Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:57 AM GMT

PDB ID	:	3NMS
Title	:	Staphylococcal Complement Inhibitor (SCIN) in complex with Human Complement C3c
Authors	:	Geisbrecht, B.V.; Garcia, B.L.
Deposited on	:	2010-06-22
Resolution	:	4.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

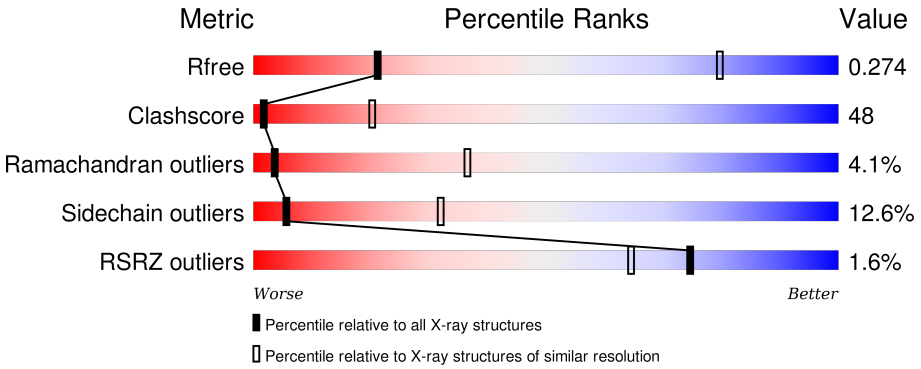
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	645	% 46% 47% 5%
2	C	343	3% 26% 47% 12% 14%
3	M	88	% 45% 38% 13% 5%
4	B	206	25% 49% 16% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9561 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			4989	3175	846	953	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	294	Total	C	N	O	S	0	0	0
			2388	1506	391	471	20			

- Molecule 3 is a protein called Staphylococcal complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

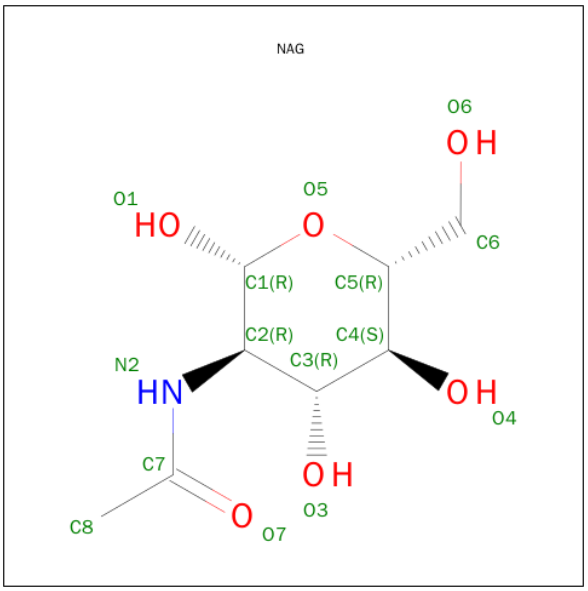
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	EXPRESSION TAG	UNP Q931M7
M	-1	THR	-	EXPRESSION TAG	UNP Q931M7
M	0	SER	-	EXPRESSION TAG	UNP Q931M7

- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	184	Total	C	N	O	S	0	0	0
			1488	956	250	277	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



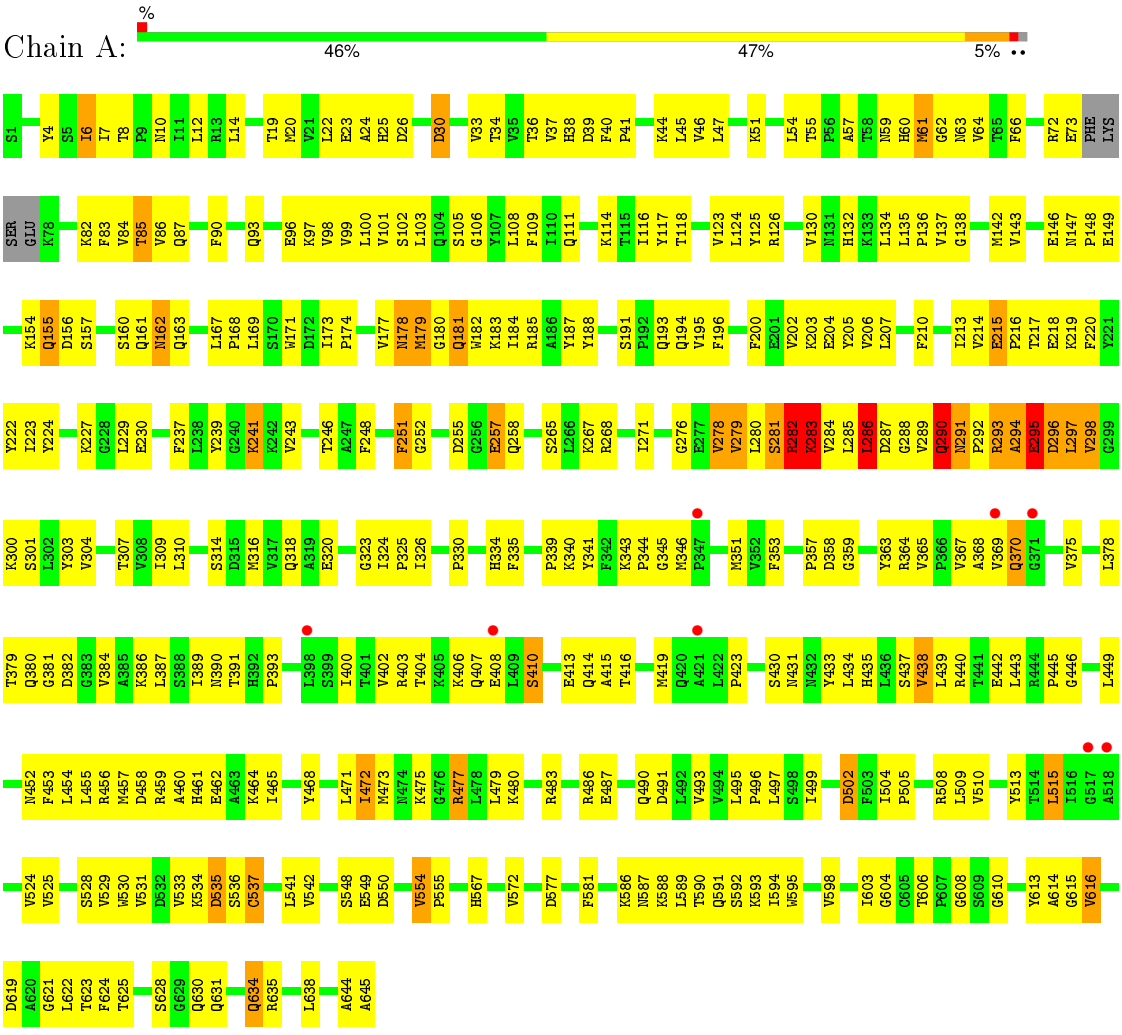
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

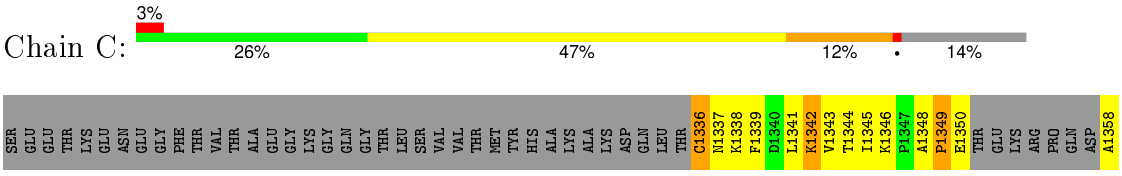
- Molecule 1: Complement C3

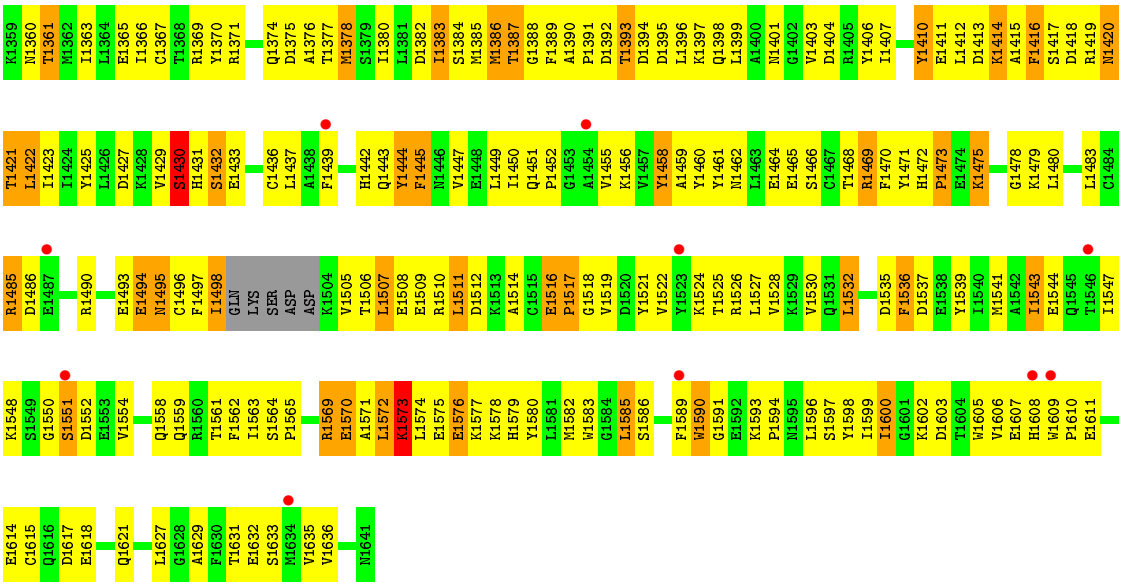
Chain A:



- Molecule 2: Complement C3

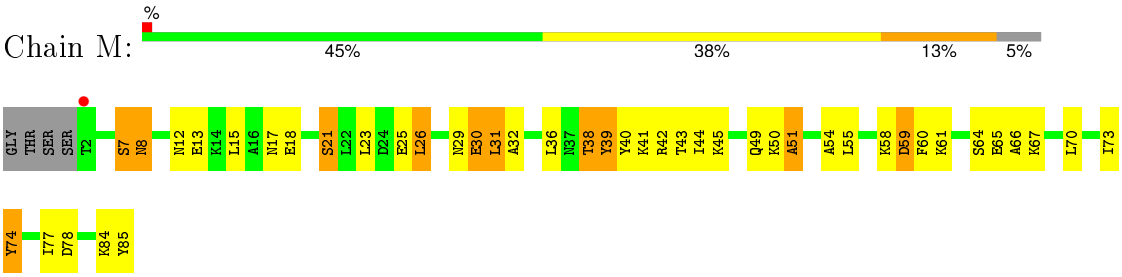
Chain C:





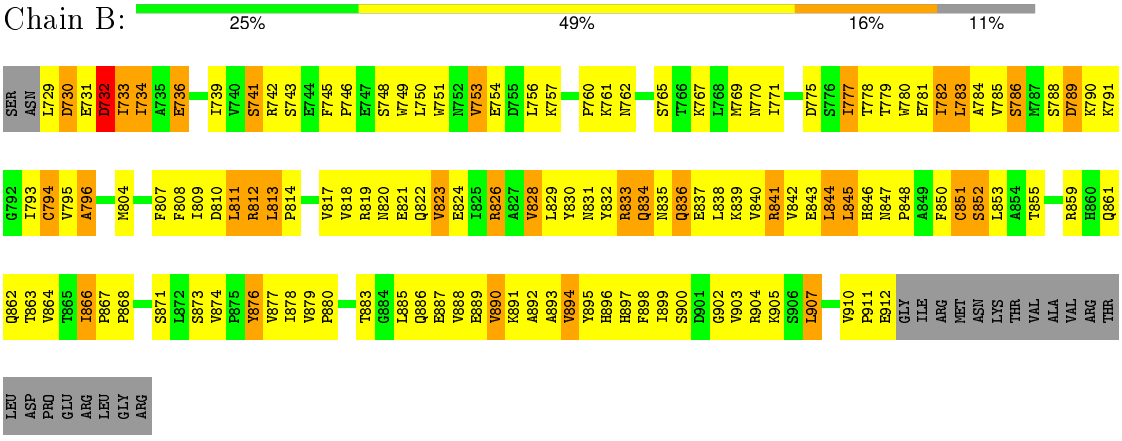
- Molecule 3: Staphylococcal complement inhibitor

