Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:23 AM GMT

PDB ID	:	2A9G
Title	:	Structure of C406A arginine deiminase in complex with L-arginine
Authors	:	Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.
Deposited on	:	2005-07-11
Resolution	:	2.30 Å(reported)

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

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

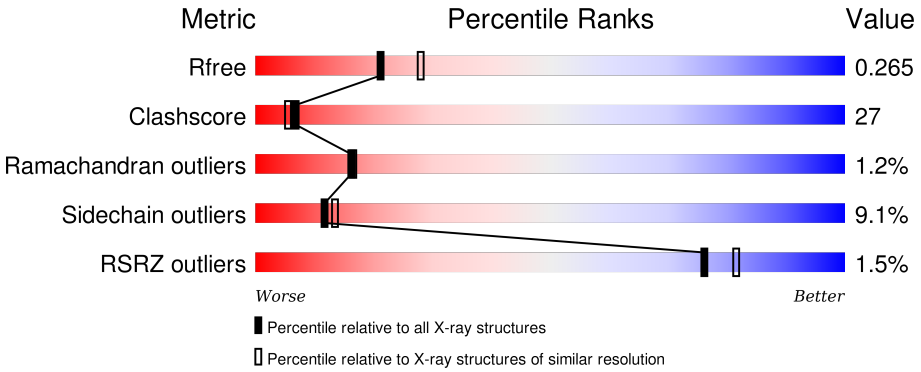
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	418	49% 42% 5%
1	B	418	61% 32%
1	C	418	59% 32% 5%
1	D	418	52% 39% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13747 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.

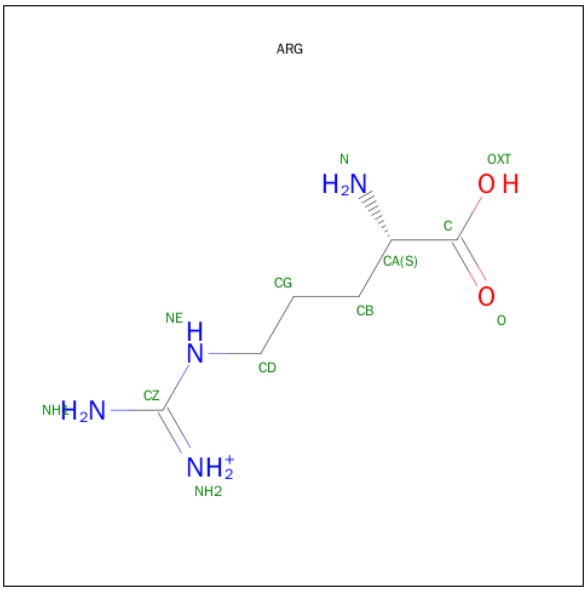
- Molecule 1 is a protein called Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3163	2001	552	594	16			
1	B	405	Total	C	N	O	S	0	0	0
			3164	2002	552	594	16			
1	C	402	Total	C	N	O	S	0	0	0
			3141	1989	546	590	16			
1	D	406	Total	C	N	O	S	0	0	0
			3167	2003	553	595	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	ALA	CYS	ENGINEERED	UNP P13981
B	406	ALA	CYS	ENGINEERED	UNP P13981
C	406	ALA	CYS	ENGINEERED	UNP P13981
D	406	ALA	CYS	ENGINEERED	UNP P13981

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 12 6 4 2	0	0
2	B	1	Total C N O 12 6 4 2	0	0
2	C	1	Total C N O 12 6 4 2	0	0
2	D	1	Total C N O 12 6 4 2	0	0

- Molecule 3 is water.

