



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:32 PM GMT

PDB ID : 3RFU
Title : Crystal structure of a copper-transporting PIB-type ATPase
Authors : Gourdon, P.; Liu, X.; Skjorringe, T.; Morth, J.P.; Birk Moller, L.; Panyella Pedersen, B.; Nissen, P.
Deposited on : 2011-04-07
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

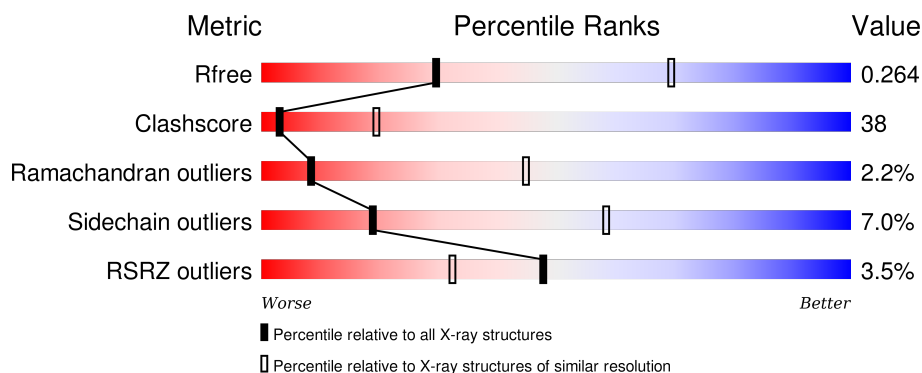
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	<div> <div>3%</div> <div>38% 47% 5% 10%</div> </div>
1	B	736	<div> <div>3%</div> <div>38% 47% 5% 10%</div> </div>
1	C	736	<div> <div>4%</div> <div>38% 47% 5% 10%</div> </div>
1	D	736	<div> <div>3%</div> <div>39% 46% 5% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ALF	A	995	-	-	X	-
4	K	A	997	-	-	-	X
4	K	B	997	-	-	-	X
4	K	C	997	-	-	-	X
4	K	D	997	-	-	-	X

2 Entry composition [i](#)

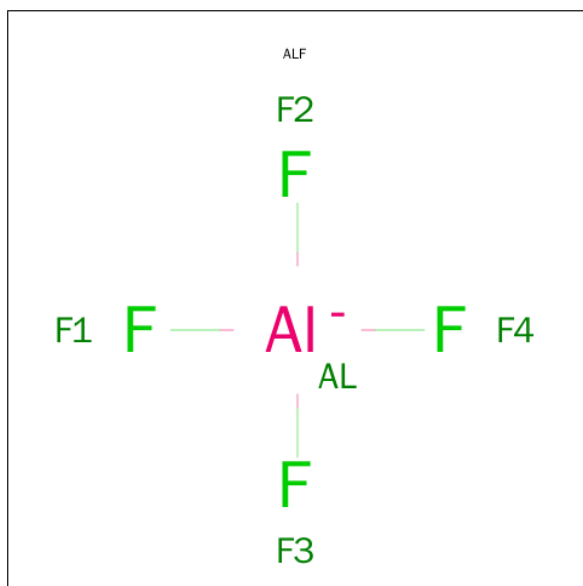
There are 4 unique types of molecules in this entry. The entry contains 19764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper efflux ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	B	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	C	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	D	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		
2	B	1	Total	Al	F	0	0
			5	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Al	F	0	0
			5	1	4		
2	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

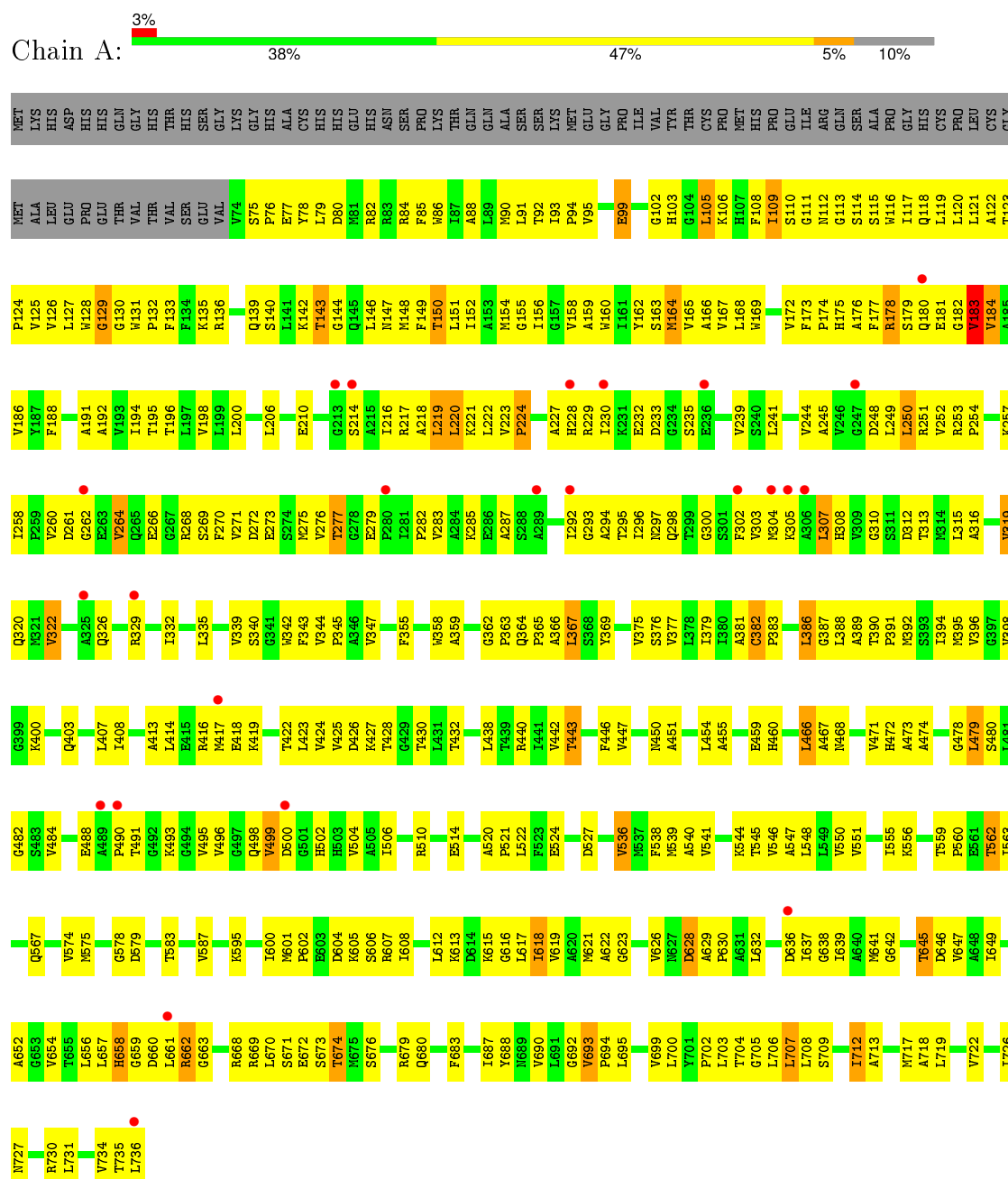
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

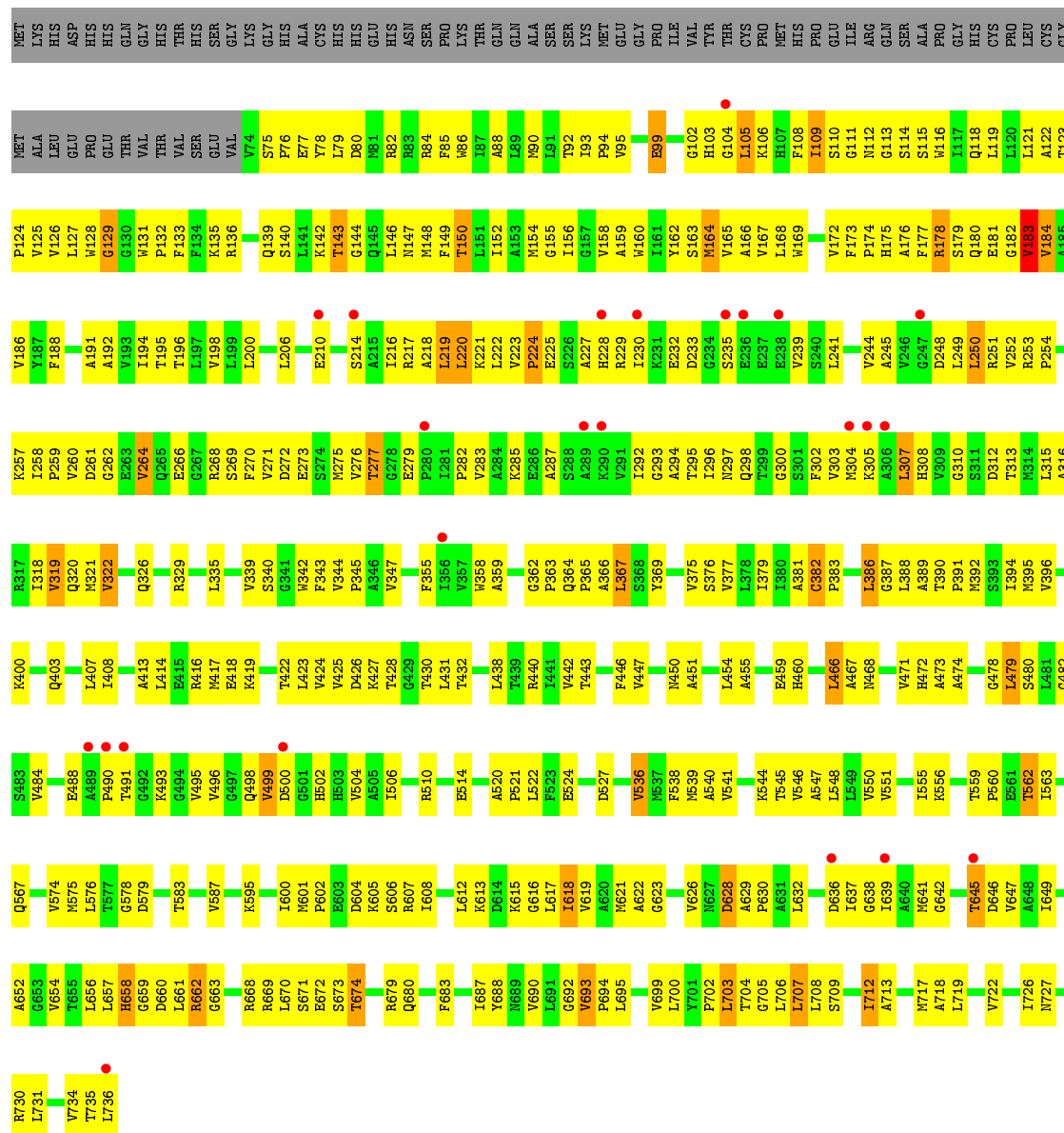
3 Residue-property plots

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.

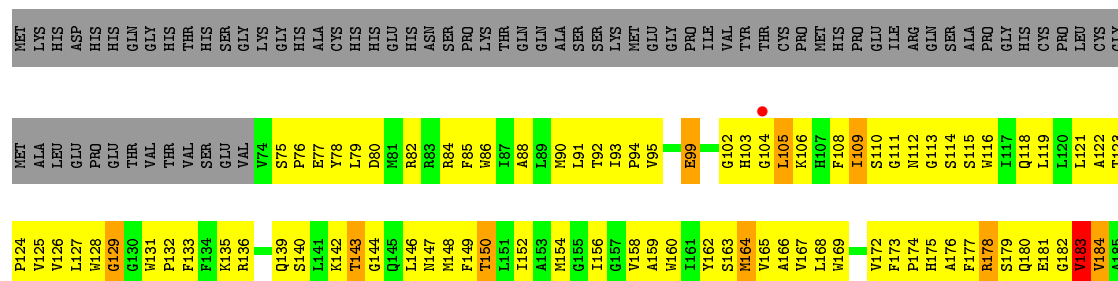
- Molecule 1: Copper efflux ATPase

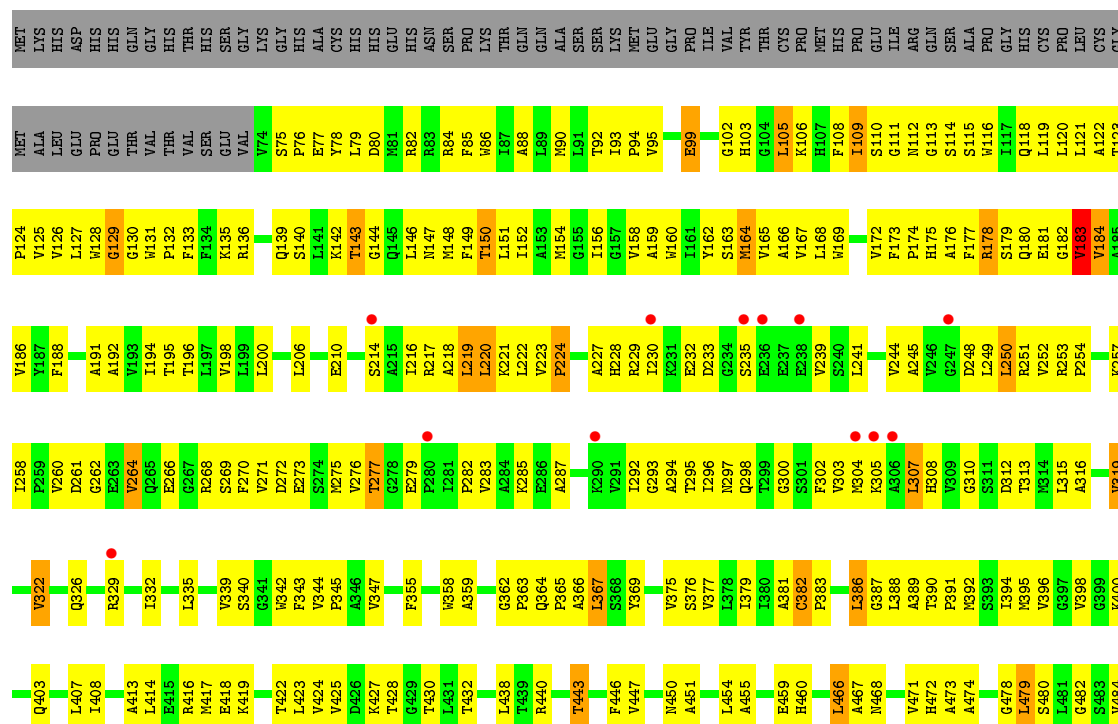


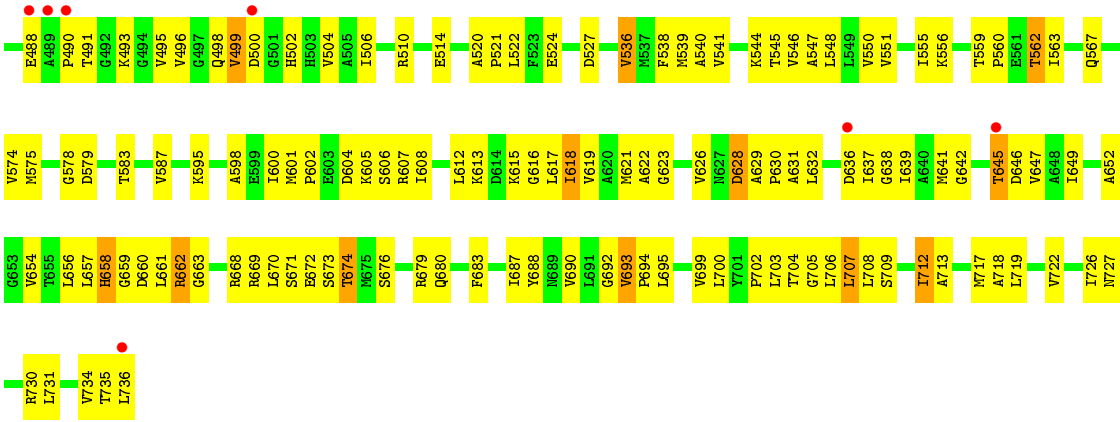
• Molecule 1: Copper efflux ATPase



• Molecule 1: Copper efflux ATPase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 72.98Å 329.95Å 89.96° 90.04° 90.22°	Depositor
Resolution (Å)	20.00 – 3.20 71.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.20) 95.5 (71.27-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.261 0.237 , 0.264	Depositor DCC
R_{free} test set	1598 reflections (2.43%)	DCC
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.6	EDS
Estimated twinning fraction	0.438 for h,-k,-l 0.428 for -h,k,-l 0.438 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 79676 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19764	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ALF, K, MG

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	0.25	0/5017	0.53	0/6812
1	B	0.25	0/5017	0.53	0/6812
1	C	0.25	0/5017	0.53	0/6812
1	D	0.25	0/5017	0.53	0/6812
All	All	0.25	0/20068	0.53	0/27248

There are no bond length outliers.

There are no bond angle outliers.

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	4934	0	5125	387	0
1	B	4934	0	5125	393	0
1	C	4934	0	5125	394	0
1	D	4934	0	5125	385	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	19764	0	20500	1547	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 38.