Chain M:



- Molecule 4: Complement C3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	214.07Å 68.43Å 114.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 4.10 49.39 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.39-4.10) 98.2 (49.39-4.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.271 , 0.289 0.252 , 0.274	Depositor DCC
R_{free} test set	1363 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	121.4	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 115.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 13635 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9561	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.43	0/5089	0.63	1/6916 (0.0%)
2	C	0.53	1/2434 (0.0%)	0.69	0/3280
3	M	0.51	0/690	0.66	0/923
4	B	0.69	0/1520	0.85	2/2066 (0.1%)
All	All	0.51	1/9733 (0.0%)	0.68	3/13185 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1496	CYS	CB-SG	5.87	1.92	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	535	ASP	CB-CA-C	-5.97	98.46	110.40
4	B	866	ILE	CB-CA-C	-5.16	101.28	111.60
4	B	730	ASP	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4989	0	5052	464	0
2	C	2388	0	2295	247	0
3	M	682	0	697	55	0
4	B	1488	0	1513	208	0
5	A	14	0	13	4	0
All	All	9561	0	9570	924	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (924) 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:280:LEU:CD2	1:A:285:LEU:HD11	1.33	1.56
1:A:230:GLU:HA	1:A:279:VAL:CG1	1.37	1.50
4:B:811:LEU:CD1	4:B:813:LEU:HD22	1.56	1.36
1:A:280:LEU:HD21	1:A:285:LEU:CD1	1.55	1.34
1:A:290:GLN:NE2	1:A:292:PRO:HG3	1.53	1.21
1:A:161:GLN:O	1:A:162:ASN:CG	1.82	1.17
2:C:1525:THR:HG22	2:C:1543:ILE:HA	1.25	1.15
1:A:287:ASP:N	1:A:291:ASN:HB3	1.61	1.13
4:B:810:ASP:HB3	4:B:828:VAL:HG23	1.30	1.13
1:A:590:THR:HG22	1:A:592:SER:H	1.13	1.13
1:A:230:GLU:CA	1:A:279:VAL:CG1	2.26	1.12
1:A:161:GLN:O	1:A:162:ASN:ND2	1.83	1.12
2:C:1497:PHE:HE2	2:C:1571:ALA:HB1	1.05	1.12
1:A:290:GLN:HE21	1:A:292:PRO:HG3	1.00	1.10
1:A:230:GLU:HG2	1:A:279:VAL:HG11	1.12	1.10
1:A:289:VAL:O	1:A:290:GLN:HB3	1.48	1.09
1:A:591:GLN:HB2	4:B:795:VAL:CB	1.82	1.08
1:A:286:LEU:HD23	1:A:286:LEU:H	1.05	1.07
4:B:811:LEU:HD12	4:B:811:LEU:C	1.75	1.07
1:A:281:SER:OG	1:A:284:VAL:HG21	1.56	1.05
1:A:230:GLU:HA	1:A:279:VAL:HG13	1.37	1.05
4:B:811:LEU:HD11	4:B:813:LEU:HD22	1.09	1.05
3:M:26:LEU:HA	3:M:74:TYR:OH	1.57	1.05
1:A:290:GLN:O	1:A:290:GLN:HG2	1.58	1.04
1:A:230:GLU:CA	1:A:279:VAL:HG12	1.85	1.04
1:A:280:LEU:CG	1:A:285:LEU:HD11	1.88	1.03
1:A:591:GLN:N	4:B:795:VAL:HG11	1.73	1.02
1:A:287:ASP:HA	1:A:291:ASN:N	1.75	1.02
1:A:287:ASP:HA	1:A:291:ASN:H	1.21	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:831:ASN:ND2	4:B:868:PRO:HA	1.74	1.02
4:B:810:ASP:CG	4:B:812:ARG:HD3	1.80	1.01
1:A:281:SER:O	1:A:284:VAL:HG23	1.60	1.01
1:A:280:LEU:HD11	1:A:285:LEU:HD12	1.40	1.01
4:B:795:VAL:HG12	4:B:795:VAL:O	1.60	1.00
1:A:206:VAL:HG11	4:B:813:LEU:O	1.61	1.00
1:A:280:LEU:CD2	1:A:285:LEU:CD1	2.27	1.00
1:A:286:LEU:HD23	1:A:286:LEU:N	1.60	0.99
2:C:1497:PHE:CE2	2:C:1571:ALA:HB1	1.97	0.99
1:A:230:GLU:HA	1:A:279:VAL:HG12	1.04	0.99
1:A:591:GLN:HB2	4:B:795:VAL:HB	1.03	0.99
4:B:811:LEU:CD1	4:B:811:LEU:C	2.29	0.99
4:B:734:ILE:HD13	4:B:893:ALA:HB1	1.44	0.99
4:B:811:LEU:HD11	4:B:813:LEU:CD2	1.93	0.98
4:B:810:ASP:OD1	4:B:812:ARG:HD3	1.64	0.98
1:A:230:GLU:CG	1:A:279:VAL:HG11	1.94	0.98
1:A:290:GLN:HE21	1:A:292:PRO:CG	1.77	0.97
1:A:541:LEU:HD22	4:B:786:SER:HB3	1.46	0.96
2:C:1343:VAL:HG21	2:C:1469:ARG:HB3	1.48	0.96
1:A:287:ASP:CA	1:A:291:ASN:HB3	1.95	0.96
1:A:161:GLN:C	1:A:162:ASN:CG	2.15	0.95
1:A:286:LEU:CD2	1:A:286:LEU:N	2.30	0.94
1:A:590:THR:HG22	1:A:592:SER:N	1.83	0.94
1:A:281:SER:CB	1:A:284:VAL:CG2	2.45	0.94
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.48	0.94
1:A:280:LEU:CG	1:A:285:LEU:CD1	2.46	0.93
3:M:39:TYR:CE1	3:M:43:THR:OG1	2.21	0.92
1:A:287:ASP:CA	1:A:291:ASN:H	1.82	0.92
4:B:734:ILE:HD12	4:B:734:ILE:H	1.35	0.92
2:C:1516:GLU:HB3	2:C:1517:PRO:HD2	1.50	0.91
2:C:1575:GLU:HB2	2:C:1578:LYS:HD2	1.49	0.91
1:A:290:GLN:C	1:A:292:PRO:HD3	1.92	0.90
1:A:591:GLN:H	4:B:795:VAL:HG11	1.30	0.89
1:A:10:ASN:HB3	1:A:635:ARG:HH11	1.37	0.89
2:C:1573:LYS:O	2:C:1574:LEU:HD23	1.73	0.88
2:C:1539:TYR:CE1	2:C:1574:LEU:HD12	2.08	0.88
4:B:811:LEU:CD1	4:B:813:LEU:CD2	2.48	0.88
1:A:591:GLN:CB	4:B:795:VAL:HB	1.99	0.87
1:A:346:MET:O	1:A:391:THR:HG22	1.74	0.86
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.10	0.86
4:B:883:THR:HG21	4:B:911:PRO:HG3	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1497:PHE:CD1	2:C:1498:ILE:HG13	2.11	0.85
1:A:287:ASP:N	1:A:291:ASN:CB	2.39	0.85
4:B:811:LEU:CG	4:B:813:LEU:HD22	2.05	0.85
4:B:822:GLN:HB2	4:B:879:VAL:HG22	1.55	0.85
4:B:733:ILE:HG12	4:B:734:ILE:N	1.90	0.85
1:A:281:SER:CB	1:A:284:VAL:HG23	2.06	0.85
1:A:280:LEU:HD11	1:A:285:LEU:CD1	2.06	0.85
1:A:281:SER:HB2	1:A:284:VAL:HG23	1.58	0.84
4:B:811:LEU:HG	4:B:813:LEU:CD2	2.08	0.84
4:B:822:GLN:HG2	4:B:822:GLN:O	1.78	0.84
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.57	0.84
1:A:126:ARG:HG3	4:B:751:TRP:CZ2	2.13	0.84
1:A:8:THR:HG22	1:A:20:MET:HB2	1.60	0.84
1:A:281:SER:C	1:A:284:VAL:HG23	1.98	0.84
4:B:811:LEU:CD1	4:B:812:ARG:N	2.41	0.84
1:A:161:GLN:C	1:A:162:ASN:OD1	2.14	0.84
4:B:833:ARG:HD2	4:B:834:GLN:HE22	1.42	0.83
1:A:229:LEU:O	1:A:279:VAL:HG12	1.78	0.83
4:B:810:ASP:OD1	4:B:812:ARG:CD	2.26	0.83
1:A:591:GLN:OE1	4:B:795:VAL:HG23	1.79	0.83
4:B:811:LEU:CG	4:B:813:LEU:CD2	2.58	0.82
4:B:833:ARG:HD2	4:B:834:GLN:NE2	1.95	0.82
1:A:223:ILE:HD11	1:A:298:VAL:HG23	1.61	0.82
2:C:1391:PRO:HB2	2:C:1396:LEU:HD11	1.61	0.82
2:C:1444:TYR:CD1	2:C:1445:PHE:HB2	2.16	0.81
1:A:590:THR:HB	1:A:593:LYS:HG3	1.61	0.81
2:C:1518:GLY:O	2:C:1585:LEU:HA	1.82	0.80
2:C:1451:GLN:HG3	2:C:1452:PRO:HD2	1.63	0.80
2:C:1497:PHE:CD1	2:C:1498:ILE:CG1	2.64	0.80
1:A:55:THR:HG22	1:A:57:ALA:H	1.45	0.80
1:A:281:SER:OG	1:A:284:VAL:CG2	2.30	0.80
1:A:161:GLN:CG	1:A:162:ASN:OD1	2.30	0.80
1:A:281:SER:O	1:A:284:VAL:CG2	2.29	0.80
1:A:161:GLN:CB	1:A:162:ASN:OD1	2.30	0.79
1:A:541:LEU:HB2	4:B:794:CYS:SG	2.23	0.79
3:M:29:ASN:ND2	3:M:44:ILE:HD12	1.97	0.79
1:A:281:SER:HB2	1:A:284:VAL:CG2	2.13	0.79
4:B:811:LEU:HD12	4:B:812:ARG:N	1.97	0.78
3:M:70:LEU:HG	3:M:74:TYR:CD1	2.17	0.78
2:C:1536:PHE:HD1	2:C:1563:ILE:HG21	1.47	0.78
4:B:831:ASN:HD21	4:B:868:PRO:HA	1.45	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:810:ASP:OD2	4:B:812:ARG:HD3	1.82	0.78
3:M:29:ASN:ND2	3:M:44:ILE:CD1	2.48	0.77
2:C:1343:VAL:HG21	2:C:1469:ARG:CB	2.14	0.77
1:A:290:GLN:O	1:A:290:GLN:CG	2.33	0.77
1:A:180:GLY:O	1:A:182:TRP:HD1	1.66	0.77
4:B:841:ARG:HG2	4:B:841:ARG:HH11	1.50	0.77
2:C:1490:ARG:NH1	2:C:1599:ILE:HG21	2.00	0.77
1:A:297:LEU:HD23	1:A:326:ILE:HD13	1.67	0.76
1:A:365:VAL:HG13	1:A:379:THR:OG1	1.85	0.76
1:A:22:LEU:HD11	1:A:64:VAL:HG23	1.67	0.75
4:B:795:VAL:CG1	4:B:795:VAL:O	2.34	0.75
4:B:810:ASP:CB	4:B:828:VAL:HG23	2.13	0.75
1:A:530:TRP:HD1	1:A:531:VAL:N	1.85	0.75
3:M:73:ILE:O	3:M:77:ILE:HG12	1.87	0.75
1:A:286:LEU:C	1:A:291:ASN:HA	2.08	0.74
1:A:290:GLN:O	1:A:292:PRO:HD3	1.86	0.74
4:B:788:SER:O	4:B:790:LYS:N	2.20	0.74
3:M:70:LEU:HG	3:M:74:TYR:CE1	2.22	0.74
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.16	0.74
1:A:610:GLY:HA3	1:A:616:VAL:N	2.02	0.74
1:A:12:LEU:HB2	1:A:101:VAL:HG22	1.70	0.74
1:A:180:GLY:O	1:A:182:TRP:CD1	2.41	0.74
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.22	0.74
1:A:223:ILE:O	1:A:282:ARG:NH1	2.21	0.74
1:A:20:MET:O	1:A:64:VAL:HB	1.87	0.74
2:C:1403:VAL:O	2:C:1404:ASP:HB2	1.88	0.74
2:C:1573:LYS:HD2	2:C:1573:LYS:N	2.02	0.73
1:A:280:LEU:CD1	1:A:285:LEU:CD1	2.65	0.73
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	0.73
4:B:822:GLN:HB2	4:B:879:VAL:CG2	2.18	0.73
4:B:813:LEU:HD12	4:B:814:PRO:CD	2.19	0.73
2:C:1444:TYR:CE1	2:C:1445:PHE:HB2	2.24	0.73
2:C:1370:TYR:CD2	2:C:1376:ALA:HB2	2.24	0.73
1:A:290:GLN:HG2	1:A:292:PRO:HD3	1.70	0.72
1:A:287:ASP:H	1:A:291:ASN:HB3	1.54	0.72
2:C:1575:GLU:O	2:C:1578:LYS:HB2	1.89	0.72
4:B:777:ILE:O	4:B:777:ILE:HG22	1.88	0.72
4:B:756:LEU:HD23	4:B:756:LEU:N	2.05	0.72
4:B:810:ASP:HB3	4:B:828:VAL:CG2	2.16	0.72
4:B:833:ARG:HH22	4:B:899:ILE:HD11	1.53	0.72
4:B:741:SER:HB3	4:B:902:GLY:C	2.09	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:749:TRP:CE3	4:B:750:LEU:HB2	2.26	0.71
4:B:874:VAL:HG12	4:B:874:VAL:O	1.90	0.71
1:A:390:ASN:OD1	1:A:390:ASN:O	2.07	0.71
1:A:289:VAL:O	1:A:290:GLN:CB	2.33	0.71
3:M:36:LEU:HD23	3:M:36:LEU:N	2.06	0.71
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.72	0.71
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.72	0.71
2:C:1497:PHE:C	2:C:1498:ILE:HG13	2.10	0.71
1:A:6:ILE:HD11	1:A:22:LEU:HD23	1.72	0.71
1:A:280:LEU:HD21	1:A:285:LEU:HD11	0.72	0.71
1:A:161:GLN:HB3	1:A:162:ASN:OD1	1.91	0.71
1:A:591:GLN:HA	4:B:795:VAL:HG21	1.72	0.70
1:A:495:LEU:HD12	1:A:496:PRO:HD2	1.73	0.70
1:A:230:GLU:HG2	1:A:279:VAL:CG1	2.07	0.70
2:C:1343:VAL:CG2	2:C:1469:ARG:HB3	2.21	0.70
2:C:1341:LEU:HD23	2:C:1469:ARG:H	1.56	0.70
2:C:1345:ILE:HD12	2:C:1363:ILE:O	1.92	0.70
1:A:239:TYR:HB2	4:B:804:MET:SD	2.32	0.69
1:A:330:PRO:O	1:A:357:PRO:HD3	1.92	0.69
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.27	0.69
1:A:281:SER:CB	1:A:284:VAL:HG21	2.16	0.69
4:B:731:GLU:O	4:B:733:ILE:N	2.25	0.69
1:A:591:GLN:OE1	4:B:795:VAL:CG2	2.39	0.69
1:A:38:HIS:CE1	1:A:45:LEU:HD12	2.27	0.69
1:A:369:VAL:HG12	1:A:370:GLN:H	1.58	0.69
4:B:811:LEU:HD13	4:B:812:ARG:N	2.06	0.69
1:A:589:LEU:HD12	1:A:590:THR:H	1.57	0.69
2:C:1510:ARG:NH1	2:C:1627:LEU:HD23	2.08	0.69
2:C:1386:MET:HE3	2:C:1389:PHE:CD1	2.28	0.69
4:B:813:LEU:HD12	4:B:814:PRO:HD3	1.74	0.69
2:C:1342:LYS:CB	2:C:1367:CYS:HB2	2.23	0.69
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.74	0.68
4:B:777:ILE:CG2	4:B:777:ILE:O	2.41	0.68
2:C:1391:PRO:CB	2:C:1396:LEU:HD11	2.24	0.68
4:B:831:ASN:HD22	4:B:868:PRO:HA	1.57	0.68
2:C:1342:LYS:HB2	2:C:1367:CYS:HB2	1.74	0.68
1:A:19:THR:HA	1:A:64:VAL:O	1.94	0.68
2:C:1590:TRP:HB3	2:C:1597:SER:HB2	1.75	0.68
1:A:180:GLY:O	1:A:181:GLN:C	2.30	0.68
1:A:280:LEU:HG	1:A:285:LEU:CD1	2.24	0.67
1:A:216:PRO:HB2	1:A:218:GLU:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1391:PRO:HB2	2:C:1396:LEU:CD1	2.24	0.67
3:M:26:LEU:CA	3:M:74:TYR:OH	2.41	0.67
1:A:286:LEU:HB3	1:A:291:ASN:HB2	1.77	0.67
4:B:734:ILE:CD1	4:B:893:ALA:HB1	2.22	0.67
3:M:70:LEU:O	3:M:74:TYR:HD1	1.77	0.66
4:B:742:ARG:HB3	4:B:775:ASP:HB3	1.78	0.66
3:M:36:LEU:HB3	3:M:40:TYR:CD2	2.30	0.66
4:B:841:ARG:NH1	4:B:841:ARG:HG2	2.09	0.66
3:M:17:ASN:O	3:M:17:ASN:CG	2.34	0.66
4:B:793:ILE:O	4:B:793:ILE:HG23	1.95	0.66
1:A:257:GLU:CD	1:A:257:GLU:N	2.49	0.66
2:C:1570:GLU:HG3	2:C:1571:ALA:H	1.61	0.66
1:A:130:VAL:HG12	1:A:136:PRO:HA	1.78	0.66
2:C:1532:LEU:HD21	2:C:1569:ARG:HE	1.60	0.66
1:A:282:ARG:O	1:A:284:VAL:N	2.29	0.66
2:C:1451:GLN:CG	2:C:1452:PRO:HD2	2.26	0.66
2:C:1600:ILE:HG22	2:C:1600:ILE:O	1.94	0.66
4:B:841:ARG:HH11	4:B:841:ARG:CG	2.08	0.66