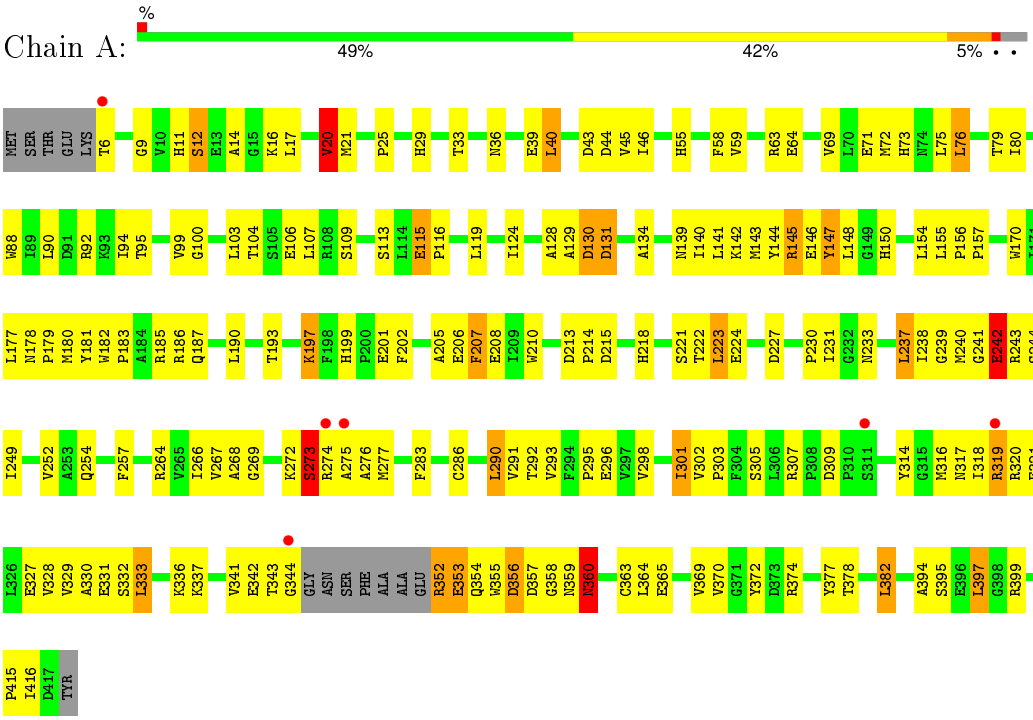
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	223	Total O 223 223	0	0
3	B	277	Total O 277 277	0	0
3	C	309	Total O 309 309	0	0
3	D	255	Total O 255 255	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

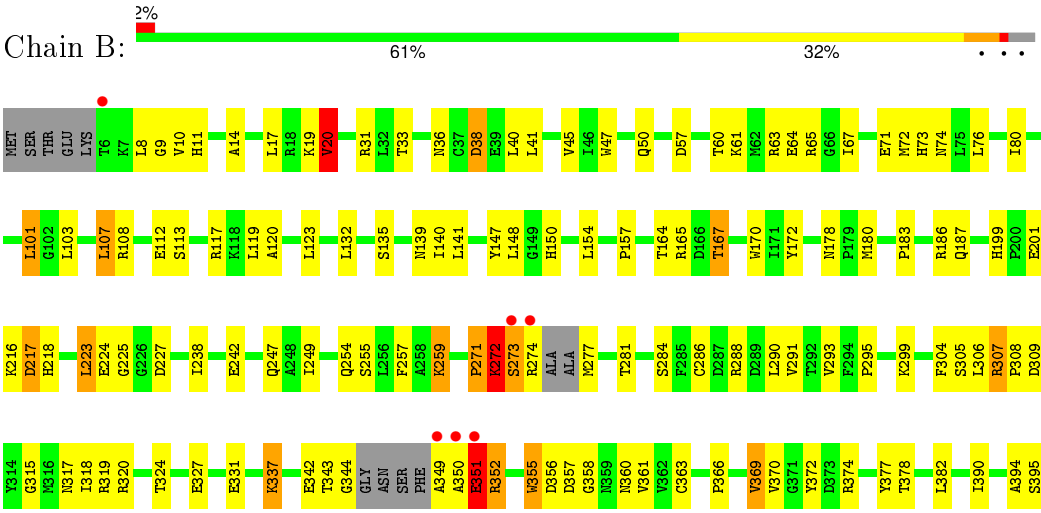
- Molecule 1: Arginine deiminase

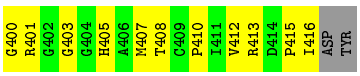
Chain A:



- Molecule 1: Arginine deiminase

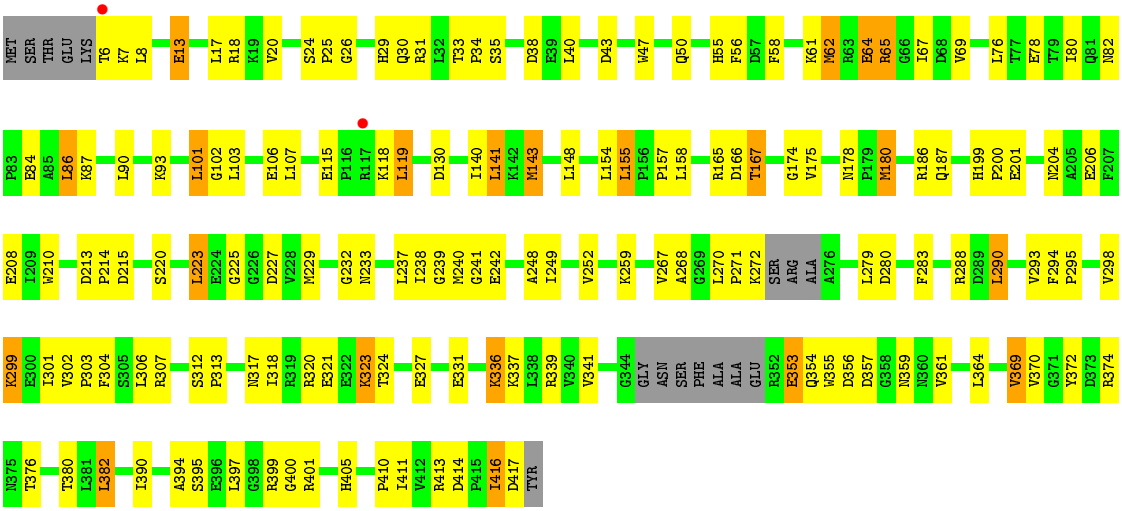
Chain B:





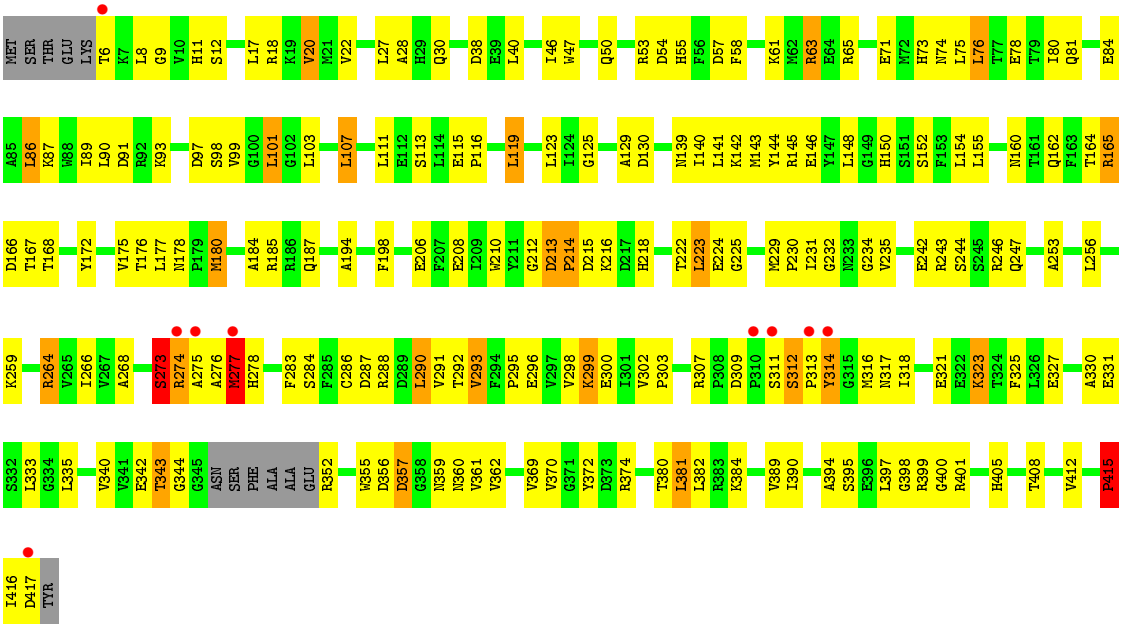
- Molecule 1: Arginine deiminase

Chain C:



- Molecule 1: Arginine deiminase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.10Å 120.70Å 151.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 99.2 (19.85-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.267 0.199 , 0.265	Depositor DCC
R_{free} test set	2001 reflections (2.71%)	DCC
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 73863 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13747	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.64	0/3230	0.89	2/4381 (0.0%)
1	B	0.68	0/3230	0.94	4/4379 (0.1%)
1	C	0.68	0/3207	0.89	1/4349 (0.0%)
1	D	0.64	0/3234	0.90	2/4386 (0.0%)
All	All	0.66	0/12901	0.90	9/17495 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	273	SER	N-CA-C	7.70	131.79	111.00
1	D	214	PRO	CA-N-CD	-6.46	102.46	111.50
1	A	20	VAL	CB-CA-C	-6.33	99.38	111.40
1	D	415	PRO	CA-N-CD	-5.89	103.25	111.50
1	B	273	SER	CA-C-N	-5.87	104.30	117.20
1	B	272	LYS	C-N-CA	5.83	136.29	121.70
1	A	237	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	20	VAL	CB-CA-C	-5.06	101.79	111.40
1	C	13	GLU	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain

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	3163	0	3151	203	0
1	B	3164	0	3152	147	0
1	C	3141	0	3127	168	0
1	D	3167	0	3154	184	0
2	A	12	0	12	0	0
2	B	12	0	12	2	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	223	0	0	54	0
3	B	277	0	0	31	0
3	C	309	0	0	46	0
3	D	255	0	0	44	0
All	All	13747	0	12632	679	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 27.