All (1547) 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:C:123:THR:HG23	1:C:124:PRO:HD3	1.31	1.12
1:B:123:THR:HG23	1:B:124:PRO:HD3	1.31	1.12
1:A:123:THR:HG23	1:A:124:PRO:HD3	1.31	1.12
1:D:123:THR:HG23	1:D:124:PRO:HD3	1.31	1.12
1:A:662:ARG:HB2	1:A:663:GLY:HA3	1.34	1.09
1:D:662:ARG:HB2	1:D:663:GLY:HA3	1.34	1.09
1:B:662:ARG:HB2	1:B:663:GLY:HA3	1.34	1.09
1:C:662:ARG:HB2	1:C:663:GLY:HA3	1.35	1.08
1:D:112:ASN:O	1:D:116:TRP:HB2	1.55	1.06
1:A:112:ASN:O	1:A:116:TRP:HB2	1.55	1.06
1:C:112:ASN:O	1:C:116:TRP:HB2	1.54	1.05
1:B:112:ASN:O	1:B:116:TRP:HB2	1.54	1.05
1:C:264:VAL:HA	1:C:303:VAL:O	1.57	1.04
1:B:264:VAL:HA	1:B:303:VAL:O	1.57	1.04
1:A:264:VAL:HA	1:A:303:VAL:O	1.57	1.02
1:D:264:VAL:HA	1:D:303:VAL:O	1.57	1.02
1:C:109:ILE:HG23	1:C:110:SER:HB3	1.41	1.00
1:B:109:ILE:HG23	1:B:110:SER:HB3	1.42	0.99
1:D:109:ILE:HG23	1:D:110:SER:HB3	1.43	0.96
1:A:109:ILE:HG23	1:A:110:SER:HB3	1.43	0.96
1:D:178:ARG:HB3	1:D:179:SER:HA	1.47	0.94
1:A:178:ARG:HB3	1:A:179:SER:HA	1.46	0.94
1:C:178:ARG:HB3	1:C:179:SER:HA	1.47	0.94
1:B:178:ARG:HB3	1:B:179:SER:HA	1.47	0.94
1:A:102:GLY:HA3	1:A:103:HIS:C	1.92	0.89
1:D:102:GLY:HA3	1:D:103:HIS:C	1.92	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:CG2	1:A:124:PRO:HD3	2.04	0.88
1:B:102:GLY:HA3	1:B:103:HIS:C	1.93	0.88
1:D:123:THR:CG2	1:D:124:PRO:HD3	2.04	0.88
1:C:102:GLY:HA3	1:C:103:HIS:C	1.92	0.88
1:C:123:THR:CG2	1:C:124:PRO:HD3	2.03	0.87
1:B:123:THR:CG2	1:B:124:PRO:HD3	2.04	0.87
1:C:482:GLY:HA3	1:C:499:VAL:HG23	1.59	0.85
1:B:482:GLY:HA3	1:B:499:VAL:HG23	1.58	0.85
1:A:482:GLY:HA3	1:A:499:VAL:HG23	1.59	0.84
1:D:482:GLY:HA3	1:D:499:VAL:HG23	1.59	0.84
1:D:229:ARG:HG2	1:D:250:LEU:HD21	1.60	0.83
1:A:229:ARG:HG2	1:A:250:LEU:HD21	1.60	0.83
1:A:416:ARG:HB2	1:A:637:ILE:HD11	1.60	0.83
1:D:416:ARG:HB2	1:D:637:ILE:HD11	1.59	0.83
1:C:229:ARG:HG2	1:C:250:LEU:HD21	1.60	0.82
1:B:229:ARG:HG2	1:B:250:LEU:HD21	1.60	0.82
1:C:416:ARG:HB2	1:C:637:ILE:HD11	1.59	0.82
1:B:416:ARG:HB2	1:B:637:ILE:HD11	1.59	0.82
1:B:232:GLU:HG3	1:B:233:ASP:H	1.43	0.81
1:C:232:GLU:HG3	1:C:233:ASP:H	1.43	0.81
1:B:222:LEU:C	1:B:224:PRO:HD2	2.01	0.81
1:C:222:LEU:C	1:C:224:PRO:HD2	2.02	0.81
1:A:563:ILE:O	1:A:567:GLN:HG2	1.81	0.81
1:D:563:ILE:O	1:D:567:GLN:HG2	1.81	0.81
1:D:232:GLU:HG3	1:D:233:ASP:H	1.43	0.81
1:A:222:LEU:C	1:A:224:PRO:HD2	2.02	0.80
1:D:222:LEU:C	1:D:224:PRO:HD2	2.02	0.80
1:B:563:ILE:O	1:B:567:GLN:HG2	1.81	0.80
1:A:232:GLU:HG3	1:A:233:ASP:H	1.43	0.80
1:D:662:ARG:HB2	1:D:663:GLY:CA	2.11	0.80
1:C:563:ILE:O	1:C:567:GLN:HG2	1.81	0.80
1:A:662:ARG:HB2	1:A:663:GLY:CA	2.12	0.80
1:D:254:PRO:HB3	1:D:300:GLY:H	1.47	0.80
1:B:662:ARG:HB2	1:B:663:GLY:CA	2.11	0.79
1:A:254:PRO:HB3	1:A:300:GLY:H	1.48	0.79
1:C:662:ARG:HB2	1:C:663:GLY:CA	2.12	0.79
1:D:708:LEU:HD21	1:D:712:ILE:HD11	1.63	0.79
1:C:254:PRO:HB3	1:C:300:GLY:H	1.47	0.79
1:A:708:LEU:HD21	1:A:712:ILE:HD11	1.64	0.78
1:B:254:PRO:HB3	1:B:300:GLY:H	1.48	0.78
1:C:708:LEU:HD21	1:C:712:ILE:HD11	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:O	1:B:123:THR:HG22	1.84	0.78
1:B:708:LEU:HD21	1:B:712:ILE:HD11	1.64	0.78
1:B:604:ASP:O	1:B:608:ILE:HG12	1.84	0.77
1:B:430:THR:HG21	1:B:623:GLY:HA2	1.66	0.77
1:C:604:ASP:O	1:C:608:ILE:HG12	1.85	0.77
1:C:119:LEU:O	1:C:123:THR:HG22	1.85	0.77
1:C:430:THR:HG21	1:C:623:GLY:HA2	1.67	0.77
1:A:119:LEU:O	1:A:123:THR:HG22	1.84	0.77
1:D:119:LEU:O	1:D:123:THR:HG22	1.84	0.77
1:D:499:VAL:HG22	1:D:500:ASP:H	1.49	0.77
1:B:499:VAL:HG22	1:B:500:ASP:H	1.49	0.77
1:D:430:THR:HG21	1:D:623:GLY:HA2	1.66	0.76
1:A:499:VAL:HG22	1:A:500:ASP:H	1.49	0.76
1:C:499:VAL:HG22	1:C:500:ASP:H	1.49	0.76
1:A:430:THR:HG21	1:A:623:GLY:HA2	1.66	0.76
1:D:604:ASP:O	1:D:608:ILE:HG12	1.84	0.76
1:A:124:PRO:O	1:A:128:TRP:HB3	1.85	0.76
1:B:662:ARG:CB	1:B:663:GLY:HA3	2.14	0.76
1:A:604:ASP:O	1:A:608:ILE:HG12	1.84	0.76
1:C:662:ARG:CB	1:C:663:GLY:HA3	2.14	0.76
1:D:124:PRO:O	1:D:128:TRP:HB3	1.86	0.75
1:A:335:LEU:O	1:A:339:VAL:HG12	1.87	0.75
1:D:335:LEU:O	1:D:339:VAL:HG12	1.87	0.75
1:C:124:PRO:O	1:C:128:TRP:HB3	1.86	0.74
1:B:124:PRO:O	1:B:128:TRP:HB3	1.86	0.74
1:C:232:GLU:CG	1:C:233:ASP:H	2.00	0.74
1:B:232:GLU:CG	1:B:233:ASP:H	2.00	0.74
1:B:159:ALA:HB2	1:B:379:ILE:HD13	1.68	0.74
1:D:232:GLU:CG	1:D:233:ASP:H	2.00	0.74
1:A:232:GLU:CG	1:A:233:ASP:H	2.00	0.74
1:B:78:TYR:HD2	1:B:79:LEU:HD12	1.53	0.74
1:D:662:ARG:CB	1:D:663:GLY:HA3	2.14	0.74
1:C:78:TYR:HD2	1:C:79:LEU:HD12	1.53	0.74
1:B:335:LEU:O	1:B:339:VAL:HG12	1.87	0.74
1:A:662:ARG:CB	1:A:663:GLY:HA3	2.14	0.73
1:C:159:ALA:HB2	1:C:379:ILE:HD13	1.68	0.73
1:D:110:SER:HB2	1:D:114:SER:HB3	1.69	0.73
1:C:147:ASN:H	1:C:150:THR:HG23	1.53	0.73
1:D:159:ALA:HB2	1:D:379:ILE:HD13	1.67	0.73
1:A:110:SER:HB2	1:A:114:SER:HB3	1.69	0.73
1:C:335:LEU:O	1:C:339:VAL:HG12	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ALA:HB1	1:C:196:THR:HG22	1.70	0.73
1:B:147:ASN:H	1:B:150:THR:HG23	1.53	0.73
1:C:110:SER:HB2	1:C:114:SER:HB3	1.69	0.73
1:B:110:SER:HB2	1:B:114:SER:HB3	1.70	0.72
1:C:152:ILE:HA	1:C:382:CYS:SG	2.29	0.72
1:B:88:ALA:HB1	1:B:196:THR:HG22	1.71	0.72
1:D:615:LYS:HG3	1:D:616:GLY:H	1.54	0.72
1:A:159:ALA:HB2	1:A:379:ILE:HD13	1.69	0.72
1:B:152:ILE:HA	1:B:382:CYS:SG	2.29	0.72
1:A:615:LYS:HG3	1:A:616:GLY:H	1.55	0.72
1:A:152:ILE:HA	1:A:382:CYS:SG	2.29	0.72
1:A:78:TYR:HD2	1:A:79:LEU:HD12	1.53	0.72
1:D:147:ASN:H	1:D:150:THR:HG23	1.53	0.72
1:D:700:LEU:HB3	1:D:704:THR:OG1	1.88	0.72
1:A:147:ASN:H	1:A:150:THR:HG23	1.53	0.72
1:C:700:LEU:HB3	1:C:704:THR:OG1	1.88	0.72
1:D:78:TYR:HD2	1:D:79:LEU:HD12	1.53	0.72
1:C:418:GLU:HG3	1:C:672:GLU:HG2	1.70	0.71
1:D:418:GLU:HG3	1:D:672:GLU:HG2	1.70	0.71
1:C:615:LYS:HG3	1:C:616:GLY:H	1.54	0.71
1:A:418:GLU:HG3	1:A:672:GLU:HG2	1.70	0.71
1:B:418:GLU:HG3	1:B:672:GLU:HG2	1.70	0.71
1:B:608:ILE:O	1:B:612:LEU:HD23	1.90	0.71
1:B:700:LEU:HB3	1:B:704:THR:OG1	1.88	0.71
1:A:413:ALA:HA	1:A:637:ILE:HD12	1.72	0.71
1:B:140:SER:OG	1:B:150:THR:HG22	1.89	0.71
1:D:152:ILE:HA	1:D:382:CYS:SG	2.30	0.71
1:B:175:HIS:HB2	1:B:176:ALA:HA	1.71	0.71
1:C:175:HIS:HB2	1:C:176:ALA:HA	1.71	0.71
1:C:608:ILE:O	1:C:612:LEU:HD23	1.90	0.71
1:A:140:SER:OG	1:A:150:THR:HG22	1.90	0.71
1:B:615:LYS:HG3	1:B:616:GLY:H	1.55	0.71
1:C:140:SER:OG	1:C:150:THR:HG22	1.90	0.71
1:A:700:LEU:HB3	1:A:704:THR:OG1	1.89	0.71
1:A:88:ALA:HB1	1:A:196:THR:HG22	1.71	0.71
1:D:413:ALA:HA	1:D:637:ILE:HD12	1.72	0.71
1:D:140:SER:OG	1:D:150:THR:HG22	1.90	0.71
1:D:175:HIS:HB2	1:D:176:ALA:HA	1.72	0.71
1:A:175:HIS:HB2	1:A:176:ALA:HA	1.72	0.71
1:C:160:TRP:O	1:C:164:MET:HB2	1.91	0.71
1:B:160:TRP:O	1:B:164:MET:HB2	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:ILE:HA	1:D:690:VAL:HG12	1.73	0.71
1:A:688:TYR:CD1	1:A:719:LEU:HD23	2.26	0.71
1:A:249:LEU:O	1:A:250:LEU:HD23	1.91	0.70
1:D:249:LEU:O	1:D:250:LEU:HD23	1.92	0.70
1:C:688:TYR:CD1	1:C:719:LEU:HD23	2.26	0.70
1:C:413:ALA:HA	1:C:637:ILE:HD12	1.72	0.70
1:D:608:ILE:O	1:D:612:LEU:HD23	1.90	0.70
1:A:687:ILE:HA	1:A:690:VAL:HG12	1.74	0.70
1:C:556:LYS:HB2	1:C:559:THR:OG1	1.92	0.70
1:D:254:PRO:HB3	1:D:300:GLY:N	2.07	0.70
1:D:121:LEU:O	1:D:124:PRO:HD2	1.92	0.70
1:B:413:ALA:HA	1:B:637:ILE:HD12	1.72	0.70
1:A:254:PRO:HB3	1:A:300:GLY:N	2.07	0.70
1:C:687:ILE:HA	1:C:690:VAL:HG12	1.74	0.70
1:B:556:LYS:HB2	1:B:559:THR:OG1	1.92	0.70
1:B:283:VAL:HG23	1:B:285:LYS:HE2	1.74	0.70
1:B:687:ILE:HA	1:B:690:VAL:HG12	1.74	0.70
1:C:432:THR:HG22	1:C:555:ILE:HA	1.74	0.70
1:C:283:VAL:HG23	1:C:285:LYS:HE2	1.74	0.70
1:B:194:ILE:O	1:B:198:VAL:HG12	1.92	0.70
1:A:432:THR:HG22	1:A:555:ILE:HA	1.74	0.70
1:B:432:THR:HG22	1:B:555:ILE:HA	1.74	0.70
1:C:254:PRO:HB3	1:C:300:GLY:N	2.07	0.69
1:A:608:ILE:O	1:A:612:LEU:HD23	1.91	0.69
1:D:432:THR:HG22	1:D:555:ILE:HA	1.74	0.69
1:D:160:TRP:O	1:D:164:MET:HB2	1.91	0.69
1:A:160:TRP:O	1:A:164:MET:HB2	1.91	0.69
1:C:661:LEU:HD23	1:C:661:LEU:O	1.92	0.69
1:B:254:PRO:HB3	1:B:300:GLY:N	2.07	0.69
1:D:93:ILE:HG23	1:D:94:PRO:HD3	1.75	0.69
1:C:121:LEU:O	1:C:124:PRO:HD2	1.92	0.69
1:C:249:LEU:O	1:C:250:LEU:HD23	1.91	0.69
1:D:688:TYR:CD1	1:D:719:LEU:HD23	2.28	0.69
1:D:661:LEU:O	1:D:661:LEU:HD23	1.92	0.69
1:A:93:ILE:HG23	1:A:94:PRO:HD3	1.75	0.69
1:B:249:LEU:O	1:B:250:LEU:HD23	1.91	0.69
1:D:122:ALA:HA	1:D:125:VAL:HG12	1.74	0.69
1:D:88:ALA:HB1	1:D:196:THR:HG22	1.72	0.69
1:B:688:TYR:CD1	1:B:719:LEU:HD23	2.27	0.69
1:C:194:ILE:O	1:C:198:VAL:HG12	1.92	0.69
1:D:194:ILE:O	1:D:198:VAL:HG12	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:O	1:B:124:PRO:HD2	1.93	0.69
1:A:556:LYS:HB2	1:A:559:THR:OG1	1.91	0.69
1:A:661:LEU:HD23	1:A:661:LEU:O	1.92	0.69
1:C:122:ALA:HA	1:C:125:VAL:HG12	1.74	0.69
1:A:122:ALA:HA	1:A:125:VAL:HG12	1.74	0.69
1:B:122:ALA:HA	1:B:125:VAL:HG12	1.75	0.69
1:A:194:ILE:O	1:A:198:VAL:HG12	1.93	0.69
1:B:661:LEU:HD23	1:B:661:LEU:O	1.93	0.69
1:A:121:LEU:O	1:A:124:PRO:HD2	1.93	0.68
1:B:93:ILE:HG23	1:B:94:PRO:HD3	1.75	0.68
1:D:283:VAL:HG23	1:D:285:LYS:HE2	1.74	0.68
1:A:283:VAL:HG23	1:A:285:LYS:HE2	1.74	0.68
1:B:273:GLU:O	1:B:273:GLU:HG2	1.93	0.68
1:C:377:VAL:HG23	1:C:693:VAL:HB	1.75	0.68
1:C:93:ILE:HG23	1:C:94:PRO:HD3	1.76	0.68
1:C:273:GLU:O	1:C:273:GLU:HG2	1.94	0.68
1:D:556:LYS:HB2	1:D:559:THR:OG1	1.92	0.68
1:B:520:ALA:HB3	1:B:521:PRO:HD3	1.76	0.68
1:D:273:GLU:O	1:D:273:GLU:HG2	1.93	0.68
1:A:273:GLU:O	1:A:273:GLU:HG2	1.93	0.67
1:C:520:ALA:HB3	1:C:521:PRO:HD3	1.76	0.67
1:B:541:VAL:HG22	1:B:546:VAL:HG11	1.77	0.67
1:A:108:PHE:O	1:A:109:ILE:HD12	1.95	0.67
1:B:377:VAL:HG23	1:B:693:VAL:HB	1.76	0.67
1:A:377:VAL:HG23	1:A:693:VAL:HB	1.75	0.67
1:A:520:ALA:HB3	1:A:521:PRO:HD3	1.76	0.67
1:C:541:VAL:HG22	1:C:546:VAL:HG11	1.77	0.67
1:D:108:PHE:O	1:D:109:ILE:HD12	1.95	0.67
1:C:110:SER:HA	1:C:114:SER:H	1.60	0.67
1:A:110:SER:HA	1:A:114:SER:H	1.60	0.67
1:D:377:VAL:HG23	1:D:693:VAL:HB	1.76	0.67
1:D:520:ALA:HB3	1:D:521:PRO:HD3	1.77	0.66
1:B:687:ILE:HD13	1:D:120:LEU:HD12	1.76	0.66
1:D:541:VAL:HG22	1:D:546:VAL:HG11	1.77	0.66
1:B:307:LEU:HD13	1:B:308:HIS:HD2	1.61	0.66
1:C:307:LEU:HD13	1:C:308:HIS:HD2	1.61	0.66
1:A:307:LEU:HD13	1:A:308:HIS:HD2	1.60	0.66
1:B:108:PHE:O	1:B:109:ILE:HD12	1.95	0.66
1:D:110:SER:HA	1:D:114:SER:H	1.61	0.66
1:A:541:VAL:HG22	1:A:546:VAL:HG11	1.77	0.66
1:C:108:PHE:O	1:C:109:ILE:HD12	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:SER:HA	1:B:114:SER:H	1.61	0.66
1:A:179:SER:HB2	1:A:183:VAL:N	2.11	0.66
1:D:307:LEU:HD13	1:D:308:HIS:HD2	1.61	0.66
1:D:179:SER:HB2	1:D:183:VAL:N	2.11	0.65
1:C:179:SER:HB2	1:C:183:VAL:N	2.11	0.65
1:A:605:LYS:HE2	1:A:628:ASP:HB3	1.79	0.65
1:D:605:LYS:HE2	1:D:628:ASP:HB3	1.79	0.65
1:B:179:SER:HB2	1:B:183:VAL:N	2.11	0.65
1:D:192:ALA:O	1:D:196:THR:HG23	1.96	0.65
1:B:605:LYS:HE2	1:B:628:ASP:HB3	1.78	0.65
1:A:490:PRO:HB2	1:A:493:LYS:HD3	1.79	0.65
1:D:490:PRO:HB2	1:D:493:LYS:HD3	1.79	0.64
1:A:192:ALA:O	1:A:196:THR:HG23	1.96	0.64
1:C:192:ALA:O	1:C:196:THR:HG23	1.98	0.64
1:B:192:ALA:O	1:B:196:THR:HG23	1.98	0.64
1:C:490:PRO:HB2	1:C:493:LYS:HD3	1.79	0.64
1:C:605:LYS:HE2	1:C:628:ASP:HB3	1.78	0.64
1:C:670:LEU:HD23	1:C:736:LEU:HD11	1.79	0.64
1:B:112:ASN:O	1:B:116:TRP:CB	2.40	0.64
1:D:93:ILE:CG2	1:D:94:PRO:HD3	2.27	0.64
1:A:93:ILE:CG2	1:A:94:PRO:HD3	2.27	0.64
1:B:490:PRO:HB2	1:B:493:LYS:HD3	1.79	0.64
1:C:112:ASN:O	1:C:116:TRP:CB	2.40	0.64
1:A:670:LEU:O	1:A:674:THR:HG23	1.98	0.64
1:B:223:VAL:O	1:B:224:PRO:C	2.37	0.64
1:D:670:LEU:O	1:D:674:THR:HG23	1.98	0.64
1:C:223:VAL:O	1:C:224:PRO:C	2.37	0.64
1:B:506:ILE:HD12	1:B:538:PHE:O	1.98	0.64
1:A:111:GLY:O	1:A:115:SER:HB2	1.98	0.63
1:B:111:GLY:O	1:B:115:SER:HB2	1.98	0.63
1:B:670:LEU:HD23	1:B:736:LEU:HD11	1.80	0.63
1:D:111:GLY:O	1:D:115:SER:HB2	1.98	0.63
1:B:93:ILE:CG2	1:B:94:PRO:HD3	2.28	0.63
1:C:93:ILE:CG2	1:C:94:PRO:HD3	2.28	0.63
1:B:275:MET:HE1	1:B:294:ALA:HB3	1.79	0.63
1:C:109:ILE:CG2	1:C:110:SER:HB3	2.22	0.63
1:C:506:ILE:HD12	1:C:538:PHE:O	1.99	0.63
1:C:275:MET:HE1	1:C:294:ALA:HB3	1.79	0.63
1:D:275:MET:HE1	1:D:294:ALA:HB3	1.80	0.63
1:A:275:MET:HE1	1:A:294:ALA:HB3	1.80	0.63
1:C:111:GLY:O	1:C:115:SER:HB2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LEU:HD23	1:A:736:LEU:HD11	1.79	0.63
1:A:506:ILE:HD12	1:A:538:PHE:O	1.98	0.63
1:D:506:ILE:HD12	1:D:538:PHE:O	1.98	0.63
1:B:109:ILE:CG2	1:B:110:SER:HB3	2.23	0.63
1:D:223:VAL:O	1:D:224:PRO:C	2.37	0.63
1:C:670:LEU:O	1:C:674:THR:HG23	1.98	0.63
1:D:670:LEU:HD23	1:D:736:LEU:HD11	1.79	0.63
1:A:223:VAL:O	1:A:224:PRO:C	2.37	0.62
1:B:670:LEU:O	1:B:674:THR:HG23	1.98	0.62
1:C:454:LEU:HD21	1:C:500:ASP:OD1	1.99	0.62
1:A:105:LEU:HD12	1:A:106:LYS:N	2.14	0.62
1:D:105:LEU:HD12	1:D:106:LYS:N	2.15	0.62
1:C:223:VAL:N	1:C:224:PRO:HD2	2.14	0.62
1:C:342:TRP:O	1:C:345:PRO:HD2	2.00	0.62
1:B:223:VAL:N	1:B:224:PRO:HD2	2.14	0.62
1:B:216:ILE:O	1:B:219:LEU:HD13	2.00	0.62
1:B:454:LEU:HD21	1:B:500:ASP:OD1	2.00	0.62
1:C:216:ILE:O	1:C:219:LEU:HD13	2.00	0.62
1:C:423:LEU:HG	1:C:425:VAL:HG13	1.81	0.62
1:A:315:LEU:O	1:A:319:VAL:HG12	2.00	0.62
1:D:109:ILE:CG2	1:D:110:SER:HB3	2.23	0.62
1:C:315:LEU:O	1:C:319:VAL:HG12	1.99	0.62
1:D:315:LEU:O	1:D:319:VAL:HG12	2.00	0.62
1:C:105:LEU:HD12	1:C:106:LYS:N	2.14	0.62
1:A:109:ILE:CG2	1:A:110:SER:HB3	2.23	0.61
1:A:454:LEU:HD21	1:A:500:ASP:OD1	2.00	0.61
1:B:105:LEU:HD12	1:B:106:LYS:N	2.14	0.61
1:D:216:ILE:O	1:D:219:LEU:HD13	2.00	0.61
1:D:342:TRP:O	1:D:345:PRO:HD2	2.00	0.61
1:A:178:ARG:CB	1:A:179:SER:HA	2.24	0.61
1:D:454:LEU:HD21	1:D:500:ASP:OD1	2.00	0.61
1:D:216:ILE:HG23	1:D:217:ARG:H	1.66	0.61
1:A:216:ILE:HG23	1:A:217:ARG:H	1.66	0.61
1:A:216:ILE:O	1:A:219:LEU:HD13	2.00	0.61
1:B:418:GLU:HB2	1:B:671:SER:OG	2.00	0.61
1:B:342:TRP:O	1:B:345:PRO:HD2	2.00	0.61
1:D:223:VAL:N	1:D:224:PRO:HD2	2.15	0.61
1:B:315:LEU:O	1:B:319:VAL:HG12	2.00	0.61
1:C:629:ALA:N	1:C:630:PRO:HD2	2.16	0.61
1:B:423:LEU:HG	1:B:425:VAL:HG13	1.81	0.61
1:A:223:VAL:N	1:A:224:PRO:HD2	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HG2	1:A:143:THR:HG23	1.82	0.61
1:B:629:ALA:N	1:B:630:PRO:HD2	2.16	0.61
1:D:142:LYS:HG2	1:D:143:THR:HG23	1.82	0.61
1:D:178:ARG:CB	1:D:179:SER:HA	2.24	0.61
1:A:342:TRP:O	1:A:345:PRO:HD2	2.01	0.61
1:A:423:LEU:HG	1:A:425:VAL:HG13	1.81	0.61
1:C:142:LYS:HG2	1:C:143:THR:HG23	1.82	0.61
1:D:418:GLU:HB2	1:D:671:SER:OG	2.00	0.61
1:D:629:ALA:N	1:D:630:PRO:HD2	2.15	0.61
1:A:120:LEU:HD12	1:C:687:ILE:HD13	1.82	0.61
1:B:142:LYS:HG2	1:B:143:THR:HG23	1.82	0.61
1:A:629:ALA:N	1:A:630:PRO:HD2	2.16	0.61
1:B:179:SER:HB3	1:B:181:GLU:N	2.16	0.60
1:C:418:GLU:HB2	1:C:671:SER:OG	2.01	0.60
1:C:344:VAL:HG22	1:C:345:PRO:HD3	1.82	0.60
1:B:662:ARG:CB	1:B:663:GLY:CA	2.77	0.60
1:D:166:ALA:HA	1:D:173:PHE:HE2	1.66	0.60
1:C:179:SER:HB3	1:C:181:GLU:N	2.16	0.60
1:B:262:GLY:HA2	1:B:307:LEU:HB2	1.83	0.60
1:D:423:LEU:HG	1:D:425:VAL:HG13	1.82	0.60
1:A:166:ALA:HA	1:A:173:PHE:HE2	1.65	0.60
1:C:662:ARG:CB	1:C:663:GLY:CA	2.78	0.60
1:C:166:ALA:HA	1:C:173:PHE:HE2	1.65	0.60
1:C:709:SER:O	1:C:712:ILE:HG13	2.01	0.60
1:C:262:GLY:HA2	1:C:307:LEU:HB2	1.83	0.60
1:D:709:SER:O	1:D:712:ILE:HG13	2.02	0.60
1:B:216:ILE:HG23	1:B:217:ARG:H	1.66	0.60
1:C:216:ILE:HG23	1:C:217:ARG:H	1.66	0.60
1:B:709:SER:O	1:B:712:ILE:HG13	2.01	0.60
1:B:344:VAL:HG22	1:B:345:PRO:HD3	1.83	0.60
1:B:191:ALA:O	1:B:195:THR:HG23	2.02	0.60
1:A:709:SER:O	1:A:712:ILE:HG13	2.02	0.60
1:B:166:ALA:HA	1:B:173:PHE:HE2	1.66	0.60
1:A:418:GLU:HB2	1:A:671:SER:OG	2.01	0.60
1:A:344:VAL:HG22	1:A:345:PRO:HD3	1.83	0.60
1:A:179:SER:HB3	1:A:181:GLU:N	2.17	0.59
1:D:262:GLY:HA2	1:D:307:LEU:HB2	1.83	0.59
1:D:179:SER:HB3	1:D:181:GLU:N	2.17	0.59
1:D:344:VAL:HG22	1:D:345:PRO:HD3	1.84	0.59
1:A:112:ASN:O	1:A:116:TRP:CB	2.40	0.59
1:C:683:PHE:CZ	1:C:687:ILE:HD12	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:PHE:CZ	1:B:687:ILE:HD12	2.37	0.59
1:A:262:GLY:HA2	1:A:307:LEU:HB2	1.83	0.59
1:B:499:VAL:HG22	1:B:500:ASP:N	2.18	0.59
1:A:646:ASP:O	1:A:649:ILE:HG22	2.03	0.59
1:D:112:ASN:O	1:D:116:TRP:CB	2.40	0.59
1:B:466:LEU:HD21	1:B:551:VAL:HG21	1.85	0.59
1:D:191:ALA:O	1:D:195:THR:HG23	2.03	0.59
1:C:268:ARG:HE	1:C:491:THR:HG21	1.68	0.59
1:B:268:ARG:HE	1:B:491:THR:HG21	1.68	0.59
1:C:499:VAL:HG22	1:C:500:ASP:N	2.18	0.58
1:D:646:ASP:O	1:D:649:ILE:HG22	2.03	0.58
1:A:683:PHE:CZ	1:A:687:ILE:HD12	2.37	0.58
1:C:646:ASP:O	1:C:649:ILE:HG22	2.03	0.58
1:D:268:ARG:HE	1:D:491:THR:HG21	1.68	0.58
1:D:662:ARG:CB	1:D:663:GLY:CA	2.77	0.58
1:D:400:LYS:O	1:D:403:GLN:HB3	2.04	0.58
1:D:683:PHE:CZ	1:D:687:ILE:HD12	2.38	0.58
1:C:466:LEU:HD21	1:C:551:VAL:HG21	1.86	0.58
1:A:147:ASN:H	1:A:150:THR:CG2	2.16	0.58
1:C:191:ALA:O	1:C:195:THR:HG23	2.04	0.58
1:A:268:ARG:HE	1:A:491:THR:HG21	1.68	0.58
1:A:662:ARG:CB	1:A:663:GLY:CA	2.77	0.58
1:A:447:VAL:CG2	1:A:450:ASN:HB2	2.34	0.58
1:A:191:ALA:O	1:A:195:THR:HG23	2.04	0.58
1:A:400:LYS:O	1:A:403:GLN:HB3	2.04	0.58
1:B:499:VAL:O	1:B:502:HIS:CG	2.56	0.58
1:D:447:VAL:CG2	1:D:450:ASN:HB2	2.34	0.58
1:B:400:LYS:O	1:B:403:GLN:HB3	2.04	0.58
1:C:400:LYS:O	1:C:403:GLN:HB3	2.04	0.58
1:D:466:LEU:HD21	1:D:551:VAL:HG21	1.85	0.58
1:C:499:VAL:O	1:C:502:HIS:CG	2.56	0.58
1:D:147:ASN:H	1:D:150:THR:CG2	2.16	0.58
1:D:119:LEU:HD12	1:D:167:VAL:HG11	1.86	0.57
