



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:58 pm BST

PDB ID : 3CQF
Title : Crystal structure of anthrolysin O (ALO)
Authors : Bourdeau, R.W.; Malito, E.; Tang, W.J.
Deposited on : 2008-04-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

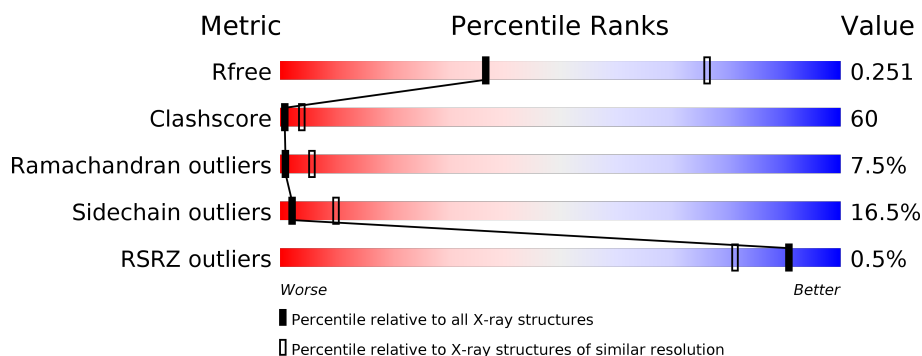
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	<div> <div></div> <div>34%45%14%• 6%</div> </div>
1	B	489	<div> <div>%</div> <div>34%46%14%• 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7101 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 Thiol-activated cytolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			
1	B	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	EXPRESSION TAG	UNP Q81N62
A	25	HIS	-	EXPRESSION TAG	UNP Q81N62
A	26	HIS	-	EXPRESSION TAG	UNP Q81N62
A	27	HIS	-	EXPRESSION TAG	UNP Q81N62
A	28	HIS	-	EXPRESSION TAG	UNP Q81N62
A	29	HIS	-	EXPRESSION TAG	UNP Q81N62
A	30	HIS	-	EXPRESSION TAG	UNP Q81N62
A	31	ALA	-	EXPRESSION TAG	UNP Q81N62
A	32	ALA	-	EXPRESSION TAG	UNP Q81N62
A	33	ALA	-	EXPRESSION TAG	UNP Q81N62
A	34	MET	-	EXPRESSION TAG	UNP Q81N62
B	24	MET	-	EXPRESSION TAG	UNP Q81N62
B	25	HIS	-	EXPRESSION TAG	UNP Q81N62
B	26	HIS	-	EXPRESSION TAG	UNP Q81N62
B	27	HIS	-	EXPRESSION TAG	UNP Q81N62
B	28	HIS	-	EXPRESSION TAG	UNP Q81N62
B	29	HIS	-	EXPRESSION TAG	UNP Q81N62
B	30	HIS	-	EXPRESSION TAG	UNP Q81N62
B	31	ALA	-	EXPRESSION TAG	UNP Q81N62
B	32	ALA	-	EXPRESSION TAG	UNP Q81N62
B	33	ALA	-	EXPRESSION TAG	UNP Q81N62
B	34	MET	-	EXPRESSION TAG	UNP Q81N62

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	16	Total 16	O 16	0	0

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

[illegible]

Chain B:

34% 46% 14% 6%

MET HIS HIS HIS HIS HIS ALA ALA MET GLU THR GLN ALA ALA ASN ALA THR GLY ALA ILE K46 M47 S49 N52 N57 Y60 D61 S62 R63 V68 N69 G70 D71 K72 V73 E74 S75 F76 I77 P78 K79 E80 S81 R82 N83 V89 V90 V91 E92 R93 I98



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.74Å 141.75Å 294.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.10) 98.4 (30.65-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.268 , 0.294 0.256 , 0.251	Depositor DCC
R_{free} test set	2675 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.66	0/3606	0.81	2/4922 (0.0%)
1	B	0.66	0/3606	0.81	2/4922 (0.0%)
All	All	0.66	0/7212	0.81	4/9844 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	481	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	149	PRO	N-CA-CB	5.34	109.71	103.30
1	A	149	PRO	N-CA-CB	5.20	109.54	103.30

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	3537	0	3406	413	0
1	B	3537	0	3406	416	0
2	A	11	0	0	1	0
2	B	16	0	0	1	0
All	All	7101	0	6812	827	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 60.

