



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1TCM
Title : CYCLODEXTRIN GLYCOSYLTRANSFERASE W616A MUTANT FROM
BACILLUS CIRCULANS STRAIN 251
Authors : Knegt, R.M.A.; Dijkstra, B.W.
Deposited on : 1996-10-07
Resolution : 2.20 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

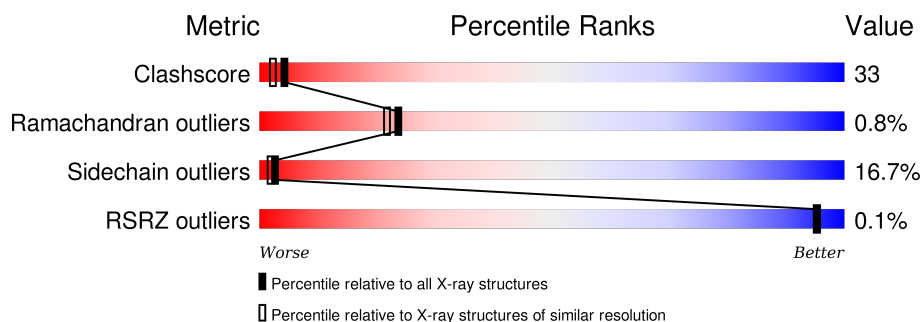
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	686	
1	B	686	

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	CA	B	688	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10779 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 CYCLODEXTRIN GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5255	3313	899	1027	16			
1	B	686	Total	C	N	O	S	0	0	0
			5255	3313	899	1027	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	ALA	TRP	ENGINEERED	UNP P43379
B	616	ALA	TRP	ENGINEERED	UNP P43379

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

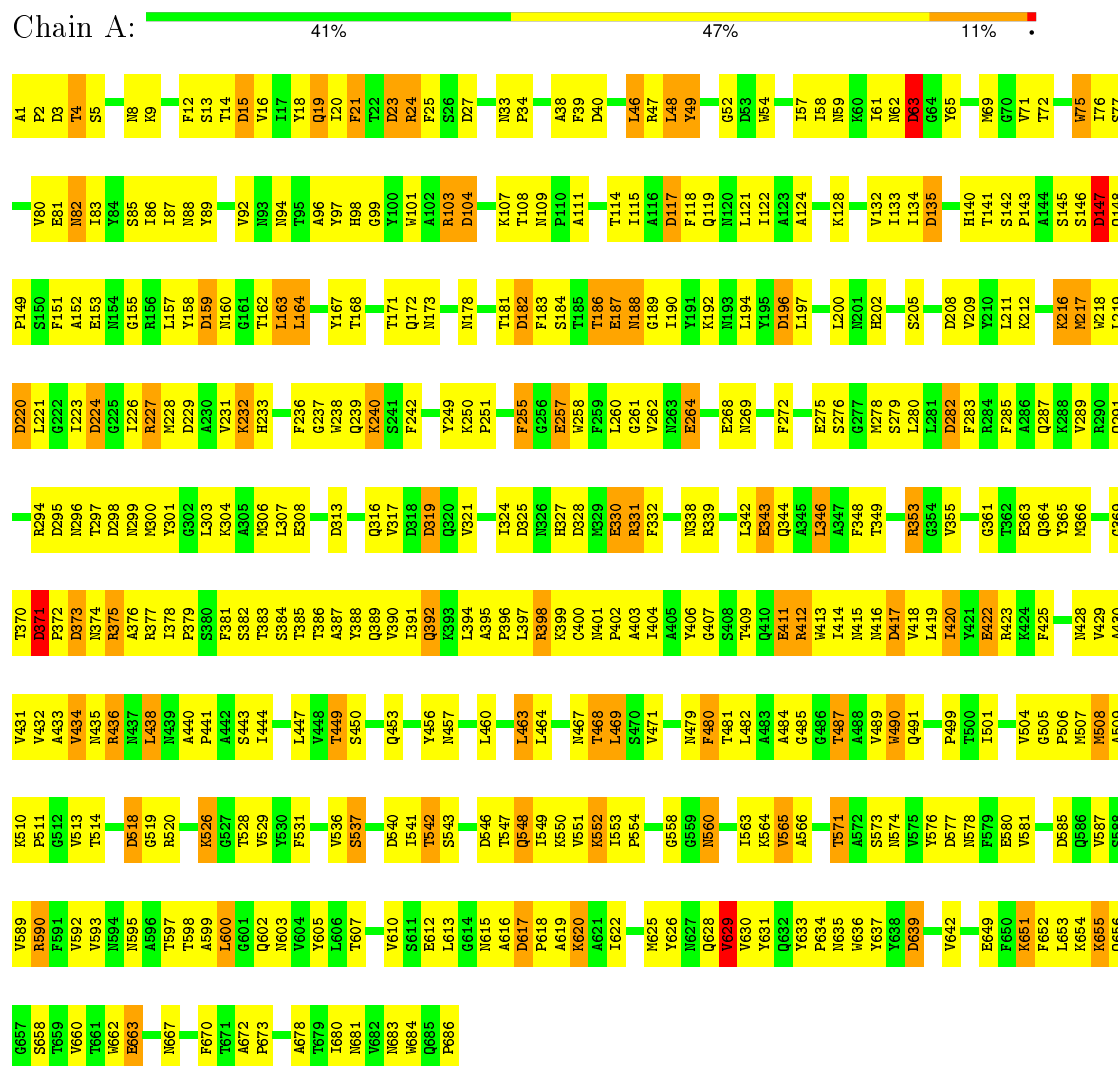
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	146	Total	O	0	0
			146	146		

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: CYCLODEXTRIN GLYCOSYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 84.80Å 118.30Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.20 6.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.20) 70.7 (6.50-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.21Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , 0.250 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.9	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48134 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10779	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	13/5383 (0.2%)	0.89	54/7336 (0.7%)
1	B	0.63	15/5383 (0.3%)	0.87	45/7336 (0.6%)
All	All	0.62	28/10766 (0.3%)	0.88	99/14672 (0.7%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	GLU	CD-OE2	5.76	1.31	1.25
1	A	363	GLU	CD-OE2	5.74	1.31	1.25
1	B	649	GLU	CD-OE2	5.55	1.31	1.25
1	A	343	GLU	CD-OE2	5.53	1.31	1.25
1	B	663	GLU	CD-OE2	5.48	1.31	1.25
1	A	330	GLU	CD-OE2	5.48	1.31	1.25
1	B	612	GLU	CD-OE2	5.48	1.31	1.25
1	B	275	GLU	CD-OE2	5.40	1.31	1.25
1	B	580	GLU	CD-OE2	5.38	1.31	1.25
1	A	268	GLU	CD-OE1	5.37	1.31	1.25
1	A	275	GLU	CD-OE2	5.37	1.31	1.25
1	A	580	GLU	CD-OE1	5.33	1.31	1.25
1	B	422	GLU	CD-OE2	5.31	1.31	1.25
1	A	153	GLU	CD-OE2	5.30	1.31	1.25
1	B	308	GLU	CD-OE2	5.26	1.31	1.25
1	B	264	GLU	CD-OE2	5.25	1.31	1.25
1	B	330	GLU	CD-OE1	5.25	1.31	1.25
1	B	545	GLU	CD-OE2	5.25	1.31	1.25
1	A	663	GLU	CD-OE2	5.23	1.31	1.25
1	A	411	GLU	CD-OE2	5.18	1.31	1.25
1	B	268	GLU	CD-OE2	5.17	1.31	1.25
1	A	649	GLU	CD-OE2	5.16	1.31	1.25
1	A	187	GLU	CD-OE2	5.13	1.31	1.25
1	A	264	GLU	CD-OE2	5.11	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	GLU	CD-OE2	5.10	1.31	1.25
1	B	187	GLU	CD-OE2	5.10	1.31	1.25
1	B	257	GLU	CD-OE2	5.09	1.31	1.25
1	B	153	GLU	CD-OE2	5.01	1.31	1.25

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	24	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	313	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	282	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	53	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	282	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	325	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	325	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	371	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	23	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	147	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	313	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	220	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	B	135	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	182	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	318	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	325	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	208	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	313	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	63	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	518	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	373	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	617	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	23	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	540	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	295	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	117	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	159	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	B	182	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	B	546	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	371	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	540	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	639	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	417	ASP	CB-CG-OD2	-5.77	113.10	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	A	147	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	458	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	458	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	147	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	B	199	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	319	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	417	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	B	313	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	208	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	117	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	24	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	373	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	B	298	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	40	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	331	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	295	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	104	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	53	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	639	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	328	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	282	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	170	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	15	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	319	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	182	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	373	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	546	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	117	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	229	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	518	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	417	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	546	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	117	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	319	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	159	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	325	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	318	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	577	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	23	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	617	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	585	ASP	CB-CG-OD1	5.25	123.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	104	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	196	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	371	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	540	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	27	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	63	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	295	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	196	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	3	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	196	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	540	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	298	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	298	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	639	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	182	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	40	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	147	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	298	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	23	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	639	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	135	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	B	282	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5255	0	5020	364	0
1	B	5255	0	5020	325	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	119	0	0	10	0
3	B	146	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10779	0	10040	685	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 33.