1:A:567:HIS:ND1	4:B:760:PRO:HG3	2.10	0.66
2:C:1585:LEU:HD21	2:C:1603:ASP:HB3	1.76	0.66
3:M:84:LYS:O	3:M:84:LYS:HG3	1.96	0.66
4:B:835:ASN:OD1	4:B:835:ASN:O	2.13	0.66
4:B:883:THR:CG2	4:B:911:PRO:HG3	2.26	0.65
2:C:1490:ARG:HH11	2:C:1599:ILE:HG21	1.61	0.65
1:A:293:ARG:NH1	1:A:295:GLU:OE2	2.29	0.65
2:C:1510:ARG:HH12	2:C:1627:LEU:CD2	2.09	0.65
4:B:843:GLU:OE2	4:B:859:ARG:HD3	1.96	0.65
1:A:281:SER:O	1:A:284:VAL:N	2.30	0.65
1:A:223:ILE:CD1	1:A:298:VAL:HG23	2.26	0.65
1:A:8:THR:HG22	1:A:20:MET:CB	2.26	0.65
2:C:1494:GLU:HB2	2:C:1602:LYS:HB3	1.79	0.65
2:C:1532:LEU:HD23	2:C:1537:ASP:HB3	1.79	0.64
1:A:161:GLN:C	1:A:163:GLN:H	1.98	0.64
3:M:38:THR:O	3:M:39:TYR:C	2.34	0.64
2:C:1590:TRP:CE3	2:C:1590:TRP:HA	2.32	0.64
2:C:1450:ILE:HG13	2:C:1450:ILE:O	1.96	0.64
2:C:1518:GLY:HA3	2:C:1585:LEU:HD22	1.80	0.64
1:A:572:VAL:HG12	4:B:753:VAL:HG22	1.79	0.64
2:C:1416:PHE:C	2:C:1416:PHE:CD2	2.70	0.64
1:A:281:SER:O	1:A:284:VAL:CB	2.45	0.64
1:A:294:ALA:O	1:A:296:ASP:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:C	1:A:279:VAL:HG12	2.18	0.64
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.79	0.64
1:A:281:SER:O	1:A:282:ARG:C	2.36	0.64
1:A:287:ASP:O	1:A:290:GLN:N	2.30	0.64
2:C:1470:PHE:CZ	4:B:822:GLN:O	2.50	0.64
4:B:833:ARG:CD	4:B:834:GLN:NE2	2.60	0.64
3:M:17:ASN:ND2	3:M:17:ASN:O	2.31	0.64
2:C:1416:PHE:HA	2:C:1419:ARG:HH12	1.62	0.64
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.33	0.64
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.64
1:A:407:GLN:O	1:A:408:GLU:HB2	1.96	0.63
4:B:811:LEU:HG	4:B:813:LEU:HD23	1.79	0.63
4:B:874:VAL:CG1	4:B:874:VAL:O	2.45	0.63
2:C:1461:TYR:CD1	2:C:1462:ASN:HB2	2.34	0.63
1:A:445:PRO:HA	1:A:499:ILE:O	1.98	0.63
1:A:295:GLU:O	1:A:298:VAL:N	2.30	0.63
1:A:610:GLY:HA3	1:A:616:VAL:H	1.63	0.63
1:A:105:SER:HB2	1:A:188:TYR:CD1	2.33	0.63
1:A:93:GLN:HA	1:A:93:GLN:OE1	1.97	0.63
2:C:1451:GLN:HB2	4:B:853:LEU:HD12	1.79	0.62
1:A:307:THR:HG23	1:A:318:GLN:HG3	1.81	0.62
1:A:294:ALA:O	1:A:295:GLU:C	2.36	0.62
1:A:287:ASP:CA	1:A:291:ASN:CB	2.74	0.62
1:A:114:LYS:HE3	1:A:116:ILE:O	1.99	0.62
1:A:340:LYS:O	1:A:341:TYR:CD1	2.53	0.62
2:C:1527:LEU:HD21	2:C:1530:VAL:CG2	2.29	0.62
1:A:136:PRO:CG	4:B:789:ASP:HA	2.30	0.62
1:A:239:TYR:HB2	4:B:804:MET:HG3	1.79	0.62
4:B:833:ARG:HG2	4:B:833:ARG:HH11	1.64	0.62
2:C:1575:GLU:OE2	2:C:1578:LYS:HD2	2.00	0.62
1:A:154:LYS:HE2	1:A:156:ASP:OD1	2.00	0.62
1:A:281:SER:CA	1:A:284:VAL:HG23	2.29	0.62
1:A:286:LEU:C	1:A:291:ASN:CA	2.68	0.62
2:C:1527:LEU:HD21	2:C:1530:VAL:HG22	1.81	0.62
4:B:745:PHE:CE2	4:B:905:LYS:HG2	2.34	0.62
1:A:251:PHE:CD1	1:A:280:LEU:HB2	2.35	0.61
1:A:126:ARG:HG3	4:B:751:TRP:CH2	2.35	0.61
1:A:433:TYR:HB2	1:A:456:ARG:HB3	1.81	0.61
4:B:907:LEU:HD23	4:B:907:LEU:H	1.64	0.61
4:B:844:LEU:HD12	4:B:845:LEU:N	2.14	0.61
2:C:1497:PHE:CD1	2:C:1498:ILE:HG12	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1506:THR:OG1	2:C:1509:GLU:HG2	2.00	0.61
4:B:840:VAL:CG1	4:B:892:ALA:HB1	2.30	0.61
2:C:1572:LEU:HD13	2:C:1574:LEU:HG	1.82	0.61
1:A:487:GLU:O	1:A:490:GLN:HB2	2.01	0.61
2:C:1358:ALA:HB1	2:C:1361:THR:CG2	2.31	0.61
2:C:1527:LEU:HD13	2:C:1541:MET:HG2	1.83	0.61
4:B:847:ASN:CB	4:B:850:PHE:HD1	2.14	0.60
1:A:438:VAL:O	1:A:440:ARG:HG3	2.00	0.60
1:A:282:ARG:O	1:A:285:LEU:N	2.26	0.60
1:A:161:GLN:C	1:A:163:GLN:N	2.54	0.60
1:A:239:TYR:CE1	4:B:832:TYR:CE1	2.89	0.60
1:A:73:GLU:HB3	1:A:82:LYS:NZ	2.16	0.60
1:A:297:LEU:HD23	1:A:326:ILE:CD1	2.31	0.60
1:A:179:MET:HG2	1:A:203:LYS:HA	1.83	0.60
1:A:513:TYR:CE1	1:A:525:VAL:HB	2.37	0.60
3:M:39:TYR:O	3:M:40:TYR:C	2.38	0.60
1:A:530:TRP:CD1	1:A:531:VAL:N	2.69	0.60
4:B:833:ARG:CD	4:B:834:GLN:HE22	2.11	0.60
1:A:160:SER:HA	1:A:167:LEU:HD21	1.82	0.60
2:C:1575:GLU:HB2	2:C:1578:LYS:CD	2.26	0.60
1:A:241:LYS:HG3	4:B:832:TYR:CE2	2.36	0.60
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.84	0.60
1:A:455:LEU:HD11	1:A:457:MET:HG2	1.82	0.60
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.83	0.60
2:C:1360:ASN:HD22	2:C:1443:GLN:HB3	1.66	0.60
1:A:285:LEU:O	1:A:286:LEU:C	2.40	0.59
4:B:808:PHE:HE1	4:B:830:TYR:CD2	2.20	0.59
2:C:1590:TRP:HE3	2:C:1590:TRP:HA	1.67	0.59
1:A:533:VAL:HG12	1:A:534:LYS:N	2.17	0.59
1:A:606:THR:HG22	1:A:608:GLY:N	2.17	0.59
1:A:591:GLN:CA	4:B:795:VAL:HG21	2.32	0.59
3:M:38:THR:O	3:M:39:TYR:O	2.20	0.59
2:C:1343:VAL:CG2	2:C:1469:ARG:CB	2.79	0.59
1:A:10:ASN:HB3	1:A:635:ARG:NH1	2.15	0.59
1:A:22:LEU:HB2	1:A:62:GLY:HA3	1.82	0.59
1:A:135:LEU:HD22	4:B:789:ASP:O	2.02	0.59
2:C:1528:VAL:HG21	2:C:1559:GLN:OE1	2.00	0.59
2:C:1530:VAL:HG23	2:C:1576:GLU:HG2	1.84	0.59
4:B:822:GLN:O	4:B:822:GLN:CG	2.48	0.59
1:A:99:VAL:HG12	1:A:100:LEU:N	2.18	0.59
4:B:808:PHE:CE1	4:B:830:TYR:HB2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLY:N	1:A:499:ILE:O	2.32	0.59
4:B:841:ARG:HG2	4:B:841:ARG:O	2.03	0.59
2:C:1589:PHE:CE1	2:C:1598:TYR:CE2	2.91	0.59
1:A:295:GLU:O	1:A:296:ASP:C	2.42	0.59
1:A:177:VAL:HG21	1:A:182:TRP:HH2	1.67	0.59
1:A:20:MET:HG2	1:A:64:VAL:HG21	1.84	0.59
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.85	0.59
2:C:1569:ARG:NH1	2:C:1569:ARG:HG3	2.17	0.58
2:C:1507:LEU:HD11	2:C:1629:ALA:HB1	1.85	0.58
1:A:589:LEU:HD12	1:A:590:THR:N	2.18	0.58
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.32	0.58
2:C:1505:VAL:HG12	2:C:1510:ARG:HE	1.68	0.58
4:B:844:LEU:HB2	4:B:876:TYR:CE2	2.39	0.58
4:B:732:ASP:O	4:B:896:HIS:N	2.33	0.58
1:A:230:GLU:CB	1:A:279:VAL:CG1	2.81	0.58
1:A:47:LEU:HD11	1:A:66:PHE:HB2	1.84	0.58
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.37	0.58
1:A:10:ASN:CG	1:A:635:ARG:HD2	2.24	0.58
1:A:345:GLY:H	1:A:391:THR:HG23	1.68	0.58
1:A:118:THR:HG23	1:A:205:TYR:CZ	2.38	0.58
2:C:1470:PHE:HB2	2:C:1478:GLY:HA3	1.85	0.57
4:B:835:ASN:O	4:B:836:GLN:CB	2.51	0.57
1:A:246:THR:OG1	2:C:1425:TYR:CZ	2.57	0.57
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.39	0.57
3:M:55:LEU:O	3:M:58:LYS:HD3	2.04	0.57
3:M:39:TYR:O	3:M:42:ARG:N	2.37	0.57
1:A:477:ARG:NH2	1:A:479:LEU:HD13	2.20	0.57
2:C:1519:VAL:HG12	2:C:1548:LYS:NZ	2.20	0.57
2:C:1617:ASP:O	2:C:1621:GLN:HG3	2.04	0.57
4:B:741:SER:HB3	4:B:903:VAL:N	2.19	0.57
1:A:282:ARG:C	1:A:284:VAL:N	2.54	0.57
2:C:1569:ARG:HG3	2:C:1569:ARG:HH11	1.70	0.57
2:C:1550:GLY:C	2:C:1552:ASP:H	2.07	0.57
1:A:99:VAL:HG12	1:A:100:LEU:H	1.70	0.57
3:M:70:LEU:O	3:M:74:TYR:CD1	2.57	0.57
1:A:541:LEU:CD2	4:B:786:SER:HB3	2.28	0.57
2:C:1536:PHE:CD1	2:C:1563:ILE:HG21	2.36	0.57
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.87	0.57
3:M:29:ASN:ND2	3:M:44:ILE:HD11	2.19	0.56
1:A:541:LEU:HD22	4:B:794:CYS:HB3	1.87	0.56
1:A:594:ILE:O	1:A:598:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:84:LYS:O	3:M:85:TYR:HB2	2.05	0.56
1:A:345:GLY:N	1:A:391:THR:HG23	2.20	0.56
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.33	0.56
1:A:292:PRO:O	1:A:293:ARG:O	2.24	0.56
1:A:287:ASP:HA	1:A:291:ASN:CB	2.36	0.56
3:M:26:LEU:HD12	3:M:26:LEU:C	2.26	0.56
3:M:70:LEU:CG	3:M:74:TYR:CE1	2.89	0.56
1:A:406:LYS:H	1:A:414:GLN:HE22	1.54	0.56
1:A:281:SER:CA	1:A:284:VAL:CG2	2.84	0.56
2:C:1572:LEU:O	2:C:1573:LYS:HB3	2.06	0.56
4:B:761:LYS:O	4:B:762:ASN:HB2	2.06	0.56
1:A:239:TYR:HE1	4:B:832:TYR:CZ	2.24	0.56
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.41	0.56
2:C:1510:ARG:NH1	2:C:1627:LEU:CD2	2.68	0.56
1:A:443:LEU:O	1:A:533:VAL:HG13	2.06	0.56
2:C:1386:MET:CE	2:C:1389:PHE:CD1	2.88	0.55
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.55
1:A:290:GLN:O	1:A:292:PRO:CD	2.55	0.55
1:A:239:TYR:HB2	4:B:804:MET:CG	2.36	0.55
1:A:230:GLU:N	1:A:279:VAL:HG12	2.22	0.55
2:C:1530:VAL:HG12	2:C:1530:VAL:O	2.07	0.55
2:C:1366:ILE:HD11	2:C:1455:VAL:HG21	1.88	0.55
3:M:64:SER:O	3:M:67:LYS:HB3	2.05	0.55
1:A:536:SER:O	1:A:537:CYS:O	2.24	0.55
1:A:142:MET:HG3	1:A:187:TYR:HE1	1.64	0.55
1:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.55
1:A:239:TYR:CB	4:B:804:MET:HG3	2.36	0.55
1:A:148:PRO:HG3	1:A:182:TRP:CD1	2.42	0.55
2:C:1389:PHE:CZ	2:C:1443:GLN:HB2	2.41	0.55
1:A:440:ARG:NH2	1:A:529:VAL:HG23	2.22	0.55
1:A:586:LYS:O	1:A:587:ASN:HB2	2.05	0.55
2:C:1421:THR:OG1	2:C:1422:LEU:N	2.39	0.55
2:C:1407:ILE:HB	2:C:1412:LEU:HD11	1.89	0.55
4:B:785:VAL:HG13	4:B:794:CYS:O	2.07	0.55
1:A:177:VAL:HG21	1:A:182:TRP:CH2	2.42	0.55
1:A:161:GLN:O	1:A:162:ASN:CB	2.46	0.55
4:B:835:ASN:O	4:B:836:GLN:CG	2.55	0.55
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	0.55
1:A:34:THR:HG22	1:A:51:LYS:HE2	1.88	0.54
1:A:577:ASP:HB2	4:B:780:TRP:CZ3	2.42	0.54
1:A:536:SER:O	1:A:537:CYS:C	2.46	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:844:LEU:HB2	4:B:876:TYR:CZ	2.43	0.54
1:A:290:GLN:C	1:A:292:PRO:CD	2.73	0.54
4:B:778:THR:HG23	4:B:779:THR:N	2.21	0.54
1:A:126:ARG:CG	4:B:751:TRP:CZ2	2.88	0.54
1:A:136:PRO:CD	4:B:789:ASP:HA	2.37	0.54
4:B:808:PHE:CD1	4:B:808:PHE:C	2.81	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.90	0.54
4:B:902:GLY:C	4:B:903:VAL:CG2	2.76	0.54
2:C:1421:THR:O	2:C:1422:LEU:CB	2.56	0.54
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.43	0.54
4:B:749:TRP:CZ3	4:B:750:LEU:HB2	2.43	0.54
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.90	0.54
2:C:1336:CYS:O	2:C:1337:ASN:CG	2.47	0.53
4:B:793:ILE:CG2	4:B:793:ILE:O	2.56	0.53
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.53
2:C:1416:PHE:HA	2:C:1419:ARG:NH1	2.23	0.53
2:C:1392:ASP:HB2	2:C:1442:HIS:NE2	2.23	0.53
1:A:577:ASP:HB2	4:B:780:TRP:HZ3	1.73	0.53
1:A:524:VAL:HB	1:A:613:TYR:CD1	2.43	0.53
1:A:287:ASP:CA	1:A:291:ASN:N	2.53	0.53
2:C:1586:SER:HA	2:C:1589:PHE:CE2	2.42	0.53
1:A:297:LEU:HA	1:A:300:LYS:HD2	1.91	0.53
1:A:567:HIS:CG	4:B:760:PRO:HG3	2.44	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
4:B:833:ARG:CG	4:B:833:ARG:HH11	2.22	0.53
1:A:239:TYR:HE1	4:B:832:TYR:CE1	2.26	0.53
2:C:1507:LEU:HD22	2:C:1511:LEU:HD12	1.91	0.53
2:C:1403:VAL:HG22	2:C:1404:ASP:N	2.23	0.53
2:C:1358:ALA:HB1	2:C:1361:THR:HG22	1.91	0.53
4:B:847:ASN:HB3	4:B:850:PHE:HD1	1.74	0.53
1:A:34:THR:CG2	1:A:51:LYS:HE2	2.38	0.53
2:C:1572:LEU:C	2:C:1573:LYS:HD2	2.28	0.53
2:C:1461:TYR:HD1	2:C:1462:ASN:HB2	1.74	0.53
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.44	0.52
2:C:1384:SER:HA	2:C:1421:THR:HA	1.91	0.52
1:A:290:GLN:HE21	1:A:292:PRO:CD	2.21	0.52
2:C:1345:ILE:HG23	2:C:1345:ILE:O	2.09	0.52
1:A:468:TYR:HE1	1:A:513:TYR:HD2	1.57	0.52
1:A:39:ASP:OD1	1:A:44:LYS:HB2	2.09	0.52
4:B:887:GLU:CG	4:B:887:GLU:O	2.57	0.52
1:A:143:VAL:O	1:A:155:GLN:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1554:VAL:HG13	2:C:1554:VAL:O	2.09	0.52
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.56	0.52
2:C:1514:ALA:HA	2:C:1519:VAL:HG21	1.92	0.52
1:A:581:PHE:CE1	1:A:588:LYS:HD2	2.45	0.52
1:A:282:ARG:C	1:A:284:VAL:H	2.12	0.52
1:A:510:VAL:HG12	1:A:528:SER:CB	2.30	0.52
2:C:1582:MET:SD	2:C:1606:VAL:HG22	2.50	0.52
1:A:468:TYR:HE1	1:A:513:TYR:CD2	2.28	0.52
2:C:1366:ILE:HD11	2:C:1455:VAL:CG2	2.39	0.52
2:C:1570:GLU:HG3	2:C:1571:ALA:N	2.23	0.52