1:D:499:VAL:O	1:D:502:HIS:CG	2.56	0.57
1:D:499:VAL:HG22	1:D:500:ASP:N	2.18	0.57
1:D:414:LEU:HD21	1:D:670:LEU:HD12	1.86	0.57
1:A:414:LEU:HD21	1:A:670:LEU:HD12	1.86	0.57
1:B:646:ASP:O	1:B:649:ILE:HG22	2.04	0.57
1:C:386:LEU:HD12	1:C:387:GLY:N	2.19	0.57
1:C:147:ASN:H	1:C:150:THR:CG2	2.17	0.57
1:B:455:ALA:O	1:B:459:GLU:HG2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:VAL:O	1:A:502:HIS:CG	2.56	0.57
1:A:499:VAL:HG22	1:A:500:ASP:N	2.18	0.57
1:B:133:PHE:CE1	1:B:198:VAL:HG13	2.39	0.57
1:C:455:ALA:O	1:C:459:GLU:HG2	2.04	0.57
1:B:147:ASN:H	1:B:150:THR:CG2	2.17	0.57
1:A:119:LEU:HD12	1:A:167:VAL:HG11	1.86	0.57
1:A:133:PHE:CE1	1:A:198:VAL:HG13	2.40	0.57
1:A:466:LEU:HD21	1:A:551:VAL:HG21	1.86	0.57
1:D:455:ALA:O	1:D:459:GLU:HG2	2.04	0.57
1:C:133:PHE:CE1	1:C:198:VAL:HG13	2.40	0.57
1:D:386:LEU:HD12	1:D:387:GLY:N	2.19	0.57
1:C:77:GLU:O	1:C:80:ASP:HB3	2.04	0.57
1:A:455:ALA:O	1:A:459:GLU:HG2	2.04	0.57
1:D:578:GLY:O	1:D:579:ASP:HB2	2.04	0.57
1:A:386:LEU:HD12	1:A:387:GLY:N	2.19	0.57
1:D:229:ARG:HD2	1:D:248:ASP:HB3	1.87	0.57
1:D:133:PHE:CE1	1:D:198:VAL:HG13	2.40	0.57
1:A:229:ARG:HD2	1:A:248:ASP:HB3	1.87	0.56
1:C:447:VAL:CG2	1:C:450:ASN:HB2	2.34	0.56
1:C:414:LEU:HD21	1:C:670:LEU:HD12	1.86	0.56
1:B:414:LEU:HD21	1:B:670:LEU:HD12	1.86	0.56
1:D:488:GLU:HB3	1:D:496:VAL:HG13	1.86	0.56
1:D:99:GLU:HG2	1:D:118:GLN:OE1	2.05	0.56
1:A:488:GLU:HB3	1:A:496:VAL:HG13	1.86	0.56
1:B:499:VAL:H	1:B:502:HIS:HA	1.70	0.56
1:B:386:LEU:HD12	1:B:387:GLY:N	2.19	0.56
1:C:119:LEU:HD12	1:C:167:VAL:HG11	1.86	0.56
1:B:662:ARG:HA	1:B:662:ARG:HH11	1.70	0.56
1:C:249:LEU:HB3	1:C:303:VAL:CG2	2.36	0.56
1:B:249:LEU:HB3	1:B:303:VAL:CG2	2.36	0.56
1:A:499:VAL:H	1:A:502:HIS:HA	1.70	0.56
1:D:499:VAL:H	1:D:502:HIS:HA	1.70	0.56
1:A:99:GLU:HG2	1:A:118:GLN:OE1	2.05	0.56
1:B:77:GLU:O	1:B:80:ASP:HB3	2.05	0.56
1:C:499:VAL:H	1:C:502:HIS:HA	1.71	0.56
1:C:99:GLU:HG2	1:C:118:GLN:OE1	2.06	0.56
1:B:390:THR:O	1:B:394:ILE:HG12	2.06	0.56
1:B:119:LEU:HD12	1:B:167:VAL:HG11	1.86	0.56
1:C:229:ARG:HD2	1:C:248:ASP:HB3	1.87	0.56
1:B:229:ARG:HD2	1:B:248:ASP:HB3	1.87	0.56
1:C:78:TYR:HA	1:C:206:LEU:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:GLU:HB3	1:C:496:VAL:HG13	1.86	0.56
1:A:662:ARG:HA	1:A:662:ARG:HH11	1.70	0.56
1:D:662:ARG:HA	1:D:662:ARG:HH11	1.70	0.56
1:C:662:ARG:HH11	1:C:662:ARG:HA	1.70	0.56
1:A:578:GLY:O	1:A:579:ASP:HB2	2.05	0.56
1:B:99:GLU:HG2	1:B:118:GLN:OE1	2.06	0.56
1:B:488:GLU:HB3	1:B:496:VAL:HG13	1.86	0.56
1:B:112:ASN:HA	1:B:116:TRP:CD1	2.41	0.56
1:B:447:VAL:CG2	1:B:450:ASN:HB2	2.35	0.56
1:A:262:GLY:HA2	1:A:305:LYS:O	2.06	0.56
1:A:390:THR:O	1:A:394:ILE:HG12	2.05	0.56
1:A:77:GLU:O	1:A:80:ASP:HB3	2.05	0.56
1:D:657:LEU:O	1:D:658:HIS:HB3	2.06	0.56
1:D:77:GLU:O	1:D:80:ASP:HB3	2.05	0.56
1:C:578:GLY:O	1:C:579:ASP:HB2	2.04	0.56
1:A:657:LEU:O	1:A:658:HIS:HB3	2.06	0.56
1:B:78:TYR:HA	1:B:206:LEU:CD1	2.36	0.56
1:D:262:GLY:HA2	1:D:305:LYS:O	2.06	0.56
1:C:112:ASN:HA	1:C:116:TRP:CD1	2.41	0.55
1:A:102:GLY:HA3	1:A:103:HIS:O	2.06	0.55
1:D:102:GLY:HA3	1:D:103:HIS:O	2.06	0.55
1:C:638:GLY:O	1:C:652:ALA:HB1	2.06	0.55
1:A:78:TYR:HA	1:A:206:LEU:CD1	2.35	0.55
1:D:390:THR:O	1:D:394:ILE:HG12	2.06	0.55
1:B:578:GLY:O	1:B:579:ASP:HB2	2.05	0.55
1:A:638:GLY:O	1:A:652:ALA:HB1	2.06	0.55
1:A:125:VAL:O	1:A:129:GLY:HA2	2.07	0.55
1:D:260:VAL:HG12	1:D:261:ASP:N	2.22	0.55
1:A:249:LEU:HB3	1:A:303:VAL:CG2	2.36	0.55
1:C:154:MET:O	1:C:158:VAL:HG12	2.07	0.55
1:D:249:LEU:HB3	1:D:303:VAL:CG2	2.36	0.55
1:C:504:VAL:HB	1:C:541:VAL:HG12	1.89	0.55
1:B:262:GLY:HA2	1:B:305:LYS:O	2.06	0.55
1:A:154:MET:O	1:A:158:VAL:HG12	2.07	0.55
1:B:154:MET:O	1:B:158:VAL:HG12	2.07	0.55
1:C:390:THR:O	1:C:394:ILE:HG12	2.07	0.55
1:D:229:ARG:HG2	1:D:250:LEU:CD2	2.34	0.55
1:C:102:GLY:HA3	1:C:103:HIS:O	2.06	0.55
1:B:657:LEU:O	1:B:658:HIS:HB3	2.06	0.55
1:C:262:GLY:HA2	1:C:305:LYS:O	2.06	0.55
1:A:504:VAL:HB	1:A:541:VAL:HG12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:HA3	1:B:103:HIS:O	2.06	0.55
1:A:559:THR:HA	1:A:562:THR:HG23	1.89	0.55
1:D:559:THR:HA	1:D:562:THR:HG23	1.89	0.55
1:A:260:VAL:HG12	1:A:261:ASP:N	2.22	0.55
1:D:112:ASN:HA	1:D:116:TRP:CD1	2.42	0.55
1:A:229:ARG:HG2	1:A:250:LEU:CD2	2.34	0.55
1:C:657:LEU:O	1:C:658:HIS:HB3	2.06	0.55
1:B:504:VAL:HB	1:B:541:VAL:HG12	1.89	0.55
1:D:388:LEU:O	1:D:392:MET:HG3	2.07	0.55
1:D:504:VAL:HB	1:D:541:VAL:HG12	1.89	0.54
1:D:310:GLY:O	1:D:313:THR:HG22	2.07	0.54
1:B:638:GLY:O	1:B:652:ALA:HB1	2.07	0.54
1:B:358:TRP:CE3	1:B:369:TYR:HB3	2.42	0.54
1:C:270:PHE:CD1	1:C:282:PRO:HB2	2.42	0.54
1:A:310:GLY:O	1:A:313:THR:HG22	2.07	0.54
1:B:718:ALA:O	1:B:722:VAL:HG12	2.06	0.54
1:D:154:MET:O	1:D:158:VAL:HG12	2.07	0.54
1:B:270:PHE:CD1	1:B:282:PRO:HB2	2.42	0.54
1:B:502:HIS:CE1	1:C:520:ALA:HA	2.42	0.54
1:D:78:TYR:HA	1:D:206:LEU:CD1	2.37	0.54
1:C:358:TRP:CE3	1:C:369:TYR:HB3	2.43	0.54
1:C:85:PHE:CZ	1:C:200:LEU:HD13	2.43	0.54
1:C:310:GLY:O	1:C:313:THR:HG22	2.07	0.54
1:C:707:LEU:HD22	1:C:707:LEU:C	2.28	0.54
1:A:388:LEU:O	1:A:392:MET:HG3	2.08	0.54
1:D:718:ALA:O	1:D:722:VAL:HG12	2.07	0.54
1:A:112:ASN:HA	1:A:116:TRP:CD1	2.43	0.54
1:D:125:VAL:O	1:D:129:GLY:HA2	2.08	0.54
1:C:718:ALA:O	1:C:722:VAL:HG12	2.07	0.54
1:D:638:GLY:O	1:D:652:ALA:HB1	2.07	0.54
1:A:229:ARG:NH1	1:A:239:VAL:HG21	2.22	0.54
1:B:310:GLY:O	1:B:313:THR:HG22	2.07	0.54
1:B:707:LEU:HD22	1:B:707:LEU:C	2.28	0.54
1:D:229:ARG:NH1	1:D:239:VAL:HG21	2.22	0.54
1:A:712:ILE:HD12	1:A:712:ILE:C	2.28	0.54
1:B:693:VAL:HG22	1:B:694:PRO:HD3	1.90	0.54
1:C:260:VAL:HG12	1:C:261:ASP:N	2.21	0.54
1:A:358:TRP:CE3	1:A:369:TYR:HB3	2.42	0.54
1:B:388:LEU:O	1:B:392:MET:HG3	2.07	0.54
1:C:121:LEU:C	1:C:124:PRO:HD2	2.28	0.54
1:A:504:VAL:HA	1:A:540:ALA:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:SER:HB2	1:C:630:PRO:HB2	1.90	0.54
1:C:709:SER:OG	1:C:712:ILE:HG23	2.08	0.54
1:C:214:SER:HB2	1:C:217:ARG:HG2	1.89	0.54
1:D:126:VAL:HG21	1:D:191:ALA:HB1	1.90	0.54
1:D:358:TRP:CE3	1:D:369:TYR:HB3	2.43	0.54
1:B:121:LEU:C	1:B:124:PRO:HD2	2.29	0.53
1:C:232:GLU:CG	1:C:233:ASP:N	2.70	0.53
1:B:559:THR:HA	1:B:562:THR:HG23	1.89	0.53
1:B:260:VAL:HG12	1:B:261:ASP:N	2.22	0.53
1:B:232:GLU:CG	1:B:233:ASP:N	2.70	0.53
1:C:559:THR:HA	1:C:562:THR:HG23	1.89	0.53
1:B:600:ILE:HB	1:B:604:ASP:OD1	2.09	0.53
1:D:504:VAL:HA	1:D:540:ALA:O	2.08	0.53
1:D:541:VAL:HG13	1:D:546:VAL:HG21	1.90	0.53
1:A:541:VAL:HG13	1:A:546:VAL:HG21	1.90	0.53
1:B:214:SER:HB2	1:B:217:ARG:HG2	1.89	0.53
1:A:126:VAL:HG21	1:A:191:ALA:HB1	1.90	0.53
1:A:85:PHE:CZ	1:A:200:LEU:HD13	2.43	0.53
1:A:613:LYS:HE2	1:A:636:ASP:OD1	2.09	0.53
1:B:712:ILE:HD12	1:B:712:ILE:C	2.28	0.53
1:C:600:ILE:HB	1:C:604:ASP:OD1	2.09	0.53
1:A:132:PRO:O	1:A:136:ARG:HG3	2.09	0.53
1:B:606:SER:HB2	1:B:630:PRO:HB2	1.91	0.53
1:A:270:PHE:CD1	1:A:282:PRO:HB2	2.42	0.53
1:D:270:PHE:CD1	1:D:282:PRO:HB2	2.42	0.53
1:C:388:LEU:O	1:C:392:MET:HG3	2.08	0.53
1:B:85:PHE:CZ	1:B:200:LEU:HD13	2.43	0.53
1:B:229:ARG:NH1	1:B:239:VAL:HG21	2.22	0.53
1:A:482:GLY:HA3	1:A:499:VAL:CG2	2.35	0.53
1:D:712:ILE:HD12	1:D:712:ILE:C	2.28	0.53
1:D:600:ILE:HB	1:D:604:ASP:OD1	2.09	0.53
1:C:229:ARG:NH1	1:C:239:VAL:HG21	2.22	0.53
1:A:227:ALA:HB1	1:A:250:LEU:HD11	1.90	0.53
1:D:227:ALA:HB1	1:D:250:LEU:HD11	1.90	0.53
1:D:160:TRP:O	1:D:164:MET:CB	2.56	0.53
1:A:160:TRP:O	1:A:164:MET:CB	2.56	0.53
1:A:707:LEU:HD22	1:A:707:LEU:C	2.28	0.53
1:D:709:SER:OG	1:D:712:ILE:HG23	2.08	0.53
1:A:600:ILE:HB	1:A:604:ASP:OD1	2.09	0.53
1:D:214:SER:HB2	1:D:217:ARG:HG2	1.89	0.53
1:D:707:LEU:HD22	1:D:707:LEU:C	2.28	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ASP:O	1:B:662:ARG:HG2	2.09	0.53
1:C:229:ARG:HG2	1:C:250:LEU:CD2	2.34	0.53
1:D:166:ALA:HA	1:D:173:PHE:CE2	2.44	0.53
1:A:499:VAL:O	1:A:502:HIS:HA	2.08	0.53
1:D:499:VAL:O	1:D:502:HIS:HA	2.08	0.53
1:C:712:ILE:HD12	1:C:712:ILE:C	2.29	0.53
1:A:214:SER:HB2	1:A:217:ARG:HG2	1.89	0.53
1:B:229:ARG:HG2	1:B:250:LEU:CD2	2.34	0.53
1:A:166:ALA:HA	1:A:173:PHE:CE2	2.44	0.53
1:C:166:ALA:HA	1:C:173:PHE:CE2	2.44	0.53
1:D:482:GLY:HA3	1:D:499:VAL:CG2	2.36	0.53
1:D:613:LYS:HE2	1:D:636:ASP:OD1	2.09	0.53
1:A:269:SER:O	1:A:285:LYS:HB2	2.09	0.53
1:C:575:MET:HE1	1:C:587:VAL:HG13	1.90	0.53
1:C:499:VAL:O	1:C:502:HIS:HA	2.09	0.53
1:B:499:VAL:O	1:B:502:HIS:HA	2.09	0.53
1:D:693:VAL:HG22	1:D:694:PRO:HD3	1.90	0.53
1:A:693:VAL:HG22	1:A:694:PRO:HD3	1.90	0.53
1:C:693:VAL:HG22	1:C:694:PRO:HD3	1.91	0.53
1:A:555:ILE:O	1:A:555:ILE:HD12	2.09	0.53
1:C:482:GLY:HA3	1:C:499:VAL:CG2	2.35	0.53
1:B:482:GLY:HA3	1:B:499:VAL:CG2	2.35	0.53
1:B:709:SER:OG	1:B:712:ILE:HG23	2.09	0.53
1:B:604:ASP:HB3	1:B:607:ARG:NH2	2.25	0.53
1:D:132:PRO:O	1:D:136:ARG:HG3	2.09	0.53
1:B:504:VAL:HA	1:B:540:ALA:O	2.09	0.53
1:A:660:ASP:O	1:A:662:ARG:HG2	2.09	0.52
1:C:613:LYS:HE2	1:C:636:ASP:OD1	2.09	0.52
1:B:613:LYS:HE2	1:B:636:ASP:OD1	2.09	0.52
1:D:269:SER:O	1:D:285:LYS:HB2	2.09	0.52
1:A:718:ALA:O	1:A:722:VAL:HG12	2.09	0.52
1:D:660:ASP:O	1:D:662:ARG:HG2	2.09	0.52
1:B:166:ALA:HA	1:B:173:PHE:CE2	2.44	0.52
1:C:604:ASP:HB3	1:C:607:ARG:NH2	2.25	0.52
1:D:604:ASP:HB3	1:D:607:ARG:NH2	2.25	0.52
1:B:541:VAL:HG13	1:B:546:VAL:HG21	1.90	0.52
1:D:391:PRO:O	1:D:395:MET:HG2	2.08	0.52
1:D:85:PHE:CZ	1:D:200:LEU:HD13	2.44	0.52
1:A:604:ASP:HB3	1:A:607:ARG:NH2	2.25	0.52
1:A:340:SER:O	1:A:344:VAL:HG13	2.09	0.52
1:D:555:ILE:HD12	1:D:555:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:VAL:HA	1:C:540:ALA:O	2.09	0.52
1:D:606:SER:HB2	1:D:630:PRO:HB2	1.91	0.52
1:B:446:PHE:HE2	1:B:451:ALA:HB2	1.75	0.52
1:A:391:PRO:O	1:A:395:MET:HG2	2.09	0.52
1:D:121:LEU:C	1:D:124:PRO:HD2	2.28	0.52
1:C:660:ASP:O	1:C:662:ARG:HG2	2.10	0.52
1:B:227:ALA:HB1	1:B:250:LEU:HD11	1.90	0.52
1:C:125:VAL:O	1:C:129:GLY:HA2	2.08	0.52
1:C:541:VAL:HG13	1:C:546:VAL:HG21	1.90	0.52
1:A:105:LEU:HD12	1:A:106:LYS:H	1.73	0.52
1:D:340:SER:O	1:D:344:VAL:HG13	2.10	0.52
1:A:575:MET:HE1	1:A:587:VAL:HG13	1.92	0.52
1:C:227:ALA:HB1	1:C:250:LEU:HD11	1.90	0.52
1:D:105:LEU:HD12	1:D:106:LYS:H	1.73	0.52
1:A:606:SER:HB2	1:A:630:PRO:HB2	1.91	0.52
1:A:474:ALA:O	1:A:478:GLY:N	2.42	0.52
1:A:266:GLU:N	1:A:303:VAL:HG12	2.25	0.52
1:B:132:PRO:O	1:B:136:ARG:HG3	2.09	0.52
1:D:474:ALA:O	1:D:478:GLY:N	2.42	0.52
1:C:266:GLU:N	1:C:303:VAL:HG12	2.25	0.52
1:B:266:GLU:N	1:B:303:VAL:HG12	2.25	0.52
1:D:266:GLU:N	1:D:303:VAL:HG12	2.25	0.52
1:C:340:SER:O	1:C:344:VAL:HG13	2.10	0.52
1:D:451:ALA:HB1	1:D:539:MET:HE1	1.92	0.52
1:A:705:GLY:O	1:A:706:LEU:HG	2.09	0.52
1:A:121:LEU:C	1:A:124:PRO:HD2	2.29	0.52
1:C:269:SER:O	1:C:285:LYS:HB2	2.09	0.52
1:B:125:VAL:O	1:B:129:GLY:HA2	2.09	0.52
1:A:78:TYR:HA	1:A:206:LEU:HD12	1.92	0.52
1:B:555:ILE:O	1:B:555:ILE:HD12	2.09	0.52
1:B:82:ARG:O	1:B:86:TRP:HD1	1.93	0.52
1:C:446:PHE:HE2	1:C:451:ALA:HB2	1.75	0.52
1:B:575:MET:HE1	1:B:587:VAL:HG13	1.91	0.52
1:B:450:ASN:HD22	1:C:513:GLN:HG3	1.75	0.52
1:D:78:TYR:HA	1:D:206:LEU:HD12	1.92	0.52
1:C:160:TRP:O	1:C:164:MET:CB	2.57	0.52
1:C:82:ARG:O	1:C:86:TRP:HD1	1.93	0.52
1:B:105:LEU:HD12	1:B:106:LYS:H	1.73	0.52
1:A:510:ARG:HG3	1:A:514:GLU:OE1	2.10	0.52
1:B:510:ARG:HG3	1:B:514:GLU:OE1	2.10	0.52
1:D:705:GLY:O	1:D:706:LEU:HG	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:SER:OG	1:A:712:ILE:HG23	2.10	0.51
1:B:269:SER:O	1:B:285:LYS:HB2	2.09	0.51
1:C:555:ILE:HD12	1:C:555:ILE:O	2.09	0.51
1:B:340:SER:O	1:B:344:VAL:HG13	2.10	0.51
1:B:391:PRO:O	1:B:395:MET:HG2	2.09	0.51
1:C:391:PRO:O	1:C:395:MET:HG2	2.08	0.51
1:B:440:ARG:HB3	1:B:550:VAL:CG2	2.40	0.51
1:C:474:ALA:O	1:C:478:GLY:N	2.42	0.51
1:C:440:ARG:HB3	1:C:550:VAL:CG2	2.40	0.51
1:D:131:TRP:HB3	1:D:132:PRO:HD3	1.92	0.51
1:D:510:ARG:HG3	1:D:514:GLU:OE1	2.10	0.51
1:B:474:ALA:O	1:B:478:GLY:N	2.42	0.51
1:C:132:PRO:O	1:C:136:ARG:HG3	2.09	0.51
1:C:105:LEU:HD12	1:C:106:LYS:H	1.73	0.51
1:A:446:PHE:HE2	1:A:451:ALA:HB2	1.74	0.51
1:B:363:PRO:HB2	1:B:364:GLN:NE2	2.26	0.51
1:C:363:PRO:HB2	1:C:364:GLN:NE2	2.26	0.51
1:A:376:SER:HA	1:A:379:ILE:HG22	1.93	0.51
1:B:160:TRP:O	1:B:164:MET:CB	2.57	0.51
1:D:363:PRO:HB2	1:D:364:GLN:NE2	2.26	0.51
1:C:510:ARG:HG3	1:C:514:GLU:OE1	2.10	0.51
1:D:261:ASP:CG	1:D:293:GLY:H	2.14	0.51
1:C:216:ILE:HG21	1:C:326:GLN:NE2	2.26	0.51
1:A:363:PRO:HB2	1:A:364:GLN:NE2	2.26	0.51
1:C:376:SER:HA	1:C:379:ILE:HG22	1.93	0.51
1:A:261:ASP:CG	1:A:293:GLY:H	2.14	0.51
1:D:446:PHE:HE2	1:D:451:ALA:HB2	1.75	0.51
1:C:705:GLY:O	1:C:706:LEU:HG	2.10	0.51
1:B:705:GLY:O	1:B:706:LEU:HG	2.10	0.51
1:D:575:MET:HE1	1:D:587:VAL:HG13	1.93	0.51
1:B:376:SER:HA	1:B:379:ILE:HG22	1.93	0.51
1:B:216:ILE:HG21	1:B:326:GLN:NE2	2.26	0.51
1:A:440:ARG:HB3	1:A:550:VAL:CG2	2.40	0.51
1:C:425:VAL:HG12	1:C:622:ALA:HB3	1.93	0.51
1:B:425:VAL:HG12	1:B:622:ALA:HB3	1.93	0.51
1:D:440:ARG:HB3	1:D:550:VAL:CG2	2.40	0.51
1:D:82:ARG:O	1:D:86:TRP:HD1	1.93	0.51
1:D:417:MET:HG3	1:D:668:ARG:HA	1.93	0.51
1:D:376:SER:HA	1:D:379:ILE:HG22	1.93	0.51
1:A:82:ARG:O	1:A:86:TRP:HD1	1.93	0.51
1:A:417:MET:HG3	1:A:668:ARG:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:VAL:HG13	1:A:550:VAL:HG12	1.93	0.50
1:A:163:SER:OG	1:A:186:VAL:HG23	2.11	0.50
1:B:447:VAL:HG13	1:C:510:ARG:HH12	1.76	0.50
1:A:75:SER:HB3	1:A:78:TYR:HB3	1.93	0.50
1:A:131:TRP:HB3	1:A:132:PRO:HD3	1.93	0.50
1:C:126:VAL:HG21	1:C:191:ALA:HB1	1.91	0.50
1:B:616:GLY:O	1:B:617:LEU:HD12	2.12	0.50
1:C:358:TRP:O	1:C:362:GLY:HA3	2.11	0.50
1:A:428:THR:O	2:A:995:ALF:F2	2.19	0.50
1:B:163:SER:OG	1:B:186:VAL:HG23	2.12	0.50
1:C:179:SER:N	1:C:180:GLN:HA	2.27	0.50
1:D:616:GLY:O	1:D:617:LEU:HD12	2.12	0.50
1:C:616:GLY:O	1:C:617:LEU:HD12	2.12	0.50
1:C:308:HIS:HB3	1:C:312:ASP:OD1	2.12	0.50
1:D:216:ILE:HG21	1:D:326:GLN:NE2	2.26	0.50
1:A:216:ILE:HG21	1:A:326:GLN:NE2	2.26	0.50
1:D:605:LYS:HD3	1:D:628:ASP:HB3	1.93	0.50
1:B:605:LYS:HD3	1:B:628:ASP:HB3	1.93	0.50
1:D:219:LEU:CD2	1:D:647:VAL:HG12	2.42	0.50
1:A:219:LEU:CD2	1:A:647:VAL:HG12	2.42	0.50
1:B:358:TRP:O	1:B:362:GLY:HA3	2.12	0.50
1:C:417:MET:HG3	1:C:668:ARG:HA	1.93	0.50
1:B:75:SER:HB3	1:B:78:TYR:HB3	1.93	0.50
1:C:131:TRP:HB3	1:C:132:PRO:HD3	1.93	0.50
1:A:616:GLY:O	1:A:617:LEU:HD12	2.12	0.50
1:B:308:HIS:HB3	1:B:312:ASP:OD1	2.12	0.50
1:C:414:LEU:HD21	1:C:670:LEU:CD1	2.42	0.50
1:C:163:SER:OG	1:C:186:VAL:HG23	2.12	0.50
1:B:179:SER:N	1:B:180:GLN:HA	2.27	0.50
1:B:131:TRP:HB3	1:B:132:PRO:HD3	1.93	0.50
1:D:75:SER:HB3	1:D:78:TYR:HB3	1.93	0.50
1:A:358:TRP:O	1:A:362:GLY:HA3	2.11	0.50
1:D:163:SER:OG	1:D:186:VAL:HG23	2.12	0.50
1:B:417:MET:HG3	1:B:668:ARG:HA	1.93	0.50
1:C:75:SER:HB3	1:C:78:TYR:HB3	1.93	0.50
1:D:358:TRP:O	1:D:362:GLY:HA3	2.11	0.50
1:C:258:ILE:HD12	1:C:295:THR:CG2	2.42	0.50
1:B:266:GLU:H	1:B:303:VAL:HG12	1.77	0.50
1:D:232:GLU:CG	1:D:233:ASP:N	2.70	0.50
1:B:414:LEU:HD21	1:B:670:LEU:CD1	2.42	0.50
1:D:425:VAL:HG12	1:D:622:ALA:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:H	1:A:367:LEU:CD1	2.25	0.50
1:A:232:GLU:CG	1:A:233:ASP:N	2.70	0.49
1:A:657:LEU:HG	1:A:658:HIS:N	2.27	0.49
1:B:90:MET:O	1:B:94:PRO:HD3	2.12	0.49
1:B:261:ASP:CG	1:B:293:GLY:H	2.14	0.49
1:C:266:GLU:H	1:C:303:VAL:HG12	1.77	0.49
1:B:78:TYR:HA	1:B:206:LEU:HD12	1.93	0.49
1:D:615:LYS:HG3	1:D:616:GLY:N	2.25	0.49
1:C:688:TYR:CE1	1:C:719:LEU:HD23	2.47	0.49
1:B:110:SER:O	1:B:111:GLY:C	2.51	0.49
1:C:78:TYR:HA	1:C:206:LEU:HD12	1.93	0.49
1:A:615:LYS:HG3	1:A:616:GLY:N	2.26	0.49
1:D:687:ILE:HA	1:D:690:VAL:CG1	2.41	0.49
1:B:680:GLN:O	1:B:683:PHE:HB3	2.12	0.49
1:A:86:TRP:HB2	1:C:703:LEU:HD21	1.93	0.49
1:B:260:VAL:CG1	1:B:261:ASP:N	2.75	0.49
1:C:260:VAL:CG1	1:C:261:ASP:N	2.75	0.49
1:C:261:ASP:CG	1:C:293:GLY:H	2.14	0.49
1:A:605:LYS:HD3	1:A:628:ASP:HB3	1.94	0.49
1:C:735:THR:O	1:C:736:LEU:C	2.51	0.49
1:B:735:THR:O	1:B:736:LEU:C	2.51	0.49
1:B:126:VAL:HG21	1:B:191:ALA:HB1	1.93	0.49
1:C:276:VAL:HG13	1:C:602:PRO:HD3	1.94	0.49
1:D:258:ILE:HD12	1:D:295:THR:CG2	2.42	0.49
1:D:367:LEU:H	1:D:367:LEU:CD1	2.26	0.49
1:D:657:LEU:HG	1:D:658:HIS:N	2.27	0.49
1:D:260:VAL:CG1	1:D:261:ASP:N	2.75	0.49
1:C:605:LYS:HD3	1:C:628:ASP:HB3	1.94	0.49
1:A:425:VAL:HG12	1:A:622:ALA:HB3	1.94	0.49
1:A:276:VAL:HG13	1:A:602:PRO:HD3	1.94	0.49
1:D:536:VAL:HG13	1:D:550:VAL:HG12	1.95	0.49
1:D:468:ASN:HA	1:D:471:VAL:HG22	1.94	0.49
1:A:468:ASN:HA	1:A:471:VAL:HG22	1.94	0.49
1:C:90:MET:O	1:C:94:PRO:HD3	2.13	0.49
1:A:260:VAL:CG1	1:A:261:ASP:N	2.75	0.49
1:D:276:VAL:HG13	1:D:602:PRO:HD3	1.94	0.49
1:C:258:ILE:HD12	1:C:295:THR:HG23	1.95	0.49
1:C:110:SER:O	1:C:111:GLY:C	2.51	0.49
1:D:159:ALA:CB	1:D:379:ILE:HD13	2.41	0.49
1:A:308:HIS:HB3	1:A:312:ASP:OD1	2.12	0.49
1:D:414:LEU:HD21	1:D:670:LEU:CD1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CD2	1:B:647:VAL:HG12	2.42	0.49
1:B:162:TYR:HB2	1:B:375:VAL:HG11	1.94	0.49
1:B:258:ILE:HD12	1:B:295:THR:CG2	2.43	0.49
1:A:266:GLU:H	1:A:303:VAL:HG12	1.77	0.49
1:A:179:SER:N	1:A:180:GLN:HA	2.27	0.49
1:D:680:GLN:O	1:D:683:PHE:HB3	2.12	0.49
1:C:693:VAL:N	1:C:694:PRO:HD2	2.28	0.49
1:B:687:ILE:HA	1:B:690:VAL:CG1	2.42	0.49
1:D:308:HIS:HB3	1:D:312:ASP:OD1	2.12	0.49
1:A:414:LEU:HD21	1:A:670:LEU:CD1	2.42	0.49
1:C:219:LEU:CD2	1:C:647:VAL:HG12	2.42	0.49
1:B:276:VAL:HG13	1:B:602:PRO:HD3	1.94	0.49