All (685) 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:413:TRP:HB3	1:A:420:ILE:HG13	1.19	1.14
1:A:38:ALA:HB2	1:A:86:ILE:HD11	1.35	1.07
1:A:285:PHE:HA	1:A:306:MET:HE1	1.40	1.04
1:A:618:PRO:HG3	1:A:662:TRP:HZ2	1.28	0.98
1:B:409:THR:HG23	1:B:423:ARG:HD3	1.48	0.95
1:B:299:ASN:HA	1:B:436:ARG:NH2	1.84	0.93
1:B:300:MET:HG3	1:B:419:LEU:HB2	1.51	0.91
1:B:383:THR:HG22	1:B:388:TYR:CZ	2.06	0.90
1:A:432:VAL:HG13	1:A:489:VAL:HG22	1.53	0.89
1:B:517:ILE:HD13	1:B:563:ILE:HD11	1.54	0.89
1:B:526:LYS:HE2	1:B:541:ILE:HB	1.56	0.86
1:B:25:PHE:CE2	1:B:60:LYS:HG3	2.10	0.86
1:B:25:PHE:HE2	1:B:60:LYS:HG3	1.37	0.86
1:B:48:LEU:HD12	1:B:95:THR:HG23	1.56	0.86
1:B:194:LEU:HB3	1:B:197:LEU:HD12	1.58	0.85
1:B:395:ALA:HB3	1:B:396:PRO:HD3	1.56	0.85
1:A:140:HIS:CD2	1:A:197:LEU:HD13	2.12	0.85
1:B:517:ILE:CD1	1:B:563:ILE:HD11	2.06	0.85
1:A:12:PHE:CE2	1:A:133:ILE:HD11	2.12	0.84
1:B:12:PHE:CE2	1:B:133:ILE:HD11	2.14	0.83
1:B:249:TYR:CE2	1:B:250:LYS:HD2	2.13	0.83
1:B:409:THR:HG23	1:B:423:ARG:CD	2.07	0.83
1:A:432:VAL:HG13	1:A:489:VAL:CG2	2.07	0.83
1:A:501:ILE:HD11	1:A:565:VAL:HG22	1.62	0.81
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.45	0.81
1:B:633:TYR:CD1	1:B:634:PRO:HA	2.16	0.80
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.62	0.80
1:A:260:LEU:HD22	1:A:264:GLU:HG2	1.63	0.79
1:A:285:PHE:HA	1:A:306:MET:CE	2.11	0.79
1:A:38:ALA:CB	1:A:86:ILE:HD11	2.12	0.79
1:A:633:TYR:CD2	1:A:634:PRO:HA	2.17	0.79
1:B:633:TYR:HA	1:B:635:ASN:H	1.46	0.79
1:B:317:VAL:HG21	1:B:353:ARG:HD2	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:PRO:HG3	1:A:662:TRP:CZ2	2.16	0.79
1:B:317:VAL:HG22	1:B:353:ARG:HG3	1.65	0.78
1:A:251:PRO:HB3	1:A:506:PRO:HG3	1.63	0.78
1:B:17:ILE:HB	1:B:357:ALA:HA	1.64	0.78
1:A:389:GLN:HA	1:A:392:GLN:HG2	1.66	0.77
1:B:554:PRO:HB2	1:B:556:VAL:HG13	1.66	0.77
1:B:299:ASN:HA	1:B:436:ARG:HH22	1.48	0.77
1:A:240:LYS:HE3	1:A:508:MET:SD	2.26	0.76
1:B:300:MET:HB3	1:B:414:ILE:HD11	1.66	0.76
1:A:361:GLY:O	1:A:366:MET:HG3	1.86	0.76
1:B:351:THR:HG22	3:B:768:HOH:O	1.86	0.75
1:B:248:ASN:OD1	1:B:510:LYS:HG2	1.86	0.75
1:B:438:LEU:HD12	1:B:485:GLY:HA3	1.68	0.75
1:B:69:MET:HG3	1:B:388:TYR:CE2	2.21	0.75
1:A:262:VAL:HG13	1:A:291:GLN:OE1	1.86	0.75
1:A:598:THR:HG22	1:A:654:LYS:HE2	1.67	0.74
1:A:183:PHE:HA	3:A:711:HOH:O	1.86	0.74
1:A:589:VAL:HG22	1:A:678:ALA:HB3	1.69	0.74
1:A:536:VAL:HG11	1:A:551:VAL:HG21	1.68	0.74
1:B:289:VAL:HG11	1:B:324:ILE:HG22	1.69	0.74
1:A:331:ARG:NH1	1:A:366:MET:HE2	2.03	0.73
1:B:251:PRO:HB3	1:B:506:PRO:HG3	1.69	0.73
1:A:386:THR:O	1:A:390:VAL:HG23	1.89	0.73
1:A:536:VAL:HG11	1:A:551:VAL:CG2	2.17	0.73
1:B:142:SER:HB2	1:B:143:PRO:HD2	1.69	0.73
1:A:520:ARG:HH11	1:A:520:ARG:HG2	1.53	0.73
1:A:38:ALA:O	1:A:49:TYR:HB2	1.89	0.72
1:A:673:PRO:HG2	1:A:678:ALA:HB2	1.71	0.72
1:B:140:HIS:CD2	1:B:197:LEU:HD22	2.25	0.72
1:B:251:PRO:HB3	1:B:506:PRO:CG	2.20	0.72
1:B:108:THR:HG23	1:B:115:ILE:HD13	1.71	0.72
1:B:108:THR:CG2	1:B:115:ILE:HD13	2.19	0.71
1:B:642:VAL:HG12	1:B:643:PRO:HD2	1.73	0.71
1:B:4:THR:HG22	1:B:399:LYS:HD2	1.70	0.71
1:B:564:LYS:HG2	1:B:565:VAL:N	2.05	0.71
1:A:543:SER:OG	1:A:550:LYS:HB2	1.91	0.71
1:A:157:LEU:O	1:A:164:LEU:HB2	1.91	0.71
1:B:594:ASN:HA	1:B:635:ASN:HD22	1.55	0.70
1:B:590:ARG:HG3	1:B:639:ASP:OD1	1.92	0.70
1:B:250:LYS:O	1:B:252:VAL:HG13	1.91	0.69
1:A:220:ASP:OD1	1:A:250:LYS:HE2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG22	1:A:218:TRP:HH2	1.58	0.69
1:B:24:ARG:HG3	1:B:375:ARG:O	1.93	0.69
1:A:143:PRO:HB3	1:A:196:ASP:OD2	1.93	0.69
1:B:8:ASN:O	1:B:131:LYS:HE2	1.92	0.69
1:A:374:ASN:OD1	1:A:375:ARG:HD2	1.93	0.69
1:A:216:LYS:HG3	1:A:249:TYR:CE2	2.26	0.69
1:B:226:ILE:HD12	1:B:252:VAL:CG2	2.22	0.68
1:A:520:ARG:HD3	1:A:547:THR:HG22	1.74	0.68
1:B:594:ASN:HA	1:B:635:ASN:ND2	2.08	0.68
1:A:590:ARG:HB2	1:A:639:ASP:OD1	1.94	0.68
1:B:389:GLN:O	1:B:393:LYS:HG2	1.94	0.68
1:A:397:LEU:HD23	1:A:400:CYS:SG	2.34	0.68
1:B:317:VAL:HG21	1:B:353:ARG:HH11	1.58	0.67
1:B:46:LEU:HD22	1:B:376:ALA:HA	1.76	0.67
1:A:75:TRP:HA	1:A:133:ILE:O	1.95	0.67
1:B:592:VAL:HG22	1:B:637:TYR:HB3	1.76	0.67
1:B:633:TYR:HA	1:B:635:ASN:N	2.09	0.67
1:A:108:THR:CG2	1:A:115:ILE:HD13	2.24	0.67
1:B:654:LYS:HE2	1:B:684:TRP:CZ2	2.30	0.67
1:A:460:LEU:CD1	1:A:464:LEU:HD12	2.24	0.67
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.60	0.67
1:B:24:ARG:HH12	1:B:46:LEU:HB3	1.58	0.67
1:B:331:ARG:HD3	3:B:790:HOH:O	1.95	0.67
1:B:394:LEU:HD21	1:B:489:VAL:HG21	1.76	0.67
1:A:518:ASP:OD1	1:A:548:GLN:HB2	1.95	0.66
1:A:12:PHE:HA	1:A:15:ASP:OD2	1.95	0.66
1:B:331:ARG:CZ	1:B:366:MET:HE2	2.26	0.66
1:B:563:ILE:HG23	1:B:576:TYR:HB3	1.76	0.66
1:A:299:ASN:OD1	1:A:301:TYR:HB2	1.94	0.66
1:B:414:ILE:HG13	1:B:415:ASN:N	2.09	0.66
1:A:316:GLN:HB2	3:A:696:HOH:O	1.95	0.66
1:A:261:GLY:O	1:A:264:GLU:HB3	1.96	0.66
1:A:12:PHE:O	1:A:355:VAL:HG13	1.96	0.66
1:B:4:THR:CG2	1:B:399:LYS:HD2	2.25	0.66
1:B:106:LYS:HB3	1:B:217:MET:HE1	1.78	0.66