4:B:895:TYR:HB3	4:B:896:HIS:CE1	2.44	0.52
2:C:1516:GLU:HB3	2:C:1517:PRO:CD	2.32	0.52
2:C:1444:TYR:CD1	2:C:1444:TYR:C	2.82	0.52
1:A:363:TYR:CE1	1:A:364:ARG:HG3	2.44	0.52
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.45	0.52
1:A:136:PRO:HD2	4:B:789:ASP:HA	1.91	0.52
2:C:1461:TYR:CD1	2:C:1462:ASN:N	2.78	0.52
1:A:268:ARG:HB2	2:C:1378:MET:HE3	1.92	0.52
1:A:257:GLU:H	1:A:257:GLU:CD	2.13	0.52
1:A:403:ARG:HG2	1:A:404:THR:O	2.10	0.52
2:C:1375:ASP:OD2	2:C:1430:SER:HA	2.10	0.52
4:B:788:SER:O	4:B:791:LYS:N	2.43	0.51
1:A:287:ASP:N	1:A:291:ASN:CA	2.72	0.51
4:B:811:LEU:HD12	4:B:813:LEU:HD22	1.77	0.51
3:M:36:LEU:HB3	3:M:40:TYR:HD2	1.73	0.51
4:B:907:LEU:HD23	4:B:907:LEU:N	2.24	0.51
1:A:193:GLN:HG2	1:A:194:GLN:N	2.24	0.51
1:A:472:ILE:HG13	1:A:480:LYS:HB3	1.92	0.51
1:A:37:VAL:HB	1:A:46:VAL:HG23	1.93	0.51
1:A:343:LYS:N	1:A:343:LYS:HD2	2.25	0.51
2:C:1410:TYR:CD2	2:C:1410:TYR:C	2.83	0.51
1:A:590:THR:HG21	1:A:592:SER:HB2	1.92	0.51
3:M:70:LEU:O	3:M:74:TYR:HB2	2.11	0.51
1:A:19:THR:HG23	1:A:64:VAL:O	2.10	0.51
1:A:591:GLN:HB2	4:B:795:VAL:CG1	2.38	0.51
2:C:1575:GLU:CB	2:C:1578:LYS:HD2	2.32	0.51
2:C:1483:LEU:HD23	2:C:1599:ILE:HD12	1.93	0.51
4:B:842:VAL:HG23	4:B:892:ALA:HB2	1.91	0.51
1:A:367:VAL:HG23	1:A:387:LEU:HD11	1.92	0.51
1:A:148:PRO:HG2	1:A:179:MET:O	2.11	0.51
1:A:468:TYR:CE1	1:A:513:TYR:HD2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TRP:CE3	1:A:595:TRP:HA	2.45	0.51
2:C:1385:MET:HG3	2:C:1390:ALA:HA	1.93	0.51
2:C:1444:TYR:CD1	2:C:1445:PHE:CB	2.93	0.51
2:C:1586:SER:O	2:C:1589:PHE:HD2	1.93	0.51
3:M:29:ASN:HD22	3:M:44:ILE:HD11	1.74	0.51
1:A:369:VAL:CG1	1:A:370:GLN:H	2.24	0.51
1:A:38:HIS:HE1	1:A:45:LEU:HD12	1.73	0.51
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.92	0.51
1:A:138:GLY:HA2	1:A:160:SER:OG	2.10	0.51
4:B:788:SER:C	4:B:790:LYS:N	2.63	0.50
2:C:1510:ARG:HH12	2:C:1627:LEU:HD23	1.68	0.50
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.11	0.50
4:B:739:ILE:O	4:B:739:ILE:HG22	2.11	0.50
1:A:4:TYR:HB3	1:A:90:PHE:CE2	2.46	0.50
1:A:285:LEU:O	1:A:286:LEU:O	2.29	0.50
2:C:1585:LEU:N	2:C:1585:LEU:HD23	2.26	0.50
2:C:1507:LEU:HD11	2:C:1629:ALA:CB	2.42	0.50
2:C:1573:LYS:CD	2:C:1573:LYS:O	2.59	0.50
2:C:1451:GLN:CG	2:C:1452:PRO:CD	2.90	0.50
2:C:1365:GLU:HG3	2:C:1437:LEU:O	2.11	0.50
1:A:291:ASN:O	1:A:291:ASN:OD1	2.29	0.50
1:A:162:ASN:OD1	1:A:162:ASN:N	2.43	0.50
1:A:495:LEU:HD12	1:A:496:PRO:CD	2.40	0.50
1:A:180:GLY:O	1:A:181:GLN:O	2.30	0.50
2:C:1360:ASN:ND2	2:C:1443:GLN:O	2.44	0.50
1:A:184:ILE:HG13	1:A:200:PHE:HE2	1.77	0.50
1:A:624:PHE:O	1:A:631:GLN:HA	2.11	0.50
1:A:462:GLU:HG3	1:A:486:ARG:HH22	1.76	0.50
1:A:63:ASN:HD21	5:A:646:NAG:C1	2.24	0.50
1:A:289:VAL:HG23	1:A:289:VAL:O	2.10	0.50
2:C:1382:ASP:HB3	2:C:1456:LYS:HB3	1.94	0.50
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.50
2:C:1578:LYS:HZ2	2:C:1608:HIS:CE1	2.28	0.50
2:C:1444:TYR:HD1	2:C:1445:PHE:HB2	1.68	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
1:A:287:ASP:O	1:A:288:GLY:C	2.51	0.50
1:A:160:SER:OG	1:A:160:SER:O	2.30	0.50
1:A:634:GLN:HG2	1:A:635:ARG:N	2.26	0.50
2:C:1338:LYS:HG3	2:C:1370:TYR:HE1	1.77	0.50
2:C:1506:THR:O	2:C:1510:ARG:HG3	2.12	0.50
2:C:1386:MET:O	2:C:1387:THR:C	2.50	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1480:LEU:HD12	4:B:851:CYS:O	2.11	0.50
3:M:18:GLU:O	3:M:21:SER:HB2	2.11	0.50
4:B:852:SER:HA	4:B:878:ILE:HG22	1.93	0.49
2:C:1393:THR:CG2	2:C:1419:ARG:HH22	2.25	0.49
1:A:588:LYS:NZ	4:B:781:GLU:OE2	2.46	0.49
2:C:1632:GLU:HA	2:C:1635:VAL:HG22	1.93	0.49
1:A:224:TYR:CD2	1:A:224:TYR:N	2.79	0.49
1:A:297:LEU:O	1:A:298:VAL:C	2.51	0.49
1:A:440:ARG:HH22	1:A:529:VAL:HG23	1.77	0.49
1:A:286:LEU:HB3	1:A:291:ASN:CB	2.42	0.49
4:B:731:GLU:CB	4:B:733:ILE:HG22	2.43	0.49
4:B:836:GLN:HE22	4:B:897:HIS:CE1	2.31	0.49
1:A:472:ILE:HA	1:A:508:ARG:O	2.11	0.49
1:A:351:MET:HE1	1:A:386:LYS:HD3	1.95	0.49
4:B:890:VAL:O	4:B:891:LYS:CG	2.60	0.49
2:C:1593:LYS:HG2	2:C:1596:LEU:HD11	1.95	0.49
3:M:26:LEU:HD12	3:M:26:LEU:O	2.13	0.49
2:C:1575:GLU:O	2:C:1576:GLU:C	2.51	0.49
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.49
1:A:406:LYS:N	1:A:414:GLN:HE22	2.10	0.49
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.95	0.49
1:A:239:TYR:HE1	4:B:832:TYR:OH	1.95	0.49
2:C:1569:ARG:CG	2:C:1569:ARG:HH11	2.24	0.49
1:A:403:ARG:NH1	1:A:416:THR:HG21	2.28	0.49
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.43	0.49
1:A:271:ILE:HD13	1:A:276:GLY:HA3	1.94	0.49
1:A:280:LEU:HD21	1:A:285:LEU:CG	2.36	0.49
1:A:281:SER:H	1:A:284:VAL:HG21	1.76	0.49
1:A:439:LEU:HD12	1:A:439:LEU:O	2.12	0.49
3:M:30:GLU:OE2	3:M:45:LYS:HE3	2.13	0.49
1:A:509:LEU:HB3	1:A:529:VAL:HG13	1.94	0.49
2:C:1413:ASP:O	2:C:1414:LYS:C	2.50	0.49
4:B:847:ASN:HB3	4:B:850:PHE:HB2	1.95	0.49
2:C:1413:ASP:O	2:C:1414:LYS:O	2.30	0.49
1:A:434:LEU:HD12	1:A:435:HIS:N	2.28	0.48
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.95	0.48
2:C:1591:GLY:O	2:C:1596:LEU:HD23	2.12	0.48
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	0.48
1:A:161:GLN:HG3	1:A:162:ASN:OD1	2.13	0.48
2:C:1497:PHE:HD1	2:C:1498:ILE:CG1	2.23	0.48
3:M:39:TYR:O	3:M:41:LYS:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1550:GLY:O	2:C:1552:ASP:N	2.46	0.48
2:C:1485:ARG:HB2	2:C:1590:TRP:HE1	1.78	0.48
2:C:1374:GLN:O	2:C:1431:HIS:HB3	2.14	0.48
1:A:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
1:A:606:THR:HG22	1:A:608:GLY:H	1.78	0.48
1:A:183:LYS:HD2	1:A:185:ARG:HD2	1.94	0.48
1:A:287:ASP:HA	1:A:291:ASN:CA	2.44	0.48
2:C:1470:PHE:CB	2:C:1478:GLY:HA3	2.43	0.48
4:B:745:PHE:CD2	4:B:905:LYS:HG2	2.49	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
2:C:1423:ILE:HG21	2:C:1425:TYR:CZ	2.48	0.48
1:A:477:ARG:HH22	1:A:479:LEU:HD13	1.78	0.48
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.48
2:C:1348:ALA:O	2:C:1349:PRO:O	2.31	0.48
1:A:20:MET:H	1:A:64:VAL:HB	1.79	0.48
1:A:183:LYS:HD3	1:A:185:ARG:CD	2.44	0.48
4:B:783:LEU:HD12	4:B:784:ALA:H	1.79	0.48
2:C:1386:MET:HE3	2:C:1389:PHE:CE1	2.49	0.48
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.48
4:B:888:VAL:HG12	4:B:889:GLU:N	2.28	0.48
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.95	0.48
4:B:902:GLY:C	4:B:903:VAL:HG23	2.32	0.48
1:A:351:MET:HE2	1:A:386:LYS:HA	1.96	0.48
2:C:1550:GLY:C	2:C:1552:ASP:N	2.67	0.48
1:A:437:SER:O	1:A:452:ASN:HB2	2.13	0.48
1:A:280:LEU:HG	1:A:285:LEU:HD13	1.94	0.48
4:B:749:TRP:O	4:B:750:LEU:HB3	2.13	0.48
1:A:403:ARG:CB	1:A:416:THR:HG22	2.44	0.48
1:A:83:PHE:HD1	1:A:99:VAL:O	1.97	0.48
1:A:603:ILE:HD12	1:A:621:GLY:HA3	1.94	0.47
1:A:364:ARG:O	1:A:378:LEU:HD22	2.14	0.47
3:M:59:ASP:OD1	3:M:59:ASP:C	2.52	0.47
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.47
1:A:171:TRP:CH2	1:A:182:TRP:CZ3	3.01	0.47
1:A:59:ASN:HB3	1:A:483:ARG:NH1	2.30	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	0.47
2:C:1563:ILE:O	2:C:1600:ILE:HB	2.15	0.47
4:B:844:LEU:HD22	4:B:876:TYR:CD2	2.49	0.47
2:C:1526:ARG:HB2	2:C:1579:HIS:CD2	2.49	0.47
1:A:97:LYS:HG3	1:A:98:VAL:N	2.30	0.47
2:C:1370:TYR:O	2:C:1431:HIS:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1544:GLU:OE1	2:C:1579:HIS:CD2	2.68	0.47
1:A:613:TYR:CE2	1:A:614:ALA:HB2	2.48	0.47
2:C:1429:VAL:O	2:C:1429:VAL:HG23	2.15	0.47
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.47
1:A:203:LYS:HG2	1:A:204:GLU:N	2.30	0.47
1:A:369:VAL:CG1	1:A:370:GLN:N	2.72	0.47
1:A:404:THR:C	1:A:414:GLN:OE1	2.53	0.47
1:A:475:LYS:HG2	1:A:598:VAL:HG11	1.96	0.47
2:C:1369:ARG:HD2	2:C:1432:SER:O	2.13	0.47
1:A:368:ALA:O	1:A:402:VAL:HG13	2.15	0.47
1:A:475:LYS:HG2	1:A:598:VAL:CG1	2.45	0.47
3:M:64:SER:O	3:M:67:LYS:N	2.47	0.47
1:A:462:GLU:HG3	1:A:486:ARG:NH2	2.29	0.47
1:A:230:GLU:CA	1:A:279:VAL:HG13	2.22	0.47
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.45	0.47
2:C:1586:SER:HA	2:C:1589:PHE:HE2	1.80	0.47
1:A:230:GLU:CB	1:A:279:VAL:HG11	2.40	0.47
2:C:1536:PHE:HD1	2:C:1563:ILE:CG2	2.20	0.47
2:C:1589:PHE:CE1	2:C:1598:TYR:CZ	3.03	0.47
2:C:1521:TYR:O	2:C:1583:TRP:HB2	2.14	0.47
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.80	0.47
3:M:66:ALA:O	3:M:67:LYS:C	2.53	0.47
1:A:251:PHE:CE1	1:A:304:VAL:CG1	2.98	0.46
1:A:591:GLN:OE1	4:B:795:VAL:CB	2.63	0.46
4:B:808:PHE:CD1	4:B:808:PHE:O	2.68	0.46
1:A:403:ARG:HB2	1:A:416:THR:HG22	1.95	0.46
1:A:105:SER:O	1:A:132:HIS:CD2	2.68	0.46
4:B:736:GLU:HA	4:B:739:ILE:HD12	1.97	0.46
3:M:23:LEU:HD11	3:M:51:ALA:HB1	1.97	0.46
1:A:111:GLN:O	1:A:125:TYR:HA	2.16	0.46
1:A:248:PHE:CZ	2:C:1380:ILE:HD11	2.49	0.46
4:B:813:LEU:CD1	4:B:814:PRO:HD3	2.45	0.46
3:M:70:LEU:CG	3:M:74:TYR:HE1	2.27	0.46
2:C:1341:LEU:HD23	2:C:1469:ARG:N	2.28	0.46
2:C:1336:CYS:O	2:C:1337:ASN:ND2	2.48	0.46
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.50	0.46
1:A:298:VAL:HG12	1:A:298:VAL:O	2.16	0.46
1:A:510:VAL:CG1	1:A:528:SER:HB3	2.33	0.46
2:C:1510:ARG:HH12	2:C:1627:LEU:HD21	1.79	0.46
2:C:1416:PHE:HD2	2:C:1416:PHE:C	2.16	0.46
4:B:885:LEU:HD12	4:B:907:LEU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1472:HIS:ND1	2:C:1473:PRO:HD2	2.31	0.46
4:B:789:ASP:OD1	4:B:790:LYS:HG3	2.16	0.46
2:C:1582:MET:CG	2:C:1606:VAL:HG22	2.45	0.46
2:C:1475:LYS:HE2	2:C:1493:GLU:OE2	2.16	0.46
3:M:8:ASN:ND2	3:M:12:ASN:OD1	2.46	0.46
2:C:1572:LEU:CD1	2:C:1574:LEU:HG	2.45	0.46
4:B:788:SER:C	4:B:790:LYS:H	2.18	0.46
1:A:239:TYR:HE1	4:B:832:TYR:HH	1.59	0.46
1:A:309:ILE:HG12	1:A:316:MET:HG3	1.97	0.46
2:C:1388:GLY:O	2:C:1443:GLN:HA	2.16	0.46
2:C:1582:MET:HG2	2:C:1605:TRP:O	2.16	0.46
2:C:1415:ALA:O	2:C:1416:PHE:C	2.54	0.46
2:C:1393:THR:HG22	2:C:1419:ARG:HH22	1.79	0.46
1:A:375:VAL:CG2	1:A:387:LEU:HD22	2.46	0.46
4:B:886:GLN:OE1	4:B:886:GLN:HA	2.15	0.46
2:C:1539:TYR:CE1	2:C:1574:LEU:CD1	2.90	0.46
1:A:85:THR:HG23	1:A:98:VAL:HG22	1.98	0.46
2:C:1342:LYS:HB2	2:C:1367:CYS:CB	2.44	0.46
2:C:1421:THR:O	2:C:1422:LEU:HB2	2.15	0.46
2:C:1451:GLN:HG3	2:C:1452:PRO:CD	2.42	0.46
1:A:185:ARG:HA	1:A:196:PHE:O	2.16	0.46
3:M:49:GLN:O	3:M:50:LYS:C	2.53	0.46
2:C:1522:VAL:O	2:C:1547:ILE:HB	2.16	0.46
2:C:1366:ILE:O	2:C:1436:CYS:HA	2.16	0.46
1:A:301:SER:HB2	1:A:323:GLY:HA2	1.98	0.46
1:A:36:THR:HA	1:A:47:LEU:O	2.17	0.45
2:C:1386:MET:SD	2:C:1471:TYR:HE1	2.39	0.45
4:B:907:LEU:N	4:B:907:LEU:CD2	2.79	0.45
1:A:73:GLU:HB3	1:A:82:LYS:HZ1	1.81	0.45
2:C:1519:VAL:HG12	2:C:1548:LYS:HZ2	1.81	0.45
1:A:40:PHE:CE2	1:A:41:PRO:HG3	2.51	0.45
2:C:1341:LEU:O	2:C:1469:ARG:HG2	2.16	0.45
1:A:379:THR:HG22	1:A:384:VAL:N	2.31	0.45
1:A:101:VAL:CG1	1:A:102:SER:N	2.80	0.45
3:M:7:SER:O	3:M:8:ASN:C	2.54	0.45
1:A:287:ASP:CB	1:A:291:ASN:HB3	2.44	0.45
1:A:6:ILE:HA	1:A:6:ILE:HD12	1.56	0.45
4:B:897:HIS:O	4:B:898:PHE:CD1	2.69	0.45
4:B:733:ILE:HB	4:B:895:TYR:HD2	1.82	0.45
1:A:271:ILE:O	1:A:271:ILE:HG22	2.16	0.45
1:A:461:HIS:O	1:A:464:LYS:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLN:OE1	4:B:795:VAL:HB	2.17	0.45
3:M:29:ASN:O	3:M:32:ALA:N	2.49	0.45
2:C:1530:VAL:HG13	2:C:1539:TYR:HE1	1.80	0.45
1:A:406:LYS:HG3	1:A:407:GLN:O	2.17	0.45
