Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:07 AM EDT

PDB ID	:	4ZPV
Title	:	Structure of MERS-Coronavirus Spike Receptor-binding Domain (England1 Strain) in Complex with Vaccine-Elicited Murine Neutralizing Antibody D12 (Crystal Form 2)
Authors	:	Joyce, M.G.; Mascola, J.R.; Graham, B.S.; Kwong, P.D.
Deposited on	:	2015-05-08
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

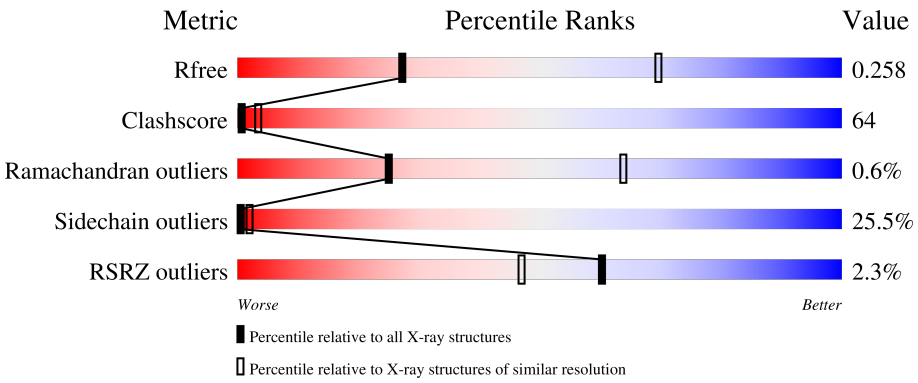
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

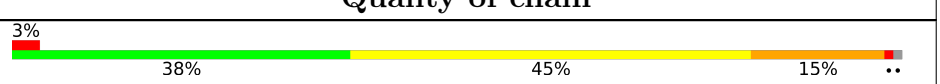
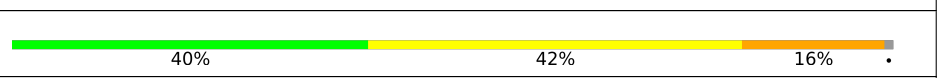
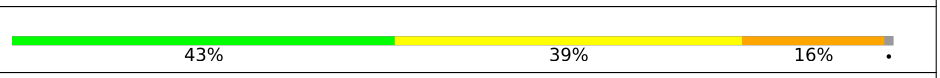
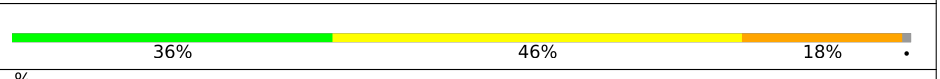
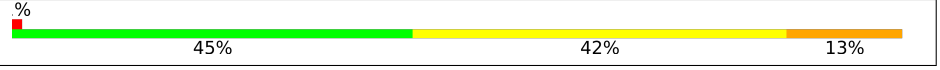
The reported resolution of this entry is 3.20 Å.

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	216	
1	H	216	
2	B	214	
2	L	214	
3	R	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	S	208	10% 36% 43% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	R	601	X	-	-	-
4	NAG	R	602	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9733 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 D12 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	213	1595	1005	259	322	9	0	0	0
1	A	213	1594	1004	260	321	9	0	0	0

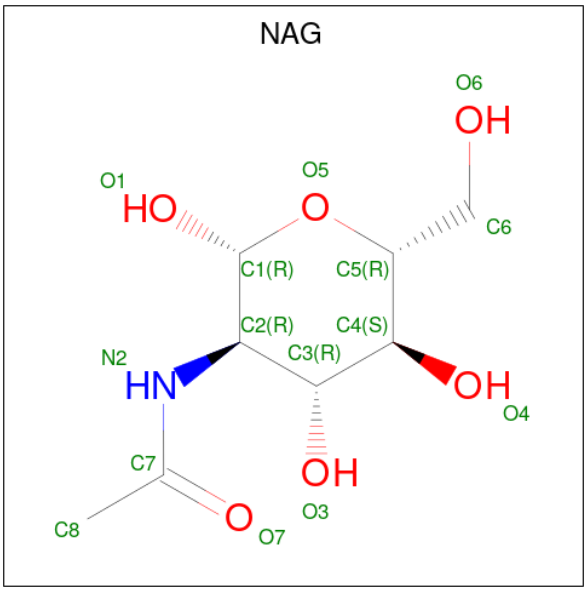
- Molecule 2 is a protein called D12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1651	1023	282	340	6	0	0	0
2	B	212	1651	1023	282	340	6	0	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S	207	1603	1023	255	314	11	0	0	0
3	R	208	1611	1029	256	315	11	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



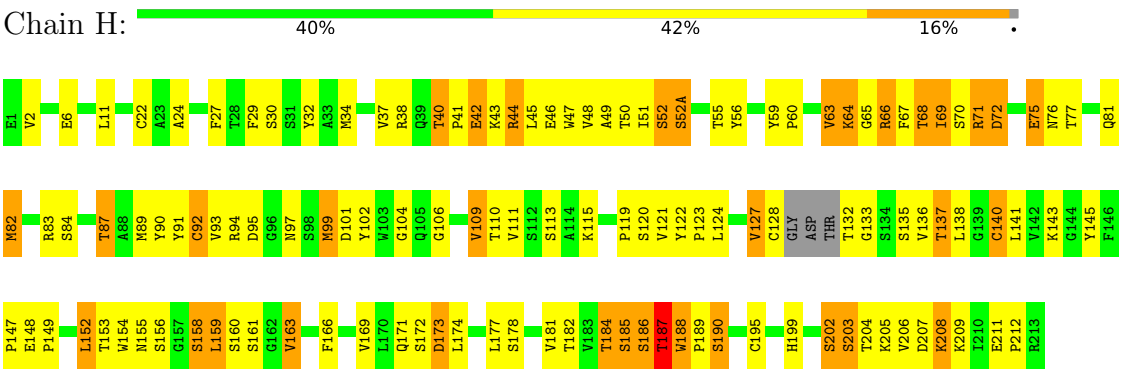
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	R	1	14	8	1	5	0	0
			Total	C	N	O		
4	R	1	14	8	1	5	0	0

3 Residue-property plots (i)

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.

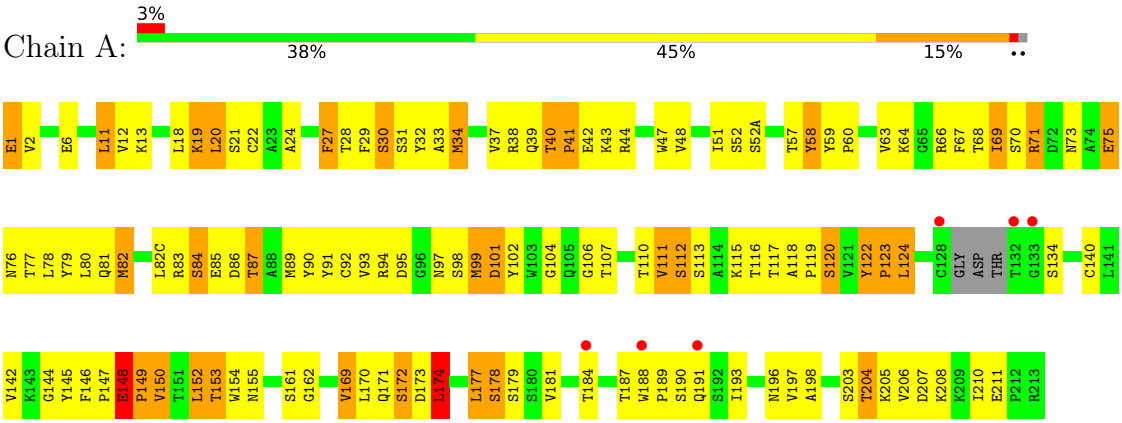
- Molecule 1: D12 Fab Heavy chain

Chain H:



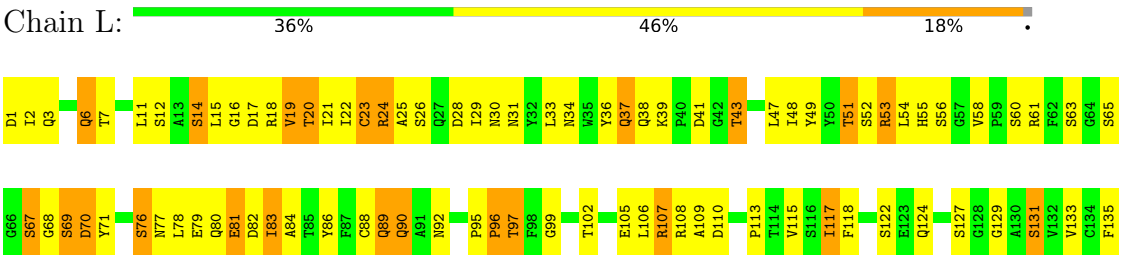
- Molecule 1: D12 Fab Heavy chain

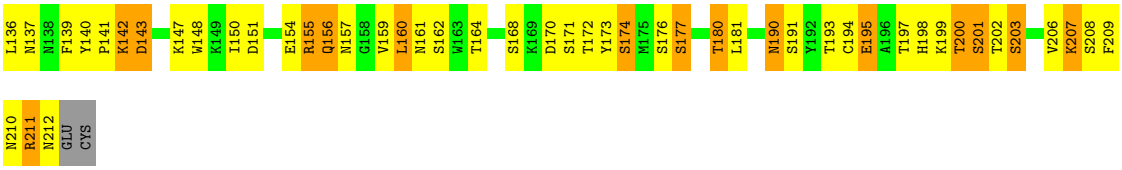
Chain A:



- Molecule 2: D12 Fab light chain

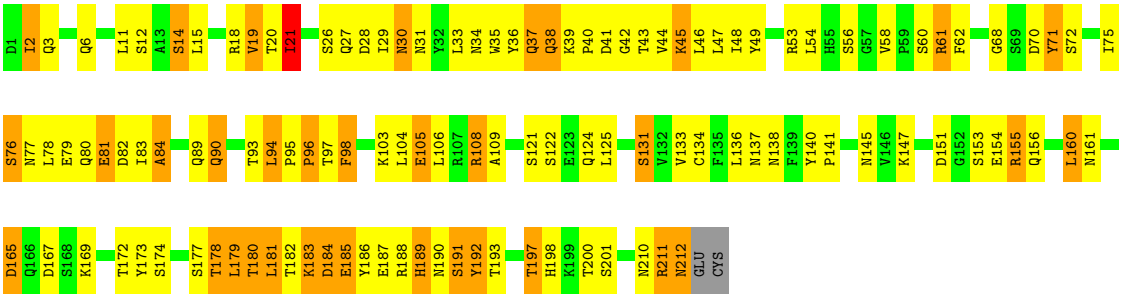
Chain L:





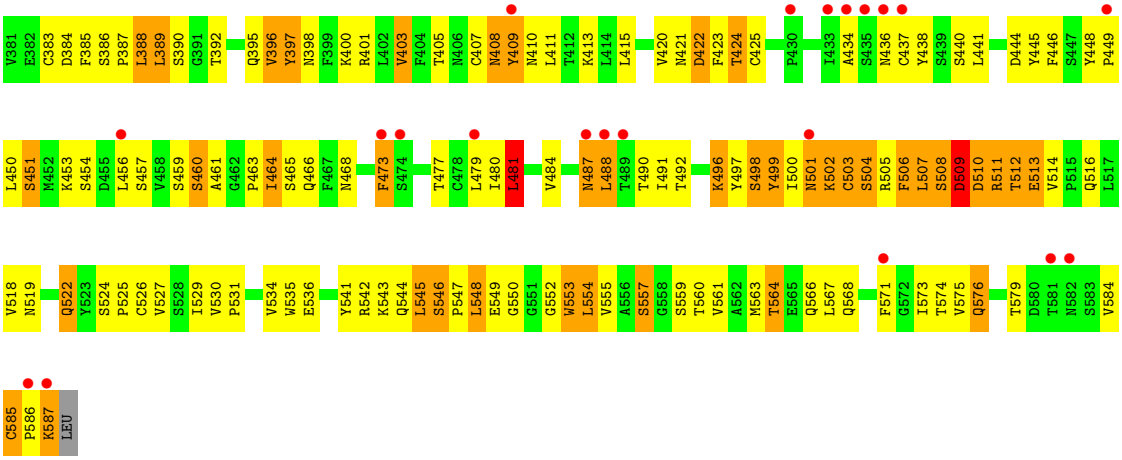
• Molecule 2: D12 Fab light chain

Chain B:



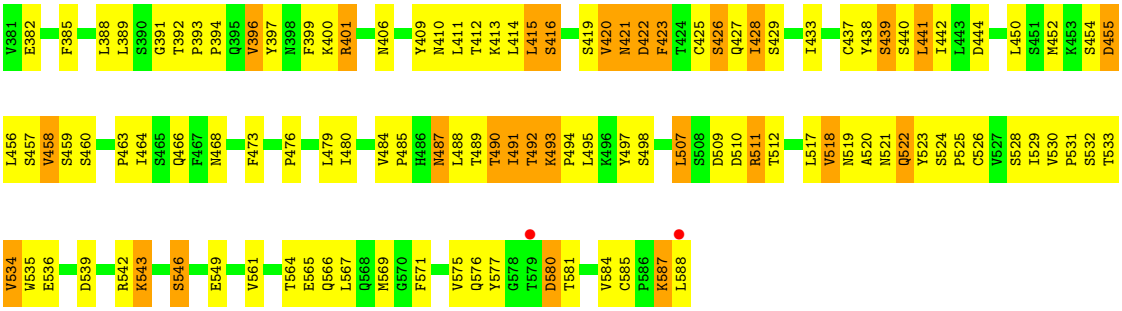
• Molecule 3: Spike glycoprotein

Chain S:



• Molecule 3: Spike glycoprotein

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.18Å 106.14Å 171.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.55 – 3.20 43.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.3 (43.55-3.20) 75.7 (43.55-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.281 0.233 , 0.258	Depositor DCC
R_{free} test set	942 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.97	0/1632	0.85	2/2226 (0.1%)
1	H	0.81	0/1633	0.76	1/2227 (0.0%)
2	B	0.98	0/1685	0.84	2/2290 (0.1%)
2	L	0.92	0/1685	0.77	1/2290 (0.0%)
3	R	0.85	0/1651	0.68	0/2254
3	S	0.66	0/1643	0.76	2/2243 (0.1%)
All	All	0.87	0/9929	0.78	8/13530 (0.1%)

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	H	0	2
3	S	0	2
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	148	GLU	C-N-CD	-11.92	94.38	120.60
2	B	96	PRO	CA-N-CD	-6.80	101.98	111.50
2	L	11	LEU	CB-CG-CD2	-6.53	99.91	111.00
3	S	509	ASP	N-CA-C	-6.43	93.64	111.00
2	B	21	ILE	CB-CA-C	-6.23	99.15	111.60
1	A	174	LEU	CB-CG-CD2	-5.37	101.87	111.00
3	S	481	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	148	GLU	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	187	THR	Peptide,Mainchain
3	S	509	ASP	Peptide
3	S	510	ASP	Peptide

5.2 Too-close contacts (i)

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	1594	0	1547	230	4
1	H	1595	0	1552	192	0
2	B	1651	0	1582	191	1
2	L	1651	0	1584	174	1
3	R	1611	0	1568	162	4
3	S	1603	0	1561	323	0
4	R	28	0	26	2	0
All	All	9733	0	9420	1230	5

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 64.

