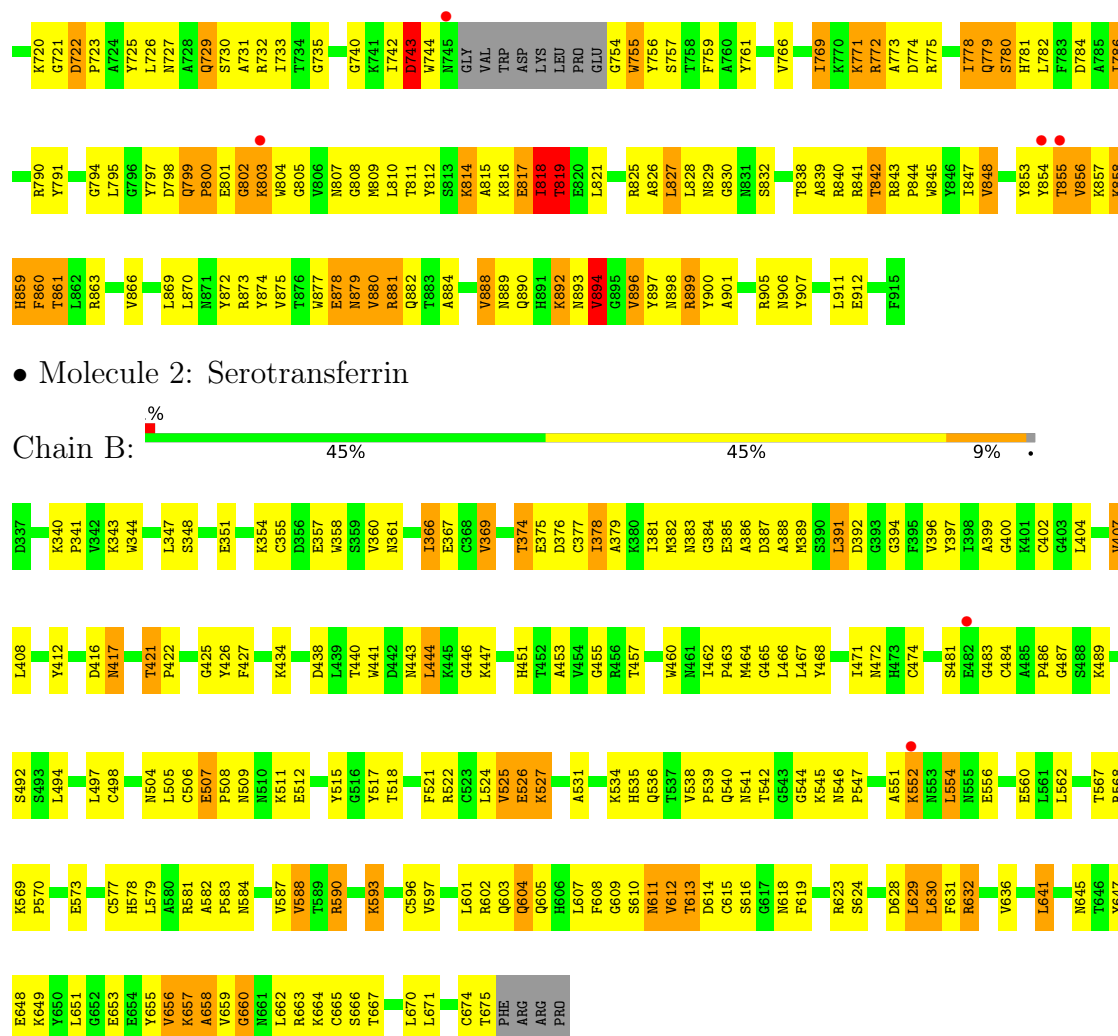
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q9JPJ0
A	13	ASP	-	expression tag	UNP Q9JPJ0
A	14	ILE	-	expression tag	UNP Q9JPJ0
A	15	HIS	-	expression tag	UNP Q9JPJ0
A	16	HIS	-	expression tag	UNP Q9JPJ0
A	17	HIS	-	expression tag	UNP Q9JPJ0
A	18	HIS	-	expression tag	UNP Q9JPJ0
A	19	HIS	-	expression tag	UNP Q9JPJ0
A	20	HIS	-	expression tag	UNP Q9JPJ0
A	21	HIS	-	expression tag	UNP Q9JPJ0
A	22	HIS	-	expression tag	UNP Q9JPJ0
A	23	HIS	-	expression tag	UNP Q9JPJ0
A	24	HIS	-	expression tag	UNP Q9JPJ0

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2552	1587	436	503	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	variant	UNP P02787



• Molecule 2: Serotransferrin

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.05Å 107.59Å 130.72Å 90.00° 94.48° 90.00°	Depositor
Resolution (Å)	29.96 – 3.10 29.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.96-3.10) 91.9 (29.96-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_865)	Depositor
R, R_{free}	0.224 , 0.287 (Not available) , 0.269	Depositor DCC
R_{free} test set	1407 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/6701	0.89	20/9081 (0.2%)
2	B	0.36	0/2605	0.83	4/3535 (0.1%)
All	All	0.38	0/9306	0.87	24/12616 (0.2%)

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	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	779	GLN	CB-CA-C	-6.93	108.59	116.63
1	A	819	THR	N-CA-C	-6.77	105.17	113.50
1	A	780	SER	N-CA-C	-6.59	99.55	108.24
2	B	507	GLU	CA-C-N	6.46	126.15	119.82
2	B	507	GLU	C-N-CA	6.46	126.15	119.82
1	A	881	ARG	N-CA-C	-6.05	105.39	112.89
1	A	729	GLN	N-CA-C	5.78	117.63	108.79
2	B	658	ALA	N-CA-C	-5.78	106.27	113.38
2	B	660	GLY	N-CA-C	-5.65	106.71	114.67
1	A	743	ASP	N-CA-C	5.46	118.94	112.72
1	A	88	VAL	N-CA-C	5.38	118.66	111.44
1	A	345	VAL	N-CA-C	5.35	112.43	107.56
1	A	289	VAL	N-CA-C	5.28	116.10	107.24
1	A	268	SER	N-CA-C	5.23	118.23	109.96
1	A	579	GLY	N-CA-C	5.14	118.08	110.63
1	A	228	GLY	N-CA-C	5.12	117.96	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	SER	N-CA-C	5.10	121.66	110.80
1	A	595	TRP	N-CA-C	5.08	116.90	111.36
1	A	817	GLU	CA-C-N	5.08	130.83	121.70
1	A	817	GLU	C-N-CA	5.08	130.83	121.70
1	A	240	VAL	N-CA-C	5.05	119.85	109.34
1	A	634	PRO	N-CA-C	-5.05	107.82	114.03
1	A	247	VAL	CA-C-N	5.01	125.16	119.90
1	A	247	VAL	C-N-CA	5.01	125.16	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	VAL	Peptide
1	A	743	ASP	Peptide

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	6558	0	6177	628	1
2	B	2552	0	2359	152	1
All	All	9110	0	8536	768	1

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 44.