1:A:304:LYS:HG2	1:A:308:GLU:OE2	1.96	0.66
1:B:26:SER:O	1:B:52:GLY:HA2	1.96	0.65
1:B:227:ARG:HG2	1:B:255:PHE:CE2	2.30	0.65
1:B:575:VAL:HG12	1:B:577:ASP:OD1	1.96	0.65
1:B:149:PRO:HG3	1:B:168:THR:HG21	1.78	0.65
1:A:308:GLU:HA	3:A:803:HOH:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HB2	1:A:283:PHE:CB	2.26	0.65
1:B:290:ARG:HH11	1:B:290:ARG:HB3	1.61	0.65
1:A:108:THR:HG23	1:A:115:ILE:HD13	1.78	0.65
1:A:19:GLN:HG3	1:A:75:TRP:CE3	2.32	0.65
1:B:106:LYS:HB3	1:B:217:MET:CE	2.27	0.65
1:B:633:TYR:CG	1:B:634:PRO:HA	2.31	0.65
1:A:260:LEU:HB2	1:A:283:PHE:HB3	1.78	0.64
1:B:4:THR:HG22	1:B:399:LYS:CD	2.28	0.64
1:A:285:PHE:O	1:A:289:VAL:HG23	1.97	0.64
1:B:48:LEU:HD12	1:B:95:THR:CG2	2.27	0.64
1:A:12:PHE:HB3	1:A:355:VAL:HG11	1.78	0.64
1:A:420:ILE:HD12	1:A:447:LEU:CD1	2.27	0.64
1:A:272:PHE:CD2	1:A:280:LEU:HD21	2.33	0.64
1:A:134:ILE:CD1	1:A:223:ILE:HG21	2.28	0.64
1:A:134:ILE:HD13	1:A:223:ILE:HG21	1.80	0.64
1:B:178:ASN:HB3	1:B:192:LYS:HE2	1.79	0.64
1:A:509:ALA:HB1	1:A:513:VAL:HG21	1.79	0.63
1:A:413:TRP:HB3	1:A:420:ILE:CG1	2.12	0.63
1:A:192:LYS:HE3	1:A:629:VAL:CG1	2.28	0.63
1:B:540:ASP:O	1:B:552:LYS:HG3	1.98	0.63
1:A:304:LYS:HE3	1:A:411:GLU:HB3	1.81	0.63
1:A:531:PHE:CD2	1:A:554:PRO:HG3	2.33	0.63
1:B:341:LYS:HG2	1:B:438:LEU:HD21	1.79	0.63
1:A:501:ILE:HD11	1:A:565:VAL:CG2	2.29	0.63
1:B:108:THR:HG23	1:B:115:ILE:CD1	2.29	0.63
1:B:226:ILE:HD12	1:B:252:VAL:HG21	1.81	0.63
1:B:410:GLN:HE21	1:B:412:ARG:HD2	1.63	0.63
1:A:513:VAL:HB	1:A:553:ILE:HD12	1.79	0.62
1:A:8:ASN:HB3	3:A:785:HOH:O	1.99	0.62
1:A:670:PHE:CE2	1:A:680:ILE:HD11	2.34	0.62
1:A:87:ILE:HD13	1:A:143:PRO:HG2	1.81	0.62
1:B:447:LEU:HB3	3:B:806:HOH:O	1.98	0.62
1:A:300:MET:SD	1:A:303:LEU:HD23	2.39	0.62
1:A:316:GLN:O	1:A:319:ASP:HB2	1.99	0.62
1:B:204:ASN:OD1	1:B:206:THR:HB	1.99	0.62
1:A:142:SER:HB2	1:A:143:PRO:HD2	1.81	0.62
1:A:560:ASN:ND2	1:A:578:ASN:HA	2.14	0.62
1:A:87:ILE:HD12	1:A:101:TRP:CZ3	2.35	0.62
1:A:192:LYS:HE3	1:A:629:VAL:HG13	1.79	0.62
1:B:673:PRO:HG3	1:B:678:ALA:HB2	1.80	0.62
1:B:585:ASP:C	1:B:586:GLN:HG2	2.20	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:MET:HE3	1:B:579:PHE:HA	1.82	0.62
1:A:178:ASN:O	1:A:192:LYS:HE2	1.99	0.62
1:A:633:TYR:CG	1:A:634:PRO:HA	2.35	0.62
1:A:217:MET:HE1	1:A:218:TRP:CE2	2.34	0.62
1:A:216:LYS:HE3	1:A:219:LEU:HD12	1.81	0.62
1:A:463:LEU:HD12	1:A:463:LEU:O	2.00	0.62
1:B:435:ASN:O	1:B:485:GLY:HA2	1.99	0.61
1:B:300:MET:CG	1:B:419:LEU:HB2	2.29	0.61
1:B:417:ASP:O	1:B:436:ARG:HG3	2.00	0.61
1:B:12:PHE:HB3	1:B:355:VAL:HG11	1.83	0.61
1:B:87:ILE:HG21	1:B:89:TYR:CE2	2.35	0.61
1:A:108:THR:HG23	1:A:115:ILE:CD1	2.30	0.61
1:A:589:VAL:HG11	1:A:680:ILE:CD1	2.30	0.61
1:A:551:VAL:HG22	1:A:552:LYS:N	2.15	0.61
1:A:537:SER:HA	1:A:541:ILE:HD11	1.82	0.61
1:B:423:ARG:HG3	1:B:423:ARG:NH1	2.15	0.61
1:A:304:LYS:HE3	1:A:411:GLU:CB	2.31	0.61
1:A:420:ILE:HG21	1:A:447:LEU:HD11	1.83	0.61
1:B:504:VAL:HB	1:B:576:TYR:CE2	2.35	0.61
1:A:383:THR:HG22	1:A:388:TYR:CZ	2.35	0.60
1:B:429:VAL:HG12	1:B:430:ALA:N	2.16	0.60
1:B:182:ASP:OD2	1:B:184:SER:HB3	2.01	0.60
1:B:300:MET:HG3	1:B:419:LEU:CB	2.29	0.60
1:A:457:ASN:HA	1:A:468:THR:HG22	1.82	0.60
1:B:82:ASN:O	1:B:103:ARG:HD2	2.01	0.60
1:B:390:VAL:HG13	1:B:394:LEU:HD12	1.83	0.60
1:B:609:SER:HA	3:B:812:HOH:O	2.01	0.60
1:A:58:ILE:HG23	1:A:124:ALA:CB	2.31	0.60
1:A:602:GLN:HB2	1:A:656:GLN:HB3	1.84	0.60
1:A:511:PRO:HA	1:A:553:ILE:HG22	1.82	0.60
1:A:285:PHE:HE2	1:A:349:THR:HG1	1.49	0.60
1:B:633:TYR:CA	1:B:635:ASN:H	2.14	0.60
1:B:603:ASN:O	1:B:654:LYS:HA	2.02	0.59
1:B:414:ILE:HG13	1:B:415:ASN:H	1.66	0.59
1:A:469:LEU:HD21	1:A:471:VAL:CG2	2.32	0.59
1:B:142:SER:HB2	1:B:143:PRO:CD	2.32	0.59
1:B:403:ALA:O	1:B:423:ARG:HB3	2.02	0.59
1:A:272:PHE:HD2	1:A:280:LEU:HD21	1.68	0.59
1:A:592:VAL:HB	1:A:681:ASN:HA	1.83	0.59
1:B:136:PHE:O	1:B:138:PRO:HD3	2.03	0.59
1:B:632:GLN:O	1:B:635:ASN:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:VAL:HG11	1:A:680:ILE:HD11	1.84	0.59
1:B:28:GLY:O	1:B:55:GLN:HG2	2.02	0.59
1:A:403:ALA:HA	1:A:425:PHE:CB	2.33	0.59
1:B:108:THR:O	1:B:110:PRO:HD3	2.03	0.59
1:B:617:ASP:OD2	1:B:620:LYS:HG3	2.03	0.59
1:B:1:ALA:HB1	1:B:2:PRO:HD2	1.85	0.59
1:A:417:ASP:OD1	1:A:436:ARG:HD2	2.03	0.59
1:B:195:TYR:HA	3:B:732:HOH:O	2.03	0.58
1:B:616:ALA:O	1:B:618:PRO:HD3	2.03	0.58
1:B:444:ILE:HD13	1:B:482:LEU:HB2	1.85	0.58
1:B:235:PRO:O	1:B:239:GLN:HG3	2.03	0.58
1:B:369:GLY:O	1:B:374:ASN:HB3	2.04	0.58
1:B:138:PRO:HB3	1:B:211:LEU:HD13	1.85	0.58
1:B:194:LEU:HD21	1:B:233:HIS:CD2	2.39	0.58
1:B:353:ARG:HG2	1:B:354:GLY:N	2.17	0.58
1:A:413:TRP:CZ3	1:A:418:VAL:HG11	2.39	0.57
1:A:364:GLN:OE1	1:A:385:THR:HG21	2.03	0.57
1:A:291:GLN:O	1:A:296:ASN:HA	2.03	0.57
1:A:653:LEU:CD1	1:A:655:LYS:HG2	2.34	0.57
1:A:514:THR:HB	3:A:746:HOH:O	2.03	0.57
1:B:57:ILE:HG21	1:B:121:LEU:HD11	1.86	0.57
1:A:435:ASN:O	1:A:485:GLY:HA2	2.03	0.57
1:A:499:PRO:O	1:A:573:SER:HB2	2.04	0.57
1:A:260:LEU:CD2	1:A:264:GLU:HG2	2.32	0.57