All (1230) 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:B:180:THR:C	2:B:181:LEU:HD23	1.18	1.54
3:S:385:PHE:CZ	3:S:409:TYR:HD2	1.22	1.52
3:S:396:VAL:HG23	3:S:446:PHE:CD1	1.46	1.49
3:S:437:CYS:SG	3:S:585:CYS:CB	2.04	1.45
3:S:383:CYS:CB	3:S:409:TYR:HB3	1.43	1.43
1:A:173:ASP:C	1:A:174:LEU:HD23	1.34	1.43
3:S:383:CYS:HB2	3:S:409:TYR:CB	1.49	1.43
3:S:385:PHE:HZ	3:S:409:TYR:CD2	1.36	1.42
3:R:488:LEU:CD2	3:R:490:THR:HG23	1.51	1.40
1:H:55:THR:HG22	1:H:56:TYR:CD1	1.55	1.40
1:A:177:LEU:HD23	1:A:178:SER:N	1.35	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:HE1	1:A:210:ILE:CD1	1.36	1.39
3:S:385:PHE:CZ	3:S:409:TYR:CD2	2.10	1.38
1:A:152:LEU:HD23	1:A:153:THR:N	1.34	1.38
1:A:67:PHE:CZ	1:A:82:MET:CE	2.08	1.37
2:B:124:GLN:HB2	1:A:122:TYR:CD1	1.58	1.36
3:S:480:ILE:C	3:S:481:LEU:HD23	1.43	1.35
3:R:437:CYS:CB	3:R:585:CYS:SG	2.14	1.35
3:S:421:ASN:OD1	3:S:450:LEU:CD2	1.73	1.34
3:S:434:ALA:HB1	3:S:587:LYS:CE	1.58	1.33
1:H:94:ARG:HH21	1:H:101:ASP:CG	1.30	1.32
3:S:503:CYS:SG	3:S:526:CYS:CB	2.17	1.32
2:L:23:CYS:SG	2:L:88:CYS:CB	2.19	1.30
2:B:151:ASP:OD2	2:B:189:HIS:CB	1.80	1.29
2:L:80:GLN:NE2	2:L:171:SER:OG	1.60	1.29
3:S:421:ASN:OD1	3:S:450:LEU:HD21	1.13	1.28
2:B:190:ASN:OD1	2:B:210:ASN:HB3	1.27	1.28
1:H:55:THR:HG22	1:H:56:TYR:CE1	1.68	1.27
1:H:140:CYS:SG	1:H:195:CYS:SG	1.41	1.27
2:B:179:LEU:HD12	2:B:180:THR:N	1.49	1.27
1:H:22:CYS:CB	1:H:92:CYS:SG	2.21	1.26
2:L:147:LYS:CD	2:L:154:GLU:OE2	1.82	1.26
3:S:389:LEU:O	3:S:491:ILE:HD12	1.29	1.25
1:H:140:CYS:SG	1:H:195:CYS:CB	2.25	1.25
3:S:563:MET:HE1	3:S:567:LEU:CD1	1.65	1.24
3:S:395:GLN:NE2	3:S:498:SER:H	1.33	1.23
1:H:152:LEU:HD23	1:H:153:THR:N	1.54	1.23
3:S:564:THR:OG1	3:S:566:GLN:O	1.52	1.22
3:S:548:LEU:HD12	3:S:548:LEU:O	1.40	1.21
3:S:544:GLN:C	3:S:545:LEU:HD23	1.60	1.20
2:L:155:ARG:HH21	2:L:155:ARG:HG3	1.05	1.19
3:S:554:LEU:HD12	3:S:555:VAL:N	1.57	1.18
3:R:457:SER:OG	3:R:458:VAL:HG23	1.41	1.18
2:B:36:TYR:OH	2:B:89:GLN:OE1	1.58	1.18
3:S:389:LEU:O	3:S:491:ILE:CD1	1.90	1.18
1:H:152:LEU:HD23	1:H:152:LEU:C	1.62	1.17
3:R:519:ASN:HB2	3:R:522:GLN:NE2	1.58	1.17
1:A:152:LEU:HD23	1:A:152:LEU:C	1.59	1.17
1:H:87:THR:HG22	1:H:110:THR:HA	1.25	1.17
3:S:411:LEU:HD21	3:S:415:LEU:CD1	1.75	1.17
2:B:151:ASP:OD2	2:B:189:HIS:HB2	1.41	1.17
2:B:180:THR:C	2:B:181:LEU:CD2	2.13	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:155:ARG:HH21	2:L:155:ARG:CG	1.57	1.16
3:S:386:SER:OG	3:S:387:PRO:HD3	1.44	1.16
2:B:103:LYS:NZ	2:B:165:ASP:OD1	1.78	1.16
3:R:437:CYS:SG	3:R:585:CYS:CB	2.32	1.16
2:B:180:THR:O	2:B:181:LEU:HD23	1.41	1.16
1:A:210:ILE:HD12	1:A:210:ILE:O	1.46	1.16
2:L:83:ILE:HG13	2:L:106:LEU:HD11	1.23	1.16
1:A:188:TRP:HE1	1:A:210:ILE:HD13	1.08	1.15
3:R:456:LEU:O	3:R:456:LEU:HD23	1.47	1.15
2:L:36:TYR:OH	2:L:89:GLN:NE2	1.79	1.15
2:L:147:LYS:HD2	2:L:154:GLU:OE2	1.01	1.15
2:L:83:ILE:HG13	2:L:106:LEU:CD1	1.75	1.15
2:B:124:GLN:HB2	1:A:122:TYR:CE1	1.82	1.15
3:S:411:LEU:HD21	3:S:415:LEU:CG	1.74	1.14
3:S:437:CYS:SG	3:S:585:CYS:HB3	1.76	1.14
3:S:401:ARG:HG3	3:S:444:ASP:OD1	1.45	1.14
3:S:507:LEU:H	3:S:507:LEU:CD1	1.57	1.13
1:H:55:THR:CG2	1:H:56:TYR:CE1	2.30	1.13
3:S:548:LEU:HD12	3:S:548:LEU:C	1.63	1.13
1:A:22:CYS:SG	1:A:92:CYS:SG	1.26	1.13
2:L:23:CYS:CB	2:L:88:CYS:SG	2.37	1.13
1:A:174:LEU:HD23	1:A:174:LEU:N	1.51	1.13
2:L:39:LYS:NZ	2:L:81:GLU:O	1.82	1.13
2:B:155:ARG:HH11	2:B:155:ARG:CG	1.62	1.13
3:S:519:ASN:HB2	3:S:522:GLN:NE2	1.62	1.12
3:S:411:LEU:HD21	3:S:415:LEU:HG	1.23	1.12
3:S:481:LEU:HD23	3:S:481:LEU:N	1.47	1.12
1:A:124:LEU:N	1:A:124:LEU:HD23	1.57	1.12
3:S:396:VAL:HG23	3:S:446:PHE:CE1	1.83	1.12
3:R:419:SER:O	3:R:421:ASN:ND2	1.81	1.12
3:R:420:VAL:C	3:R:421:ASN:HD22	1.51	1.12
1:A:177:LEU:HD23	1:A:177:LEU:C	1.65	1.11
3:S:437:CYS:CB	3:S:585:CYS:HB3	1.81	1.11
1:H:22:CYS:SG	1:H:92:CYS:SG	1.20	1.11
3:S:438:TYR:CG	3:S:575:VAL:HG21	1.85	1.11
3:R:519:ASN:HB2	3:R:522:GLN:HE21	0.94	1.10
3:S:507:LEU:N	3:S:507:LEU:HD12	1.52	1.09
3:R:488:LEU:HD21	3:R:490:THR:HG23	1.13	1.09
1:H:67:PHE:CE1	1:H:82:MET:HB3	1.86	1.09
3:S:503:CYS:SG	3:S:526:CYS:SG	1.10	1.09
1:H:63:VAL:HG22	1:H:67:PHE:CD2	1.86	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HA	1:A:111:VAL:HG12	1.32	1.08
2:B:160:LEU:HD13	1:A:169:VAL:HG11	1.36	1.08
1:A:207:ASP:O	1:A:208:LYS:HD3	1.53	1.08
1:A:123:PRO:C	1:A:124:LEU:HD23	1.74	1.08
2:B:124:GLN:CB	1:A:122:TYR:CE1	2.35	1.08
1:H:87:THR:CG2	1:H:110:THR:HA	1.82	1.07
3:R:411:LEU:O	3:R:415:LEU:HD23	1.53	1.07
3:S:563:MET:HE1	3:S:567:LEU:HD13	1.14	1.07
3:S:519:ASN:CB	3:S:522:GLN:HE21	1.66	1.07
3:S:436:ASN:O	3:S:586:PRO:HD2	1.55	1.07
3:S:437:CYS:CA	3:S:585:CYS:HB3	1.84	1.07
1:A:188:TRP:HE1	1:A:210:ILE:HD11	1.17	1.07
3:S:545:LEU:HD23	3:S:545:LEU:N	1.57	1.07
3:S:411:LEU:CD2	3:S:415:LEU:HG	1.85	1.06
3:S:437:CYS:HA	3:S:585:CYS:HB3	1.37	1.06
2:B:151:ASP:OD2	2:B:189:HIS:HB3	1.53	1.06
1:H:93:VAL:HG11	1:H:99:MET:HG2	1.35	1.06
3:S:411:LEU:O	3:S:411:LEU:HD23	1.56	1.05
1:A:188:TRP:NE1	1:A:210:ILE:CD1	2.19	1.05
1:A:188:TRP:NE1	1:A:210:ILE:HD13	1.69	1.05
1:H:63:VAL:CG2	1:H:67:PHE:CD2	2.39	1.05
3:R:389:LEU:O	3:R:491:ILE:CD1	2.05	1.05
1:A:57:THR:C	1:A:58:TYR:CD2	2.30	1.05
1:H:75:GLU:OE2	1:H:75:GLU:HA	1.50	1.04
3:S:434:ALA:HB1	3:S:587:LYS:HE2	1.07	1.04
3:S:563:MET:CE	3:S:567:LEU:HD13	1.86	1.04
1:A:22:CYS:CB	1:A:92:CYS:SG	2.45	1.04
3:S:563:MET:CE	3:S:567:LEU:CD1	2.34	1.03
1:A:207:ASP:O	1:A:208:LYS:CD	2.05	1.03
3:S:392:THR:OG1	3:S:492:THR:OG1	1.73	1.03
2:B:198:HIS:ND1	2:B:200:THR:HG23	1.73	1.03
3:S:409:TYR:HD1	3:S:409:TYR:H	1.05	1.03
3:S:448:TYR:CE1	3:S:464:ILE:CD1	2.41	1.03
3:S:584:VAL:O	3:S:584:VAL:HG13	1.55	1.03
3:R:488:LEU:HD23	3:R:490:THR:HG23	1.40	1.03
1:A:84:SER:O	1:A:87:THR:OG1	1.76	1.03
2:B:105:GLU:OE1	2:B:173:TYR:OH	1.75	1.02
2:L:83:ILE:HD11	2:L:106:LEU:HD13	1.40	1.02
3:S:396:VAL:CG2	3:S:446:PHE:CD1	2.41	1.02
3:S:506:PHE:HD2	3:S:506:PHE:N	1.58	1.02
3:R:382:GLU:OE2	3:R:587:LYS:NZ	1.91	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CZ	1:A:82:MET:HE3	1.91	1.02
2:B:181:LEU:HD23	2:B:181:LEU:N	1.53	1.01
3:R:389:LEU:HA	3:R:491:ILE:HD11	1.40	1.01
3:R:411:LEU:O	3:R:415:LEU:CD2	2.08	1.01
2:B:211:ARG:HG3	2:B:211:ARG:NH1	1.65	1.01
3:R:382:GLU:OE2	3:R:413:LYS:NZ	1.93	1.01
3:S:437:CYS:SG	3:S:585:CYS:HB2	1.98	1.00
3:S:505:ARG:C	3:S:506:PHE:CD2	2.34	1.00
2:B:211:ARG:HG3	2:B:211:ARG:HH11	0.85	1.00
2:B:211:ARG:HH11	2:B:211:ARG:CG	1.73	1.00
1:H:169:VAL:HG11	2:L:160:LEU:HD23	1.42	1.00
2:B:30:ASN:O	2:B:31:ASN:HB2	1.57	1.00
1:A:173:ASP:O	1:A:174:LEU:HD23	1.61	1.00
2:L:198:HIS:ND1	2:L:200:THR:HG23	1.76	1.00
2:B:188:ARG:HB2	2:B:189:HIS:CE1	1.96	1.00
1:A:173:ASP:C	1:A:174:LEU:CD2	2.30	1.00
3:S:505:ARG:C	3:S:506:PHE:HD2	1.64	1.00
2:B:190:ASN:OD1	2:B:210:ASN:CB	2.09	1.00
1:H:55:THR:CG2	1:H:56:TYR:CD1	2.44	0.99
2:B:21:ILE:HG22	2:B:21:ILE:O	1.60	0.99
3:S:519:ASN:HD22	3:S:522:GLN:NE2	1.60	0.99
1:A:67:PHE:CZ	1:A:82:MET:HE1	1.97	0.99
1:A:152:LEU:C	1:A:152:LEU:CD2	2.30	0.99
3:S:507:LEU:H	3:S:507:LEU:HD12	0.83	0.99
1:H:94:ARG:NH2	1:H:101:ASP:CG	2.15	0.99
2:L:195:GLU:HG3	2:L:206:VAL:HG22	1.44	0.99
3:S:395:GLN:NE2	3:S:498:SER:N	2.08	0.99
3:R:415:LEU:HD23	3:R:415:LEU:H	1.27	0.98
2:B:90:GLN:HG3	2:B:90:GLN:O	1.64	0.98
2:B:124:GLN:HA	1:A:122:TYR:HE1	1.26	0.98
2:B:160:LEU:CD1	1:A:169:VAL:HG11	1.93	0.98
2:B:179:LEU:HD12	2:B:179:LEU:C	1.71	0.98
1:H:152:LEU:C	1:H:152:LEU:CD2	2.30	0.98
3:S:434:ALA:O	3:S:587:LYS:HE3	1.61	0.98
1:A:152:LEU:CD2	1:A:153:THR:N	2.26	0.97
1:A:87:THR:HG23	1:A:111:VAL:H	1.27	0.97
2:L:83:ILE:CG1	2:L:106:LEU:CD1	2.42	0.97
3:S:448:TYR:HE1	3:S:464:ILE:CD1	1.76	0.97
1:A:177:LEU:HD23	1:A:178:SER:CA	1.94	0.97
3:S:497:TYR:CE1	3:S:563:MET:SD	2.58	0.97
1:H:22:CYS:SG	1:H:92:CYS:CB	2.51	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:554:LEU:HD12	3:S:554:LEU:C	1.80	0.97
2:L:124:GLN:NE2	2:L:131:SER:OG	1.96	0.96
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.47	0.96
3:S:545:LEU:HB2	3:S:552:GLY:O	1.65	0.96
3:R:388:LEU:HD11	3:R:571:PHE:HE1	1.30	0.96
1:H:55:THR:CG2	1:H:56:TYR:HE1	1.72	0.96
2:B:133:VAL:HG22	2:B:178:THR:HG23	1.46	0.96
3:R:452:MET:O	3:R:455:ASP:OD2	1.82	0.95
1:A:84:SER:HA	1:A:111:VAL:CG1	1.95	0.95
3:R:415:LEU:CD2	3:R:415:LEU:N	2.29	0.95
3:R:437:CYS:HG	3:R:585:CYS:CB	1.73	0.95
1:A:87:THR:CG2	1:A:110:THR:HA	1.97	0.95
2:B:180:THR:O	2:B:181:LEU:CD2	2.14	0.95
2:B:124:GLN:CB	1:A:122:TYR:CD1	2.49	0.95
1:A:177:LEU:C	1:A:177:LEU:CD2	2.29	0.95
2:L:36:TYR:HE2	2:L:89:GLN:HE21	1.02	0.95
3:S:480:ILE:C	3:S:481:LEU:CD2	2.34	0.95
3:R:421:ASN:HD22	3:R:421:ASN:N	1.59	0.94
2:B:183:LYS:HZ2	2:B:183:LYS:HB2	1.29	0.94
3:R:439:SER:OG	3:R:576:GLN:O	1.82	0.94
1:A:152:LEU:HD23	1:A:153:THR:CA	1.96	0.94
1:H:55:THR:HG22	1:H:56:TYR:HD1	1.18	0.94
3:S:396:VAL:CG2	3:S:446:PHE:CE1	2.49	0.94
3:S:448:TYR:CE1	3:S:464:ILE:HD13	2.02	0.94
1:A:58:TYR:HD2	1:A:58:TYR:N	1.62	0.94
1:A:177:LEU:CD2	1:A:178:SER:N	2.30	0.94
3:S:408:ASN:HD22	3:S:408:ASN:N	1.63	0.94
3:R:456:LEU:HD23	3:R:456:LEU:C	1.88	0.94
2:B:124:GLN:CA	1:A:122:TYR:HE1	1.81	0.94
1:H:186:SER:O	1:H:190:SER:OG	1.86	0.94
3:R:488:LEU:CD2	3:R:490:THR:CG2	2.43	0.93
1:H:64:LYS:CD	1:H:65:GLY:N	2.30	0.93
3:S:438:TYR:CB	3:S:575:VAL:HG21	1.98	0.93
1:H:51:ILE:CG2	1:H:69:ILE:HD13	1.98	0.93
3:S:481:LEU:N	3:S:481:LEU:CD2	2.30	0.93
3:S:545:LEU:N	3:S:545:LEU:CD2	2.30	0.93
3:R:519:ASN:CB	3:R:522:GLN:HE21	1.80	0.93
1:A:124:LEU:N	1:A:124:LEU:CD2	2.29	0.93
2:L:147:LYS:HD2	2:L:154:GLU:CD	1.88	0.93
1:H:63:VAL:HG13	1:H:63:VAL:O	1.64	0.93
2:L:36:TYR:CE2	2:L:89:GLN:NE2	2.36	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:411:LEU:HD23	3:S:411:LEU:C	1.88	0.93
3:S:504:SER:HB3	3:S:506:PHE:CE2	2.03	0.92
3:S:519:ASN:HD22	3:S:522:GLN:HE22	1.02	0.92
3:S:385:PHE:HE2	3:S:409:TYR:HB2	1.34	0.92
3:S:395:GLN:HE22	3:S:498:SER:N	1.67	0.92
2:B:155:ARG:HH11	2:B:155:ARG:HG3	1.35	0.92
1:H:137:THR:HG23	1:H:182:THR:OG1	1.70	0.92
3:R:415:LEU:CD2	3:R:415:LEU:H	1.81	0.92
2:L:110:ASP:OD2	2:L:199:LYS:NZ	2.03	0.92
1:H:94:ARG:HH21	1:H:101:ASP:CB	1.82	0.92
1:A:75:GLU:OE1	1:A:75:GLU:HA	1.70	0.91
3:S:496:LYS:NZ	3:S:535:TRP:O	2.03	0.91
3:S:448:TYR:CE1	3:S:464:ILE:HD11	2.05	0.91
3:S:448:TYR:OH	3:S:464:ILE:CD1	2.19	0.91
3:R:414:LEU:HB3	3:R:415:LEU:HD22	1.51	0.91
2:B:160:LEU:HD13	1:A:169:VAL:CG1	2.00	0.91
2:L:124:GLN:HE22	2:L:131:SER:HG	1.19	0.90
2:L:36:TYR:CZ	2:L:89:GLN:NE2	2.40	0.90
3:S:434:ALA:HB1	3:S:587:LYS:HE3	1.51	0.90
1:A:174:LEU:N	1:A:174:LEU:CD2	2.32	0.90
2:L:83:ILE:CD1	2:L:106:LEU:HD13	2.01	0.90
2:L:198:HIS:ND1	2:L:200:THR:CG2	2.34	0.89
2:B:183:LYS:HG3	2:B:184:ASP:N	1.78	0.89
1:H:52(A):SER:OG	3:R:539:ASP:OD1	1.89	0.89
2:L:80:GLN:O	2:L:83:ILE:HD12	1.71	0.89