1:A:339:PRO:O	1:A:340:LYS:HD3	2.16	0.45
2:C:1399:LEU:HD23	2:C:1399:LEU:HA	1.80	0.45
2:C:1524:LYS:HA	2:C:1580:TYR:O	2.16	0.45
4:B:894:VAL:HG23	4:B:899:ILE:O	2.16	0.45
2:C:1383:ILE:CD1	2:C:1439:PHE:HZ	2.30	0.45
1:A:20:MET:HG2	1:A:64:VAL:CB	2.47	0.45
2:C:1605:TRP:HE1	2:C:1607:GLU:CD	2.20	0.45
2:C:1505:VAL:HG11	2:C:1607:GLU:OE2	2.16	0.45
2:C:1361:THR:HB	2:C:1442:HIS:HD1	1.82	0.45
1:A:644:ALA:O	1:A:645:ALA:HB3	2.16	0.45
4:B:823:VAL:HG23	4:B:824:GLU:N	2.32	0.45
4:B:866:ILE:HG22	4:B:867:PRO:O	2.16	0.45
1:A:591:GLN:CB	4:B:795:VAL:CB	2.74	0.45
1:A:251:PHE:CD2	1:A:251:PHE:N	2.85	0.45
4:B:910:VAL:HA	4:B:911:PRO:HD3	1.82	0.45
1:A:210:PHE:HB3	1:A:237:PHE:HA	1.99	0.45
2:C:1505:VAL:CG1	2:C:1510:ARG:HE	2.28	0.45
3:M:64:SER:O	3:M:65:GLU:C	2.55	0.45
1:A:380:GLN:O	1:A:382:ASP:N	2.50	0.45
3:M:26:LEU:O	3:M:29:ASN:N	2.50	0.44
2:C:1386:MET:CE	2:C:1389:PHE:CG	2.99	0.44
1:A:30:ASP:N	1:A:30:ASP:OD1	2.50	0.44
4:B:813:LEU:HA	4:B:814:PRO:HD3	1.88	0.44
4:B:734:ILE:HD13	4:B:893:ALA:CB	2.32	0.44
1:A:346:MET:O	1:A:391:THR:CG2	2.57	0.44
4:B:853:LEU:HD23	4:B:853:LEU:HA	1.57	0.44
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.68	0.44
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.81	0.44
1:A:281:SER:O	1:A:284:VAL:HB	2.16	0.44
2:C:1543:ILE:HD11	2:C:1554:VAL:HG21	1.99	0.44
2:C:1497:PHE:CE1	2:C:1498:ILE:CG1	3.01	0.44
3:M:70:LEU:HG	3:M:74:TYR:HD1	1.77	0.44
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.52	0.44
3:M:29:ASN:O	3:M:30:GLU:C	2.55	0.44
2:C:1573:LYS:O	2:C:1574:LEU:CD2	2.56	0.44
2:C:1539:TYR:CZ	2:C:1574:LEU:HD12	2.49	0.44
1:A:179:MET:CG	1:A:202:VAL:O	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1509:GLU:HA	2:C:1509:GLU:OE1	2.16	0.44
4:B:822:GLN:CB	4:B:879:VAL:HG22	2.39	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
2:C:1617:ASP:OD1	2:C:1618:GLU:N	2.48	0.44
2:C:1631:THR:O	2:C:1635:VAL:HG22	2.18	0.44
1:A:278:VAL:C	1:A:279:VAL:HG22	2.38	0.44
2:C:1575:GLU:N	2:C:1575:GLU:OE2	2.50	0.44
1:A:604:GLY:HA2	1:A:619:ASP:O	2.18	0.44
2:C:1472:HIS:CG	2:C:1473:PRO:HD2	2.52	0.44
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.18	0.44
2:C:1404:ASP:O	2:C:1427:ASP:HB2	2.18	0.44
4:B:830:TYR:CD1	4:B:871:SER:HB3	2.53	0.44
1:A:38:HIS:HE1	1:A:45:LEU:CD1	2.31	0.44
2:C:1494:GLU:HG3	2:C:1602:LYS:HB3	2.00	0.44
2:C:1411:GLU:OE2	2:C:1414:LYS:HD2	2.17	0.44
1:A:465:ILE:HD11	1:A:515:LEU:HD13	2.00	0.44
2:C:1336:CYS:HB3	2:C:1337:ASN:H	1.57	0.44
2:C:1508:GLU:C	2:C:1510:ARG:N	2.69	0.44
1:A:86:VAL:O	1:A:96:GLU:HB2	2.18	0.44
2:C:1464:GLU:O	2:C:1466:SER:N	2.45	0.44
1:A:251:PHE:CE1	1:A:280:LEU:HB2	2.52	0.44
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.44
2:C:1514:ALA:HB2	2:C:1583:TRP:CE2	2.53	0.44
2:C:1383:ILE:HG23	2:C:1455:VAL:HG22	1.99	0.44
2:C:1410:TYR:O	2:C:1410:TYR:CD2	2.71	0.44
2:C:1610:PRO:HB2	2:C:1615:CYS:SG	2.57	0.44
1:A:161:GLN:HG2	1:A:162:ASN:OD1	2.17	0.43
2:C:1415:ALA:O	2:C:1417:SER:N	2.51	0.43
2:C:1589:PHE:CZ	2:C:1598:TYR:CE2	3.05	0.43
2:C:1589:PHE:CZ	2:C:1598:TYR:HE2	2.36	0.43
2:C:1511:LEU:HD11	2:C:1633:SER:OG	2.17	0.43
1:A:40:PHE:HA	1:A:41:PRO:HA	1.69	0.43
1:A:410:SER:OG	1:A:413:GLU:HG3	2.18	0.43
4:B:784:ALA:HB3	4:B:796:ALA:HB3	2.00	0.43
2:C:1337:ASN:O	2:C:1371:ARG:HD2	2.19	0.43
4:B:840:VAL:HG11	4:B:892:ALA:HB1	1.99	0.43
4:B:795:VAL:O	4:B:796:ALA:C	2.54	0.43
1:A:453:PHE:CE2	1:A:495:LEU:HB2	2.53	0.43
4:B:808:PHE:CE1	4:B:830:TYR:CD2	3.03	0.43
3:M:15:LEU:HD22	3:M:60:PHE:CE1	2.53	0.43
3:M:51:ALA:O	3:M:54:ALA:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1632:GLU:O	2:C:1636:VAL:HG12	2.17	0.43
1:A:458:ASP:OD2	1:A:460:ALA:HB3	2.18	0.43
4:B:746:PRO:HB3	4:B:748:SER:O	2.19	0.43
1:A:227:LYS:HE2	1:A:227:LYS:HB2	1.64	0.43
1:A:287:ASP:N	1:A:287:ASP:OD1	2.50	0.43
4:B:734:ILE:N	4:B:734:ILE:HD12	2.17	0.43
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.43
4:B:771:ILE:O	4:B:771:ILE:HG13	2.18	0.43
1:A:161:GLN:HB3	1:A:162:ASN:CG	2.39	0.43
1:A:541:LEU:HA	1:A:541:LEU:HD12	1.77	0.43
1:A:148:PRO:HG3	1:A:182:TRP:NE1	2.33	0.43
2:C:1429:VAL:O	2:C:1430:SER:C	2.56	0.43
1:A:283:LYS:O	1:A:287:ASP:OD1	2.36	0.43
2:C:1342:LYS:HB3	2:C:1367:CYS:HB2	1.98	0.43
2:C:1397:LYS:O	2:C:1401:ASN:ND2	2.40	0.43
1:A:590:THR:HB	1:A:593:LYS:CG	2.39	0.43
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.01	0.43
1:A:458:ASP:O	1:A:460:ALA:N	2.52	0.43
1:A:454:LEU:HA	1:A:491:ASP:O	2.18	0.43
1:A:255:ASP:O	1:A:258:GLN:HB3	2.18	0.43
2:C:1444:TYR:HD1	2:C:1444:TYR:C	2.20	0.43
2:C:1380:ILE:HB	2:C:1458:TYR:CE1	2.54	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.71	0.43
1:A:20:MET:HG2	1:A:64:VAL:CG2	2.47	0.43
4:B:894:VAL:HG21	4:B:899:ILE:HB	2.01	0.43
5:A:646:NAG:H62	5:A:646:NAG:O3	2.19	0.43
3:M:15:LEU:O	3:M:18:GLU:HB2	2.19	0.43
2:C:1577:LYS:HA	2:C:1577:LYS:HD3	1.77	0.43
4:B:807:PHE:CD2	4:B:807:PHE:C	2.92	0.43
1:A:282:ARG:O	1:A:283:LYS:C	2.58	0.42
1:A:281:SER:N	1:A:284:VAL:HG21	2.34	0.42
4:B:899:ILE:HG22	4:B:900:SER:N	2.35	0.42
2:C:1460:TYR:CG	2:C:1461:TYR:N	2.86	0.42
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.31	0.42
4:B:731:GLU:HB3	4:B:733:ILE:HG22	1.98	0.42
3:M:43:THR:HG21	3:M:73:ILE:HD13	2.01	0.42
1:A:182:TRP:CD1	1:A:182:TRP:N	2.86	0.42
4:B:835:ASN:O	4:B:836:GLN:HB3	2.19	0.42
2:C:1526:ARG:NH1	2:C:1526:ARG:HB3	2.34	0.42
4:B:894:VAL:CG2	4:B:899:ILE:O	2.67	0.42
1:A:87:GLN:HG3	1:A:96:GLU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:O	1:A:169:LEU:HG	2.20	0.42
4:B:819:ARG:NE	4:B:883:THR:HG23	2.35	0.42
2:C:1341:LEU:HB3	2:C:1469:ARG:HG2	2.02	0.42
4:B:750:LEU:HG	4:B:750:LEU:O	2.20	0.42
2:C:1386:MET:HG3	2:C:1386:MET:H	1.34	0.42
1:A:402:VAL:HG12	1:A:403:ARG:H	1.84	0.42
4:B:907:LEU:CD2	4:B:907:LEU:H	2.28	0.42
1:A:442:GLU:OE1	1:A:534:LYS:HD3	2.18	0.42
1:A:290:GLN:O	1:A:291:ASN:C	2.57	0.42
1:A:177:VAL:HG22	1:A:178:ASN:N	2.34	0.42
1:A:468:TYR:CE1	1:A:513:TYR:CD2	3.05	0.42
1:A:455:LEU:HB2	1:A:468:TYR:OH	2.19	0.42
2:C:1472:HIS:CE1	2:C:1473:PRO:HD2	2.55	0.42
4:B:838:LEU:HA	4:B:838:LEU:HD23	1.77	0.42
4:B:783:LEU:HD12	4:B:784:ALA:N	2.34	0.42
3:M:29:ASN:O	3:M:31:LEU:N	2.53	0.42
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.42
4:B:819:ARG:O	4:B:820:ASN:HB2	2.20	0.42
1:A:203:LYS:HG2	1:A:204:GLU:H	1.85	0.42
1:A:533:VAL:CG1	1:A:534:LYS:N	2.81	0.42
2:C:1483:LEU:HD23	2:C:1599:ILE:HG23	2.01	0.42
2:C:1472:HIS:HA	2:C:1473:PRO:HD3	1.81	0.42
2:C:1524:LYS:HD2	2:C:1609:TRP:CH2	2.54	0.42
4:B:829:LEU:N	4:B:829:LEU:HD12	2.35	0.42
1:A:613:TYR:CD2	1:A:614:ALA:N	2.88	0.42
1:A:504:ILE:HG23	1:A:505:PRO:HA	2.02	0.42
2:C:1341:LEU:HD12	2:C:1341:LEU:HA	1.84	0.42
2:C:1403:VAL:CG2	2:C:1404:ASP:N	2.82	0.42
2:C:1337:ASN:OD1	2:C:1338:LYS:N	2.52	0.42
1:A:61:MET:CE	1:A:483:ARG:HG2	2.50	0.42
1:A:101:VAL:HG12	1:A:102:SER:N	2.35	0.41
1:A:239:TYR:CE1	4:B:832:TYR:HE1	2.35	0.41
1:A:4:TYR:HB3	1:A:90:PHE:CZ	2.55	0.41
4:B:890:VAL:O	4:B:891:LYS:HG3	2.20	0.41
1:A:195:VAL:CG1	1:A:196:PHE:N	2.82	0.41
3:M:23:LEU:HD23	3:M:23:LEU:HA	1.81	0.41
2:C:1564:SER:OG	2:C:1565:PRO:HD2	2.19	0.41
4:B:821:GLU:O	4:B:880:PRO:HD3	2.20	0.41
1:A:207:LEU:O	4:B:812:ARG:NH2	2.53	0.41
1:A:20:MET:HG2	1:A:64:VAL:HG11	2.01	0.41
2:C:1445:PHE:C	2:C:1445:PHE:CD1	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.41
2:C:1419:ARG:O	2:C:1421:THR:N	2.52	0.41
3:M:13:GLU:O	3:M:13:GLU:HG2	2.20	0.41
4:B:786:SER:O	4:B:794:CYS:N	2.33	0.41
1:A:179:MET:CB	1:A:202:VAL:O	2.69	0.41
4:B:804:MET:HE3	4:B:804:MET:HB2	1.90	0.41
1:A:219:LYS:HD2	1:A:358:ASP:OD2	2.19	0.41
2:C:1494:GLU:CB	2:C:1602:LYS:HB3	2.47	0.41
2:C:1632:GLU:HA	2:C:1635:VAL:CG2	2.49	0.41
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.41
2:C:1554:VAL:CG2	2:C:1558:GLN:HB2	2.50	0.41
2:C:1497:PHE:HD1	2:C:1498:ILE:HG12	1.84	0.41
1:A:106:GLY:HA2	1:A:132:HIS:CD2	2.55	0.41
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.92	0.41
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.76	0.41
4:B:813:LEU:HA	4:B:813:LEU:HD13	1.28	0.41
4:B:839:LYS:HE2	4:B:895:TYR:HD1	1.85	0.41
1:A:171:TRP:HH2	1:A:182:TRP:CZ3	2.39	0.41
4:B:841:ARG:HD2	4:B:861:GLN:OE1	2.20	0.41
1:A:73:GLU:HB3	1:A:82:LYS:HZ3	1.84	0.41
1:A:14:LEU:HD11	1:A:103:LEU:CD2	2.51	0.41
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.85	0.41
1:A:289:VAL:HG23	1:A:290:GLN:NE2	2.36	0.41
2:C:1543:ILE:CD1	2:C:1554:VAL:HG11	2.50	0.41
2:C:1404:ASP:O	2:C:1427:ASP:N	2.51	0.41
1:A:404:THR:HG1	1:A:415:ALA:H	1.66	0.41
1:A:83:PHE:CD1	1:A:100:LEU:HA	2.56	0.41
1:A:33:VAL:HG22	1:A:90:PHE:HA	2.03	0.41
2:C:1495:ASN:OD1	2:C:1495:ASN:N	2.54	0.41
4:B:811:LEU:HD13	4:B:812:ARG:H	1.85	0.41
2:C:1530:VAL:HG13	2:C:1539:TYR:CE1	2.54	0.41
4:B:847:ASN:HB3	4:B:850:PHE:CD1	2.55	0.41
1:A:533:VAL:HG12	1:A:534:LYS:H	1.86	0.41
3:M:58:LYS:HD2	3:M:58:LYS:HA	1.75	0.41
1:A:343:LYS:N	1:A:343:LYS:CD	2.83	0.41
1:A:63:ASN:ND2	5:A:646:NAG:C1	2.84	0.41
3:M:15:LEU:HD12	3:M:15:LEU:HA	1.82	0.41
4:B:841:ARG:HA	4:B:862:GLN:O	2.20	0.41
3:M:84:LYS:O	3:M:85:TYR:CB	2.69	0.41
4:B:889:GLU:HB2	4:B:904:ARG:HG3	2.03	0.41
1:A:265:SER:O	1:A:267:LYS:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:812:ARG:HD2	4:B:812:ARG:HA	1.58	0.41
1:A:114:LYS:HE2	1:A:117:TYR:CD1	2.56	0.41
2:C:1386:MET:HE3	2:C:1389:PHE:CG	2.56	0.41
4:B:897:HIS:O	4:B:898:PHE:HD1	2.04	0.41
4:B:847:ASN:HA	4:B:848:PRO:HD2	1.77	0.41
1:A:509:LEU:HB3	1:A:529:VAL:CG1	2.50	0.41
1:A:508:ARG:CZ	1:A:604:GLY:HA3	2.51	0.41
4:B:754:GLU:HB3	4:B:767:LYS:HE3	2.02	0.41
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.03	0.41
1:A:278:VAL:O	1:A:279:VAL:HG13	2.21	0.41
2:C:1497:PHE:HE2	2:C:1571:ALA:CB	1.99	0.41
2:C:1497:PHE:O	2:C:1498:ILE:HG13	2.20	0.41
4:B:839:LYS:HG2	4:B:863:THR:HG23	2.03	0.41
1:A:453:PHE:HE2	1:A:495:LEU:HB2	1.85	0.41
2:C:1459:ALA:O	2:C:1460:TYR:C	2.58	0.41
2:C:1339:PHE:HE2	2:C:1429:VAL:HG21	1.85	0.41
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.41
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.56	0.41
2:C:1395:ASP:O	2:C:1398:GLN:HB3	2.21	0.41
4:B:846:HIS:CE1	4:B:855:THR:HA	2.56	0.40
2:C:1611:GLU:HB3	2:C:1614:GLU:HB2	2.03	0.40
1:A:400:ILE:HD12	1:A:400:ILE:N	2.35	0.40
1:A:590:THR:HG22	1:A:591:GLN:N	2.35	0.40
2:C:1384:SER:HB3	4:B:826:ARG:HH12	1.87	0.40
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.57	0.40
2:C:1544:GLU:OE1	2:C:1579:HIS:HD2	2.03	0.40
1:A:345:GLY:HA2	1:A:393:PRO:HD3	2.04	0.40
4:B:852:SER:O	4:B:853:LEU:HD23	2.21	0.40
4:B:808:PHE:HD1	4:B:808:PHE:C	2.25	0.40
1:A:239:TYR:CZ	4:B:808:PHE:HZ	2.39	0.40
1:A:502:ASP:OD1	1:A:502:ASP:N	2.53	0.40
4:B:750:LEU:HD23	4:B:782:ILE:HD13	2.04	0.40
2:C:1562:PHE:CE2	2:C:1582:MET:HE1	2.57	0.40
2:C:1590:TRP:N	2:C:1597:SER:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/645 (99%)	545 (86%)	73 (12%)	19 (3%)	5	45
2	C	288/343 (84%)	232 (81%)	39 (14%)	17 (6%)	2	28
3	M	82/88 (93%)	56 (68%)	22 (27%)	4 (5%)	3	32
4	B	182/206 (88%)	145 (80%)	28 (15%)	9 (5%)	3	32
All	All	1189/1282 (93%)	978 (82%)	162 (14%)	49 (4%)	3	36