All (768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:TYR:CE1	1:A:856:VAL:HG12	1.47	1.46
1:A:855:THR:CG2	1:A:861:THR:HB	1.43	1.45
1:A:52:ASP:HB3	1:A:53:ASN:CB	1.51	1.40
1:A:854:TYR:CD1	1:A:856:VAL:HG12	1.60	1.37
1:A:75:ASN:ND2	1:A:77:ARG:H	1.19	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:ARG:HG3	2:B:590:ARG:HH11	1.06	1.15
1:A:75:ASN:ND2	1:A:77:ARG:N	1.95	1.14
1:A:530:PRO:HA	1:A:531:GLN:HB3	1.21	1.12
1:A:854:TYR:CE1	1:A:856:VAL:CG1	2.30	1.12
1:A:855:THR:HG23	1:A:861:THR:CB	1.78	1.11
1:A:52:ASP:CB	1:A:53:ASN:HB3	1.82	1.10
1:A:52:ASP:CB	1:A:53:ASN:CB	2.30	1.09
1:A:75:ASN:C	1:A:75:ASN:HD22	1.61	1.07
1:A:553:ARG:HG2	1:A:553:ARG:HH21	0.96	1.04
1:A:805:GLY:HA3	1:A:853:TYR:CE2	1.95	1.02
1:A:75:ASN:ND2	1:A:76:ILE:N	2.09	1.01
1:A:854:TYR:CD1	1:A:856:VAL:CG1	2.40	1.01
1:A:717:GLU:OE2	1:A:829:ASN:N	1.94	1.00
1:A:52:ASP:OD1	1:A:53:ASN:HB2	1.61	1.00
1:A:855:THR:CG2	1:A:861:THR:CB	2.37	0.99
1:A:395:THR:HG23	1:A:445:HIS:HB2	1.46	0.97
1:A:635:THR:HG22	1:A:637:TRP:H	1.27	0.97
1:A:134:ALA:HB2	1:A:441:PHE:HB3	1.45	0.96
1:A:75:ASN:HD22	1:A:76:ILE:N	1.63	0.95
1:A:854:TYR:HE1	1:A:856:VAL:CB	1.81	0.93
1:A:855:THR:HG23	1:A:861:THR:HB	0.96	0.93
1:A:553:ARG:HG2	1:A:553:ARG:NH2	1.76	0.93
1:A:206:SER:HB2	1:A:223:THR:HG23	1.52	0.92
1:A:530:PRO:HA	1:A:531:GLN:CB	2.00	0.91
2:B:384:GLY:HA2	2:B:590:ARG:HH21	1.34	0.91
1:A:103:GLY:HA2	1:A:786:ILE:HG22	1.53	0.91
1:A:294:TYR:OH	1:A:297:PRO:O	1.88	0.91
1:A:585:ALA:HB2	1:A:603:ARG:HG3	1.53	0.91
1:A:778:ILE:HD11	1:A:826:ALA:HB3	1.50	0.91
2:B:590:ARG:HG3	2:B:590:ARG:NH1	1.80	0.90
2:B:379:ALA:HA	2:B:382:MET:HG3	1.54	0.90
1:A:349:LEU:HA	1:A:350:THR:HG22	1.54	0.90
1:A:150:ALA:H	1:A:174:GLN:HG3	1.35	0.89
1:A:638:LEU:HD22	1:A:639:ASP:H	1.36	0.89
1:A:805:GLY:HA3	1:A:853:TYR:HE2	1.37	0.89
1:A:291:THR:O	1:A:294:TYR:N	2.06	0.88
1:A:821:LEU:HD21	1:A:877:TRP:CH2	2.08	0.88
1:A:869:LEU:O	1:A:905:ARG:NH1	2.08	0.87
1:A:754:GLY:O	1:A:797:TYR:HD1	1.58	0.86
1:A:553:ARG:HH21	1:A:553:ARG:CG	1.87	0.86
1:A:52:ASP:HB3	1:A:53:ASN:HB3	0.86	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG22	1:A:861:THR:HB	1.55	0.85
1:A:854:TYR:HE1	1:A:856:VAL:CA	1.89	0.85
1:A:510:LEU:HB3	1:A:575:ARG:HG3	1.59	0.85
1:A:854:TYR:HE1	1:A:856:VAL:CG1	1.84	0.85
1:A:854:TYR:HE1	1:A:856:VAL:HG12	1.35	0.84
1:A:143:ILE:HD13	1:A:143:ILE:H	1.42	0.84
1:A:81:ARG:HD3	1:A:82:TYR:CZ	2.13	0.84
1:A:97:SER:HA	1:A:140:ILE:HG13	1.58	0.84
1:A:516:TYR:HA	1:A:561:ILE:HG13	1.59	0.84
2:B:497:LEU:O	2:B:527:LYS:NZ	2.09	0.84
1:A:52:ASP:CB	1:A:53:ASN:HB2	2.07	0.83
1:A:456:ARG:O	1:A:461:LYS:NZ	2.10	0.83
1:A:896:VAL:HG13	1:A:898:ASN:H	1.44	0.83
1:A:771:LYS:HZ3	1:A:773:ALA:HA	1.44	0.82
2:B:375:GLU:O	2:B:378:ILE:HG12	1.78	0.82
1:A:635:THR:O	1:A:636:ASP:HB3	1.78	0.82
2:B:624:SER:HB3	2:B:629:LEU:HD22	1.62	0.82
1:A:75:ASN:HD21	1:A:77:ARG:H	0.83	0.82
1:A:659:TRP:CZ3	1:A:661:ALA:HB2	2.15	0.82
1:A:638:LEU:HD22	1:A:639:ASP:N	1.94	0.82
1:A:714:ASP:N	1:A:715:GLY:HA2	1.93	0.82
2:B:628:ASP:HB3	2:B:632:ARG:HA	1.62	0.82
1:A:854:TYR:CE1	1:A:856:VAL:CA	2.63	0.81
1:A:240:VAL:C	1:A:241:GLN:HG2	2.06	0.81
1:A:649:ARG:HH21	1:A:652:SER:HB3	1.46	0.80
2:B:615:CYS:SG	2:B:623:ARG:HG3	2.21	0.80
1:A:161:GLU:O	1:A:162:GLN:NE2	2.16	0.79
1:A:75:ASN:HD22	1:A:77:ARG:N	1.77	0.78
1:A:52:ASP:CG	1:A:53:ASN:HB2	2.08	0.78
1:A:754:GLY:O	1:A:755:TRP:HB2	1.82	0.78
1:A:829:ASN:CG	1:A:830:GLY:H	1.90	0.78
1:A:194:THR:OG1	1:A:205:GLN:OE1	2.02	0.78
1:A:364:LEU:O	1:A:367:ASN:ND2	2.15	0.78
1:A:643:ARG:HG2	1:A:643:ARG:HH21	1.48	0.77
1:A:779:GLN:OE1	1:A:780:SER:N	2.18	0.77
1:A:60:LYS:HB2	1:A:153:ILE:O	1.83	0.77
1:A:157:SER:HB3	1:A:647:GLY:HA3	1.66	0.77
1:A:92:GLY:HA2	1:A:882:GLN:NE2	2.00	0.77
1:A:179:ASP:OD1	1:A:212:ARG:NH2	2.15	0.77
1:A:219:LEU:HD11	1:A:221:ILE:HD11	1.66	0.77
1:A:713:LYS:C	1:A:715:GLY:HA2	2.10	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ASN:ND2	1:A:570:THR:HG23	2.00	0.76
1:A:150:ALA:H	1:A:174:GLN:CG	1.98	0.76
1:A:571:ASP:OD1	1:A:573:THR:HG23	1.86	0.76
1:A:838:THR:HG22	1:A:840:ARG:H	1.49	0.76
1:A:64:SER:H	1:A:67:THR:HB	1.50	0.76
1:A:393:TYR:HB2	1:A:445:HIS:CD2	2.21	0.76
1:A:54:GLU:O	1:A:55:VAL:CB	2.34	0.75
1:A:75:ASN:HD21	1:A:77:ARG:N	1.67	0.75
1:A:162:GLN:HG2	1:A:170:SER:OG	1.86	0.75
1:A:174:GLN:N	1:A:174:GLN:OE1	2.20	0.75
1:A:181:VAL:HG12	1:A:189:GLY:N	2.01	0.75
2:B:590:ARG:HH11	2:B:590:ARG:CG	1.95	0.75
1:A:55:VAL:HA	1:A:587:ARG:HH22	1.52	0.75
1:A:602:LEU:HD23	1:A:626:TRP:HB3	1.68	0.75
1:A:778:ILE:H	1:A:778:ILE:CD1	1.99	0.75
1:A:817:GLU:HA	1:A:818:ILE:HB	1.68	0.74
1:A:67:THR:O	1:A:71:GLU:HG3	1.87	0.74
1:A:717:GLU:CD	1:A:829:ASN:H	1.95	0.74
1:A:754:GLY:O	1:A:797:TYR:CD1	2.39	0.74
1:A:105:ASP:OD2	1:A:881:ARG:NH2	2.21	0.74
1:A:502:GLY:HA3	1:A:583:TYR:HE2	1.52	0.74
1:A:802:GLY:O	1:A:803:LYS:CB	2.36	0.74
1:A:896:VAL:O	1:A:897:TYR:HB2	1.87	0.74
1:A:412:TYR:C	1:A:412:TYR:HD2	1.95	0.74
1:A:479:LEU:HD13	1:A:504:ASP:HB3	1.70	0.74
1:A:598:VAL:HG12	1:A:630:ILE:HG22	1.70	0.74
2:B:551:ALA:HA	2:B:554:LEU:HD22	1.68	0.73
1:A:178:ALA:O	1:A:181:VAL:HG22	1.88	0.73
1:A:616:VAL:HA	1:A:667:ALA:HB1	1.68	0.73
1:A:376:TYR:HB3	1:A:392:GLU:HB3	1.70	0.73
1:A:240:VAL:O	1:A:241:GLN:HG2	1.89	0.73
1:A:114:ASP:OD2	1:A:175:THR:OG1	2.04	0.73
1:A:412:TYR:C	1:A:412:TYR:CD2	2.67	0.72
1:A:659:TRP:HZ3	1:A:661:ALA:HB2	1.54	0.72
1:A:268:SER:OG	1:A:269:TYR:N	2.19	0.72
