Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 09:49 PM EDT

PDB ID	:	3L3O / pdb_00003l3o
Title	:	Staphylococcal Complement Inhibitor (SCIN) in complex with Human Complement Component C3c
Authors	:	Geisbrecht, B.V.; Garcia, B.G.
Deposited on	:	2009-12-17
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

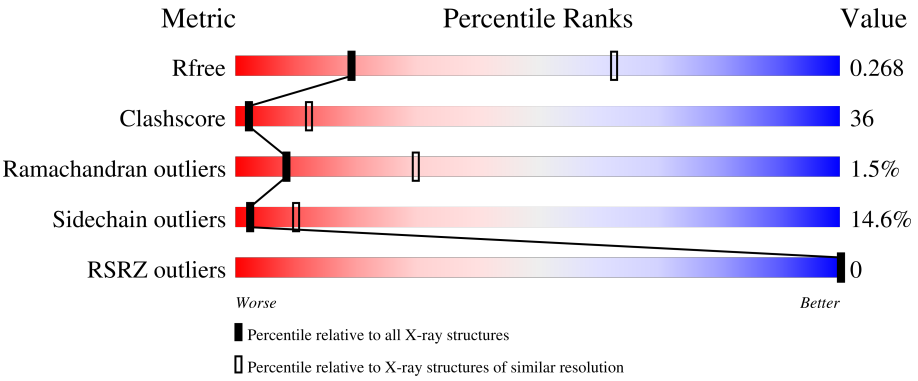
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	645	42% 50% 6% ·
1	D	645	44% 49% 6% ·
2	B	206	35% 39% 16% 11%
2	E	206	35% 39% 15% 11%
3	M	88	40% 44% 11% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	88	39% 45% 11% 5%
4	C	343	37% 38% 10% 14%
4	F	343	38% 38% 10% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19090 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	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			
1	D	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			

- Molecule 2 is a protein called Complement C3.

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

- 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			
3	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

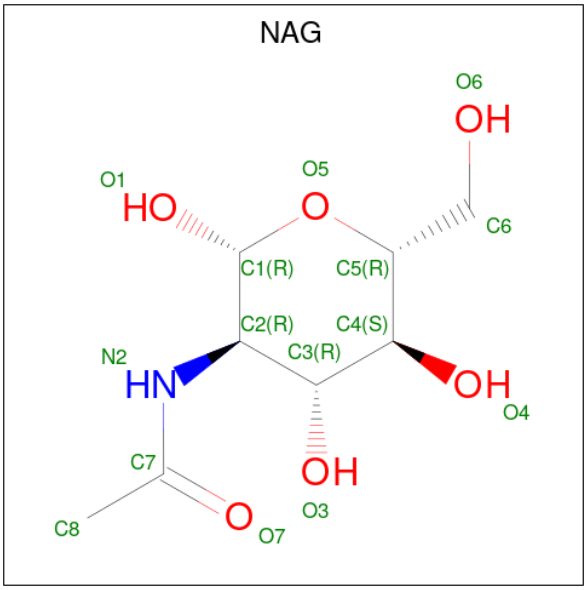
There are 6 discrepancies between the modelled and reference sequences:

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
P	-2	GLY	-	expression tag	UNP Q931M7
P	-1	THR	-	expression tag	UNP Q931M7
P	0	SER	-	expression tag	UNP Q931M7

- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	294	Total	C	N	O	S	0	0	0
			2382	1500	391	471	20			
4	C	294	Total	C	N	O	S	0	0	0
			2382	1500	391	471	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



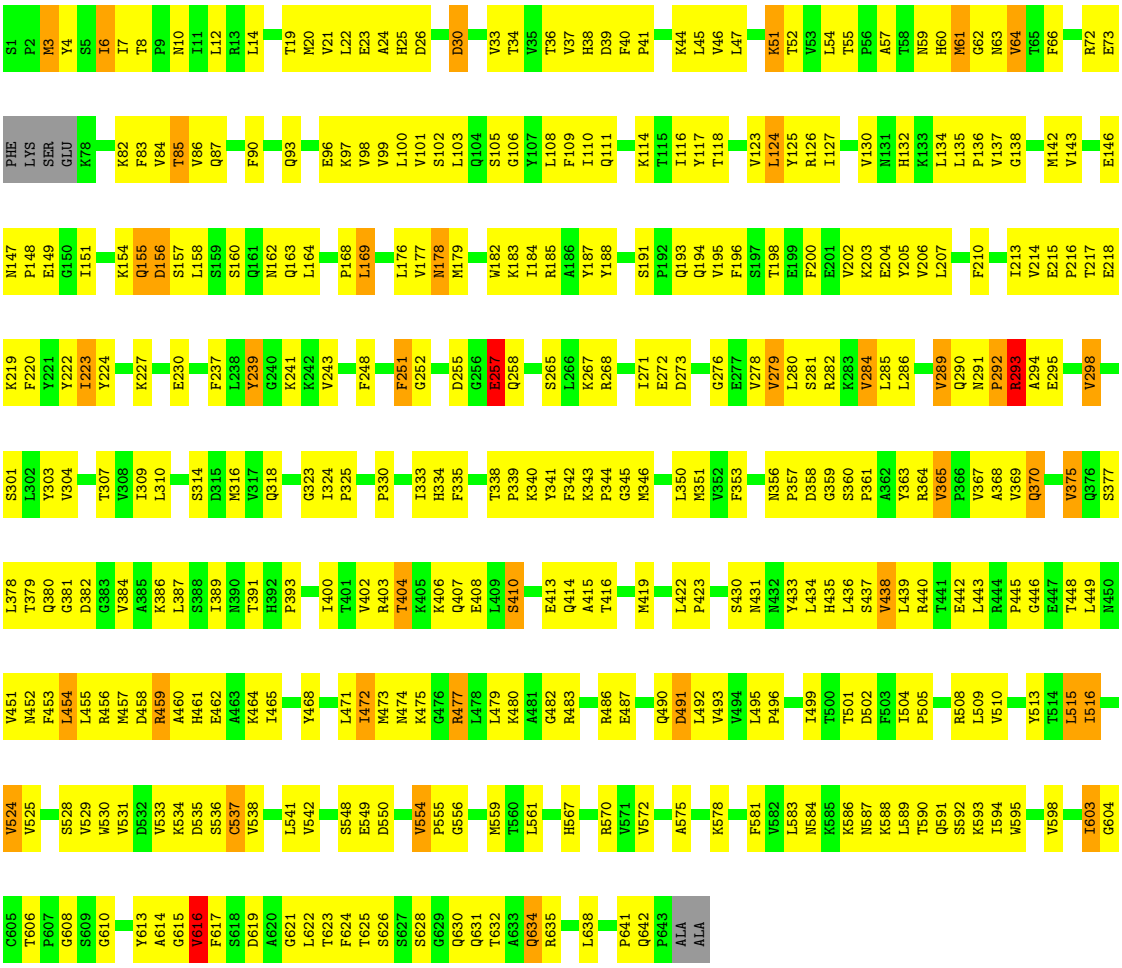
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

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.

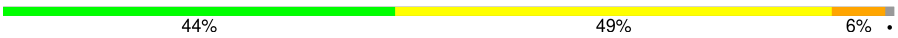
• Molecule 1: Complement C3

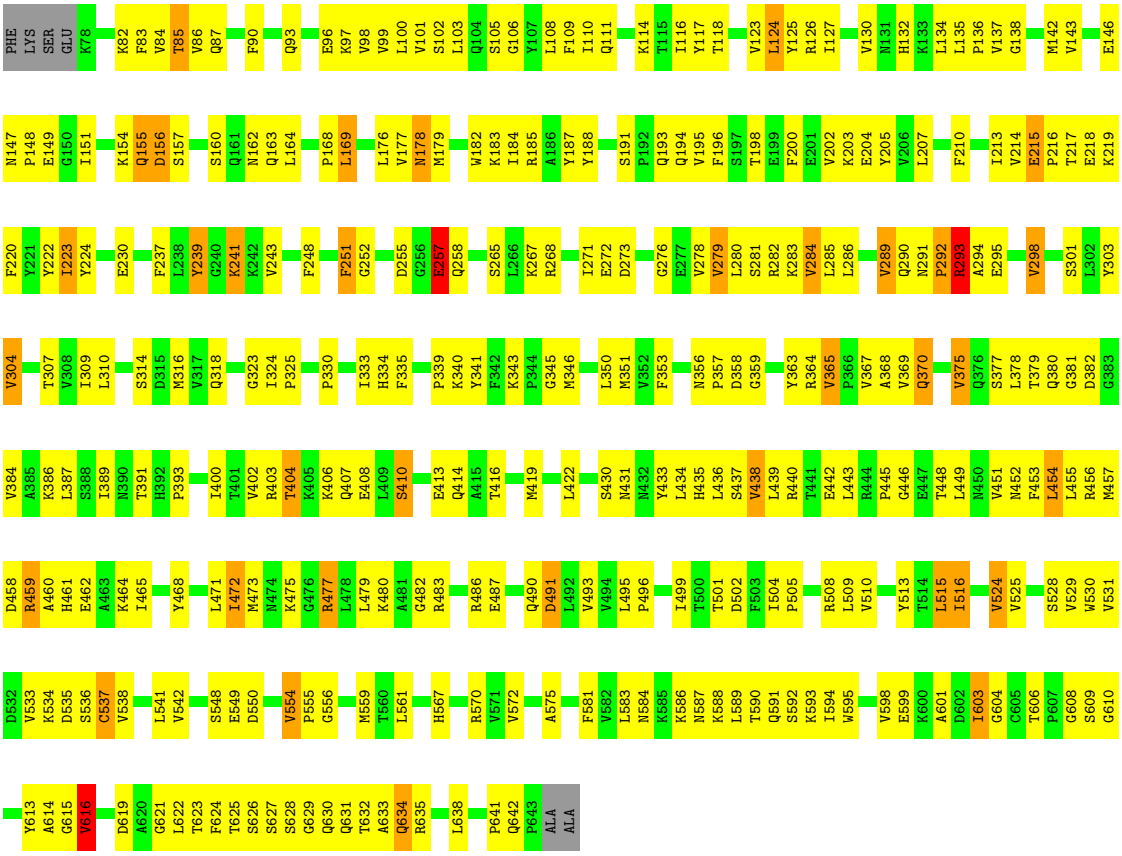
Chain A:



• Molecule 1: Complement C3

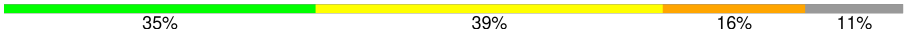
Chain D:

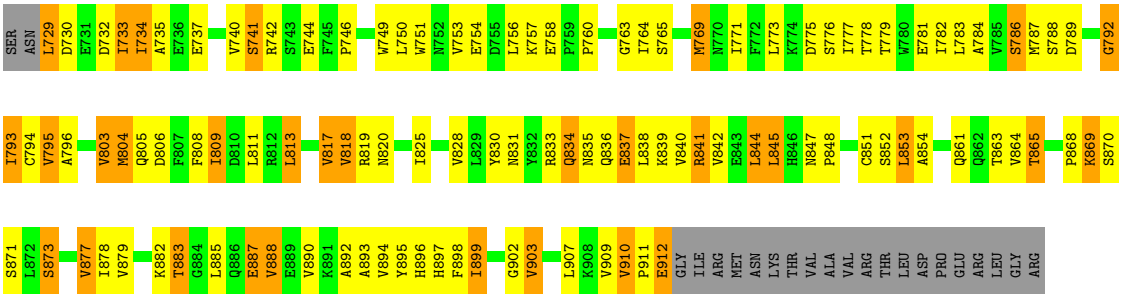




• Molecule 2: Complement C3

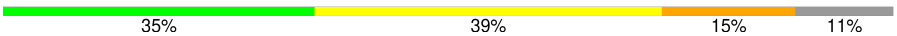
Chain B:

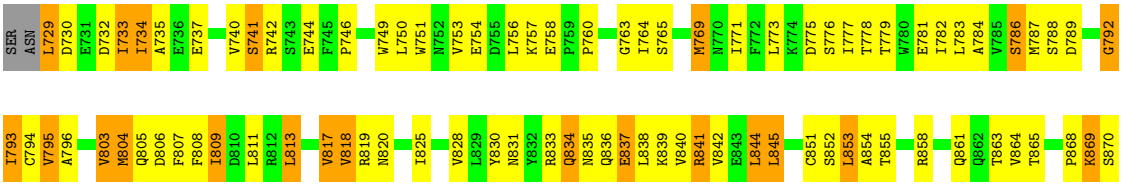


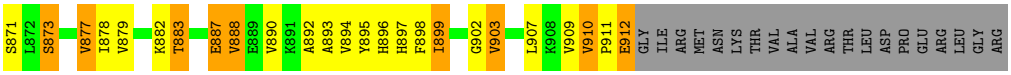


• Molecule 2: Complement C3

Chain E:

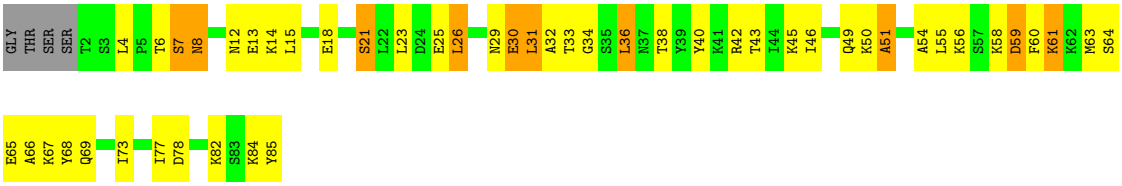






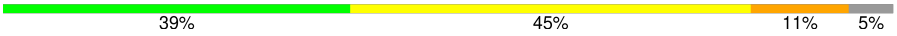
• Molecule 3: Staphylococcal complement inhibitor

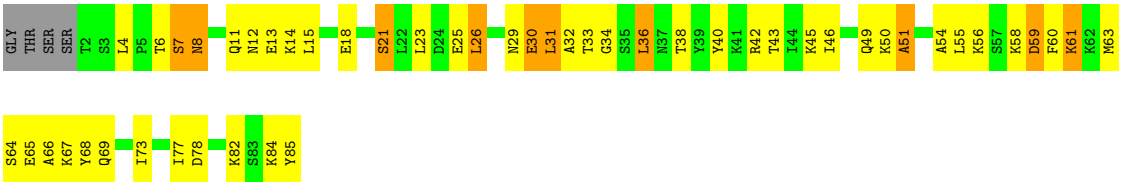
Chain M:



• Molecule 3: Staphylococcal complement inhibitor

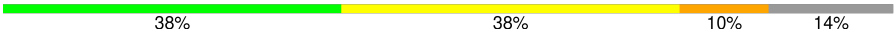
Chain P:

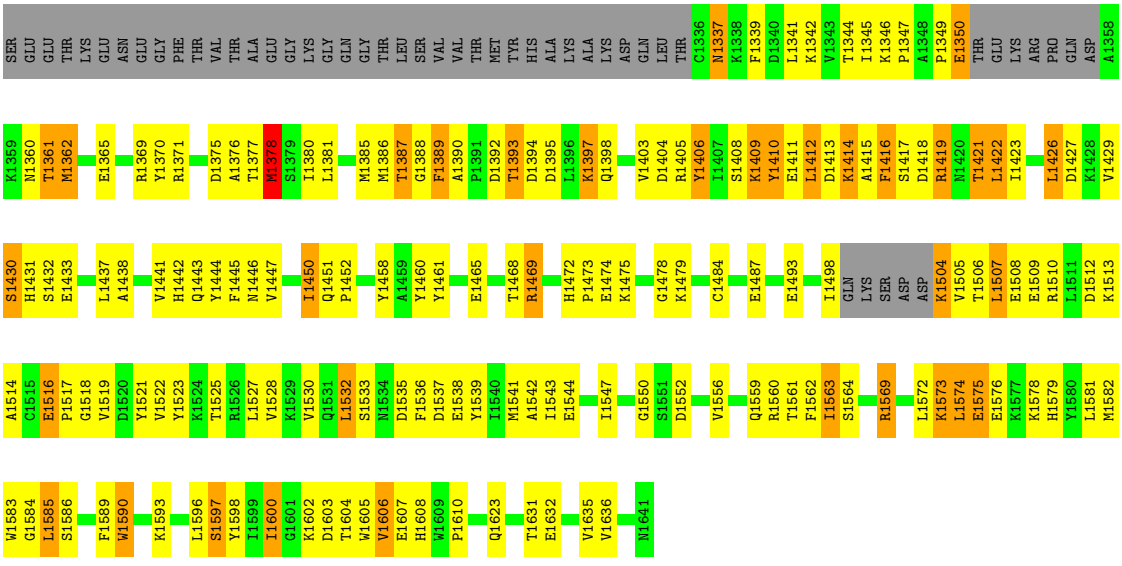




• Molecule 4: Complement C3

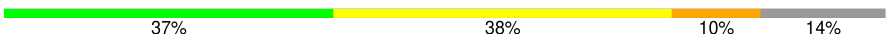
Chain F:

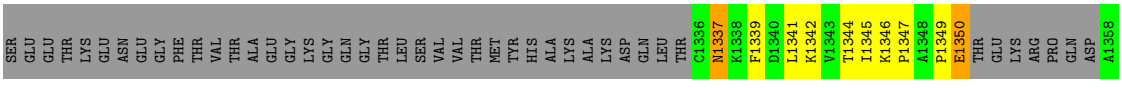


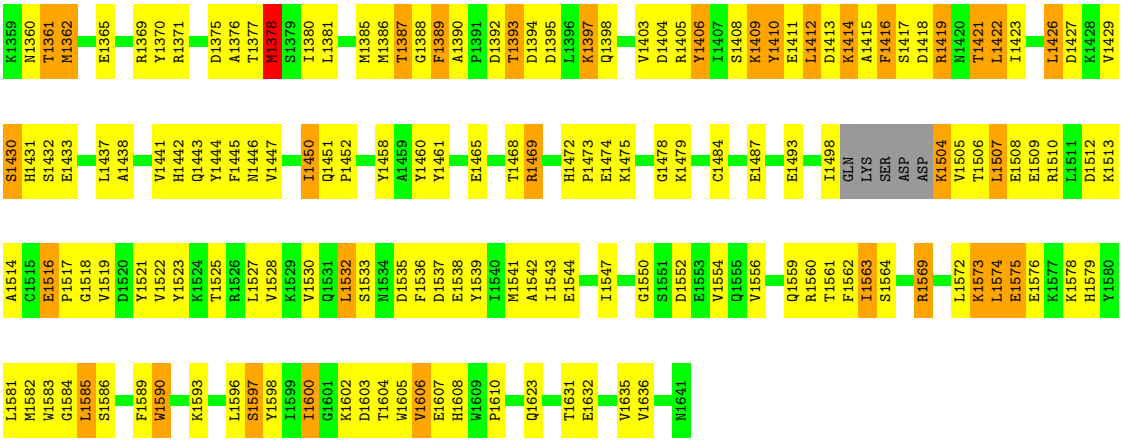


• Molecule 4: Complement C3

Chain C:






K1359 N1360 T1361 M1362 E1365 R1369 Y1370 R1371 D1375 A1376 T1377 M1378 S1379 I1380 L1381 M1385 M1386 T1387 G1388 F1389 A1390 P1391 D1392 T1393 D1394 D1395 L1396 K1397 Q1398 V1403 D1404 R1405 Y1406 I1407 S1408 K1409 Y1410 E1411 L1412 D1413 K1414 A1415 F1416 S1417 D1418 R1419 N1420 T1421 L1422 I1423 L1426 D1427 K1428 V1429
S1430 H1431 S1432 E1433 L1437 A1438 V1441 H1442 Q1443 Y1444 F1445 N1446 V1447 I1450 Q1451 P1452 Y1458 A1459 Y1460 Y1461 E1465 T1468 R1469 H1472 P1473 E1474 K1475 G1478 K1479 C1484 E1487 E1493 I1498 GLN LYS SER ASP ASP K1504 V1505 T1506 L1507 E1508 E1509 R1510 L1511 D1512 K1513
A1514 G1515 E1516 P1517 G1518 V1519 D1520 Y1521 V1522 Y1523 K1524 T1525 R1526 L1527 V1528 K1529 V1530 Q1531 L1532 S1533 N1534 D1535 F1536 D1537 E1538 Y1539 I1540 M1541 A1542 I1543 E1544 I1547 G1550 S1551 D1552 E1553 V1554 Q1555 V1556 Q1559 R1560 T1561 F1562 I1563 S1564 R1569 L1572 K1573 L1574 E1575 E1576 K1577 K1578 H1579 Y1580
L1581 M1582 W1583 G1584 L1585 S1586 F1589 W1590 K1593 L1596 S1597 Y1598 I1599 I1600 G1601 K1602 D1603 T1604 W1605 V1606 E1607 H1608 W1609 P1610 Q1623 T1631 E1632 V1635 V1636 N1641

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.11Å 217.03Å 115.65Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	34.52 – 3.40 34.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (34.52-3.40) 91.1 (34.52-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.271 0.216 , 0.268	Depositor DCC
R_{free} test set	1857 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19090	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.52	0/5079	0.95	10/6902 (0.1%)
1	D	0.53	0/5079	0.95	10/6902 (0.1%)
2	B	0.63	0/1520	0.97	5/2066 (0.2%)
2	E	0.63	0/1520	0.97	5/2066 (0.2%)
3	M	0.51	0/690	0.85	1/923 (0.1%)
3	P	0.51	0/690	0.84	1/923 (0.1%)
4	C	0.45	0/2427	0.87	3/3271 (0.1%)
4	F	0.45	0/2427	0.87	3/3271 (0.1%)
All	All	0.52	0/19432	0.93	38/26324 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	535	ASP	CB-CA-C	-7.24	98.42	110.29
1	D	535	ASP	CB-CA-C	-7.23	98.44	110.29
4	F	1606	VAL	N-CA-C	6.95	118.12	108.12
4	C	1606	VAL	N-CA-C	6.95	118.12	108.12
1	D	151	ILE	N-CA-C	6.65	114.14	107.55
1	A	151	ILE	N-CA-C	6.63	114.11	107.55
1	D	279	VAL	N-CA-C	6.59	118.20	108.45
1	A	279	VAL	N-CA-C	6.58	118.18	108.45
1	A	239	TYR	N-CA-C	-6.57	100.58	110.24
1	D	239	TYR	N-CA-C	-6.57	100.59	110.24
1	A	535	ASP	N-CA-C	6.46	119.13	109.25
1	D	535	ASP	N-CA-C	6.45	119.11	109.25
2	E	733	ILE	N-CA-C	6.33	116.74	107.75
2	B	733	ILE	N-CA-C	6.31	116.72	107.75
2	E	887	GLU	N-CA-C	6.00	118.19	108.34
2	B	887	GLU	N-CA-C	5.99	118.16	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	804	MET	N-CA-C	5.85	115.82	108.45
2	E	804	MET	N-CA-C	5.84	115.81	108.45
1	A	257	GLU	N-CA-C	-5.83	106.02	114.12
1	D	257	GLU	N-CA-C	-5.79	106.07	114.12
4	F	1409	LYS	N-CA-C	-5.75	104.00	111.02
4	C	1409	LYS	N-CA-C	-5.75	104.00	111.02
1	A	333	ILE	N-CA-C	5.65	116.13	107.77
1	D	333	ILE	N-CA-C	5.64	116.12	107.77
3	M	46	ILE	CB-CA-C	-5.39	104.79	112.22
3	P	46	ILE	CB-CA-C	-5.35	104.83	112.22
1	D	491	ASP	N-CA-C	-5.32	107.33	113.88
1	A	491	ASP	N-CA-C	-5.31	107.35	113.88
1	D	356	ASN	CA-C-N	-5.23	113.30	119.84
1	D	356	ASN	C-N-CA	-5.23	113.30	119.84
1	A	356	ASN	CA-C-N	-5.22	113.31	119.84
1	A	356	ASN	C-N-CA	-5.22	113.31	119.84
2	B	792	GLY	N-CA-C	5.21	121.28	112.22
2	E	792	GLY	N-CA-C	5.20	121.27	112.22
2	E	803	VAL	CB-CA-C	-5.12	104.77	110.96
4	F	1478	GLY	N-CA-C	-5.11	107.03	114.90
4	C	1478	GLY	N-CA-C	-5.11	107.03	114.90
2	B	803	VAL	CB-CA-C	-5.08	104.81	110.96

There are no chirality outliers.

There are no planarity outliers.

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	4979	0	5041	349	0
1	D	4979	0	5041	345	0
2	B	1488	0	1512	123	0
2	E	1488	0	1512	124	0
3	M	682	0	697	57	0
3	P	682	0	697	56	0
4	C	2382	0	2288	204	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2382	0	2288	205	0
5	A	14	0	13	4	0
5	D	14	0	13	4	0
All	All	19090	0	19102	1360	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 36.