1:A:258:ILE:HD12	1:A:295:THR:CG2	2.43	0.49
1:B:163:SER:O	1:B:167:VAL:HG12	2.13	0.49
1:D:179:SER:N	1:D:180:GLN:HA	2.27	0.49
1:B:152:ILE:O	1:B:156:ILE:HG12	2.13	0.49
1:B:703:LEU:HD21	1:D:86:TRP:HB2	1.95	0.49
1:D:342:TRP:C	1:D:345:PRO:HD2	2.33	0.49
1:B:468:ASN:HA	1:B:471:VAL:HG22	1.94	0.49
1:D:266:GLU:H	1:D:303:VAL:HG12	1.77	0.49
1:A:152:ILE:O	1:A:156:ILE:HG12	2.13	0.49
1:A:78:TYR:CD2	1:A:79:LEU:HD12	2.42	0.49
1:D:152:ILE:O	1:D:156:ILE:HG12	2.13	0.49
1:B:693:VAL:N	1:B:694:PRO:HD2	2.28	0.49
1:A:735:THR:O	1:A:736:LEU:C	2.51	0.49
1:D:735:THR:O	1:D:736:LEU:C	2.51	0.49
1:C:468:ASN:HA	1:C:471:VAL:HG22	1.94	0.49
1:B:367:LEU:CD1	1:B:367:LEU:H	2.25	0.49
1:B:657:LEU:HG	1:B:658:HIS:N	2.27	0.49
1:C:657:LEU:HG	1:C:658:HIS:N	2.27	0.49
1:C:152:ILE:O	1:C:156:ILE:HG12	2.13	0.49
1:B:605:LYS:CD	1:B:628:ASP:HB3	2.43	0.49
1:B:447:VAL:HG22	1:C:513:GLN:OE1	2.12	0.48
1:A:680:GLN:O	1:A:683:PHE:HB3	2.13	0.48
1:C:687:ILE:HA	1:C:690:VAL:CG1	2.42	0.48
1:A:220:LEU:HG	1:A:647:VAL:HG11	1.96	0.48
1:A:342:TRP:C	1:A:345:PRO:HD2	2.34	0.48
1:C:536:VAL:HG13	1:C:550:VAL:HG12	1.95	0.48
1:C:367:LEU:CD1	1:C:367:LEU:H	2.25	0.48
1:D:430:THR:HG22	1:D:641:MET:HG3	1.94	0.48
1:A:688:TYR:CE1	1:A:719:LEU:HD23	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HA	1:A:690:VAL:CG1	2.42	0.48
1:A:90:MET:O	1:A:94:PRO:HD3	2.13	0.48
1:D:605:LYS:CD	1:D:628:ASP:HB3	2.43	0.48
1:B:639:ILE:CG2	1:B:656:LEU:HD13	2.43	0.48
1:D:90:MET:O	1:D:94:PRO:HD3	2.13	0.48
1:C:342:TRP:C	1:C:345:PRO:HD2	2.33	0.48
1:D:220:LEU:HG	1:D:647:VAL:HG11	1.96	0.48
1:A:426:ASP:OD2	2:A:995:ALF:F2	2.20	0.48
1:B:258:ILE:HD12	1:B:295:THR:HG23	1.95	0.48
1:D:162:TYR:HB2	1:D:375:VAL:HG11	1.95	0.48
1:D:110:SER:O	1:D:111:GLY:C	2.50	0.48
1:C:639:ILE:CG2	1:C:656:LEU:HD13	2.43	0.48
1:A:269:SER:HB3	1:A:300:GLY:HA3	1.96	0.48
1:D:78:TYR:CD2	1:D:79:LEU:HD12	2.43	0.48
1:C:680:GLN:O	1:C:683:PHE:HB3	2.13	0.48
1:B:143:THR:OG1	1:B:144:GLY:N	2.47	0.48
1:A:163:SER:O	1:A:167:VAL:HG12	2.13	0.48
1:A:510:ARG:O	1:A:514:GLU:HG3	2.13	0.48
1:A:162:TYR:HB2	1:A:375:VAL:HG11	1.95	0.48
1:B:224:PRO:O	1:B:241:LEU:HD22	2.14	0.48
1:C:224:PRO:O	1:C:241:LEU:HD22	2.14	0.48
1:D:269:SER:HB3	1:D:300:GLY:HA3	1.96	0.48
1:A:605:LYS:CD	1:A:628:ASP:HB3	2.44	0.48
1:B:220:LEU:HG	1:B:647:VAL:HG11	1.95	0.48
1:A:143:THR:OG1	1:A:144:GLY:N	2.47	0.48
1:D:143:THR:OG1	1:D:144:GLY:N	2.47	0.48
1:C:143:THR:OG1	1:C:144:GLY:N	2.47	0.48
1:B:510:ARG:O	1:B:514:GLU:HG3	2.13	0.48
1:D:510:ARG:O	1:D:514:GLU:HG3	2.13	0.48
1:C:162:TYR:HB2	1:C:375:VAL:HG11	1.95	0.48
1:C:636:ASP:O	1:C:637:ILE:HD13	2.14	0.48
1:C:657:LEU:O	1:C:658:HIS:CB	2.61	0.48
1:D:693:VAL:N	1:D:694:PRO:HD2	2.29	0.48
1:C:220:LEU:HG	1:C:647:VAL:HG11	1.96	0.48
1:D:390:THR:N	1:D:391:PRO:HD2	2.29	0.48
1:B:536:VAL:HG13	1:B:550:VAL:HG12	1.96	0.48
1:C:163:SER:O	1:C:167:VAL:HG12	2.14	0.48
1:D:163:SER:O	1:D:167:VAL:HG12	2.14	0.48
1:A:224:PRO:O	1:A:241:LEU:HD22	2.14	0.48
1:B:657:LEU:O	1:B:658:HIS:CB	2.61	0.48
1:B:544:LYS:O	1:B:546:VAL:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TRP:C	1:B:345:PRO:HD2	2.34	0.48
1:D:692:GLY:O	1:D:695:LEU:HG	2.14	0.48
1:B:440:ARG:HB3	1:B:550:VAL:HG21	1.96	0.48
1:D:136:ARG:HD2	1:D:149:PHE:CE2	2.49	0.48
1:C:605:LYS:CD	1:C:628:ASP:HB3	2.44	0.48
1:A:110:SER:O	1:A:111:GLY:C	2.51	0.48
1:C:510:ARG:O	1:C:514:GLU:HG3	2.13	0.48
1:B:636:ASP:O	1:B:637:ILE:HD13	2.14	0.48
1:A:159:ALA:CB	1:A:379:ILE:HD13	2.42	0.48
1:B:702:PRO:O	1:B:703:LEU:C	2.52	0.48
1:A:390:THR:N	1:A:391:PRO:HD2	2.29	0.48
1:C:269:SER:HB3	1:C:300:GLY:HA3	1.96	0.47
1:D:657:LEU:O	1:D:658:HIS:CB	2.61	0.47
1:A:657:LEU:O	1:A:658:HIS:CB	2.61	0.47
1:A:693:VAL:N	1:A:694:PRO:HD2	2.29	0.47
1:A:636:ASP:O	1:A:637:ILE:HD13	2.14	0.47
1:D:224:PRO:O	1:D:241:LEU:HD22	2.14	0.47
1:B:269:SER:HB3	1:B:300:GLY:HA3	1.96	0.47
1:C:430:THR:HG22	1:C:641:MET:HG3	1.95	0.47
1:B:688:TYR:CE1	1:B:719:LEU:HD23	2.49	0.47
1:C:440:ARG:HB3	1:C:550:VAL:HG21	1.97	0.47
1:D:440:ARG:HB3	1:D:550:VAL:HG21	1.96	0.47
1:A:136:ARG:HD2	1:A:149:PHE:CE2	2.50	0.47
1:A:692:GLY:O	1:A:695:LEU:HG	2.14	0.47
1:A:440:ARG:HB3	1:A:550:VAL:HG21	1.96	0.47
1:C:297:ASN:O	1:C:298:GLN:HG3	2.14	0.47
1:C:702:PRO:O	1:C:703:LEU:C	2.52	0.47
1:C:146:LEU:HD13	1:C:344:VAL:HG22	1.97	0.47
1:C:692:GLY:O	1:C:695:LEU:HG	2.14	0.47
1:D:258:ILE:HD12	1:D:295:THR:HG23	1.96	0.47
1:D:92:THR:O	1:D:95:VAL:HB	2.15	0.47
1:D:224:PRO:HD3	1:D:257:LYS:HD2	1.97	0.47
1:A:430:THR:HG22	1:A:641:MET:HG3	1.95	0.47
1:C:164:MET:HE2	1:C:164:MET:HA	1.97	0.47
1:C:216:ILE:HD11	1:C:322:VAL:HG21	1.97	0.47
1:A:216:ILE:HG21	1:A:326:GLN:HE22	1.79	0.47
1:A:146:LEU:HD13	1:A:344:VAL:HG22	1.97	0.47
1:B:692:GLY:O	1:B:695:LEU:HG	2.15	0.47
1:A:258:ILE:HD12	1:A:295:THR:HG23	1.96	0.47
1:B:297:ASN:O	1:B:298:GLN:HG3	2.14	0.47
1:B:224:PRO:HD3	1:B:257:LYS:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:PRO:HD3	1:C:257:LYS:HD2	1.97	0.47
1:A:224:PRO:HD3	1:A:257:LYS:HD2	1.97	0.47
1:B:708:LEU:HD13	1:B:709:SER:N	2.30	0.47
1:B:159:ALA:CB	1:B:379:ILE:HD13	2.41	0.47
1:D:616:GLY:C	1:D:617:LEU:HD12	2.35	0.47
1:A:419:LYS:C	1:A:618:ILE:HD12	2.34	0.47
1:D:179:SER:HB3	1:D:181:GLU:C	2.34	0.47
1:D:636:ASP:O	1:D:637:ILE:HD13	2.15	0.47
1:C:708:LEU:HD13	1:C:709:SER:N	2.30	0.47
1:B:430:THR:HG22	1:B:641:MET:HG3	1.95	0.47
1:B:641:MET:HE1	1:B:659:GLY:O	2.15	0.47
1:B:657:LEU:O	1:B:659:GLY:HA2	2.14	0.47
1:C:641:MET:HE1	1:C:659:GLY:O	2.15	0.47
1:A:430:THR:HA	1:A:641:MET:HE2	1.95	0.47
1:A:616:GLY:C	1:A:617:LEU:HD12	2.35	0.47
1:C:615:LYS:HG3	1:C:616:GLY:N	2.25	0.47
1:D:131:TRP:N	1:D:132:PRO:CD	2.77	0.47
1:B:615:LYS:HG3	1:B:616:GLY:N	2.25	0.47
1:B:616:GLY:C	1:B:617:LEU:HD12	2.35	0.47
1:B:216:ILE:HD11	1:B:322:VAL:HG21	1.97	0.47
1:D:216:ILE:HG21	1:D:326:GLN:HE22	1.79	0.47
1:A:539:MET:CE	1:A:547:ALA:HB3	2.45	0.47
1:C:657:LEU:O	1:C:659:GLY:HA2	2.14	0.47
1:C:616:GLY:C	1:C:617:LEU:HD12	2.35	0.47
1:D:605:LYS:CE	1:D:628:ASP:HB3	2.44	0.47
1:A:297:ASN:O	1:A:298:GLN:HG3	2.14	0.47
1:D:297:ASN:O	1:D:298:GLN:HG3	2.14	0.47
1:D:479:LEU:HD22	1:D:479:LEU:C	2.35	0.47
1:D:713:ALA:O	1:D:717:MET:HG3	2.15	0.47
1:D:407:LEU:HD23	1:D:407:LEU:N	2.28	0.47
1:A:92:THR:O	1:A:95:VAL:HB	2.15	0.47
1:B:179:SER:HB3	1:B:181:GLU:C	2.35	0.47
1:A:690:VAL:HA	1:A:693:VAL:HG13	1.97	0.47
1:D:540:ALA:HB2	1:D:545:THR:HA	1.97	0.47
1:D:216:ILE:HD11	1:D:322:VAL:HG21	1.97	0.47
1:D:539:MET:CE	1:D:547:ALA:HB3	2.45	0.47
1:C:92:THR:O	1:C:95:VAL:HB	2.15	0.47
1:B:479:LEU:HD22	1:B:479:LEU:C	2.35	0.47
1:B:179:SER:CB	1:B:183:VAL:HG22	2.45	0.47
1:D:639:ILE:CG2	1:D:656:LEU:HD13	2.44	0.47
1:B:562:THR:OG1	1:B:661:LEU:HD22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:LEU:O	1:D:659:GLY:HA2	2.14	0.47
1:C:136:ARG:HD2	1:C:149:PHE:CE2	2.49	0.47
1:D:690:VAL:HA	1:D:693:VAL:HG13	1.97	0.47
1:A:605:LYS:CE	1:A:628:ASP:HB3	2.44	0.47
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.74	0.47
1:B:146:LEU:HD13	1:B:344:VAL:HG22	1.97	0.47
1:C:419:LYS:C	1:C:618:ILE:HD12	2.35	0.47
1:C:479:LEU:HD22	1:C:479:LEU:C	2.35	0.47
1:B:186:VAL:HG22	1:B:188:PHE:H	1.80	0.46
1:D:119:LEU:HD12	1:D:167:VAL:CG1	2.45	0.46
1:C:109:ILE:HG23	1:C:110:SER:CB	2.29	0.46
1:C:179:SER:HB3	1:C:181:GLU:C	2.35	0.46
1:A:639:ILE:CG2	1:A:656:LEU:HD13	2.44	0.46
1:A:131:TRP:N	1:A:132:PRO:CD	2.78	0.46
1:C:544:LYS:O	1:C:546:VAL:HG13	2.15	0.46
1:B:261:ASP:HB3	1:B:307:LEU:HB3	1.97	0.46
1:A:540:ALA:HB2	1:A:545:THR:HA	1.97	0.46
1:A:479:LEU:HD22	1:A:479:LEU:C	2.35	0.46
1:A:407:LEU:HD23	1:A:407:LEU:N	2.29	0.46
1:A:657:LEU:O	1:A:659:GLY:HA2	2.14	0.46
1:B:605:LYS:CE	1:B:628:ASP:HB3	2.43	0.46
1:C:216:ILE:HG21	1:C:326:GLN:HE22	1.79	0.46
1:D:146:LEU:HD13	1:D:344:VAL:HG22	1.97	0.46
1:A:216:ILE:HD11	1:A:322:VAL:HG21	1.97	0.46
1:C:539:MET:CE	1:C:547:ALA:HB3	2.45	0.46
1:A:702:PRO:O	1:A:703:LEU:C	2.52	0.46
1:D:702:PRO:O	1:D:703:LEU:C	2.52	0.46
1:A:119:LEU:HD12	1:A:167:VAL:CG1	2.46	0.46
1:C:562:THR:OG1	1:C:661:LEU:HD22	2.16	0.46
1:C:159:ALA:CB	1:C:379:ILE:HD13	2.42	0.46
1:B:131:TRP:N	1:B:132:PRO:CD	2.78	0.46
1:C:540:ALA:HB2	1:C:545:THR:HA	1.97	0.46
1:C:261:ASP:HB3	1:C:307:LEU:HB3	1.98	0.46
1:D:414:LEU:HA	1:D:414:LEU:HD23	1.73	0.46
1:B:390:THR:N	1:B:391:PRO:HD2	2.30	0.46
1:B:460:HIS:HA	1:B:471:VAL:HG11	1.97	0.46
1:B:136:ARG:HD2	1:B:149:PHE:CE2	2.50	0.46
1:A:88:ALA:CB	1:A:125:VAL:HG23	2.46	0.46
1:D:544:LYS:O	1:D:546:VAL:HG13	2.15	0.46
1:D:490:PRO:HB2	1:D:493:LYS:HB2	1.98	0.46
1:C:390:THR:N	1:C:391:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LYS:C	1:B:618:ILE:HD12	2.35	0.46
1:C:574:VAL:HG22	1:C:595:LYS:HB2	1.97	0.46
1:C:119:LEU:HD12	1:C:167:VAL:CG1	2.45	0.46
1:D:109:ILE:HG23	1:D:110:SER:CB	2.30	0.46
1:A:179:SER:HB3	1:A:181:GLU:C	2.36	0.46
1:D:708:LEU:HD13	1:D:709:SER:N	2.30	0.46
1:C:88:ALA:CB	1:C:125:VAL:HG23	2.46	0.46
1:B:621:MET:CE	1:B:628:ASP:HB2	2.46	0.46
1:D:455:ALA:HB2	1:D:539:MET:SD	2.55	0.46
1:A:713:ALA:O	1:A:717:MET:HG3	2.16	0.46
1:C:186:VAL:HG22	1:C:188:PHE:H	1.81	0.46
1:C:621:MET:CE	1:C:628:ASP:HB2	2.46	0.46
1:C:460:HIS:HA	1:C:471:VAL:HG11	1.97	0.46
1:A:574:VAL:HG22	1:A:595:LYS:HB2	1.98	0.46
1:A:186:VAL:HG22	1:A:188:PHE:H	1.80	0.46
1:A:109:ILE:HG23	1:A:110:SER:CB	2.30	0.46
1:A:708:LEU:HD13	1:A:709:SER:N	2.30	0.46
1:C:131:TRP:N	1:C:132:PRO:CD	2.78	0.46
1:B:540:ALA:HB2	1:B:545:THR:HA	1.97	0.46
1:A:490:PRO:HB2	1:A:493:LYS:HB2	1.98	0.46
1:C:605:LYS:CE	1:C:628:ASP:HB3	2.44	0.46
1:B:216:ILE:HG21	1:B:326:GLN:HE22	1.79	0.46
1:D:419:LYS:C	1:D:618:ILE:HD12	2.35	0.46
1:C:713:ALA:O	1:C:717:MET:HG3	2.16	0.46
1:D:186:VAL:HG22	1:D:188:PHE:H	1.80	0.46
1:B:109:ILE:HG23	1:B:110:SER:CB	2.30	0.46
1:D:178:ARG:HB2	1:D:184:VAL:HA	1.98	0.46
1:C:179:SER:CB	1:C:183:VAL:HG22	2.46	0.46
1:C:559:THR:N	1:C:560:PRO:HD2	2.31	0.46
1:B:164:MET:HE2	1:B:164:MET:HA	1.98	0.46
1:B:446:PHE:CE2	1:B:451:ALA:HB2	2.51	0.46
1:B:727:ASN:O	1:B:730:ARG:HB3	2.16	0.46
1:B:381:ALA:O	1:B:383:PRO:HD3	2.15	0.46
1:A:178:ARG:HB2	1:A:184:VAL:HA	1.98	0.46
1:D:430:THR:HA	1:D:641:MET:HE2	1.96	0.46
1:A:688:TYR:CD2	1:A:719:LEU:HB3	2.51	0.46
1:C:490:PRO:HB2	1:C:493:LYS:HB2	1.98	0.46
1:B:490:PRO:HB2	1:B:493:LYS:HB2	1.98	0.46
1:D:601:MET:HB3	1:D:602:PRO:HD2	1.97	0.46
1:B:574:VAL:HG22	1:B:595:LYS:HB2	1.98	0.46
1:C:381:ALA:O	1:C:383:PRO:HD3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD12	1:B:167:VAL:CG1	2.46	0.46
1:B:447:VAL:HG13	1:C:510:ARG:NH1	2.31	0.46
1:D:88:ALA:CB	1:D:125:VAL:HG23	2.46	0.46
1:C:164:MET:HA	1:C:164:MET:CE	2.46	0.46
1:D:688:TYR:CD2	1:D:719:LEU:HB3	2.51	0.46
1:D:688:TYR:CE1	1:D:719:LEU:HD23	2.50	0.46
1:A:621:MET:CE	1:A:628:ASP:HB2	2.46	0.46
1:D:621:MET:CE	1:D:628:ASP:HB2	2.46	0.46
1:B:670:LEU:O	1:B:673:SER:HB3	2.16	0.46
1:C:626:VAL:HA	1:C:647:VAL:HG22	1.98	0.46
1:C:695:LEU:HD12	1:C:695:LEU:C	2.37	0.46
1:B:92:THR:O	1:B:95:VAL:HB	2.16	0.46
1:A:422:THR:HG23	1:A:619:VAL:HG23	1.98	0.46
1:D:574:VAL:HG22	1:D:595:LYS:HB2	1.98	0.46
1:C:427:LYS:HG3	1:C:428:THR:N	2.31	0.46
1:D:179:SER:CB	1:D:183:VAL:HG22	2.45	0.45
1:C:178:ARG:HB2	1:C:184:VAL:HA	1.98	0.45
1:A:544:LYS:O	1:A:546:VAL:HG13	2.15	0.45
1:C:414:LEU:HD23	1:C:414:LEU:HA	1.73	0.45
1:A:629:ALA:HA	1:A:632:LEU:HD23	1.98	0.45
1:A:446:PHE:CE2	1:A:451:ALA:HB2	2.51	0.45
1:B:695:LEU:C	1:B:695:LEU:HD12	2.37	0.45
1:B:135:LYS:HG2	1:B:139:GLN:NE2	2.31	0.45
1:B:713:ALA:O	1:B:717:MET:HG3	2.16	0.45
1:B:690:VAL:HA	1:B:693:VAL:HG13	1.97	0.45
1:A:261:ASP:HB3	1:A:307:LEU:HB3	1.97	0.45
1:D:261:ASP:HB3	1:D:307:LEU:HB3	1.97	0.45
1:B:626:VAL:HA	1:B:647:VAL:HG22	1.98	0.45
1:B:539:MET:CE	1:B:547:ALA:HB3	2.46	0.45
1:D:446:PHE:CE2	1:D:451:ALA:HB2	2.51	0.45
1:A:601:MET:HB3	1:A:602:PRO:HD2	1.98	0.45
1:A:427:LYS:HG3	1:A:428:THR:N	2.30	0.45
1:C:135:LYS:HG2	1:C:139:GLN:NE2	2.31	0.45
1:D:422:THR:HG23	1:D:619:VAL:HG23	1.98	0.45
1:B:178:ARG:HB2	1:B:184:VAL:HA	1.98	0.45
1:B:164:MET:CE	1:B:164:MET:HA	2.46	0.45
1:B:690:VAL:O	1:B:694:PRO:HD3	2.16	0.45
1:D:670:LEU:O	1:D:673:SER:HB3	2.16	0.45
1:B:219:LEU:HD22	1:B:219:LEU:C	2.36	0.45
1:D:219:LEU:HD22	1:D:219:LEU:C	2.36	0.45
1:A:219:LEU:HD22	1:A:219:LEU:C	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:O	1:A:550:VAL:HG22	2.16	0.45
1:B:427:LYS:HG3	1:B:428:THR:N	2.31	0.45
1:C:178:ARG:HA	1:C:178:ARG:HD3	1.73	0.45
1:C:600:ILE:HD12	1:C:600:ILE:O	2.16	0.45
1:C:629:ALA:HA	1:C:632:LEU:HD23	1.99	0.45
1:C:446:PHE:CE2	1:C:451:ALA:HB2	2.51	0.45
1:B:440:ARG:O	1:B:550:VAL:HG22	2.16	0.45
1:D:440:ARG:O	1:D:550:VAL:HG22	2.16	0.45
1:A:479:LEU:HD13	1:A:480:SER:H	1.81	0.45
1:C:218:ALA:O	1:C:221:LYS:HB2	2.17	0.45
1:D:727:ASN:O	1:D:730:ARG:HB3	2.16	0.45
1:A:562:THR:OG1	1:A:661:LEU:HD22	2.16	0.45
1:D:562:THR:OG1	1:D:661:LEU:HD22	2.16	0.45
1:D:657:LEU:C	1:D:659:GLY:HA2	2.37	0.45
1:C:219:LEU:C	1:C:219:LEU:HD22	2.36	0.45
1:C:292:ILE:O	1:C:295:THR:HG22	2.16	0.45
1:D:460:HIS:HA	1:D:471:VAL:HG11	1.97	0.45
1:A:460:HIS:HA	1:A:471:VAL:HG11	1.97	0.45
1:B:292:ILE:O	1:B:295:THR:HG22	2.16	0.45
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.77	0.45
1:C:407:LEU:HD23	1:C:407:LEU:N	2.29	0.45
1:B:218:ALA:O	1:B:221:LYS:HB2	2.17	0.45
1:A:179:SER:CB	1:A:183:VAL:HG22	2.46	0.45
1:A:559:THR:N	1:A:560:PRO:HD2	2.32	0.45
1:B:559:THR:N	1:B:560:PRO:HD2	2.32	0.45
1:C:656:LEU:HD22	1:C:661:LEU:HA	1.98	0.45
1:D:629:ALA:HA	1:D:632:LEU:HD23	1.99	0.45
1:C:392:MET:O	1:C:396:VAL:HG12	2.16	0.45
1:D:135:LYS:HG2	1:D:139:GLN:NE2	2.31	0.45
1:B:178:ARG:HD3	1:B:178:ARG:HA	1.73	0.45
1:B:600:ILE:O	1:B:600:ILE:HD12	2.17	0.45
1:A:657:LEU:C	1:A:659:GLY:HA2	2.37	0.45
1:C:690:VAL:O	1:C:694:PRO:HD3	2.17	0.45
1:A:626:VAL:HA	1:A:647:VAL:HG22	1.97	0.45
1:B:629:ALA:HA	1:B:632:LEU:HD23	1.99	0.45
1:B:455:ALA:HB2	1:B:539:MET:SD	2.57	0.45
1:C:706:LEU:HB3	1:C:707:LEU:H	1.42	0.45
1:B:706:LEU:HB3	1:B:707:LEU:H	1.42	0.45
1:D:695:LEU:C	1:D:695:LEU:HD12	2.37	0.45
1:B:479:LEU:HD13	1:B:480:SER:H	1.82	0.45
1:D:427:LYS:HG3	1:D:428:THR:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:GLN:HG2	1:C:502:HIS:O	2.17	0.45
1:A:417:MET:HE1	1:A:637:ILE:HG21	1.98	0.45
1:A:600:ILE:HD12	1:A:600:ILE:O	2.16	0.45
1:C:688:TYR:CD2	1:C:719:LEU:HB3	2.51	0.45
1:A:690:VAL:O	1:A:694:PRO:HD3	2.17	0.45
1:C:670:LEU:O	1:C:673:SER:HB3	2.17	0.45
1:D:626:VAL:HA	1:D:647:VAL:HG22	1.98	0.45
1:D:539:MET:HE2	1:D:547:ALA:HB3	1.99	0.45
1:D:343:PHE:O	1:D:347:VAL:HG23	2.17	0.45
1:C:140:SER:HG	1:C:150:THR:HG22	1.82	0.45
1:A:670:LEU:O	1:A:673:SER:HB3	2.17	0.45
1:A:695:LEU:C	1:A:695:LEU:HD12	2.37	0.45
1:C:440:ARG:O	1:C:550:VAL:HG22	2.16	0.45
1:D:479:LEU:HD13	1:D:480:SER:H	1.82	0.45
1:A:135:LYS:HG2	1:A:139:GLN:NE2	2.31	0.45
1:B:656:LEU:HD22	1:B:661:LEU:HA	1.98	0.45
1:C:690:VAL:HA	1:C:693:VAL:HG13	1.98	0.45
1:C:479:LEU:HD13	1:C:480:SER:H	1.82	0.45
1:A:343:PHE:O	1:A:347:VAL:HG23	2.17	0.45
1:A:365:PRO:HA	1:A:366:ALA:C	2.37	0.45
1:C:524:GLU:HA	1:C:527:ASP:OD2	2.17	0.45
1:C:343:PHE:O	1:C:347:VAL:HG23	2.16	0.45
1:D:548:LEU:HD12	1:D:548:LEU:HA	1.77	0.45
1:A:656:LEU:HD22	1:A:661:LEU:HA	1.98	0.44
1:D:559:THR:N	1:D:560:PRO:HD2	2.32	0.44
1:B:657:LEU:C	1:B:659:GLY:HA2	2.37	0.44
1:D:600:ILE:HD12	1:D:600:ILE:O	2.17	0.44
1:B:122:ALA:O	1:B:125:VAL:HG12	2.17	0.44
1:B:688:TYR:CD2	1:B:719:LEU:HB3	2.51	0.44
1:D:261:ASP:HA	1:D:293:GLY:N	2.33	0.44
1:A:451:ALA:HB1	1:A:539:MET:HE1	1.98	0.44
1:D:392:MET:O	1:D:396:VAL:HG12	2.17	0.44
1:B:407:LEU:HD23	1:B:407:LEU:N	2.30	0.44
1:C:727:ASN:O	1:C:730:ARG:HB3	2.17	0.44
1:C:230:ILE:HG12	1:C:235:SER:O	2.17	0.44
1:C:657:LEU:C	1:C:659:GLY:HA2	2.37	0.44
1:D:430:THR:HG21	1:D:623:GLY:CA	2.43	0.44
1:A:261:ASP:HA	1:A:293:GLY:N	2.33	0.44
1:C:576:LEU:HB3	1:C:605:LYS:HZ2	1.83	0.44
1:C:601:MET:HB3	1:C:602:PRO:HD2	1.98	0.44
1:B:601:MET:HB3	1:B:602:PRO:HD2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LEU:HD13	1:B:480:SER:N	2.33	0.44
1:C:450:ASN:O	1:C:454:LEU:HG	2.17	0.44
1:B:498:GLN:HG2	1:B:502:HIS:O	2.17	0.44
1:B:230:ILE:HG12	1:B:235:SER:O	2.17	0.44
1:B:88:ALA:CB	1:B:125:VAL:HG23	2.47	0.44
1:D:690:VAL:O	1:D:694:PRO:HD3	2.17	0.44
1:B:422:THR:HG23	1:B:619:VAL:HG23	1.98	0.44
1:A:727:ASN:O	1:A:730:ARG:HB3	2.17	0.44
1:B:365:PRO:HA	1:B:366:ALA:C	2.37	0.44
1:D:365:PRO:HA	1:D:366:ALA:C	2.37	0.44
1:B:450:ASN:O	1:B:454:LEU:HG	2.17	0.44
1:A:450:ASN:O	1:A:454:LEU:HG	2.18	0.44
1:A:498:GLN:HG2	1:A:502:HIS:O	2.17	0.44
1:D:498:GLN:HG2	1:D:502:HIS:O	2.17	0.44
1:D:413:ALA:HB1	1:D:654:VAL:HG23	1.99	0.44
1:D:656:LEU:HD22	1:D:661:LEU:HA	1.98	0.44
1:B:392:MET:O	1:B:396:VAL:HG12	2.17	0.44
1:D:468:ASN:O	1:D:472:HIS:HB2	2.18	0.44
1:A:292:ILE:O	1:A:295:THR:HG22	2.17	0.44
1:D:381:ALA:O	1:D:383:PRO:HD3	2.16	0.44
1:D:218:ALA:O	1:D:221:LYS:HB2	2.17	0.44
1:A:218:ALA:O	1:A:221:LYS:HB2	2.17	0.44
1:C:365:PRO:HA	1:C:366:ALA:C	2.37	0.44
1:D:450:ASN:O	1:D:454:LEU:HG	2.18	0.44
1:A:122:ALA:O	1:A:125:VAL:HG12	2.17	0.44
1:A:392:MET:O	1:A:396:VAL:HG12	2.17	0.44
1:A:468:ASN:O	1:A:472:HIS:HB2	2.18	0.44
1:B:343:PHE:O	1:B:347:VAL:HG23	2.17	0.44
1:A:430:THR:HG21	1:A:623:GLY:CA	2.44	0.44
1:C:122:ALA:O	1:C:125:VAL:HG12	2.18	0.44
1:B:219:LEU:HD22	1:B:647:VAL:HG12	2.00	0.44
1:D:292:ILE:O	1:D:295:THR:HG22	2.17	0.44