1:A:53:ASN:OD1	1:A:53:ASN:C	2.33	0.72
1:A:81:ARG:HD3	1:A:82:TYR:CE2	2.25	0.72
1:A:771:LYS:HE2	1:A:775:ARG:O	1.89	0.72
1:A:187:GLN:HG3	1:A:187:GLN:O	1.87	0.72
1:A:233:HIS:CD2	1:A:235:ASP:HB2	2.24	0.72
1:A:771:LYS:NZ	1:A:773:ALA:HA	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PRO:CA	1:A:531:GLN:HB3	2.13	0.71
1:A:141:ASN:OD1	1:A:435:VAL:HG13	1.89	0.71
1:A:805:GLY:CA	1:A:853:TYR:CE2	2.73	0.71
1:A:55:VAL:HA	1:A:587:ARG:NH2	2.05	0.71
2:B:663:ARG:HA	2:B:664:LYS:C	2.16	0.71
1:A:75:ASN:ND2	1:A:75:ASN:C	2.30	0.71
1:A:807:ASN:OD1	1:A:808:GLY:N	2.23	0.71
2:B:629:LEU:C	2:B:631:PHE:H	1.99	0.70
2:B:547:PRO:HA	2:B:552:LYS:HE2	1.73	0.70
1:A:778:ILE:H	1:A:778:ILE:HD13	1.56	0.70
1:A:314:PHE:HE1	1:A:316:PRO:HG3	1.57	0.70
1:A:673:GLU:HG2	1:A:703:LEU:HA	1.72	0.70
1:A:421:THR:HG22	1:A:422:TRP:H	1.56	0.70
1:A:575:ARG:HB3	1:A:657:TYR:CE2	2.27	0.70
1:A:845:TRP:HB2	1:A:872:TYR:HE2	1.56	0.70
1:A:754:GLY:O	1:A:755:TRP:CB	2.39	0.69
1:A:143:ILE:HD13	1:A:143:ILE:N	2.07	0.69
1:A:318:PHE:HD2	1:A:318:PHE:N	1.90	0.69
1:A:314:PHE:CE1	1:A:316:PRO:HG3	2.28	0.69
1:A:105:ASP:O	1:A:108:ARG:HB2	1.93	0.69
1:A:613:ASP:OD1	1:A:614:GLY:N	2.26	0.69
1:A:755:TRP:HB2	1:A:797:TYR:HD1	1.56	0.69
1:A:318:PHE:N	1:A:318:PHE:CD2	2.60	0.69
1:A:149:LYS:N	1:A:174:GLN:HE21	1.91	0.68
1:A:325:HIS:CD2	1:A:414:TYR:HD1	2.10	0.68
1:A:402:THR:HG23	1:A:438:ASP:HB3	1.75	0.68
1:A:484:PHE:HB2	1:A:499:VAL:HG13	1.74	0.68
1:A:854:TYR:CE1	1:A:856:VAL:HA	2.28	0.68
1:A:291:THR:O	1:A:293:ASP:N	2.26	0.68
2:B:568:ARG:O	2:B:569:LYS:HD2	1.93	0.67
2:B:671:LEU:O	2:B:675:THR:HG23	1.94	0.67
1:A:261:LYS:HG2	1:A:548:TRP:CZ2	2.29	0.67
1:A:818:ILE:HB	1:A:841:ARG:HD3	1.75	0.67
1:A:86:ILE:HD11	1:A:155:LYS:HE2	1.77	0.67
1:A:143:ILE:HG12	1:A:145:TYR:HE1	1.60	0.67
1:A:635:THR:HG22	1:A:637:TRP:N	2.07	0.67
2:B:407:VAL:O	2:B:641:LEU:HD11	1.95	0.67
1:A:149:LYS:H	1:A:174:GLN:HG2	1.59	0.67
1:A:817:GLU:HA	1:A:818:ILE:CB	2.25	0.66
2:B:542:THR:HG22	2:B:554:LEU:HB3	1.75	0.66
1:A:129:GLY:HA2	2:B:636:VAL:CG1	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:LYS:O	1:A:841:ARG:HD2	1.96	0.65
1:A:119:ILE:O	1:A:140:ILE:HG23	1.96	0.65
1:A:89:VAL:CG2	1:A:881:ARG:HH21	2.09	0.65
1:A:756:TYR:O	1:A:795:LEU:HD12	1.96	0.65
1:A:801:GLU:O	1:A:802:GLY:C	2.39	0.65
2:B:462:ILE:O	2:B:466:LEU:HD13	1.97	0.65
2:B:524:LEU:HB2	2:B:531:ALA:HB2	1.77	0.65
1:A:801:GLU:O	1:A:803:LYS:N	2.30	0.65
1:A:827:LEU:HD13	2:B:360:VAL:HG12	1.78	0.65
1:A:799:GLN:O	1:A:802:GLY:N	2.30	0.65
1:A:52:ASP:HB3	1:A:53:ASN:HB2	1.61	0.65
2:B:655:TYR:CE2	2:B:659:VAL:HG11	2.31	0.65
2:B:663:ARG:HA	2:B:665:CYS:N	2.11	0.65
1:A:89:VAL:HG12	1:A:89:VAL:O	1.97	0.64
1:A:854:TYR:HD1	1:A:856:VAL:CG1	2.02	0.64
1:A:433:GLN:HG2	1:A:434:GLY:N	2.12	0.64
1:A:459:ALA:HB1	1:A:553:ARG:HD3	1.80	0.64
1:A:614:GLY:O	1:A:667:ALA:HB2	1.96	0.64
2:B:656:VAL:O	2:B:657:LYS:HB3	1.97	0.64
1:A:92:GLY:HA2	1:A:882:GLN:HE21	1.61	0.64
1:A:349:LEU:HD13	1:A:354:PHE:HE1	1.62	0.64
1:A:446:CYS:HB3	1:A:464:SER:HB3	1.78	0.64
1:A:688:PHE:N	1:A:688:PHE:CD2	2.63	0.64
1:A:810:LEU:HD23	1:A:810:LEU:O	1.97	0.64
1:A:273:LYS:HD2	1:A:273:LYS:O	1.97	0.64
1:A:502:GLY:HA3	1:A:583:TYR:CE2	2.33	0.64
1:A:608:SER:HA	1:A:619:GLY:HA2	1.80	0.64
1:A:821:LEU:CD2	1:A:877:TRP:CH2	2.80	0.63
1:A:104:MET:HE3	1:A:108:ARG:HG2	1.79	0.63
1:A:89:VAL:O	1:A:89:VAL:CG1	2.46	0.63
1:A:130:GLY:HA3	1:A:131:THR:HB	1.80	0.63
1:A:688:PHE:O	1:A:743:ASP:N	2.31	0.63
1:A:817:GLU:CB	1:A:818:ILE:HG22	2.29	0.63
2:B:546:ASN:O	2:B:552:LYS:CG	2.47	0.63
1:A:799:GLN:O	1:A:800:PRO:C	2.42	0.63
1:A:643:ARG:HG2	1:A:643:ARG:NH2	2.14	0.63
1:A:269:TYR:OH	1:A:546:PRO:O	2.11	0.62
1:A:742:ILE:HD11	1:A:744:TRP:NE1	2.14	0.62
1:A:190:ILE:HG12	1:A:209:LEU:HB3	1.81	0.62
1:A:350:THR:HG23	1:A:353:VAL:HB	1.81	0.62
1:A:688:PHE:HD2	1:A:689:GLY:H	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG22	1:A:173:PHE:HB2	1.81	0.62
1:A:825:ARG:HH21	1:A:825:ARG:HG2	1.64	0.62
1:A:314:PHE:HD1	1:A:316:PRO:HD3	1.65	0.62
2:B:544:GLY:O	2:B:552:LYS:NZ	2.32	0.62
1:A:461:LYS:O	1:A:464:SER:OG	2.16	0.62
1:A:182:ILE:HG13	1:A:183:GLY:C	2.25	0.62
1:A:778:ILE:CD1	1:A:826:ALA:HB3	2.27	0.62
2:B:453:ALA:HB2	2:B:515:TYR:HE1	1.63	0.62
2:B:608:PHE:CD1	2:B:619:PHE:HD2	2.18	0.62
1:A:842:THR:HB	1:A:877:TRP:HB2	1.82	0.62
2:B:357:GLU:O	2:B:361:ASN:ND2	2.29	0.61
1:A:622:ARG:HD2	1:A:622:ARG:N	2.16	0.61
1:A:441:PHE:C	1:A:441:PHE:CD2	2.78	0.61
1:A:160:VAL:O	1:A:603:ARG:NH2	2.32	0.61
1:A:242:SER:O	1:A:287:GLN:O	2.17	0.61
1:A:817:GLU:HB3	1:A:818:ILE:HG22	1.80	0.61
1:A:854:TYR:CE1	1:A:856:VAL:N	2.69	0.61
1:A:358:LYS:CB	2:B:545:LYS:HE2	2.31	0.61
1:A:603:ARG:HD3	1:A:605:ASP:OD2	2.01	0.61
1:A:878:GLU:H	1:A:879:ASN:C	2.08	0.61
1:A:341:ARG:NH1	1:A:451:SER:HB2	2.15	0.61
2:B:551:ALA:O	2:B:552:LYS:HB2	1.98	0.61
2:B:611:ASN:HA	2:B:612:VAL:C	2.25	0.61
1:A:215:GLY:HA2	1:A:319:ARG:HB3	1.83	0.61
1:A:691:LEU:HD13	1:A:740:GLY:HA3	1.82	0.61
1:A:818:ILE:CG1	1:A:841:ARG:HD3	2.31	0.61
1:A:342:ASP:OD2	1:A:344:THR:N	2.34	0.60
2:B:358:TRP:HE1	2:B:604:GLN:HG3	1.65	0.60
2:B:466:LEU:HD11	2:B:658:ALA:HB1	1.83	0.60
1:A:613:ASP:CG	1:A:614:GLY:H	2.09	0.60
2:B:498:CYS:HB3	2:B:512:GLU:OE2	2.01	0.60
1:A:755:TRP:O	1:A:756:TYR:HB3	2.01	0.60
1:A:160:VAL:HG23	1:A:161:GLU:H	1.64	0.60
1:A:167:LEU:HG	1:A:675:SER:HB3	1.83	0.60
2:B:343:LYS:HA	2:B:367:GLU:O	2.01	0.60
1:A:508:SER:CB	1:A:653:PHE:HD2	2.14	0.60