3:S:438:TYR:HB3	3:S:575:VAL:CG2	2.01	0.89
1:H:185:SER:O	1:H:188:TRP:O	1.88	0.89
3:S:434:ALA:O	3:S:587:LYS:HG3	1.73	0.89
1:H:63:VAL:CG2	1:H:67:PHE:CE2	2.55	0.89
2:B:96:PRO:HD3	1:A:47:TRP:CE3	2.08	0.89
3:S:395:GLN:NE2	3:S:498:SER:OG	2.05	0.89
2:B:179:LEU:HD12	2:B:180:THR:H	1.38	0.89
1:H:38:ARG:NH2	1:H:46:GLU:OE2	2.04	0.88
1:A:67:PHE:CZ	1:A:82:MET:HE2	2.07	0.88
3:R:488:LEU:HD21	3:R:490:THR:CG2	2.02	0.88
3:S:544:GLN:C	3:S:545:LEU:CD2	2.41	0.88
2:B:38:GLN:O	2:B:84:ALA:HB1	1.73	0.88
1:A:60:PRO:HD2	1:A:63:VAL:CG2	2.04	0.88
1:A:57:THR:C	1:A:58:TYR:HD2	1.70	0.88
2:B:192:TYR:N	2:B:192:TYR:HD1	1.72	0.87
3:R:509:ASP:O	3:R:510:ASP:HB2	1.71	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:O	1:A:111:VAL:HG11	1.74	0.87
3:S:497:TYR:HB2	3:S:561:VAL:O	1.75	0.87
2:B:155:ARG:HH11	2:B:155:ARG:HG2	1.36	0.87
3:S:449:PRO:HB3	3:S:497:TYR:CD2	2.10	0.87
3:S:434:ALA:CB	3:S:587:LYS:CE	2.50	0.87
3:S:548:LEU:C	3:S:548:LEU:CD1	2.40	0.87
3:R:389:LEU:CA	3:R:491:ILE:HD11	2.04	0.87
2:B:38:GLN:NE2	2:B:42:GLY:HA2	1.90	0.87
1:H:169:VAL:HG11	2:L:160:LEU:CD2	2.04	0.86
3:S:480:ILE:O	3:S:481:LEU:HD23	1.75	0.86
2:B:33:LEU:HD12	2:B:89:GLN:O	1.74	0.86
2:B:89:GLN:HG2	2:B:90:GLN:N	1.90	0.86
2:B:124:GLN:HB2	1:A:122:TYR:HD1	1.31	0.86
1:H:64:LYS:HD2	1:H:65:GLY:N	1.91	0.86
3:S:501:ASN:ND2	3:S:557:SER:OG	2.09	0.85
1:H:87:THR:HG23	1:H:111:VAL:H	1.40	0.85
3:S:450:LEU:HD12	3:S:568:GLN:OE1	1.76	0.85
2:B:137:ASN:OD1	2:B:174:SER:HB3	1.76	0.85
1:A:67:PHE:CE2	1:A:82:MET:CE	2.58	0.85
2:B:61:ARG:NH2	2:B:79:GLU:OE1	2.08	0.85
2:B:183:LYS:CB	2:B:183:LYS:NZ	2.37	0.85
1:A:40:THR:O	1:A:42:GLU:N	2.10	0.85
3:S:434:ALA:CB	3:S:587:LYS:HE2	2.02	0.85
3:R:410:ASN:O	3:R:413:LYS:N	2.08	0.85
2:B:188:ARG:HB2	2:B:189:HIS:ND1	1.92	0.85
1:H:55:THR:HG21	1:H:56:TYR:HE1	1.42	0.85
3:S:508:SER:O	3:S:509:ASP:C	2.12	0.85
1:A:87:THR:HG23	1:A:111:VAL:N	1.90	0.85
3:S:519:ASN:HB2	3:S:522:GLN:HE21	0.76	0.85
3:S:563:MET:CE	3:S:567:LEU:HD12	2.05	0.85
3:R:498:SER:HB3	3:R:534:VAL:HG23	1.57	0.85
2:B:160:LEU:CD1	1:A:169:VAL:CG1	2.54	0.85
1:A:67:PHE:CE2	1:A:82:MET:HE3	2.11	0.85
3:R:488:LEU:HD23	3:R:490:THR:CG2	2.07	0.84
2:L:155:ARG:HG3	2:L:155:ARG:NH2	1.78	0.84
1:A:60:PRO:HD2	1:A:63:VAL:HG22	1.57	0.84
3:S:499:TYR:C	3:S:499:TYR:CD2	2.50	0.84
1:A:58:TYR:CD2	1:A:58:TYR:N	2.31	0.84
1:H:72:ASP:CG	1:H:75:GLU:HB2	1.97	0.84
3:S:395:GLN:HE22	3:S:498:SER:H	0.87	0.84
2:B:179:LEU:HD11	2:B:181:LEU:HD21	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:586:PRO:O	3:S:587:LYS:HG3	1.78	0.83
1:H:67:PHE:HE1	1:H:82:MET:HB3	1.43	0.83
1:H:166:PHE:O	1:H:177:LEU:CD1	2.26	0.83
2:B:183:LYS:HZ2	2:B:183:LYS:CB	1.91	0.83
3:S:499:TYR:C	3:S:499:TYR:HD2	1.82	0.83
3:S:448:TYR:OH	3:S:464:ILE:HD12	1.79	0.83
2:L:155:ARG:CG	2:L:155:ARG:NH2	2.31	0.82
1:A:11:LEU:O	1:A:12:VAL:HG12	1.79	0.82
3:S:440:SER:O	3:S:575:VAL:HG23	1.79	0.82
1:A:188:TRP:CG	1:A:189:PRO:HA	2.14	0.82
3:S:411:LEU:CD2	3:S:415:LEU:CD1	2.56	0.82
3:S:545:LEU:HG	3:S:552:GLY:O	1.80	0.82
1:H:29:PHE:CE2	1:H:71:ARG:NH1	2.47	0.82
2:B:49:TYR:OH	2:B:53:ARG:NH1	2.12	0.82
1:H:48:VAL:O	1:H:60:PRO:HD2	1.79	0.82
1:H:63:VAL:HG21	1:H:67:PHE:CD2	2.13	0.82
3:S:437:CYS:HA	3:S:585:CYS:CB	2.09	0.82
2:B:192:TYR:N	2:B:192:TYR:CD1	2.47	0.82
3:R:388:LEU:HD11	3:R:571:PHE:CE1	2.15	0.82
1:H:64:LYS:HD3	1:H:65:GLY:N	1.95	0.81
1:H:51:ILE:HG22	1:H:69:ILE:CD1	2.09	0.81
2:L:108:ARG:HD2	2:L:171:SER:HB2	1.61	0.81
1:H:42:GLU:O	1:H:43:LYS:HB2	1.81	0.81
1:A:83:ARG:C	1:A:111:VAL:HG11	1.99	0.81
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.63	0.81
2:B:47:LEU:O	2:B:48:ILE:HD12	1.81	0.81
1:A:173:ASP:O	1:A:174:LEU:CD2	2.29	0.81
1:H:55:THR:HG21	1:H:56:TYR:CE1	2.16	0.80
1:H:94:ARG:NH2	1:H:101:ASP:CB	2.43	0.80
3:R:389:LEU:O	3:R:491:ILE:HD12	1.78	0.80
2:B:124:GLN:CA	1:A:122:TYR:CE1	2.61	0.80
3:S:450:LEU:CD1	3:S:568:GLN:CD	2.49	0.80
2:L:22:ILE:O	2:L:22:ILE:CG1	2.30	0.80
3:S:438:TYR:CB	3:S:575:VAL:CG2	2.59	0.80
3:S:461:ALA:O	3:S:466:GLN:NE2	2.14	0.80
1:A:11:LEU:O	1:A:12:VAL:CG1	2.30	0.80
1:A:75:GLU:OE1	1:A:75:GLU:CA	2.30	0.80
1:H:75:GLU:OE2	1:H:75:GLU:CA	2.30	0.80
3:S:503:CYS:SG	3:S:526:CYS:HB2	2.21	0.80
3:S:526:CYS:SG	3:S:554:LEU:HD11	2.22	0.80
3:S:496:LYS:NZ	3:S:534:VAL:O	2.14	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:545:LEU:CB	3:S:552:GLY:O	2.30	0.79
3:S:586:PRO:O	3:S:587:LYS:CG	2.30	0.79
3:R:518:VAL:HG23	3:R:519:ASN:O	1.81	0.79
2:B:79:GLU:O	2:B:82:ASP:HB2	1.82	0.79
1:A:120:SER:OG	1:A:122:TYR:CE2	2.36	0.79
2:B:124:GLN:HA	1:A:122:TYR:CE1	2.14	0.79
1:H:69:ILE:O	1:H:69:ILE:CG2	2.30	0.79
2:L:81:GLU:O	2:L:81:GLU:HG3	1.82	0.79
3:S:385:PHE:CE2	3:S:409:TYR:HB2	2.17	0.79
3:S:448:TYR:CZ	3:S:464:ILE:CD1	2.66	0.79
3:S:499:TYR:CZ	3:S:559:SER:HB2	2.18	0.79
2:B:131:SER:HB3	2:B:180:THR:HG23	1.64	0.79
2:L:21:ILE:HD13	2:L:102:THR:HG21	1.65	0.79
3:S:480:ILE:O	3:S:481:LEU:CD2	2.30	0.79
2:B:189:HIS:ND1	2:B:189:HIS:N	2.30	0.79
1:A:207:ASP:O	1:A:208:LYS:HD2	1.83	0.79
2:L:211:ARG:O	2:L:212:ASN:HB2	1.81	0.78
3:R:423:PHE:HD1	3:R:423:PHE:C	1.86	0.78
3:R:493:LYS:NZ	3:R:565:GLU:O	2.15	0.78
2:L:20:THR:HG22	2:L:20:THR:O	1.82	0.78
2:L:22:ILE:O	2:L:22:ILE:HG13	1.83	0.78
3:S:408:ASN:HD22	3:S:408:ASN:H	1.32	0.78
3:S:506:PHE:HB3	3:S:511:ARG:HG3	1.65	0.78
3:R:421:ASN:ND2	3:R:421:ASN:N	2.29	0.78
1:A:87:THR:HG22	1:A:110:THR:HA	1.64	0.78
2:B:124:GLN:CB	1:A:122:TYR:HE1	1.91	0.78
3:S:499:TYR:CE2	3:S:559:SER:HB2	2.18	0.78
3:S:584:VAL:O	3:S:584:VAL:CG1	2.30	0.78
3:S:553:TRP:N	3:S:553:TRP:CD1	2.48	0.78
1:H:37:VAL:HG21	1:H:99:MET:CE	2.14	0.78
2:B:68:GLY:O	2:B:71:TYR:OH	2.00	0.78
2:L:211:ARG:O	2:L:212:ASN:CB	2.32	0.78
3:R:415:LEU:N	3:R:415:LEU:HD22	1.98	0.77
3:S:448:TYR:HE1	3:S:464:ILE:HD11	1.41	0.77
3:S:504:SER:HB3	3:S:506:PHE:CZ	2.19	0.77
3:S:388:LEU:HG	3:S:389:LEU:N	2.00	0.77
1:A:210:ILE:HD12	1:A:210:ILE:C	2.05	0.77
3:S:389:LEU:O	3:S:491:ILE:HD11	1.84	0.77
3:R:456:LEU:C	3:R:456:LEU:CD2	2.53	0.77
2:L:105:GLU:OE1	2:L:142:LYS:HE3	1.85	0.77
3:S:548:LEU:O	3:S:548:LEU:CD1	2.30	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:564:THR:OG1	3:S:566:GLN:N	2.18	0.77
3:S:395:GLN:CD	3:S:498:SER:OG	2.23	0.76
3:S:409:TYR:HD1	3:S:409:TYR:N	1.83	0.76
3:R:519:ASN:CB	3:R:522:GLN:NE2	2.44	0.76
1:A:111:VAL:HG12	1:A:111:VAL:O	1.85	0.76
1:A:210:ILE:CD1	1:A:210:ILE:O	2.30	0.76
3:S:411:LEU:CD2	3:S:411:LEU:C	2.54	0.76
1:H:69:ILE:O	1:H:69:ILE:HG23	1.85	0.76
2:L:51:THR:HG23	2:L:71:TYR:HD1	1.49	0.76
1:H:55:THR:C	1:H:56:TYR:HD1	1.90	0.76
3:R:457:SER:OG	3:R:458:VAL:CG2	2.30	0.76
3:S:408:ASN:N	3:S:408:ASN:ND2	2.30	0.76
1:H:160:SER:C	1:H:163:VAL:CG2	2.54	0.75
2:B:2:ILE:HD11	2:B:27:GLN:OE1	1.86	0.75
1:A:71:ARG:HD2	1:A:73:ASN:OD1	1.86	0.75
3:S:456:LEU:HD13	3:S:479:LEU:HD21	1.66	0.75
3:S:464:ILE:HG22	3:S:465:SER:N	1.99	0.75
3:S:545:LEU:CG	3:S:552:GLY:O	2.35	0.75
2:L:2:ILE:O	2:L:97:THR:HG21	1.87	0.75
3:R:423:PHE:C	3:R:423:PHE:CD1	2.58	0.75
3:S:408:ASN:H	3:S:408:ASN:ND2	1.85	0.75
2:B:133:VAL:CG2	2:B:178:THR:HG23	2.17	0.75
1:H:140:CYS:CB	1:H:195:CYS:SG	2.74	0.74
3:R:498:SER:HB3	3:R:534:VAL:CG2	2.17	0.74
3:S:564:THR:OG1	3:S:566:GLN:C	2.26	0.74
1:H:160:SER:C	1:H:163:VAL:HG21	2.08	0.74
3:S:506:PHE:N	3:S:506:PHE:CD2	2.30	0.74
3:R:456:LEU:HD22	3:R:479:LEU:HD21	1.69	0.74
3:S:386:SER:OG	3:S:387:PRO:CD	2.30	0.74
2:B:191:SER:C	2:B:192:TYR:HD1	1.91	0.74
3:S:386:SER:HG	3:S:387:PRO:HD3	1.50	0.74
1:H:63:VAL:O	1:H:63:VAL:CG1	2.34	0.73
3:R:420:VAL:C	3:R:421:ASN:ND2	2.36	0.73
1:H:52:SER:HB3	3:R:536:GLU:HB2	1.70	0.73
3:S:519:ASN:ND2	3:S:522:GLN:NE2	2.34	0.73
1:H:93:VAL:CG1	1:H:99:MET:HG2	2.14	0.73
1:H:166:PHE:O	1:H:177:LEU:HD12	1.87	0.73
2:L:28:ASP:OD1	2:L:29:ILE:N	2.22	0.73
3:S:497:TYR:HE1	3:S:563:MET:SD	2.11	0.73
2:B:138:ASN:ND2	2:B:172:THR:OG1	2.22	0.73
2:L:195:GLU:CG	2:L:206:VAL:HG22	2.18	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HH22	1:A:86:ASP:CG	1.91	0.72
1:H:64:LYS:HD3	1:H:65:GLY:H	1.53	0.72
3:S:463:PRO:HA	3:S:466:GLN:HB2	1.71	0.72
1:A:40:THR:O	1:A:43:LYS:N	2.22	0.72
1:A:123:PRO:CA	1:A:124:LEU:HD23	2.19	0.72
2:L:136:LEU:C	2:L:137:ASN:HD22	1.93	0.72
1:A:20:LEU:HB2	1:A:80:LEU:HB3	1.71	0.72
3:R:392:THR:HG1	3:R:492:THR:CB	2.02	0.72
2:L:33:LEU:HD23	2:L:34:ASN:N	2.05	0.72
1:A:123:PRO:C	1:A:124:LEU:CD2	2.54	0.72
2:L:29:ILE:HA	2:L:92:ASN:HD22	1.55	0.72
2:L:19:VAL:CG1	2:L:78:LEU:HD21	2.20	0.71
3:S:449:PRO:HB3	3:S:497:TYR:CE2	2.24	0.71
3:S:586:PRO:O	3:S:587:LYS:CB	2.36	0.71
1:A:87:THR:HG23	1:A:110:THR:HA	1.72	0.71
2:B:185:GLU:O	2:B:188:ARG:HG2	1.90	0.71
2:B:155:ARG:CG	2:B:155:ARG:NH1	2.35	0.71
1:A:188:TRP:CE2	1:A:210:ILE:HD13	2.24	0.71
1:H:67:PHE:CD1	1:H:82:MET:HB3	2.26	0.71
3:S:553:TRP:HD1	3:S:553:TRP:H	1.38	0.71
1:A:29:PHE:CE2	1:A:71:ARG:NH1	2.58	0.71
1:H:87:THR:CG2	1:H:111:VAL:H	2.02	0.71
1:A:169:VAL:HG12	1:A:169:VAL:O	1.90	0.71
3:R:389:LEU:C	3:R:491:ILE:CD1	2.59	0.71
1:H:63:VAL:HG22	1:H:67:PHE:CE2	2.20	0.70
1:A:111:VAL:CG1	1:A:111:VAL:O	2.38	0.70
4:R:602:NAG:C1	4:R:602:NAG:O7	2.39	0.70
2:L:124:GLN:HG2	2:L:129:GLY:O	1.91	0.70
3:S:421:ASN:C	3:S:422:ASP:OD2	2.30	0.70
3:R:569:MET:CE	3:R:571:PHE:CZ	2.74	0.70
2:L:156:GLN:O	2:L:159:VAL:HG23	1.90	0.70
2:B:124:GLN:CG	1:A:122:TYR:CE1	2.74	0.70
2:B:211:ARG:NH1	2:B:211:ARG:CG	2.39	0.70
1:H:94:ARG:NH2	1:H:101:ASP:HB3	2.07	0.70
1:H:155:ASN:O	1:H:158:SER:HB3	1.92	0.70
3:S:501:ASN:OD1	3:S:501:ASN:C	2.30	0.70
3:S:504:SER:HB3	3:S:506:PHE:HE2	1.56	0.70
3:S:448:TYR:CZ	3:S:464:ILE:HD13	2.27	0.70
3:R:494:PRO:HD2	3:R:567:LEU:HD13	1.73	0.69
1:H:37:VAL:HG21	1:H:99:MET:HE1	1.75	0.69
2:L:90:GLN:C	2:L:90:GLN:OE1	2.30	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:421:ASN:OD1	3:S:450:LEU:HD22	1.86	0.69
1:A:206:VAL:HG12	1:A:207:ASP:N	2.07	0.69
3:R:389:LEU:C	3:R:491:ILE:HD11	2.12	0.69
1:A:18:LEU:CD2	1:A:20:LEU:HD21	2.22	0.69
1:H:42:GLU:O	1:H:43:LYS:CB	2.37	0.69
2:L:83:ILE:CD1	2:L:106:LEU:CD1	2.68	0.69
1:H:63:VAL:HG21	1:H:67:PHE:HD2	1.58	0.69
3:S:385:PHE:CE2	3:S:409:TYR:HD2	2.03	0.69
3:S:411:LEU:CD2	3:S:415:LEU:HD12	2.22	0.69
3:R:522:GLN:HG3	3:R:523:TYR:N	2.07	0.69
2:B:96:PRO:HD2	2:B:96:PRO:O	1.90	0.69
2:L:20:THR:O	2:L:20:THR:CG2	2.38	0.69
3:R:487:ASN:OD1	3:R:487:ASN:N	2.26	0.69
2:B:124:GLN:HG3	1:A:122:TYR:CE1	2.28	0.69
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.23	0.69
1:H:72:ASP:OD1	1:H:72:ASP:C	2.29	0.68
3:S:563:MET:HE3	3:S:567:LEU:HD12	1.74	0.68
2:B:96:PRO:CD	1:A:47:TRP:CE3	2.76	0.68
1:H:172:SER:O	1:H:173:ASP:HB2	1.92	0.68
2:B:186:TYR:HE1	2:B:192:TYR:CE2	2.10	0.68
1:A:171:GLN:O	1:A:172:SER:C	2.30	0.68
2:L:155:ARG:HH21	2:L:155:ARG:HG2	1.56	0.68
3:S:411:LEU:HD21	3:S:415:LEU:HD12	1.74	0.68
3:S:508:SER:O	3:S:510:ASP:HA	1.92	0.68