All (679) 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:B:14:ALA:O	1:B:366:PRO:HD3	1.34	1.22
1:D:276:ALA:HA	3:D:4622:HOH:O	1.42	1.19
1:B:242:GLU:OE2	1:B:273:SER:HB3	1.42	1.19
1:A:247:GLN:HG2	3:D:4733:HOH:O	1.42	1.16
1:B:73:HIS:HB3	1:B:117:ARG:HH12	1.04	1.14
1:A:317:ASN:HB2	3:A:1699:HOH:O	1.47	1.13
1:C:410:PRO:HD2	3:C:3796:HOH:O	1.48	1.09
1:C:331:GLU:HB2	3:C:3771:HOH:O	1.55	1.07
1:C:33:THR:HG22	1:C:35:SER:H	1.22	1.04
1:D:416:ILE:HG23	1:D:417:ASP:H	1.22	1.04
1:B:101:LEU:HD12	1:B:101:LEU:H	1.19	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD11	3:A:1709:HOH:O	1.62	0.98
1:C:199:HIS:HD2	1:C:201:GLU:H	1.10	0.98
1:D:293:VAL:HG22	1:D:298:VAL:HG21	1.44	0.97
1:C:354:GLN:HE22	1:D:47:TRP:HA	1.31	0.95
1:A:267:VAL:HG13	3:A:1703:HOH:O	1.66	0.95
1:D:63:ARG:HG2	3:D:4730:HOH:O	1.65	0.94
1:D:357:ASP:HB2	3:D:4613:HOH:O	1.68	0.94
1:B:304:PHE:HB3	1:B:318:ILE:HD11	1.50	0.93
1:B:8:LEU:HB2	3:B:2760:HOH:O	1.69	0.93
1:B:207:PHE:HB3	3:B:2760:HOH:O	1.66	0.93
1:D:76:LEU:O	1:D:80:ILE:HG12	1.69	0.91
1:A:80:ILE:HB	1:A:86:LEU:HD13	1.51	0.91
1:A:104:THR:HG22	3:A:1721:HOH:O	1.71	0.90
1:B:73:HIS:HB3	1:B:117:ARG:NH1	1.85	0.90
1:D:323:LYS:HG2	1:D:327:GLU:HB3	1.53	0.90
1:D:103:LEU:HD13	1:D:154:LEU:HD11	1.54	0.90
1:C:416:ILE:HG22	1:C:417:ASP:OD1	1.71	0.90
1:A:395:SER:OG	1:B:395:SER:HB3	1.71	0.89
1:A:286:CYS:HB2	1:A:290:LEU:HD13	1.54	0.89
1:B:242:GLU:OE2	1:B:273:SER:CB	2.22	0.87
1:D:231:ILE:HD13	1:D:333:LEU:HD21	1.56	0.86
1:B:286:CYS:HB2	1:B:290:LEU:HD12	1.58	0.86
1:B:101:LEU:CD1	1:B:101:LEU:H	1.90	0.85
1:D:231:ILE:HD13	1:D:333:LEU:CD2	2.07	0.85
1:D:333:LEU:HB2	1:D:335:LEU:HD12	1.57	0.84
1:C:208:GLU:HG2	1:C:210:TRP:CZ3	2.12	0.84
1:B:349:ALA:HA	3:B:2749:HOH:O	1.78	0.84
1:D:416:ILE:HA	3:D:4739:HOH:O	1.77	0.83
1:C:33:THR:HG22	1:C:35:SER:N	1.93	0.83
1:D:65:ARG:HG3	1:D:65:ARG:HH11	1.43	0.82
1:A:83:PRO:HA	3:A:1563:HOH:O	1.78	0.82
1:D:17:LEU:HD21	1:D:20:VAL:CG1	2.09	0.82
1:B:374:ARG:HD2	3:B:2538:HOH:O	1.80	0.82
1:D:142:LYS:HA	3:D:4751:HOH:O	1.79	0.82
1:C:199:HIS:CD2	1:C:201:GLU:H	1.97	0.82
1:C:323:LYS:HB3	1:C:327:GLU:OE1	1.80	0.81
1:A:344:GLY:HA3	3:A:1689:HOH:O	1.79	0.81
1:D:416:ILE:HG23	1:D:417:ASP:N	1.96	0.81
1:A:134:ALA:HA	3:A:1648:HOH:O	1.81	0.81
1:B:165:ARG:HD3	1:B:405:HIS:O	1.81	0.80
1:D:76:LEU:HD22	1:D:80:ILE:HD11	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD13	3:A:1717:HOH:O	1.82	0.79
1:C:240:MET:HG2	1:C:241:GLY:N	1.97	0.79