1:A:635:THR:CG2	1:A:637:TRP:H	2.10	0.60
1:A:818:ILE:CB	1:A:841:ARG:HD3	2.32	0.60
1:A:892:LYS:HB2	1:A:893:ASN:HA	1.82	0.60
1:A:119:ILE:HB	1:A:435:VAL:HG11	1.83	0.60
2:B:583:PRO:HG3	2:B:651:LEU:HD23	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:TYR:CB	1:A:392:GLU:HB3	2.31	0.60
1:A:407:ARG:HG3	1:A:407:ARG:O	2.02	0.60
1:A:567:ASN:O	1:A:662:GLY:HA2	2.02	0.59
1:A:578:ASN:OD1	1:A:579:GLY:N	2.34	0.59
1:A:673:GLU:HG3	1:A:704:ILE:HG13	1.84	0.59
1:A:815:ALA:HA	1:A:843:ARG:CA	2.33	0.59
1:A:829:ASN:CG	1:A:830:GLY:N	2.57	0.59
2:B:384:GLY:HA2	2:B:590:ARG:NH2	2.13	0.59
1:A:243:PHE:CD2	1:A:243:PHE:O	2.56	0.59
1:A:604:TYR:HD1	1:A:624:LEU:HD12	1.66	0.59
1:A:818:ILE:HG12	1:A:841:ARG:HD3	1.85	0.59
2:B:614:ASP:O	2:B:618:ASN:HB2	2.03	0.59
1:A:56:THR:OG1	1:A:57:GLY:N	2.31	0.59
1:A:148:VAL:HB	1:A:174:GLN:NE2	2.18	0.59
1:A:233:HIS:CD2	1:A:873:ARG:HB2	2.38	0.59
1:A:228:GLY:O	1:A:231:ARG:NH1	2.36	0.59
2:B:399:ALA:HB1	2:B:404:LEU:HD12	1.85	0.59
1:A:670:ILE:HG21	1:A:726:LEU:HA	1.85	0.58
1:A:684:PHE:O	1:A:690:ASN:HA	2.02	0.58
1:A:717:GLU:HB2	1:A:828:LEU:HD22	1.83	0.58
1:A:778:ILE:HD13	1:A:778:ILE:N	2.18	0.58
1:A:875:VAL:HG22	1:A:901:ALA:HA	1.84	0.58
1:A:80:THR:HG21	1:A:86:ILE:HG21	1.84	0.58
1:A:319:ARG:NH1	1:A:326:TYR:HB2	2.18	0.58
1:A:97:SER:CA	1:A:140:ILE:HG13	2.32	0.58
1:A:262:GLU:H	1:A:262:GLU:CD	2.11	0.58
2:B:386:ALA:O	2:B:590:ARG:NH2	2.35	0.58
1:A:187:GLN:OE1	1:A:212:ARG:O	2.21	0.58
2:B:546:ASN:O	2:B:552:LYS:HG3	2.03	0.58
1:A:91:GLN:HG2	1:A:95:ALA:O	2.03	0.58
2:B:389:MET:HE2	2:B:391:LEU:HD23	1.86	0.58
2:B:412:TYR:CE1	2:B:632:ARG:HD3	2.39	0.58
2:B:505:LEU:HD23	2:B:506:CYS:HB2	1.86	0.57
1:A:302:ALA:O	1:A:303:ASP:HB2	2.03	0.57
1:A:755:TRP:HB2	1:A:797:TYR:CD1	2.38	0.57
1:A:742:ILE:C	1:A:742:ILE:HD12	2.29	0.57
1:A:127:ALA:HB2	1:A:569:TYR:CG	2.40	0.57
2:B:655:TYR:O	2:B:659:VAL:HG12	2.05	0.57
1:A:260:VAL:HG22	1:A:263:GLU:HG3	1.87	0.57
1:A:349:LEU:HA	1:A:350:THR:CG2	2.31	0.57
1:A:742:ILE:HD12	1:A:742:ILE:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:PHE:N	1:A:860:PHE:CD2	2.73	0.57
2:B:468:TYR:O	2:B:472:ASN:N	2.33	0.57
1:A:731:ALA:HB2	1:A:769:ILE:HG22	1.87	0.57
1:A:743:ASP:O	1:A:744:TRP:C	2.48	0.57
1:A:174:GLN:N	1:A:174:GLN:CD	2.62	0.57
1:A:866:VAL:HG22	1:A:907:TYR:CD1	2.39	0.57
1:A:114:ASP:OD2	1:A:407:ARG:NH2	2.38	0.56
1:A:142:GLU:HB2	1:A:336:GLN:HE22	1.70	0.56
1:A:296:GLY:HA3	1:A:344:THR:HA	1.86	0.56
1:A:854:TYR:CD1	1:A:856:VAL:N	2.73	0.56
1:A:896:VAL:CG1	1:A:897:TYR:N	2.68	0.56
1:A:95:ALA:HB2	1:A:338:PHE:CE1	2.40	0.56
1:A:510:LEU:HB3	1:A:575:ARG:CG	2.35	0.56
1:A:696:PHE:CZ	1:A:735:GLY:HA3	2.40	0.56
1:A:860:PHE:H	1:A:860:PHE:HD2	1.53	0.56
1:A:896:VAL:HG12	1:A:897:TYR:N	2.19	0.56
1:A:89:VAL:HG22	1:A:881:ARG:HH21	1.69	0.56
2:B:387:ASP:O	2:B:388:ALA:HB2	2.04	0.56
1:A:74:LEU:O	1:A:225:ARG:NH1	2.38	0.56
1:A:162:GLN:CG	1:A:170:SER:OG	2.54	0.56
1:A:299:ARG:NE	1:A:343:MET:HB2	2.20	0.56
1:A:240:VAL:O	1:A:241:GLN:CG	2.53	0.56
1:A:243:PHE:O	1:A:243:PHE:CG	2.58	0.56
2:B:489:LYS:O	2:B:492:SER:HB3	2.05	0.56
1:A:319:ARG:HD3	1:A:325:HIS:O	2.06	0.56
1:A:358:LYS:HB2	2:B:545:LYS:HE2	1.87	0.56
1:A:810:LEU:HD23	1:A:810:LEU:C	2.31	0.56
1:A:634:PRO:HG2	1:A:638:LEU:CD1	2.36	0.55
1:A:445:HIS:CD2	1:A:445:HIS:O	2.60	0.55
1:A:613:ASP:CG	1:A:614:GLY:N	2.64	0.55
1:A:809:MET:O	1:A:848:VAL:HA	2.07	0.55
1:A:878:GLU:N	1:A:879:ASN:O	2.29	0.55
1:A:150:ALA:N	1:A:174:GLN:NE2	2.54	0.55
1:A:221:ILE:HD13	1:A:313:LEU:HD23	1.89	0.55
1:A:668:VAL:HG13	1:A:668:VAL:O	2.07	0.55
1:A:815:ALA:HA	1:A:843:ARG:C	2.31	0.55
1:A:259:ILE:HG22	1:A:548:TRP:HZ3	1.71	0.55
2:B:546:ASN:O	2:B:552:LYS:HG2	2.07	0.55
1:A:757:SER:HB2	1:A:794:GLY:O	2.06	0.55
2:B:354:LYS:HD3	2:B:629:LEU:HB3	1.88	0.55
1:A:273:LYS:HE2	1:A:543:GLU:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ASN:HD21	1:A:732:ARG:HE	1.53	0.55
2:B:383:ASN:OD1	2:B:385:GLU:HG3	2.06	0.55
1:A:134:ALA:CB	1:A:441:PHE:HB3	2.30	0.54
2:B:663:ARG:CB	2:B:666:SER:HB2	2.37	0.54
1:A:209:LEU:N	1:A:209:LEU:HD23	2.23	0.54
1:A:825:ARG:HG2	1:A:825:ARG:NH2	2.21	0.54
2:B:538:VAL:HB	2:B:539:PRO:HD3	1.89	0.54
1:A:233:HIS:CD2	1:A:235:ASP:H	2.24	0.54
2:B:466:LEU:CD1	2:B:658:ALA:HB1	2.37	0.54
2:B:517:TYR:CD2	2:B:534:LYS:HG2	2.41	0.54
1:A:317:GLY:C	1:A:318:PHE:HD2	2.15	0.54
1:A:575:ARG:HB3	1:A:657:TYR:HE2	1.73	0.54
1:A:708:TYR:HE1	1:A:722:ASP:C	2.15	0.54
1:A:877:TRP:O	1:A:877:TRP:CD1	2.61	0.54
1:A:215:GLY:CA	1:A:319:ARG:HB3	2.38	0.54
1:A:238:ARG:O	1:A:240:VAL:CG2	2.54	0.54
1:A:508:SER:CB	1:A:653:PHE:CD2	2.90	0.54
2:B:660:GLY:HA2	2:B:663:ARG:O	2.07	0.54
1:A:77:ARG:NH2	1:A:90:GLU:OE2	2.36	0.54
1:A:294:TYR:CG	1:A:295:THR:N	2.75	0.54
1:A:784:ASP:OD1	1:A:881:ARG:NH1	2.40	0.54
2:B:605:GLN:O	2:B:609:GLY:HA3	2.08	0.54
1:A:65:SER:N	1:A:149:LYS:O	2.41	0.54
1:A:688:PHE:O	1:A:743:ASP:HB2	2.07	0.54
1:A:779:GLN:HA	1:A:825:ARG:HA	1.89	0.54
1:A:106:LYS:HE2	1:A:888:VAL:HG12	1.89	0.53
1:A:816:LYS:HG3	1:A:817:GLU:N	2.22	0.53
1:A:313:LEU:HD11	1:A:330:ILE:HD11	1.91	0.53
1:A:148:VAL:HG11	1:A:173:PHE:HD1	1.74	0.53
1:A:273:LYS:HD3	1:A:546:PRO:CD	2.38	0.53
1:A:421:THR:HG22	1:A:422:TRP:N	2.23	0.53
1:A:598:VAL:CG1	1:A:630:ILE:HG22	2.38	0.53
1:A:649:ARG:NH2	1:A:655:GLU:OE1	2.41	0.53
1:A:247:VAL:HG12	1:A:376:TYR:OH	2.08	0.53
1:A:308:GLU:OE2	1:A:310:ARG:NH2	2.42	0.53
1:A:688:PHE:N	1:A:688:PHE:HD2	2.06	0.53
2:B:570:PRO:HD2	2:B:573:GLU:HG3	1.90	0.53