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	LEU
1	A	290	GLN
1	A	293	ARG
1	A	294	ALA
1	A	295	GLU
1	A	537	CYS
2	C	1494	GLU
2	C	1573	LYS
4	B	730	ASP
4	B	789	ASP
4	B	836	GLN
1	A	282	ARG
2	C	1377	THR
2	C	1414	LYS
2	C	1430	SER
3	M	51	ALA
4	B	732	ASP
4	B	852	SER
1	A	181	GLN
1	A	283	LYS
1	A	296	ASP
2	C	1349	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1422	LEU
2	C	1432	SER
2	C	1458	TYR
2	C	1551	SER
2	C	1576	GLU
3	M	30	GLU
3	M	61	LYS
4	B	743	SER
4	B	837	GLU
1	A	179	MET
2	C	1420	ASN
2	C	1486	ASP
3	M	39	TYR
4	B	753	VAL
4	B	796	ALA
1	A	72	ARG
1	A	291	ASN
1	A	370	GLN
1	A	459	ARG
2	C	1406	TYR
2	C	1517	PRO
1	A	298	VAL
1	A	381	GLY
2	C	1516	GLU
1	A	616	VAL
1	A	359	GLY
2	C	1473	PRO

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	563/567 (99%)	523 (93%)	40 (7%)	18 58
2	C	267/309 (86%)	219 (82%)	48 (18%)	2 17
3	M	76/79 (96%)	66 (87%)	10 (13%)	5 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	B	172/191 (90%)	134 (78%)	38 (22%)	1 10
All	All	1078/1146 (94%)	942 (87%)	136 (13%)	5 32