All (1360) 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)
4:C:1569:ARG:HG3	4:C:1569:ARG:HH11	0.99	1.15
4:C:1505:VAL:HG11	4:C:1510:ARG:HH21	1.06	1.14
2:E:912:GLU:H	2:E:912:GLU:CD	1.52	1.12
4:F:1349:PRO:O	4:F:1350:GLU:HB2	1.47	1.12
4:F:1569:ARG:HG3	4:F:1569:ARG:HH11	0.99	1.11
4:C:1349:PRO:O	4:C:1350:GLU:HB2	1.47	1.10
1:A:590:THR:HG22	1:A:592:SER:H	1.13	1.10
2:B:912:GLU:CD	2:B:912:GLU:H	1.52	1.10
4:F:1505:VAL:HG11	4:F:1510:ARG:HH21	1.06	1.09
4:C:1605:TRP:HE1	4:C:1607:GLU:CD	1.60	1.08
4:F:1605:TRP:HE1	4:F:1607:GLU:CD	1.60	1.08
1:D:590:THR:HG22	1:D:592:SER:H	1.13	1.07
2:B:841:ARG:HG2	2:B:841:ARG:HH11	1.22	1.05
4:F:1582:MET:HG2	4:F:1606:VAL:HG22	1.38	1.04
2:E:841:ARG:HH11	2:E:841:ARG:HG2	1.22	1.03
4:C:1504:LYS:NZ	4:C:1504:LYS:HB2	1.75	1.02
4:C:1582:MET:HG2	4:C:1606:VAL:HG22	1.38	1.02
4:F:1360:ASN:ND2	4:F:1443:GLN:HB3	1.75	1.01
4:C:1360:ASN:ND2	4:C:1443:GLN:HB3	1.75	1.01
4:F:1504:LYS:HB2	4:F:1504:LYS:NZ	1.75	1.01
4:F:1505:VAL:HG11	4:F:1510:ARG:NH2	1.75	1.01
4:C:1505:VAL:HG11	4:C:1510:ARG:NH2	1.75	1.00
2:B:853:LEU:HD11	4:C:1451:GLN:HB2	1.46	0.97
4:C:1569:ARG:HG3	4:C:1569:ARG:NH1	1.72	0.96
4:F:1569:ARG:HG3	4:F:1569:ARG:NH1	1.72	0.95
4:F:1451:GLN:HB2	2:E:853:LEU:HD11	1.46	0.94
1:D:590:THR:HG22	1:D:592:SER:N	1.83	0.94
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.48	0.93
4:F:1360:ASN:HD22	4:F:1443:GLN:HB3	1.30	0.93
4:C:1504:LYS:NZ	4:C:1504:LYS:CB	2.30	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1582:MET:CG	4:C:1606:VAL:HG22	1.98	0.92
1:A:590:THR:HG22	1:A:592:SER:N	1.83	0.92
4:F:1582:MET:CG	4:F:1606:VAL:HG22	1.98	0.92
1:D:510:VAL:HG12	1:D:528:SER:HB3	1.48	0.92
1:A:223:ILE:HD11	1:A:298:VAL:HG23	1.53	0.91
4:F:1504:LYS:NZ	4:F:1504:LYS:CB	2.30	0.91
1:D:10:ASN:HB3	1:D:635:ARG:HH11	1.37	0.90
4:C:1360:ASN:HD22	4:C:1443:GLN:HB3	1.30	0.90
2:B:912:GLU:CD	2:B:912:GLU:N	2.30	0.89
4:C:1450:ILE:HG13	4:C:1450:ILE:O	1.72	0.89
1:D:223:ILE:HD11	1:D:298:VAL:HG23	1.53	0.89
1:A:10:ASN:HB3	1:A:635:ARG:HH11	1.37	0.89
4:F:1450:ILE:HG13	4:F:1450:ILE:O	1.72	0.89
1:D:291:ASN:N	1:D:292:PRO:HD3	1.88	0.88
1:D:138:GLY:HA2	1:D:160:SER:OG	1.74	0.88
1:A:138:GLY:HA2	1:A:160:SER:OG	1.74	0.87
2:E:912:GLU:CD	2:E:912:GLU:N	2.30	0.87
1:D:346:MET:O	1:D:391:THR:HG22	1.74	0.87
1:A:346:MET:O	1:A:391:THR:HG22	1.74	0.87
1:A:291:ASN:N	1:A:292:PRO:HD3	1.87	0.87
3:M:4:LEU:HB2	4:F:1446:ASN:HB2	1.55	0.87
4:F:1527:LEU:HD13	4:F:1541:MET:HG2	1.56	0.86
4:F:1504:LYS:HB2	4:F:1504:LYS:HZ2	1.41	0.86
4:C:1527:LEU:HD13	4:C:1541:MET:HG2	1.56	0.86
1:D:142:MET:HG3	1:D:187:TYR:CE1	2.10	0.85
4:C:1600:ILE:O	4:C:1600:ILE:HG22	1.77	0.85
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.10	0.85
2:B:734:ILE:HD12	2:B:734:ILE:H	1.42	0.85
4:C:1504:LYS:HB2	4:C:1504:LYS:HZ3	1.40	0.85
1:D:453:PHE:HB2	1:D:493:VAL:HG23	1.57	0.84
2:E:734:ILE:HD12	2:E:734:ILE:H	1.42	0.84
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.57	0.84
1:D:8:THR:HG22	1:D:20:MET:HB2	1.60	0.83
2:B:853:LEU:CD1	4:C:1451:GLN:HB2	2.08	0.83
4:F:1593:LYS:HG2	4:F:1596:LEU:HD11	1.59	0.83
4:C:1593:LYS:HG2	4:C:1596:LEU:HD11	1.59	0.83
1:A:8:THR:HG22	1:A:20:MET:HB2	1.60	0.82
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.60	0.82
4:F:1516:GLU:HB3	4:F:1517:PRO:HD2	1.61	0.82
3:P:6:THR:HA	4:C:1445:PHE:HE1	1.43	0.82
4:F:1451:GLN:HB2	2:E:853:LEU:CD1	2.08	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1600:ILE:O	4:F:1600:ILE:HG22	1.77	0.82
4:C:1578:LYS:HD3	4:C:1608:HIS:CD2	2.15	0.82
4:F:1578:LYS:HD3	4:F:1608:HIS:CD2	2.15	0.81
1:A:590:THR:HB	1:A:593:LYS:HG3	1.62	0.81
4:C:1516:GLU:HB3	4:C:1517:PRO:HD2	1.62	0.81
1:D:400:ILE:HD13	1:D:419:MET:HE3	1.60	0.81
1:A:55:THR:HG22	1:A:57:ALA:H	1.45	0.81
4:C:1532:LEU:HD11	4:C:1569:ARG:HE	1.47	0.80
1:D:590:THR:HB	1:D:593:LYS:HG3	1.61	0.80
4:C:1504:LYS:CB	4:C:1504:LYS:HZ3	1.92	0.79
2:E:833:ARG:HH22	2:E:899:ILE:HD11	1.47	0.79
3:P:4:LEU:HB2	4:C:1446:ASN:HB2	1.63	0.79
4:C:1475:LYS:HE2	4:C:1493:GLU:OE2	1.83	0.79
4:F:1475:LYS:HE2	4:F:1493:GLU:OE2	1.83	0.78
4:C:1337:ASN:O	4:C:1371:ARG:HD2	1.84	0.78
4:F:1532:LEU:HD11	4:F:1569:ARG:HE	1.47	0.78
2:B:833:ARG:HH22	2:B:899:ILE:HD11	1.47	0.77
4:F:1337:ASN:O	4:F:1371:ARG:HD2	1.84	0.77
4:C:1569:ARG:HH11	4:C:1569:ARG:CG	1.88	0.77
2:B:819:ARG:HH21	2:B:911:PRO:HB3	1.49	0.77
1:D:55:THR:HG22	1:D:57:ALA:H	1.45	0.77
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.65	0.77
1:A:365:VAL:HG13	1:A:379:THR:OG1	1.85	0.76
1:D:22:LEU:HD11	1:D:64:VAL:HG23	1.67	0.76
4:F:1569:ARG:HH11	4:F:1569:ARG:CG	1.88	0.76
1:D:365:VAL:HG13	1:D:379:THR:OG1	1.85	0.76
1:D:47:LEU:CD1	1:D:66:PHE:HB2	2.16	0.76
4:C:1582:MET:SD	4:C:1606:VAL:HG22	2.26	0.75
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.16	0.75
1:D:20:MET:O	1:D:64:VAL:HB	1.87	0.75
3:M:6:THR:HA	4:F:1445:PHE:HE1	1.49	0.75
1:D:117:TYR:CZ	1:D:123:VAL:HG13	2.22	0.75
4:C:1563:ILE:O	4:C:1600:ILE:HB	1.87	0.75
1:A:20:MET:O	1:A:64:VAL:HB	1.87	0.75
1:A:530:TRP:HD1	1:A:531:VAL:N	1.85	0.75
1:D:530:TRP:HD1	1:D:531:VAL:N	1.85	0.75
1:A:22:LEU:HD11	1:A:64:VAL:HG23	1.67	0.75
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.22	0.74
4:F:1582:MET:SD	4:F:1606:VAL:HG22	2.26	0.74
1:D:610:GLY:HA3	1:D:616:VAL:N	2.02	0.74
4:C:1600:ILE:O	4:C:1600:ILE:CG2	2.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:819:ARG:HH21	2:E:911:PRO:HB3	1.49	0.74
4:F:1563:ILE:O	4:F:1600:ILE:HB	1.87	0.74
1:D:541:LEU:HD22	2:E:786:SER:HB3	1.67	0.74
2:E:733:ILE:HG12	2:E:734:ILE:N	2.01	0.74
4:C:1504:LYS:O	4:C:1504:LYS:CG	2.36	0.74
4:F:1605:TRP:CZ2	4:F:1607:GLU:OE2	2.41	0.74
4:F:1605:TRP:NE1	4:F:1607:GLU:CD	2.43	0.74
2:B:733:ILE:HD11	2:B:893:ALA:HB3	1.70	0.74
4:C:1525:THR:HG22	4:C:1543:ILE:HA	1.70	0.74
1:A:12:LEU:HB2	1:A:101:VAL:HG22	1.70	0.74
2:E:733:ILE:HD11	2:E:893:ALA:HB3	1.70	0.74
2:B:733:ILE:HG12	2:B:734:ILE:N	2.01	0.74
4:F:1504:LYS:HB2	4:F:1504:LYS:HZ3	1.52	0.74
4:F:1600:ILE:O	4:F:1600:ILE:CG2	2.35	0.73
4:C:1416:PHE:HE2	4:C:1444:TYR:HD2	1.36	0.73
1:A:610:GLY:HA3	1:A:616:VAL:N	2.02	0.73
4:F:1525:THR:HG22	4:F:1543:ILE:HA	1.70	0.73
4:F:1504:LYS:CG	4:F:1504:LYS:O	2.36	0.73
4:F:1347:PRO:HA	4:F:1362:MET:HB3	1.71	0.73
1:D:12:LEU:HB2	1:D:101:VAL:HG22	1.70	0.73
4:C:1605:TRP:CZ2	4:C:1607:GLU:OE2	2.41	0.73
4:C:1347:PRO:HA	4:C:1362:MET:HB3	1.71	0.73
4:F:1416:PHE:HE2	4:F:1444:TYR:HD2	1.36	0.72
3:P:6:THR:CA	4:C:1445:PHE:HE1	2.03	0.72
4:F:1543:ILE:HD11	4:F:1560:ARG:HG3	1.71	0.72
2:B:840:VAL:HG11	2:B:892:ALA:HB1	1.72	0.72
4:C:1543:ILE:HD11	4:C:1560:ARG:HG3	1.71	0.72
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	0.71
1:D:369:VAL:HG12	1:D:370:GLN:N	2.03	0.71
4:F:1388:GLY:O	4:F:1443:GLN:HA	1.89	0.71
2:B:733:ILE:HG12	2:B:734:ILE:H	1.55	0.71
2:B:841:ARG:HG2	2:B:841:ARG:NH1	1.95	0.71
3:P:7:SER:N	4:C:1445:PHE:CE1	2.58	0.71
1:D:6:ILE:HD11	1:D:22:LEU:HD23	1.72	0.71
1:D:223:ILE:CD1	1:D:298:VAL:HG23	2.21	0.71
4:C:1388:GLY:O	4:C:1443:GLN:HA	1.89	0.71
4:C:1605:TRP:NE1	4:C:1607:GLU:CD	2.43	0.71
2:E:733:ILE:HG12	2:E:734:ILE:H	1.55	0.71
2:E:840:VAL:HG11	2:E:892:ALA:HB1	1.72	0.71
1:A:281:SER:OG	1:A:284:VAL:HG23	1.90	0.71
1:D:257:GLU:N	1:D:257:GLU:CD	2.49	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:SER:OG	1:D:284:VAL:HG23	1.90	0.70
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.73	0.70
1:A:223:ILE:CD1	1:A:298:VAL:HG23	2.21	0.70
1:A:495:LEU:HD12	1:A:496:PRO:HD2	1.74	0.70
1:D:24:ALA:HB3	1:D:60:HIS:HB3	1.72	0.70
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.27	0.70
3:P:36:LEU:HB3	3:P:40:TYR:CD2	2.27	0.70
1:D:6:ILE:HD11	1:D:20:MET:HE3	1.73	0.70
1:A:257:GLU:N	1:A:257:GLU:CD	2.49	0.70
1:D:237:PHE:CE2	1:D:243:VAL:HG22	2.27	0.70
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.72	0.70
4:F:1504:LYS:CB	4:F:1504:LYS:HZ3	2.03	0.70
1:A:6:ILE:HD11	1:A:22:LEU:HD23	1.72	0.70
4:C:1504:LYS:HB2	4:C:1504:LYS:HZ2	1.52	0.70
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.74	0.70
1:D:589:LEU:HD12	1:D:590:THR:H	1.57	0.70
4:C:1389:PHE:HD1	4:C:1441:VAL:HG23	1.57	0.70
3:M:36:LEU:HD23	3:M:36:LEU:N	2.05	0.69
1:D:38:HIS:CE1	1:D:45:LEU:HD12	2.27	0.69
1:D:495:LEU:HD12	1:D:496:PRO:HD2	1.73	0.69
4:F:1389:PHE:HD1	4:F:1441:VAL:HG23	1.57	0.69
4:F:1605:TRP:HE1	4:F:1607:GLU:CG	2.06	0.69
1:A:38:HIS:CE1	1:A:45:LEU:HD12	2.28	0.69
3:P:36:LEU:N	3:P:36:LEU:HD23	2.07	0.69
4:C:1605:TRP:HE1	4:C:1607:GLU:CG	2.06	0.69
1:A:588:LYS:NZ	2:B:781:GLU:OE2	2.26	0.69
1:D:369:VAL:HG12	1:D:370:GLN:H	1.58	0.69
1:A:330:PRO:O	1:A:357:PRO:HD3	1.93	0.68
2:B:825:ILE:CD1	2:B:888:VAL:HG11	2.24	0.68
2:E:825:ILE:CD1	2:E:888:VAL:HG11	2.24	0.68
3:P:6:THR:C	4:C:1445:PHE:CE1	2.72	0.68
1:D:330:PRO:O	1:D:357:PRO:HD3	1.93	0.68
1:A:19:THR:HA	1:A:64:VAL:O	1.94	0.68
1:D:19:THR:HA	1:D:64:VAL:O	1.94	0.68
1:D:588:LYS:NZ	2:E:781:GLU:OE2	2.26	0.68
2:E:841:ARG:HG2	2:E:841:ARG:NH1	1.95	0.68
1:A:216:PRO:HB2	1:A:218:GLU:O	1.95	0.67
1:D:47:LEU:HD13	1:D:66:PHE:HB2	1.74	0.67
3:M:7:SER:N	4:F:1445:PHE:CE1	2.63	0.67
1:A:589:LEU:HD12	1:A:590:THR:H	1.58	0.67
4:F:1519:VAL:HA	4:F:1584:GLY:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:PRO:HB2	1:D:218:GLU:O	1.95	0.67
1:A:369:VAL:HG12	1:A:370:GLN:H	1.58	0.67
2:B:837:GLU:HG2	3:P:64:SER:OG	1.95	0.67
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.77	0.67
3:M:36:LEU:HB3	3:M:40:TYR:CD2	2.30	0.67
1:D:130:VAL:HG12	1:D:136:PRO:HA	1.78	0.66
1:A:130:VAL:HG12	1:A:136:PRO:HA	1.78	0.66
4:F:1504:LYS:O	4:F:1504:LYS:HG2	1.94	0.66
3:P:6:THR:C	4:C:1445:PHE:HE1	2.03	0.66
3:P:84:LYS:O	3:P:84:LYS:HG3	1.96	0.66
2:E:742:ARG:HB3	2:E:775:ASP:HB3	1.77	0.66
4:C:1504:LYS:O	4:C:1504:LYS:HG2	1.94	0.66
1:A:8:THR:HG22	1:A:20:MET:CB	2.26	0.66
4:F:1582:MET:HG2	4:F:1606:VAL:CG2	2.21	0.65
1:D:8:THR:HG22	1:D:20:MET:CB	2.26	0.65
4:C:1385:MET:HG3	4:C:1390:ALA:HA	1.79	0.65
4:C:1519:VAL:HA	4:C:1584:GLY:O	1.95	0.65
3:M:64:SER:OG	2:E:837:GLU:HG2	1.97	0.65
4:C:1605:TRP:HZ2	4:C:1607:GLU:OE2	1.79	0.65
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.78	0.65
4:F:1632:GLU:O	4:F:1636:VAL:HG12	1.96	0.65
2:E:793:ILE:HG13	2:E:794:CYS:H	1.61	0.65
2:B:793:ILE:HG13	2:B:794:CYS:H	1.62	0.65
2:B:795:VAL:HG12	2:B:795:VAL:O	1.96	0.65
2:B:839:LYS:NZ	3:P:12:ASN:OD1	2.30	0.65
3:M:6:THR:CA	4:F:1445:PHE:HE1	2.09	0.65
4:C:1416:PHE:C	4:C:1416:PHE:CD2	2.75	0.65
1:D:407:GLN:O	1:D:408:GLU:HB2	1.96	0.65
1:D:567:HIS:ND1	2:E:760:PRO:HG3	2.12	0.64
3:M:84:LYS:O	3:M:84:LYS:HG3	1.96	0.64
4:F:1416:PHE:C	4:F:1416:PHE:CD2	2.75	0.64
4:F:1385:MET:HG3	4:F:1390:ALA:HA	1.79	0.64
1:D:6:ILE:HG22	1:D:625:THR:HB	1.80	0.64
1:D:93:GLN:OE1	1:D:93:GLN:HA	1.97	0.64
1:D:445:PRO:HA	1:D:499:ILE:O	1.98	0.64
4:C:1505:VAL:CG1	4:C:1510:ARG:HE	2.11	0.64
3:M:6:THR:C	4:F:1445:PHE:CE1	2.76	0.64
1:D:554:VAL:HG13	1:D:555:PRO:HD2	1.79	0.64
1:A:105:SER:HB2	1:A:188:TYR:CD1	2.33	0.64
2:B:819:ARG:HG2	2:B:820:ASN:ND2	2.13	0.64
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HA	1:A:499:ILE:O	1.98	0.64
1:A:610:GLY:HA3	1:A:616:VAL:H	1.63	0.64
4:C:1632:GLU:O	4:C:1636:VAL:HG12	1.96	0.64
2:B:840:VAL:CG1	2:B:892:ALA:HB1	2.28	0.64
1:D:335:PHE:CD2	1:D:419:MET:HB3	2.33	0.63
1:D:610:GLY:HA3	1:D:616:VAL:H	1.63	0.63
4:C:1527:LEU:CD1	4:C:1541:MET:HG2	2.27	0.63
1:A:407:GLN:O	1:A:408:GLU:HB2	1.96	0.63
1:A:93:GLN:OE1	1:A:93:GLN:HA	1.97	0.63
1:A:433:TYR:HB2	1:A:456:ARG:HB3	1.81	0.63
4:F:1505:VAL:CG1	4:F:1510:ARG:HE	2.11	0.63
2:E:841:ARG:HH11	2:E:841:ARG:CG	2.06	0.63
4:F:1532:LEU:HD23	4:F:1533:SER:H	1.63	0.63
4:F:1605:TRP:HZ2	4:F:1607:GLU:OE2	1.79	0.63
4:F:1369:ARG:HD2	4:F:1432:SER:O	1.98	0.63
1:D:105:SER:HB2	1:D:188:TYR:CD1	2.33	0.63
1:D:293:ARG:CZ	1:D:293:ARG:HB3	2.28	0.63
2:E:840:VAL:CG1	2:E:892:ALA:HB1	2.28	0.63
1:A:114:LYS:HE3	1:A:116:ILE:O	1.99	0.63
4:F:1542:ALA:HB2	4:F:1559:GLN:HG2	1.80	0.63
1:D:10:ASN:CG	1:D:635:ARG:HD2	2.24	0.63
2:E:795:VAL:HG12	2:E:795:VAL:O	1.96	0.63
4:C:1532:LEU:HD23	4:C:1537:ASP:HB3	1.81	0.63
2:E:819:ARG:HG2	2:E:820:ASN:ND2	2.13	0.63
3:M:6:THR:C	4:F:1445:PHE:HE1	2.06	0.62
4:C:1369:ARG:HD2	4:C:1432:SER:O	1.98	0.62
4:C:1542:ALA:HB2	4:C:1559:GLN:HG2	1.80	0.62
1:A:293:ARG:CZ	1:A:293:ARG:HB3	2.28	0.62
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.06	0.62
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.62
1:A:340:LYS:O	1:A:341:TYR:CD1	2.53	0.62
1:D:340:LYS:O	1:D:341:TYR:CD1	2.53	0.62
4:C:1582:MET:HG2	4:C:1606:VAL:CG2	2.21	0.62
1:A:346:MET:HE1	1:A:454:LEU:HG	1.82	0.62
4:F:1532:LEU:HD23	4:F:1537:ASP:HB3	1.81	0.62
1:D:154:LYS:HE2	1:D:156:ASP:OD1	2.00	0.62
4:C:1532:LEU:HD23	4:C:1533:SER:H	1.63	0.62
1:A:295:GLU:O	1:A:298:VAL:HB	2.00	0.62
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.15	0.62
4:F:1378:MET:HE3	1:D:248:PHE:HD1	1.63	0.62
4:F:1610:PRO:HD3	4:F:1623:GLN:NE2	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:THR:HG23	1:D:318:GLN:HG3	1.81	0.62
1:A:307:THR:HG23	1:A:318:GLN:HG3	1.81	0.62
2:B:912:GLU:N	2:B:912:GLU:OE1	2.30	0.62
4:C:1605:TRP:NE1	4:C:1607:GLU:HG3	2.14	0.62
2:B:842:VAL:HG23	2:B:892:ALA:HB2	1.82	0.62
3:P:6:THR:HA	4:C:1445:PHE:CE1	2.31	0.62
4:F:1605:TRP:NE1	4:F:1607:GLU:HG3	2.14	0.62
1:D:346:MET:HE1	1:D:454:LEU:HG	1.82	0.62
1:D:433:TYR:HB2	1:D:456:ARG:HB3	1.81	0.62
1:A:248:PHE:HD1	4:C:1378:MET:HE3	1.64	0.61
1:A:10:ASN:CG	1:A:635:ARG:HD2	2.24	0.61
1:A:292:PRO:O	1:A:293:ARG:C	2.43	0.61
1:A:438:VAL:O	1:A:440:ARG:HG3	2.00	0.61
4:F:1405:ARG:NE	4:F:1437:LEU:HD23	2.15	0.61
3:M:26:LEU:C	3:M:26:LEU:HD12	2.26	0.61
1:D:179:MET:HG3	1:D:203:LYS:HA	1.82	0.61
1:A:136:PRO:HD2	2:B:789:ASP:HA	1.83	0.61
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.83	0.61
3:M:12:ASN:OD1	2:E:839:LYS:NZ	2.32	0.61
4:F:1590:TRP:HA	4:F:1590:TRP:CE3	2.36	0.61
1:D:292:PRO:O	1:D:293:ARG:C	2.43	0.61
1:A:22:LEU:HB2	1:A:62:GLY:HA3	1.83	0.61
1:A:154:LYS:HE2	1:A:156:ASP:OD1	2.00	0.61
1:A:179:MET:HG3	1:A:203:LYS:HA	1.82	0.61
1:A:487:GLU:O	1:A:490:GLN:HB2	2.01	0.61
1:D:438:VAL:O	1:D:440:ARG:HG3	2.00	0.61
1:D:455:LEU:HD11	1:D:457:MET:HG2	1.82	0.61
4:C:1602:LYS:HG3	4:C:1603:ASP:N	2.16	0.61
1:D:114:LYS:HE3	1:D:116:ILE:O	1.99	0.61
1:D:570:ARG:O	2:E:786:SER:HA	2.01	0.61
2:B:741:SER:HB3	2:B:902:GLY:C	2.26	0.61
3:P:26:LEU:C	3:P:26:LEU:HD12	2.26	0.61
4:F:1505:VAL:CG1	4:F:1510:ARG:NH2	2.58	0.61
2:E:842:VAL:HG23	2:E:892:ALA:HB2	1.82	0.61
4:F:1527:LEU:CD1	4:F:1541:MET:HG2	2.27	0.61
1:D:295:GLU:O	1:D:298:VAL:HB	2.00	0.61
1:D:487:GLU:O	1:D:490:GLN:HB2	2.01	0.61
1:A:73:GLU:HB3	1:A:82:LYS:NZ	2.16	0.60
1:A:455:LEU:HD11	1:A:457:MET:HG2	1.82	0.60
4:C:1590:TRP:HA	4:C:1590:TRP:CE3	2.36	0.60
4:F:1602:LYS:HG3	4:F:1603:ASP:N	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LEU:HB2	1:D:62:GLY:HA3	1.83	0.60
1:D:513:TYR:CE1	1:D:525:VAL:HB	2.36	0.60
4:C:1610:PRO:HD3	4:C:1623:GLN:NE2	2.15	0.60
1:A:446:GLY:N	1:A:499:ILE:O	2.32	0.60
4:F:1602:LYS:HG3	4:F:1603:ASP:H	1.66	0.60
4:C:1405:ARG:NE	4:C:1437:LEU:HD23	2.15	0.60
1:A:533:VAL:HG12	1:A:534:LYS:N	2.17	0.60
2:E:741:SER:HB3	2:E:902:GLY:C	2.26	0.60
3:P:36:LEU:HB3	3:P:40:TYR:HD2	1.65	0.60
4:F:1422:LEU:HD12	4:F:1423:ILE:N	2.17	0.60
4:C:1339:PHE:HE2	4:C:1429:VAL:HG21	1.67	0.60
4:C:1422:LEU:HD12	4:C:1423:ILE:N	2.17	0.59
4:C:1505:VAL:CG1	4:C:1510:ARG:NH2	2.58	0.59
1:D:334:HIS:HB2	1:D:353:PHE:HB3	1.83	0.59
1:A:448:THR:HG21	1:D:377:SER:HB2	1.84	0.59
1:A:513:TYR:CE1	1:A:525:VAL:HB	2.36	0.59
1:A:606:THR:HG22	1:A:608:GLY:N	2.17	0.59
4:F:1339:PHE:HE2	4:F:1429:VAL:HG21	1.67	0.59
4:F:1527:LEU:HD21	4:F:1574:LEU:CD1	2.32	0.59
1:D:117:TYR:CG	1:D:123:VAL:HG22	2.38	0.59
4:C:1341:LEU:O	4:C:1469:ARG:HG2	2.03	0.59
2:B:734:ILE:HD12	2:B:734:ILE:N	2.16	0.59
1:D:134:LEU:HD11	1:D:598:VAL:HG21	1.84	0.59
4:C:1518:GLY:HA3	4:C:1585:LEU:HD22	1.84	0.59
2:E:831:ASN:ND2	2:E:868:PRO:HA	2.18	0.59
2:E:841:ARG:HG2	2:E:841:ARG:O	2.01	0.59
2:B:852:SER:C	2:B:854:ALA:H	2.10	0.59
1:D:73:GLU:HB3	1:D:82:LYS:NZ	2.16	0.59
2:B:831:ASN:ND2	2:B:868:PRO:HA	2.18	0.59
1:A:99:VAL:HG12	1:A:100:LEU:N	2.18	0.59
4:C:1527:LEU:HD21	4:C:1574:LEU:CD1	2.32	0.59
2:E:852:SER:C	2:E:854:ALA:H	2.10	0.59
2:B:825:ILE:HD13	2:B:888:VAL:HG11	1.84	0.59
1:D:61:MET:HE2	1:D:483:ARG:HG2	1.85	0.59
1:D:530:TRP:CD1	1:D:531:VAL:N	2.69	0.59
4:C:1360:ASN:HD22	4:C:1443:GLN:CB	2.11	0.59
4:C:1602:LYS:HG3	4:C:1603:ASP:H	1.67	0.59
2:E:912:GLU:N	2:E:912:GLU:OE1	2.30	0.59
1:A:61:MET:HE2	1:A:483:ARG:HG2	1.85	0.59
1:D:606:THR:HG22	1:D:608:GLY:N	2.17	0.59
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.85	0.58
4:F:1377:THR:O	4:F:1378:MET:C	2.46	0.58
1:D:20:MET:HG2	1:D:64:VAL:HG21	1.84	0.58
1:D:99:VAL:HG12	1:D:100:LEU:N	2.18	0.58
1:D:443:LEU:HD11	1:D:449:LEU:HD22	1.85	0.58
4:F:1518:GLY:HA3	4:F:1585:LEU:HD22	1.84	0.58
4:F:1590:TRP:HA	4:F:1590:TRP:HE3	1.67	0.58
1:D:47:LEU:HD11	1:D:66:PHE:HB2	1.84	0.58
1:D:345:GLY:H	1:D:391:THR:HG23	1.68	0.58
4:C:1510:ARG:O	4:C:1514:ALA:HB3	2.03	0.58
1:A:20:MET:HG2	1:A:64:VAL:HG21	1.84	0.58
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.37	0.58
2:B:841:ARG:HG2	2:B:841:ARG:O	2.01	0.58
1:D:118:THR:HG23	1:D:205:TYR:CZ	2.38	0.58
4:C:1397:LYS:O	4:C:1398:GLN:C	2.46	0.58
2:E:734:ILE:HD12	2:E:734:ILE:N	2.16	0.58
1:A:377:SER:HB2	1:D:448:THR:HG21	1.85	0.58
4:F:1341:LEU:O	4:F:1469:ARG:HG2	2.03	0.58
4:F:1527:LEU:HD13	4:F:1541:MET:CG	2.32	0.58
4:C:1590:TRP:HA	4:C:1590:TRP:HE3	1.67	0.58
1:A:345:GLY:H	1:A:391:THR:HG23	1.68	0.58
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.39	0.58
2:B:804:MET:HG2	2:B:805:GLN:H	1.68	0.58
2:B:833:ARG:NH2	2:B:899:ILE:HD11	2.17	0.58
1:D:533:VAL:HG12	1:D:534:LYS:N	2.17	0.58
4:C:1377:THR:O	4:C:1378:MET:C	2.46	0.58
4:C:1408:SER:O	4:C:1409:LYS:C	2.45	0.58
2:E:833:ARG:NH2	2:E:899:ILE:HD11	2.17	0.58
1:A:47:LEU:HD11	1:A:66:PHE:HB2	1.84	0.58
1:A:530:TRP:CD1	1:A:531:VAL:N	2.69	0.58
1:A:589:LEU:HD12	1:A:590:THR:N	2.18	0.58
4:F:1341:LEU:HD23	4:F:1469:ARG:HB2	1.86	0.58
4:F:1510:ARG:O	4:F:1514:ALA:HB3	2.03	0.58
1:D:589:LEU:HD12	1:D:590:THR:N	2.18	0.58
1:A:118:THR:HG23	1:A:205:TYR:CZ	2.38	0.58
4:C:1605:TRP:NE1	4:C:1607:GLU:OE2	2.37	0.58
4:F:1550:GLY:C	4:F:1552:ASP:H	2.12	0.58
2:E:825:ILE:HD13	2:E:888:VAL:HG11	1.84	0.58
4:F:1408:SER:O	4:F:1409:LYS:C	2.45	0.57
4:F:1584:GLY:C	4:F:1585:LEU:HD23	2.29	0.57
1:D:453:PHE:HB2	1:D:493:VAL:CG2	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1584:GLY:C	4:C:1585:LEU:HD23	2.29	0.57
4:C:1365:GLU:HG3	4:C:1438:ALA:HB2	1.85	0.57
3:M:55:LEU:O	3:M:58:LYS:HD3	2.04	0.57
4:F:1365:GLU:HG3	4:F:1438:ALA:HB2	1.85	0.57
2:E:804:MET:HG2	2:E:805:GLN:H	1.68	0.57
4:F:1397:LYS:O	4:F:1398:GLN:C	2.46	0.57
1:A:477:ARG:NH2	1:A:479:LEU:HD13	2.20	0.57
4:F:1505:VAL:HG11	4:F:1510:ARG:CZ	2.34	0.57
4:F:1605:TRP:NE1	4:F:1607:GLU:OE2	2.36	0.57
1:D:10:ASN:HB3	1:D:635:ARG:NH1	2.15	0.57
1:D:136:PRO:HD2	2:E:789:ASP:HA	1.86	0.57
4:C:1345:ILE:HG23	4:C:1345:ILE:O	2.04	0.57
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.33	0.57
4:F:1421:THR:HG21	2:E:873:SER:HB3	1.86	0.57
1:D:23:GLU:HG2	1:D:61:MET:HG2	1.87	0.57
1:A:594:ILE:O	1:A:598:VAL:HG23	2.05	0.57
4:F:1393:THR:CG2	4:F:1419:ARG:HH22	2.17	0.57
4:F:1416:PHE:HE2	4:F:1444:TYR:CD2	2.21	0.57
1:D:99:VAL:HG12	1:D:100:LEU:H	1.70	0.57
1:D:513:TYR:CZ	1:D:525:VAL:HB	2.39	0.57
4:C:1393:THR:CG2	4:C:1419:ARG:HH22	2.17	0.57
4:C:1550:GLY:C	4:C:1552:ASP:H	2.12	0.57
3:P:84:LYS:O	3:P:85:TYR:HB2	2.05	0.57
1:D:477:ARG:NH2	1:D:479:LEU:HD13	2.20	0.57
1:A:570:ARG:O	2:B:786:SER:HA	2.05	0.57
2:B:873:SER:HB3	4:C:1421:THR:HG21	1.86	0.57
3:M:84:LYS:O	3:M:85:TYR:HB2	2.05	0.57
3:P:55:LEU:O	3:P:58:LYS:HD3	2.04	0.57
4:F:1506:THR:OG1	4:F:1509:GLU:HG2	2.04	0.57
4:F:1345:ILE:HG23	4:F:1345:ILE:O	2.04	0.57
4:C:1506:THR:OG1	4:C:1509:GLU:HG2	2.04	0.57
1:A:142:MET:HG3	1:A:187:TYR:HE1	1.65	0.56
1:A:345:GLY:N	1:A:391:THR:HG23	2.20	0.56
1:A:536:SER:O	1:A:537:CYS:C	2.48	0.56
2:B:788:SER:O	2:B:792:GLY:N	2.35	0.56
2:B:819:ARG:HG2	2:B:820:ASN:CG	2.31	0.56
4:F:1505:VAL:CG1	4:F:1510:ARG:NE	2.68	0.56
1:D:34:THR:HG22	1:D:51:LYS:HE2	1.88	0.56
1:D:406:LYS:H	1:D:414:GLN:HE22	1.53	0.56
1:D:567:HIS:CG	2:E:760:PRO:HG3	2.40	0.56
1:D:594:ILE:O	1:D: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)
4:C:1416:PHE:HE2	4:C:1444:TYR:CD2	2.21	0.56
1:A:567:HIS:CG	2:B:760:PRO:HG3	2.40	0.56
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.87	0.56
3:P:64:SER:O	3:P:67:LYS:HB3	2.05	0.56
1:D:446:GLY:N	1:D:499:ILE:O	2.32	0.56
2:B:734:ILE:H	2:B:734:ILE:CD1	2.16	0.56
1:A:34:THR:HG22	1:A:51:LYS:HE2	1.88	0.56
1:A:99:VAL:HG12	1:A:100:LEU:H	1.70	0.56
4:F:1360:ASN:HD22	4:F:1443:GLN:CB	2.11	0.56
4:F:1409:LYS:HG2	4:F:1413:ASP:OD2	2.06	0.56
1:D:6:ILE:CD1	1:D:22:LEU:HD23	2.33	0.56
1:D:536:SER:O	1:D:537:CYS:C	2.48	0.56
4:C:1349:PRO:O	4:C:1350:GLU:CB	2.34	0.56
2:E:819:ARG:HG2	2:E:820:ASN:CG	2.31	0.56