1:D:234:GLY:HA2	3:D:4578:HOH:O	1.81	0.79
1:A:33:THR:HG22	1:A:36:ASN:CG	2.04	0.79
1:C:140:ILE:HG22	1:C:143:MET:HE1	1.66	0.78
1:D:17:LEU:HD21	1:D:20:VAL:HG11	1.64	0.77
1:D:97:ASP:C	3:D:4733:HOH:O	2.22	0.77
1:D:111:LEU:O	1:D:119:LEU:HD22	1.85	0.77
1:D:38:ASP:HB3	3:D:4743:HOH:O	1.85	0.77
1:A:72:MET:HE3	3:A:1615:HOH:O	1.84	0.77
1:C:270:LEU:HD21	3:C:3786:HOH:O	1.84	0.76
1:C:279:LEU:HA	3:C:3786:HOH:O	1.86	0.76
1:A:238:ILE:HG21	1:A:249:ILE:HG12	1.68	0.76
1:D:288:ARG:HD2	3:D:4600:HOH:O	1.86	0.75
1:B:17:LEU:HD11	1:B:20:VAL:HG13	1.67	0.75
1:A:248:ALA:O	1:A:252:VAL:HG23	1.87	0.74
1:D:357:ASP:OD1	1:D:357:ASP:N	2.20	0.74
1:B:304:PHE:HE1	1:C:143:MET:HE2	1.52	0.74
1:C:240:MET:CE	1:C:267:VAL:HG11	2.18	0.74
1:B:361:VAL:HB	1:B:369:VAL:HG13	1.70	0.73
1:A:318:ILE:HD12	1:D:140:ILE:HD13	1.68	0.73
1:A:103:LEU:HD13	1:A:154:LEU:HD11	1.70	0.73
1:C:376:THR:O	1:C:380:THR:HG23	1.88	0.73
1:A:140:ILE:HD12	1:A:144:TYR:CE2	2.23	0.73
1:A:186:ARG:NH1	3:A:1645:HOH:O	2.21	0.73
1:A:377:TYR:CE2	3:A:1531:HOH:O	2.42	0.73
1:B:342:GLU:O	1:B:352:ARG:NH2	2.22	0.73
1:D:145:ARG:HD2	3:D:4644:HOH:O	1.87	0.73
1:C:31:ARG:HD2	1:C:157:PRO:HB3	1.71	0.72
1:A:240:MET:HB2	3:A:1703:HOH:O	1.89	0.72
1:B:255:SER:O	1:B:259:LYS:HD3	1.89	0.72
1:D:129:ALA:HB2	1:D:141:LEU:HD12	1.71	0.72
1:B:352:ARG:NE	3:B:2667:HOH:O	2.21	0.72
1:B:60:THR:HA	3:B:2772:HOH:O	1.90	0.72
1:A:298:VAL:O	1:A:301:ILE:HG22	1.90	0.72
1:A:303:PRO:HG2	1:A:321:GLU:HB2	1.71	0.72
1:A:178:ASN:HB3	1:A:223:LEU:O	1.89	0.72
1:B:363:CYS:O	1:B:413:ARG:NH2	2.23	0.72
1:A:63:ARG:C	3:A:1504:HOH:O	2.28	0.72
1:A:183:PRO:HA	1:A:186:ARG:HD2	1.73	0.71
1:C:103:LEU:HD22	1:C:154:LEU:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:CYS:HB2	1:B:290:LEU:CD1	2.20	0.71
1:B:119:LEU:O	1:B:119:LEU:HD23	1.90	0.71
1:C:240:MET:HE1	1:C:267:VAL:HG11	1.71	0.71
1:A:156:PRO:HG3	1:A:187:GLN:NE2	2.05	0.70
1:A:143:MET:O	1:A:147:TYR:HB2	1.91	0.70
1:C:214:PRO:HD2	3:C:3697:HOH:O	1.91	0.70
1:A:372:TYR:CG	1:A:394:ALA:HB2	2.27	0.70
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.74	0.70
1:A:72:MET:CE	3:A:1615:HOH:O	2.38	0.70
1:C:87:LYS:HE2	3:C:3804:HOH:O	1.92	0.70
1:C:101:LEU:HG	3:C:3775:HOH:O	1.91	0.70
1:B:352:ARG:CZ	3:B:2667:HOH:O	2.40	0.70
1:B:216:LYS:HE2	3:B:2651:HOH:O	1.91	0.70
1:C:232:GLY:O	1:C:233:ASN:HB2	1.92	0.69
1:D:416:ILE:CG2	1:D:417:ASP:H	2.02	0.69
1:D:416:ILE:HG13	3:D:4739:HOH:O	1.90	0.69
1:D:323:LYS:HG3	1:D:327:GLU:OE1	1.93	0.69