1:A:63:LYS:NZ	1:A:79:LEU:HD22	2.24	0.53
1:A:518:GLN:HG2	1:A:558:THR:HB	1.91	0.53
1:A:744:TRP:CD1	1:A:756:TYR:HA	2.44	0.53
1:A:815:ALA:HA	1:A:843:ARG:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:HB3	1:A:230:ILE:HG12	1.90	0.53
1:A:566:ASN:HD22	1:A:570:THR:HG23	1.74	0.53
1:A:566:ASN:HD21	1:A:570:THR:HG23	1.73	0.53
1:A:472:ILE:O	1:A:510:LEU:HD23	2.09	0.53
1:A:632:LEU:O	1:A:639:ASP:HB2	2.09	0.53
1:A:70:LYS:HA	1:A:863:ARG:CZ	2.39	0.52
1:A:860:PHE:N	1:A:860:PHE:HD2	2.08	0.52
2:B:453:ALA:HB2	2:B:515:TYR:CE1	2.43	0.52
1:A:821:LEU:CD2	1:A:877:TRP:HH2	2.21	0.52
2:B:358:TRP:CZ2	2:B:366:ILE:HD12	2.43	0.52
2:B:518:THR:HG23	2:B:541:ASN:OD1	2.09	0.52
1:A:528:THR:HG23	1:A:539:PRO:HD3	1.91	0.52
1:A:88:VAL:O	1:A:98:GLY:O	2.26	0.52
1:A:317:GLY:C	1:A:318:PHE:CD2	2.87	0.52
1:A:638:LEU:O	1:A:639:ASP:HB3	2.10	0.52
1:A:273:LYS:HZ2	1:A:274:ALA:HA	1.75	0.52
1:A:508:SER:HB3	1:A:653:PHE:CD2	2.45	0.52
1:A:772:ARG:C	1:A:774:ASP:H	2.18	0.52
1:A:131:THR:CG2	1:A:133:THR:HG23	2.40	0.52
2:B:522:ARG:O	2:B:525:VAL:HG13	2.10	0.52
1:A:305:LEU:HD13	1:A:340:THR:HG22	1.90	0.52
1:A:395:THR:HG23	1:A:445:HIS:CB	2.29	0.52
2:B:447:LYS:N	2:B:447:LYS:HD2	2.25	0.52
2:B:451:HIS:HE1	2:B:464:MET:HE3	1.74	0.52
1:A:857:LYS:O	1:A:859:HIS:N	2.43	0.52
1:A:81:ARG:CD	1:A:82:TYR:CE2	2.92	0.51
1:A:616:VAL:HG12	1:A:616:VAL:O	2.09	0.51
1:A:771:LYS:HG2	1:A:773:ALA:H	1.74	0.51
2:B:374:THR:O	2:B:378:ILE:HG23	2.10	0.51
2:B:444:LEU:O	2:B:447:LYS:HB2	2.10	0.51
1:A:131:THR:HG23	1:A:133:THR:HG23	1.91	0.51
1:A:350:THR:CG2	1:A:353:VAL:HB	2.40	0.51
1:A:671:ASP:O	1:A:727:ASN:ND2	2.39	0.51
2:B:374:THR:O	2:B:377:CYS:HB3	2.10	0.51
1:A:178:ALA:C	1:A:180:ASP:H	2.19	0.51
1:A:872:TYR:O	1:A:874:TYR:HD2	1.92	0.51
1:A:66:ASP:OD1	1:A:66:ASP:N	2.42	0.51
1:A:246:LEU:HD13	1:A:351:LYS:HB2	1.93	0.51
1:A:294:TYR:CD1	1:A:295:THR:N	2.79	0.51
2:B:521:PHE:O	2:B:525:VAL:HG12	2.10	0.51
1:A:159:SER:HB2	1:A:647:GLY:HA2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG21	1:A:330:ILE:HD11	1.93	0.51
1:A:440:HIS:HB2	1:A:470:ARG:NH1	2.25	0.51
1:A:536:LYS:HE2	2:B:567:THR:CG2	2.41	0.51
1:A:797:TYR:HE2	1:A:804:TRP:CZ2	2.29	0.51
1:A:845:TRP:HZ3	1:A:847:ILE:HG12	1.75	0.51
1:A:877:TRP:O	1:A:878:GLU:CD	2.54	0.51
1:A:854:TYR:HD1	1:A:856:VAL:HG13	1.76	0.51
1:A:878:GLU:CB	1:A:879:ASN:HB2	2.40	0.51
1:A:446:CYS:SG	1:A:455:CYS:C	2.94	0.51
2:B:391:LEU:HD11	2:B:588:VAL:HG21	1.93	0.51
1:A:520:ALA:HA	1:A:555:ASN:O	2.11	0.51
1:A:894:VAL:HG11	1:A:900:TYR:CE2	2.46	0.51
1:A:181:VAL:HG12	1:A:188:TRP:C	2.35	0.50
1:A:602:LEU:CD2	1:A:626:TRP:HB3	2.40	0.50
1:A:686:GLY:HA3	1:A:688:PHE:HE2	1.74	0.50
1:A:814:LYS:HA	1:A:844:PRO:HB3	1.93	0.50
2:B:655:TYR:O	2:B:658:ALA:HB3	2.11	0.50
1:A:129:GLY:HA2	2:B:636:VAL:HG12	1.93	0.50
1:A:289:VAL:HG23	1:A:289:VAL:O	2.10	0.50
1:A:706:ARG:HB2	1:A:725:TYR:CE1	2.47	0.50
1:A:884:ALA:HA	1:A:890:GLN:NE2	2.27	0.50
1:A:89:VAL:O	1:A:96:SER:O	2.29	0.50
1:A:143:ILE:HG12	1:A:145:TYR:CE1	2.42	0.50
1:A:350:THR:HG23	1:A:350:THR:O	2.12	0.50
1:A:781:HIS:O	1:A:782:LEU:HB2	2.10	0.50
1:A:70:LYS:HA	1:A:863:ARG:NH1	2.27	0.50
1:A:502:GLY:CA	1:A:583:TYR:CE2	2.95	0.50
1:A:818:ILE:HD12	1:A:818:ILE:O	2.11	0.50
1:A:51:ARG:O	1:A:52:ASP:O	2.30	0.50
1:A:817:GLU:HA	1:A:818:ILE:CG2	2.41	0.50
2:B:441:TRP:HA	2:B:444:LEU:CD2	2.42	0.50
1:A:174:GLN:CD	1:A:174:GLN:H	2.20	0.50
1:A:470:ARG:HB3	1:A:513:GLN:O	2.12	0.50
2:B:381:ILE:O	2:B:590:ARG:CZ	2.60	0.50
2:B:522:ARG:O	2:B:526:GLU:HG3	2.11	0.50
1:A:370:TYR:HB2	1:A:374:HIS:O	2.11	0.50
2:B:590:ARG:HB2	2:B:593:LYS:HZ3	1.77	0.50
2:B:629:LEU:C	2:B:631:PHE:N	2.67	0.50
1:A:518:GLN:CG	1:A:558:THR:HB	2.40	0.50
1:A:524:TYR:C	1:A:524:TYR:CD2	2.90	0.50
2:B:462:ILE:HD11	2:B:655:TYR:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:504:ASN:HB2	2:B:511:LYS:CB	2.42	0.50
1:A:815:ALA:H	1:A:844:PRO:CA	2.25	0.50
1:A:53:ASN:OD1	1:A:53:ASN:O	2.30	0.49
2:B:462:ILE:N	2:B:463:PRO:HD2	2.27	0.49
1:A:130:GLY:HA3	1:A:131:THR:CB	2.36	0.49
1:A:150:ALA:C	1:A:174:GLN:CD	2.79	0.49
1:A:812:TYR:HE1	1:A:814:LYS:HE2	1.77	0.49
2:B:441:TRP:O	2:B:444:LEU:HD22	2.12	0.49
1:A:277:LYS:HD2	1:A:370:TYR:CE1	2.48	0.49
2:B:382:MET:CE	2:B:402:CYS:HB3	2.43	0.49
1:A:122:TYR:C	1:A:122:TYR:CD2	2.91	0.49
2:B:505:LEU:HD23	2:B:505:LEU:C	2.37	0.49
1:A:634:PRO:HG2	1:A:638:LEU:HD12	1.94	0.49
2:B:378:ILE:HG22	2:B:389:MET:SD	2.52	0.49
1:A:587:ARG:HG2	1:A:600:ALA:O	2.13	0.49
1:A:670:ILE:HD13	1:A:725:TYR:O	2.13	0.49
1:A:247:VAL:HG22	1:A:283:LYS:O	2.13	0.49
2:B:547:PRO:HA	2:B:552:LYS:CE	2.40	0.49
1:A:102:ARG:O	1:A:733:ILE:HD13	2.13	0.49
1:A:547:TYR:CE1	2:B:570:PRO:HG3	2.47	0.49
1:A:408:TYR:CE2	1:A:432:ARG:HD3	2.47	0.49
1:A:497:LEU:C	1:A:497:LEU:HD23	2.38	0.49
1:A:104:MET:HB2	1:A:168:ALA:HB2	1.95	0.49
1:A:880:VAL:HG13	1:A:897:TYR:HE1	1.77	0.49
2:B:425:GLY:HA2	2:B:584:ASN:OD1	2.13	0.49
1:A:311:SER:HB2	1:A:334:THR:HG23	1.95	0.48
1:A:756:TYR:CD1	1:A:757:SER:N	2.81	0.48
1:A:55:VAL:O	1:A:56:THR:O	2.30	0.48
1:A:259:ILE:CD1	1:A:276:PRO:HA	2.43	0.48
1:A:603:ARG:HG2	1:A:604:TYR:N	2.28	0.48
1:A:688:PHE:CD2	1:A:689:GLY:N	2.80	0.48
1:A:161:GLU:O	1:A:161:GLU:HG3	2.13	0.48
1:A:855:THR:HG22	1:A:861:THR:CB	2.28	0.48
1:A:93:ARG:NH1	1:A:889:ASN:ND2	2.62	0.48
1:A:317:GLY:HA3	1:A:326:TYR:OH	2.14	0.48
2:B:656:VAL:C	2:B:658:ALA:H	2.20	0.48
1:A:91:GLN:HB3	1:A:97:SER:HB2	1.96	0.48
1:A:291:THR:O	1:A:292:ARG:C	2.57	0.48
1:A:659:TRP:CZ3	1:A:723:PRO:HG2	2.49	0.48