All (827) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:NH2	1:A:178:TRP:HB2	1.46	1.30
1:B:504:LEU:C	1:B:504:LEU:HD23	1.54	1.26
1:B:152:ARG:NH2	1:B:178:TRP:HB2	1.47	1.26
1:A:504:LEU:HD23	1:A:504:LEU:C	1.56	1.18
1:A:433:LYS:HA	1:A:433:LYS:CE	1.71	1.17
1:B:181:LYS:O	1:B:182:TYR:CD2	1.98	1.17
1:A:181:LYS:O	1:A:182:TYR:CD2	1.98	1.16
1:B:433:LYS:HA	1:B:433:LYS:CE	1.73	1.15
1:B:234:VAL:HG22	1:B:295:GLU:HB2	1.25	1.15
1:A:433:LYS:CA	1:A:433:LYS:HE2	1.77	1.14
1:B:152:ARG:HH21	1:B:178:TRP:CB	1.61	1.14
1:B:433:LYS:HE2	1:B:433:LYS:CA	1.78	1.13
1:A:152:ARG:HH21	1:A:178:TRP:CB	1.61	1.12
1:A:135:LEU:CD2	1:A:135:LEU:O	1.98	1.11
1:A:332:THR:CG2	1:A:347:VAL:HG23	1.82	1.10
1:B:251:PRO:HD3	1:B:280:MET:HE1	1.33	1.10
1:B:465:ILE:HG22	1:B:466:LYS:H	1.12	1.10
1:B:332:THR:CG2	1:B:347:VAL:HG23	1.82	1.10
1:A:239:TYR:CE1	1:A:358:ILE:HD13	1.88	1.09
1:A:406:LYS:HZ2	1:A:406:LYS:HA	1.16	1.08
1:A:334:VAL:HG12	1:A:345:LYS:HG3	1.35	1.08
1:A:234:VAL:HG22	1:A:295:GLU:HB2	1.24	1.08
1:B:239:TYR:CE1	1:B:358:ILE:HD13	1.88	1.08
1:B:465:ILE:HG22	1:B:466:LYS:N	1.67	1.07
1:B:388:VAL:CG1	1:B:388:VAL:O	2.01	1.07
1:A:200:TYR:HD1	1:A:394:TYR:CE1	1.73	1.07
1:A:332:THR:HG23	1:A:347:VAL:CG2	1.85	1.07
1:B:200:TYR:HD1	1:B:394:TYR:CE1	1.72	1.06
1:A:465:ILE:HG22	1:A:466:LYS:H	1.15	1.06
1:B:332:THR:HG23	1:B:347:VAL:CG2	1.86	1.06
1:B:334:VAL:HG12	1:B:345:LYS:HG3	1.35	1.05
1:B:465:ILE:HG21	1:B:489:VAL:HB	1.33	1.05
1:A:251:PRO:HD3	1:A:280:MET:HE1	1.34	1.04
1:B:135:LEU:CD2	1:B:135:LEU:O	2.04	1.04
1:A:388:VAL:CG1	1:A:388:VAL:O	2.01	1.04
1:A:465:ILE:HG21	1:A:489:VAL:HB	1.35	1.04
1:A:406:LYS:HZ3	1:A:406:LYS:HB2	1.15	1.03
1:B:200:TYR:CD1	1:B:394:TYR:HE1	1.77	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CD1	1:A:394:TYR:HE1	1.77	1.03
1:A:230:GLY:O	1:A:299:LYS:HE2	1.58	1.02
1:B:406:LYS:HZ3	1:B:406:LYS:HB2	1.18	1.02
1:A:504:LEU:HD23	1:A:504:LEU:O	1.58	1.02
1:B:406:LYS:HZ2	1:B:406:LYS:HA	1.21	1.02
1:A:465:ILE:HG22	1:A:466:LYS:N	1.69	1.01
1:B:504:LEU:O	1:B:504:LEU:HD23	1.57	1.01
1:B:230:GLY:O	1:B:299:LYS:HE2	1.60	1.01
1:A:135:LEU:C	1:A:135:LEU:HD23	1.79	1.01
1:A:135:LEU:HD23	1:A:135:LEU:O	1.57	1.00
1:B:203:SER:HB2	1:B:392:THR:HG23	1.41	1.00
1:B:388:VAL:HG12	1:B:388:VAL:O	1.59	1.00
1:A:294:LEU:HD23	1:A:331:PHE:HD1	1.26	0.99
1:A:433:LYS:NZ	1:A:434:GLU:H	1.58	0.99
1:A:388:VAL:HG12	1:A:388:VAL:O	1.61	0.99
1:B:327:GLU:OE2	1:B:327:GLU:HA	1.62	0.99
1:A:209:LEU:HD11	1:A:236:VAL:HG12	1.42	0.99
1:B:135:LEU:HD23	1:B:135:LEU:C	1.81	0.99
1:B:71:ASP:O	1:B:72:LYS:O	1.79	0.98
1:A:327:GLU:OE2	1:A:327:GLU:HA	1.58	0.98
1:B:209:LEU:HD11	1:B:236:VAL:HG12	1.40	0.98
1:B:433:LYS:NZ	1:B:434:GLU:H	1.60	0.98
1:A:203:SER:HB2	1:A:392:THR:HG23	1.42	0.98
1:A:310:LEU:HD23	1:A:310:LEU:O	1.64	0.98
1:B:294:LEU:HD23	1:B:331:PHE:HD1	1.26	0.97
1:B:428:PHE:HA	1:B:433:LYS:O	1.63	0.97
1:B:294:LEU:HD23	1:B:331:PHE:CD1	2.00	0.97
1:B:233:LYS:HE3	1:B:399:THR:HB	1.47	0.97
1:A:252:ASN:N	1:A:252:ASN:HD22	1.61	0.97
1:B:411:HIS:CD2	1:B:413:GLY:H	1.81	0.96
1:A:71:ASP:O	1:A:72:LYS:O	1.81	0.96
1:B:465:ILE:CG2	1:B:466:LYS:N	2.29	0.96
1:B:203:SER:HB2	1:B:392:THR:CG2	1.95	0.95
1:B:310:LEU:HD23	1:B:310:LEU:O	1.65	0.95
1:A:294:LEU:HD23	1:A:331:PHE:CD1	1.99	0.95
1:A:411:HIS:CD2	1:A:413:GLY:H	1.82	0.95
1:B:135:LEU:HD23	1:B:135:LEU:O	1.65	0.95
1:B:411:HIS:HD2	1:B:413:GLY:H	1.08	0.94
1:A:411:HIS:HD2	1:A:413:GLY:H	1.08	0.94
1:B:209:LEU:HD11	1:B:236:VAL:CG1	1.97	0.94
1:A:200:TYR:HD1	1:A:394:TYR:HE1	0.98	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:THR:HG22	1:B:504:LEU:N	1.83	0.93
1:B:109:ASP:OD1	1:B:338:GLY:HA2	1.69	0.93
1:B:252:ASN:N	1:B:252:ASN:HD22	1.61	0.93
1:A:209:LEU:HD11	1:A:236:VAL:CG1	1.98	0.92
1:A:203:SER:HB2	1:A:392:THR:CG2	1.98	0.92
1:A:504:LEU:CD2	1:A:504:LEU:C	2.37	0.92
1:A:233:LYS:HE3	1:A:399:THR:HB	1.50	0.92
1:B:200:TYR:HD1	1:B:394:TYR:HE1	0.98	0.92
1:B:504:LEU:C	1:B:504:LEU:CD2	2.35	0.92
1:A:465:ILE:CG2	1:A:466:LYS:N	2.31	0.91
1:B:332:THR:HG23	1:B:347:VAL:HG23	0.95	0.91
1:A:428:PHE:HA	1:A:433:LYS:O	1.69	0.91
1:A:109:ASP:OD1	1:A:338:GLY:HA2	1.70	0.91
1:B:111:VAL:HG13	1:B:114:ARG:HD3	1.51	0.91
1:A:502:THR:HG22	1:A:504:LEU:N	1.85	0.90
1:A:149:PRO:O	1:A:151:MET:N	2.05	0.90
1:A:406:LYS:CB	1:A:406:LYS:HZ3	1.84	0.90
1:A:111:VAL:O	1:A:111:VAL:HG12	1.73	0.89
1:A:473:THR:HG22	1:A:479:TRP:C	1.93	0.89
1:A:334:VAL:HG12	1:A:345:LYS:CG	2.03	0.88
1:A:111:VAL:HG13	1:A:114:ARG:HD3	1.55	0.88
1:B:73:VAL:O	1:B:74:GLU:HB3	1.72	0.88
1:B:149:PRO:O	1:B:151:MET:N	2.05	0.88
1:B:473:THR:HG22	1:B:479:TRP:C	1.93	0.88
1:B:406:LYS:CB	1:B:406:LYS:HZ3	1.85	0.88
1:A:234:VAL:CG2	1:A:295:GLU:HB2	2.04	0.88
1:A:406:LYS:NZ	1:A:406:LYS:CB	2.37	0.87
1:A:234:VAL:HG22	1:A:295:GLU:CB	2.03	0.87
1:B:234:VAL:HG22	1:B:295:GLU:CB	2.03	0.87
1:B:100:THR:HG22	1:B:101:SER:H	1.39	0.87
1:B:234:VAL:CG2	1:B:295:GLU:HB2	2.05	0.87
1:B:150:GLY:H	1:B:178:TRP:HE1	1.22	0.87
1:A:191:ARG:HD3	2:A:514:HOH:O	1.74	0.86
1:A:406:LYS:NZ	1:A:406:LYS:HA	1.90	0.86
1:B:252:ASN:N	1:B:252:ASN:ND2	2.19	0.86
1:B:139:ARG:NH1	1:B:257:LEU:HD22	1.90	0.86
1:A:100:THR:HG22	1:A:101:SER:H	1.40	0.86
1:A:332:THR:HG23	1:A:347:VAL:HG23	0.93	0.86
1:A:99:THR:HG22	1:A:99:THR:O	1.74	0.86
1:B:99:THR:O	1:B:99:THR:HG22	1.74	0.86
1:B:334:VAL:HG12	1:B:345:LYS:CG	2.06	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD22	1:A:135:LEU:O	1.73	0.85
1:A:73:VAL:O	1:A:74:GLU:HB3	1.76	0.85
1:A:150:GLY:H	1:A:178:TRP:HE1	1.21	0.85
1:A:406:LYS:NZ	1:A:406:LYS:HB2	1.89	0.85
1:B:135:LEU:O	1:B:135:LEU:HD22	1.76	0.84
1:B:406:LYS:NZ	1:B:406:LYS:HB2	1.93	0.84
1:A:406:LYS:NZ	1:A:406:LYS:CA	2.41	0.83
1:B:252:ASN:H	1:B:252:ASN:ND2	1.75	0.83
1:B:406:LYS:NZ	1:B:406:LYS:HA	1.92	0.83
1:B:502:THR:HG22	1:B:504:LEU:H	1.43	0.83
1:A:252:ASN:ND2	1:A:252:ASN:N	2.20	0.83
1:B:228:ALA:O	1:B:397:THR:HG21	1.78	0.83
1:A:202:LYS:N	1:A:224:PHE:CE1	2.47	0.82
1:B:111:VAL:HG12	1:B:111:VAL:O	1.78	0.82
1:A:406:LYS:HZ2	1:A:406:LYS:CA	1.91	0.82
1:B:202:LYS:N	1:B:224:PHE:CE1	2.48	0.82
1:A:228:ALA:O	1:A:397:THR:HG21	1.80	0.81
1:B:406:LYS:NZ	1:B:406:LYS:CA	2.43	0.81
1:B:406:LYS:CB	1:B:406:LYS:NZ	2.41	0.81
1:B:442:GLU:OE2	1:B:442:GLU:HA	1.80	0.81
1:A:139:ARG:NH1	1:A:257:LEU:HD22	1.95	0.80
1:A:442:GLU:OE2	1:A:442:GLU:HA	1.81	0.80
1:A:201:SER:C	1:A:224:PHE:HE1	1.85	0.80
1:B:157:ILE:CG2	1:B:158:THR:N	2.45	0.80
1:A:200:TYR:CD1	1:A:394:TYR:CE1	2.60	0.79
1:A:93:ARG:HH11	1:A:229:ASN:HA	1.46	0.79
1:A:157:ILE:CG2	1:A:158:THR:N	2.45	0.79
1:B:93:ARG:HH11	1:B:229:ASN:HA	1.45	0.79
1:A:116:TYR:CE2	1:A:119:ALA:HB2	2.18	0.79
1:A:334:VAL:CG1	1:A:345:LYS:HG3	2.12	0.79
1:B:201:SER:C	1:B:224:PHE:HE1	1.86	0.79
1:A:252:ASN:H	1:A:252:ASN:ND2	1.77	0.78
1:A:205:ILE:CG2	1:A:206:ALA:N	2.46	0.78
1:A:232:LYS:HE2	1:A:295:GLU:HG3	1.66	0.78
1:B:89:VAL:HG12	1:B:90:VAL:O	1.84	0.78
1:B:123:ALA:HB3	1:B:277:PRO:HD2	1.65	0.78
1:B:220:LEU:O	1:B:221:ASN:HB2	1.85	0.77
1:B:504:LEU:HD22	1:B:505:TYR:CD1	2.19	0.77
1:B:504:LEU:CD2	1:B:505:TYR:CG	2.67	0.77
1:A:388:VAL:HG13	1:A:388:VAL:O	1.84	0.77
1:A:288:ARG:HE	1:A:368:ASN:HB3	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:CG1	1:B:345:LYS:HG3	2.14	0.76
1:B:433:LYS:HA	1:B:433:LYS:HE2	0.84	0.76
1:B:465:ILE:CG2	1:B:489:VAL:HB	2.14	0.76