1:B:417:ASP:HA	1:B:436:ARG:HD2	1.86	0.57
1:A:422:GLU:HB2	1:A:431:VAL:HG22	1.87	0.57
1:B:517:ILE:HB	1:B:549:ILE:HB	1.87	0.57
1:A:361:GLY:HA3	1:A:366:MET:SD	2.44	0.57
1:B:317:VAL:CG2	1:B:353:ARG:HD2	2.34	0.57
1:B:630:VAL:HG23	1:B:637:TYR:OH	2.03	0.57
1:B:403:ALA:O	1:B:407:GLY:HA3	2.04	0.57
1:A:511:PRO:HA	1:A:553:ILE:CG2	2.35	0.57
1:B:318:ASP:HB2	3:B:722:HOH:O	2.03	0.57
1:A:34:PRO:HG2	1:A:49:TYR:CG	2.39	0.57
1:A:307:LEU:HD13	1:A:409:THR:HG21	1.86	0.57
1:A:464:LEU:HD12	1:A:487:THR:HG21	1.87	0.57
1:A:403:ALA:HB2	1:A:428:ASN:O	2.05	0.56
1:B:421:TYR:CZ	1:B:432:VAL:HB	2.40	0.56
1:A:122:ILE:HD13	1:A:132:VAL:HG21	1.85	0.56
1:B:366:MET:SD	1:B:379:PRO:HD3	2.46	0.56
1:B:398:ARG:NH1	1:B:404:ILE:HG22	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HG2	1:A:224:ASP:HA	1.86	0.56
1:A:566:ALA:HA	1:A:571:THR:O	2.05	0.56
1:A:505:GLY:HA2	1:A:506:PRO:C	2.24	0.56
1:A:188:ASN:O	1:A:192:LYS:HG3	2.06	0.56
1:A:205:SER:O	1:A:209:VAL:HG23	2.05	0.56
1:B:517:ILE:HD11	1:B:563:ILE:HD11	1.87	0.56
1:B:219:LEU:HD13	1:B:250:LYS:HB2	1.88	0.56
1:A:599:ALA:O	1:A:602:GLN:HB3	2.05	0.56
1:A:285:PHE:CA	1:A:306:MET:HE1	2.24	0.56
1:A:654:LYS:HG3	1:A:684:TRP:CH2	2.41	0.56
1:A:19:GLN:HG3	1:A:75:TRP:CZ3	2.41	0.56
1:B:630:VAL:HG12	1:B:631:TYR:CE1	2.41	0.56
1:B:531:PHE:CE2	1:B:554:PRO:HD3	2.41	0.56
1:A:397:LEU:HA	1:A:400:CYS:SG	2.45	0.56
1:A:403:ALA:HA	1:A:425:PHE:HB3	1.88	0.56
1:A:467:ASN:HD21	1:A:480:PHE:HD2	1.52	0.56
1:A:504:VAL:HG11	1:A:563:ILE:HD12	1.88	0.56
1:A:403:ALA:O	1:A:423:ARG:HB3	2.06	0.56
1:A:670:PHE:CZ	1:A:680:ILE:HD11	2.41	0.55
1:A:520:ARG:NH1	1:A:520:ARG:HG2	2.19	0.55
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.87	0.55
1:B:237:GLY:HA3	1:B:639:ASP:O	2.06	0.55
1:A:218:TRP:CE3	1:A:221:LEU:HD12	2.42	0.55
1:B:243:MET:SD	1:B:254:THR:HG21	2.47	0.55
1:A:402:PRO:HG3	1:A:520:ARG:NH2	2.21	0.55
1:A:81:GLU:CD	1:A:103:ARG:HD3	2.27	0.55
1:A:414:ILE:HG13	1:A:418:VAL:O	2.06	0.55
1:A:19:GLN:HG3	1:A:75:TRP:CD2	2.41	0.55
1:A:403:ALA:O	1:A:407:GLY:HA3	2.06	0.55
1:B:187:GLU:OE2	1:B:626:TYR:HB3	2.07	0.55
1:A:415:ASN:OD1	1:A:418:VAL:HB	2.07	0.54
1:A:460:LEU:O	1:A:463:LEU:HB2	2.07	0.54
1:A:227:ARG:NH1	1:A:257:GLU:HB2	2.22	0.54
1:B:406:TYR:HB2	1:B:425:PHE:CD2	2.42	0.54
1:B:147:ASP:C	1:B:149:PRO:HD3	2.28	0.54
1:B:188:ASN:O	1:B:192:LYS:HB2	2.07	0.54
1:A:605:TYR:CD1	1:A:655:LYS:HG3	2.42	0.54
1:A:558:GLY:HA2	1:A:581:VAL:O	2.08	0.54
1:A:444:ILE:HD12	1:A:444:ILE:N	2.22	0.54
1:B:290:ARG:CB	1:B:290:ARG:HH11	2.20	0.54
1:A:307:LEU:HD11	3:A:693:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:THR:OG1	1:A:552:LYS:HG3	2.08	0.54
1:B:1:ALA:HB1	1:B:2:PRO:CD	2.38	0.54
1:A:282:ASP:OD2	1:A:285:PHE:HB2	2.08	0.54
1:A:24:ARG:NH1	1:A:46:LEU:HD22	2.22	0.54
1:A:630:VAL:HB	1:A:637:TYR:CE2	2.43	0.54
1:B:511:PRO:HA	1:B:553:ILE:HB	1.89	0.54
1:B:552:LYS:HB3	1:B:552:LYS:NZ	2.22	0.53
1:B:339:ARG:HD3	3:B:781:HOH:O	2.07	0.53
1:A:300:MET:HB3	1:A:414:ILE:HD11	1.90	0.53
1:B:303:LEU:HD23	1:B:419:LEU:CD2	2.39	0.53
1:B:223:ILE:HD12	1:B:225:GLY:O	2.08	0.53
1:B:650:PHE:CE1	1:B:670:PHE:HD1	2.26	0.53
1:B:330:GLU:HB3	1:B:369:GLY:HA2	1.89	0.53
1:B:585:ASP:HA	3:B:766:HOH:O	2.07	0.53
1:A:158:TYR:CE2	1:A:163:LEU:HG	2.44	0.53
1:B:418:VAL:HG13	1:B:434:VAL:O	2.07	0.53
1:A:54:TRP:HE1	1:A:76:ILE:HD12	1.73	0.53
1:A:62:ASN:HD22	1:A:128:LYS:HD2	1.73	0.53
1:B:585:ASP:O	1:B:586:GLN:HG2	2.08	0.53
1:A:92:VAL:HG23	1:A:94:ASN:HD21	1.73	0.53
1:A:223:ILE:O	1:A:223:ILE:HG13	2.07	0.53
1:A:135:ASP:OD1	1:A:227:ARG:HB3	2.09	0.53
1:A:560:ASN:HD21	1:A:578:ASN:HA	1.72	0.53
1:A:429:VAL:HG12	1:A:430:ALA:H	1.73	0.53
1:A:429:VAL:HG12	1:A:430:ALA:N	2.24	0.53
1:B:88:ASN:HB3	3:B:721:HOH:O	2.07	0.53
1:B:414:ILE:HD12	1:B:419:LEU:HD13	1.89	0.53
1:B:652:PHE:HB3	1:B:684:TRP:HZ3	1.74	0.53
1:B:526:LYS:O	1:B:568:ALA:HB2	2.09	0.53
1:B:317:VAL:HG22	1:B:353:ARG:CG	2.37	0.53
1:B:290:ARG:HH11	1:B:290:ARG:CG	2.22	0.53
1:B:317:VAL:CG2	1:B:353:ARG:HH11	2.21	0.52
1:A:383:THR:HG22	1:A:388:TYR:CE2	2.45	0.52
1:A:324:ILE:HD12	1:A:332:PHE:CD2	2.44	0.52
1:B:651:LYS:HG3	1:B:652:PHE:H	1.74	0.52
1:A:653:LEU:HD12	1:A:653:LEU:C	2.29	0.52
1:A:231:VAL:HG12	1:A:239:GLN:OE1	2.09	0.52
1:A:339:ARG:O	1:A:343:GLU:HG3	2.10	0.52
1:A:81:GLU:CG	1:A:103:ARG:HD3	2.40	0.52
1:B:136:PHE:C	1:B:138:PRO:HD3	2.29	0.52
1:A:186:THR:O	1:A:190:ILE:HG13	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:VAL:O	1:B:553:ILE:HG13	2.09	0.52
1:B:615:ASN:HA	3:B:812:HOH:O	2.09	0.52
1:A:303:LEU:HD11	1:A:348:PHE:CZ	2.45	0.52
1:B:289:VAL:CG1	1:B:324:ILE:HG22	2.38	0.52
1:B:181:THR:HG22	1:B:193:ASN:O	2.10	0.52
1:A:147:ASP:O	1:A:148:GLN:HG2	2.10	0.52
1:B:506:PRO:HD2	1:B:515:ILE:HG22	1.91	0.52
1:A:142:SER:HB2	1:A:143:PRO:CD	2.39	0.52
1:A:371:ASP:HB2	1:A:375:ARG:CZ	2.40	0.52
1:B:243:MET:HE2	1:B:254:THR:HB	1.92	0.52
1:A:504:VAL:HG11	1:A:563:ILE:CD1	2.40	0.51
1:A:61:ILE:HG22	1:A:62:ASN:N	2.24	0.51
1:B:53:ASP:HB2	1:B:112:TYR:O	2.10	0.51