1:C:479:LEU:HD13	1:C:480:SER:N	2.33	0.44
1:C:417:MET:HE1	1:C:637:ILE:HG21	2.00	0.44
1:B:413:ALA:HB1	1:B:654:VAL:HG23	1.99	0.44
1:A:230:ILE:HG12	1:A:235:SER:O	2.17	0.44
1:B:430:THR:HG21	1:B:623:GLY:CA	2.43	0.44
1:A:156:ILE:HD11	1:A:194:ILE:CG2	2.48	0.44
1:D:156:ILE:HD11	1:D:194:ILE:CG2	2.48	0.44
1:A:699:VAL:HG23	1:A:700:LEU:HD23	1.99	0.44
1:D:164:MET:CE	1:D:164:MET:HA	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:THR:CG2	1:B:578:GLY:O	2.66	0.44
1:B:524:GLU:HA	1:B:527:ASP:OD2	2.18	0.44
1:B:168:LEU:HA	1:B:168:LEU:HD12	1.86	0.44
1:A:381:ALA:O	1:A:383:PRO:HD3	2.17	0.44
1:C:119:LEU:C	1:C:119:LEU:HD23	2.38	0.44
1:D:179:SER:N	1:D:180:GLN:CA	2.81	0.44
1:A:179:SER:N	1:A:180:GLN:CA	2.81	0.44
1:C:178:ARG:CB	1:C:179:SER:HA	2.24	0.44
1:D:498:GLN:HA	1:D:502:HIS:O	2.18	0.44
1:D:230:ILE:HG12	1:D:235:SER:O	2.17	0.44
1:B:78:TYR:CD2	1:B:79:LEU:HD12	2.42	0.44
1:B:261:ASP:HA	1:B:293:GLY:N	2.33	0.44
1:C:261:ASP:HA	1:C:293:GLY:N	2.33	0.44
1:B:490:PRO:HD2	1:B:495:VAL:HA	1.99	0.44
1:C:219:LEU:HD22	1:C:647:VAL:HG12	2.00	0.44
1:A:277:THR:CG2	1:A:578:GLY:O	2.66	0.44
1:A:313:THR:HG22	1:A:316:ALA:HB3	1.98	0.44
1:C:313:THR:HG22	1:C:316:ALA:HB3	1.98	0.44
1:B:178:ARG:CB	1:B:179:SER:HA	2.24	0.44
1:B:103:HIS:HA	1:B:104:GLY:HA3	1.78	0.44
1:B:498:GLN:HA	1:B:502:HIS:O	2.18	0.44
1:C:413:ALA:HB1	1:C:654:VAL:HG23	1.99	0.44
1:C:78:TYR:CD2	1:C:79:LEU:HD12	2.42	0.44
1:B:140:SER:HG	1:B:150:THR:HG22	1.83	0.44
1:B:703:LEU:CD2	1:D:86:TRP:HB2	2.48	0.44
1:D:326:GLN:O	1:D:329:ARG:HG3	2.18	0.44
1:B:313:THR:HG22	1:B:316:ALA:HB3	1.98	0.44
1:A:228:HIS:O	1:A:250:LEU:HD22	2.18	0.43
1:C:103:HIS:HA	1:C:104:GLY:HA3	1.78	0.43
1:D:699:VAL:HG23	1:D:700:LEU:HD23	2.00	0.43
1:D:122:ALA:O	1:D:125:VAL:HG12	2.18	0.43
1:A:326:GLN:O	1:A:329:ARG:HG3	2.18	0.43
1:C:455:ALA:HB2	1:C:539:MET:SD	2.58	0.43
1:A:455:ALA:HB2	1:A:539:MET:SD	2.58	0.43
1:D:277:THR:CG2	1:D:578:GLY:O	2.66	0.43
1:C:422:THR:HG23	1:C:619:VAL:HG23	1.99	0.43
1:D:228:HIS:O	1:D:250:LEU:HD22	2.18	0.43
1:D:417:MET:HE1	1:D:637:ILE:HG21	1.99	0.43
1:B:416:ARG:HG2	1:B:416:ARG:HH11	1.82	0.43
1:C:430:THR:HG21	1:C:623:GLY:CA	2.43	0.43
1:B:122:ALA:HA	1:B:125:VAL:CG1	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:PRO:HD2	1:C:495:VAL:HA	2.00	0.43
1:B:414:LEU:HA	1:B:414:LEU:HD23	1.73	0.43
1:D:313:THR:HG23	1:D:316:ALA:H	1.83	0.43
1:D:313:THR:HG22	1:D:316:ALA:HB3	1.98	0.43
1:A:313:THR:HG23	1:A:316:ALA:H	1.83	0.43
1:B:468:ASN:O	1:B:472:HIS:HB2	2.18	0.43
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.86	0.43
1:A:498:GLN:HA	1:A:502:HIS:O	2.18	0.43
1:C:122:ALA:HA	1:C:125:VAL:CG1	2.47	0.43
1:D:206:LEU:O	1:D:210:GLU:HB2	2.19	0.43
1:D:276:VAL:O	1:D:277:THR:CB	2.67	0.43
1:A:524:GLU:HA	1:A:527:ASP:OD2	2.17	0.43
1:A:416:ARG:HG2	1:A:416:ARG:HH11	1.82	0.43
1:A:413:ALA:HB1	1:A:654:VAL:HG23	2.00	0.43
1:A:164:MET:CE	1:A:164:MET:HA	2.48	0.43
1:B:307:LEU:HD13	1:B:308:HIS:CD2	2.49	0.43
1:C:307:LEU:HD13	1:C:308:HIS:CD2	2.49	0.43
1:D:490:PRO:HD2	1:D:495:VAL:HA	1.99	0.43
1:A:479:LEU:HD13	1:A:480:SER:N	2.33	0.43
1:B:447:VAL:HG23	1:B:450:ASN:H	1.83	0.43
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.82	0.43
1:A:206:LEU:O	1:A:210:GLU:HB2	2.19	0.43
1:C:699:VAL:HG23	1:C:700:LEU:HD23	1.99	0.43
1:C:86:TRP:O	1:C:90:MET:HG3	2.18	0.43
1:A:490:PRO:HD2	1:A:495:VAL:HA	2.00	0.43
1:C:468:ASN:O	1:C:472:HIS:HB2	2.18	0.43
1:D:119:LEU:HD23	1:D:119:LEU:C	2.39	0.43
1:D:179:SER:HB3	1:D:182:GLY:N	2.34	0.43
1:A:183:VAL:HG23	1:A:184:VAL:N	2.33	0.43
1:C:156:ILE:HD11	1:C:194:ILE:CG2	2.48	0.43
1:D:86:TRP:O	1:D:90:MET:HG3	2.18	0.43
1:C:326:GLN:O	1:C:329:ARG:HG3	2.18	0.43
1:A:276:VAL:O	1:A:277:THR:CB	2.67	0.43
1:B:119:LEU:C	1:B:119:LEU:HD23	2.39	0.43
1:C:166:ALA:HB1	1:C:184:VAL:CG2	2.49	0.43
1:C:447:VAL:HG23	1:C:450:ASN:H	1.84	0.43
1:A:447:VAL:HG23	1:A:450:ASN:H	1.84	0.43
1:D:447:VAL:HG23	1:D:450:ASN:H	1.84	0.43
1:B:156:ILE:HD11	1:B:194:ILE:CG2	2.48	0.43
1:B:326:GLN:O	1:B:329:ARG:HG3	2.18	0.43
1:D:479:LEU:HD13	1:D:480:SER:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HD23	1:C:169:TRP:CZ3	2.54	0.43
1:D:524:GLU:HA	1:D:527:ASP:OD2	2.17	0.43
1:B:249:LEU:HA	1:B:304:MET:O	2.19	0.43
1:D:249:LEU:HA	1:D:304:MET:O	2.19	0.43
1:C:179:SER:N	1:C:180:GLN:CA	2.80	0.43
1:B:417:MET:HE1	1:B:637:ILE:HG21	2.01	0.43
1:A:671:SER:O	1:A:672:GLU:C	2.57	0.43
1:B:699:VAL:HG23	1:B:700:LEU:HD23	2.00	0.43
1:A:86:TRP:O	1:A:90:MET:HG3	2.18	0.43
1:A:669:ARG:CZ	1:A:736:LEU:O	2.67	0.43
1:D:669:ARG:CZ	1:D:736:LEU:O	2.67	0.43
1:D:277:THR:HG23	1:D:578:GLY:O	2.19	0.43
1:C:249:LEU:HA	1:C:304:MET:O	2.19	0.43
1:D:671:SER:O	1:D:672:GLU:C	2.57	0.43
1:A:277:THR:HG23	1:A:578:GLY:O	2.19	0.43
1:B:168:LEU:HD23	1:B:169:TRP:CZ3	2.54	0.43
1:A:249:LEU:HA	1:A:304:MET:O	2.19	0.43
1:C:498:GLN:HA	1:C:502:HIS:O	2.19	0.43
1:C:416:ARG:HH11	1:C:416:ARG:HG2	1.83	0.43
1:D:233:ASP:C	1:D:235:SER:H	2.23	0.43
1:A:122:ALA:HA	1:A:125:VAL:CG1	2.46	0.43
1:C:277:THR:CG2	1:C:578:GLY:O	2.67	0.43
1:A:168:LEU:HD23	1:A:169:TRP:CZ3	2.54	0.43
1:A:119:LEU:C	1:A:119:LEU:HD23	2.40	0.42
1:C:228:HIS:O	1:C:250:LEU:HD22	2.18	0.42
1:B:228:HIS:O	1:B:250:LEU:HD22	2.18	0.42
1:D:183:VAL:HG23	1:D:184:VAL:N	2.34	0.42
1:B:179:SER:N	1:B:180:GLN:CA	2.81	0.42
1:B:559:THR:O	1:B:563:ILE:HG12	2.19	0.42
1:D:122:ALA:HA	1:D:125:VAL:CG1	2.46	0.42
1:B:86:TRP:O	1:B:90:MET:HG3	2.19	0.42
1:B:262:GLY:CA	1:B:307:LEU:HB2	2.49	0.42
1:A:262:GLY:CA	1:A:305:LYS:O	2.67	0.42
1:A:539:MET:HE2	1:A:547:ALA:HB3	2.01	0.42
1:B:277:THR:HG23	1:B:578:GLY:O	2.19	0.42
1:D:168:LEU:HD23	1:D:169:TRP:CZ3	2.54	0.42
1:C:179:SER:HB3	1:C:182:GLY:N	2.34	0.42
1:D:559:THR:O	1:D:563:ILE:HG12	2.19	0.42
1:A:233:ASP:C	1:A:235:SER:H	2.23	0.42
1:C:559:THR:O	1:C:563:ILE:HG12	2.19	0.42
1:D:262:GLY:CA	1:D:305:LYS:O	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD22	1:D:647:VAL:HG12	2.00	0.42
1:B:148:MET:SD	1:B:386:LEU:HD13	2.59	0.42
1:A:179:SER:HB3	1:A:182:GLY:N	2.35	0.42
1:C:183:VAL:HG23	1:C:184:VAL:N	2.33	0.42
1:C:148:MET:SD	1:C:386:LEU:HD13	2.59	0.42
1:D:148:MET:SD	1:D:386:LEU:HD13	2.59	0.42
1:C:313:THR:HG23	1:C:316:ALA:H	1.83	0.42
1:C:244:VAL:HG12	1:C:245:ALA:N	2.35	0.42
1:D:272:ASP:HB3	1:D:296:ILE:HG23	2.01	0.42
1:C:731:LEU:O	1:C:731:LEU:HD13	2.20	0.42
1:B:179:SER:HB3	1:B:182:GLY:N	2.35	0.42
1:C:122:ALA:CA	1:C:125:VAL:HG12	2.47	0.42
1:A:219:LEU:HD22	1:A:647:VAL:HG12	2.00	0.42
1:B:313:THR:HG23	1:B:316:ALA:H	1.83	0.42
1:C:730:ARG:HG3	1:C:730:ARG:HH11	1.84	0.42
1:B:244:VAL:HG12	1:B:245:ALA:N	2.35	0.42
1:C:264:VAL:HG22	1:C:287:ALA:HA	2.01	0.42
1:B:264:VAL:HG22	1:B:287:ALA:HA	2.01	0.42
1:B:166:ALA:HB1	1:B:184:VAL:CG2	2.50	0.42
1:D:262:GLY:CA	1:D:307:LEU:HB2	2.49	0.42
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.86	0.42
1:A:244:VAL:HG12	1:A:245:ALA:N	2.35	0.42
1:A:641:MET:HE1	1:A:659:GLY:O	2.18	0.42
1:B:122:ALA:CA	1:B:125:VAL:HG12	2.48	0.42
1:D:277:THR:HG22	1:D:279:GLU:HG2	2.02	0.42
1:C:276:VAL:O	1:C:277:THR:CB	2.66	0.42
1:B:367:LEU:C	1:B:367:LEU:HD22	2.40	0.42
1:D:244:VAL:HG12	1:D:245:ALA:N	2.35	0.42
1:A:332:ILE:HA	1:A:332:ILE:HD12	1.93	0.42
1:D:119:LEU:HA	1:D:188:PHE:CE2	2.55	0.42
1:C:454:LEU:HD22	1:C:499:VAL:CG1	2.50	0.42
1:B:233:ASP:C	1:B:235:SER:H	2.23	0.42
1:B:206:LEU:O	1:B:210:GLU:HB2	2.19	0.42
1:C:418:GLU:CG	1:C:672:GLU:HG2	2.47	0.42
1:D:418:GLU:CG	1:D:672:GLU:HG2	2.47	0.42
1:B:418:GLU:CG	1:B:672:GLU:HG2	2.47	0.42
1:A:262:GLY:CA	1:A:307:LEU:HB2	2.50	0.42
1:B:605:LYS:HD3	1:B:628:ASP:CB	2.50	0.42
1:B:669:ARG:CZ	1:B:736:LEU:O	2.67	0.42
1:B:271:VAL:HA	1:B:297:ASN:HA	2.02	0.42
1:B:730:ARG:HH11	1:B:730:ARG:HG3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:THR:O	2:D:995:ALF:F2	2.28	0.42
1:D:642:GLY:O	1:D:645:THR:HG22	2.20	0.42
1:C:233:ASP:C	1:C:235:SER:H	2.23	0.42
1:A:559:THR:O	1:A:563:ILE:HG12	2.19	0.42
1:B:430:THR:HA	1:B:641:MET:HE2	2.02	0.42
1:C:88:ALA:HB1	1:C:125:VAL:HG23	2.02	0.42
1:B:308:HIS:HB3	1:B:312:ASP:CG	2.40	0.42
1:C:308:HIS:HB3	1:C:312:ASP:CG	2.40	0.42
1:C:669:ARG:CZ	1:C:736:LEU:O	2.67	0.42
1:B:451:ALA:HB1	1:B:539:MET:CE	2.50	0.42
1:D:451:ALA:HB1	1:D:539:MET:CE	2.49	0.42
1:B:467:ALA:O	1:B:471:VAL:HG13	2.20	0.42
1:C:367:LEU:C	1:C:367:LEU:HD22	2.40	0.42
1:C:91:LEU:O	1:C:95:VAL:HG23	2.20	0.42
1:A:272:ASP:HB3	1:A:296:ILE:HG23	2.02	0.42
1:C:734:VAL:HG22	1:C:734:VAL:O	2.20	0.42
1:D:332:ILE:HA	1:D:332:ILE:HD12	1.93	0.42
1:B:454:LEU:HD22	1:B:499:VAL:CG1	2.50	0.42
1:C:127:LEU:O	1:C:131:TRP:HB2	2.19	0.42
1:D:676:SER:O	1:D:680:GLN:HG3	2.20	0.42
1:A:148:MET:SD	1:A:386:LEU:HD13	2.60	0.42
1:C:271:VAL:HA	1:C:297:ASN:HA	2.02	0.42
1:A:642:GLY:O	1:A:645:THR:HG22	2.20	0.42
1:A:734:VAL:HG22	1:A:734:VAL:O	2.20	0.42
1:B:731:LEU:HD13	1:B:731:LEU:O	2.20	0.42
1:C:642:GLY:O	1:C:645:THR:HG22	2.20	0.42
1:B:173:PHE:HA	1:B:174:PRO:HD3	1.87	0.42
1:B:183:VAL:HG23	1:B:184:VAL:N	2.34	0.42
1:B:499:VAL:O	1:B:502:HIS:ND1	2.53	0.42
1:D:499:VAL:O	1:D:502:HIS:ND1	2.53	0.42
1:B:224:PRO:HG3	1:B:257:LYS:HD2	2.01	0.42
1:C:224:PRO:HG3	1:C:257:LYS:HD2	2.01	0.42
1:A:86:TRP:HB2	1:C:703:LEU:CD2	2.50	0.42
1:A:443:THR:HG21	1:A:446:PHE:O	2.20	0.42
1:A:271:VAL:HA	1:A:297:ASN:HA	2.02	0.42
1:A:422:THR:O	1:A:619:VAL:HG23	2.20	0.42
1:A:730:ARG:HH11	1:A:730:ARG:HG3	1.85	0.42
1:B:355:PHE:O	1:B:359:ALA:HB2	2.20	0.42
1:A:119:LEU:HA	1:A:188:PHE:CE2	2.55	0.41
1:A:264:VAL:HG22	1:A:287:ALA:HA	2.01	0.41
1:D:264:VAL:HG22	1:D:287:ALA:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PHE:HA	1:C:174:PRO:HD3	1.87	0.41
1:D:500:ASP:C	1:D:502:HIS:H	2.23	0.41
1:C:671:SER:O	1:C:672:GLU:C	2.57	0.41
1:A:127:LEU:O	1:A:131:TRP:HB2	2.19	0.41
1:A:84:ARG:NH1	1:A:132:PRO:HD3	2.35	0.41
1:D:271:VAL:HA	1:D:297:ASN:HA	2.02	0.41
1:A:355:PHE:O	1:A:359:ALA:HB2	2.20	0.41
1:B:642:GLY:O	1:B:645:THR:HG22	2.20	0.41
1:D:731:LEU:HD13	1:D:731:LEU:O	2.20	0.41
1:A:500:ASP:C	1:A:502:HIS:H	2.23	0.41
1:D:641:MET:HE1	1:D:659:GLY:O	2.19	0.41
1:D:84:ARG:NH1	1:D:132:PRO:HD3	2.36	0.41
1:A:129:GLY:HA3	1:A:130:GLY:HA3	1.70	0.41
1:A:308:HIS:HB3	1:A:312:ASP:CG	2.40	0.41
1:C:605:LYS:HD3	1:C:628:ASP:CB	2.51	0.41
1:A:151:LEU:HD13	1:A:344:VAL:HG12	2.02	0.41
1:C:442:VAL:HG23	1:C:548:LEU:HB3	2.02	0.41
1:D:355:PHE:O	1:D:359:ALA:HB2	2.20	0.41
1:A:166:ALA:HB1	1:A:184:VAL:CG2	2.50	0.41
1:C:499:VAL:O	1:C:502:HIS:ND1	2.53	0.41
1:B:500:ASP:C	1:B:502:HIS:H	2.23	0.41
1:A:454:LEU:HD22	1:A:499:VAL:CG1	2.50	0.41
1:A:224:PRO:HG3	1:A:257:LYS:HD2	2.01	0.41
1:D:224:PRO:HG3	1:D:257:LYS:HD2	2.01	0.41
1:B:127:LEU:O	1:B:131:TRP:HB2	2.20	0.41
1:B:262:GLY:CA	1:B:305:LYS:O	2.67	0.41
1:D:151:LEU:HD13	1:D:344:VAL:HG12	2.02	0.41
1:B:695:LEU:O	1:B:707:LEU:HG	2.20	0.41
1:A:467:ALA:O	1:A:471:VAL:HG13	2.21	0.41
1:C:355:PHE:O	1:C:359:ALA:HB2	2.21	0.41
1:D:734:VAL:HG22	1:D:734:VAL:O	2.20	0.41
1:B:734:VAL:HG22	1:B:734:VAL:O	2.20	0.41
1:A:499:VAL:O	1:A:502:HIS:CA	2.69	0.41
1:D:499:VAL:O	1:D:502:HIS:CA	2.69	0.41
1:A:253:ARG:HD2	1:A:254:PRO:O	2.21	0.41
1:C:430:THR:HA	1:C:641:MET:HE2	2.02	0.41
1:C:262:GLY:CA	1:C:305:LYS:O	2.67	0.41
1:D:308:HIS:HB3	1:D:312:ASP:CG	2.40	0.41
1:C:277:THR:HG23	1:C:578:GLY:O	2.20	0.41
1:B:276:VAL:O	1:B:277:THR:CB	2.67	0.41
1:D:168:LEU:HA	1:D:168:LEU:HD12	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:HA	1:B:321:MET:HE2	2.02	0.41
1:B:499:VAL:O	1:B:502:HIS:CA	2.69	0.41
1:D:605:LYS:HD3	1:D:628:ASP:CB	2.50	0.41
1:A:277:THR:HG22	1:A:279:GLU:HG2	2.03	0.41
1:B:442:VAL:HG23	1:B:548:LEU:HB3	2.03	0.41
1:B:272:ASP:HB3	1:B:296:ILE:HG23	2.01	0.41
1:A:408:ILE:HD12	1:A:408:ILE:N	2.35	0.41
1:C:408:ILE:HD12	1:C:408:ILE:N	2.36	0.41
1:A:731:LEU:HD13	1:A:731:LEU:O	2.20	0.41
1:A:249:LEU:HD12	1:A:249:LEU:N	2.36	0.41
1:D:249:LEU:HD12	1:D:249:LEU:N	2.36	0.41
1:C:500:ASP:C	1:C:502:HIS:H	2.23	0.41
1:A:499:VAL:O	1:A:502:HIS:ND1	2.53	0.41
1:B:253:ARG:HD2	1:B:254:PRO:O	2.20	0.41
1:D:127:LEU:O	1:D:131:TRP:HB2	2.20	0.41
1:D:629:ALA:N	1:D:630:PRO:CD	2.82	0.41
1:D:443:THR:HG21	1:D:446:PHE:O	2.20	0.41
1:D:695:LEU:O	1:D:707:LEU:HG	2.21	0.41
1:B:363:PRO:HB2	1:B:364:GLN:CD	2.41	0.41
1:D:467:ALA:O	1:D:471:VAL:HG13	2.21	0.41
1:C:467:ALA:O	1:C:471:VAL:HG13	2.21	0.41
1:D:730:ARG:HH11	1:D:730:ARG:HG3	1.86	0.41
1:C:318:ILE:HA	1:C:321:MET:HE2	2.02	0.41
1:C:499:VAL:O	1:C:502:HIS:CA	2.69	0.41
1:D:253:ARG:HD2	1:D:254:PRO:O	2.21	0.41
1:C:206:LEU:O	1:C:210:GLU:HB2	2.20	0.41
1:B:84:ARG:NH1	1:B:132:PRO:HD3	2.35	0.41
1:B:671:SER:O	1:B:672:GLU:C	2.57	0.41
1:A:605:LYS:HD3	1:A:628:ASP:CB	2.51	0.41
1:C:490:PRO:CB	1:C:493:LYS:HD3	2.49	0.41
1:A:629:ALA:N	1:A:630:PRO:CD	2.82	0.41
1:C:277:THR:HG22	1:C:279:GLU:HG2	2.03	0.41
1:C:363:PRO:HB2	1:C:364:GLN:CD	2.41	0.41
1:D:367:LEU:C	1:D:367:LEU:HD22	2.40	0.41
1:B:119:LEU:HA	1:B:188:PHE:CE2	2.55	0.41
1:D:454:LEU:HD22	1:D:499:VAL:CG1	2.51	0.41
1:C:253:ARG:HD2	1:C:254:PRO:O	2.21	0.41
1:D:93:ILE:HG23	1:D:94:PRO:CD	2.48	0.41
1:B:312:ASP:N	1:B:312:ASP:OD2	2.53	0.41
1:B:490:PRO:CB	1:B:493:LYS:HD3	2.49	0.41
1:B:219:LEU:HD21	1:B:647:VAL:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:THR:O	1:C:619:VAL:HG23	2.21	0.41
1:B:431:LEU:HA	1:B:431:LEU:HD12	1.93	0.41
1:D:166:ALA:HB1	1:D:184:VAL:CG2	2.51	0.41
1:D:173:PHE:HA	1:D:174:PRO:HD3	1.87	0.41
1:A:173:PHE:HA	1:A:174:PRO:HD3	1.87	0.41
1:C:84:ARG:NH1	1:C:132:PRO:HD3	2.36	0.41
1:D:129:GLY:HA3	1:D:130:GLY:HA3	1.70	0.41
1:A:127:LEU:C	1:A:129:GLY:N	2.73	0.41
1:A:93:ILE:HG23	1:A:94:PRO:CD	2.49	0.41
1:A:307:LEU:HD13	1:A:308:HIS:CD2	2.48	0.41
1:C:312:ASP:N	1:C:312:ASP:OD2	2.53	0.41
1:D:307:LEU:HD13	1:D:308:HIS:CD2	2.49	0.41
1:B:426:ASP:HA	1:B:576:LEU:O	2.21	0.41
1:C:628:ASP:O	1:C:631:ALA:HB3	2.20	0.41
1:C:219:LEU:HD21	1:C:647:VAL:HA	2.02	0.41
1:B:451:ALA:HB1	1:B:539:MET:HE1	2.03	0.41
1:C:695:LEU:O	1:C:707:LEU:HG	2.21	0.41
1:A:695:LEU:O	1:A:707:LEU:HG	2.21	0.41
1:D:297:ASN:C	1:D:298:GLN:HG3	2.41	0.41
1:D:574:VAL:HG12	1:D:574:VAL:O	2.21	0.41
1:B:438:LEU:HD12	1:B:473:ALA:CB	2.51	0.41
1:B:408:ILE:N	1:B:408:ILE:HD12	2.36	0.41
1:C:431:LEU:HD12	1:C:431:LEU:HA	1.93	0.41
1:C:119:LEU:HA	1:C:188:PHE:CE2	2.56	0.41
1:C:127:LEU:C	1:C:129:GLY:N	2.72	0.41
1:A:155:GLY:O	1:A:159:ALA:HB2	2.21	0.41
1:D:127:LEU:C	1:D:129:GLY:N	2.73	0.41
1:A:117:ILE:HG12	1:C:687:ILE:HD11	2.03	0.41
1:C:451:ALA:HB1	1:C:539:MET:CE	2.51	0.41
1:B:277:THR:HG22	1:B:279:GLU:HG2	2.03	0.41
1:A:297:ASN:C	1:A:298:GLN:HG3	2.41	0.41
1:B:297:ASN:C	1:B:298:GLN:HG3	2.41	0.41
1:B:574:VAL:O	1:B:574:VAL:HG12	2.21	0.41
1:C:272:ASP:HB3	1:C:296:ILE:HG23	2.02	0.41
1:C:249:LEU:HD12	1:C:249:LEU:N	2.36	0.40
1:B:249:LEU:HD12	1:B:249:LEU:N	2.36	0.40
1:B:223:VAL:HG12	1:B:225:GLU:HB3	2.03	0.40
1:C:223:VAL:HG12	1:C:225:GLU:HB3	2.03	0.40
1:A:676:SER:O	1:A:680:GLN:HG3	2.21	0.40
1:C:576:LEU:HB3	1:C:605:LYS:NZ	2.36	0.40
1:C:426:ASP:OD2	2:C:995:ALF:F2	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD21	1:D:647:VAL:HA	2.02	0.40
1:C:443:THR:HG21	1:C:446:PHE:O	2.20	0.40
1:A:85:PHE:CE1	1:A:200:LEU:HB2	2.56	0.40
1:D:85:PHE:CE1	1:D:200:LEU:HB2	2.56	0.40
1:D:363:PRO:HB2	1:D:364:GLN:CD	2.41	0.40
1:C:297:ASN:C	1:C:298:GLN:HG3	2.41	0.40
1:A:442:VAL:HG23	1:A:548:LEU:HB3	2.03	0.40
1:A:251:ARG:HA	1:A:302:PHE:O	2.21	0.40
1:D:408:ILE:N	1:D:408:ILE:HD12	2.36	0.40
1:B:251:ARG:HA	1:B:302:PHE:O	2.21	0.40
1:B:155:GLY:O	1:B:159:ALA:HB2	2.21	0.40
1:B:131:TRP:N	1:B:132:PRO:HD2	2.36	0.40
1:D:131:TRP:N	1:D:132:PRO:HD2	2.35	0.40
1:C:522:LEU:HD12	1:C:545:THR:HG22	2.03	0.40
1:D:522:LEU:HD12	1:D:545:THR:HG22	2.03	0.40
1:B:576:LEU:HB3	1:B:605:LYS:NZ	2.36	0.40
1:A:367:LEU:C	1:A:367:LEU:HD22	2.40	0.40
1:B:422:THR:O	1:B:619:VAL:HG23	2.22	0.40
1:C:251:ARG:HA	1:C:302:PHE:O	2.21	0.40
1:C:438:LEU:HD12	1:C:473:ALA:CB	2.51	0.40
1:C:131:TRP:N	1:C:132:PRO:HD2	2.36	0.40
1:A:522:LEU:HD12	1:A:545:THR:HG22	2.03	0.40
1:C:426:ASP:HA	1:C:576:LEU:O	2.21	0.40
1:A:451:ALA:HB1	1:A:539:MET:CE	2.51	0.40
1:B:85:PHE:CE1	1:B:200:LEU:HB2	2.57	0.40
1:D:422:THR:O	1:D:619:VAL:HG23	2.22	0.40
1:D:251:ARG:HA	1:D:302:PHE:O	2.22	0.40
1:B:127:LEU:C	1:B:129:GLY:N	2.73	0.40
1:B:522:LEU:HD12	1:B:545:THR:HG22	2.04	0.40
1:A:219:LEU:HD21	1:A:647:VAL:HA	2.03	0.40
1:A:394:ILE:O	1:A:398:VAL:HG13	2.22	0.40
1:A:91:LEU:O	1:A:95:VAL:HG23	2.21	0.40
1:C:574:VAL:O	1:C:574:VAL:HG12	2.21	0.40
1:D:438:LEU:HD12	1:D:473:ALA:CB	2.51	0.40
1:D:598:ALA:O	1:D:600:ILE:HG23	2.22	0.40
1:B:88:ALA:HB1	1:B:125:VAL:HG23	2.04	0.40
1:D:130:GLY:HA2	1:D:133:PHE:CD1	2.57	0.40
1:A:88:ALA:HB1	1:A:125:VAL:HG23	2.02	0.40
1:A:131:TRP:N	1:A:132:PRO:HD2	2.36	0.40
1:D:628:ASP:O	1:D:631:ALA:HB3	2.21	0.40
1:D:394:ILE:O	1:D:398:VAL:HG13	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:HB2	1:A:364:GLN:CD	2.41	0.40
1:B:258:ILE:HA	1:B:259:PRO:HD3	1.82	0.40
1:A:258:ILE:HD11	1:A:297:ASN:HB3	2.03	0.40
1:A:438:LEU:HD12	1:A:473:ALA:CB	2.51	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	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	9	46
1	B	661/736 (90%)	578 (87%)	68 (10%)	15 (2%)	8	44
1	C	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	9	46
1	D	661/736 (90%)	579 (88%)	68 (10%)	14 (2%)	9	46
All	All	2644/2944 (90%)	2313 (88%)	274 (10%)	57 (2%)	8	45