1:A:756:TYR:CD1	1:A:756:TYR:C	2.92	0.48
1:A:879:ASN:O	1:A:880:VAL:HB	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG23	1:A:73:VAL:O	2.14	0.48
1:A:181:VAL:HG11	1:A:188:TRP:HA	1.96	0.48
2:B:457:THR:O	2:B:462:ILE:HG12	2.14	0.48
1:A:678:LYS:C	1:A:678:LYS:HD2	2.39	0.48
2:B:446:GLY:O	2:B:481:SER:OG	2.20	0.48
1:A:407:ARG:HB2	1:A:433:GLN:HB2	1.96	0.47
1:A:496:ASN:HB2	1:A:589:ASN:OD1	2.13	0.47
1:A:540:ASN:O	2:B:434:LYS:NZ	2.44	0.47
1:A:52:ASP:CA	1:A:53:ASN:CB	2.91	0.47
1:A:182:ILE:HG13	1:A:183:GLY:CA	2.44	0.47
1:A:240:VAL:C	1:A:241:GLN:CG	2.83	0.47
1:A:242:SER:O	1:A:243:PHE:CD1	2.67	0.47
1:A:800:PRO:O	1:A:801:GLU:CB	2.62	0.47
1:A:704:ILE:HA	1:A:726:LEU:O	2.14	0.47
2:B:560:GLU:CD	2:B:568:ARG:HD2	2.39	0.47
1:A:259:ILE:HD11	1:A:276:PRO:HA	1.96	0.47
1:A:759:PHE:CD2	1:A:759:PHE:C	2.92	0.47
1:A:160:VAL:HG11	1:A:626:TRP:C	2.39	0.47
1:A:256:ALA:HB1	1:A:279:ASP:HB2	1.95	0.47
1:A:317:GLY:HA3	1:A:326:TYR:CE1	2.48	0.47
1:A:418:ASP:OD1	1:A:419:LYS:N	2.39	0.47
1:A:468:SER:O	1:A:515:TYR:HA	2.14	0.47
1:A:786:ILE:O	1:A:786:ILE:HG13	2.14	0.47
2:B:417:ASN:O	2:B:421:THR:HG23	2.14	0.47
1:A:137:SER:C	1:A:139:ALA:H	2.23	0.47
1:A:246:LEU:HA	1:A:284:ASP:HA	1.96	0.47
1:A:299:ARG:CD	1:A:343:MET:HB2	2.45	0.47
1:A:713:LYS:C	1:A:715:GLY:CA	2.85	0.47
1:A:325:HIS:CD2	1:A:414:TYR:CD1	2.97	0.47
2:B:340:LYS:CB	2:B:341:PRO:HD2	2.44	0.47
1:A:144:GLU:OE1	1:A:225:ARG:NH2	2.43	0.47
1:A:854:TYR:HD1	1:A:856:VAL:H	1.62	0.47
1:A:224:GLY:HA2	1:A:309:SER:O	2.15	0.47
1:A:433:GLN:CG	1:A:434:GLY:N	2.78	0.47
1:A:649:ARG:NH1	1:A:673:GLU:OE1	2.40	0.47
2:B:382:MET:HE2	2:B:382:MET:HB3	1.87	0.47
1:A:799:GLN:O	1:A:801:GLU:N	2.47	0.46
2:B:394:GLY:O	2:B:397:TYR:HB3	2.14	0.46
2:B:441:TRP:HA	2:B:444:LEU:HD22	1.95	0.46
2:B:653:GLU:O	2:B:656:VAL:O	2.32	0.46
1:A:229:GLU:H	1:A:305:LEU:HD23	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:OD1	1:A:416:ASN:C	2.57	0.46
1:A:640:LEU:HD22	1:A:682:ILE:HG22	1.97	0.46
1:A:63:LYS:HB2	1:A:151:VAL:HG13	1.96	0.46
1:A:97:SER:HA	1:A:140:ILE:H	1.80	0.46
1:A:97:SER:C	1:A:140:ILE:HG13	2.41	0.46
1:A:292:ARG:HA	1:A:301:LEU:HD23	1.97	0.46
1:A:436:GLY:O	1:A:437:LEU:HD23	2.15	0.46
1:A:582:TYR:CD1	1:A:582:TYR:C	2.93	0.46
1:A:636:ASP:O	1:A:637:TRP:CB	2.63	0.46
1:A:854:TYR:HE1	1:A:856:VAL:HA	1.65	0.46
1:A:884:ALA:H	1:A:890:GLN:HG3	1.80	0.46
1:A:280:VAL:HG21	1:A:375:LYS:HB3	1.96	0.46
1:A:416:ASN:OD1	1:A:417:ALA:N	2.48	0.46
1:A:606:TYR:CD2	1:A:606:TYR:C	2.92	0.46
1:A:709:GLU:HB2	1:A:720:LYS:O	2.14	0.46
2:B:451:HIS:CE1	2:B:464:MET:HE3	2.50	0.46
1:A:183:GLY:HA2	1:A:184:GLU:O	2.15	0.46
1:A:670:ILE:CG2	1:A:726:LEU:HA	2.46	0.46
1:A:686:GLY:HA3	1:A:688:PHE:CE2	2.50	0.46
1:A:899:ARG:HD2	1:A:900:TYR:CZ	2.50	0.46
1:A:412:TYR:HD2	1:A:413:VAL:N	2.13	0.46
1:A:428:LEU:C	1:A:428:LEU:HD12	2.41	0.46
1:A:445:HIS:O	1:A:445:HIS:HD2	1.98	0.46
1:A:698:ASN:HB2	1:A:733:ILE:HG12	1.98	0.46
1:A:742:ILE:HD11	1:A:757:SER:OG	2.15	0.46
1:A:842:THR:CB	1:A:877:TRP:HB2	2.45	0.46
1:A:855:THR:HA	1:A:861:THR:HA	1.97	0.46
1:A:150:ALA:N	1:A:174:GLN:CG	2.72	0.46
1:A:712:ILE:HG23	1:A:715:GLY:O	2.15	0.46
1:A:838:THR:CG2	1:A:839:ALA:N	2.78	0.46
2:B:483:GLY:HA2	2:B:497:LEU:HD12	1.98	0.46
1:A:122:TYR:C	1:A:122:TYR:HD2	2.24	0.46
1:A:181:VAL:CG1	1:A:188:TRP:HA	2.45	0.46
1:A:182:ILE:HG13	1:A:183:GLY:HA3	1.98	0.46
1:A:342:ASP:OD2	1:A:342:ASP:C	2.58	0.46
1:A:354:PHE:CE1	1:A:381:THR:HB	2.51	0.46
1:A:430:TYR:HA	1:A:479:LEU:O	2.16	0.46
1:A:731:ALA:CB	1:A:769:ILE:HG22	2.46	0.46
2:B:602:ARG:O	2:B:605:GLN:HG2	2.16	0.46
1:A:175:THR:HG21	1:A:330:ILE:CD1	2.46	0.46
1:A:821:LEU:HD21	1:A:877:TRP:CZ2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:O	1:A:856:VAL:C	2.59	0.46
2:B:343:LYS:HB3	2:B:369:VAL:HG22	1.98	0.46
2:B:376:ASP:OD1	2:B:377:CYS:N	2.49	0.46
2:B:605:GLN:O	2:B:609:GLY:N	2.49	0.46
2:B:611:ASN:HA	2:B:613:THR:N	2.31	0.46
1:A:111:LEU:HD23	1:A:118:GLN:HB2	1.98	0.45
1:A:857:LYS:O	1:A:858:LYS:C	2.58	0.45
1:A:649:ARG:NH1	1:A:673:GLU:CD	2.74	0.45
2:B:610:SER:O	2:B:613:THR:HG23	2.17	0.45
1:A:636:ASP:O	1:A:636:ASP:CG	2.59	0.45
1:A:756:TYR:HD1	1:A:757:SER:N	2.14	0.45
2:B:590:ARG:HB2	2:B:593:LYS:NZ	2.31	0.45
1:A:585:ALA:CB	1:A:603:ARG:HG3	2.36	0.45
1:A:299:ARG:CG	1:A:299:ARG:HH11	2.29	0.45
1:A:390:GLY:N	1:A:463:PHE:HB3	2.32	0.45
1:A:531:GLN:OE1	1:A:531:GLN:HA	2.16	0.45
1:A:714:ASP:N	1:A:715:GLY:CA	2.74	0.45
2:B:427:PHE:HB2	2:B:535:HIS:HD2	1.81	0.45
2:B:484:CYS:HA	2:B:494:LEU:O	2.15	0.45
1:A:638:LEU:HD13	1:A:639:ASP:HA	1.98	0.45
1:A:817:GLU:HA	1:A:818:ILE:HG22	1.98	0.45
2:B:641:LEU:HD12	2:B:641:LEU:N	2.32	0.45
1:A:123:THR:O	1:A:123:THR:HG22	2.16	0.45
1:A:291:THR:C	1:A:293:ASP:N	2.73	0.45
1:A:896:VAL:HG12	1:A:897:TYR:H	1.82	0.45
1:A:663:VAL:HG23	1:A:664:GLN:O	2.16	0.45
1:A:712:ILE:O	1:A:713:LYS:NZ	2.36	0.45
1:A:273:LYS:NZ	1:A:274:ALA:HA	2.30	0.45
1:A:729:GLN:HG2	1:A:730:SER:H	1.82	0.45
1:A:826:ALA:H	1:A:832:SER:HB2	1.82	0.45
1:A:892:LYS:CB	1:A:893:ASN:HA	2.42	0.45
1:A:183:GLY:HA2	1:A:184:GLU:C	2.42	0.44
1:A:257:TYR:CE2	1:A:278:LYS:HD2	2.52	0.44
1:A:160:VAL:HG23	1:A:161:GLU:N	2.30	0.44
1:A:178:ALA:O	1:A:181:VAL:CG2	2.61	0.44
1:A:815:ALA:HB2	1:A:844:PRO:HD3	1.97	0.44
1:A:894:VAL:HG11	1:A:900:TYR:HE2	1.82	0.44
1:A:896:VAL:CG1	1:A:898:ASN:H	2.24	0.44
1:A:86:ILE:CD1	1:A:155:LYS:HE2	2.47	0.44
1:A:884:ALA:HA	1:A:890:GLN:CD	2.42	0.44