2:B:773:LEU:HD13	2:B:803:VAL:CG2	2.35	0.56
3:M:64:SER:O	3:M:67:LYS:HB3	2.05	0.56
2:B:741:SER:HB3	2:B:902:GLY:O	2.06	0.56
1:D:364:ARG:HG2	1:D:378:LEU:HD23	1.87	0.56
1:D:471:LEU:O	1:D:509:LEU:HD12	2.06	0.56
4:C:1411:GLU:O	4:C:1414:LYS:HG3	2.06	0.56
2:E:773:LEU:HD13	2:E:803:VAL:CG2	2.35	0.56
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.87	0.56
1:A:179:MET:HG3	1:A:202:VAL:O	2.06	0.56
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.41	0.56
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.56
1:A:443:LEU:O	1:A:533:VAL:HG13	2.06	0.56
1:D:179:MET:HG3	1:D:202:VAL:O	2.06	0.56
1:D:443:LEU:O	1:D:533:VAL:HG13	2.06	0.56
1:D:575:ALA:HB2	2:E:782:ILE:HG12	1.87	0.56
4:C:1409:LYS:HG2	4:C:1413:ASP:OD2	2.06	0.56
1:D:210:PHE:CE2	1:D:310:LEU:HD21	2.41	0.56
1:D:345:GLY:N	1:D:391:THR:HG23	2.20	0.56
1:D:586:LYS:O	1:D:587:ASN:HB2	2.05	0.56
2:E:741:SER:HB3	2:E:902:GLY:O	2.06	0.56
1:A:406:LYS:H	1:A:414:GLN:HE22	1.53	0.55
1:A:257:GLU:CD	1:A:257:GLU:H	2.14	0.55
4:C:1341:LEU:HD23	4:C:1469:ARG:HB2	1.86	0.55
4:F:1444:TYR:CD1	4:F:1445:PHE:HB2	2.42	0.55
4:C:1505:VAL:CG1	4:C:1510:ARG:NE	2.69	0.55
4:F:1389:PHE:N	4:F:1389:PHE:CD2	2.75	0.55
4:C:1605:TRP:NE1	4:C:1607:GLU:CG	2.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:732:ASP:OD1	2:E:896:HIS:HA	2.06	0.55
1:A:364:ARG:HG2	1:A:378:LEU:HD23	1.87	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
1:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.55
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.55
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.32	0.55
4:F:1404:ASP:HA	4:F:1427:ASP:HB2	1.88	0.55
1:D:142:MET:HG3	1:D:187:TYR:HE1	1.65	0.55
1:D:440:ARG:NH2	1:D:529:VAL:HG23	2.22	0.55
4:C:1505:VAL:HG11	4:C:1510:ARG:CZ	2.34	0.55
4:C:1527:LEU:HD13	4:C:1541:MET:CG	2.32	0.55
1:D:54:LEU:HB3	1:D:60:HIS:HA	1.89	0.55
2:B:734:ILE:HD13	2:B:893:ALA:HB1	1.88	0.55
4:F:1562:PHE:CE1	4:F:1598:TYR:CD1	2.95	0.55
1:D:610:GLY:N	1:D:616:VAL:HG23	2.22	0.55
4:C:1562:PHE:CE1	4:C:1598:TYR:CD1	2.95	0.55
2:E:808:PHE:C	2:E:808:PHE:CD1	2.85	0.55
2:E:851:CYS:HB3	2:E:879:VAL:HB	1.87	0.55
4:C:1444:TYR:CD1	4:C:1445:PHE:HB2	2.42	0.54
2:B:732:ASP:OD1	2:B:896:HIS:HA	2.06	0.54
2:B:883:THR:HA	2:B:909:VAL:HG12	1.88	0.54
4:F:1411:GLU:O	4:F:1414:LYS:HG3	2.06	0.54
1:D:147:ASN:HB2	1:D:148:PRO:HD3	1.90	0.54
1:D:257:GLU:CD	1:D:257:GLU:H	2.14	0.54
1:A:10:ASN:HB3	1:A:635:ARG:NH1	2.15	0.54
4:F:1583:TRP:O	4:F:1604:THR:HG23	2.08	0.54
1:D:38:HIS:HE1	1:D:45:LEU:HD12	1.73	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.90	0.54
2:E:734:ILE:HD13	2:E:893:ALA:HB1	1.88	0.54
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	0.54
1:A:575:ALA:HB2	2:B:782:ILE:HG12	1.89	0.54
1:D:430:SER:O	1:D:431:ASN:HB2	2.06	0.54
2:B:793:ILE:HG13	2:B:794:CYS:N	2.23	0.54
1:D:34:THR:CG2	1:D:51:LYS:HE2	2.38	0.54
4:C:1404:ASP:HA	4:C:1427:ASP:HB2	1.88	0.54
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	0.54
4:C:1389:PHE:N	4:C:1389:PHE:CD2	2.75	0.54
2:B:907:LEU:HD23	2:B:907:LEU:H	1.73	0.54
4:F:1605:TRP:CE2	4:F:1607:GLU:OE2	2.61	0.54
2:E:788:SER:O	2:E:792:GLY:N	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:HB	1:A:613:TYR:CD1	2.43	0.54
1:D:363:TYR:CZ	1:D:364:ARG:HG3	2.43	0.54
4:C:1504:LYS:HZ3	4:C:1504:LYS:HB3	1.72	0.54
2:E:844:LEU:HD12	2:E:844:LEU:C	2.33	0.54
1:A:282:ARG:O	1:A:286:LEU:HD12	2.08	0.53
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.89	0.53
2:B:844:LEU:C	2:B:844:LEU:HD12	2.33	0.53
4:F:1381:LEU:HD12	4:F:1426:LEU:HD11	1.91	0.53
1:D:510:VAL:HG12	1:D:528:SER:CB	2.30	0.53
2:E:883:THR:HA	2:E:909:VAL:HG12	1.88	0.53
1:D:468:TYR:HE1	1:D:513:TYR:HD2	1.57	0.53
2:E:819:ARG:HH21	2:E:911:PRO:CB	2.19	0.53
1:A:591:GLN:HB2	2:B:795:VAL:HB	1.91	0.53
2:B:808:PHE:CD1	2:B:808:PHE:C	2.85	0.53
4:F:1360:ASN:ND2	4:F:1443:GLN:CB	2.60	0.53
2:E:836:GLN:C	2:E:868:PRO:HG3	2.33	0.53
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.56	0.53
2:B:763:GLY:O	2:B:764:ILE:HD13	2.09	0.53
2:B:836:GLN:C	2:B:868:PRO:HG3	2.34	0.53
4:C:1409:LYS:O	4:C:1412:LEU:N	2.42	0.53
1:A:34:THR:CG2	1:A:51:LYS:HE2	2.38	0.53
4:F:1581:LEU:O	4:F:1582:MET:HG3	2.09	0.53
1:D:73:GLU:HB3	1:D:82:LYS:HZ3	1.74	0.53
1:D:146:GLU:CD	1:D:185:ARG:HD2	2.33	0.53
4:C:1381:LEU:HD12	4:C:1426:LEU:HD11	1.91	0.53
4:C:1583:TRP:O	4:C:1604:THR:HG23	2.08	0.53
3:M:36:LEU:HB3	3:M:40:TYR:HD2	1.73	0.53
1:D:477:ARG:HG2	1:D:477:ARG:HH11	1.72	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
3:P:59:ASP:OD1	3:P:59:ASP:C	2.52	0.53
1:D:124:LEU:N	1:D:124:LEU:HD23	2.24	0.53
1:D:365:VAL:CG1	1:D:379:THR:OG1	2.56	0.53
1:D:524:VAL:HB	1:D:613:TYR:CD1	2.43	0.53
4:C:1346:LYS:O	4:C:1362:MET:HB2	2.09	0.53
2:E:793:ILE:HG13	2:E:794:CYS:N	2.23	0.53
2:E:808:PHE:CE1	2:E:830:TYR:HB2	2.44	0.53
2:E:852:SER:HB3	2:E:878:ILE:HG22	1.91	0.53
1:A:39:ASP:OD1	1:A:44:LYS:HB2	2.09	0.53
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.43	0.53
1:D:282:ARG:O	1:D:286:LEU:HD12	2.08	0.53
1:D:468:TYR:HE1	1:D:513:TYR:CD2	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:763:GLY:O	2:E:764:ILE:HD13	2.09	0.53
2:B:808:PHE:CE1	2:B:830:TYR:HB2	2.44	0.52
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.91	0.52
1:D:363:TYR:CE1	1:D:364:ARG:HG3	2.44	0.52
1:A:363:TYR:CE1	1:A:364:ARG:HG3	2.44	0.52
4:F:1525:THR:HG22	4:F:1543:ILE:HG23	1.91	0.52
1:D:39:ASP:OD1	1:D:44:LYS:HB2	2.09	0.52
3:M:59:ASP:C	3:M:59:ASP:OD1	2.52	0.52
4:F:1409:LYS:O	4:F:1412:LEU:N	2.42	0.52
4:C:1605:TRP:CE2	4:C:1607:GLU:OE2	2.61	0.52
2:E:907:LEU:H	2:E:907:LEU:HD23	1.73	0.52
1:A:468:TYR:CE1	1:A:513:TYR:HD2	2.28	0.52
3:P:49:GLN:O	3:P:50:LYS:C	2.52	0.52
2:E:777:ILE:HD13	2:E:808:PHE:CD2	2.44	0.52
1:A:143:VAL:O	1:A:155:GLN:HA	2.10	0.52
1:A:343:LYS:HD2	1:A:343:LYS:N	2.25	0.52
2:B:740:VAL:HB	3:M:42:ARG:HA	1.91	0.52
2:B:783:LEU:HD12	2:B:784:ALA:N	2.24	0.52
4:F:1346:LYS:O	4:F:1362:MET:HB2	2.09	0.52
1:D:343:LYS:HD2	1:D:343:LYS:N	2.25	0.52
2:B:777:ILE:HD13	2:B:808:PHE:CD2	2.44	0.52
2:B:907:LEU:HD23	2:B:907:LEU:O	2.10	0.52
4:F:1409:LYS:O	4:F:1411:GLU:N	2.43	0.52
1:D:19:THR:HG23	1:D:64:VAL:O	2.10	0.52
4:C:1525:THR:HG22	4:C:1543:ILE:HG23	1.91	0.52
4:C:1581:LEU:O	4:C:1582:MET:HG3	2.09	0.52
2:E:907:LEU:HD23	2:E:907:LEU:O	2.10	0.52
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.44	0.52
1:A:404:THR:C	1:A:414:GLN:OE1	2.53	0.52
1:A:19:THR:HG23	1:A:64:VAL:O	2.10	0.52
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.92	0.52
1:A:581:PHE:CE1	1:A:588:LYS:HD2	2.45	0.52
3:M:49:GLN:O	3:M:50:LYS:C	2.52	0.52
1:D:117:TYR:CD1	1:D:123:VAL:HG22	2.44	0.52
1:D:193:GLN:HG2	1:D:194:GLN:N	2.25	0.52
2:E:783:LEU:HD12	2:E:784:ALA:N	2.24	0.52
1:A:367:VAL:HG23	1:A:387:LEU:HD11	1.92	0.52
1:D:404:THR:C	1:D:414:GLN:OE1	2.53	0.52
1:D:581:PHE:CE1	1:D:588:LYS:HD2	2.45	0.52
1:A:248:PHE:HD1	4:C:1378:MET:CE	2.23	0.52
1:A:468:TYR:HE1	1:A:513:TYR:CD2	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:HE1	1:A:513:TYR:HD2	1.57	0.51
1:D:403:ARG:HG2	1:D:404:THR:O	2.10	0.51
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.45	0.51
1:A:595:TRP:CE3	1:A:595:TRP:HA	2.45	0.51
2:B:819:ARG:NH1	4:C:1487:GLU:O	2.43	0.51
4:F:1378:MET:HE3	1:D:248:PHE:CD1	2.45	0.51
1:D:143:VAL:O	1:D:155:GLN:HA	2.10	0.51
4:F:1593:LYS:HG2	4:F:1596:LEU:CD1	2.37	0.51
1:D:505:PRO:HG3	1:D:595:TRP:CE3	2.45	0.51
1:D:634:GLN:HG2	1:D:635:ARG:N	2.26	0.51
2:B:819:ARG:HH21	2:B:911:PRO:CB	2.19	0.51
3:M:61:LYS:HD3	2:E:896:HIS:CB	2.40	0.51
4:F:1403:VAL:C	4:F:1405:ARG:H	2.18	0.51
4:F:1451:GLN:HG3	4:F:1452:PRO:HD2	1.92	0.51
1:D:357:PRO:O	1:D:358:ASP:C	2.53	0.51
4:C:1360:ASN:ND2	4:C:1443:GLN:CB	2.60	0.51
2:E:773:LEU:HD13	2:E:803:VAL:HG22	1.92	0.51
1:A:37:VAL:HB	1:A:46:VAL:HG23	1.93	0.51
1:A:248:PHE:CD1	4:C:1378:MET:HE3	2.44	0.51
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.51
1:A:590:THR:HG21	1:A:592:SER:HB2	1.92	0.51
1:A:624:PHE:O	1:A:631:GLN:HA	2.11	0.51
3:M:66:ALA:O	3:M:67:LYS:C	2.53	0.51
1:D:4:TYR:HB3	1:D:90:PHE:CE2	2.46	0.51
1:A:193:GLN:HG2	1:A:194:GLN:N	2.24	0.51
1:A:462:GLU:HG3	1:A:486:ARG:HH22	1.76	0.51
1:D:37:VAL:HB	1:D:46:VAL:HG23	1.93	0.51
4:C:1409:LYS:O	4:C:1411:GLU:N	2.43	0.51
4:F:1487:GLU:O	2:E:819:ARG:NH1	2.43	0.51
4:C:1386:MET:O	4:C:1387:THR:C	2.54	0.51
4:C:1405:ARG:CZ	4:C:1437:LEU:HD23	2.40	0.51
1:A:403:ARG:HG2	1:A:404:THR:O	2.10	0.51
1:D:438:VAL:HG13	1:D:449:LEU:HD11	1.92	0.51
1:D:472:ILE:HG13	1:D:480:LYS:HB3	1.92	0.51
1:D:595:TRP:CE3	1:D:595:TRP:HA	2.45	0.51
1:A:3:MET:HE2	1:A:626:SER:CB	2.41	0.51
1:A:4:TYR:HB3	1:A:90:PHE:CE2	2.46	0.51
1:A:495:LEU:HD12	1:A:496:PRO:CD	2.40	0.51
4:F:1386:MET:O	4:F:1387:THR:C	2.53	0.51
4:F:1405:ARG:CZ	4:F:1437:LEU:HD23	2.40	0.51
4:F:1451:GLN:CB	2:E:853:LEU:HD11	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:GLU:HA	1:D:279:VAL:HG22	1.92	0.51
4:C:1451:GLN:HG3	4:C:1452:PRO:HD2	1.92	0.51
1:A:472:ILE:HG13	1:A:480:LYS:HB3	1.92	0.51
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.11	0.51
1:D:369:VAL:CG1	1:D:370:GLN:H	2.24	0.51
1:D:472:ILE:HA	1:D:508:ARG:O	2.11	0.51
1:D:628:SER:HB2	1:D:630:GLN:OE1	2.11	0.51
2:E:744:GLU:C	2:E:746:PRO:HD3	2.37	0.51
1:A:73:GLU:HB3	1:A:82:LYS:HZ3	1.74	0.50
2:B:744:GLU:C	2:B:746:PRO:HD3	2.37	0.50
2:B:773:LEU:HD13	2:B:803:VAL:HG22	1.92	0.50
1:D:3:MET:HE2	1:D:626:SER:CB	2.41	0.50
1:D:468:TYR:CE1	1:D:513:TYR:HD2	2.28	0.50
1:A:136:PRO:CD	2:B:789:ASP:HA	2.41	0.50
1:A:472:ILE:HA	1:A:508:ARG:O	2.11	0.50
1:A:634:GLN:HG2	1:A:635:ARG:N	2.26	0.50
2:B:806:ASP:HB3	2:B:833:ARG:HH11	1.76	0.50
4:C:1532:LEU:CD2	4:C:1537:ASP:HB3	2.41	0.50
1:A:63:ASN:HD21	5:A:646:NAG:C1	2.24	0.50
3:P:18:GLU:O	3:P:21:SER:HB2	2.12	0.50
3:P:42:ARG:HA	2:E:740:VAL:HB	1.93	0.50
4:F:1450:ILE:O	4:F:1450:ILE:CG1	2.55	0.50
4:C:1519:VAL:HG22	4:C:1583:TRP:HD1	1.77	0.50
2:B:853:LEU:HD11	4:C:1451:GLN:CB	2.30	0.50
3:M:7:SER:O	3:M:8:ASN:C	2.54	0.50
4:F:1519:VAL:HG22	4:F:1583:TRP:HD1	1.77	0.50
1:D:590:THR:HG21	1:D:592:SER:HB2	1.92	0.50
1:D:624:PHE:O	1:D:631:GLN:HA	2.11	0.50
3:P:7:SER:O	3:P:8:ASN:C	2.54	0.50
3:P:29:ASN:O	3:P:30:GLU:C	2.55	0.50
4:F:1337:ASN:OD1	4:F:1337:ASN:C	2.55	0.50
2:E:806:ASP:HB3	2:E:833:ARG:HH11	1.76	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
1:A:459:ARG:HH22	1:D:458:ASP:HA	1.77	0.50
1:A:184:ILE:HG13	1:A:200:PHE:HE2	1.77	0.50
1:A:406:LYS:N	1:A:414:GLN:HE22	2.10	0.50
1:A:440:ARG:HH22	1:A:529:VAL:HG23	1.77	0.50
1:A:510:VAL:HG12	1:A:528:SER:CB	2.30	0.50
4:F:1378:MET:CE	1:D:248:PHE:HD1	2.23	0.50
4:F:1544:GLU:OE1	4:F:1579:HIS:CD2	2.64	0.50
1:D:179:MET:CG	1:D:203:LYS:HA	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1444:TYR:CE1	4:C:1445:PHE:HB2	2.46	0.50
2:E:734:ILE:H	2:E:734:ILE:CD1	2.16	0.50
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.50
3:M:18:GLU:O	3:M:21:SER:HB2	2.12	0.50
4:F:1532:LEU:CD2	4:F:1537:ASP:HB3	2.41	0.50
1:D:351:MET:SD	1:D:440:ARG:HD3	2.52	0.50
1:D:367:VAL:HG23	1:D:387:LEU:HD11	1.92	0.50
1:D:462:GLU:HG3	1:D:486:ARG:HH22	1.76	0.50
1:D:495:LEU:HD12	1:D:496:PRO:CD	2.40	0.50
1:A:230:GLU:HA	1:A:279:VAL:HG22	1.92	0.50
4:F:1602:LYS:HE3	4:F:1603:ASP:OD1	2.12	0.50
1:A:38:HIS:HE1	1:A:45:LEU:HD12	1.73	0.49
1:A:509:LEU:HB3	1:A:529:VAL:HG13	1.94	0.49
4:F:1444:TYR:CE1	4:F:1445:PHE:HB2	2.46	0.49
4:F:1578:LYS:HD3	4:F:1608:HIS:NE2	2.27	0.49
1:D:63:ASN:HD21	5:D:646:NAG:C1	2.24	0.49
4:C:1403:VAL:C	4:C:1405:ARG:H	2.18	0.49
2:E:836:GLN:O	2:E:836:GLN:HG3	2.12	0.49
3:M:61:LYS:HD3	2:E:896:HIS:HB3	1.93	0.49
4:F:1416:PHE:C	4:F:1416:PHE:HD2	2.20	0.49
4:F:1525:THR:OG1	4:F:1541:MET:HE3	2.12	0.49
1:D:184:ILE:HG13	1:D:200:PHE:HE2	1.77	0.49
4:C:1593:LYS:HG2	4:C:1596:LEU:CD1	2.37	0.49
1:A:459:ARG:NH2	1:D:458:ASP:HA	2.27	0.49
1:A:536:SER:O	1:A:537:CYS:O	2.30	0.49
2:B:883:THR:HA	2:B:909:VAL:CG1	2.42	0.49
1:D:509:LEU:HB3	1:D:529:VAL:HG13	1.94	0.49
4:C:1525:THR:OG1	4:C:1541:MET:HE3	2.12	0.49
4:C:1602:LYS:HE3	4:C:1603:ASP:OD1	2.12	0.49
3:M:30:GLU:OE2	3:M:45:LYS:HE3	2.12	0.49
4:F:1416:PHE:CE2	4:F:1444:TYR:HD2	2.25	0.49
1:D:164:LEU:O	2:E:787:MET:HG2	2.11	0.49
1:D:402:VAL:HG12	1:D:403:ARG:N	2.27	0.49
1:D:439:LEU:HD12	1:D:439:LEU:O	2.13	0.49
1:D:603:ILE:HD12	1:D:621:GLY:HA3	1.94	0.49
3:M:29:ASN:O	3:M:30:GLU:C	2.55	0.49
1:D:406:LYS:N	1:D:414:GLN:HE22	2.10	0.49
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.49
2:B:896:HIS:CB	3:P:61:LYS:HD3	2.41	0.49
4:C:1544:GLU:OE1	4:C:1579:HIS:CD2	2.64	0.49
3:M:64:SER:O	3:M:65:GLU:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1550:GLY:C	4:F:1552:ASP:N	2.71	0.49
4:F:1605:TRP:NE1	4:F:1607:GLU:CG	2.70	0.49
1:D:63:ASN:OD1	5:D:646:NAG:N2	2.46	0.49
4:C:1337:ASN:OD1	4:C:1337:ASN:C	2.55	0.49
4:C:1416:PHE:C	4:C:1416:PHE:HD2	2.20	0.49
4:C:1523:TYR:HB3	4:C:1525:THR:HG23	1.95	0.49
1:A:271:ILE:HD13	1:A:276:GLY:HA3	1.94	0.49
1:D:369:VAL:CG1	1:D:370:GLN:N	2.72	0.49
1:D:536:SER:O	1:D:537:CYS:O	2.30	0.49
1:D:613:TYR:CE2	1:D:614:ALA:HB2	2.48	0.49
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.95	0.49
1:A:179:MET:CG	1:A:203:LYS:HA	2.42	0.49
1:A:403:ARG:NH1	1:A:416:THR:HG21	2.27	0.49
1:A:459:ARG:NH2	1:D:459:ARG:H	2.11	0.49
3:P:64:SER:O	3:P:65:GLU:C	2.55	0.49
1:D:445:PRO:HA	1:D:499:ILE:HG22	1.95	0.49
4:C:1393:THR:HG22	4:C:1419:ARG:HH22	1.78	0.49
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.49
3:P:8:ASN:ND2	3:P:12:ASN:OD1	2.46	0.49
1:D:271:ILE:HD13	1:D:276:GLY:HA3	1.94	0.49
1:D:530:TRP:CD1	1:D:530:TRP:C	2.91	0.49
1:A:434:LEU:HD12	1:A:435:HIS:N	2.28	0.48
1:D:25:HIS:O	1:D:26:ASP:HB2	2.12	0.48
1:D:136:PRO:CD	2:E:789:ASP:HA	2.43	0.48
1:D:183:LYS:HD2	1:D:185:ARG:HD2	1.94	0.48
1:D:440:ARG:HH22	1:D:529:VAL:HG23	1.77	0.48
1:D:590:THR:HB	1:D:593:LYS:CG	2.39	0.48
4:C:1562:PHE:CD1	4:C:1598:TYR:HB2	2.48	0.48
3:P:26:LEU:HD12	3:P:26:LEU:O	2.13	0.48
3:P:66:ALA:O	3:P:67:LYS:C	2.53	0.48
4:F:1393:THR:HG22	4:F:1419:ARG:HH22	1.78	0.48
4:F:1504:LYS:NZ	4:F:1504:LYS:HB3	2.25	0.48
1:D:100:LEU:HD21	1:D:638:LEU:HD23	1.95	0.48
1:D:504:ILE:CG2	1:D:505:PRO:HA	2.43	0.48
2:E:730:ASP:CG	2:E:730:ASP:O	2.56	0.48
2:E:883:THR:HA	2:E:909:VAL:CG1	2.42	0.48
4:F:1523:TYR:HB3	4:F:1525:THR:HG23	1.95	0.48
1:D:109:PHE:CZ	1:D:594:ILE:HG23	2.49	0.48
1:D:437:SER:O	1:D:452:ASN:HB2	2.13	0.48
4:C:1578:LYS:HD3	4:C:1608:HIS:NE2	2.27	0.48
2:E:839:LYS:HG2	2:E:895:TYR:HD1	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:O	1:A:290:GLN:CD	2.57	0.48
1:A:458:ASP:HA	1:D:459:ARG:NH2	2.28	0.48
2:B:836:GLN:O	2:B:836:GLN:HG3	2.12	0.48
2:B:896:HIS:HB3	3:P:61:LYS:HD3	1.96	0.48
1:D:434:LEU:HD12	1:D:435:HIS:N	2.28	0.48
1:D:606:THR:HG22	1:D:608:GLY:H	1.78	0.48
4:C:1444:TYR:CD1	4:C:1444:TYR:C	2.92	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
2:B:730:ASP:CG	2:B:730:ASP:O	2.56	0.48
4:F:1528:VAL:HG21	4:F:1559:GLN:OE1	2.14	0.48
1:D:289:VAL:O	1:D:290:GLN:CD	2.57	0.48
1:D:403:ARG:HB2	1:D:416:THR:HG22	1.95	0.48
1:D:591:GLN:HB2	2:E:795:VAL:HB	1.94	0.48
4:C:1360:ASN:OD1	4:C:1361:THR:N	2.47	0.48
4:C:1586:SER:HA	4:C:1589:PHE:CD2	2.48	0.48
1:A:459:ARG:H	1:D:459:ARG:NH2	2.12	0.48
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.95	0.48
3:M:8:ASN:ND2	3:M:12:ASN:OD1	2.46	0.48
4:F:1409:LYS:O	4:F:1410:TYR:C	2.56	0.48
1:D:403:ARG:NH1	1:D:416:THR:HG21	2.27	0.48
4:C:1409:LYS:O	4:C:1410:TYR:C	2.56	0.48
1:A:351:MET:HE1	1:A:386:LYS:HB2	1.96	0.48
1:A:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
1:A:458:ASP:HA	1:D:459:ARG:HH22	1.78	0.48
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.95	0.48
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.48
4:C:1381:LEU:CD1	4:C:1426:LEU:HD11	2.43	0.48
1:A:183:LYS:HD2	1:A:185:ARG:HD2	1.94	0.48
1:A:462:GLU:HG3	1:A:486:ARG:NH2	2.29	0.48
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.48
2:B:839:LYS:HG2	2:B:895:TYR:HD1	1.79	0.48
2:B:877:VAL:HG13	4:C:1451:GLN:CD	2.39	0.48
1:D:138:GLY:HA2	1:D:160:SER:HG	1.75	0.48
1:D:403:ARG:CB	1:D:416:THR:HG22	2.44	0.48
2:E:809:ILE:HD12	2:E:903:VAL:HG23	1.96	0.48
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.43	0.48
1:A:541:LEU:CD2	2:B:786:SER:HB3	2.39	0.48
3:P:30:GLU:OE2	3:P:45:LYS:HE3	2.13	0.48
4:F:1360:ASN:OD1	4:F:1361:THR:N	2.46	0.48
1:D:183:LYS:HD3	1:D:185:ARG:CD	2.44	0.48
1:D:462:GLU:HG3	1:D:486:ARG:NH2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:MET:HB2	1:D:508:ARG:HB2	1.95	0.48
4:C:1506:THR:C	4:C:1508:GLU:N	2.70	0.48
1:A:6:ILE:HD12	1:A:6:ILE:HA	1.56	0.48
1:A:59:ASN:HB3	1:A:483:ARG:NH1	2.29	0.48
1:A:183:LYS:HD3	1:A:185:ARG:CD	2.44	0.48
1:A:510:VAL:CG1	1:A:528:SER:HB3	2.33	0.48
4:F:1380:ILE:HG21	4:F:1458:TYR:CZ	2.48	0.48
4:F:1381:LEU:CD1	4:F:1426:LEU:HD11	2.43	0.48
4:F:1444:TYR:CD1	4:F:1444:TYR:C	2.92	0.48
4:F:1562:PHE:CD1	4:F:1598:TYR:HB2	2.48	0.48
1:D:61:MET:HE2	1:D:483:ARG:CG	2.44	0.48
4:C:1380:ILE:HG21	4:C:1458:TYR:CZ	2.48	0.48
4:C:1528:VAL:HG21	4:C:1559:GLN:OE1	2.14	0.48
1:A:203:LYS:HG2	1:A:204:GLU:N	2.29	0.47
1:A:403:ARG:HB2	1:A:416:THR:HG22	1.96	0.47
1:A:613:TYR:CE2	1:A:614:ALA:HB2	2.48	0.47
4:F:1518:GLY:O	4:F:1585:LEU:HA	2.14	0.47
1:D:59:ASN:HB3	1:D:483:ARG:NH1	2.29	0.47
1:D:285:LEU:O	1:D:285:LEU:HG	2.14	0.47
1:A:369:VAL:CG1	1:A:370:GLN:N	2.72	0.47
1:A:439:LEU:HD12	1:A:439:LEU:O	2.13	0.47
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.47
1:A:603:ILE:HD12	1:A:621:GLY:HA3	1.94	0.47
3:M:6:THR:HA	4:F:1445:PHE:CE1	2.38	0.47
4:F:1341:LEU:HD23	4:F:1469:ARG:N	2.29	0.47
4:F:1506:THR:C	4:F:1508:GLU:N	2.70	0.47
1:A:61:MET:HE2	1:A:483:ARG:CG	2.44	0.47
1:A:477:ARG:HH22	1:A:479:LEU:HD13	1.78	0.47
1:D:510:VAL:HG21	1:D:622:LEU:HD12	1.95	0.47
1:D:549:GLU:O	1:D:550:ASP:HB2	2.14	0.47
4:C:1550:GLY:C	4:C:1552:ASP:N	2.71	0.47
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.50	0.47
1:A:437:SER:O	1:A:452:ASN:HB2	2.13	0.47
2:B:756:LEU:HA	2:B:758:GLU:OE1	2.14	0.47
3:M:64:SER:O	3:M:67:LYS:N	2.47	0.47
1:D:83:PHE:HD1	1:D:99:VAL:O	1.97	0.47
1:A:606:THR:HG22	1:A:608:GLY:H	1.78	0.47
1:D:20:MET:H	1:D:64:VAL:HB	1.79	0.47
1:D:477:ARG:HH22	1:D:479:LEU:HD13	1.78	0.47
1:D:541:LEU:HD23	2:E:796:ALA:HB2	1.97	0.47
1:A:148:PRO:HG3	1:A:182:TRP:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ALA:O	1:A:402:VAL:HG13	2.15	0.47
2:B:735:ALA:HB1	2:B:737:GLU:OE2	2.15	0.47
2:B:897:HIS:HB3	2:B:899:ILE:HG13	1.97	0.47
3:M:26:LEU:HD12	3:M:26:LEU:O	2.13	0.47
4:F:1586:SER:HA	4:F:1589:PHE:CD2	2.49	0.47
1:D:7:ILE:HA	1:D:623:THR:O	2.14	0.47
4:C:1341:LEU:HD23	4:C:1469:ARG:N	2.29	0.47
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.80	0.47
1:A:97:LYS:HG3	1:A:98:VAL:N	2.30	0.47
1:A:135:LEU:HD22	2:B:789:ASP:O	2.14	0.47
2:B:754:GLU:HG3	2:B:769:MET:SD	2.55	0.47
4:F:1451:GLN:CD	2:E:877:VAL:HG13	2.39	0.47
4:F:1475:LYS:CE	4:F:1493:GLU:OE2	2.61	0.47
1:D:97:LYS:HG3	1:D:98:VAL:N	2.30	0.47
1:D:97:LYS:NZ	1:D:632:THR:O	2.48	0.47
1:D:615:GLY:O	1:D:616:VAL:C	2.57	0.47
4:C:1519:VAL:HG22	4:C:1583:TRP:CD1	2.50	0.47
2:E:852:SER:C	2:E:854:ALA:N	2.73	0.47
1:A:83:PHE:HD1	1:A:99:VAL:O	1.97	0.47
1:A:97:LYS:NZ	1:A:632:THR:O	2.48	0.47
1:A:403:ARG:CB	1:A:416:THR:HG22	2.44	0.47
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.45	0.47
4:F:1392:ASP:HB2	4:F:1442:HIS:NE2	2.30	0.47
4:F:1522:VAL:O	4:F:1547:ILE:HB	2.15	0.47
1:D:148:PRO:HG3	1:D:182:TRP:CD1	2.50	0.47
1:D:309:ILE:HG12	1:D:316:MET:HG3	1.97	0.47
2:E:894:VAL:CG2	2:E:899:ILE:HB	2.45	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	0.47
1:A:105:SER:O	1:A:132:HIS:CD2	2.68	0.47
1:A:285:LEU:O	1:A:285:LEU:HG	2.14	0.47
1:A:475:LYS:HG2	1:A:598:VAL:CG1	2.45	0.47
1:A:475:LYS:HG2	1:A:598:VAL:HG11	1.96	0.47
3:P:64:SER:O	3:P:67:LYS:N	2.47	0.47
1:D:510:VAL:CG1	1:D:528:SER:HB3	2.33	0.47
1:A:20:MET:H	1:A:64:VAL:HB	1.79	0.47
1:A:251:PHE:CE1	1:A:304:VAL:CG1	2.98	0.47
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.45	0.47
1:D:294:ALA:O	1:D:295:GLU:C	2.58	0.47
4:C:1631:THR:O	4:C:1635:VAL:HG22	2.15	0.47
2:E:735:ALA:HB1	2:E:737:GLU:OE2	2.15	0.47
2:E:756:LEU:HA	2:E:758:GLU:OE1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.46
2:B:809:ILE:HD12	2:B:903:VAL:HG23	1.96	0.46
1:D:203:LYS:HG2	1:D:204:GLU:N	2.29	0.46
1:D:222:TYR:CE2	1:D:224:TYR:HB2	2.50	0.46
1:D:475:LYS:HG2	1:D:598:VAL:HG11	1.96	0.46
4:C:1389:PHE:HD1	4:C:1441:VAL:CG2	2.26	0.46
2:E:754:GLU:HG3	2:E:769:MET:SD	2.54	0.46
4:F:1406:TYR:CZ	4:F:1408:SER:HA	2.51	0.46
1:D:351:MET:HE1	1:D:386:LYS:HB2	1.96	0.46
1:D:461:HIS:O	1:D:464:LYS:HB2	2.16	0.46
1:A:309:ILE:HG12	1:A:316:MET:HG3	1.97	0.46
3:M:7:SER:HG	4:F:1445:PHE:HZ	1.64	0.46
4:F:1376:ALA:HB3	4:F:1429:VAL:HG22	1.97	0.46
4:F:1521:TYR:CD1	4:F:1521:TYR:O	2.68	0.46
1:A:289:VAL:O	1:A:290:GLN:OE1	2.34	0.46
2:B:733:ILE:CG1	2:B:734:ILE:N	2.75	0.46
1:D:289:VAL:O	1:D:290:GLN:OE1	2.34	0.46
4:C:1518:GLY:O	4:C:1585:LEU:HA	2.14	0.46