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO
1	A	662	ARG
1	B	224	PRO
1	C	224	PRO
1	C	662	ARG
1	D	224	PRO
1	D	662	ARG
1	A	129	GLY
1	A	618	ILE
1	A	658	HIS
1	B	129	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	618	ILE
1	B	658	HIS
1	B	662	ARG
1	C	129	GLY
1	C	618	ILE
1	C	658	HIS
1	D	129	GLY
1	D	618	ILE
1	D	658	HIS
1	A	389	ALA
1	B	389	ALA
1	C	389	ALA
1	D	389	ALA
1	A	76	PRO
1	A	499	VAL
1	B	76	PRO
1	B	499	VAL
1	B	628	ASP
1	C	76	PRO
1	C	499	VAL
1	D	76	PRO
1	D	499	VAL
1	D	628	ASP
1	A	143	THR
1	A	628	ASP
1	B	113	GLY
1	B	143	THR
1	C	628	ASP
1	D	143	THR
1	A	113	GLY
1	A	177	PHE
1	B	177	PHE
1	B	703	LEU
1	C	113	GLY
1	C	143	THR
1	C	177	PHE
1	D	113	GLY
1	D	177	PHE
1	A	484	VAL
1	B	183	VAL
1	B	484	VAL
1	C	183	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	484	VAL
1	D	183	VAL
1	D	484	VAL
1	A	183	VAL