3:R:411:LEU:O	3:R:415:LEU:HD21	1.92	0.68
2:B:19:VAL:HG12	2:B:19:VAL:O	1.93	0.68
1:A:119:PRO:CA	1:A:145:TYR:HB3	2.24	0.68
1:H:38:ARG:NE	1:H:46:GLU:OE2	2.26	0.68
2:L:28:ASP:OD1	2:L:28:ASP:C	2.30	0.68
3:S:450:LEU:CD1	3:S:568:GLN:CG	2.72	0.68
1:H:63:VAL:CG2	1:H:67:PHE:HD2	2.05	0.68
1:H:166:PHE:O	1:H:177:LEU:HD11	1.92	0.68
1:A:11:LEU:C	1:A:12:VAL:HG13	2.12	0.68
3:R:438:TYR:CD1	3:R:575:VAL:HG21	2.28	0.68
3:R:569:MET:HE2	3:R:571:PHE:CZ	2.29	0.68
3:S:449:PRO:HB3	3:S:497:TYR:HD2	1.57	0.68
2:L:136:LEU:N	2:L:136:LEU:HD12	2.08	0.67
2:L:106:LEU:N	2:L:106:LEU:HD12	2.09	0.67
2:B:155:ARG:HG3	2:B:155:ARG:NH1	2.04	0.67
1:A:188:TRP:NE1	1:A:210:ILE:HD11	1.94	0.67
2:B:80:GLN:O	2:B:82:ASP:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HB2	1:A:147:PRO:HG3	1.75	0.67
3:R:485:PRO:HB3	4:R:601:NAG:O7	1.95	0.67
2:B:38:GLN:HE21	2:B:42:GLY:HA2	1.56	0.67
2:L:48:ILE:HG23	2:L:53:ARG:O	1.94	0.67
1:H:34:MET:CE	1:H:94:ARG:HG3	2.24	0.67
3:S:388:LEU:H	3:S:388:LEU:HD23	1.60	0.67
1:H:154:TRP:HB3	1:H:159:LEU:HD23	1.77	0.67
1:A:145:TYR:CZ	1:A:150:VAL:HG11	2.31	0.66
1:H:29:PHE:CD2	1:H:71:ARG:NH1	2.64	0.66
3:S:450:LEU:HD13	3:S:568:GLN:CD	2.14	0.66
1:H:51:ILE:HG21	1:H:69:ILE:HD13	1.77	0.66
1:A:11:LEU:C	1:A:12:VAL:CG1	2.63	0.66
1:H:51:ILE:CG2	1:H:69:ILE:CD1	2.67	0.66
3:S:395:GLN:CG	3:S:498:SER:OG	2.44	0.66
1:H:184:THR:OG1	1:H:187:THR:OG1	2.12	0.65
2:L:206:VAL:O	2:L:207:LYS:HD2	1.95	0.65
3:S:543:LYS:HG2	2:B:49:TYR:CZ	2.32	0.65
3:R:456:LEU:CD2	3:R:479:LEU:HD21	2.25	0.65
1:A:67:PHE:CE1	1:A:82:MET:CE	2.77	0.65
1:H:87:THR:HG23	1:H:111:VAL:N	2.09	0.65
3:S:434:ALA:CB	3:S:587:LYS:HE3	2.20	0.65
3:S:448:TYR:OH	3:S:464:ILE:HD13	1.96	0.65
3:R:498:SER:CB	3:R:534:VAL:HG23	2.26	0.65
3:R:509:ASP:OD2	3:R:510:ASP:N	2.30	0.65
2:B:186:TYR:CE1	2:B:192:TYR:CE2	2.84	0.65
3:S:501:ASN:OD1	3:S:502:LYS:N	2.30	0.65
2:B:70:ASP:C	2:B:71:TYR:CD2	2.70	0.65
3:S:507:LEU:O	3:S:509:ASP:O	2.15	0.65
2:L:81:GLU:O	2:L:81:GLU:CG	2.44	0.65
3:S:450:LEU:HD12	3:S:450:LEU:H	1.62	0.65
2:B:160:LEU:HD21	1:A:171:GLN:NE2	2.11	0.65
2:L:190:ASN:O	2:L:190:ASN:ND2	2.30	0.65
3:R:456:LEU:HD22	3:R:479:LEU:CD2	2.27	0.65
2:B:80:GLN:C	2:B:82:ASP:H	2.00	0.65
1:H:42:GLU:N	1:H:42:GLU:OE1	2.30	0.64
3:S:422:ASP:OD2	3:S:422:ASP:N	2.30	0.64
1:A:101:ASP:OD2	1:A:101:ASP:N	2.30	0.64
3:S:450:LEU:CD1	3:S:568:GLN:OE1	2.42	0.64
1:A:67:PHE:HZ	1:A:82:MET:CE	1.97	0.64
3:R:426:SER:O	3:R:427:GLN:HB2	1.96	0.64
3:R:452:MET:C	3:R:455:ASP:OD2	2.35	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH2	1:A:86:ASP:OD1	2.29	0.64
2:L:108:ARG:NH1	2:L:109:ALA:O	2.30	0.64
1:A:87:THR:CG2	1:A:111:VAL:H	2.04	0.64
3:S:505:ARG:N	3:S:514:VAL:O	2.27	0.64
2:B:77:ASN:O	2:B:77:ASN:ND2	2.30	0.64
1:A:145:TYR:CZ	1:A:150:VAL:CG1	2.80	0.64
2:L:105:GLU:OE1	2:L:142:LYS:CE	2.46	0.64
3:S:395:GLN:HG3	3:S:498:SER:OG	1.97	0.64
3:S:397:TYR:CD1	3:S:500:ILE:HG13	2.33	0.64
3:S:409:TYR:N	3:S:409:TYR:CD1	2.56	0.64
2:L:14:SER:N	2:L:17:ASP:OD2	2.30	0.64
3:S:554:LEU:C	3:S:554:LEU:CD1	2.56	0.64
1:A:67:PHE:CE2	1:A:82:MET:HE1	2.30	0.64
2:L:108:ARG:HD3	2:L:172:THR:HG22	1.81	0.63
1:A:51:ILE:HB	1:A:69:ILE:HD13	1.80	0.63
3:S:411:LEU:CD2	3:S:415:LEU:CG	2.54	0.63
1:H:37:VAL:HG21	1:H:99:MET:HE2	1.79	0.63
1:A:22:CYS:SG	1:A:92:CYS:CB	2.77	0.63
3:S:473:PHE:HD2	3:S:473:PHE:H	1.45	0.63
3:R:437:CYS:SG	3:R:585:CYS:SG	0.64	0.63
3:R:441:LEU:HB2	3:R:584:VAL:HG11	1.81	0.63
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.81	0.63
3:S:480:ILE:HB	3:S:571:PHE:HB2	1.79	0.63
1:H:119:PRO:CB	1:H:145:TYR:HB3	2.27	0.63
2:B:160:LEU:HD12	1:A:169:VAL:HG11	1.81	0.63
3:S:408:ASN:HB3	3:S:585:CYS:O	1.99	0.63
2:B:183:LYS:CD	2:B:187:GLU:CD	2.68	0.63
1:A:19:LYS:C	1:A:20:LEU:HD23	2.19	0.63
1:H:152:LEU:HD23	1:H:153:THR:CA	2.29	0.62
3:R:518:VAL:CG2	3:R:519:ASN:O	2.47	0.62
3:R:580:ASP:OD1	3:R:580:ASP:N	2.29	0.62
2:B:98:PHE:N	2:B:98:PHE:CD1	2.66	0.62
1:A:119:PRO:HB3	1:A:145:TYR:CB	2.29	0.62
2:B:183:LYS:CG	2:B:184:ASP:N	2.56	0.62
3:S:383:CYS:SG	3:S:409:TYR:HB3	2.40	0.62
1:A:152:LEU:HA	1:A:196:ASN:O	2.00	0.62
2:L:89:GLN:HG2	2:L:90:GLN:N	2.13	0.62
2:B:71:TYR:CD2	2:B:71:TYR:N	2.66	0.62
2:B:131:SER:CB	2:B:180:THR:HG23	2.27	0.62
3:R:396:VAL:CG2	3:R:468:ASN:HB3	2.30	0.62
3:R:491:ILE:CD1	3:R:491:ILE:N	2.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:VAL:CG1	2:B:134:CYS:N	2.62	0.62
2:L:33:LEU:HD12	2:L:71:TYR:CD2	2.34	0.62
2:L:76:SER:O	2:L:77:ASN:C	2.32	0.62
3:R:428:ILE:CG2	3:R:429:SER:N	2.62	0.62
1:H:132:THR:OG1	1:H:133:GLY:N	2.30	0.62
3:S:438:TYR:CD1	3:S:575:VAL:HG21	2.31	0.62
1:A:19:LYS:HD2	1:A:81:GLN:OE1	2.00	0.62
2:L:118:PHE:HE2	2:L:135:PHE:CD2	2.18	0.62
1:A:70:SER:OG	1:A:79:TYR:HB2	2.00	0.62
3:S:407:CYS:O	3:S:584:VAL:HA	2.00	0.61
2:L:161:ASN:OD1	2:L:177:SER:HB2	1.99	0.61
3:S:386:SER:O	3:S:389:LEU:HB2	2.00	0.61
2:L:49:TYR:O	2:L:53:ARG:HB2	2.00	0.61
2:B:76:SER:O	2:B:77:ASN:C	2.35	0.61
2:L:131:SER:HB3	2:L:180:THR:HG23	1.82	0.61
3:S:463:PRO:O	3:S:464:ILE:C	2.36	0.61
1:H:38:ARG:CZ	1:H:46:GLU:OE2	2.48	0.61
2:L:117:ILE:HG13	2:L:194:CYS:HB2	1.82	0.61
3:R:427:GLN:HB2	3:R:476:PRO:HA	1.81	0.61
3:R:509:ASP:O	3:R:510:ASP:CB	2.42	0.61
2:B:78:LEU:HD12	2:B:82:ASP:OD2	1.99	0.61
2:B:155:ARG:HG2	2:B:155:ARG:NH1	2.07	0.61
2:L:23:CYS:SG	2:L:88:CYS:SG	0.61	0.61
2:L:70:ASP:OD1	2:L:70:ASP:N	2.30	0.61
3:R:507:LEU:HB2	3:R:512:THR:HB	1.82	0.61
3:R:399:PHE:HE2	3:R:401:ARG:HH21	1.49	0.61
2:B:62:PHE:CE1	2:B:75:ILE:HG12	2.36	0.61
2:B:54:LEU:HD11	2:B:58:VAL:HG12	1.83	0.61
1:H:52:SER:HB2	3:R:536:GLU:OE1	1.99	0.61
3:R:488:LEU:HD22	3:R:491:ILE:H	1.65	0.61
2:L:33:LEU:HD12	2:L:71:TYR:CG	2.35	0.61
3:S:504:SER:C	3:S:506:PHE:HE2	2.04	0.61
2:B:183:LYS:HD2	2:B:187:GLU:CD	2.21	0.60
1:A:148:GLU:OE1	1:A:148:GLU:HA	2.01	0.60
1:H:47:TRP:CZ3	1:H:60:PRO:HD3	2.36	0.60
2:L:51:THR:HG23	2:L:71:TYR:CD1	2.35	0.60
3:S:436:ASN:O	3:S:586:PRO:CD	2.39	0.60
1:A:11:LEU:HG	1:A:12:VAL:N	2.13	0.60
1:H:52:SER:OG	1:H:56:TYR:HB2	2.02	0.60
1:H:37:VAL:CG2	1:H:99:MET:CE	2.79	0.60
3:S:389:LEU:HA	3:S:491:ILE:HD11	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:434:ALA:C	3:S:587:LYS:HE3	2.21	0.60
2:B:179:LEU:CD1	2:B:181:LEU:HD21	2.31	0.60
1:A:28:THR:HG21	1:A:31:SER:OG	2.01	0.60
3:S:411:LEU:HD23	3:S:415:LEU:HG	1.81	0.60
3:S:450:LEU:HD12	3:S:568:GLN:CD	2.19	0.60
2:B:183:LYS:O	2:B:186:TYR:HB3	2.02	0.60
2:L:95:PRO:O	2:L:96:PRO:C	2.39	0.60
3:S:385:PHE:CE2	3:S:409:TYR:CD2	2.85	0.60
3:S:564:THR:CB	3:S:566:GLN:O	2.48	0.60
2:B:190:ASN:OD1	2:B:211:ARG:N	2.32	0.60
2:L:33:LEU:CD1	2:L:71:TYR:CG	2.84	0.60
3:S:383:CYS:CB	3:S:409:TYR:CB	2.36	0.60
3:S:574:THR:CG2	3:S:575:VAL:N	2.64	0.60
3:S:491:ILE:CG2	3:S:492:THR:N	2.65	0.59
3:S:586:PRO:O	3:S:587:LYS:HB2	2.02	0.59
2:B:30:ASN:O	2:B:31:ASN:CB	2.38	0.59
1:H:64:LYS:CD	1:H:64:LYS:C	2.66	0.59
1:H:140:CYS:SG	1:H:195:CYS:HB3	2.37	0.59
3:R:396:VAL:O	3:R:399:PHE:HD1	1.85	0.59
3:R:401:ARG:NE	3:R:444:ASP:OD1	2.35	0.59
1:H:90:TYR:O	1:H:106:GLY:HA2	2.03	0.59
3:R:410:ASN:O	3:R:413:LYS:CB	2.49	0.59
2:B:96:PRO:O	2:B:96:PRO:CD	2.50	0.59
2:B:47:LEU:C	2:B:48:ILE:HD12	2.23	0.59
2:B:184:ASP:O	2:B:188:ARG:CD	2.50	0.59
2:B:190:ASN:CG	2:B:210:ASN:HB3	2.18	0.59
3:R:491:ILE:N	3:R:491:ILE:HD13	2.17	0.59
1:A:18:LEU:HD23	1:A:20:LEU:HD21	1.84	0.59
3:R:410:ASN:O	3:R:413:LYS:HB3	2.03	0.59
3:S:403:VAL:HG12	3:S:403:VAL:O	1.99	0.58
3:S:437:CYS:HA	3:S:585:CYS:HA	1.84	0.58
3:S:438:TYR:HE2	3:S:586:PRO:HG3	1.67	0.58
3:R:520:ALA:O	3:R:521:ASN:HB2	2.03	0.58
1:A:188:TRP:CD1	1:A:189:PRO:HA	2.38	0.58
2:L:30:ASN:O	2:L:31:ASN:HB2	2.02	0.58
3:S:388:LEU:HG	3:S:389:LEU:HD13	1.84	0.58
2:B:29:ILE:HG21	2:B:90:GLN:OE1	2.03	0.58
1:H:160:SER:C	1:H:163:VAL:HG23	2.24	0.58
3:R:509:ASP:OD2	3:R:511:ARG:N	2.29	0.58
2:L:69:SER:C	2:L:70:ASP:OD1	2.41	0.58
3:S:409:TYR:CE1	3:S:586:PRO:HB3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:NZ	1:A:113:SER:O	2.35	0.58
3:R:399:PHE:HE2	3:R:401:ARG:NH2	2.02	0.58
1:A:118:ALA:HB1	1:A:204:THR:HG21	1.84	0.58
1:H:188:TRP:CG	1:H:189:PRO:HA	2.38	0.58
3:S:438:TYR:HB3	3:S:575:VAL:HG21	1.66	0.58
1:A:18:LEU:HD21	1:A:20:LEU:HD21	1.86	0.58
1:A:19:LYS:CD	1:A:81:GLN:OE1	2.52	0.58
1:H:87:THR:CG2	1:H:110:THR:CA	2.71	0.58
3:R:564:THR:OG1	3:R:566:GLN:O	2.22	0.58
1:H:42:GLU:OE1	1:H:42:GLU:CA	2.52	0.58
1:H:55:THR:CG2	1:H:56:TYR:HD1	2.01	0.57
3:S:397:TYR:HD1	3:S:500:ILE:HG13	1.67	0.57
3:S:505:ARG:HG3	3:S:506:PHE:N	2.18	0.57
1:H:64:LYS:HD2	1:H:65:GLY:CA	2.34	0.57
2:B:198:HIS:ND1	2:B:200:THR:CG2	2.59	0.57
1:A:82(C):LEU:HB3	1:A:111:VAL:HG21	1.85	0.57
1:A:169:VAL:CG1	1:A:169:VAL:O	2.49	0.57
2:B:108:ARG:HH11	2:B:108:ARG:CG	2.16	0.57
1:H:64:LYS:CD	1:H:65:GLY:H	2.13	0.57
1:H:122:TYR:HD2	1:H:141:LEU:HD23	1.67	0.57
3:S:434:ALA:O	3:S:587:LYS:CG	2.49	0.57
3:S:496:LYS:NZ	3:S:535:TRP:C	2.57	0.57
1:H:121:VAL:HG12	1:H:208:LYS:HD3	1.87	0.57
1:H:136:VAL:HG23	1:H:136:VAL:O	2.04	0.57
1:A:119:PRO:CD	1:A:119:PRO:O	2.51	0.57
2:L:7:THR:HG21	2:L:22:ILE:HD11	1.87	0.57
2:B:80:GLN:C	2:B:82:ASP:N	2.56	0.57
3:S:508:SER:O	3:S:510:ASP:CA	2.53	0.56
1:A:33:ALA:C	1:A:34:MET:HG2	2.26	0.56
1:H:199:HIS:ND1	1:H:202:SER:HB3	2.20	0.56
1:H:37:VAL:CG2	1:H:99:MET:HE2	2.35	0.56
2:L:53:ARG:HD3	3:R:528:SER:HB2	1.87	0.56
3:S:449:PRO:CB	3:S:497:TYR:CD2	2.85	0.56
2:B:184:ASP:O	2:B:188:ARG:HG2	2.04	0.56
1:A:1:GLU:O	1:A:1:GLU:HG3	2.04	0.56
3:S:397:TYR:C	3:S:397:TYR:CD2	2.79	0.56
1:H:93:VAL:HG11	1:H:99:MET:CG	2.21	0.56
2:L:148:TRP:HE1	2:L:177:SER:HG	1.54	0.56
3:S:505:ARG:CA	3:S:506:PHE:HD2	2.19	0.56
2:B:121:SER:OG	1:A:122:TYR:HB3	2.06	0.56
1:H:34:MET:HE1	1:H:94:ARG:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:VAL:HG21	1:H:67:PHE:CE2	2.34	0.56
3:S:411:LEU:HD21	3:S:415:LEU:HD11	1.77	0.56
2:L:90:GLN:CD	2:L:90:GLN:O	2.44	0.56
3:R:399:PHE:CE2	3:R:401:ARG:NH2	2.73	0.56
3:R:463:PRO:HA	3:R:466:GLN:HB2	1.88	0.56
2:B:179:LEU:C	2:B:179:LEU:CD1	2.49	0.56
1:H:34:MET:HE2	1:H:94:ARG:HG3	1.88	0.56
2:B:108:ARG:NH1	2:B:108:ARG:HG3	2.20	0.55
1:H:22:CYS:HB2	1:H:92:CYS:SG	2.40	0.55
3:S:499:TYR:CE2	3:S:559:SER:CB	2.88	0.55
3:S:505:ARG:CG	3:S:506:PHE:N	2.69	0.55
2:B:190:ASN:OD1	2:B:210:ASN:CA	2.53	0.55
2:L:118:PHE:HE2	2:L:135:PHE:HD2	1.52	0.55
1:A:40:THR:C	1:A:42:GLU:H	2.09	0.55
3:R:401:ARG:HD3	3:R:442:ILE:CG2	2.36	0.55
1:H:40:THR:OG1	1:H:42:GLU:HG2	2.05	0.55
2:L:117:ILE:O	2:L:117:ILE:CG2	2.54	0.55
3:S:415:LEU:HD21	3:S:480:ILE:HD13	1.89	0.55
3:S:487:ASN:N	3:S:487:ASN:OD1	2.39	0.55
2:B:95:PRO:O	2:B:97:THR:HG23	2.07	0.55
2:B:183:LYS:HB2	2:B:183:LYS:NZ	1.98	0.55
1:A:37:VAL:O	1:A:91:TYR:HB2	2.07	0.55
1:H:87:THR:HG22	1:H:109:VAL:O	2.06	0.55
3:S:563:MET:HE3	3:S:567:LEU:HA	1.89	0.55
1:H:47:TRP:HE1	1:H:50:THR:HG1	1.54	0.55