1:A:217:GLU:HG2	1:A:317:GLY:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LYS:HB2	1:A:580:LYS:NZ	2.32	0.44
1:A:814:LYS:HE2	1:A:814:LYS:HB3	1.62	0.44
2:B:392:ASP:O	2:B:396:VAL:HG23	2.17	0.44
2:B:426:TYR:CE2	2:B:582:ALA:HB3	2.53	0.44
2:B:590:ARG:NE	2:B:593:LYS:NZ	2.65	0.44
1:A:156:GLY:O	1:A:169:GLY:HA2	2.17	0.44
1:A:484:PHE:HB2	1:A:499:VAL:CG1	2.44	0.44
1:A:798:ASP:HB3	1:A:799:GLN:H	1.58	0.44
1:A:817:GLU:HB3	1:A:819:THR:H	1.82	0.44
2:B:438:ASP:O	2:B:440:THR:HG23	2.18	0.44
2:B:536:GLN:O	2:B:540:GLN:HG3	2.18	0.44
2:B:629:LEU:C	2:B:630:LEU:HG	2.42	0.44
1:A:228:GLY:HA3	1:A:305:LEU:O	2.17	0.44
1:A:296:GLY:HA2	1:A:297:PRO:O	2.18	0.44
1:A:316:PRO:HD2	1:A:329:GLY:O	2.17	0.44
1:A:563:ARG:O	1:A:564:LEU:HD12	2.18	0.44
2:B:603:GLN:O	2:B:607:LEU:HG	2.17	0.44
1:A:106:LYS:HB3	1:A:107:ASN:H	1.52	0.44
1:A:178:ALA:C	1:A:180:ASP:N	2.75	0.44
1:A:794:GLY:HA2	1:A:808:GLY:O	2.18	0.44
2:B:517:TYR:CZ	2:B:534:LYS:HE3	2.53	0.44
1:A:349:LEU:H	1:A:349:LEU:HG	1.55	0.44
1:A:880:VAL:O	1:A:880:VAL:HG12	2.18	0.44
1:A:95:ALA:O	1:A:96:SER:C	2.61	0.44
1:A:273:LYS:O	1:A:273:LYS:CD	2.64	0.44
1:A:412:TYR:CD2	1:A:413:VAL:N	2.85	0.44
1:A:725:TYR:O	1:A:726:LEU:HD23	2.17	0.44
1:A:817:GLU:CA	1:A:818:ILE:HG22	2.48	0.44
2:B:408:LEU:HB2	2:B:587:VAL:CG2	2.47	0.44
2:B:455:GLY:H	2:B:460:TRP:CD1	2.36	0.44
1:A:617:SER:HA	1:A:656:MET:HE3	2.00	0.43
1:A:78:ASP:O	1:A:81:ARG:HB3	2.18	0.43
1:A:185:GLY:O	1:A:186:ARG:C	2.61	0.43
1:A:510:LEU:HD22	1:A:511:ARG:N	2.32	0.43
1:A:649:ARG:HH11	1:A:673:GLU:CD	2.25	0.43
1:A:679:GLU:HG3	1:A:696:PHE:HB3	2.01	0.43
1:A:102:ARG:HD2	1:A:698:ASN:ND2	2.33	0.43
1:A:363:SER:OG	2:B:539:PRO:HG3	2.18	0.43
1:A:376:TYR:CG	1:A:392:GLU:HB3	2.53	0.43
1:A:542:SER:O	1:A:545:SER:N	2.48	0.43
1:A:553:ARG:NH2	1:A:553:ARG:CG	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD21	1:A:220:LEU:HD23	2.01	0.43
1:A:239:GLY:C	1:A:240:VAL:HG22	2.43	0.43
2:B:378:ILE:O	2:B:381:ILE:HB	2.19	0.43
1:A:75:ASN:HD22	1:A:76:ILE:C	2.26	0.43
1:A:720:LYS:HA	1:A:721:GLY:HA2	1.66	0.43
1:A:622:ARG:HD2	1:A:622:ARG:H	1.82	0.43
2:B:381:ILE:HG23	2:B:590:ARG:NH1	2.33	0.43
1:A:95:ALA:HB2	1:A:338:PHE:CD1	2.54	0.43
1:A:202:GLY:HA3	1:A:227:ALA:HB2	2.01	0.43
1:A:233:HIS:HD2	1:A:235:ASP:HB2	1.76	0.43
1:A:618:THR:HG22	1:A:619:GLY:N	2.33	0.43
1:A:653:PHE:N	1:A:653:PHE:CD1	2.86	0.43
1:A:700:TYR:C	1:A:701:ARG:HG3	2.44	0.43
1:A:467:LYS:HE2	2:B:416:ASP:OD2	2.18	0.43
1:A:616:VAL:HG23	1:A:656:MET:O	2.19	0.43
2:B:344:TRP:HB3	2:B:355:CYS:SG	2.59	0.43
1:A:604:TYR:OH	1:A:622:ARG:HB3	2.18	0.43
1:A:814:LYS:O	1:A:815:ALA:C	2.62	0.43
1:A:134:ALA:HB2	1:A:441:PHE:CB	2.31	0.43
1:A:143:ILE:N	1:A:143:ILE:CD1	2.75	0.43
2:B:379:ALA:O	2:B:382:MET:N	2.52	0.43
1:A:149:LYS:C	1:A:174:GLN:HE21	2.26	0.42
1:A:294:TYR:CZ	1:A:297:PRO:O	2.71	0.42
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.84	0.42
1:A:317:GLY:HA3	1:A:326:TYR:HE1	1.84	0.42
1:A:582:TYR:CE1	1:A:606:TYR:HB3	2.53	0.42
1:A:120:GLN:NE2	1:A:653:PHE:CZ	2.87	0.42
1:A:142:GLU:HB2	1:A:336:GLN:NE2	2.34	0.42
1:A:238:ARG:O	1:A:240:VAL:HG23	2.18	0.42
1:A:294:TYR:OH	1:A:298:ASN:HB2	2.19	0.42
1:A:455:CYS:O	1:A:456:ARG:HD2	2.18	0.42
1:A:761:TYR:CE1	1:A:791:TYR:CZ	3.07	0.42
1:A:911:LEU:HD23	1:A:911:LEU:O	2.19	0.42
1:A:230:ILE:O	1:A:230:ILE:HG22	2.19	0.42
1:A:327:ILE:HD12	1:A:411:GLU:O	2.20	0.42
1:A:564:LEU:HG	1:A:573:THR:HG22	2.01	0.42
1:A:602:LEU:HD23	1:A:626:TRP:CB	2.42	0.42
1:A:790:ARG:HA	1:A:812:TYR:O	2.19	0.42
2:B:427:PHE:CE2	2:B:578:HIS:CE1	3.08	0.42
2:B:465:GLY:HA3	2:B:658:ALA:O	2.18	0.42
1:A:502:GLY:N	1:A:583:TYR:CE2	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:GLY:C	1:A:809:MET:HG2	2.45	0.42
2:B:426:TYR:CZ	2:B:582:ALA:HB3	2.54	0.42
1:A:454:TYR:O	1:A:455:CYS:C	2.63	0.42
1:A:566:ASN:OD1	1:A:566:ASN:N	2.37	0.42
1:A:878:GLU:HB3	1:A:879:ASN:HB2	2.02	0.42
1:A:75:ASN:ND2	1:A:76:ILE:CA	2.80	0.42
1:A:93:ARG:NH1	1:A:889:ASN:HD21	2.17	0.42
1:A:355:ASP:OD1	2:B:545:LYS:HE3	2.20	0.42
2:B:507:GLU:HA	2:B:508:PRO:HD3	1.91	0.42
1:A:331:LEU:C	1:A:331:LEU:HD23	2.45	0.42
1:A:638:LEU:HD13	1:A:638:LEU:C	2.44	0.42
2:B:508:PRO:O	2:B:515:TYR:CE1	2.73	0.42
1:A:75:ASN:HD21	1:A:77:ARG:HD2	1.84	0.42
1:A:233:HIS:NE2	1:A:873:ARG:HB2	2.35	0.42
2:B:467:LEU:O	2:B:471:ILE:HG13	2.19	0.42
1:A:326:TYR:CD1	1:A:327:ILE:N	2.88	0.42
1:A:713:LYS:O	1:A:714:ASP:HB2	2.19	0.42
1:A:778:ILE:HD11	1:A:826:ALA:CB	2.35	0.42
1:A:120:GLN:HG3	1:A:475:GLU:OE2	2.20	0.41
1:A:457:PRO:HA	1:A:464:SER:HB2	2.02	0.41
1:A:87:ALA:HB3	1:A:100:SER:HB3	2.02	0.41
1:A:120:GLN:NE2	1:A:653:PHE:CE2	2.89	0.41
2:B:389:MET:CE	2:B:391:LEU:HD23	2.49	0.41
2:B:391:LEU:HD11	2:B:588:VAL:CG2	2.50	0.41
2:B:570:PRO:HD2	2:B:573:GLU:CG	2.50	0.41
2:B:610:SER:O	2:B:613:THR:OG1	2.25	0.41
2:B:421:THR:HA	2:B:422:PRO:HD3	1.95	0.41
1:A:148:VAL:HA	1:A:174:GLN:O	2.20	0.41
1:A:190:ILE:HD13	1:A:191:GLN:N	2.36	0.41
1:A:412:TYR:HB3	1:A:428:LEU:HG	2.02	0.41
1:A:289:VAL:HB	1:A:290:SER:HB2	2.03	0.41
1:A:668:VAL:HG11	1:A:726:LEU:HD21	2.03	0.41
1:A:51:ARG:O	1:A:52:ASP:C	2.63	0.41
1:A:91:GLN:O	1:A:889:ASN:HB2	2.21	0.41
1:A:354:PHE:O	1:A:358:LYS:HD3	2.21	0.41
1:A:500:ASN:HB2	1:A:585:ALA:HB3	2.02	0.41
1:A:618:THR:OG1	1:A:669:LYS:HD2	2.21	0.41
2:B:394:GLY:HA2	2:B:655:TYR:OH	2.21	0.41
1:A:209:LEU:HD23	1:A:209:LEU:H	1.84	0.41
1:A:273:LYS:CD	1:A:273:LYS:C	2.94	0.41
1:A:290:SER:O	1:A:291:THR:OG1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HB3	1:A:391:ALA:CB	2.51	0.41