1:A:205:ILE:HG22	1:A:206:ALA:H	1.51	0.76
1:A:490:PRO:HG2	1:A:512:HIS:CE1	2.21	0.76
1:B:406:LYS:HZ2	1:B:406:LYS:CA	1.97	0.76
1:A:420:ASP:HB2	1:A:468:VAL:HG23	1.66	0.76
1:A:123:ALA:HB3	1:A:277:PRO:HD2	1.66	0.76
1:B:79:LYS:HD2	1:B:92:GLU:HG3	1.68	0.76
1:B:116:TYR:CE2	1:B:119:ALA:HB2	2.21	0.76
1:A:502:THR:HG22	1:A:504:LEU:H	1.47	0.76
1:A:504:LEU:HD22	1:A:505:TYR:CD1	2.21	0.76
1:B:205:ILE:CG2	1:B:206:ALA:N	2.48	0.75
1:B:225:ASN:O	1:B:228:ALA:N	2.19	0.75
1:B:223:ASP:OD1	1:B:223:ASP:O	2.05	0.75
1:A:171:VAL:CG2	1:A:246:VAL:HG21	2.17	0.75
1:B:232:LYS:HE2	1:B:295:GLU:HG3	1.67	0.75
1:A:504:LEU:CD2	1:A:505:TYR:CG	2.70	0.75
1:B:388:VAL:HG13	1:B:388:VAL:O	1.86	0.75
1:B:364:LEU:HD12	1:B:365:SER:H	1.52	0.74
1:A:239:TYR:CE1	1:A:358:ILE:CD1	2.70	0.74
1:A:225:ASN:O	1:A:228:ALA:N	2.19	0.74
1:B:484:ILE:HD11	1:B:508:ALA:HB1	1.68	0.74
1:A:73:VAL:O	1:A:74:GLU:CB	2.35	0.74
1:A:223:ASP:OD1	1:A:223:ASP:O	2.05	0.74
1:A:220:LEU:O	1:A:221:ASN:HB2	1.88	0.74
1:A:89:VAL:HG12	1:A:90:VAL:O	1.87	0.74
1:A:465:ILE:CG2	1:A:489:VAL:HB	2.15	0.74
1:B:107:ILE:HD11	1:B:375:TYR:HD2	1.53	0.74
1:A:201:SER:C	1:A:224:PHE:CE1	2.61	0.73
1:B:222:ILE:HB	1:B:224:PHE:CE2	2.22	0.73
1:B:73:VAL:O	1:B:74:GLU:CB	2.35	0.73
1:A:79:LYS:HD2	1:A:92:GLU:HG3	1.70	0.73
1:B:251:PRO:HD3	1:B:280:MET:CE	2.17	0.73
1:A:299:LYS:HB3	1:A:399:THR:HG21	1.70	0.73
1:A:222:ILE:HB	1:A:224:PHE:CE2	2.24	0.73
1:A:433:LYS:HZ1	1:A:434:GLU:H	1.35	0.73
1:B:200:TYR:CD1	1:B:394:TYR:CE1	2.60	0.73
1:B:378:THR:HG22	1:B:383:ASN:HA	1.70	0.72
1:B:484:ILE:CD1	1:B:508:ALA:HB1	2.19	0.72
1:B:201:SER:C	1:B:224:PHE:CE1	2.62	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LYS:HZ1	1:B:434:GLU:H	1.37	0.72
1:A:199:VAL:O	1:A:199:VAL:HG23	1.88	0.71
1:B:299:LYS:HB3	1:B:399:THR:HG21	1.71	0.71
1:B:205:ILE:HG22	1:B:206:ALA:H	1.55	0.71
1:B:63:ARG:HA	1:B:389:HIS:CD2	2.25	0.71
1:A:279:VAL:HG12	1:A:379:PHE:CD2	2.25	0.71
1:A:364:LEU:HD12	1:A:365:SER:H	1.54	0.71
1:A:107:ILE:HD11	1:A:375:TYR:HD2	1.56	0.71
1:A:484:ILE:HD11	1:A:508:ALA:HB1	1.71	0.71
1:A:251:PRO:HD3	1:A:280:MET:CE	2.17	0.71
1:B:279:VAL:HG12	1:B:379:PHE:CD2	2.25	0.71
1:A:100:THR:HG22	1:A:101:SER:N	2.06	0.71
1:A:266:GLU:O	1:A:270:LYS:HB2	1.90	0.71
1:A:378:THR:HG22	1:A:383:ASN:HA	1.72	0.71
1:B:100:THR:HG22	1:B:101:SER:N	2.05	0.71
1:B:200:TYR:O	1:B:224:PHE:HD1	1.74	0.71
1:A:171:VAL:HG22	1:A:246:VAL:HG21	1.73	0.70
1:A:63:ARG:HA	1:A:389:HIS:CD2	2.27	0.70
1:A:395:ILE:HG22	1:A:395:ILE:O	1.91	0.70
1:B:171:VAL:CG2	1:B:246:VAL:HG21	2.21	0.70
1:B:395:ILE:HG22	1:B:395:ILE:O	1.91	0.70
1:A:200:TYR:O	1:A:224:PHE:HD1	1.74	0.70
1:A:484:ILE:CD1	1:A:508:ALA:HB1	2.21	0.70
1:B:139:ARG:HD2	1:B:257:LEU:O	1.92	0.70
1:A:214:LYS:NZ	1:A:214:LYS:HB3	2.07	0.70
1:B:420:ASP:HB2	1:B:468:VAL:HG23	1.72	0.70
1:B:473:THR:HG22	1:B:479:TRP:O	1.91	0.70
1:B:502:THR:CG2	1:B:504:LEU:H	2.04	0.69
1:A:433:LYS:HA	1:A:433:LYS:HE2	0.83	0.69
1:B:291:TYR:HB2	1:B:334:VAL:HG22	1.72	0.69
1:B:288:ARG:HE	1:B:368:ASN:HB3	1.57	0.69
1:A:171:VAL:HG12	1:A:172:ASP:N	2.08	0.69
1:B:433:LYS:HZ3	1:B:434:GLU:H	1.40	0.69
1:A:310:LEU:O	1:A:310:LEU:CD2	2.39	0.69
1:B:239:TYR:CE1	1:B:358:ILE:CD1	2.70	0.69
1:A:420:ASP:OD2	1:A:470:ARG:NH2	2.24	0.69
1:A:139:ARG:HD2	1:A:257:LEU:O	1.93	0.69
1:A:410:ASP:HB3	1:A:412:TYR:HE2	1.58	0.69
1:B:157:ILE:HG22	1:B:158:THR:N	2.06	0.69
1:A:473:THR:HG22	1:A:479:TRP:O	1.91	0.69
1:A:157:ILE:HG22	1:A:158:THR:N	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:OD1	1:B:158:THR:HB	1.92	0.68
1:B:199:VAL:HG23	1:B:199:VAL:O	1.92	0.68
1:B:490:PRO:HG2	1:B:512:HIS:CE1	2.28	0.68
1:B:266:GLU:O	1:B:270:LYS:HB2	1.94	0.68
1:B:71:ASP:O	1:B:72:LYS:C	2.31	0.68
1:A:71:ASP:O	1:A:72:LYS:C	2.32	0.67
1:B:504:LEU:HD22	1:B:505:TYR:CG	2.28	0.67
1:A:107:ILE:HD11	1:A:375:TYR:CD2	2.30	0.67
1:A:433:LYS:HZ3	1:A:434:GLU:H	1.38	0.67
1:B:107:ILE:HD11	1:B:375:TYR:CD2	2.28	0.67
1:B:492:THR:HG21	1:B:512:HIS:CD2	2.30	0.67
1:B:310:LEU:CD2	1:B:310:LEU:O	2.40	0.67
1:A:198:MET:HE3	1:A:234:VAL:O	1.94	0.67
1:A:291:TYR:HB2	1:A:334:VAL:HG22	1.76	0.67
1:A:429:ASP:OD1	1:A:433:LYS:N	2.23	0.67
1:B:222:ILE:O	1:B:224:PHE:HD2	1.78	0.67
1:B:429:ASP:OD1	1:B:433:LYS:N	2.22	0.67
1:A:222:ILE:O	1:A:224:PHE:HD2	1.78	0.66
1:A:409:LEU:HD11	1:A:456:ILE:HD11	1.76	0.66
1:B:364:LEU:HD12	1:B:365:SER:N	2.09	0.66
1:B:411:HIS:CD2	1:B:413:GLY:N	2.62	0.66
1:B:420:ASP:OD2	1:B:470:ARG:NH2	2.25	0.66
1:A:205:ILE:CG2	1:A:206:ALA:H	2.08	0.66
1:B:135:LEU:CD2	1:B:135:LEU:C	2.49	0.66
1:B:82:ILE:HD13	1:B:83:ASN:N	2.10	0.66
1:A:143:ASN:OD1	1:A:158:THR:HB	1.95	0.66
1:A:223:ASP:O	1:A:225:ASN:N	2.28	0.66
1:A:82:ILE:HD13	1:A:83:ASN:N	2.10	0.66
1:B:459:PRO:O	1:B:462:SER:OG	2.12	0.66
1:B:223:ASP:O	1:B:225:ASN:N	2.28	0.66
1:A:100:THR:HG22	1:A:102:PRO:HD3	1.78	0.66
1:A:364:LEU:HD12	1:A:365:SER:N	2.11	0.66
1:B:214:LYS:NZ	1:B:214:LYS:HB3	2.11	0.65
1:A:459:PRO:O	1:A:462:SER:OG	2.14	0.65
1:B:410:ASP:HB3	1:B:412:TYR:HE2	1.59	0.65
1:B:100:THR:HG22	1:B:102:PRO:HD3	1.78	0.65
1:A:299:LYS:HB3	1:A:399:THR:CG2	2.27	0.65
1:B:352:ASN:HA	1:B:355:ARG:HG3	1.78	0.65
1:A:411:HIS:CD2	1:A:413:GLY:N	2.62	0.65
1:B:171:VAL:HG22	1:B:246:VAL:HG21	1.78	0.65
1:B:502:THR:HG22	1:B:503:THR:N	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD12	1:B:454:THR:CG2	2.27	0.64
1:A:504:LEU:HD22	1:A:505:TYR:CG	2.32	0.64
1:B:310:LEU:HD23	1:B:310:LEU:C	2.17	0.64
1:A:181:LYS:C	1:A:182:TYR:CD2	2.71	0.64
1:B:198:MET:HE3	1:B:234:VAL:O	1.98	0.64
1:A:135:LEU:C	1:A:135:LEU:CD2	2.49	0.64
1:A:441:TRP:O	1:A:444:SER:HB2	1.97	0.64
1:A:478:GLU:O	1:A:479:TRP:CD1	2.49	0.64
1:B:171:VAL:HG12	1:B:172:ASP:N	2.12	0.64
1:B:299:LYS:HB3	1:B:399:THR:CG2	2.26	0.64
1:B:409:LEU:HD11	1:B:456:ILE:HD11	1.78	0.64
1:B:502:THR:CG2	1:B:503:THR:N	2.61	0.64
1:A:352:ASN:HA	1:A:355:ARG:HG3	1.78	0.64
1:A:99:THR:CG2	1:A:99:THR:O	2.46	0.64
1:B:427:THR:O	1:B:435:VAL:N	2.21	0.64
1:A:239:TYR:HE1	1:A:358:ILE:HD13	1.58	0.64
1:A:492:THR:HG21	1:A:512:HIS:CD2	2.34	0.63
1:A:214:LYS:NZ	1:A:214:LYS:CB	2.61	0.63
1:B:233:LYS:CE	1:B:399:THR:HB	2.26	0.63
1:B:93:ARG:NH1	1:B:229:ASN:HA	2.14	0.63
1:B:478:GLU:O	1:B:479:TRP:CD1	2.51	0.63
1:B:504:LEU:CD2	1:B:505:TYR:CD1	2.83	0.62
1:A:469:ALA:HB3	1:A:484:ILE:HB	1.81	0.62
1:B:181:LYS:C	1:B:182:TYR:CD2	2.70	0.62
1:A:300:SER:O	1:A:302:ASP:N	2.32	0.62
1:A:205:ILE:HG23	1:A:206:ALA:N	2.15	0.62
1:A:427:THR:O	1:A:435:VAL:N	2.22	0.62
1:A:502:THR:CG2	1:A:504:LEU:H	2.10	0.62
1:B:225:ASN:O	1:B:226:ALA:C	2.38	0.62
1:B:307:PHE:O	1:B:309:ALA:N	2.32	0.62
1:B:466:LYS:HG3	1:B:487:GLN:HB3	1.81	0.62
1:A:233:LYS:CE	1:A:399:THR:HB	2.29	0.61
1:A:411:HIS:HD2	1:A:413:GLY:N	1.90	0.61
1:B:239:TYR:HE1	1:B:358:ILE:HD13	1.57	0.61
1:B:211:VAL:HG23	1:B:212:ASN:N	2.15	0.61
1:A:111:VAL:O	1:A:111:VAL:CG1	2.48	0.61
1:B:296:THR:HA	1:B:328:GLU:O	2.00	0.61
1:B:423:TRP:CD2	1:B:458:LEU:HD21	2.35	0.61
1:A:127:PHE:C	1:A:129:ASP:H	2.03	0.61
1:A:127:PHE:O	1:A:129:ASP:N	2.34	0.61
1:A:423:TRP:CD2	1:A:458:LEU:HD21	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HA	1:A:328:GLU:O	2.00	0.61
1:A:281:VAL:O	1:A:281:VAL:HG12	2.01	0.61
1:B:200:TYR:HB2	1:B:394:TYR:HD1	1.66	0.61
1:B:469:ALA:HB3	1:B:484:ILE:HB	1.83	0.61
1:A:181:LYS:O	1:A:182:TYR:HD2	1.76	0.61
1:B:100:THR:HB	1:B:390:ASN:HB3	1.83	0.61