4:C:1521:TYR:O	4:C:1521:TYR:CD1	2.68	0.46
1:A:40:PHE:CE2	1:A:41:PRO:HG3	2.51	0.46
3:P:23:LEU:HD11	3:P:51:ALA:HB1	1.97	0.46
4:F:1389:PHE:HD1	4:F:1441:VAL:CG2	2.26	0.46
4:F:1395:ASP:O	4:F:1398:GLN:HB3	2.15	0.46
1:D:105:SER:O	1:D:132:HIS:CD2	2.68	0.46
4:C:1406:TYR:CZ	4:C:1408:SER:HA	2.51	0.46
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.46
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.46
2:B:852:SER:C	2:B:854:ALA:N	2.73	0.46
1:D:368:ALA:O	1:D:402:VAL:HG13	2.15	0.46
4:C:1403:VAL:O	4:C:1404:ASP:HB2	2.15	0.46
4:C:1564:SER:HB2	4:C:1600:ILE:HD13	1.97	0.46
1:A:461:HIS:O	1:A:464:LYS:HB2	2.16	0.46
1:D:251:PHE:CE1	1:D:304:VAL:CG1	2.98	0.46
4:C:1376:ALA:HB3	4:C:1429:VAL:HG22	1.97	0.46
4:C:1395:ASP:O	4:C:1398:GLN:HB3	2.15	0.46
1:A:185:ARG:HA	1:A:196:PHE:O	2.16	0.46
4:F:1631:THR:O	4:F:1635:VAL:HG22	2.15	0.46
1:D:47:LEU:C	1:D:47:LEU:HD23	2.41	0.46
1:D:214:VAL:HG11	1:D:304:VAL:CG2	2.45	0.46
1:D:375:VAL:CG2	1:D:387:LEU:HD22	2.46	0.46
2:E:855:THR:HG1	2:E:858:ARG:H	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG22	1:A:384:VAL:N	2.31	0.46
1:D:6:ILE:HA	1:D:6:ILE:HD12	1.56	0.46
1:D:185:ARG:HA	1:D:196:PHE:O	2.16	0.46
1:D:475:LYS:HG2	1:D:598:VAL:CG1	2.45	0.46
1:D:541:LEU:CD2	2:E:786:SER:HB3	2.40	0.46
4:C:1392:ASP:HB2	4:C:1442:HIS:NE2	2.30	0.46
4:C:1522:VAL:O	4:C:1547:ILE:HB	2.15	0.46
4:C:1530:VAL:HG23	4:C:1576:GLU:HG2	1.98	0.46
1:A:369:VAL:CG1	1:A:370:GLN:H	2.24	0.46
1:A:406:LYS:HG3	1:A:407:GLN:O	2.16	0.46
2:B:804:MET:CG	2:B:805:GLN:H	2.29	0.46
4:F:1451:GLN:NE2	2:E:877:VAL:HG13	2.31	0.46
4:F:1544:GLU:OE1	4:F:1579:HIS:HD2	1.98	0.46
1:D:40:PHE:CE2	1:D:41:PRO:HG3	2.51	0.46
1:D:59:ASN:HB3	1:D:483:ARG:HH12	1.80	0.46
1:D:224:TYR:N	1:D:224:TYR:CD2	2.84	0.46
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.81	0.46
2:E:897:HIS:HB3	2:E:899:ILE:HG13	1.97	0.46
1:A:164:LEU:O	2:B:787:MET:HG2	2.15	0.45
4:F:1403:VAL:O	4:F:1404:ASP:HB2	2.15	0.45
4:F:1519:VAL:HG22	4:F:1583:TRP:CD1	2.50	0.45
1:D:85:THR:HG23	1:D:98:VAL:HG22	1.98	0.45
1:A:111:GLN:O	1:A:125:TYR:HA	2.16	0.45
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.45	0.45
1:A:224:TYR:N	1:A:224:TYR:CD2	2.84	0.45
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.81	0.45
1:A:541:LEU:HD23	2:B:796:ALA:HB2	1.98	0.45
3:M:23:LEU:HD11	3:M:51:ALA:HB1	1.97	0.45
1:D:111:GLN:O	1:D:125:TYR:HA	2.16	0.45
1:D:215:GLU:HA	1:D:216:PRO:HD3	1.68	0.45
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.52	0.45
1:D:136:PRO:CG	2:E:789:ASP:HA	2.46	0.45
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.45
1:D:118:THR:HG23	1:D:205:TYR:CE2	2.52	0.45
1:D:339:PRO:O	1:D:340:LYS:HD3	2.16	0.45
4:C:1544:GLU:OE1	4:C:1579:HIS:HD2	1.98	0.45
1:A:30:ASP:OD1	1:A:30:ASP:N	2.50	0.45
1:A:36:THR:HA	1:A:47:LEU:O	2.17	0.45
1:A:339:PRO:O	1:A:340:LYS:HD3	2.16	0.45
2:B:877:VAL:HG13	4:C:1451:GLN:NE2	2.31	0.45
3:P:29:ASN:O	3:P:32:ALA:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:PHE:N	1:D:251:PHE:CD2	2.85	0.45
1:D:406:LYS:HG3	1:D:407:GLN:O	2.17	0.45
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.77	0.45
2:B:733:ILE:HB	2:B:895:TYR:CD2	2.51	0.45
1:D:301:SER:HB2	1:D:323:GLY:HA2	1.98	0.45
1:D:641:PRO:O	1:D:642:GLN:C	2.59	0.45
1:A:85:THR:HG23	1:A:98:VAL:HG22	1.98	0.45
1:A:101:VAL:CG1	1:A:102:SER:N	2.80	0.45
1:A:138:GLY:HA2	1:A:160:SER:HG	1.77	0.45
1:A:210:PHE:HB3	1:A:237:PHE:HA	1.99	0.45
1:A:351:MET:HE2	1:A:351:MET:HA	1.99	0.45
1:A:375:VAL:CG2	1:A:387:LEU:HD22	2.46	0.45
4:F:1389:PHE:N	4:F:1389:PHE:HD2	2.14	0.45
4:F:1564:SER:HB2	4:F:1600:ILE:HD13	1.97	0.45
4:F:1575:GLU:CB	4:F:1578:LYS:HD2	2.47	0.45
1:D:30:ASP:OD1	1:D:30:ASP:N	2.50	0.45
1:D:295:GLU:H	1:D:295:GLU:CD	2.25	0.45
4:C:1389:PHE:N	4:C:1389:PHE:HD2	2.14	0.45
1:A:271:ILE:O	1:A:271:ILE:HG22	2.16	0.45
1:A:516:ILE:C	1:A:516:ILE:HD12	2.42	0.45
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.77	0.45
2:B:817:VAL:HG22	2:B:907:LEU:HD12	1.99	0.45
3:M:7:SER:HB2	2:E:863:THR:HB	1.99	0.45
3:P:36:LEU:N	3:P:36:LEU:CD2	2.78	0.45
4:F:1513:LYS:O	4:F:1516:GLU:HG3	2.16	0.45
1:D:379:THR:HG22	1:D:384:VAL:N	2.31	0.45
4:C:1406:TYR:OH	4:C:1408:SER:HA	2.16	0.45
2:E:811:LEU:HG	2:E:813:LEU:HD13	1.98	0.45
1:A:251:PHE:CD2	1:A:251:PHE:N	2.85	0.45
1:A:290:GLN:OE1	1:A:290:GLN:HA	2.17	0.45
1:A:468:TYR:CE1	1:A:513:TYR:CD2	3.05	0.45
4:C:1341:LEU:HD23	4:C:1469:ARG:H	1.82	0.45
4:C:1513:LYS:O	4:C:1516:GLU:HG3	2.17	0.45
4:C:1575:GLU:HB2	4:C:1578:LYS:HD2	1.99	0.45
1:D:36:THR:HA	1:D:47:LEU:O	2.17	0.45
1:A:301:SER:HB2	1:A:323:GLY:HA2	1.98	0.44
3:P:26:LEU:O	3:P:29:ASN:N	2.50	0.44
4:F:1349:PRO:O	4:F:1350:GLU:CB	2.34	0.44
1:D:20:MET:HG2	1:D:64:VAL:CB	2.47	0.44
1:D:290:GLN:OE1	1:D:290:GLN:HA	2.17	0.44
1:D:380:GLN:C	1:D:382:ASP:H	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1575:GLU:CB	4:C:1578:LYS:HD2	2.47	0.44
1:A:380:GLN:O	1:A:382:ASP:N	2.51	0.44
2:B:835:ASN:O	2:B:836:GLN:HB3	2.17	0.44
2:B:844:LEU:HD12	2:B:845:LEU:N	2.33	0.44
3:P:29:ASN:C	3:P:31:LEU:N	2.76	0.44
3:P:58:LYS:HA	3:P:58:LYS:HD2	1.75	0.44
4:F:1504:LYS:HZ3	4:F:1504:LYS:HB3	1.80	0.44
4:C:1504:LYS:O	4:C:1504:LYS:HG3	2.17	0.44
4:C:1505:VAL:CG1	4:C:1510:ARG:CZ	2.95	0.44
2:E:804:MET:CG	2:E:805:GLN:H	2.29	0.44
1:A:20:MET:HG2	1:A:64:VAL:CB	2.47	0.44
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.18	0.44
1:A:294:ALA:O	1:A:295:GLU:C	2.58	0.44
1:A:641:PRO:O	1:A:642:GLN:C	2.59	0.44
3:M:29:ASN:O	3:M:32:ALA:N	2.49	0.44
4:F:1341:LEU:HD23	4:F:1469:ARG:H	1.82	0.44
4:F:1406:TYR:OH	4:F:1408:SER:HA	2.17	0.44
4:F:1416:PHE:CD2	4:F:1417:SER:N	2.85	0.44
1:D:101:VAL:CG1	1:D:102:SER:N	2.80	0.44
4:C:1410:TYR:C	4:C:1410:TYR:CD2	2.95	0.44
2:E:817:VAL:HG22	2:E:907:LEU:HD12	1.99	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
1:A:453:PHE:CE2	1:A:495:LEU:HB2	2.53	0.44
3:P:73:ILE:O	3:P:77:ILE:HG13	2.18	0.44
4:F:1410:TYR:C	4:F:1410:TYR:CD2	2.95	0.44
1:D:38:HIS:HE1	1:D:45:LEU:CD1	2.30	0.44
1:A:590:THR:HB	1:A:593:LYS:CG	2.39	0.44
2:B:863:THR:HB	3:P:7:SER:HB2	1.99	0.44
3:M:15:LEU:HD12	3:M:15:LEU:HA	1.82	0.44
3:P:7:SER:HG	4:C:1445:PHE:HZ	1.65	0.44
1:D:210:PHE:HB3	1:D:237:PHE:HA	1.99	0.44
1:D:239:TYR:HB2	2:E:804:MET:HE2	1.99	0.44
1:D:380:GLN:O	1:D:382:ASP:N	2.51	0.44
1:D:465:ILE:HD11	1:D:515:LEU:HD13	2.00	0.44
1:A:136:PRO:CG	2:B:789:ASP:HA	2.47	0.44
1:A:604:GLY:HA2	1:A:619:ASP:O	2.18	0.44
3:M:23:LEU:HD23	3:M:23:LEU:HA	1.81	0.44
4:F:1375:ASP:CG	4:F:1430:SER:HA	2.43	0.44
4:F:1472:HIS:CE1	4:F:1474:GLU:H	2.35	0.44
4:F:1530:VAL:HG23	4:F:1576:GLU:HG2	1.98	0.44
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:O	1:D:271:ILE:HG22	2.16	0.44
1:D:604:GLY:HA2	1:D:619:ASP:O	2.18	0.44
1:A:239:TYR:HB2	2:B:804:MET:HE2	2.00	0.44
1:A:458:ASP:OD2	1:A:460:ALA:HB3	2.18	0.44
1:A:86:VAL:O	1:A:96:GLU:HB2	2.18	0.44
2:B:840:VAL:HG13	2:B:893:ALA:O	2.18	0.44
3:M:26:LEU:O	3:M:29:ASN:N	2.50	0.44
4:F:1341:LEU:CD2	4:F:1469:ARG:HB2	2.48	0.44
4:F:1421:THR:CG2	2:E:873:SER:HB3	2.48	0.44
4:F:1521:TYR:HB2	4:F:1523:TYR:CZ	2.53	0.44
1:D:351:MET:HA	1:D:351:MET:HE2	1.99	0.44
1:D:458:ASP:OD2	1:D:460:ALA:HB3	2.18	0.44
1:D:516:ILE:HD12	1:D:516:ILE:C	2.42	0.44
4:C:1451:GLN:HA	4:C:1452:PRO:HD3	1.81	0.44
4:C:1521:TYR:HB2	4:C:1523:TYR:CZ	2.53	0.44
2:E:733:ILE:HB	2:E:895:TYR:CD2	2.51	0.44
1:A:295:GLU:CD	1:A:295:GLU:H	2.25	0.44
4:C:1527:LEU:HB2	4:C:1541:MET:SD	2.58	0.44
2:E:840:VAL:HG13	2:E:893:ALA:O	2.18	0.44
1:A:38:HIS:HE1	1:A:45:LEU:CD1	2.31	0.43
3:M:14:LYS:O	3:M:15:LEU:C	2.61	0.43
3:M:73:ILE:O	3:M:77:ILE:HG13	2.18	0.43
4:F:1575:GLU:HB2	4:F:1578:LYS:HD2	1.99	0.43
1:D:97:LYS:HD3	1:D:625:THR:OG1	2.17	0.43
1:D:290:GLN:O	1:D:291:ASN:HB2	2.18	0.43
1:D:583:LEU:HA	1:D:583:LEU:HD23	1.76	0.43
1:D:584:ASN:C	1:D:584:ASN:OD1	2.61	0.43
4:C:1416:PHE:CD2	4:C:1417:SER:N	2.85	0.43
4:C:1460:TYR:CG	4:C:1461:TYR:N	2.86	0.43
4:C:1576:GLU:C	4:C:1578:LYS:H	2.25	0.43
1:A:124:LEU:HD12	2:B:751:TRP:CG	2.53	0.43
1:A:298:VAL:HG12	1:A:298:VAL:O	2.18	0.43
1:A:454:LEU:HA	1:A:491:ASP:O	2.19	0.43
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.43
1:D:86:VAL:O	1:D:96:GLU:HB2	2.18	0.43
1:D:410:SER:OG	1:D:413:GLU:HG3	2.18	0.43
4:C:1472:HIS:CE1	4:C:1474:GLU:H	2.35	0.43
4:C:1475:LYS:CE	4:C:1493:GLU:OE2	2.61	0.43
4:C:1590:TRP:HB3	4:C:1597:SER:HB2	2.00	0.43
1:A:578:LYS:HB3	1:A:578:LYS:HE2	1.86	0.43
4:F:1576:GLU:C	4:F:1578:LYS:H	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:MET:HG2	1:D:64:VAL:CG2	2.47	0.43
1:D:124:LEU:HD12	2:E:751:TRP:CG	2.52	0.43
1:D:271:ILE:HD13	1:D:271:ILE:HA	1.74	0.43
1:D:442:GLU:OE1	1:D:534:LYS:HD3	2.19	0.43
4:C:1538:GLU:O	4:C:1539:TYR:CD1	2.71	0.43
2:E:835:ASN:O	2:E:836:GLN:HB3	2.17	0.43
1:A:271:ILE:HD13	1:A:271:ILE:HA	1.74	0.43
1:A:290:GLN:O	1:A:291:ASN:HB2	2.17	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
3:M:68:TYR:O	3:M:69:GLN:C	2.61	0.43
3:P:15:LEU:HD22	3:P:60:PHE:CE1	2.53	0.43
1:D:255:ASP:O	1:D:258:GLN:HB3	2.18	0.43
4:F:1506:THR:O	4:F:1507:LEU:C	2.62	0.43
4:F:1590:TRP:HB3	4:F:1597:SER:HB2	2.00	0.43
1:D:40:PHE:HA	1:D:41:PRO:HA	1.69	0.43
1:D:324:ILE:HA	1:D:325:PRO:HD3	1.85	0.43
2:E:833:ARG:HH22	2:E:899:ILE:CD1	2.24	0.43
2:E:844:LEU:HD12	2:E:845:LEU:N	2.32	0.43
1:A:268:ARG:HB2	4:C:1378:MET:HE3	2.00	0.43
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.31	0.43
2:B:778:THR:OG1	2:B:779:THR:N	2.52	0.43
3:M:29:ASN:C	3:M:31:LEU:N	2.76	0.43
3:M:33:THR:O	3:M:34:GLY:C	2.61	0.43
3:P:14:LYS:O	3:P:15:LEU:C	2.61	0.43
4:C:1375:ASP:CG	4:C:1430:SER:HA	2.43	0.43
2:E:749:TRP:CE3	2:E:750:LEU:HB2	2.54	0.43
1:A:410:SER:OG	1:A:413:GLU:HG3	2.18	0.43
1:A:465:ILE:HD11	1:A:515:LEU:HD13	2.00	0.43
3:P:15:LEU:O	3:P:18:GLU:HB2	2.19	0.43
3:P:51:ALA:O	3:P:54:ALA:N	2.52	0.43
2:B:898:PHE:CE2	3:M:50:LYS:HA	2.54	0.43
4:F:1378:MET:HA	4:F:1426:LEU:O	2.19	0.43
1:D:454:LEU:HA	1:D:491:ASP:O	2.18	0.43
1:D:541:LEU:HD12	1:D:541:LEU:HA	1.77	0.43
4:C:1337:ASN:O	4:C:1371:ARG:CD	2.60	0.43
1:A:20:MET:HG2	1:A:64:VAL:CG2	2.47	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.43
2:B:865:THR:OG1	3:P:11:GLN:HG2	2.18	0.43
4:F:1337:ASN:O	4:F:1371:ARG:CD	2.60	0.43
4:F:1527:LEU:HB2	4:F:1541:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:PHE:CE2	1:D:495:LEU:HB2	2.53	0.43
4:C:1505:VAL:HG12	4:C:1510:ARG:NE	2.34	0.43
2:E:729:LEU:CD1	2:E:737:GLU:OE2	2.67	0.43
1:A:177:VAL:HG22	1:A:178:ASN:N	2.34	0.43
2:B:729:LEU:CD1	2:B:737:GLU:OE2	2.67	0.43
2:B:885:LEU:HD12	2:B:885:LEU:HA	1.74	0.43
3:P:15:LEU:HA	3:P:15:LEU:HD12	1.82	0.43
3:P:68:TYR:O	3:P:69:GLN:C	2.61	0.43
4:F:1460:TYR:CG	4:F:1461:TYR:N	2.86	0.43
4:F:1538:GLU:O	4:F:1539:TYR:CD1	2.71	0.43
4:F:1632:GLU:HA	4:F:1635:VAL:HG22	2.00	0.43
1:D:458:ASP:O	1:D:460:ALA:N	2.52	0.43
1:A:442:GLU:OE1	1:A:534:LYS:HD3	2.19	0.42
1:A:458:ASP:O	1:A:460:ALA:N	2.52	0.42
3:P:82:LYS:C	3:P:84:LYS:H	2.27	0.42
4:F:1574:LEU:HA	4:F:1574:LEU:HD22	1.78	0.42
1:D:477:ARG:HH11	1:D:477:ARG:CG	2.31	0.42
4:C:1472:HIS:ND1	4:C:1473:PRO:HD2	2.34	0.42
1:A:87:GLN:HG3	1:A:96:GLU:HB3	2.01	0.42
1:A:455:LEU:HB2	1:A:468:TYR:OH	2.19	0.42
4:F:1585:LEU:HD21	4:F:1603:ASP:HB3	2.00	0.42
1:D:20:MET:HG2	1:D:64:VAL:HG11	2.01	0.42
5:D:646:NAG:H62	5:D:646:NAG:O3	2.19	0.42
4:C:1506:THR:O	4:C:1509:GLU:N	2.52	0.42
1:A:255:ASP:O	1:A:258:GLN:HB3	2.18	0.42
2:B:873:SER:HB3	4:C:1421:THR:CG2	2.48	0.42
3:M:7:SER:CB	2:E:863:THR:HB	2.50	0.42
4:F:1506:THR:O	4:F:1509:GLU:N	2.52	0.42
1:D:195:VAL:CG1	1:D:196:PHE:N	2.82	0.42
1:D:220:PHE:HB3	1:D:357:PRO:HG2	2.01	0.42
1:D:298:VAL:O	1:D:298:VAL:HG12	2.18	0.42
4:C:1415:ALA:O	4:C:1416:PHE:C	2.62	0.42
2:E:729:LEU:HD13	2:E:737:GLU:OE2	2.20	0.42
1:A:219:LYS:HD2	1:A:358:ASP:OD2	2.19	0.42
2:B:729:LEU:HD13	2:B:737:GLU:OE2	2.20	0.42
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.54	0.42
3:M:58:LYS:HD2	3:M:58:LYS:HA	1.75	0.42
4:F:1414:LYS:HD3	4:F:1419:ARG:HG3	2.02	0.42
1:D:603:ILE:HB	1:D:635:ARG:HH12	1.84	0.42
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.01	0.42
1:A:251:PHE:CD1	1:A:280:LEU:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:15:LEU:O	3:M:18:GLU:HB2	2.19	0.42
3:P:29:ASN:O	3:P:31:LEU:N	2.52	0.42
4:F:1505:VAL:HG11	4:F:1510:ARG:NE	2.35	0.42
1:D:3:MET:HE2	1:D:626:SER:HB2	2.01	0.42
1:D:177:VAL:HG22	1:D:178:ASN:N	2.34	0.42
1:D:203:LYS:HG2	1:D:204:GLU:H	1.85	0.42
1:D:219:LYS:HD2	1:D:358:ASP:OD2	2.19	0.42
4:C:1573:LYS:HA	4:C:1573:LYS:HD3	1.28	0.42
2:E:778:THR:OG1	2:E:779:THR:N	2.52	0.42
1:A:446:GLY:O	1:D:378:LEU:HD13	2.20	0.42
3:M:29:ASN:O	3:M:31:LEU:N	2.53	0.42
4:F:1370:TYR:O	4:F:1431:HIS:HA	2.19	0.42
4:F:1516:GLU:CB	4:F:1517:PRO:HD2	2.42	0.42
1:D:168:PRO:O	1:D:169:LEU:HG	2.20	0.42
1:D:241:LYS:HA	1:D:241:LYS:HD3	1.83	0.42
1:D:251:PHE:CD1	1:D:280:LEU:HB2	2.55	0.42
1:D:468:TYR:CE1	1:D:513:TYR:CD2	3.05	0.42
4:C:1574:LEU:HD22	4:C:1574:LEU:HA	1.78	0.42
4:C:1585:LEU:HD21	4:C:1603:ASP:HB3	2.00	0.42
2:E:733:ILE:CG1	2:E:734:ILE:H	2.28	0.42
2:B:778:THR:HG23	2:B:779:THR:N	2.34	0.42
4:F:1378:MET:HE3	1:D:268:ARG:HB2	2.02	0.42
4:F:1437:LEU:HD12	4:F:1437:LEU:C	2.45	0.42
4:F:1573:LYS:HA	4:F:1573:LYS:HD3	1.28	0.42
4:C:1370:TYR:O	4:C:1431:HIS:HA	2.19	0.42
4:C:1416:PHE:CE2	4:C:1444:TYR:HD2	2.25	0.42
4:C:1632:GLU:HA	4:C:1635:VAL:HG22	2.00	0.42
1:A:4:TYR:HB3	1:A:90:PHE:CZ	2.55	0.42
1:A:360:SER:HA	1:A:361:PRO:HD2	1.81	0.42
1:A:584:ASN:OD1	1:A:584:ASN:C	2.61	0.42
3:M:13:GLU:O	3:M:13:GLU:HG2	2.20	0.42
3:P:26:LEU:O	3:P:29:ASN:HB2	2.19	0.42
3:P:33:THR:O	3:P:34:GLY:C	2.61	0.42
4:F:1505:VAL:CG1	4:F:1510:ARG:CZ	2.95	0.42
1:D:61:MET:CE	1:D:483:ARG:HG2	2.50	0.42
1:D:455:LEU:HB2	1:D:468:TYR:OH	2.19	0.42
1:D:556:GLY:HA2	2:E:773:LEU:O	2.18	0.42
2:E:734:ILE:HD11	2:E:898:PHE:HA	2.02	0.42
1:A:101:VAL:HG12	1:A:102:SER:N	2.35	0.42
1:A:203:LYS:HG2	1:A:204:GLU:H	1.85	0.42
3:P:13:GLU:O	3:P:13:GLU:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1505:VAL:HG12	4:F:1510:ARG:NE	2.34	0.42
1:D:350:LEU:O	1:D:351:MET:HE2	2.19	0.42
4:C:1378:MET:HA	4:C:1426:LEU:O	2.19	0.42
1:A:20:MET:HG2	1:A:64:VAL:HG11	2.01	0.42
3:P:58:LYS:C	3:P:63:MET:HE2	2.45	0.42
4:F:1415:ALA:O	4:F:1416:PHE:C	2.62	0.42
4:F:1562:PHE:CG	4:F:1598:TYR:HB2	2.55	0.42
1:D:87:GLN:HG3	1:D:96:GLU:HB3	2.01	0.42
1:D:135:LEU:HD22	2:E:789:ASP:O	2.19	0.42
4:C:1562:PHE:CG	4:C:1598:TYR:HB2	2.55	0.42
1:A:195:VAL:CG1	1:A:196:PHE:N	2.82	0.41
1:A:402:VAL:HG12	1:A:403:ARG:H	1.84	0.41
3:M:43:THR:HG21	3:M:73:ILE:HD13	2.01	0.41
1:D:613:TYR:CD2	1:D:614:ALA:N	2.88	0.41
4:C:1437:LEU:HD12	4:C:1437:LEU:C	2.45	0.41
2:E:733:ILE:CG1	2:E:734:ILE:N	2.75	0.41
1:A:61:MET:HE1	1:A:482:GLY:HA2	2.01	0.41
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.85	0.41
2:B:734:ILE:HD11	2:B:898:PHE:HA	2.02	0.41
2:B:897:HIS:CB	2:B:899:ILE:HG13	2.50	0.41
1:D:33:VAL:HG22	1:D:90:PHE:HA	2.02	0.41
4:C:1586:SER:HA	4:C:1589:PHE:CE2	2.55	0.41
1:A:168:PRO:O	1:A:169:LEU:HG	2.20	0.41
1:A:343:LYS:N	1:A:343:LYS:CD	2.83	0.41
1:A:533:VAL:CG1	1:A:534:LYS:N	2.81	0.41
1:A:561:LEU:HB3	2:B:769:MET:HB2	2.02	0.41
1:A:613:TYR:CD2	1:A:614:ALA:N	2.88	0.41
2:B:818:VAL:HA	2:B:910:VAL:O	2.20	0.41
2:B:833:ARG:HD2	2:B:834:GLN:NE2	2.35	0.41
3:M:26:LEU:O	3:M:29:ASN:HB2	2.19	0.41
3:M:82:LYS:C	3:M:84:LYS:H	2.27	0.41
4:F:1472:HIS:CE1	4:F:1473:PRO:HD2	2.55	0.41
4:F:1586:SER:HA	4:F:1589:PHE:CE2	2.55	0.41
1:D:265:SER:O	1:D:267:LYS:HG2	2.21	0.41
1:D:346:MET:O	1:D:391:THR:CG2	2.57	0.41
4:C:1341:LEU:CD2	4:C:1469:ARG:HB2	2.48	0.41
4:C:1472:HIS:CE1	4:C:1473:PRO:HD2	2.55	0.41
1:A:492:LEU:HA	1:A:492:LEU:HD12	1.87	0.41
2:B:786:SER:O	2:B:793:ILE:HA	2.21	0.41
1:D:61:MET:HE1	1:D:482:GLY:HA2	2.01	0.41
1:D:106:GLY:HA2	1:D:132:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:O	1:A:475:LYS:C	2.64	0.41
1:A:502:ASP:N	1:A:502:ASP:OD1	2.54	0.41
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.90	0.41
3:P:43:THR:HG21	3:P:73:ILE:HD13	2.01	0.41
4:F:1472:HIS:ND1	4:F:1473:PRO:HD2	2.34	0.41
1:D:14:LEU:HD11	1:D:103:LEU:CD2	2.51	0.41
1:D:83:PHE:CD1	1:D:100:LEU:HA	2.56	0.41
1:D:402:VAL:HG12	1:D:403:ARG:H	1.84	0.41
1:D:455:LEU:CD1	1:D:457:MET:HG2	2.49	0.41
1:A:3:MET:HE2	1:A:626:SER:HB2	2.01	0.41
1:A:14:LEU:HD11	1:A:103:LEU:CD2	2.51	0.41
1:A:227:LYS:HB2	1:A:227:LYS:HE2	1.64	0.41
1:A:265:SER:O	1:A:267:LYS:HG2	2.21	0.41
1:A:350:LEU:O	1:A:351:MET:HE2	2.19	0.41
1:A:378:LEU:HD13	1:D:446:GLY:O	2.20	0.41
5:A:646:NAG:H62	5:A:646:NAG:O3	2.19	0.41
2:B:833:ARG:HH22	2:B:899:ILE:CD1	2.24	0.41
1:D:4:TYR:HB3	1:D:90:PHE:CZ	2.55	0.41
1:D:502:ASP:OD1	1:D:502:ASP:N	2.54	0.41
4:C:1554:VAL:O	4:C:1554:VAL:HG13	2.21	0.41
2:E:833:ARG:HD2	2:E:834:GLN:NE2	2.35	0.41
1:A:400:ILE:HD12	1:A:400:ILE:N	2.36	0.41
1:A:509:LEU:HB3	1:A:529:VAL:CG1	2.50	0.41
1:D:101:VAL:HG12	1:D:102:SER:N	2.35	0.41
1:D:389:ILE:O	1:D:389:ILE:HG13	2.20	0.41
1:D:453:PHE:HE2	1:D:495:LEU:HB2	1.86	0.41
1:D:453:PHE:CB	1:D:493:VAL:HG23	2.41	0.41
4:C:1414:LYS:HD3	4:C:1419:ARG:HG3	2.02	0.41
4:C:1516:GLU:HB3	4:C:1517:PRO:CD	2.43	0.41
4:C:1542:ALA:HA	4:C:1559:GLN:HA	2.03	0.41
1:A:61:MET:CE	1:A:483:ARG:HG2	2.50	0.41
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.89	0.41
2:B:733:ILE:CG1	2:B:734:ILE:H	2.28	0.41
3:M:58:LYS:C	3:M:63:MET:HE2	2.45	0.41
3:P:82:LYS:HB2	3:P:82:LYS:HE3	1.97	0.41
4:F:1527:LEU:HD23	4:F:1575:GLU:O	2.21	0.41
1:D:114:LYS:HE2	1:D:117:TYR:CD1	2.56	0.41
1:D:343:LYS:N	1:D:343:LYS:CD	2.83	0.41
1:D:400:ILE:N	1:D:400:ILE:HD12	2.36	0.41
4:C:1506:THR:O	4:C:1507:LEU:C	2.62	0.41
2:E:804:MET:HG2	2:E:805:GLN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG22	1:A:90:PHE:HA	2.02	0.41
1:A:106:GLY:HA2	1:A:132:HIS:CD2	2.55	0.41
1:A:206:VAL:HG11	2:B:813:LEU:O	2.20	0.41
1:A:342:PHE:HD1	1:A:391:THR:HG21	1.86	0.41
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.03	0.41
1:A:404:THR:HG1	1:A:415:ALA:H	1.65	0.41
1:A:504:ILE:HG23	1:A:505:PRO:HA	2.02	0.41
1:A:508:ARG:CZ	1:A:604:GLY:HA3	2.51	0.41
1:D:272:GLU:O	1:D:273:ASP:C	2.64	0.41
1:D:283:LYS:HZ2	1:D:283:LYS:HG2	1.77	0.41
1:D:345:GLY:HA2	1:D:393:PRO:HD3	2.03	0.41
1:D:508:ARG:CZ	1:D:604:GLY:HA3	2.51	0.41
1:D:561:LEU:HB3	2:E:769:MET:HB2	2.03	0.41
4:C:1450:ILE:O	4:C:1450:ILE:CG1	2.55	0.41
4:C:1527:LEU:HD23	4:C:1575:GLU:O	2.21	0.41
2:E:734:ILE:N	2:E:734:ILE:CD1	2.81	0.41
2:E:869:LYS:O	2:E:870:SER:HB3	2.21	0.41
2:E:897:HIS:CB	2:E:899:ILE:HG13	2.50	0.41
1:A:272:GLU:O	1:A:273:ASP:C	2.64	0.41
2:B:869:LYS:O	2:B:870:SER:HB3	2.21	0.41
1:D:252:GLY:HA3	1:D:303:TYR:CZ	2.56	0.41
2:E:786:SER:O	2:E:793:ILE:HA	2.21	0.41
2:E:807:PHE:CD2	2:E:807:PHE:C	2.98	0.41
2:E:838:LEU:HD23	2:E:838:LEU:HA	1.84	0.41
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.40
1:A:556:GLY:HA2	2:B:773:LEU:O	2.21	0.40
1:A:615:GLY:C	1:A:617:PHE:N	2.79	0.40
3:M:84:LYS:O	3:M:85:TYR:CB	2.69	0.40
1:D:533:VAL:CG1	1:D:534:LYS:N	2.81	0.40
2:E:818:VAL:HA	2:E:910:VAL:O	2.20	0.40
2:E:837:GLU:HG2	2:E:837:GLU:H	1.72	0.40
1:A:345:GLY:HA2	1:A:393:PRO:HD3	2.03	0.40
1:A:346:MET:O	1:A:391:THR:CG2	2.57	0.40
1:D:627:SER:C	1:D:629:GLY:H	2.30	0.40
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.57	0.40
3:P:23:LEU:HD23	3:P:23:LEU:HA	1.81	0.40
4:F:1380:ILE:HD11	1:D:248:PHE:CZ	2.56	0.40
1:D:63:ASN:ND2	5:D:646:NAG:C1	2.84	0.40
1:D:436:LEU:HA	1:D:452:ASN:O	2.21	0.40
1:D:504:ILE:HG23	1:D:505:PRO:HA	2.02	0.40
1:D:595:TRP:HA	1:D:595:TRP:HE3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:778:THR:HG23	2:E:779:THR:N	2.34	0.40
1:A:63:ASN:ND2	5:A:646:NAG:C1	2.84	0.40
1:A:83:PHE:CD1	1:A:100:LEU:HA	2.56	0.40
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.56	0.40
1:A:338:THR:HG23	1:A:339:PRO:HD2	2.03	0.40
1:A:533:VAL:HG12	1:A:534:LYS:H	1.85	0.40
3:M:4:LEU:HB2	4:F:1446:ASN:CB	2.39	0.40
1:D:599:GLU:C	1:D:601:ALA:N	2.79	0.40
1:D:609:SER:C	1:D:616:VAL:HG22	2.47	0.40
2:E:806:ASP:CB	2:E:833:ARG:HH11	2.35	0.40
1:A:114:LYS:HE2	1:A:117:TYR:CD1	2.56	0.40
1:A:125:TYR:CZ	1:A:169:LEU:HB3	2.57	0.40
1:A:436:LEU:HA	1:A:452:ASN:O	2.21	0.40
1:A:590:THR:HG22	1:A:591:GLN:N	2.35	0.40
2:B:838:LEU:HA	2:B:838:LEU:HD23	1.84	0.40
4:F:1472:HIS:CG	4:F:1473:PRO:HD2	2.57	0.40
1:D:108:LEU:HB2	1:D:196:PHE:CG	2.57	0.40
1:D:632:THR:O	1:D:633:ALA:C	2.63	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	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	8 29
1	D	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	8 29
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	12 37
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	12 37
3	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2 16
3	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	C	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	13 39
4	F	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	13 39
All	All	2374/2564 (93%)	2042 (86%)	296 (12%)	36 (2%)	8 30