1:A:19:LYS:HB2	1:A:81:GLN:OE1	2.06	0.55
1:A:67:PHE:CE1	1:A:82:MET:HE2	2.41	0.55
1:H:6:GLU:OE1	1:H:92:CYS:N	2.31	0.55
1:A:120:SER:OG	1:A:122:TYR:HE2	1.88	0.55
2:B:183:LYS:HD3	2:B:187:GLU:CD	2.27	0.54
1:H:136:VAL:O	1:H:136:VAL:CG2	2.54	0.54
1:H:68:THR:O	1:H:68:THR:HG22	2.06	0.54
1:H:127:VAL:HG11	2:L:209:PHE:HB2	1.88	0.54
1:A:20:LEU:HD23	1:A:20:LEU:N	2.23	0.54
2:L:105:GLU:OE2	2:L:142:LYS:CE	2.55	0.54
3:S:409:TYR:CZ	3:S:441:LEU:HD22	2.40	0.54
3:S:573:ILE:CG2	3:S:574:THR:N	2.70	0.54
1:A:28:THR:CG2	1:A:31:SER:OG	2.56	0.54
3:S:396:VAL:HG23	3:S:446:PHE:HD1	1.54	0.54
3:S:397:TYR:HD2	3:S:398:ASN:N	2.06	0.54
3:R:439:SER:OG	3:R:577:TYR:HA	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:457:SER:HG	3:R:458:VAL:HG23	1.67	0.54
1:A:148:GLU:OE1	1:A:149:PRO:HA	2.07	0.54
1:H:97:ASN:N	1:H:97:ASN:OD1	2.39	0.54
1:H:160:SER:O	1:H:163:VAL:HG23	2.08	0.54
1:A:87:THR:HG23	1:A:110:THR:CA	2.38	0.54
1:A:101:ASP:HB2	1:A:102:TYR:CD2	2.42	0.54
2:L:147:LYS:HD3	2:L:154:GLU:OE2	1.99	0.54
2:B:188:ARG:C	2:B:189:HIS:ND1	2.61	0.54
1:H:160:SER:O	1:H:163:VAL:CG2	2.55	0.54
2:B:183:LYS:HD2	2:B:187:GLU:OE1	2.08	0.54
1:A:19:LYS:CE	1:A:81:GLN:OE1	2.55	0.54
1:A:84:SER:CA	1:A:111:VAL:CG1	2.78	0.54
3:S:421:ASN:N	3:S:421:ASN:HD22	2.05	0.53
1:A:6:GLU:HG3	1:A:92:CYS:HB2	1.90	0.53
3:S:437:CYS:HA	3:S:585:CYS:CA	2.38	0.53
3:S:448:TYR:HE1	3:S:464:ILE:HD13	1.47	0.53
3:R:426:SER:O	3:R:427:GLN:CB	2.55	0.53
3:S:574:THR:HG22	3:S:575:VAL:N	2.22	0.53
2:B:36:TYR:CZ	2:B:89:GLN:OE1	2.56	0.53
1:H:56:TYR:CD1	1:H:56:TYR:N	2.76	0.53
2:L:37:GLN:HB2	2:L:86:TYR:CE1	2.43	0.53
2:L:137:ASN:HA	2:L:174:SER:HB3	1.89	0.53
3:S:397:TYR:HE2	3:S:398:ASN:ND2	2.05	0.53
1:H:56:TYR:HD1	1:H:56:TYR:N	2.06	0.53
2:L:107:ARG:NH1	2:L:107:ARG:HG3	2.23	0.53
2:L:139:PHE:O	2:L:139:PHE:CD1	2.61	0.53
2:B:184:ASP:O	2:B:188:ARG:HD3	2.08	0.53
2:L:105:GLU:OE2	2:L:142:LYS:NZ	2.41	0.53
3:S:385:PHE:HB3	3:S:388:LEU:HD21	1.90	0.53
2:B:38:GLN:HE21	2:B:42:GLY:CA	2.21	0.53
2:L:19:VAL:HG23	2:L:20:THR:N	2.23	0.53
1:H:177:LEU:HG	1:H:178:SER:N	2.23	0.53
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.42	0.53
2:L:148:TRP:CD1	2:L:159:VAL:CG1	2.91	0.53
3:S:450:LEU:HD12	3:S:450:LEU:N	2.24	0.53
2:B:41:ASP:OD1	2:B:43:THR:OG1	2.22	0.53
1:H:94:ARG:NH2	1:H:101:ASP:OD2	2.39	0.53
2:B:108:ARG:NH1	2:B:109:ALA:O	2.42	0.53
1:A:32:TYR:O	1:A:71:ARG:NH2	2.37	0.53
1:H:55:THR:C	1:H:56:TYR:CD1	2.79	0.53
3:S:397:TYR:C	3:S:397:TYR:HD2	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:PRO:HG2	1:A:47:TRP:CG	2.43	0.53
2:L:105:GLU:CD	2:L:173:TYR:OH	2.47	0.52
2:B:160:LEU:HD12	1:A:169:VAL:CG1	2.38	0.52
1:H:101:ASP:HB3	1:H:102:TYR:CD2	2.44	0.52
1:H:186:SER:C	1:H:188:TRP:O	2.47	0.52
2:L:61:ARG:HH12	2:L:82:ASP:CG	2.13	0.52
1:H:32:TYR:O	1:H:71:ARG:NH2	2.42	0.52
3:R:458:VAL:HG12	3:R:459:SER:N	2.25	0.52
1:A:40:THR:C	1:A:42:GLU:N	2.62	0.52
1:A:210:ILE:CD1	1:A:210:ILE:C	2.73	0.52
2:L:67:SER:OG	2:L:68:GLY:N	2.40	0.52
3:S:450:LEU:HD11	3:S:568:GLN:HG2	1.90	0.52
2:B:183:LYS:CB	2:B:183:LYS:HZ3	2.21	0.52
1:A:119:PRO:HB3	1:A:145:TYR:CD1	2.44	0.52
1:H:119:PRO:HB3	1:H:145:TYR:CB	2.28	0.52
3:S:449:PRO:CA	3:S:497:TYR:HE2	2.22	0.52
1:H:72:ASP:OD1	1:H:75:GLU:N	2.29	0.52
2:L:147:LYS:HD2	2:L:154:GLU:CG	2.40	0.52
3:S:449:PRO:CB	3:S:497:TYR:CE2	2.93	0.52
3:S:497:TYR:HE1	3:S:563:MET:CE	2.22	0.52
1:A:119:PRO:O	1:A:119:PRO:CG	2.58	0.52
1:H:109:VAL:O	1:H:109:VAL:HG12	2.10	0.52
3:R:396:VAL:HG22	3:R:397:TYR:N	2.24	0.52
3:R:414:LEU:HB3	3:R:415:LEU:CD2	2.34	0.52
1:A:90:TYR:O	1:A:106:GLY:HA2	2.08	0.52
2:L:41:ASP:OD1	2:L:43:THR:OG1	2.28	0.52
2:B:28:ASP:OD1	2:B:28:ASP:C	2.47	0.52
2:B:37:GLN:O	2:B:37:GLN:HG3	2.07	0.52
2:B:190:ASN:O	2:B:210:ASN:HA	2.09	0.52
2:B:198:HIS:CE1	2:B:200:THR:HG23	2.40	0.52
1:A:71:ARG:CD	1:A:73:ASN:OD1	2.56	0.52
1:H:206:VAL:C	1:H:207:ASP:OD1	2.49	0.52
3:R:494:PRO:HD2	3:R:567:LEU:CD1	2.40	0.52
1:A:67:PHE:HZ	1:A:82:MET:HE1	1.62	0.52
2:L:19:VAL:CG2	2:L:20:THR:N	2.68	0.51
3:S:450:LEU:CD1	3:S:568:GLN:HG2	2.41	0.51
2:B:212:ASN:OD1	2:B:212:ASN:C	2.47	0.51
2:B:103:LYS:HZ1	2:B:165:ASP:CG	1.95	0.51
2:B:98:PHE:HD1	2:B:98:PHE:H	1.58	0.51
1:A:29:PHE:CD2	1:A:71:ARG:NH1	2.78	0.51
1:A:210:ILE:O	1:A:211:GLU:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:TRP:CD1	1:H:189:PRO:HA	2.46	0.51
1:A:177:LEU:CD2	1:A:178:SER:CA	2.80	0.51
1:H:159:LEU:HG	1:H:159:LEU:O	2.08	0.51
2:L:95:PRO:C	2:L:96:PRO:O	2.46	0.51
1:A:27:PHE:CD1	1:A:27:PHE:N	2.78	0.51
2:L:140:TYR:CG	2:L:141:PRO:HA	2.46	0.51
2:B:191:SER:C	2:B:192:TYR:CD1	2.79	0.51
3:R:463:PRO:O	3:R:464:ILE:C	2.50	0.51
3:R:413:LYS:O	3:R:416:SER:OG	2.29	0.50
2:B:136:LEU:N	2:B:136:LEU:HD12	2.26	0.50
2:L:108:ARG:HH11	2:L:108:ARG:HG3	1.76	0.50
3:S:506:PHE:HD1	3:S:511:ARG:CG	2.24	0.50
3:R:421:ASN:O	3:R:422:ASP:OD2	2.29	0.50
2:B:167:ASP:OD1	2:B:169:LYS:HG2	2.11	0.50
1:H:169:VAL:CG1	2:L:160:LEU:CD2	2.83	0.50
3:S:396:VAL:CG1	3:S:397:TYR:N	2.74	0.50
3:R:428:ILE:HG21	3:R:433:ILE:HB	1.92	0.50
2:B:108:ARG:CG	2:B:109:ALA:N	2.75	0.50
3:S:388:LEU:HG	3:S:389:LEU:H	1.76	0.50
2:B:49:TYR:CZ	2:B:53:ARG:HB3	2.47	0.50
1:A:117:THR:CG2	1:A:118:ALA:N	2.74	0.50
2:L:76:SER:O	2:L:77:ASN:O	2.30	0.50
1:A:57:THR:O	1:A:58:TYR:CD2	2.64	0.50
2:L:148:TRP:HD1	2:L:159:VAL:HG11	1.76	0.50
2:B:39:LYS:HE2	2:B:81:GLU:O	2.11	0.50
1:A:67:PHE:CE1	1:A:82:MET:HE3	2.42	0.50
1:H:40:THR:OG1	1:H:41:PRO:N	2.39	0.50
2:L:90:GLN:OE1	2:L:90:GLN:O	2.30	0.50
3:R:452:MET:CA	3:R:455:ASP:OD2	2.59	0.50
1:A:173:ASP:O	1:A:173:ASP:OD1	2.30	0.50
1:A:189:PRO:O	1:A:191:GLN:O	2.30	0.50
2:L:108:ARG:NH1	2:L:108:ARG:HG3	2.26	0.50
2:L:210:ASN:O	2:L:212:ASN:OD1	2.30	0.50
3:S:398:ASN:OD1	3:S:398:ASN:O	2.30	0.50
3:S:506:PHE:CZ	3:S:513:GLU:OE2	2.64	0.50
2:B:49:TYR:O	2:B:53:ARG:HB2	2.12	0.50
2:L:105:GLU:OE2	2:L:142:LYS:HE2	2.13	0.49
2:L:211:ARG:O	2:L:212:ASN:CG	2.51	0.49
3:S:410:ASN:OD1	3:S:410:ASN:O	2.30	0.49
3:S:553:TRP:N	3:S:553:TRP:HD1	2.01	0.49
3:S:586:PRO:C	3:S:587:LYS:CG	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ILE:O	2:B:84:ALA:HB2	2.12	0.49
2:B:103:LYS:CE	2:B:165:ASP:OD1	2.59	0.49
3:R:382:GLU:CD	3:R:587:LYS:NZ	2.63	0.49
3:R:428:ILE:HG13	3:R:476:PRO:HB2	1.92	0.49
3:R:488:LEU:HD21	3:R:491:ILE:HD13	1.94	0.49
2:L:95:PRO:O	2:L:96:PRO:O	2.30	0.49
3:S:499:TYR:HE2	3:S:559:SER:HG	1.60	0.49
3:R:423:PHE:HE1	3:R:425:CYS:SG	2.35	0.49
1:A:97:ASN:OD1	1:A:97:ASN:N	2.33	0.49
1:A:28:THR:HG22	1:A:31:SER:HB2	1.95	0.49
2:L:18:ARG:HG3	2:L:76:SER:HB3	1.95	0.49
2:L:148:TRP:CD1	2:L:159:VAL:HG11	2.47	0.49
2:L:201:SER:OG	2:L:203:SER:O	2.30	0.49
3:S:438:TYR:HB3	3:S:575:VAL:HG22	1.88	0.49
2:B:212:ASN:OD1	2:B:212:ASN:O	2.30	0.49
1:A:75:GLU:OE1	1:A:75:GLU:O	2.29	0.49
1:H:160:SER:HA	1:H:163:VAL:HG21	1.94	0.49
2:L:21:ILE:HD13	2:L:102:THR:CG2	2.38	0.49
2:L:211:ARG:O	2:L:212:ASN:OD1	2.30	0.49
3:S:449:PRO:CB	3:S:497:TYR:HD2	2.21	0.49
3:S:506:PHE:HD1	3:S:511:ARG:HG2	1.77	0.49
3:R:389:LEU:O	3:R:491:ILE:HD13	2.08	0.49
1:A:29:PHE:HE2	1:A:71:ARG:HD3	1.78	0.49
3:S:546:SER:OG	3:S:549:GLU:OE2	2.30	0.49
1:H:44:ARG:HH21	1:H:45:LEU:H	1.60	0.49
1:H:202:SER:C	1:H:203:SER:OG	2.50	0.49
2:L:14:SER:O	2:L:17:ASP:OD2	2.30	0.49
2:B:71:TYR:N	2:B:71:TYR:HD2	2.09	0.49
3:R:480:ILE:HB	3:R:571:PHE:HB2	1.95	0.49
3:R:529:ILE:HG22	3:R:543:LYS:HG2	1.95	0.49
3:R:546:SER:OG	3:R:549:GLU:OE2	2.30	0.49
1:A:38:ARG:CG	1:A:38:ARG:O	2.60	0.49
1:A:75:GLU:O	1:A:77:THR:HG23	2.13	0.49
1:A:76:ASN:O	1:A:77:THR:HG22	2.12	0.49
1:A:145:TYR:CZ	1:A:150:VAL:HG12	2.48	0.49
3:S:421:ASN:N	3:S:421:ASN:ND2	2.61	0.48
3:S:499:TYR:CD2	3:S:499:TYR:O	2.64	0.48
3:R:463:PRO:O	3:R:466:GLN:N	2.46	0.48
1:A:28:THR:HG22	1:A:31:SER:CB	2.43	0.48
1:A:67:PHE:CE1	1:A:82:MET:HB3	2.48	0.48
1:A:142:VAL:HG12	1:A:145:TYR:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:CZ2	1:A:210:ILE:HD13	2.48	0.48
2:L:136:LEU:C	2:L:137:ASN:ND2	2.65	0.48
3:S:397:TYR:CE2	3:S:398:ASN:ND2	2.80	0.48
3:R:509:ASP:OD2	3:R:509:ASP:C	2.52	0.48
2:L:190:ASN:C	2:L:190:ASN:HD22	2.16	0.48
3:S:449:PRO:HA	3:S:497:TYR:HE2	1.78	0.48
2:B:37:GLN:O	2:B:37:GLN:CG	2.59	0.48
1:H:207:ASP:OD1	1:H:207:ASP:N	2.45	0.48
3:S:388:LEU:HA	3:S:445:TYR:CZ	2.48	0.48
2:L:211:ARG:C	2:L:212:ASN:OD1	2.52	0.48
3:S:511:ARG:C	3:S:512:THR:HG22	2.32	0.48
1:A:152:LEU:CD2	1:A:153:THR:CA	2.83	0.48
3:R:575:VAL:HG23	3:R:576:GLN:N	2.27	0.48
1:A:30:SER:O	1:A:52(A):SER:HB2	2.14	0.48
1:H:87:THR:HG23	1:H:111:VAL:HG23	1.95	0.48
2:L:24:ARG:HG3	2:L:25:ALA:N	2.28	0.48
3:S:508:SER:O	3:S:510:ASP:N	2.47	0.48
1:A:38:ARG:HA	1:A:89:MET:O	2.14	0.48
1:H:171:GLN:O	1:H:172:SER:HB2	2.14	0.48
2:L:3:GLN:H	2:L:26:SER:HB2	1.79	0.48
2:L:170:ASP:O	2:L:171:SER:HB2	2.13	0.48
3:S:575:VAL:HG22	3:S:576:GLN:N	2.28	0.48
3:R:522:GLN:HG3	3:R:523:TYR:H	1.79	0.48
2:B:89:GLN:HG2	2:B:90:GLN:H	1.76	0.48
1:H:22:CYS:HB3	1:H:92:CYS:SG	2.43	0.48
3:S:512:THR:O	3:S:512:THR:OG1	2.30	0.48
1:A:20:LEU:N	1:A:80:LEU:O	2.24	0.48
2:L:16:GLY:HA2	2:L:77:ASN:HA	1.95	0.48
3:S:385:PHE:CB	3:S:388:LEU:HD21	2.39	0.48
2:L:139:PHE:CD1	2:L:139:PHE:C	2.87	0.47
1:A:206:VAL:CG1	1:A:207:ASP:N	2.73	0.47
1:H:52:SER:HG	1:H:56:TYR:HB2	1.78	0.47
2:L:3:GLN:H	2:L:26:SER:CB	2.27	0.47
2:B:147:LYS:NZ	2:B:154:GLU:OE2	2.40	0.47
1:A:122:TYR:N	1:A:122:TYR:CD2	2.82	0.47
3:S:423:PHE:CD1	3:S:480:ILE:HG12	2.48	0.47
3:R:456:LEU:CD2	3:R:479:LEU:CD2	2.90	0.47
2:L:49:TYR:CZ	2:L:53:ARG:HB3	2.50	0.47
3:R:546:SER:O	3:R:549:GLU:N	2.30	0.47
1:A:13:LYS:HA	1:A:112:SER:O	2.14	0.47
3:S:554:LEU:CD1	3:S:555:VAL:N	2.51	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:THR:O	2:B:94:LEU:HD23	2.15	0.47
1:H:202:SER:OG	1:H:204:THR:OG1	2.30	0.47
2:L:38:GLN:O	2:L:84:ALA:HB1	2.14	0.47
2:L:148:TRP:CD1	2:L:159:VAL:HG13	2.50	0.47
2:B:83:ILE:HG23	2:B:104:LEU:O	2.14	0.47
2:B:96:PRO:CD	1:A:47:TRP:CD2	2.98	0.47
1:A:48:VAL:O	1:A:60:PRO:HD3	2.14	0.47
1:A:155:ASN:HD21	1:A:193:ILE:HA	1.80	0.47
2:L:107:ARG:CG	2:L:107:ARG:HH11	2.28	0.47
2:B:211:ARG:O	2:B:212:ASN:C	2.52	0.47
1:A:146:PHE:CG	1:A:147:PRO:HA	2.50	0.47
2:B:189:HIS:O	2:B:211:ARG:NH1	2.48	0.47
2:L:90:GLN:O	2:L:90:GLN:CG	2.62	0.47
3:S:395:GLN:HG3	3:S:498:SER:HG	1.80	0.47
3:R:531:PRO:O	3:R:532:SER:C	2.50	0.47
2:B:96:PRO:HD3	1:A:47:TRP:CD2	2.50	0.47
1:A:184:THR:HG1	1:A:187:THR:HG1	1.59	0.47
2:L:1:ASP:OD1	2:L:1:ASP:N	2.36	0.46
3:S:501:ASN:OD1	3:S:502:LYS:HB3	2.15	0.46
1:A:145:TYR:CE1	1:A:150:VAL:HG11	2.49	0.46
1:H:140:CYS:SG	1:H:195:CYS:HB2	2.42	0.46
2:L:92:ASN:O	3:R:532:SER:OG	2.12	0.46
2:L:108:ARG:HD2	2:L:171:SER:CB	2.39	0.46
2:L:143:ASP:OD1	2:L:143:ASP:N	2.46	0.46
3:R:518:VAL:HG23	3:R:519:ASN:N	2.30	0.46
3:R:411:LEU:HG	3:R:415:LEU:HD21	1.97	0.46
3:S:409:TYR:CE2	3:S:441:LEU:HD22	2.51	0.46