1:D:216:LYS:HD3	1:D:218:HIS:CE1	2.27	0.69
1:C:206:GLU:HG2	3:C:3688:HOH:O	1.91	0.69
1:D:107:LEU:HD22	1:D:111:LEU:CD1	2.23	0.69
1:A:140:ILE:HD12	1:A:144:TYR:CZ	2.28	0.69
1:B:295:PRO:O	1:B:299:LYS:HG2	1.93	0.69
1:A:364:LEU:HD11	1:A:370:VAL:CG2	2.23	0.69
1:A:178:ASN:HB2	1:A:180:MET:CE	2.23	0.68
1:B:401:ARG:NH2	3:B:2736:HOH:O	2.24	0.68
1:B:208:GLU:OE1	1:B:208:GLU:HA	1.92	0.68
1:C:18:ARG:NH1	1:C:414:ASP:OD2	2.27	0.68
1:D:361:VAL:HG22	3:D:4725:HOH:O	1.91	0.68
1:D:111:LEU:HD22	1:D:119:LEU:HD13	1.76	0.68
1:C:175:VAL:HG12	3:C:3784:HOH:O	1.93	0.68
1:A:363:CYS:O	1:A:413:ARG:NH2	2.27	0.68
1:D:318:ILE:HG23	1:D:318:ILE:O	1.94	0.68
1:C:178:ASN:HB3	1:C:223:LEU:O	1.94	0.68
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.59	0.67
1:B:14:ALA:O	1:B:366:PRO:CD	2.27	0.67
1:D:99:VAL:HG13	1:D:154:LEU:HD12	1.76	0.67
1:D:370:VAL:HG22	1:D:390:ILE:HB	1.75	0.67
1:D:98:SER:N	3:D:4733:HOH:O	2.26	0.67
1:C:140:ILE:HA	1:C:143:MET:HE1	1.75	0.67
1:D:57:ASP:OD1	1:D:61:LYS:HE3	1.95	0.67
1:D:288:ARG:HB3	1:D:416:ILE:HD11	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:NE2	3:A:1717:HOH:O	2.27	0.67
1:D:103:LEU:CD1	1:D:154:LEU:HD11	2.25	0.67
1:A:94:ILE:CG2	3:A:1721:HOH:O	2.42	0.67
1:D:256:LEU:HD12	3:D:4747:HOH:O	1.94	0.66
1:D:65:ARG:CG	1:D:65:ARG:HH11	2.08	0.66
1:A:25:PRO:HA	1:A:29:HIS:CE1	2.31	0.66
1:C:17:LEU:HD21	1:C:20:VAL:HG11	1.77	0.66
1:D:12:SER:HB2	3:D:4599:HOH:O	1.94	0.66
1:A:94:ILE:HG22	3:A:1721:HOH:O	1.96	0.66
1:C:355:TRP:CH2	1:C:357:ASP:HB2	2.31	0.66
1:C:405:HIS:HE1	3:C:3781:HOH:O	1.78	0.66
1:A:174:GLY:HA3	1:A:210:TRP:CE2	2.32	0.65
1:D:235:VAL:HG13	1:D:264:ARG:HG2	1.79	0.65
1:C:354:GLN:NE2	1:D:47:TRP:HA	2.06	0.65
1:C:341:VAL:HG21	1:C:382:LEU:HD12	1.78	0.65
1:B:293:VAL:O	1:B:295:PRO:HD3	1.97	0.65
1:C:242:GLU:OE2	1:C:272:LYS:HG2	1.97	0.65
1:A:182:TRP:HB3	3:A:1515:HOH:O	1.96	0.65
1:B:307:ARG:HD2	3:B:2582:HOH:O	1.96	0.64
1:A:80:ILE:HD11	1:A:116:PRO:HA	1.77	0.64
1:D:187:GLN:HG3	3:D:4542:HOH:O	1.98	0.64
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.61	0.64
1:A:352:ARG:O	1:A:353:GLU:HB2	1.98	0.64
1:D:307:ARG:HD2	3:D:4741:HOH:O	1.97	0.64
1:A:318:ILE:HG22	1:A:319:ARG:N	2.12	0.64
1:C:165:ARG:NH1	3:C:3796:HOH:O	2.29	0.64
1:D:93:LYS:HE2	3:D:4723:HOH:O	1.98	0.63
1:D:274:ARG:HB3	3:D:4666:HOH:O	1.98	0.63
1:B:73:HIS:CB	1:B:117:ARG:HH12	1.96	0.63
1:A:364:LEU:HD11	1:A:370:VAL:HG23	1.81	0.63
1:B:107:LEU:HG	1:B:154:LEU:HD13	1.81	0.63