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	D	292	PRO
1	A	289	VAL
1	A	293	ARG
1	A	537	CYS
3	M	51	ALA
3	P	51	ALA
1	D	289	VAL
1	D	293	ARG
1	D	537	CYS
2	B	853	LEU
2	B	883	THR
3	M	30	GLU
3	M	61	LYS
3	P	30	GLU
3	P	61	LYS
4	F	1410	TYR
4	C	1410	TYR
2	E	853	LEU
2	E	883	THR
4	F	1378	MET
4	C	1378	MET
1	A	72	ARG
1	A	370	GLN
1	A	459	ARG
1	D	72	ARG
1	D	370	GLN
1	D	459	ARG
1	A	381	GLY
4	F	1516	GLU
1	D	381	GLY
4	C	1516	GLU
1	A	616	VAL
1	D	616	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	GLY
1	D	359	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	563/567 (99%)	503 (89%)	60 (11%)	5 20
1	D	563/567 (99%)	502 (89%)	61 (11%)	5 20
2	B	172/191 (90%)	135 (78%)	37 (22%)	1 2
2	E	172/191 (90%)	135 (78%)	37 (22%)	1 2
3	M	76/79 (96%)	65 (86%)	11 (14%)	2 10
3	P	76/79 (96%)	65 (86%)	11 (14%)	2 10
4	C	266/309 (86%)	217 (82%)	49 (18%)	1 5
4	F	266/309 (86%)	217 (82%)	49 (18%)	1 5
All	All	2154/2292 (94%)	1839 (85%)	315 (15%)	2 10