2:B:348:SER:H	2:B:351:GLU:HB2	1.86	0.41
1:A:326:TYR:CD1	1:A:326:TYR:C	2.99	0.41
1:A:818:ILE:HA	1:A:818:ILE:HD13	1.75	0.41
2:B:378:ILE:HD11	2:B:670:LEU:HD23	2.02	0.41
2:B:400:GLY:HA3	2:B:647:TYR:CG	2.56	0.41
2:B:542:THR:HB	2:B:554:LEU:O	2.21	0.41
2:B:659:VAL:HG22	2:B:660:GLY:N	2.34	0.41
1:A:350:THR:CG2	1:A:350:THR:O	2.69	0.41
2:B:486:PRO:HA	2:B:506:CYS:O	2.21	0.41
1:A:239:GLY:C	1:A:240:VAL:CG2	2.93	0.40
1:A:258:PHE:CD1	1:A:369:LYS:HD2	2.56	0.40
1:A:673:GLU:CG	1:A:704:ILE:HG13	2.49	0.40
2:B:427:PHE:HE2	2:B:578:HIS:CE1	2.38	0.40
2:B:487:GLY:HA2	2:B:508:PRO:HG3	2.03	0.40
1:A:143:ILE:CG1	1:A:145:TYR:HE1	2.31	0.40
1:A:150:ALA:N	1:A:174:GLN:CD	2.79	0.40
1:A:343:MET:HE3	1:A:343:MET:HB3	1.94	0.40
1:A:742:ILE:C	1:A:742:ILE:CD1	2.94	0.40
2:B:465:GLY:HA2	2:B:662:LEU:HB2	2.02	0.40
1:A:188:TRP:HE3	1:A:189:GLY:N	2.19	0.40
1:A:438:ASP:OD2	1:A:470:ARG:NH1	2.55	0.40
1:A:561:ILE:HD13	2:B:416:ASP:OD2	2.22	0.40
1:A:299:ARG:CG	1:A:299:ARG:NH1	2.84	0.40
1:A:826:ALA:HA	1:A:832:SER:HB3	2.02	0.40

All (1) 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:290:SER:OG	2:B:438:ASP:O[2_454]	2.02	0.18

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	847/904 (94%)	757 (89%)	72 (8%)	18 (2%)	5	25
2	B	337/343 (98%)	311 (92%)	26 (8%)	0	100	100
All	All	1184/1247 (95%)	1068 (90%)	98 (8%)	18 (2%)	8	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	55	VAL
1	A	56	THR
1	A	58	LEU
1	A	800	PRO
1	A	818	ILE
1	A	880	VAL
1	A	240	VAL
1	A	292	ARG
1	A	802	GLY
1	A	803	LYS
1	A	755	TRP
1	A	799	GLN
1	A	858	LYS
1	A	89	VAL
1	A	230	ILE
1	A	894	VAL
1	A	303	ASP

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	662/741 (89%)	521 (79%)	141 (21%)	1	5
2	B	271/292 (93%)	226 (83%)	45 (17%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	933/1033 (90%)	747 (80%)	186 (20%)	1 6

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	56	THR
1	A	61	LEU
1	A	63	LYS
1	A	65	SER
1	A	66	ASP
1	A	67	THR
1	A	68	LEU
1	A	75	ASN
1	A	76	ILE
1	A	79	LEU
1	A	81	ARG
1	A	83	ASP
1	A	89	VAL
1	A	91	GLN
1	A	106	LYS
1	A	109	VAL
1	A	112	THR
1	A	120	GLN
1	A	122	TYR
1	A	123	THR
1	A	128	LEU
1	A	132	ARG
1	A	140	ILE
1	A	141	ASN
1	A	143	ILE
1	A	151	VAL
1	A	157	SER
1	A	158	ASN
1	A	162	GLN
1	A	179	ASP
1	A	180	ASP
1	A	181	VAL
1	A	182	ILE
1	A	186	ARG
1	A	187	GLN
1	A	190	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	SER
1	A	203	LEU
1	A	204	THR
1	A	207	ILE
1	A	209	LEU
1	A	220	LEU
1	A	226	ARG
1	A	240	VAL
1	A	243	PHE
1	A	250	GLU
1	A	260	VAL
1	A	273	LYS
1	A	275	ASN
1	A	280	VAL
1	A	290	SER
1	A	291	THR
1	A	299	ARG
1	A	301	LEU
1	A	309	SER
1	A	318	PHE
1	A	320	PHE
1	A	330	ILE
1	A	344	THR
1	A	349	LEU
1	A	350	THR
1	A	353	VAL
1	A	358	LYS
1	A	359	LYS
1	A	379	LEU
1	A	392	GLU
1	A	395	THR
1	A	402	THR
1	A	407	ARG
1	A	412	TYR
1	A	419	LYS
1	A	428	LEU
1	A	429	SER
1	A	441	PHE
1	A	444	THR
1	A	460	ASP
1	A	464	SER
1	A	478	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	495	HIS
1	A	498	SER
1	A	499	VAL
1	A	508	SER
1	A	510	LEU
1	A	524	TYR
1	A	533	ASN
1	A	535	LYS
1	A	550	THR
1	A	553	ARG
1	A	556	VAL
1	A	557	VAL
1	A	558	THR
1	A	564	LEU
1	A	566	ASN
1	A	575	ARG
1	A	588	ASP
1	A	597	ASP
1	A	603	ARG
1	A	620	THR
1	A	622	ARG
1	A	623	THR
1	A	625	SER
1	A	631	VAL
1	A	636	ASP
1	A	638	LEU
1	A	663	VAL
1	A	670	ILE
1	A	683	VAL
1	A	688	PHE
1	A	712	ILE
1	A	716	LYS
1	A	717	GLU
1	A	722	ASP
1	A	766	VAL
1	A	769	ILE
1	A	771	LYS
1	A	772	ARG
1	A	778	ILE
1	A	786	ILE
1	A	811	THR
1	A	814	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	818	ILE
1	A	819	THR
1	A	827	LEU
1	A	842	THR
1	A	848	VAL
1	A	855	THR
1	A	856	VAL
1	A	859	HIS
1	A	860	PHE
1	A	861	THR
1	A	870	LEU
1	A	878	GLU
1	A	879	ASN
1	A	888	VAL
1	A	892	LYS
1	A	894	VAL
1	A	896	VAL
1	A	899	ARG
1	A	906	ASN
1	A	912	GLU
2	B	347	LEU
2	B	366	ILE
2	B	369	VAL
2	B	374	THR
2	B	378	ILE
2	B	391	LEU
2	B	407	VAL
2	B	417	ASN
2	B	421	THR
2	B	443	ASN
2	B	444	LEU
2	B	474	CYS
2	B	509	ASN
2	B	525	VAL
2	B	526	GLU
2	B	527	LYS
2	B	552	LYS
2	B	554	LEU
2	B	556	GLU
2	B	562	LEU
2	B	577	CYS
2	B	579	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	581	ARG
2	B	588	VAL
2	B	590	ARG
2	B	593	LYS
2	B	596	CYS
2	B	597	VAL
2	B	601	LEU
2	B	604	GLN
2	B	611	ASN
2	B	612	VAL
2	B	613	THR
2	B	616	SER
2	B	629	LEU
2	B	630	LEU
2	B	632	ARG
2	B	641	LEU
2	B	645	ASN
2	B	648	GLU
2	B	649	LYS
2	B	656	VAL
2	B	657	LYS
2	B	667	THR
2	B	674	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	120	GLN
1	A	147	ASN
1	A	174	GLN
1	A	233	HIS
1	A	241	GLN
1	A	254	ASN
1	A	439	ASN
1	A	440	HIS
1	A	442	GLN
1	A	519	HIS
1	A	697	ASN
1	A	698	ASN
1	A	729	GLN
1	A	829	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	882	GLN
1	A	906	ASN
2	B	443	ASN
2	B	535	HIS
2	B	555	ASN
2	B	606	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	853/904 (94%)	0.20	16 (1%) 66 45	24, 73, 122, 160	0
2	B	339/343 (98%)	-0.04	2 (0%) 85 70	31, 69, 112, 126	0
All	All	1192/1247 (95%)	0.14	18 (1%) 72 52	24, 72, 118, 160	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	745	ASN	5.7
1	A	57	GLY	4.1
1	A	854	TYR	3.5
1	A	855	THR	3.0
1	A	237	GLY	2.9
1	A	58	LEU	2.8
1	A	54	GLU	2.5
1	A	56	THR	2.5
1	A	710	ALA	2.4
1	A	180	ASP	2.4
1	A	408	TYR	2.3
1	A	489	ASP	2.3
1	A	234	GLU	2.3
2	B	482	GLU	2.2
1	A	619	GLY	2.2
2	B	552	LYS	2.1
1	A	163	GLY	2.1
1	A	803	LYS	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.