1:B:178:ASN:HB3	1:B:223:LEU:O	1.99	0.63
1:B:218:HIS:N	3:B:2640:HOH:O	2.26	0.63
1:D:369:VAL:CG2	1:D:389:VAL:HG22	2.29	0.63
1:C:33:THR:CG2	3:C:3691:HOH:O	2.45	0.63
1:B:372:TYR:CG	1:B:394:ALA:HB2	2.34	0.63
1:D:184:ALA:HA	3:D:4614:HOH:O	1.98	0.63
1:A:273:SER:OG	1:A:275:ALA:N	2.30	0.63
1:A:268:ALA:HB1	1:A:301:ILE:CD1	2.29	0.63
1:A:44:ASP:OD1	1:A:45:VAL:N	2.32	0.63
1:D:107:LEU:HD22	1:D:111:LEU:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:O	1:A:44:ASP:HB2	1.98	0.62
1:D:286:CYS:SG	1:D:292:THR:HG23	2.39	0.62
1:A:90:LEU:HB3	1:A:94:ILE:HD12	1.81	0.62
1:A:223:LEU:HD23	1:A:224:GLU:N	2.14	0.62
1:B:183:PRO:HA	1:B:186:ARG:HG3	1.81	0.62
1:B:337:LYS:HB2	1:B:337:LYS:NZ	2.14	0.62
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.64	0.62
1:D:17:LEU:HD21	1:D:20:VAL:HG13	1.80	0.62
1:A:183:PRO:HA	1:A:186:ARG:CD	2.29	0.62
1:A:241:GLY:O	1:A:242:GLU:HB2	1.98	0.61
1:A:268:ALA:HB1	1:A:301:ILE:HD11	1.81	0.61
1:B:167:THR:HG21	3:B:2617:HOH:O	1.99	0.61
1:B:19:LYS:HB3	1:B:412:VAL:HG23	1.80	0.61
1:D:243:ARG:HG2	3:D:4722:HOH:O	2.00	0.61
1:C:359:ASN:HA	3:C:3798:HOH:O	1.99	0.61
1:A:100:GLY:O	1:A:104:THR:HG23	2.00	0.61
1:A:343:THR:OG1	1:A:359:ASN:ND2	2.32	0.61
1:C:336:LYS:HE3	3:C:3787:HOH:O	2.00	0.61
1:A:95:THR:N	3:A:1721:HOH:O	2.33	0.61
1:D:6:THR:N	3:D:4718:HOH:O	2.33	0.61
1:C:331:GLU:HG2	3:C:3728:HOH:O	2.01	0.61
1:A:273:SER:OG	1:A:275:ALA:HB3	2.01	0.61
1:B:271:PRO:HD3	1:C:148:LEU:HD22	1.82	0.61
1:A:157:PRO:HB2	3:A:1709:HOH:O	2.00	0.60
1:C:180:MET:HA	1:C:180:MET:HE2	1.81	0.60
1:C:206:GLU:HB2	3:C:3789:HOH:O	2.00	0.60
1:C:118:LYS:HD3	3:C:3679:HOH:O	2.00	0.60
1:A:157:PRO:HD2	3:A:1709:HOH:O	2.01	0.60
1:A:268:ALA:CB	1:A:301:ILE:HD11	2.31	0.60
1:B:183:PRO:HA	1:B:186:ARG:CG	2.31	0.60
1:D:107:LEU:HD11	1:D:155:LEU:HD13	1.82	0.60
1:A:128:ALA:HB3	1:A:131:ASP:OD1	2.02	0.60
1:B:135:SER:O	1:B:139:ASN:ND2	2.30	0.60
1:D:119:LEU:HD12	1:D:119:LEU:O	2.01	0.60
1:D:165:ARG:HD2	1:D:405:HIS:O	2.03	0.59
1:A:331:GLU:HG3	1:A:332:SER:N	2.17	0.59
1:A:327:GLU:O	1:A:330:ALA:HB3	2.02	0.59
1:A:277:MET:HE2	3:A:1702:HOH:O	2.02	0.59
1:D:65:ARG:NH1	1:D:65:ARG:HG3	2.17	0.59
1:A:269:GLY:HA3	1:D:148:LEU:HD11	1.85	0.59
1:A:190:LEU:HD23	3:A:1579:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:PRO:HG2	1:C:321:GLU:HB2	1.84	0.59
1:D:307:ARG:HB2	3:D:4741:HOH:O	2.03	0.59
1:A:222:THR:O	1:A:244:SER:HA	2.03	0.59
1:C:65:ARG:NH1	3:C:3538:HOH:O	2.35	0.59