1:A:300:MET:SD	1:A:419:LEU:HB2	2.50	0.51
1:B:562:ASN:OD1	1:B:577:ASP:HB3	2.09	0.51
1:A:187:GLU:OE2	1:A:629:VAL:HG23	2.11	0.51
1:B:339:ARG:HB3	1:B:365:TYR:CE2	2.46	0.51
1:A:5:SER:HA	3:A:801:HOH:O	2.10	0.51
1:B:607:THR:OG1	1:B:616:ALA:HA	2.11	0.51
1:B:73:ALA:HA	1:B:130:ILE:HG23	1.93	0.51
1:B:251:PRO:CB	1:B:506:PRO:HG3	2.40	0.51
1:B:592:VAL:HG22	1:B:637:TYR:CB	2.39	0.51
1:B:290:ARG:O	1:B:294:ARG:HB3	2.11	0.51
1:B:652:PHE:HB2	1:B:684:TRP:CZ3	2.46	0.50
1:B:526:LYS:HE2	1:B:541:ILE:CB	2.36	0.50
1:A:38:ALA:CA	1:A:86:ILE:HD11	2.42	0.50
1:A:260:LEU:HB2	1:A:283:PHE:HB2	1.92	0.50
1:A:87:ILE:CD1	1:A:143:PRO:HG2	2.41	0.50
1:B:361:GLY:O	1:B:366:MET:HG3	2.10	0.50
1:B:223:ILE:HD11	1:B:226:ILE:HD11	1.94	0.50
1:A:331:ARG:CD	1:A:366:MET:HB2	2.41	0.50
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.92	0.50
1:A:16:VAL:O	1:A:16:VAL:HG12	2.11	0.50
1:A:65:TYR:HB2	3:A:761:HOH:O	2.12	0.50
1:A:464:LEU:HD12	1:A:487:THR:CG2	2.42	0.50
1:B:19:GLN:NE2	1:B:359:TYR:CD1	2.80	0.50
1:A:553:ILE:HG23	1:A:554:PRO:HD2	1.93	0.50
1:B:653:LEU:HD12	1:B:660:VAL:HB	1.92	0.50
1:A:236:PHE:CZ	1:A:258:TRP:CZ3	3.00	0.50
1:A:617:ASP:HB3	1:A:620:LYS:HG3	1.92	0.50
1:A:662:TRP:CH2	1:B:662:TRP:CD1	3.00	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:PRO:HB2	1:B:646:LYS:HG2	1.93	0.50
1:A:342:LEU:C	1:A:342:LEU:HD23	2.31	0.50
1:A:633:TYR:HA	1:A:635:ASN:N	2.26	0.50
1:A:605:TYR:CE1	1:A:655:LYS:HG3	2.47	0.50
1:A:236:PHE:N	1:A:236:PHE:CD1	2.80	0.50
1:B:251:PRO:HB3	1:B:506:PRO:HG2	1.92	0.49
1:A:480:PHE:CD1	1:A:480:PHE:N	2.80	0.49
1:B:395:ALA:HB3	1:B:396:PRO:CD	2.36	0.49
1:A:378:ILE:HG21	1:A:381:PHE:CZ	2.47	0.49
1:B:427:SER:H	1:B:496:THR:HG23	1.77	0.49
1:A:549:ILE:HG22	1:A:550:LYS:N	2.26	0.49
1:A:617:ASP:OD2	1:A:619:ALA:HB3	2.12	0.49
1:B:34:PRO:HG2	1:B:49:TYR:CG	2.46	0.49
1:A:140:HIS:HD2	1:A:197:LEU:HD22	1.76	0.49
1:A:226:ILE:HG22	1:A:227:ARG:N	2.27	0.49
1:B:101:TRP:HB3	1:B:142:SER:CB	2.42	0.49
1:B:564:LYS:HD2	1:B:572:ALA:HB1	1.94	0.49
1:A:172:GLN:O	1:A:173:ASN:HB2	2.12	0.49
1:A:625:MET:HE1	1:A:652:PHE:HE2	1.77	0.49
1:A:432:VAL:HG13	1:A:489:VAL:HG23	1.94	0.49
1:B:17:ILE:CD1	1:B:133:ILE:HD12	2.42	0.49
1:A:411:GLU:C	1:A:412:ARG:HG2	2.33	0.49
1:A:457:ASN:HA	1:A:468:THR:CG2	2.42	0.49
1:B:201:ASN:OD1	1:B:203:ASN:HB3	2.12	0.49
1:B:636:TRP:N	1:B:636:TRP:CD1	2.80	0.49
1:A:4:THR:HG22	1:A:399:LYS:HD2	1.93	0.49
1:A:464:LEU:CD1	1:A:487:THR:HG21	2.43	0.49
1:A:227:ARG:HD2	1:A:227:ARG:C	2.32	0.49
1:A:87:ILE:HG21	1:A:89:TYR:CZ	2.48	0.49
1:A:339:ARG:HB3	1:A:365:TYR:CE2	2.47	0.49
1:B:330:GLU:CB	1:B:369:GLY:HA2	2.43	0.48
1:B:567:ASN:C	1:B:569:ALA:H	2.16	0.48
1:A:602:GLN:HA	1:A:655:LYS:O	2.13	0.48
1:A:82:ASN:OD1	1:A:99:GLY:HA2	2.13	0.48
1:B:139:ASN:HB3	3:B:695:HOH:O	2.12	0.48
1:B:509:ALA:HA	1:B:582:LEU:HD12	1.94	0.48
1:B:383:THR:HG22	1:B:388:TYR:CE2	2.48	0.48
1:A:610:VAL:CG2	1:A:613:LEU:HB2	2.42	0.48
1:A:75:TRP:CE2	1:A:227:ARG:HG3	2.48	0.48
1:B:101:TRP:HB3	1:B:142:SER:HB3	1.96	0.48
1:A:504:VAL:HB	1:A:576:TYR:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:PHE:O	1:A:663:GLU:HB2	2.12	0.48
1:B:610:VAL:HG11	1:B:648:ILE:HG13	1.96	0.48
1:A:202:HIS:HB3	1:A:238:TRP:CD1	2.48	0.48
1:A:662:TRP:CZ3	1:B:662:TRP:CD1	3.02	0.48
1:A:531:PHE:CE2	1:A:554:PRO:HD3	2.48	0.48
1:A:118:PHE:O	1:A:121:LEU:HB3	2.14	0.48
1:A:420:ILE:HG23	1:A:433:ALA:HB2	1.95	0.48
1:B:642:VAL:HG12	1:B:643:PRO:CD	2.43	0.48
1:A:108:THR:HG22	1:A:218:TRP:CH2	2.43	0.48
1:A:18:TYR:CE1	1:A:20:ILE:HG12	2.48	0.48
1:A:33:ASN:ND2	1:A:39:PHE:CZ	2.81	0.48
1:B:659:THR:HG22	1:B:659:THR:O	2.14	0.48
1:B:598:THR:HG23	1:B:636:TRP:HZ2	1.78	0.48
1:A:47:ARG:NE	1:A:372:PRO:HG3	2.29	0.48
1:B:652:PHE:CB	1:B:684:TRP:HZ3	2.27	0.48
1:A:287:GLN:OE1	1:A:287:GLN:HA	2.14	0.48
1:B:610:VAL:HG11	1:B:648:ILE:CG1	2.44	0.48
1:B:38:ALA:O	1:B:49:TYR:HB2	2.14	0.47
1:B:288:LYS:HE3	1:B:298:ASP:OD2	2.14	0.47
1:A:316:GLN:HE21	1:A:507:MET:HG3	1.79	0.47
1:A:181:THR:OG1	1:A:189:GLY:HA2	2.15	0.47
1:B:172:GLN:HB3	1:B:174:LEU:HD21	1.95	0.47
1:A:134:ILE:HD11	1:A:223:ILE:HD13	1.95	0.47
1:B:159:ASP:OD1	1:B:210:TYR:HE1	1.97	0.47
1:B:300:MET:CE	1:B:436:ARG:HG2	2.44	0.47
1:A:262:VAL:HG13	1:A:291:GLN:CD	2.34	0.47
1:A:519:GLY:O	1:A:547:THR:HA	2.14	0.47
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.55	0.47
1:A:440:ALA:O	1:A:484:ALA:HA	2.14	0.47
1:B:12:PHE:O	1:B:355:VAL:HG13	2.15	0.47
1:A:389:GLN:CA	1:A:392:GLN:HG2	2.42	0.47
1:A:464:LEU:HB3	1:A:487:THR:HB	1.97	0.47
1:B:650:PHE:CD1	1:B:650:PHE:N	2.83	0.47
1:B:333:HIS:HE1	1:B:337:ALA:O	1.95	0.47
1:A:456:TYR:HB3	1:A:490:TRP:HB3	1.96	0.47
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.80	0.47
1:B:502:GLY:O	1:B:503:HIS:HB2	2.13	0.47
1:B:459:VAL:HG23	1:B:489:VAL:O	2.14	0.47
1:B:504:VAL:HG12	1:B:505:GLY:N	2.30	0.47
1:B:434:VAL:HG12	1:B:435:ASN:N	2.30	0.46
1:A:317:VAL:C	1:A:319:ASP:H	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LYS:HB2	1:A:651:LYS:HE2	1.60	0.46