1:A:200:TYR:HB2	1:A:394:TYR:HD1	1.65	0.61
1:A:423:TRP:CE3	1:A:458:LEU:HD21	2.36	0.61
1:B:203:SER:C	1:B:392:THR:HG21	2.21	0.61
1:B:259:ASP:OD1	1:B:260:ASN:N	2.34	0.61
1:A:297:THR:OG1	1:A:328:GLU:HB3	2.02	0.60
1:B:107:ILE:HD11	1:B:115:THR:HG21	1.83	0.60
1:B:187:THR:HB	2:B:515:HOH:O	2.00	0.60
1:A:225:ASN:O	1:A:226:ALA:C	2.39	0.60
1:B:91:VAL:O	1:B:91:VAL:HG12	2.01	0.60
1:B:205:ILE:CG2	1:B:206:ALA:H	2.13	0.60
1:A:409:LEU:HD12	1:A:454:THR:CG2	2.31	0.60
1:A:73:VAL:HG22	1:A:393:ASP:HB3	1.82	0.60
1:B:107:ILE:CD1	1:B:375:TYR:HD2	2.15	0.60
1:B:73:VAL:HG22	1:B:393:ASP:HB3	1.83	0.60
1:A:504:LEU:CD2	1:A:505:TYR:CD1	2.84	0.60
1:B:307:PHE:C	1:B:309:ALA:N	2.53	0.59
1:A:420:ASP:HA	1:A:444:SER:OG	2.03	0.59
1:B:233:LYS:HE3	1:B:399:THR:CB	2.29	0.59
1:B:310:LEU:CD2	1:B:310:LEU:C	2.71	0.59
1:B:423:TRP:CE3	1:B:458:LEU:HD21	2.36	0.59
1:A:291:TYR:CE2	1:A:336:LEU:HD21	2.37	0.59
1:B:205:ILE:HG23	1:B:206:ALA:N	2.17	0.59
1:B:441:TRP:O	1:B:444:SER:HB2	2.03	0.59
1:A:107:ILE:HD11	1:A:115:THR:HG21	1.84	0.59
1:B:281:VAL:O	1:B:281:VAL:HG12	2.02	0.59
1:A:472:CYS:HB2	1:A:477:TRP:CZ2	2.37	0.59
1:B:127:PHE:C	1:B:129:ASP:H	2.05	0.59
1:B:152:ARG:NH2	1:B:178:TRP:CB	2.38	0.59
1:A:307:PHE:O	1:A:309:ALA:N	2.36	0.59
1:B:109:ASP:CG	1:B:338:GLY:HA2	2.23	0.59
1:A:466:LYS:HG3	1:A:487:GLN:HB3	1.85	0.59
1:B:106:LEU:HD11	1:B:212:ASN:HB2	1.85	0.59
1:B:113:ASN:N	1:B:113:ASN:HD22	2.01	0.59
1:A:152:ARG:HH21	1:A:178:TRP:HB2	0.65	0.59
1:A:106:LEU:HD11	1:A:212:ASN:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:O	1:B:129:ASP:N	2.36	0.58
1:A:91:VAL:HG12	1:A:91:VAL:O	2.02	0.58
1:B:291:TYR:CE2	1:B:336:LEU:HD21	2.38	0.58
1:A:211:VAL:HG23	1:A:212:ASN:N	2.18	0.58
1:A:229:ASN:O	1:A:231:GLU:N	2.36	0.58
1:B:420:ASP:HA	1:B:444:SER:OG	2.03	0.58
1:A:294:LEU:HD22	1:A:307:PHE:CD1	2.39	0.58
1:A:477:TRP:HE3	1:A:480:TRP:CD1	2.21	0.58
1:B:297:THR:OG1	1:B:328:GLU:HB3	2.03	0.58
1:A:152:ARG:NH2	1:A:178:TRP:CB	2.38	0.58
1:A:208:ALA:C	1:A:210:ASN:H	2.06	0.58
1:A:150:GLY:O	1:A:152:ARG:HG3	2.04	0.58
1:A:310:LEU:C	1:A:310:LEU:CD2	2.71	0.58
1:B:423:TRP:CD2	1:B:458:LEU:CD2	2.87	0.58
1:A:100:THR:HB	1:A:390:ASN:HB3	1.84	0.58
1:B:122:LEU:HD11	1:B:271:GLY:HA3	1.86	0.58
1:B:197:SER:O	1:B:235:MET:HB2	2.03	0.58
1:B:492:THR:CG2	1:B:512:HIS:CD2	2.87	0.58
1:A:307:PHE:C	1:A:309:ALA:N	2.55	0.57
1:B:472:CYS:HB2	1:B:477:TRP:CZ2	2.38	0.57
1:A:206:ALA:O	1:A:207:SER:C	2.41	0.57
1:A:279:VAL:HG12	1:A:379:PHE:HD2	1.69	0.57
1:A:502:THR:HG22	1:A:503:THR:N	2.20	0.57
1:B:229:ASN:O	1:B:231:GLU:N	2.34	0.57
1:B:411:HIS:HD2	1:B:413:GLY:N	1.91	0.57
1:A:109:ASP:CG	1:A:338:GLY:HA2	2.24	0.57
1:B:107:ILE:CG1	1:B:375:TYR:HD2	2.18	0.57
1:A:107:ILE:CD1	1:A:375:TYR:HD2	2.17	0.57
1:A:423:TRP:CD2	1:A:458:LEU:CD2	2.87	0.57
1:A:199:VAL:O	1:A:199:VAL:CG2	2.52	0.57
1:A:203:SER:C	1:A:392:THR:HG21	2.24	0.57
1:B:279:VAL:HG12	1:B:379:PHE:HD2	1.68	0.57
1:A:113:ASN:N	1:A:113:ASN:HD22	2.03	0.57
1:A:93:ARG:NH1	1:A:229:ASN:HA	2.17	0.57
1:B:300:SER:O	1:B:302:ASP:N	2.37	0.56
1:B:214:LYS:NZ	1:B:214:LYS:CB	2.67	0.56
1:A:283:ASN:OD1	1:A:283:ASN:C	2.43	0.56
1:A:288:ARG:NE	1:A:368:ASN:HB3	2.18	0.56
1:A:122:LEU:HD11	1:A:271:GLY:HA3	1.87	0.56
1:B:157:ILE:HG23	1:B:158:THR:N	2.21	0.56
1:B:403:SER:HA	1:B:460:PRO:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:THR:CG2	1:A:512:HIS:CD2	2.89	0.56
1:A:347:VAL:O	1:A:347:VAL:CG1	2.54	0.56
1:B:52:ASN:OD1	1:B:255:SER:HB3	2.05	0.56
1:A:502:THR:CG2	1:A:503:THR:N	2.68	0.56
1:B:283:ASN:OD1	1:B:283:ASN:C	2.43	0.56
1:B:359:LYS:C	1:B:361:ASN:H	2.09	0.56
1:A:107:ILE:CG1	1:A:375:TYR:HD2	2.17	0.56
1:B:307:PHE:C	1:B:309:ALA:H	2.08	0.56
1:B:118:GLY:O	1:B:139:ARG:NH2	2.35	0.56
1:B:99:THR:O	1:B:99:THR:CG2	2.46	0.56
1:B:203:SER:HB2	1:B:392:THR:HG21	1.83	0.56
1:B:406:LYS:HZ3	1:B:406:LYS:CA	2.14	0.56
1:B:411:HIS:C	1:B:411:HIS:CD2	2.79	0.56
1:A:209:LEU:HD11	1:A:236:VAL:HG11	1.87	0.55
1:A:239:TYR:HE1	1:A:358:ILE:CD1	2.16	0.55
1:B:209:LEU:HD11	1:B:236:VAL:HG11	1.87	0.55
1:B:477:TRP:HE3	1:B:480:TRP:CD1	2.24	0.55
1:A:310:LEU:C	1:A:310:LEU:HD23	2.17	0.55
1:A:491:LEU:C	1:A:492:THR:HG22	2.26	0.55
1:B:150:GLY:O	1:B:152:ARG:HG3	2.05	0.55
1:B:139:ARG:HH12	1:B:257:LEU:HD22	1.70	0.55
1:B:288:ARG:HD3	1:B:361:ASN:OD1	2.06	0.55
1:B:63:ARG:HA	1:B:389:HIS:HD2	1.71	0.55
1:A:472:CYS:HB2	1:A:477:TRP:CE2	2.41	0.55
1:A:504:LEU:HD23	1:A:505:TYR:N	2.19	0.55
1:A:148:LEU:HD13	1:A:178:TRP:CD2	2.41	0.55
1:A:470:ARG:NH1	1:A:470:ARG:HB2	2.22	0.55
1:B:181:LYS:O	1:B:182:TYR:HD2	1.75	0.55
1:B:148:LEU:HD13	1:B:178:TRP:CD2	2.42	0.55
1:B:472:CYS:HB2	1:B:477:TRP:CE2	2.41	0.55
1:B:347:VAL:O	1:B:347:VAL:CG1	2.54	0.55
1:A:411:HIS:C	1:A:411:HIS:CD2	2.80	0.55
1:B:76:PHE:O	1:B:78:PRO:HD3	2.07	0.55
1:A:288:ARG:HD3	1:A:361:ASN:OD1	2.07	0.55
1:A:466:LYS:HA	1:A:486:GLU:O	2.06	0.55
1:A:359:LYS:C	1:A:361:ASN:H	2.10	0.54
1:B:223:ASP:C	1:B:225:ASN:H	2.11	0.54
1:A:76:PHE:O	1:A:78:PRO:HD3	2.07	0.54
1:B:152:ARG:HH21	1:B:178:TRP:HB2	0.65	0.54
1:A:157:ILE:HG23	1:A:158:THR:N	2.21	0.54
1:A:197:SER:O	1:A:235:MET:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:C	1:A:225:ASN:H	2.11	0.54
1:B:359:LYS:O	1:B:361:ASN:N	2.41	0.54
1:B:206:ALA:O	1:B:207:SER:C	2.45	0.54
1:B:208:ALA:C	1:B:210:ASN:H	2.11	0.54
1:A:52:ASN:OD1	1:A:255:SER:HB3	2.07	0.54
1:A:409:LEU:HD23	1:A:497:VAL:CG2	2.37	0.54
1:B:100:THR:CG2	1:B:101:SER:H	2.17	0.54
1:B:504:LEU:HD23	1:B:505:TYR:N	2.17	0.54
1:B:222:ILE:O	1:B:224:PHE:CD2	2.60	0.53
1:B:504:LEU:CD2	1:B:505:TYR:CD2	2.90	0.53
1:A:222:ILE:O	1:A:224:PHE:CD2	2.60	0.53
1:A:307:PHE:C	1:A:309:ALA:H	2.11	0.53
1:B:216:LEU:CD2	1:B:220:LEU:HD12	2.39	0.53
1:A:101:SER:N	1:A:102:PRO:HD3	2.23	0.53
1:A:63:ARG:HA	1:A:389:HIS:HD2	1.71	0.53
1:A:203:SER:HB2	1:A:392:THR:HG21	1.85	0.53
1:A:113:ASN:HD22	1:A:113:ASN:H	1.57	0.53
1:A:504:LEU:CD2	1:A:505:TYR:CD2	2.92	0.53
1:B:504:LEU:HD21	1:B:505:TYR:CD2	2.43	0.53
1:A:177:THR:HG22	1:A:178:TRP:N	2.23	0.53
1:A:259:ASP:OD1	1:A:260:ASN:N	2.39	0.53
1:A:206:ALA:O	1:A:208:ALA:N	2.42	0.53
1:A:334:VAL:HG12	1:A:345:LYS:CB	2.39	0.53
1:B:101:SER:N	1:B:102:PRO:HD3	2.23	0.53
1:B:504:LEU:HD21	1:B:505:TYR:CE2	2.44	0.53
1:B:155:ASN:O	1:B:174:LEU:HD11	2.09	0.53
1:B:283:ASN:OD1	1:B:284:VAL:N	2.41	0.53
1:B:466:LYS:HA	1:B:486:GLU:O	2.08	0.53
1:A:299:LYS:CB	1:A:399:THR:HG21	2.30	0.52
1:B:111:VAL:CG1	1:B:111:VAL:O	2.53	0.52
1:A:504:LEU:HD21	1:A:505:TYR:CD2	2.44	0.52
1:A:222:ILE:O	1:A:224:PHE:N	2.42	0.52
1:A:371:TYR:HE1	1:A:373:ILE:HD11	1.74	0.52
1:B:155:ASN:O	1:B:174:LEU:CD1	2.58	0.52
1:B:279:VAL:CG1	1:B:379:PHE:CD2	2.92	0.52
1:A:283:ASN:OD1	1:A:284:VAL:N	2.42	0.52
1:A:359:LYS:O	1:A:361:ASN:N	2.42	0.52
1:A:279:VAL:CG1	1:A:379:PHE:CD2	2.92	0.52
1:B:491:LEU:C	1:B:492:THR:HG22	2.30	0.52
1:A:116:TYR:CE1	1:A:164:TYR:HB2	2.45	0.52
1:B:181:LYS:C	1:B:182:TYR:HD2	2.11	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:HB3	1:A:154:GLU:HG2	1.92	0.52
1:B:199:VAL:O	1:B:199:VAL:CG2	2.57	0.52
1:B:214:LYS:HZ1	1:B:214:LYS:HB3	1.75	0.52
1:A:181:LYS:O	1:A:182:TYR:CG	2.59	0.52
1:A:181:LYS:C	1:A:182:TYR:HD2	2.12	0.52
1:B:116:TYR:CE1	1:B:164:TYR:HB2	2.44	0.52
1:B:359:LYS:C	1:B:361:ASN:N	2.64	0.52
1:A:163:THR:O	1:A:164:TYR:C	2.47	0.52
1:A:403:SER:HA	1:A:460:PRO:HB3	1.91	0.52
1:B:113:ASN:H	1:B:113:ASN:HD22	1.58	0.52