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	30	ASP
1	A	61	MET
1	A	84	VAL
1	A	85	THR
1	A	137	VAL
1	A	149	GLU
1	A	155	GLN
1	A	157	SER
1	A	162	ASN
1	A	178	ASN
1	A	191	SER
1	A	213	ILE
1	A	215	GLU
1	A	217	THR
1	A	241	LYS
1	A	251	PHE
1	A	257	GLU
1	A	278	VAL
1	A	279	VAL
1	A	281	SER
1	A	282	ARG
1	A	283	LYS
1	A	286	LEU
1	A	290	GLN
1	A	295	GLU
1	A	297	LEU
1	A	314	SER
1	A	320	GLU
1	A	410	SER
1	A	438	VAL
1	A	472	ILE
1	A	477	ARG
1	A	502	ASP
1	A	515	LEU
1	A	535	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	542	VAL
1	A	548	SER
1	A	554	VAL
1	A	634	GLN
2	C	1336	CYS
2	C	1342	LYS
2	C	1344	THR
2	C	1346	LYS
2	C	1350	GLU
2	C	1361	THR
2	C	1378	MET
2	C	1383	ILE
2	C	1386	MET
2	C	1387	THR
2	C	1393	THR
2	C	1394	ASP
2	C	1410	TYR
2	C	1416	PHE
2	C	1418	ASP
2	C	1420	ASN
2	C	1421	THR
2	C	1430	SER
2	C	1433	GLU
2	C	1444	TYR
2	C	1445	PHE
2	C	1447	VAL
2	C	1449	LEU
2	C	1465	GLU
2	C	1468	THR
2	C	1469	ARG
2	C	1475	LYS
2	C	1479	LYS
2	C	1485	ARG
2	C	1495	ASN
2	C	1498	ILE
2	C	1507	LEU
2	C	1511	LEU
2	C	1512	ASP
2	C	1532	LEU
2	C	1535	ASP
2	C	1536	PHE
2	C	1543	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1551	SER
2	C	1561	THR
2	C	1569	ARG
2	C	1570	GLU
2	C	1572	LEU
2	C	1573	LYS
2	C	1585	LEU
2	C	1590	TRP
2	C	1594	PRO
2	C	1600	ILE
3	M	7	SER
3	M	8	ASN
3	M	21	SER
3	M	25	GLU
3	M	26	LEU
3	M	31	LEU
3	M	38	THR
3	M	59	ASP
3	M	74	TYR
3	M	78	ASP
4	B	729	LEU
4	B	732	ASP
4	B	733	ILE
4	B	734	ILE
4	B	736	GLU
4	B	741	SER
4	B	757	LYS
4	B	765	SER
4	B	769	MET
4	B	770	ASN
4	B	777	ILE
4	B	782	ILE
4	B	783	LEU
4	B	786	SER
4	B	794	CYS
4	B	809	ILE
4	B	811	LEU
4	B	812	ARG
4	B	813	LEU
4	B	817	VAL
4	B	818	VAL
4	B	823	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	826	ARG
4	B	828	VAL
4	B	833	ARG
4	B	834	GLN
4	B	841	ARG
4	B	844	LEU
4	B	845	LEU
4	B	851	CYS
4	B	864	VAL
4	B	873	SER
4	B	876	TYR
4	B	877	VAL
4	B	890	VAL
4	B	894	VAL
4	B	907	LEU
4	B	912	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	290	GLN
1	A	390	ASN
1	A	552	GLN
2	C	1579	HIS
3	M	17	ASN
4	B	897	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	NAG	A	646	-	14,14,15	0.45	0	15,19,21	1.53	1 (6%)