1:B:219:LEU:HD12	1:B:249:TYR:HD2	1.80	0.46
1:A:536:VAL:O	1:A:541:ILE:HD11	2.14	0.46
1:B:506:PRO:O	1:B:579:PHE:HE2	1.98	0.46
1:A:413:TRP:CE3	1:A:418:VAL:HG11	2.50	0.46
1:A:108:THR:HG21	1:A:115:ILE:HD13	1.94	0.46
1:B:541:ILE:O	1:B:541:ILE:HG22	2.16	0.46
1:A:589:VAL:CG1	1:A:680:ILE:HD12	2.45	0.46
1:B:564:LYS:HG2	1:B:565:VAL:H	1.75	0.46
1:B:75:TRP:CZ2	1:B:227:ARG:HG3	2.50	0.46
1:B:187:GLU:CD	1:B:626:TYR:HB3	2.36	0.46
1:A:236:PHE:N	1:A:236:PHE:HD1	2.13	0.46
1:A:447:LEU:HD21	1:A:449:THR:CG2	2.46	0.46
1:B:651:LYS:HE3	1:B:663:GLU:O	2.16	0.46
1:A:14:THR:O	1:A:398:ARG:HB2	2.16	0.46
1:B:24:ARG:NH1	1:B:46:LEU:HB3	2.28	0.46
1:A:600:LEU:C	1:A:602:GLN:H	2.18	0.46
1:A:398:ARG:HE	1:A:398:ARG:HB3	1.48	0.46
1:A:369:GLY:H	1:A:373:ASP:HB2	1.79	0.46
1:A:285:PHE:CE1	1:A:348:PHE:HE1	2.33	0.46
1:A:140:HIS:CD2	1:A:197:LEU:HD22	2.51	0.46
1:B:19:GLN:HG3	1:B:75:TRP:CE3	2.50	0.46
1:A:83:ILE:HD12	1:A:85:SER:OG	2.16	0.46
1:A:528:THR:OG1	1:A:537:SER:HB3	2.15	0.46
1:B:146:SER:O	1:B:168:THR:HG23	2.16	0.46
1:A:417:ASP:O	1:A:436:ARG:HG3	2.16	0.46
1:A:610:VAL:HG23	1:A:613:LEU:H	1.81	0.46
1:A:300:MET:CE	1:A:434:VAL:HG12	2.45	0.46
1:B:510:LYS:O	1:B:513:VAL:HG23	2.15	0.46
1:B:673:PRO:CG	1:B:678:ALA:HB2	2.44	0.46
1:B:610:VAL:CG1	1:B:648:ILE:HG13	2.46	0.46
1:A:202:HIS:HB3	1:A:238:TRP:NE1	2.31	0.46
1:A:182:ASP:OD2	1:A:184:SER:HB3	2.15	0.46
1:A:25:PHE:HD2	1:A:57:ILE:HG13	1.81	0.46
1:B:600:LEU:HD22	1:B:600:LEU:HA	1.71	0.46
1:A:61:ILE:HG22	1:A:62:ASN:ND2	2.30	0.46
1:B:98:HIS:ND1	1:B:100:TYR:HB2	2.31	0.46
1:A:467:ASN:ND2	1:A:480:PHE:HD2	2.14	0.45
1:A:430:ALA:HA	1:A:491:GLN:HA	1.98	0.45
1:B:134:ILE:HD12	1:B:135:ASP:O	2.16	0.45
1:A:285:PHE:CZ	1:A:348:PHE:HE1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:HG22	1:A:613:LEU:HB2	1.98	0.45
1:B:322:THR:O	1:B:323:PHE:HB3	2.16	0.45
1:A:38:ALA:HB2	1:A:86:ILE:CD1	2.25	0.45
1:B:397:LEU:O	1:B:401:ASN:HB3	2.17	0.45
1:A:187:GLU:OE1	1:A:626:TYR:HB3	2.16	0.45
1:B:236:PHE:CD1	1:B:236:PHE:N	2.80	0.45
1:A:438:LEU:HD12	1:A:438:LEU:HA	1.82	0.45
1:A:526:LYS:HE2	1:A:541:ILE:HB	1.97	0.45
1:A:216:LYS:CE	1:A:219:LEU:HD12	2.44	0.45
1:B:444:ILE:HD12	1:B:444:ILE:N	2.30	0.45
1:B:336:ASN:HD22	1:B:336:ASN:N	2.14	0.45
1:A:103:ARG:HG2	1:A:104:ASP:N	2.32	0.45
1:B:290:ARG:HH12	1:B:294:ARG:NH1	2.14	0.45
1:A:630:VAL:HB	1:A:637:TYR:CZ	2.52	0.45
1:A:593:VAL:HG12	1:A:636:TRP:HB2	1.97	0.45
1:B:215:ILE:O	1:B:219:LEU:HG	2.17	0.45
1:A:81:GLU:HB2	1:A:108:THR:O	2.17	0.45
1:A:653:LEU:HD13	1:A:655:LYS:HG2	1.97	0.45
1:A:14:THR:O	1:A:399:LYS:HD3	2.16	0.45
1:A:200:LEU:HD13	1:A:211:LEU:HD11	1.98	0.45
1:A:615:ASN:O	1:A:616:ALA:HB3	2.17	0.45
1:B:224:ASP:O	1:B:252:VAL:HB	2.17	0.45
1:B:57:ILE:HG13	3:B:764:HOH:O	2.17	0.45
1:B:365:TYR:HE1	1:B:385:THR:HB	1.82	0.45
1:B:652:PHE:CB	1:B:684:TRP:CZ3	3.00	0.45
1:B:548:GLN:HG2	1:B:549:ILE:N	2.32	0.45
1:B:331:ARG:NH1	1:B:366:MET:CE	2.80	0.45
1:A:655:LYS:HE2	1:A:655:LYS:HB3	1.46	0.45
1:B:452:PRO:HD2	1:B:456:TYR:OH	2.17	0.45
1:B:530:TYR:O	1:B:563:ILE:HA	2.17	0.45
1:A:101:TRP:HA	1:A:141:THR:O	2.17	0.45
1:A:406:TYR:HB2	1:A:425:PHE:CD2	2.52	0.45
1:B:426:GLY:HA3	1:B:496:THR:HG21	1.99	0.45
1:B:648:ILE:HG22	1:B:649:GLU:N	2.31	0.45
1:B:317:VAL:CG2	1:B:353:ARG:NH1	2.80	0.44
1:B:397:LEU:HD11	1:B:459:VAL:HG11	1.99	0.44
1:A:387:ALA:O	1:A:391:ILE:HG13	2.17	0.44
1:A:662:TRP:CH2	1:B:662:TRP:NE1	2.86	0.44
1:A:15:ASP:HB3	1:A:72:THR:OG1	2.16	0.44
1:A:444:ILE:CD1	1:A:444:ILE:N	2.80	0.44
1:B:520:ARG:HD3	1:B:547:THR:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PHE:HE2	1:B:60:LYS:CG	2.19	0.44
1:A:610:VAL:HG23	1:A:613:LEU:N	2.32	0.44
1:A:59:ASN:O	1:A:63:ASP:HB3	2.17	0.44
1:A:420:ILE:HG21	1:A:447:LEU:CD1	2.48	0.44
1:B:429:VAL:HG12	1:B:430:ALA:H	1.79	0.44
1:A:58:ILE:HG23	1:A:124:ALA:HB1	2.00	0.44
1:B:648:ILE:CG2	1:B:649:GLU:N	2.80	0.44
1:B:98:HIS:HB2	1:B:100:TYR:CD2	2.52	0.44
1:B:240:LYS:HG2	1:B:508:MET:HE3	2.00	0.44
1:A:551:VAL:CG2	1:A:552:LYS:N	2.80	0.44
1:A:81:GLU:HG2	1:A:103:ARG:HD3	2.00	0.44
1:A:92:VAL:HG23	1:A:94:ASN:ND2	2.32	0.44
1:A:228:MET:CE	1:A:242:PHE:CD2	3.01	0.44
1:B:290:ARG:HH12	1:B:294:ARG:HH11	1.66	0.44
1:A:407:GLY:HA2	1:A:425:PHE:HB2	1.99	0.44
1:B:269:ASN:C	1:B:269:ASN:HD22	2.21	0.44
1:B:647:THR:HG22	1:B:647:THR:O	2.17	0.44
1:B:383:THR:HG22	1:B:388:TYR:CE1	2.51	0.44
1:B:630:VAL:CG2	1:B:637:TYR:CE2	3.01	0.44
1:A:440:ALA:HA	1:A:441:PRO:HD3	1.73	0.44
1:B:71:VAL:O	1:B:71:VAL:HG12	2.18	0.44
1:B:78:GLN:HA	1:B:79:PRO:HD3	1.72	0.44
1:A:662:TRP:CD1	1:B:651:LYS:HE2	2.53	0.44
1:B:504:VAL:CG1	1:B:505:GLY:N	2.80	0.44
1:A:24:ARG:NH2	1:A:97:TYR:CE2	2.85	0.44
1:B:426:GLY:HA3	1:B:496:THR:CG2	2.47	0.44
1:A:481:THR:HG22	1:A:481:THR:O	2.17	0.44
1:A:149:PRO:HG3	1:A:168:THR:HG21	2.00	0.44
1:A:520:ARG:CD	1:A:547:THR:HG22	2.47	0.44
1:A:54:TRP:O	1:A:58:ILE:HG13	2.18	0.44
1:A:303:LEU:HD21	1:A:348:PHE:CE2	2.53	0.43
1:A:537:SER:HA	1:A:541:ILE:CD1	2.47	0.43
1:B:87:ILE:CG2	1:B:89:TYR:CE2	3.01	0.43