3:S:544:GLN:O	3:S:545:LEU:CD2	2.63	0.46
3:R:488:LEU:HD23	3:R:490:THR:H	1.80	0.46
3:R:497:TYR:HB2	3:R:561:VAL:HB	1.97	0.46
3:S:397:TYR:CD2	3:S:398:ASN:N	2.84	0.46
3:R:428:ILE:HG22	3:R:429:SER:N	2.29	0.46
2:B:184:ASP:O	2:B:188:ARG:CG	2.64	0.46
1:H:202:SER:O	1:H:203:SER:OG	2.30	0.46
2:L:36:TYR:HE2	2:L:89:GLN:HB3	1.79	0.46
1:H:87:THR:CG2	1:H:111:VAL:N	2.72	0.46
3:S:505:ARG:CA	3:S:506:PHE:CD2	2.96	0.46
3:R:427:GLN:O	3:R:428:ILE:HG12	2.15	0.46
2:B:93:THR:C	2:B:94:LEU:HD23	2.36	0.46
1:A:152:LEU:HD23	1:A:153:THR:HA	1.93	0.46
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LEU:HD22	2:B:95:PRO:HA	1.97	0.46
2:B:137:ASN:OD1	2:B:174:SER:CB	2.58	0.46
1:H:160:SER:CA	1:H:163:VAL:HG21	2.46	0.46
2:L:198:HIS:CG	2:L:200:THR:HG23	2.48	0.46
3:S:386:SER:N	3:S:387:PRO:CD	2.78	0.46
3:S:573:ILE:HG22	3:S:574:THR:N	2.27	0.46
1:A:71:ARG:O	1:A:71:ARG:HG3	2.15	0.46
1:H:91:TYR:HD1	1:H:104:GLY:O	1.99	0.45
3:S:457:SER:O	3:S:460:SER:OG	2.30	0.45
3:S:547:PRO:O	3:S:550:GLY:N	2.49	0.45
1:A:172:SER:HB3	1:A:173:ASP:H	1.37	0.45
3:S:385:PHE:CZ	3:S:409:TYR:CE2	2.93	0.45
3:S:516:GLN:HB3	3:S:525:PRO:HG2	1.98	0.45
3:R:428:ILE:HG13	3:R:476:PRO:CB	2.46	0.45
3:R:439:SER:OG	3:R:576:GLN:C	2.54	0.45
2:B:28:ASP:OD1	2:B:30:ASN:N	2.48	0.45
1:A:206:VAL:HG12	1:A:207:ASP:H	1.76	0.45
2:B:40:PRO:C	2:B:42:GLY:H	2.19	0.45
2:B:189:HIS:C	2:B:211:ARG:HH12	2.19	0.45
3:S:389:LEU:HA	3:S:389:LEU:HD12	1.43	0.45
2:B:133:VAL:HG12	2:B:134:CYS:N	2.27	0.45
1:A:171:GLN:O	1:A:173:ASP:N	2.49	0.45
1:H:42:GLU:N	1:H:42:GLU:CD	2.68	0.45
3:S:411:LEU:HD22	3:S:415:LEU:HD12	1.95	0.45
3:S:491:ILE:HG22	3:S:492:THR:N	2.30	0.45
2:L:6:GLN:OE1	2:L:99:GLY:HA3	2.17	0.45
2:L:24:ARG:HE	2:L:24:ARG:HB2	1.24	0.45
3:S:383:CYS:CB	3:S:409:TYR:CG	2.98	0.45
3:S:388:LEU:CD1	3:S:389:LEU:HD13	2.47	0.45
3:S:449:PRO:CA	3:S:497:TYR:CE2	3.00	0.45
3:R:542:ARG:O	3:R:543:LYS:HD2	2.16	0.45
1:H:37:VAL:CG2	1:H:99:MET:HE1	2.43	0.45
1:H:161:SER:CA	1:H:163:VAL:HG23	2.47	0.45
3:R:385:PHE:CD1	3:R:414:LEU:HD22	2.51	0.45
3:R:543:LYS:HD2	3:R:543:LYS:HA	1.73	0.45
3:S:450:LEU:HD11	3:S:568:GLN:CG	2.46	0.45
3:R:409:TYR:CD1	3:R:409:TYR:N	2.84	0.45
1:H:159:LEU:HD21	1:H:181:VAL:HG21	1.99	0.45
3:S:410:ASN:ND2	3:S:413:LYS:HB2	2.32	0.45
3:S:473:PHE:CD2	3:S:473:PHE:N	2.84	0.45
2:B:90:GLN:O	2:B:90:GLN:CG	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:N	1:A:27:PHE:HD1	2.15	0.45
1:A:52(A):SER:HA	1:A:71:ARG:NH2	2.32	0.45
1:H:38:ARG:HA	1:H:89:MET:O	2.17	0.44
1:H:121:VAL:HG12	1:H:121:VAL:O	2.16	0.44
1:H:172:SER:O	1:H:173:ASP:CB	2.55	0.44
2:L:150:ILE:O	2:L:151:ASP:C	2.55	0.44
3:S:497:TYR:CE1	3:S:563:MET:CE	2.99	0.44
1:A:94:ARG:HD2	1:A:101:ASP:OD1	2.17	0.44
3:S:397:TYR:HE2	3:S:398:ASN:HD22	1.64	0.44
3:S:438:TYR:HE2	3:S:586:PRO:CG	2.30	0.44
3:S:450:LEU:O	3:S:451:SER:C	2.55	0.44
3:S:395:GLN:O	3:S:398:ASN:OD1	2.35	0.44
3:R:389:LEU:C	3:R:491:ILE:HD12	2.34	0.44
1:A:28:THR:CG2	1:A:31:SER:HB2	2.47	0.44
1:H:124:LEU:HD11	2:L:133:VAL:HG21	2.00	0.44
1:H:169:VAL:HG11	2:L:160:LEU:HD21	1.95	0.44
3:S:564:THR:HG21	3:S:568:GLN:HG3	1.99	0.44
1:A:145:TYR:OH	1:A:150:VAL:CG1	2.66	0.44
1:H:66:ARG:CB	1:H:66:ARG:HH11	2.30	0.44
1:H:122:TYR:CD2	1:H:141:LEU:HD23	2.51	0.44
3:S:477:THR:HG22	3:S:574:THR:OG1	2.16	0.44
3:S:484:VAL:HG13	3:S:488:LEU:HD13	1.99	0.44
3:S:501:ASN:OD1	3:S:502:LYS:CB	2.66	0.44
3:S:554:LEU:HD12	3:S:555:VAL:H	1.67	0.44
2:B:47:LEU:HD13	2:B:62:PHE:CD1	2.52	0.44
1:A:119:PRO:HA	1:A:145:TYR:HB3	1.99	0.44
1:H:69:ILE:O	1:H:69:ILE:HG22	2.16	0.44
2:L:105:GLU:CD	2:L:142:LYS:CE	2.85	0.44
1:H:40:THR:CG2	1:H:44:ARG:HB2	2.48	0.44
2:L:90:GLN:C	2:L:90:GLN:CD	2.76	0.44
1:A:93:VAL:CG1	1:A:99:MET:HB3	2.48	0.44
1:H:84:SER:O	1:H:87:THR:OG1	2.35	0.44
1:H:97:ASN:OD1	3:R:543:LYS:NZ	2.48	0.44
2:L:37:GLN:O	2:L:37:GLN:CG	2.64	0.44
2:B:76:SER:O	2:B:77:ASN:O	2.35	0.44
2:L:29:ILE:O	2:L:30:ASN:C	2.55	0.44
2:L:15:LEU:HD12	2:L:15:LEU:H	1.82	0.43
1:A:40:THR:O	1:A:41:PRO:C	2.55	0.43
3:S:513:GLU:HG3	3:S:514:VAL:N	2.33	0.43
3:S:585:CYS:HA	3:S:586:PRO:HD2	1.70	0.43
1:H:94:ARG:HE	1:H:101:ASP:HB2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:434:ALA:O	3:S:586:PRO:O	2.36	0.43
3:S:524:SER:O	3:S:527:VAL:HG23	2.18	0.43
1:A:188:TRP:HA	1:A:189:PRO:C	2.39	0.43
2:L:36:TYR:HH	2:L:89:GLN:HE22	1.46	0.43
3:R:414:LEU:HA	3:R:414:LEU:HD12	1.56	0.43
3:R:491:ILE:CG2	3:R:492:THR:N	2.80	0.43
1:H:24:ALA:HB3	1:H:29:PHE:CD1	2.54	0.43
2:L:61:ARG:NH2	2:L:79:GLU:OE1	2.52	0.43
3:S:385:PHE:HB3	3:S:388:LEU:CD2	2.49	0.43
3:S:407:CYS:O	3:S:584:VAL:HG23	2.19	0.43
3:R:428:ILE:HG23	3:R:429:SER:N	2.32	0.43
3:R:519:ASN:H	3:R:522:GLN:HE21	1.65	0.43
1:A:162:GLY:O	1:A:181:VAL:HA	2.18	0.43
1:H:72:ASP:OD2	1:H:75:GLU:HB2	2.18	0.43
3:S:519:ASN:CB	3:S:522:GLN:NE2	2.47	0.43
3:S:544:GLN:HG3	3:S:545:LEU:H	1.83	0.43
2:B:80:GLN:O	2:B:81:GLU:C	2.54	0.43
3:S:536:GLU:HB2	1:A:52:SER:HB2	2.01	0.43
3:R:519:ASN:H	3:R:522:GLN:NE2	2.16	0.43
2:B:19:VAL:HG13	2:B:20:THR:N	2.29	0.43
2:B:39:LYS:CE	2:B:81:GLU:O	2.67	0.43
2:L:19:VAL:HG11	2:L:78:LEU:HD21	1.99	0.43
2:L:76:SER:O	2:L:77:ASN:HB3	2.18	0.43
2:L:155:ARG:CD	2:L:157:ASN:O	2.66	0.43
3:S:449:PRO:CG	3:S:497:TYR:HD2	2.31	0.43
3:R:569:MET:HE3	3:R:569:MET:HB3	1.93	0.43
2:L:33:LEU:HD13	2:L:71:TYR:CB	2.48	0.43
3:S:395:GLN:NE2	3:S:498:SER:CA	2.81	0.43
1:A:40:THR:O	1:A:40:THR:OG1	2.36	0.43
1:H:72:ASP:OD1	1:H:75:GLU:HB2	2.17	0.43
2:L:55:HIS:O	2:L:58:VAL:HB	2.19	0.43
1:A:28:THR:CG2	1:A:31:SER:CB	2.97	0.43
1:A:76:ASN:C	1:A:77:THR:CG2	2.87	0.43
1:H:50:THR:HG21	3:R:535:TRP:CH2	2.54	0.42
3:S:389:LEU:C	3:S:491:ILE:HD11	2.39	0.42
3:S:397:TYR:OH	3:S:531:PRO:O	2.33	0.42
3:S:499:TYR:CZ	3:S:559:SER:CB	2.95	0.42
3:S:560:THR:C	3:S:561:VAL:HG23	2.39	0.42
3:R:420:VAL:CA	3:R:421:ASN:HD22	2.28	0.42
3:R:511:ARG:CZ	3:R:511:ARG:CB	2.96	0.42
2:B:93:THR:HB	2:B:94:LEU:H	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:GLU:C	2:B:188:ARG:HG2	2.38	0.42
2:L:124:GLN:HG2	2:L:129:GLY:C	2.39	0.42
2:L:164:THR:HG23	2:L:174:SER:O	2.18	0.42
3:S:564:THR:CG2	3:S:566:GLN:O	2.67	0.42
3:R:391:GLY:O	3:R:393:PRO:HD3	2.19	0.42
3:R:414:LEU:CB	3:R:415:LEU:HD22	2.36	0.42
2:B:11:LEU:CD2	2:B:19:VAL:HG22	2.49	0.42
1:A:28:THR:O	1:A:31:SER:HB2	2.20	0.42
1:H:45:LEU:HD23	1:H:45:LEU:HA	1.79	0.42
2:B:169:LYS:NZ	1:A:161:SER:O	2.49	0.42
1:A:82:MET:HE3	1:A:82:MET:HB3	1.54	0.42
1:A:150:VAL:HG23	1:A:198:ALA:O	2.19	0.42
2:L:83:ILE:CG1	2:L:106:LEU:HD12	2.44	0.42
3:R:498:SER:OG	3:R:533:THR:CG2	2.68	0.42
2:B:145:ASN:HB2	2:B:197:THR:HB	2.00	0.42
1:H:40:THR:HG23	1:H:44:ARG:HB2	2.01	0.42
1:H:51:ILE:CB	1:H:69:ILE:HD13	2.49	0.42
1:H:211:GLU:HA	1:H:212:PRO:HD3	1.90	0.42
3:S:563:MET:HG3	3:S:564:THR:N	2.34	0.42
1:A:84:SER:CA	1:A:111:VAL:HG11	2.48	0.42
3:S:466:GLN:O	3:S:518:VAL:HG12	2.19	0.42
3:R:388:LEU:HD21	3:R:569:MET:HE1	2.01	0.42
3:R:507:LEU:O	3:R:510:ASP:N	2.50	0.42
3:R:569:MET:HE2	3:R:571:PHE:CE2	2.54	0.42
3:S:400:LYS:HD3	2:B:30:ASN:HD21	1.84	0.42
3:S:464:ILE:O	3:S:468:ASN:HB2	2.18	0.42
3:S:504:SER:CB	3:S:506:PHE:CE2	2.91	0.42
3:S:508:SER:C	3:S:509:ASP:O	2.52	0.42
1:H:51:ILE:HG22	1:H:69:ILE:HD11	1.97	0.42
2:L:71:TYR:CD2	2:L:71:TYR:N	2.87	0.42
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.55	0.42
1:A:91:TYR:HD1	1:A:104:GLY:O	2.03	0.42
1:A:150:VAL:HG21	1:A:197:VAL:HG13	2.02	0.42
3:S:386:SER:N	3:S:387:PRO:HD2	2.34	0.42
1:H:199:HIS:HB3	1:H:204:THR:HB	2.01	0.42
3:S:448:TYR:CZ	3:S:456:LEU:HG	2.55	0.42
1:H:6:GLU:OE1	1:H:104:GLY:HA3	2.20	0.41
3:S:383:CYS:HB2	3:S:409:TYR:HB3	0.56	0.41
3:S:384:ASP:OD1	3:S:386:SER:HB3	2.20	0.41
3:R:392:THR:OG1	3:R:492:THR:OG1	2.07	0.41
1:A:19:LYS:HE3	1:A:81:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:392:THR:OG1	3:R:492:THR:CB	2.65	0.41
3:R:393:PRO:HA	3:R:394:PRO:HD3	1.85	0.41
3:R:491:ILE:HG22	3:R:492:THR:N	2.34	0.41
2:L:33:LEU:HD23	2:L:33:LEU:C	2.39	0.41
2:L:107:ARG:HG3	2:L:107:ARG:HH11	1.82	0.41
2:B:35:TRP:O	2:B:46:LEU:HD12	2.20	0.41
2:B:44:VAL:HG12	2:B:45:LYS:H	1.84	0.41
1:H:47:TRP:CE3	1:H:60:PRO:HD3	2.55	0.41
1:H:137:THR:O	1:H:138:LEU:HD23	2.20	0.41
1:H:184:THR:O	1:H:185:SER:C	2.59	0.41
2:L:115:VAL:HA	2:L:135:PHE:O	2.20	0.41
3:R:484:VAL:HG13	3:R:488:LEU:HD13	2.02	0.41
2:B:108:ARG:HH11	2:B:108:ARG:HG3	1.82	0.41
2:B:122:SER:HA	2:B:125:LEU:HD12	2.03	0.41
1:H:75:GLU:O	1:H:76:ASN:HB2	2.19	0.41
3:S:410:ASN:OD1	3:S:413:LYS:HB3	2.20	0.41
3:R:412:THR:O	3:R:416:SER:OG	2.29	0.41
2:B:124:GLN:HE22	2:B:131:SER:HG	1.64	0.41
1:A:57:THR:CA	1:A:58:TYR:HD2	2.33	0.41
1:A:120:SER:HG	1:A:122:TYR:HE2	1.55	0.41
3:S:424:THR:O	3:S:425:CYS:SG	2.79	0.41
3:S:383:CYS:SG	3:S:409:TYR:CG	3.13	0.41
1:A:6:GLU:CG	1:A:92:CYS:HB2	2.51	0.41
1:A:59:TYR:HA	1:A:60:PRO:HD3	1.82	0.41
2:L:80:GLN:C	2:L:82:ASP:H	2.23	0.41
1:H:6:GLU:HG3	1:H:92:CYS:HB2	2.03	0.41
2:B:34:ASN:ND2	1:A:98:SER:HA	2.35	0.41
2:B:89:GLN:CG	2:B:90:GLN:N	2.73	0.41
2:B:200:THR:OG1	2:B:201:SER:N	2.53	0.41
2:L:190:ASN:ND2	2:L:190:ASN:C	2.74	0.41
3:S:499:TYR:HD2	3:S:500:ILE:N	2.16	0.41
3:S:507:LEU:O	3:S:508:SER:C	2.58	0.41
3:S:529:ILE:HD12	3:S:541:TYR:O	2.20	0.41
3:S:544:GLN:CA	3:S:545:LEU:HD23	2.45	0.41
3:R:522:GLN:CG	3:R:523:TYR:N	2.71	0.41
2:B:28:ASP:OD1	2:B:29:ILE:N	2.54	0.41
1:A:57:THR:CA	1:A:58:TYR:CD2	3.04	0.41
1:H:135:SER:C	1:H:136:VAL:CG1	2.90	0.40
2:L:83:ILE:O	2:L:84:ALA:HB2	2.21	0.40
3:S:415:LEU:HD21	3:S:480:ILE:CD1	2.51	0.40
2:B:38:GLN:HG2	2:B:44:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HG13	1:H:27:PHE:CD1	2.56	0.40
2:L:118:PHE:CE2	2:L:135:PHE:CD2	3.04	0.40
3:S:389:LEU:CA	3:S:491:ILE:HD11	2.48	0.40
3:S:481:LEU:HD22	3:S:481:LEU:HA	1.73	0.40
1:A:140:CYS:HB2	1:A:154:TRP:CH2	2.55	0.40
1:H:48:VAL:HG12	1:H:49:ALA:N	2.36	0.40
1:H:123:PRO:O	1:H:124:LEU:HD23	2.21	0.40
1:H:137:THR:HG23	1:H:182:THR:HG1	1.81	0.40
2:L:76:SER:O	2:L:77:ASN:CB	2.66	0.40
3:R:488:LEU:CD2	3:R:491:ILE:H	2.32	0.40
3:R:526:CYS:O	3:R:530:VAL:HG23	2.21	0.40
1:A:24:ALA:HB1	1:A:27:PHE:CE1	2.57	0.40
1:A:116:THR:HG23	1:A:147:PRO:HD2	2.03	0.40
2:L:14:SER:CA	2:L:17:ASP:OD2	2.69	0.40
2:L:33:LEU:HD23	2:L:34:ASN:H	1.84	0.40
3:R:524:SER:HA	3:R:525:PRO:HD3	1.90	0.40
2:B:14:SER:O	2:B:15:LEU:C	2.57	0.40
2:B:108:ARG:HG3	2:B:109:ALA:N	2.36	0.40
2:B:189:HIS:O	2:B:192:TYR:CE1	2.75	0.40
1:A:66:ARG:NH2	1:A:86:ASP:OD2	2.51	0.40
1:H:59:TYR:HB3	1:H:63:VAL:HG12	2.04	0.40
2:L:33:LEU:HD13	2:L:71:TYR:CG	2.56	0.40
2:L:47:LEU:HD11	2:L:86:TYR:CE1	2.56	0.40
3:S:388:LEU:CG	3:S:389:LEU:HD13	2.49	0.40
3:R:530:VAL:HA	3:R:531:PRO:HD3	1.69	0.40
2:B:140:TYR:CG	2:B:141:PRO:HA	2.57	0.40
2:B:161:ASN:HD22	2:B:177:SER:HA	1.86	0.40
2:B:191:SER:O	2:B:191:SER:OG	2.30	0.40
1:A:144:GLY:HA2	1:A:174:LEU:HB3	2.04	0.40
1:A:188:TRP:CG	1:A:189:PRO:CA	2.96	0.40