1:B:216:LEU:HD21	1:B:220:LEU:HD12	1.91	0.52
1:B:239:TYR:HE1	1:B:358:ILE:CD1	2.15	0.52
1:A:214:LYS:HZ1	1:A:214:LYS:HB3	1.75	0.51
1:A:409:LEU:HD12	1:A:454:THR:HG21	1.93	0.51
1:A:490:PRO:O	1:A:492:THR:HG23	2.10	0.51
1:A:105:ILE:N	1:A:105:ILE:HD13	2.24	0.51
1:A:504:LEU:HD21	1:A:505:TYR:CE2	2.45	0.51
1:B:409:LEU:HD23	1:B:497:VAL:CG2	2.41	0.51
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.45	0.51
1:A:127:PHE:HD1	1:A:127:PHE:C	2.14	0.51
1:A:473:THR:HG22	1:A:480:TRP:N	2.25	0.51
1:B:177:THR:HG22	1:B:178:TRP:N	2.25	0.51
1:B:294:LEU:HD22	1:B:307:PHE:CD1	2.45	0.51
1:B:371:TYR:HE1	1:B:373:ILE:HD11	1.74	0.51
1:A:139:ARG:CB	1:A:162:PRO:HD2	2.41	0.51
1:A:406:LYS:HZ3	1:A:406:LYS:CA	2.17	0.51
1:B:105:ILE:N	1:B:105:ILE:HD13	2.24	0.51
1:B:226:ALA:HB1	1:B:232:LYS:HB2	1.93	0.51
1:B:463:LYS:O	1:B:464:ASN:HB2	2.11	0.51
1:B:127:PHE:HD1	1:B:127:PHE:C	2.14	0.51
1:B:433:LYS:CE	1:B:433:LYS:CA	2.59	0.51
1:B:492:THR:CG2	1:B:512:HIS:HD2	2.24	0.51
1:A:149:PRO:C	1:A:151:MET:H	2.09	0.51
1:B:124:ASN:O	1:B:127:PHE:HB3	2.11	0.51
1:B:291:TYR:HB2	1:B:334:VAL:CG2	2.40	0.50
1:B:409:LEU:HD12	1:B:454:THR:HG21	1.92	0.50
1:B:127:PHE:CD1	1:B:127:PHE:C	2.83	0.50
1:A:216:LEU:CD2	1:A:220:LEU:HD12	2.41	0.50
1:A:472:CYS:HB2	1:A:477:TRP:CH2	2.46	0.50
1:A:118:GLY:O	1:A:139:ARG:NH2	2.38	0.50
1:A:359:LYS:C	1:A:361:ASN:N	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:O	1:A:174:LEU:HD11	2.11	0.50
1:A:226:ALA:HB1	1:A:232:LYS:HB2	1.94	0.50
1:B:466:LYS:HA	1:B:487:GLN:HA	1.94	0.50
1:B:490:PRO:O	1:B:492:THR:HG23	2.10	0.50
1:A:100:THR:CG2	1:A:101:SER:H	2.18	0.50
1:A:127:PHE:CD1	1:A:127:PHE:C	2.83	0.50
1:B:472:CYS:HB2	1:B:477:TRP:CH2	2.47	0.50
1:A:216:LEU:HD21	1:A:220:LEU:HD12	1.93	0.50
1:A:246:VAL:HG12	1:A:247:SER:N	2.25	0.50
1:B:98:LEU:HD11	1:B:208:ALA:HB2	1.93	0.50
1:A:171:VAL:HG21	1:A:246:VAL:HG21	1.94	0.50
1:B:139:ARG:CB	1:B:162:PRO:HD2	2.42	0.50
1:A:294:LEU:CD2	1:A:331:PHE:CD1	2.85	0.49
1:B:223:ASP:OD1	1:B:223:ASP:C	2.49	0.49
1:A:141:PRO:HB3	1:A:160:GLN:HA	1.94	0.49
1:A:326:PHE:HA	1:A:329:SER:HB2	1.94	0.49
1:A:98:LEU:HD11	1:A:208:ALA:HB2	1.94	0.49
1:B:260:ASN:C	1:B:262:VAL:H	2.14	0.49
1:A:116:TYR:CD2	1:A:119:ALA:HB2	2.47	0.49
1:A:199:VAL:HG12	1:A:205:ILE:HG12	1.95	0.49
1:A:200:TYR:O	1:A:224:PHE:CD1	2.59	0.49
1:A:466:LYS:HA	1:A:487:GLN:HA	1.94	0.49
1:B:222:ILE:O	1:B:224:PHE:N	2.41	0.49
1:B:326:PHE:HA	1:B:329:SER:HB2	1.95	0.49
1:A:223:ASP:OD1	1:A:223:ASP:C	2.50	0.49
1:B:112:VAL:HG13	1:B:113:ASN:N	2.28	0.49
1:A:327:GLU:CA	1:A:327:GLU:OE2	2.37	0.49
1:B:127:PHE:C	1:B:129:ASP:N	2.66	0.49
1:B:163:THR:O	1:B:164:TYR:C	2.48	0.49
1:B:335:VAL:O	1:B:336:LEU:C	2.50	0.49
1:B:394:TYR:CD2	1:B:394:TYR:N	2.80	0.49
1:A:415:TYR:CD1	1:A:415:TYR:O	2.65	0.49
1:B:409:LEU:HD12	1:B:454:THR:HG22	1.93	0.49
1:B:470:ARG:HB2	1:B:470:ARG:NH1	2.27	0.49
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.47	0.49
1:A:127:PHE:C	1:A:129:ASP:N	2.65	0.49
1:B:327:GLU:OE2	1:B:327:GLU:CA	2.40	0.49
1:B:465:ILE:HG21	1:B:489:VAL:CB	2.24	0.49
1:A:463:LYS:O	1:A:464:ASN:HB2	2.12	0.49
1:B:100:THR:CG2	1:B:101:SER:N	2.75	0.49
1:B:181:LYS:O	1:B:182:TYR:CG	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:MET:CE	1:B:467:ILE:HD11	2.42	0.49
1:B:307:PHE:O	1:B:308:LYS:C	2.50	0.49
1:A:233:LYS:HE3	1:A:399:THR:CB	2.32	0.48
1:B:200:TYR:O	1:B:224:PHE:CD1	2.60	0.48
1:B:294:LEU:CD2	1:B:331:PHE:CD1	2.86	0.48
1:A:134:LEU:HD23	1:A:135:LEU:H	1.78	0.48
1:B:288:ARG:NE	1:B:368:ASN:HB3	2.25	0.48
1:B:79:LYS:HD2	1:B:92:GLU:CG	2.42	0.48
1:B:411:HIS:HD2	1:B:412:TYR:N	2.11	0.48
1:A:345:LYS:HG2	1:A:346:VAL:N	2.28	0.48
1:B:116:TYR:CD2	1:B:119:ALA:HB2	2.49	0.48
1:A:124:ASN:O	1:A:127:PHE:HB3	2.13	0.48
1:A:152:ARG:HD3	1:A:155:ASN:HB3	1.94	0.48
1:A:499:ILE:HA	1:A:507:THR:O	2.13	0.48
1:B:152:ARG:HB3	1:B:154:GLU:HG2	1.95	0.48
1:B:296:THR:HB	1:B:329:SER:OG	2.14	0.48
1:B:421:VAL:HG22	1:B:467:ILE:HG12	1.95	0.48
1:A:155:ASN:O	1:A:174:LEU:CD1	2.61	0.48
1:A:179:ASN:O	1:A:183:SER:HB2	2.13	0.48
1:A:394:TYR:N	1:A:394:TYR:CD2	2.80	0.48
1:A:491:LEU:C	1:A:492:THR:CG2	2.81	0.48
1:A:60:TYR:CE1	1:A:277:PRO:HG2	2.49	0.48
1:B:473:THR:HG22	1:B:480:TRP:N	2.27	0.48
1:A:267:LEU:O	1:A:270:LYS:N	2.45	0.48
1:A:105:ILE:HD13	1:A:105:ILE:H	1.79	0.48
1:A:473:THR:HG22	1:A:480:TRP:HA	1.96	0.48
1:B:423:TRP:CE2	1:B:458:LEU:CD2	2.96	0.48
1:A:304:GLN:HG3	1:A:305:ALA:N	2.29	0.48
1:B:149:PRO:C	1:B:151:MET:H	2.09	0.48
1:B:74:GLU:HG3	1:B:75:SER:N	2.28	0.48
1:A:208:ALA:O	1:A:210:ASN:N	2.46	0.47
1:A:294:LEU:HD23	1:A:331:PHE:CE1	2.48	0.47
1:A:409:LEU:HD23	1:A:497:VAL:HG21	1.94	0.47
1:B:93:ARG:NH1	1:B:229:ASN:HB3	2.29	0.47
1:A:334:VAL:HG12	1:A:345:LYS:HB2	1.96	0.47
1:A:408:THR:HG22	1:A:408:THR:O	2.13	0.47
1:A:324:ASP:O	1:A:327:GLU:HB2	2.14	0.47
1:A:423:TRP:CE2	1:A:458:LEU:CD2	2.97	0.47
1:A:414:ALA:HB2	1:B:270:LYS:HE3	1.95	0.47
1:B:419:PHE:CZ	1:B:499:ILE:HD13	2.47	0.47
1:B:246:VAL:HG12	1:B:247:SER:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:TYR:O	1:B:415:TYR:CD1	2.68	0.47
1:B:90:VAL:HG12	1:B:91:VAL:N	2.29	0.47
1:A:395:ILE:CG2	1:A:395:ILE:O	2.61	0.47
1:A:421:VAL:HG22	1:A:467:ILE:HG12	1.96	0.47
1:B:141:PRO:HB3	1:B:160:GLN:HA	1.95	0.47
1:A:171:VAL:CG1	1:A:172:ASP:N	2.78	0.47
1:A:115:THR:HG21	1:A:375:TYR:CD2	2.49	0.47
1:B:105:ILE:HD13	1:B:105:ILE:H	1.78	0.47
1:A:411:HIS:HD2	1:A:412:TYR:N	2.12	0.47
1:A:420:ASP:HB2	1:A:468:VAL:CG2	2.41	0.47
1:B:304:GLN:HG3	1:B:305:ALA:N	2.30	0.47
1:B:426:PHE:CE1	1:B:461:ASN:HB2	2.49	0.47
1:A:111:VAL:HG13	1:A:114:ARG:CD	2.38	0.47
1:B:150:GLY:HA3	1:B:182:TYR:CD1	2.50	0.47
1:B:68:VAL:CG1	1:B:69:ASN:N	2.77	0.47
1:A:93:ARG:NH1	1:A:229:ASN:HB3	2.29	0.47
1:A:375:TYR:HE1	1:A:377:SER:OG	1.97	0.47
1:A:79:LYS:HD2	1:A:92:GLU:CG	2.43	0.47
1:B:156:THR:O	1:B:156:THR:HG22	2.13	0.47
1:B:198:MET:HA	1:B:198:MET:HE3	1.97	0.47
1:B:199:VAL:HG12	1:B:205:ILE:HG12	1.97	0.47
1:B:345:LYS:HG2	1:B:346:VAL:N	2.30	0.47
1:B:484:ILE:CG1	1:B:508:ALA:HB1	2.44	0.47
1:A:484:ILE:CG1	1:A:508:ALA:HB1	2.45	0.47
1:B:179:ASN:O	1:B:183:SER:HB2	2.15	0.47
1:B:491:LEU:C	1:B:492:THR:CG2	2.84	0.47
1:A:184:THR:C	1:A:186:HIS:N	2.66	0.46
1:A:139:ARG:HH12	1:A:257:LEU:HD22	1.78	0.46
1:A:489:VAL:HA	1:A:490:PRO:HD2	1.64	0.46
1:B:223:ASP:C	1:B:225:ASN:N	2.69	0.46
1:B:334:VAL:HG12	1:B:345:LYS:CB	2.45	0.46
1:A:208:ALA:C	1:A:210:ASN:N	2.69	0.46
1:A:307:PHE:O	1:A:308:LYS:C	2.52	0.46
1:B:257:LEU:HA	1:B:257:LEU:HD23	1.68	0.46
1:A:150:GLY:HA3	1:A:182:TYR:CD1	2.50	0.46
1:A:291:TYR:HB2	1:A:334:VAL:CG2	2.43	0.46
1:A:407:MET:CE	1:A:467:ILE:HD11	2.45	0.46
1:B:152:ARG:HD3	1:B:155:ASN:HB3	1.97	0.46
1:B:249:GLU:O	1:B:250:LEU:C	2.51	0.46
1:B:375:TYR:HE1	1:B:377:SER:OG	1.99	0.46
1:A:157:ILE:HG23	1:A:158:THR:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:TRP:O	1:A:478:GLU:C	2.53	0.46
1:A:469:ALA:CB	1:A:484:ILE:HB	2.44	0.46
1:A:335:VAL:O	1:A:336:LEU:C	2.52	0.46
1:B:112:VAL:HG13	1:B:113:ASN:H	1.80	0.46
1:B:111:VAL:CG1	1:B:114:ARG:HD3	2.36	0.46
1:A:112:VAL:HG13	1:A:113:ASN:N	2.31	0.46
1:B:408:THR:HG22	1:B:408:THR:O	2.15	0.46
1:B:418:GLN:NE2	1:B:445:GLY:O	2.49	0.46
1:B:267:LEU:O	1:B:270:LYS:N	2.48	0.46
1:B:395:ILE:O	1:B:395:ILE:CG2	2.62	0.46
1:A:260:ASN:C	1:A:262:VAL:H	2.19	0.46
1:A:294:LEU:HD22	1:A:307:PHE:CE1	2.50	0.46