1:B:201:ASN:C	1:B:203:ASN:H	2.21	0.43
1:A:82:ASN:N	1:A:82:ASN:HD22	2.16	0.43
1:A:413:TRP:CZ3	1:A:418:VAL:CG1	3.01	0.43
1:A:251:PRO:HB3	1:A:506:PRO:CG	2.42	0.43
1:B:598:THR:HG23	1:B:636:TRP:CZ2	2.53	0.43
1:A:114:THR:H	1:A:117:ASP:HB2	1.83	0.43
1:A:651:LYS:HB2	3:A:765:HOH:O	2.17	0.43
1:B:219:LEU:HD13	1:B:250:LYS:CB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HG3	1:A:258:TRP:CE2	2.53	0.43
1:B:464:LEU:O	1:B:465:ASN:HB2	2.17	0.43
1:B:6:VAL:O	1:B:6:VAL:HG22	2.18	0.43
1:A:413:TRP:CE3	1:A:418:VAL:CG1	3.01	0.43
1:B:429:VAL:CG1	1:B:430:ALA:N	2.80	0.43
1:A:403:ALA:HA	1:A:425:PHE:HB2	1.99	0.43
1:B:86:ILE:HG21	1:B:93:ASN:ND2	2.33	0.43
1:A:285:PHE:CD1	1:A:306:MET:HE1	2.54	0.43
1:B:69:MET:HE3	1:B:69:MET:HB3	1.86	0.43
1:B:331:ARG:NH1	1:B:366:MET:HE2	2.34	0.43
1:B:536:VAL:CG1	1:B:540:ASP:HB2	2.48	0.43
1:B:617:ASP:HB2	1:B:620:LYS:NZ	2.34	0.43
1:A:46:LEU:HD11	1:A:376:ALA:HB2	2.01	0.43
1:B:339:ARG:O	1:B:343:GLU:HG3	2.18	0.43
1:A:23:ASP:HA	1:A:52:GLY:HA3	1.99	0.43
1:A:151:PHE:O	1:A:152:ALA:HB3	2.19	0.43
1:B:12:PHE:HA	1:B:15:ASP:OD1	2.19	0.43
1:B:554:PRO:HB2	1:B:556:VAL:CG1	2.44	0.43
1:B:331:ARG:HB3	1:B:331:ARG:HE	1.45	0.43
1:B:187:GLU:OE1	1:B:628:GLN:HG3	2.19	0.43
1:B:684:TRP:O	1:B:686:PRO:HD3	2.19	0.42
1:A:115:ILE:O	1:A:119:GLN:HG3	2.19	0.42
1:A:272:PHE:O	1:A:276:SER:HB3	2.19	0.42
1:B:278:MET:HG2	1:B:278:MET:O	2.19	0.42
1:B:290:ARG:NH1	1:B:290:ARG:CG	2.81	0.42
1:B:185:THR:OG1	1:B:188:ASN:HB2	2.19	0.42
1:A:467:ASN:ND2	1:A:480:PHE:CD2	2.81	0.42
1:B:339:ARG:HB3	1:B:365:TYR:CD2	2.54	0.42
1:A:378:ILE:HG21	1:A:381:PHE:CE1	2.53	0.42
1:B:49:TYR:CE1	1:B:97:TYR:HA	2.54	0.42
1:B:468:THR:CG2	1:B:469:LEU:N	2.82	0.42
1:B:366:MET:HE3	1:B:366:MET:HB3	1.96	0.42
1:B:439:ASN:O	1:B:440:ALA:HB2	2.19	0.42
1:B:680:ILE:H	1:B:680:ILE:HG12	1.53	0.42
1:A:549:ILE:CG2	1:A:550:LYS:N	2.81	0.42
1:A:460:LEU:HD11	1:A:464:LEU:HD12	2.00	0.42
1:B:19:GLN:HG3	1:B:75:TRP:CD2	2.54	0.42
1:B:82:ASN:OD1	1:B:99:GLY:HA2	2.18	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.77	0.42
1:B:526:LYS:HA	1:B:544:TRP:CD2	2.54	0.42
1:A:565:VAL:HG23	1:A:573:SER:OG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LYS:HG2	1:B:393:LYS:H	1.60	0.42
1:B:176:HIS:HB3	1:B:178:ASN:ND2	2.34	0.42
1:B:122:ILE:HD12	1:B:122:ILE:HA	1.74	0.42
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.80	0.42
1:A:21:PHE:CE2	1:A:327:HIS:HB3	2.47	0.42
1:B:257:GLU:HB2	1:B:281:LEU:HD12	2.01	0.42
1:A:479:ASN:N	1:A:479:ASN:HD22	2.18	0.42
1:A:159:ASP:O	1:A:160:ASN:HB3	2.20	0.42
1:A:300:MET:HE3	1:A:434:VAL:HG12	2.02	0.42
1:B:548:GLN:O	1:B:549:ILE:HG13	2.20	0.42
1:A:388:TYR:O	1:A:392:GLN:HB3	2.19	0.42
1:B:507:MET:CE	1:B:579:PHE:HA	2.47	0.42
1:B:240:LYS:HD3	1:B:641:SER:HB3	2.01	0.42
1:A:283:PHE:O	1:A:287:GLN:HG2	2.20	0.42
1:B:646:LYS:HA	1:B:646:LYS:HD3	1.39	0.42
1:A:371:ASP:HA	1:A:374:ASN:OD1	2.20	0.42
1:A:401:ASN:OD1	1:A:428:ASN:HB3	2.20	0.42
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.50	0.42
1:A:631:TYR:HB2	1:A:637:TYR:CD1	2.55	0.41
1:B:654:LYS:CE	1:B:684:TRP:CZ2	3.00	0.41
1:B:17:ILE:HB	1:B:357:ALA:CA	2.43	0.41
1:A:251:PRO:CB	1:A:506:PRO:HG3	2.44	0.41
1:B:374:ASN:HA	3:B:790:HOH:O	2.21	0.41
1:B:157:LEU:HD11	1:B:210:TYR:CE2	2.54	0.41
1:A:667:ASN:HA	3:A:765:HOH:O	2.19	0.41
1:A:142:SER:OG	1:A:155:GLY:HA2	2.20	0.41
1:A:216:LYS:HA	1:A:219:LEU:HB2	2.02	0.41
1:A:613:LEU:HA	1:A:622:ILE:HD11	2.02	0.41
1:A:285:PHE:CZ	1:A:348:PHE:CE1	3.09	0.41
1:B:548:GLN:HG2	1:B:549:ILE:H	1.84	0.41
1:A:226:ILE:CG2	1:A:227:ARG:N	2.84	0.41
1:B:255:PHE:CD2	1:B:321:VAL:HG21	2.55	0.41
1:A:228:MET:HE2	1:A:242:PHE:CD2	2.55	0.41
1:A:69:MET:HB2	1:A:69:MET:HE3	1.88	0.41
1:A:96:ALA:HA	1:A:98:HIS:CE1	2.55	0.41
1:B:393:LYS:HE3	1:B:393:LYS:HB3	1.97	0.41
1:B:87:ILE:HD11	1:B:152:ALA:HB2	2.01	0.41
1:B:339:ARG:H	1:B:339:ARG:HG3	1.62	0.41
1:A:236:PHE:HZ	1:A:258:TRP:CH2	2.38	0.41
1:B:417:ASP:CB	1:B:436:ARG:HD2	2.51	0.41
1:A:672:ALA:HA	1:A:673:PRO:HD3	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HE	1:A:412:ARG:HB3	1.45	0.41
1:A:420:ILE:HD12	1:A:447:LEU:HD13	2.01	0.41
1:B:101:TRP:HA	1:B:141:THR:O	2.21	0.41
1:B:210:TYR:CD2	1:B:211:LEU:HD23	2.55	0.41
1:A:114:THR:O	1:A:117:ASP:HB2	2.21	0.41
1:A:75:TRP:HB2	1:A:133:ILE:HB	2.01	0.41
1:A:418:VAL:CG1	1:A:419:LEU:N	2.84	0.41
1:B:409:THR:HG23	1:B:423:ARG:HD2	1.96	0.41
1:B:618:PRO:O	1:B:655:LYS:HE3	2.20	0.41
1:A:617:ASP:CG	1:A:620:LYS:HZ2	2.24	0.41
1:A:378:ILE:HG23	1:A:378:ILE:O	2.21	0.41
1:A:228:MET:CE	1:A:242:PHE:CE2	3.03	0.41
1:B:517:ILE:HD13	1:B:563:ILE:CD1	2.39	0.41
1:A:435:ASN:HB2	1:A:482:LEU:CD2	2.51	0.41
1:A:378:ILE:HA	1:A:379:PRO:HD3	1.93	0.41
1:A:385:THR:O	1:A:389:GLN:HG3	2.20	0.40
1:A:402:PRO:HG3	1:A:520:ARG:CZ	2.51	0.40
1:B:411:GLU:HA	1:B:421:TYR:HA	2.02	0.40
1:B:170:ASP:HB3	1:B:177:HIS:NE2	2.36	0.40
1:B:237:GLY:HA2	3:B:762:HOH:O	2.21	0.40
1:B:605:TYR:CE1	1:B:655:LYS:HB2	2.56	0.40
1:B:180:GLY:HA2	1:B:193:ASN:HB2	2.03	0.40