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	523/586 (89%)	486 (93%)	37 (7%)	18	57
1	B	523/586 (89%)	486 (93%)	37 (7%)	18	57
1	C	523/586 (89%)	486 (93%)	37 (7%)	18	57
1	D	523/586 (89%)	487 (93%)	36 (7%)	19	59
All	All	2092/2344 (89%)	1945 (93%)	147 (7%)	19	58

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	105	LEU
1	A	109	ILE
1	A	150	THR
1	A	164	MET
1	A	165	VAL
1	A	172	VAL
1	A	178	ARG
1	A	183	VAL
1	A	184	VAL
1	A	219	LEU
1	A	220	LEU
1	A	250	LEU
1	A	252	VAL
1	A	264	VAL
1	A	277	THR
1	A	307	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	VAL
1	A	320	GLN
1	A	322	VAL
1	A	367	LEU
1	A	382	CYS
1	A	386	LEU
1	A	424	VAL
1	A	443	THR
1	A	466	LEU
1	A	479	LEU
1	A	536	VAL
1	A	562	THR
1	A	583	THR
1	A	645	THR
1	A	674	THR
1	A	679	ARG
1	A	693	VAL
1	A	707	LEU
1	A	712	ILE
1	A	726	ILE
1	B	99	GLU
1	B	105	LEU
1	B	109	ILE
1	B	150	THR
1	B	164	MET
1	B	165	VAL
1	B	172	VAL
1	B	178	ARG
1	B	183	VAL
1	B	184	VAL
1	B	219	LEU
1	B	220	LEU
1	B	250	LEU
1	B	252	VAL
1	B	264	VAL
1	B	277	THR
1	B	307	LEU
1	B	319	VAL
1	B	320	GLN
1	B	322	VAL
1	B	367	LEU
1	B	382	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	386	LEU
1	B	424	VAL
1	B	443	THR
1	B	466	LEU
1	B	479	LEU
1	B	536	VAL
1	B	562	THR
1	B	583	THR
1	B	645	THR
1	B	674	THR
1	B	679	ARG
1	B	693	VAL
1	B	707	LEU
1	B	712	ILE
1	B	726	ILE
1	C	99	GLU
1	C	105	LEU
1	C	109	ILE
1	C	150	THR
1	C	164	MET
1	C	165	VAL
1	C	172	VAL
1	C	178	ARG
1	C	183	VAL
1	C	184	VAL
1	C	219	LEU
1	C	220	LEU
1	C	250	LEU
1	C	252	VAL
1	C	264	VAL
1	C	277	THR
1	C	307	LEU
1	C	319	VAL
1	C	320	GLN
1	C	322	VAL
1	C	367	LEU
1	C	382	CYS
1	C	386	LEU
1	C	424	VAL
1	C	443	THR
1	C	466	LEU
1	C	479	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	536	VAL
1	C	562	THR
1	C	583	THR
1	C	645	THR
1	C	674	THR
1	C	679	ARG
1	C	693	VAL
1	C	707	LEU
1	C	712	ILE
1	C	726	ILE
1	D	99	GLU
1	D	105	LEU
1	D	109	ILE
1	D	150	THR
1	D	164	MET
1	D	165	VAL
1	D	172	VAL
1	D	178	ARG
1	D	183	VAL
1	D	184	VAL
1	D	219	LEU
1	D	220	LEU
1	D	250	LEU
1	D	252	VAL
1	D	264	VAL
1	D	277	THR
1	D	307	LEU
1	D	319	VAL
1	D	322	VAL
1	D	367	LEU
1	D	382	CYS
1	D	386	LEU
1	D	424	VAL
1	D	443	THR
1	D	466	LEU
1	D	479	LEU
1	D	536	VAL
1	D	562	THR
1	D	583	THR
1	D	645	THR
1	D	674	THR
1	D	679	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	693	VAL
1	D	707	LEU
1	D	712	ILE
1	D	726	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS
1	A	498	GLN
1	A	727	ASN
1	B	308	HIS
1	B	450	ASN
1	B	498	GLN
1	B	502	HIS
1	B	727	ASN
1	C	308	HIS
1	C	498	GLN
1	C	727	ASN
1	D	308	HIS
1	D	498	GLN
1	D	727	ASN