1:B:157:ILE:HG23	1:B:158:THR:H	1.80	0.46
1:B:477:TRP:O	1:B:478:GLU:C	2.54	0.46
1:B:499:ILE:HA	1:B:507:THR:O	2.16	0.46
1:B:160:GLN:NE2	1:B:160:GLN:HA	2.30	0.46
1:B:484:ILE:HD11	1:B:508:ALA:CB	2.41	0.46
1:A:205:ILE:HA	1:A:205:ILE:HD12	1.62	0.45
1:B:409:LEU:HD23	1:B:497:VAL:HG21	1.97	0.45
1:A:184:THR:O	1:A:186:HIS:N	2.49	0.45
1:A:465:ILE:HG21	1:A:489:VAL:CB	2.26	0.45
1:A:492:THR:CG2	1:A:512:HIS:HD2	2.27	0.45
1:A:68:VAL:CG1	1:A:69:ASN:N	2.79	0.45
1:A:74:GLU:HG3	1:A:75:SER:N	2.30	0.45
1:A:223:ASP:C	1:A:225:ASN:N	2.68	0.45
1:B:294:LEU:HD23	1:B:331:PHE:CE1	2.49	0.45
1:B:60:TYR:CE1	1:B:277:PRO:HG2	2.52	0.45
1:B:442:GLU:OE2	1:B:442:GLU:CA	2.56	0.45
1:A:426:PHE:CE1	1:A:461:ASN:HB2	2.51	0.45
1:A:155:ASN:OD1	1:A:156:THR:N	2.49	0.45
1:A:442:GLU:CA	1:A:442:GLU:OE2	2.56	0.45
1:B:324:ASP:O	1:B:327:GLU:HB2	2.16	0.45
1:B:469:ALA:CB	1:B:484:ILE:HB	2.45	0.45
1:A:296:THR:HG21	1:A:303:VAL:HG22	1.99	0.45
1:B:184:THR:C	1:B:186:HIS:N	2.70	0.45
1:B:206:ALA:O	1:B:208:ALA:N	2.50	0.45
1:B:171:VAL:HG21	1:B:246:VAL:HG21	1.97	0.45
1:A:184:THR:O	1:A:185:THR:C	2.55	0.45
1:A:144:ILE:CG1	1:A:144:ILE:O	2.65	0.44
1:A:81:SER:O	1:A:82:ILE:HB	2.17	0.44
1:B:291:TYR:O	1:B:333:ALA:HA	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:THR:CG2	1:B:383:ASN:HA	2.45	0.44
1:B:473:THR:HG22	1:B:480:TRP:HA	1.99	0.44
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.80	0.44
1:A:192:MET:HE3	1:A:194:TYR:HB2	1.99	0.44
1:A:300:SER:O	1:A:301:LYS:C	2.56	0.44
1:A:291:TYR:O	1:A:333:ALA:HA	2.18	0.44
1:A:156:THR:HG22	1:A:156:THR:O	2.13	0.44
1:A:484:ILE:HG12	1:A:508:ALA:HB1	1.98	0.44
1:B:200:TYR:HD1	1:B:394:TYR:CD1	2.30	0.44
1:A:188:LEU:HA	1:A:189:PRO:HD3	1.83	0.44
1:A:450:ALA:HB1	1:B:136:VAL:HG11	1.99	0.44
1:B:115:THR:HG21	1:B:375:TYR:CD2	2.52	0.44
1:A:433:LYS:CA	1:A:433:LYS:CE	2.58	0.44
1:A:148:LEU:HB3	1:A:178:TRP:CD1	2.52	0.44
1:A:210:ASN:O	1:A:210:ASN:CG	2.55	0.44
1:B:484:ILE:HG12	1:B:508:ALA:HB1	1.98	0.44
1:B:81:SER:O	1:B:82:ILE:HB	2.17	0.44
1:A:296:THR:HB	1:A:329:SER:OG	2.17	0.44
1:A:471:GLU:HG2	1:A:471:GLU:O	2.15	0.44
1:A:472:CYS:HA	1:A:480:TRP:HB3	2.00	0.44
1:A:90:VAL:HG12	1:A:91:VAL:N	2.31	0.44
1:B:188:LEU:HA	1:B:189:PRO:HD3	1.82	0.44
1:A:310:LEU:HD21	1:A:351:PHE:CD2	2.52	0.44
1:B:146:ILE:HG23	1:B:148:LEU:H	1.83	0.44
1:B:155:ASN:OD1	1:B:156:THR:N	2.51	0.44
1:B:205:ILE:O	1:B:209:LEU:HB2	2.18	0.44
1:A:300:SER:C	1:A:302:ASP:N	2.70	0.43
1:B:134:LEU:HD23	1:B:135:LEU:H	1.83	0.43
1:B:265:ASP:O	1:B:266:GLU:C	2.57	0.43
1:A:424:ASP:HB2	1:A:463:LYS:O	2.18	0.43
1:B:346:VAL:HG12	1:B:348:THR:HG23	2.01	0.43
1:B:415:TYR:HB3	1:B:503:THR:HG23	2.00	0.43
1:A:300:SER:C	1:A:302:ASP:H	2.21	0.43
1:B:489:VAL:HA	1:B:490:PRO:HD2	1.67	0.43
1:B:107:ILE:CD1	1:B:115:THR:HG21	2.46	0.43
1:A:160:GLN:NE2	1:A:160:GLN:HA	2.33	0.43
1:B:210:ASN:CG	1:B:210:ASN:O	2.57	0.43
1:A:314:ASN:N	1:A:314:ASN:ND2	2.67	0.43
1:A:484:ILE:HD11	1:A:508:ALA:CB	2.43	0.43
1:A:73:VAL:O	1:A:74:GLU:HG2	2.19	0.43
1:A:287:GLY:O	1:A:370:ALA:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:HG13	1:B:114:ARG:CD	2.34	0.43
1:A:80:GLU:HG2	1:A:81:SER:N	2.33	0.42
1:A:100:THR:HG22	1:A:102:PRO:CD	2.47	0.42
1:B:296:THR:HG21	1:B:303:VAL:HG22	2.01	0.42
1:A:192:MET:HE3	1:A:192:MET:HB3	1.92	0.42
1:A:214:LYS:HZ2	1:A:214:LYS:HB3	1.83	0.42
1:A:269:ARG:HE	1:A:269:ARG:HB2	1.61	0.42
1:A:352:ASN:O	1:A:352:ASN:ND2	2.53	0.42
1:A:377:SER:HB2	1:A:386:ALA:HB3	2.00	0.42
1:B:196:GLU:HG2	1:B:196:GLU:O	2.20	0.42
1:B:220:LEU:HA	1:B:220:LEU:HD23	1.83	0.42
1:A:198:MET:HA	1:A:198:MET:HE3	2.01	0.42
1:A:294:LEU:HB3	1:A:307:PHE:CE1	2.53	0.42
1:A:409:LEU:HD12	1:A:454:THR:HG22	2.01	0.42
1:B:197:SER:OG	1:B:198:MET:N	2.52	0.42
1:B:209:LEU:CD1	1:B:236:VAL:CG1	2.84	0.42
1:B:279:VAL:HG12	1:B:379:PHE:HA	2.02	0.42
1:A:244:TYR:CE2	1:A:286:TYR:HB2	2.55	0.42
1:A:346:VAL:HG12	1:A:348:THR:HG23	2.02	0.42
1:B:377:SER:HB2	1:B:386:ALA:HB3	2.01	0.42
1:A:152:ARG:H	1:A:152:ARG:HD2	1.85	0.42
1:B:192:MET:HE3	1:B:194:TYR:HB2	2.02	0.42
1:B:200:TYR:HB2	1:B:394:TYR:CD1	2.51	0.42
1:B:408:THR:O	1:B:497:VAL:HG23	2.20	0.42
1:A:112:VAL:HG13	1:A:113:ASN:H	1.84	0.41
1:B:260:ASN:C	1:B:262:VAL:N	2.73	0.41
1:B:399:THR:HG23	1:B:400:THR:N	2.35	0.41
1:B:47:ASN:C	1:B:49:SER:N	2.73	0.41
1:A:418:GLN:NE2	1:A:445:GLY:O	2.53	0.41
1:B:139:ARG:NH1	1:B:257:LEU:CD2	2.74	0.41
1:B:144:ILE:CG1	1:B:144:ILE:O	2.68	0.41
1:B:205:ILE:HA	1:B:205:ILE:HD12	1.63	0.41
1:B:352:ASN:O	1:B:352:ASN:ND2	2.53	0.41
1:B:508:ALA:C	1:B:509:THR:HG23	2.40	0.41
1:B:68:VAL:HG12	1:B:69:ASN:N	2.35	0.41
1:A:205:ILE:O	1:A:209:LEU:HB2	2.21	0.41
1:A:433:LYS:CE	1:A:434:GLU:H	2.32	0.41
1:A:508:ALA:C	1:A:509:THR:HG23	2.41	0.41
1:B:114:ARG:NH1	1:B:132:PRO:O	2.53	0.41
1:B:468:VAL:HA	1:B:484:ILE:O	2.20	0.41
1:A:139:ARG:HB2	1:A:162:PRO:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:HG23	1:A:400:THR:N	2.36	0.41
1:B:412:TYR:N	1:B:412:TYR:CD2	2.89	0.41
1:B:420:ASP:HB2	1:B:468:VAL:CG2	2.45	0.41
1:B:471:GLU:HG2	1:B:471:GLU:O	2.13	0.41
1:A:364:LEU:O	1:A:365:SER:HB3	2.20	0.41
1:B:71:ASP:OD2	1:B:71:ASP:N	2.53	0.41
1:A:134:LEU:HD23	1:A:135:LEU:N	2.36	0.41
1:A:436:LEU:HA	1:A:436:LEU:HD12	1.58	0.41
1:A:73:VAL:O	1:A:74:GLU:CG	2.68	0.41
1:A:304:GLN:CG	1:A:305:ALA:N	2.81	0.41
1:B:472:CYS:HA	1:B:480:TRP:HB3	2.03	0.41
1:A:116:TYR:CD1	1:A:164:TYR:HB2	2.55	0.41
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.70	0.41
1:B:202:LYS:O	1:B:203:SER:C	2.59	0.41
1:B:287:GLY:O	1:B:370:ALA:HA	2.21	0.41
1:B:304:GLN:CG	1:B:305:ALA:N	2.82	0.41
1:B:334:VAL:HG12	1:B:345:LYS:HB2	2.02	0.41
1:B:424:ASP:HB2	1:B:463:LYS:O	2.21	0.41
1:A:407:MET:HA	1:A:495:ILE:O	2.20	0.41
1:B:300:SER:C	1:B:302:ASP:N	2.72	0.41
1:B:106:LEU:HD23	1:B:106:LEU:H	1.86	0.41
1:B:148:LEU:HB3	1:B:178:TRP:CD1	2.55	0.41
1:B:325:ILE:C	1:B:327:GLU:H	2.25	0.41
1:A:146:ILE:HG23	1:A:148:LEU:H	1.86	0.41
1:B:116:TYR:CD1	1:B:164:TYR:HB2	2.56	0.41
1:B:364:LEU:O	1:B:365:SER:HB3	2.21	0.41
1:A:205:ILE:O	1:A:206:ALA:C	2.59	0.40
1:A:429:ASP:N	1:A:429:ASP:OD1	2.50	0.40
1:A:473:THR:HG22	1:A:480:TRP:CA	2.51	0.40
1:A:408:THR:O	1:A:497:VAL:HG23	2.20	0.40
1:B:436:LEU:HA	1:B:436:LEU:HD12	1.60	0.40
1:A:193:GLN:O	1:A:240:LYS:HB2	2.22	0.40
1:A:502:THR:CG2	1:A:504:LEU:N	2.68	0.40
1:B:407:MET:HA	1:B:495:ILE:O	2.20	0.40
1:B:437:THR:O	1:B:437:THR:HG22	2.22	0.40
1:A:419:PHE:CZ	1:A:499:ILE:HD13	2.56	0.40
1:B:184:THR:O	1:B:185:THR:C	2.59	0.40
1:B:208:ALA:C	1:B:210:ASN:N	2.73	0.40
1:B:429:ASP:OD1	1:B:429:ASP:N	2.53	0.40
1:A:106:LEU:HD23	1:A:106:LEU:H	1.87	0.40
1:B:106:LEU:CD1	1:B:212:ASN:HB2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:SER:O	1:B:301:LYS:C	2.59	0.40
1:A:265:ASP:O	1:A:266:GLU:C	2.59	0.40
1:A:378:THR:HG22	1:A:383:ASN:CA	2.47	0.40
1:A:415:TYR:HB3	1:A:503:THR:HG23	2.02	0.40
1:B:223:ASP:CG	1:B:223:ASP:O	2.60	0.40
1:B:300:SER:C	1:B:302:ASP:H	2.24	0.40
1:B:294:LEU:HD22	1:B:307:PHE:CE1	2.57	0.40
1:B:434:GLU:HG2	1:B:436:LEU:HD13	2.04	0.40
1:B:425:GLU:OE2	1:B:459:PRO:HG3	2.21	0.40
1:B:80:GLU:HG2	1:B:81:SER:N	2.35	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	458/489 (94%)	358 (78%)	66 (14%)	34 (7%)	1	6
1	B	458/489 (94%)	357 (78%)	66 (14%)	35 (8%)	1	5
All	All	916/978 (94%)	715 (78%)	132 (14%)	69 (8%)	1	6