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	6	ILE
1	A	21	VAL
1	A	30	ASP
1	A	51	LYS
1	A	52	THR
1	A	61	MET
1	A	64	VAL
1	A	84	VAL
1	A	85	THR
1	A	110	ILE
1	A	124	LEU
1	A	127	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	VAL
1	A	149	GLU
1	A	155	GLN
1	A	156	ASP
1	A	157	SER
1	A	162	ASN
1	A	163	GLN
1	A	169	LEU
1	A	176	LEU
1	A	178	ASN
1	A	191	SER
1	A	198	THR
1	A	207	LEU
1	A	213	ILE
1	A	215	GLU
1	A	217	THR
1	A	223	ILE
1	A	241	LYS
1	A	251	PHE
1	A	257	GLU
1	A	278	VAL
1	A	284	VAL
1	A	293	ARG
1	A	298	VAL
1	A	314	SER
1	A	365	VAL
1	A	375	VAL
1	A	404	THR
1	A	410	SER
1	A	422	LEU
1	A	438	VAL
1	A	451	VAL
1	A	454	LEU
1	A	472	ILE
1	A	477	ARG
1	A	501	THR
1	A	515	LEU
1	A	516	ILE
1	A	524	VAL
1	A	538	VAL
1	A	542	VAL
1	A	548	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	554	VAL
1	A	559	MET
1	A	603	ILE
1	A	616	VAL
1	A	634	GLN
2	B	729	LEU
2	B	734	ILE
2	B	741	SER
2	B	753	VAL
2	B	757	LYS
2	B	765	SER
2	B	769	MET
2	B	771	ILE
2	B	776	SER
2	B	786	SER
2	B	793	ILE
2	B	795	VAL
2	B	809	ILE
2	B	813	LEU
2	B	817	VAL
2	B	818	VAL
2	B	828	VAL
2	B	834	GLN
2	B	837	GLU
2	B	841	ARG
2	B	844	LEU
2	B	845	LEU
2	B	861	GLN
2	B	864	VAL
2	B	865	THR
2	B	869	LYS
2	B	871	SER
2	B	873	SER
2	B	877	VAL
2	B	882	LYS
2	B	887	GLU
2	B	888	VAL
2	B	890	VAL
2	B	899	ILE
2	B	903	VAL
2	B	910	VAL
2	B	912	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	36	LEU
3	M	38	THR
3	M	56	LYS
3	M	59	ASP
3	M	78	ASP
3	P	7	SER
3	P	8	ASN
3	P	21	SER
3	P	25	GLU
3	P	26	LEU
3	P	31	LEU
3	P	36	LEU
3	P	38	THR
3	P	56	LYS
3	P	59	ASP
3	P	78	ASP
4	F	1337	ASN
4	F	1342	LYS
4	F	1344	THR
4	F	1350	GLU
4	F	1361	THR
4	F	1362	MET
4	F	1378	MET
4	F	1387	THR
4	F	1389	PHE
4	F	1393	THR
4	F	1394	ASP
4	F	1397	LYS
4	F	1406	TYR
4	F	1412	LEU
4	F	1414	LYS
4	F	1416	PHE
4	F	1418	ASP
4	F	1419	ARG
4	F	1421	THR
4	F	1422	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	1426	LEU
4	F	1430	SER
4	F	1433	GLU
4	F	1447	VAL
4	F	1450	ILE
4	F	1465	GLU
4	F	1468	THR
4	F	1469	ARG
4	F	1479	LYS
4	F	1484	CYS
4	F	1498	ILE
4	F	1504	LYS
4	F	1507	LEU
4	F	1512	ASP
4	F	1532	LEU
4	F	1535	ASP
4	F	1536	PHE
4	F	1556	VAL
4	F	1561	THR
4	F	1563	ILE
4	F	1569	ARG
4	F	1572	LEU
4	F	1573	LYS
4	F	1574	LEU
4	F	1575	GLU
4	F	1585	LEU
4	F	1590	TRP
4	F	1597	SER
4	F	1600	ILE
1	D	3	MET
1	D	6	ILE
1	D	21	VAL
1	D	30	ASP
1	D	51	LYS
1	D	52	THR
1	D	61	MET
1	D	64	VAL
1	D	84	VAL
1	D	85	THR
1	D	110	ILE
1	D	124	LEU
1	D	127	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	137	VAL
1	D	149	GLU
1	D	155	GLN
1	D	156	ASP
1	D	157	SER
1	D	162	ASN
1	D	163	GLN
1	D	169	LEU
1	D	176	LEU
1	D	178	ASN
1	D	191	SER
1	D	198	THR
1	D	207	LEU
1	D	213	ILE
1	D	215	GLU
1	D	217	THR
1	D	223	ILE
1	D	241	LYS
1	D	251	PHE
1	D	257	GLU
1	D	278	VAL
1	D	284	VAL
1	D	293	ARG
1	D	298	VAL
1	D	304	VAL
1	D	314	SER
1	D	365	VAL
1	D	375	VAL
1	D	404	THR
1	D	410	SER
1	D	422	LEU
1	D	438	VAL
1	D	451	VAL
1	D	454	LEU
1	D	472	ILE
1	D	477	ARG
1	D	501	THR
1	D	515	LEU
1	D	516	ILE
1	D	524	VAL
1	D	538	VAL
1	D	542	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	548	SER
1	D	554	VAL
1	D	559	MET
1	D	603	ILE
1	D	616	VAL
1	D	634	GLN
4	C	1337	ASN
4	C	1342	LYS
4	C	1344	THR
4	C	1350	GLU
4	C	1361	THR
4	C	1362	MET
4	C	1378	MET
4	C	1387	THR
4	C	1389	PHE
4	C	1393	THR
4	C	1394	ASP
4	C	1397	LYS
4	C	1406	TYR
4	C	1412	LEU
4	C	1414	LYS
4	C	1416	PHE
4	C	1418	ASP
4	C	1419	ARG
4	C	1421	THR
4	C	1422	LEU
4	C	1426	LEU
4	C	1430	SER
4	C	1433	GLU
4	C	1447	VAL
4	C	1450	ILE
4	C	1465	GLU
4	C	1468	THR
4	C	1469	ARG
4	C	1479	LYS
4	C	1484	CYS
4	C	1498	ILE
4	C	1504	LYS
4	C	1507	LEU
4	C	1512	ASP
4	C	1532	LEU
4	C	1535	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	1536	PHE
4	C	1556	VAL
4	C	1561	THR
4	C	1563	ILE
4	C	1569	ARG
4	C	1572	LEU
4	C	1573	LYS
4	C	1574	LEU
4	C	1575	GLU
4	C	1585	LEU
4	C	1590	TRP
4	C	1597	SER
4	C	1600	ILE
2	E	729	LEU
2	E	734	ILE
2	E	741	SER
2	E	753	VAL
2	E	757	LYS
2	E	765	SER
2	E	769	MET
2	E	771	ILE
2	E	776	SER
2	E	786	SER
2	E	793	ILE
2	E	795	VAL
2	E	809	ILE
2	E	813	LEU
2	E	817	VAL
2	E	818	VAL
2	E	828	VAL
2	E	834	GLN
2	E	837	GLU
2	E	841	ARG
2	E	844	LEU
2	E	845	LEU
2	E	861	GLN
2	E	864	VAL
2	E	865	THR
2	E	869	LYS
2	E	871	SER
2	E	873	SER
2	E	877	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	882	LYS
2	E	887	GLU
2	E	888	VAL
2	E	890	VAL
2	E	899	ILE
2	E	903	VAL
2	E	910	VAL
2	E	912	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN
1	A	356	ASN
1	A	392	HIS
3	M	8	ASN
3	M	29	ASN
3	M	69	GLN
3	P	8	ASN
3	P	29	ASN
3	P	69	GLN
3	P	71	GLN
1	D	132	HIS
1	D	144	ASN
1	D	155	GLN
1	D	163	GLN
1	D	392	HIS
4	C	1531	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	NAG	A	646	-	14,14,15	0.44	0	17,19,21	1.45	1 (5%)
5	NAG	D	646	-	14,14,15	0.44	0	17,19,21	1.45	1 (5%)