1:A:236:PHE:CZ	1:A:258:TRP:HZ3	2.39	0.40
1:B:54:TRP:CZ3	1:B:118:PHE:HB2	2.56	0.40
1:B:69:MET:O	1:B:391:ILE:HG22	2.22	0.40
1:A:237:GLY:HA3	1:A:639:ASP:O	2.22	0.40
1:B:280:LEU:H	1:B:320:GLN:HE21	1.68	0.40
1:A:278:MET:HG3	1:A:279:SER:O	2.22	0.40
1:B:371:ASP:HA	1:B:372:PRO:HA	1.54	0.40
1:A:109:ASN:OD1	1:A:111:ALA:HB3	2.22	0.40
1:A:353:ARG:HG2	1:A:353:ARG:O	2.21	0.40
1:A:194:LEU:HD21	1:A:233:HIS:CE1	2.56	0.40
1:A:603:ASN:O	1:A:654:LYS:HA	2.21	0.40
1:B:564:LYS:HB3	1:B:564:LYS:HE2	1.78	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.86	0.40
1:B:106:LYS:HB3	1:B:217:MET:HE3	2.02	0.40
1:A:255:PHE:CD2	1:A:321:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	684/686 (100%)	608 (89%)	72 (10%)	4 (1%)	30	29
1	B	684/686 (100%)	602 (88%)	75 (11%)	7 (1%)	19	16
All	All	1368/1372 (100%)	1210 (88%)	147 (11%)	11 (1%)	24	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	B	22	THR
1	B	539	ALA
1	A	46	LEU
1	A	629	VAL
1	B	585	ASP
1	A	542	THR
1	B	46	LEU
1	B	195	TYR
1	B	627	ASN
1	B	629	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	555/555 (100%)	456 (82%)	99 (18%)	2	1
1	B	555/555 (100%)	469 (84%)	86 (16%)	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1110/1110 (100%)	925 (83%)	185 (17%)	3 2

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	13	SER
1	A	19	GLN
1	A	21	PHE
1	A	48	LEU
1	A	49	TYR
1	A	63	ASP
1	A	71	VAL
1	A	75	TRP
1	A	77	SER
1	A	80	VAL
1	A	82	ASN
1	A	88	ASN
1	A	103	ARG
1	A	107	LYS
1	A	145	SER
1	A	146	SER
1	A	147	ASP
1	A	162	THR
1	A	163	LEU
1	A	164	LEU
1	A	167	TYR
1	A	171	THR
1	A	186	THR
1	A	188	ASN
1	A	212	LYS
1	A	216	LYS
1	A	217	MET
1	A	224	ASP
1	A	227	ARG
1	A	232	LYS
1	A	240	LYS
1	A	255	PHE
1	A	257	GLU
1	A	269	ASN
1	A	294	ARG
1	A	297	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	330	GLU
1	A	331	ARG
1	A	344	GLN
1	A	346	LEU
1	A	353	ARG
1	A	370	THR
1	A	371	ASP
1	A	375	ARG
1	A	377	ARG
1	A	382	SER
1	A	384	SER
1	A	392	GLN
1	A	394	LEU
1	A	398	ARG
1	A	404	ILE
1	A	412	ARG
1	A	416	ASN
1	A	420	ILE
1	A	422	GLU
1	A	434	VAL
1	A	436	ARG
1	A	438	LEU
1	A	443	SER
1	A	449	THR
1	A	450	SER
1	A	453	GLN
1	A	463	LEU
1	A	468	THR
1	A	469	LEU
1	A	480	PHE
1	A	487	THR
1	A	490	TRP
1	A	508	MET
1	A	510	LYS
1	A	526	LYS
1	A	529	VAL
1	A	537	SER
1	A	542	THR
1	A	548	GLN
1	A	552	LYS
1	A	560	ASN
1	A	564	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	565	VAL
1	A	571	THR
1	A	574	ASN
1	A	577	ASP
1	A	587	VAL
1	A	590	ARG
1	A	595	ASN
1	A	597	THR
1	A	600	LEU
1	A	607	THR
1	A	620	LYS
1	A	628	GLN
1	A	629	VAL
1	A	642	VAL
1	A	651	LYS
1	A	655	LYS
1	A	658	SER
1	A	660	VAL
1	A	683	ASN
1	A	686	PRO
1	B	4	THR
1	B	5	SER
1	B	19	GLN
1	B	21	PHE
1	B	24	ARG
1	B	26	SER
1	B	46	LEU
1	B	48	LEU
1	B	69	MET
1	B	75	TRP
1	B	76	ILE
1	B	78	GLN
1	B	82	ASN
1	B	87	ILE
1	B	90	SER
1	B	122	ILE
1	B	134	ILE
1	B	135	ASP
1	B	145	SER
1	B	147	ASP
1	B	163	LEU
1	B	169	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	ASN
1	B	194	LEU
1	B	199	ASP
1	B	200	LEU
1	B	205	SER
1	B	213	ASP
1	B	216	LYS
1	B	234	MET
1	B	257	GLU
1	B	269	ASN
1	B	271	LYS
1	B	278	MET
1	B	279	SER
1	B	288	LYS
1	B	290	ARG
1	B	300	MET
1	B	316	GLN
1	B	331	ARG
1	B	335	SER
1	B	336	ASN
1	B	339	ARG
1	B	341	LYS
1	B	342	LEU
1	B	353	ARG
1	B	375	ARG
1	B	377	ARG
1	B	378	ILE
1	B	382	SER
1	B	383	THR
1	B	393	LYS
1	B	400	CYS
1	B	409	THR
1	B	412	ARG
1	B	414	ILE
1	B	415	ASN
1	B	427	SER
1	B	436	ARG
1	B	438	LEU
1	B	443	SER
1	B	445	SER
1	B	450	SER
1	B	493	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	496	THR
1	B	514	THR
1	B	537	SER
1	B	542	THR
1	B	543	SER
1	B	552	LYS
1	B	571	THR
1	B	577	ASP
1	B	588	SER
1	B	597	THR
1	B	600	LEU
1	B	613	LEU
1	B	632	GLN
1	B	642	VAL
1	B	646	LYS
1	B	651	LYS
1	B	658	SER
1	B	660	VAL
1	B	666	SER
1	B	670	PHE
1	B	680	ILE
1	B	681	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	33	ASN
1	A	62	ASN
1	A	88	ASN
1	A	94	ASN
1	A	120	ASN
1	A	173	ASN
1	A	188	ASN
1	A	269	ASN
1	A	333	HIS
1	A	344	GLN
1	A	416	ASN
1	A	439	ASN
1	A	479	ASN
1	A	548	GLN
1	A	560	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	603	ASN
1	B	19	GLN
1	B	32	ASN
1	B	62	ASN
1	B	93	ASN
1	B	94	ASN
1	B	119	GLN
1	B	120	ASN
1	B	169	ASN
1	B	173	ASN
1	B	176	HIS
1	B	178	ASN
1	B	202	HIS
1	B	233	HIS
1	B	269	ASN
1	B	316	GLN
1	B	320	GLN
1	B	336	ASN
1	B	410	GLN
1	B	416	ASN
1	B	479	ASN
1	B	578	ASN
1	B	594	ASN
1	B	632	GLN
1	B	635	ASN
1	B	681	ASN
1	B	685	GLN

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	686/686 (100%)	-0.51	0 100 100	2, 18, 35, 64	0
1	B	686/686 (100%)	-0.56	1 (0%) 95 95	2, 16, 33, 53	0
All	All	1372/1372 (100%)	-0.53	1 (0%) 95 95	2, 17, 34, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	CA	B	688	1/1	0.95	0.17	2.55	11,11,11,11	0
2	CA	A	687	1/1	0.97	0.05	-3.00	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	688	1/1	0.99	0.04	-3.05	12,12,12,12	0
2	CA	B	687	1/1	0.99	0.04	-3.78	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.