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	73	VAL
1	A	74	GLU
1	A	100	THR
1	A	151	MET
1	A	209	LEU
1	A	230	GLY
1	A	259	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	304	GLN
1	A	319	SER
1	A	465	ILE
1	B	72	LYS
1	B	73	VAL
1	B	74	GLU
1	B	100	THR
1	B	151	MET
1	B	209	LEU
1	B	224	PHE
1	B	230	GLY
1	B	259	ASP
1	B	304	GLN
1	B	319	SER
1	B	465	ILE
1	A	109	ASP
1	A	113	ASN
1	A	128	ALA
1	A	150	GLY
1	A	182	TYR
1	A	185	THR
1	A	206	ALA
1	A	221	ASN
1	A	223	ASP
1	A	224	PHE
1	A	301	LYS
1	A	308	LYS
1	B	113	ASN
1	B	128	ALA
1	B	150	GLY
1	B	182	TYR
1	B	221	ASN
1	B	223	ASP
1	B	301	LYS
1	B	308	LYS
1	B	370	ALA
1	A	101	SER
1	A	370	ALA
1	B	101	SER
1	B	109	ASP
1	B	206	ALA
1	B	338	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	ILE
1	A	172	ASP
1	A	338	GLY
1	A	391	ASN
1	A	414	ALA
1	B	172	ASP
1	B	185	THR
1	B	414	ALA
1	A	249	GLU
1	A	466	LYS
1	B	82	ILE
1	B	249	GLU
1	B	360	ASP
1	B	391	ASN
1	B	466	LYS
1	A	360	ASP
1	A	111	VAL
1	B	111	VAL
1	B	105	ILE