All (5) 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)
3:R:511:ARG:NH2	1:A:115:LYS:CE[4_455]	0.40	1.80
3:R:511:ARG:NH2	1:A:115:LYS:CD[4_455]	1.61	0.59
3:R:511:ARG:CZ	1:A:115:LYS:NZ[4_455]	1.78	0.42
3:R:511:ARG:NE	1:A:115:LYS:CE[4_455]	1.93	0.27
2:L:53:ARG:NH2	2:B:18:ARG:NH1[2_455]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/216 (97%)	203 (97%)	3 (1%)	3 (1%)	11	46
1	H	209/216 (97%)	205 (98%)	3 (1%)	1 (0%)	29	67
2	B	210/214 (98%)	202 (96%)	6 (3%)	2 (1%)	15	54
2	L	210/214 (98%)	202 (96%)	7 (3%)	1 (0%)	29	67
3	R	206/208 (99%)	196 (95%)	9 (4%)	1 (0%)	29	67
3	S	205/208 (99%)	196 (96%)	9 (4%)	0	100	100
All	All	1249/1276 (98%)	1204 (96%)	37 (3%)	8 (1%)	25	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	149	PRO
1	A	149	PRO
2	B	81	GLU
1	A	123	PRO
3	R	458	VAL
2	B	84	ALA
1	A	41	PRO
2	L	96	PRO