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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
2	ALF	A	995	-	0,4,4	0.00	-	0,6,6	0.00	-
2	ALF	B	995	-	0,4,4	0.00	-	0,6,6	0.00	-
2	ALF	C	995	-	0,4,4	0.00	-	0,6,6	0.00	-
2	ALF	D	995	-	0,4,4	0.00	-	0,6,6	0.00	-

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
2	ALF	A	995	-	-	0/0/0/0	0/0/0/0
2	ALF	B	995	-	-	0/0/0/0	0/0/0/0
2	ALF	C	995	-	-	0/0/0/0	0/0/0/0
2	ALF	D	995	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	995	ALF	2	0
2	C	995	ALF	1	0
2	D	995	ALF	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	663/736 (90%)	0.04	24 (3%)	46 31	56, 106, 243, 371	0
1	B	663/736 (90%)	0.03	24 (3%)	46 31	55, 106, 244, 373	0
1	C	663/736 (90%)	0.05	27 (4%)	41 27	55, 106, 244, 371	0
1	D	663/736 (90%)	-0.02	19 (2%)	55 41	56, 106, 244, 369	0
All	All	2652/2944 (90%)	0.03	94 (3%)	48 32	55, 106, 244, 373	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	500	ASP	10.1
1	A	500	ASP	9.0
1	B	490	PRO	8.0
1	B	214	SER	7.7
1	D	489	ALA	7.7
1	D	247	GLY	7.2
1	A	736	LEU	7.0
1	B	489	ALA	6.7
1	D	736	LEU	6.5
1	C	490	PRO	6.3
1	B	500	ASP	6.1
1	C	214	SER	6.1
1	D	280	PRO	6.0
1	D	490	PRO	5.8
1	B	290	LYS	5.7
1	B	104	GLY	5.6
1	A	489	ALA	5.6
1	A	214	SER	5.5
1	D	500	ASP	5.5
1	A	247	GLY	5.3
1	A	490	PRO	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	489	ALA	5.1
1	A	305	LYS	5.0
1	D	290	LYS	4.9
1	A	304	MET	4.6
1	C	736	LEU	4.5
1	C	236	GLU	4.3
1	B	736	LEU	4.3
1	C	305	LYS	4.2
1	B	236	GLU	3.9
1	B	247	GLY	3.6
1	D	214	SER	3.6
1	A	289	ALA	3.4
1	B	238	GLU	3.4
1	C	289	ALA	3.4
1	B	304	MET	3.3
1	D	238	GLU	3.3
1	A	280	PRO	3.3
1	B	280	PRO	3.2
1	A	306	ALA	3.2
1	B	305	LYS	3.2
1	D	306	ALA	3.2
1	B	235	SER	3.2
1	D	236	GLU	3.1
1	D	645	THR	3.1
1	D	636	ASP	3.0
1	D	305	LYS	3.0
1	A	636	ASP	3.0
1	C	302	PHE	2.9
1	C	290	LYS	2.8
1	C	304	MET	2.8
1	A	230	ILE	2.8
1	A	180	GLN	2.7
1	A	329	ARG	2.7
1	C	306	ALA	2.7
1	A	302	PHE	2.7
1	A	325	ALA	2.7
1	C	247	GLY	2.7
1	A	236	GLU	2.6
1	C	288	SER	2.6
1	C	661	LEU	2.6
1	D	230	ILE	2.6
1	B	230	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	HIS	2.5
1	B	645	THR	2.5
1	C	653	GLY	2.5
1	C	211	GLN	2.5
1	C	230	ILE	2.5
1	C	213	GLY	2.5
1	B	306	ALA	2.5
1	D	329	ARG	2.5
1	B	639	ILE	2.4
1	A	262	GLY	2.4
1	C	483	SER	2.3
1	B	289	ALA	2.3
1	C	104	GLY	2.3
1	C	501	GLY	2.3
1	A	417	MET	2.3
1	B	491	THR	2.3
1	C	292	ILE	2.2
1	D	304	MET	2.2
1	B	228	HIS	2.2
1	B	356	ILE	2.2
1	D	235	SER	2.1
1	D	488	GLU	2.1
1	A	292	ILE	2.1
1	B	210	GLU	2.1
1	A	661	LEU	2.1
1	B	636	ASP	2.1
1	A	213	GLY	2.1
1	C	445	ASP	2.1
1	C	238	GLU	2.1
1	C	360	LEU	2.0
1	C	296	ILE	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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	K	A	997	1/1	0.59	0.40	10.02	141,141,141,141	0
4	K	C	997	1/1	0.72	0.38	6.50	144,144,144,144	0
4	K	B	997	1/1	0.90	0.33	2.95	154,154,154,154	0
4	K	D	997	1/1	0.84	0.27	2.15	160,160,160,160	0
3	MG	C	996	1/1	0.99	0.22	1.84	58,58,58,58	0
2	ALF	B	995	5/5	0.96	0.20	0.85	48,60,80,130	0
2	ALF	D	995	5/5	0.95	0.21	0.61	57,62,80,127	0
2	ALF	A	995	5/5	0.98	0.21	0.59	37,50,60,136	0
2	ALF	C	995	5/5	0.98	0.19	0.59	45,57,62,117	0
3	MG	D	996	1/1	0.98	0.21	0.51	77,77,77,77	0
3	MG	B	996	1/1	0.97	0.19	0.45	67,67,67,67	0
3	MG	A	996	1/1	0.98	0.17	-0.02	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.