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	-	-	4/6/23/26	0/1/1/1
5	NAG	D	646	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	646	NAG	C1-O5-C5	4.92	118.78	112.19
5	A	646	NAG	C1-O5-C5	4.91	118.76	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	646	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	646	NAG	O5-C5-C6-O6
5	A	646	NAG	C8-C7-N2-C2
5	A	646	NAG	O7-C7-N2-C2
5	D	646	NAG	C8-C7-N2-C2
5	D	646	NAG	O7-C7-N2-C2
5	A	646	NAG	C4-C5-C6-O6
5	D	646	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

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	639/645 (99%)	-1.72	0	100	100	20, 103, 160, 191	0
1	D	639/645 (99%)	-1.72	0	100	100	20, 103, 160, 191	0
2	B	184/206 (89%)	-1.75	0	100	100	52, 77, 109, 129	0
2	E	184/206 (89%)	-1.78	0	100	100	52, 77, 109, 129	0
3	M	84/88 (95%)	-1.78	0	100	100	68, 87, 139, 187	0
3	P	84/88 (95%)	-1.77	0	100	100	68, 87, 139, 187	0
4	C	294/343 (85%)	-1.58	0	100	100	20, 134, 208, 240	0
4	F	294/343 (85%)	-1.58	0	100	100	20, 134, 208, 240	0
All	All	2402/2564 (93%)	-1.70	0	100	100	20, 97, 182, 240	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
5	NAG	A	646	14/15	0.98	0.04	90,126,144,147	0
5	NAG	D	646	14/15	0.98	0.03	90,126,144,147	0

6.5 Other polymers (i)

There are no such residues in this entry.