5.3.2 Protein sidechains (i)

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	182/186 (98%)	135 (74%)	47 (26%)	0 2
1	H	182/186 (98%)	132 (72%)	50 (28%)	0 1
2	B	190/192 (99%)	145 (76%)	45 (24%)	1 3
2	L	190/192 (99%)	135 (71%)	55 (29%)	0 1
3	R	190/190 (100%)	151 (80%)	39 (20%)	1 6
3	S	189/190 (100%)	139 (74%)	50 (26%)	0 2
All	All	1123/1136 (99%)	837 (74%)	286 (26%)	0 2

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	SER
1	H	40	THR
1	H	42	GLU
1	H	44	ARG
1	H	52	SER
1	H	52(A)	SER
1	H	63	VAL
1	H	64	LYS
1	H	66	ARG
1	H	68	THR
1	H	69	ILE
1	H	70	SER
1	H	71	ARG
1	H	72	ASP
1	H	75	GLU
1	H	77	THR
1	H	81	GLN
1	H	82	MET
1	H	83	ARG
1	H	87	THR
1	H	92	CYS
1	H	95	ASP
1	H	99	MET
1	H	109	VAL
1	H	113	SER
1	H	115	LYS
1	H	120	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	127	VAL
1	H	128	CYS
1	H	137	THR
1	H	140	CYS
1	H	143	LYS
1	H	152	LEU
1	H	156	SER
1	H	158	SER
1	H	159	LEU
1	H	163	VAL
1	H	173	ASP
1	H	174	LEU
1	H	184	THR
1	H	185	SER
1	H	186	SER
1	H	187	THR
1	H	188	TRP
1	H	190	SER
1	H	202	SER
1	H	203	SER
1	H	205	LYS
1	H	208	LYS
1	H	209	LYS
2	L	6	GLN
2	L	12	SER
2	L	14	SER
2	L	19	VAL
2	L	20	THR
2	L	23	CYS
2	L	24	ARG
2	L	37	GLN
2	L	43	THR
2	L	51	THR
2	L	52	SER
2	L	53	ARG
2	L	54	LEU
2	L	56	SER
2	L	60	SER
2	L	63	SER
2	L	65	SER
2	L	67	SER
2	L	69	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	70	ASP
2	L	76	SER
2	L	81	GLU
2	L	83	ILE
2	L	89	GLN
2	L	90	GLN
2	L	97	THR
2	L	107	ARG
2	L	117	ILE
2	L	122	SER
2	L	127	SER
2	L	131	SER
2	L	142	LYS
2	L	143	ASP
2	L	155	ARG
2	L	156	GLN
2	L	160	LEU
2	L	162	SER
2	L	168	SER
2	L	174	SER
2	L	176	SER
2	L	177	SER
2	L	180	THR
2	L	181	LEU
2	L	190	ASN
2	L	191	SER
2	L	193	THR
2	L	195	GLU
2	L	197	THR
2	L	200	THR
2	L	201	SER
2	L	202	THR
2	L	203	SER
2	L	207	LYS
2	L	208	SER
2	L	211	ARG
3	S	388	LEU
3	S	389	LEU
3	S	390	SER
3	S	396	VAL
3	S	397	TYR
3	S	403	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S	405	THR
3	S	408	ASN
3	S	409	TYR
3	S	420	VAL
3	S	422	ASP
3	S	424	THR
3	S	451	SER
3	S	453	LYS
3	S	454	SER
3	S	459	SER
3	S	460	SER
3	S	464	ILE
3	S	473	PHE
3	S	481	LEU
3	S	487	ASN
3	S	488	LEU
3	S	490	THR
3	S	496	LYS
3	S	498	SER
3	S	499	TYR
3	S	501	ASN
3	S	502	LYS
3	S	503	CYS
3	S	504	SER
3	S	506	PHE
3	S	507	LEU
3	S	508	SER
3	S	511	ARG
3	S	512	THR
3	S	513	GLU
3	S	522	GLN
3	S	530	VAL
3	S	542	ARG
3	S	545	LEU
3	S	546	SER
3	S	548	LEU
3	S	553	TRP
3	S	554	LEU
3	S	557	SER
3	S	564	THR
3	S	576	GLN
3	S	579	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S	585	CYS
3	S	587	LYS
3	R	396	VAL
3	R	400	LYS
3	R	401	ARG
3	R	406	ASN
3	R	415	LEU
3	R	416	SER
3	R	420	VAL
3	R	421	ASN
3	R	422	ASP
3	R	423	PHE
3	R	426	SER
3	R	428	ILE
3	R	439	SER
3	R	440	SER
3	R	441	LEU
3	R	450	LEU
3	R	454	SER
3	R	455	ASP
3	R	460	SER
3	R	473	PHE
3	R	487	ASN
3	R	489	THR
3	R	490	THR
3	R	491	ILE
3	R	492	THR
3	R	493	LYS
3	R	495	LEU
3	R	507	LEU
3	R	511	ARG
3	R	517	LEU
3	R	518	VAL
3	R	522	GLN
3	R	534	VAL
3	R	543	LYS
3	R	546	SER
3	R	580	ASP
3	R	581	THR
3	R	587	LYS
3	R	588	LEU
2	B	2	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3	GLN
2	B	6	GLN
2	B	12	SER
2	B	14	SER
2	B	19	VAL
2	B	21	ILE
2	B	26	SER
2	B	30	ASN
2	B	37	GLN
2	B	38	GLN
2	B	45	LYS
2	B	56	SER
2	B	60	SER
2	B	61	ARG
2	B	71	TYR
2	B	72	SER
2	B	76	SER
2	B	90	GLN
2	B	94	LEU
2	B	98	PHE
2	B	105	GLU
2	B	106	LEU
2	B	108	ARG
2	B	131	SER
2	B	153	SER
2	B	155	ARG
2	B	156	GLN
2	B	160	LEU
2	B	165	ASP
2	B	178	THR
2	B	179	LEU
2	B	180	THR
2	B	181	LEU
2	B	182	THR
2	B	183	LYS
2	B	184	ASP
2	B	185	GLU
2	B	189	HIS
2	B	191	SER
2	B	192	TYR
2	B	193	THR
2	B	197	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	211	ARG
2	B	212	ASN
1	A	1	GLU
1	A	11	LEU
1	A	19	LYS
1	A	20	LEU
1	A	21	SER
1	A	27	PHE
1	A	30	SER
1	A	34	MET
1	A	39	GLN
1	A	40	THR
1	A	44	ARG
1	A	58	TYR
1	A	64	LYS
1	A	68	THR
1	A	69	ILE
1	A	71	ARG
1	A	75	GLU
1	A	78	LEU
1	A	82	MET
1	A	84	SER
1	A	85	GLU
1	A	87	THR
1	A	95	ASP
1	A	99	MET
1	A	101	ASP
1	A	107	THR
1	A	111	VAL
1	A	112	SER
1	A	120	SER
1	A	122	TYR
1	A	124	LEU
1	A	134	SER
1	A	148	GLU
1	A	150	VAL
1	A	152	LEU
1	A	153	THR
1	A	169	VAL
1	A	170	LEU
1	A	172	SER
1	A	174	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	LEU
1	A	178	SER
1	A	179	SER
1	A	190	SER
1	A	203	SER
1	A	204	THR
1	A	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	81	GLN
2	L	34	ASN
2	L	37	GLN
2	L	55	HIS
2	L	89	GLN
2	L	92	ASN
2	L	124	GLN
2	L	137	ASN
2	L	156	GLN
2	L	190	ASN
3	S	395	GLN
3	S	408	ASN
3	S	471	GLN
3	S	522	GLN
3	R	408	ASN
3	R	421	ASN
3	R	522	GLN
2	B	30	ASN
2	B	38	GLN
2	B	77	ASN
2	B	138	ASN
2	B	161	ASN
1	A	171	GLN
1	A	191	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	R	602	3	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	R	601	3	14,14,15	0.29	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	602	3	-	1/6/23/26	0/1/1/1
4	NAG	R	601	3	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	R	601	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	601	NAG	C8-C7-N2-C2
4	R	601	NAG	O7-C7-N2-C2
4	R	602	NAG	C1-C2-N2-C7
4	R	601	NAG	C4-C5-C6-O6
4	R	601	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	602	NAG	1	0
4	R	601	NAG	1	0

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	213/216 (98%)	0.10	6 (2%) 53 37	39, 73, 119, 169	0
1	H	213/216 (98%)	-0.34	0 100 100	26, 49, 84, 133	0
2	B	212/214 (99%)	-0.16	0 100 100	25, 57, 96, 135	0
2	L	212/214 (99%)	-0.39	0 100 100	25, 47, 77, 92	0
3	R	208/208 (100%)	-0.10	2 (0%) 82 72	28, 68, 121, 228	0
3	S	207/208 (99%)	0.58	21 (10%) 7 4	53, 102, 183, 294	0
All	All	1265/1276 (99%)	-0.06	29 (2%) 60 47	25, 63, 126, 294	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	434	ALA	6.4
3	S	582	ASN	4.9
3	S	433	ILE	4.4
3	S	571	PHE	3.7
1	A	128	CYS	3.6
3	S	436	ASN	3.6
3	S	409	TYR	3.5
1	A	133	GLY	3.1
3	S	488	LEU	2.8
1	A	188	TRP	2.5
3	S	430	PRO	2.5
3	S	449	PRO	2.5
3	S	487	ASN	2.4
3	S	581	THR	2.4
1	A	184	THR	2.4
3	S	456	LEU	2.4
3	S	435	SER	2.4
3	S	586	PRO	2.4
3	S	437	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	S	474	SER	2.3
3	R	588	LEU	2.3
1	A	132	THR	2.2
3	S	587	LYS	2.2
3	S	501	ASN	2.1
3	S	473	PHE	2.1
1	A	191	GLN	2.1
3	R	579	THR	2.1
3	S	489	THR	2.0
3	S	479	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	R	602	14/15	0.75	0.52	20,20,20,20	0
4	NAG	R	601	14/15	0.80	0.43	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.