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
5	NAG	A	646	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	646	NAG	C1-O5-C5	5.19	118.83	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	646	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	641/645 (99%)	-0.12	8 (1%) 81 73	26, 151, 213, 245	0
2	C	294/343 (85%)	0.17	10 (3%) 49 38	118, 187, 274, 305	0
3	M	84/88 (95%)	-0.16	1 (1%) 81 73	121, 146, 199, 261	0
4	B	184/206 (89%)	-0.27	0 100 100	99, 130, 161, 183	0
All	All	1203/1282 (93%)	-0.08	19 (1%) 74 64	26, 151, 238, 305	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	2	THR	4.0
1	A	408	GLU	3.3
2	C	1454	ALA	3.3
2	C	1487	GLU	3.2
1	A	517	GLY	2.8
1	A	518	ALA	2.6
2	C	1546	THR	2.5
2	C	1608	HIS	2.5
1	A	398	LEU	2.4
2	C	1634	MET	2.4
2	C	1551	SER	2.3
2	C	1589	PHE	2.3
2	C	1609	TRP	2.3
2	C	1523	TYR	2.3
2	C	1439	PHE	2.2
1	A	369	VAL	2.1
1	A	347	PRO	2.1
1	A	421	ALA	2.0
1	A	371	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	646	14/15	0.83	0.53	-	159,175,186,189	0

6.5 Other polymers (i)

There are no such residues in this entry.