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	387/423 (92%)	323 (84%)	64 (16%)	2	10
1	B	387/423 (92%)	323 (84%)	64 (16%)	2	10
All	All	774/846 (92%)	646 (84%)	128 (16%)	2	10

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	61	ASP
1	A	62	SER
1	A	71	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	GLU
1	A	82	ILE
1	A	98	LEU
1	A	106	LEU
1	A	109	ASP
1	A	113	ASN
1	A	114	ARG
1	A	125	LYS
1	A	127	PHE
1	A	129	ASP
1	A	134	LEU
1	A	135	LEU
1	A	142	LEU
1	A	152	ARG
1	A	156	THR
1	A	158	THR
1	A	171	VAL
1	A	184	THR
1	A	187	THR
1	A	203	SER
1	A	205	ILE
1	A	211	VAL
1	A	216	LEU
1	A	219	SER
1	A	225	ASN
1	A	235	MET
1	A	252	ASN
1	A	261	SER
1	A	269	ARG
1	A	275	SER
1	A	282	SER
1	A	286	TYR
1	A	295	GLU
1	A	300	SER
1	A	301	LYS
1	A	314	ASN
1	A	319	SER
1	A	327	GLU
1	A	330	THR
1	A	332	THR
1	A	347	VAL
1	A	348	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	364	LEU
1	A	366	PHE
1	A	397	THR
1	A	399	THR
1	A	406	LYS
1	A	410	ASP
1	A	426	PHE
1	A	433	LYS
1	A	436	LEU
1	A	449	THR
1	A	465	ILE
1	A	468	VAL
1	A	491	LEU
1	A	492	THR
1	A	497	VAL
1	A	498	SER
1	A	503	THR
1	A	504	LEU
1	B	57	ASN
1	B	61	ASP
1	B	62	SER
1	B	71	ASP
1	B	74	GLU
1	B	82	ILE
1	B	98	LEU
1	B	106	LEU
1	B	109	ASP
1	B	113	ASN
1	B	114	ARG
1	B	125	LYS
1	B	127	PHE
1	B	129	ASP
1	B	134	LEU
1	B	135	LEU
1	B	142	LEU
1	B	152	ARG
1	B	156	THR
1	B	158	THR
1	B	184	THR
1	B	187	THR
1	B	203	SER
1	B	205	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	211	VAL
1	B	216	LEU
1	B	219	SER
1	B	225	ASN
1	B	235	MET
1	B	247	SER
1	B	252	ASN
1	B	261	SER
1	B	269	ARG
1	B	275	SER
1	B	282	SER
1	B	286	TYR
1	B	295	GLU
1	B	300	SER
1	B	301	LYS
1	B	314	ASN
1	B	319	SER
1	B	327	GLU
1	B	330	THR
1	B	332	THR
1	B	347	VAL
1	B	348	THR
1	B	364	LEU
1	B	366	PHE
1	B	397	THR
1	B	399	THR
1	B	406	LYS
1	B	410	ASP
1	B	426	PHE
1	B	433	LYS
1	B	436	LEU
1	B	449	THR
1	B	465	ILE
1	B	468	VAL
1	B	491	LEU
1	B	492	THR
1	B	497	VAL
1	B	498	SER
1	B	503	THR
1	B	504	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	113	ASN
1	A	160	GLN
1	A	193	GLN
1	A	225	ASN
1	A	252	ASN
1	A	314	ASN
1	A	352	ASN
1	A	389	HIS
1	A	391	ASN
1	A	411	HIS
1	A	418	GLN
1	A	512	HIS
1	B	83	ASN
1	B	113	ASN
1	B	160	GLN
1	B	193	GLN
1	B	225	ASN
1	B	252	ASN
1	B	314	ASN
1	B	352	ASN
1	B	389	HIS
1	B	391	ASN
1	B	411	HIS
1	B	418	GLN
1	B	512	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/489 (94%)	0.22	2 (0%) 92 84	51, 76, 99, 105	0
1	B	462/489 (94%)	0.22	3 (0%) 89 78	51, 76, 99, 105	0
All	All	924/978 (94%)	0.22	5 (0%) 91 81	51, 76, 99, 105	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LYS	2.8
1	B	242	ILE	2.5
1	B	79	LYS	2.5
1	A	230	GLY	2.4
1	B	144	ILE	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.