1:A:264:ARG:NH1	1:A:305:SER:OG	2.35	0.59
1:B:400:GLY:O	1:B:401:ARG:HB2	2.03	0.58
1:D:231:ILE:HD12	1:D:232:GLY:N	2.18	0.58
1:A:80:ILE:HD11	1:A:116:PRO:CA	2.33	0.58
1:C:270:LEU:HD11	3:C:3786:HOH:O	2.04	0.58
1:C:324:THR:OG1	1:C:327:GLU:HG3	2.03	0.58
1:A:64:GLU:N	3:A:1504:HOH:O	2.36	0.58
1:A:174:GLY:HA3	1:A:210:TRP:NE1	2.18	0.58
1:A:277:MET:CE	3:A:1702:HOH:O	2.52	0.58
1:A:103:LEU:HD13	1:A:154:LEU:CD1	2.32	0.58
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.69	0.58
1:A:150:HIS:CE1	3:A:1717:HOH:O	2.57	0.58
1:A:63:ARG:NH2	1:A:69:VAL:O	2.37	0.58
1:C:359:ASN:N	3:C:3785:HOH:O	2.37	0.57
1:B:284:SER:O	1:B:291:VAL:HA	2.03	0.57
1:A:243:ARG:HE	1:A:276:ALA:HB1	1.68	0.57
1:A:293:VAL:O	1:A:295:PRO:HD3	2.04	0.57
1:A:295:PRO:HG2	1:A:342:GLU:HB3	1.84	0.57
1:B:165:ARG:O	1:B:225:GLY:HA3	2.05	0.57
1:D:314:TYR:HD1	1:D:314:TYR:H	1.50	0.57
1:C:20:VAL:HG12	1:C:410:PRO:HA	1.86	0.57
1:D:288:ARG:CB	1:D:416:ILE:HD11	2.35	0.57
1:A:75:LEU:HD23	1:A:199:HIS:NE2	2.19	0.57
1:C:33:THR:HG23	3:C:3691:HOH:O	2.03	0.57
1:D:71:GLU:OE1	1:D:73:HIS:HB2	2.04	0.57
1:C:271:PRO:O	1:C:272:LYS:HB3	2.04	0.57
1:B:372:TYR:CD2	1:B:394:ALA:HB2	2.40	0.57
1:A:177:LEU:HD13	1:A:193:THR:OG1	2.05	0.57
1:D:87:LYS:NZ	3:D:4641:HOH:O	2.36	0.57
1:D:55:HIS:O	1:D:58:PHE:HB3	2.05	0.57
1:D:139:ASN:O	1:D:143:MET:HG3	2.05	0.56
1:A:372:TYR:CD2	1:A:394:ALA:HB2	2.39	0.56
1:B:324:THR:OG1	1:B:327:GLU:HG3	2.06	0.56
1:A:218:HIS:HB2	3:A:1558:HOH:O	2.05	0.56
1:D:224:GLU:OE1	1:D:278:HIS:NE2	2.37	0.56
1:A:206:GLU:O	1:A:207:PHE:HB3	2.05	0.56
1:C:56:PHE:HA	3:C:3556:HOH:O	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:VAL:HA	1:C:390:ILE:O	2.05	0.56
1:B:140:ILE:HD13	1:C:318:ILE:HG21	1.86	0.56
1:C:336:LYS:HG3	3:C:3760:HOH:O	2.05	0.56
1:D:89:ILE:HD11	1:D:194:ALA:CB	2.36	0.56
1:B:277:MET:N	3:B:2769:HOH:O	2.39	0.56
1:C:80:ILE:HD12	1:C:119:LEU:HD13	1.86	0.56
1:C:187:GLN:HE21	1:C:187:GLN:HA	1.70	0.56
1:D:398:GLY:C	1:D:400:GLY:H	2.08	0.56
1:C:26:GLY:O	1:C:30:GLN:HG3	2.05	0.56
1:C:353:GLU:CD	3:C:3801:HOH:O	2.45	0.56
1:C:93:LYS:HE3	1:C:155:LEU:HG	1.87	0.56
1:C:399:ARG:NH2	3:C:3595:HOH:O	2.39	0.56
1:C:33:THR:HG23	1:C:34:PRO:HD2	1.86	0.56
1:B:227:ASP:O	1:B:238:ILE:HA	2.05	0.56
1:A:130:ASP:HB3	1:A:142:LYS:NZ	2.22	0.56
1:D:374:ARG:NH2	3:D:4738:HOH:O	2.39	0.55
1:C:323:LYS:NZ	3:C:3791:HOH:O	2.39	0.55
1:D:295:PRO:HG3	1:D:342:GLU:HG2	1.88	0.55
1:C:65:ARG:NH2	1:C:390:ILE:HD11	2.20	0.55
1:D:17:LEU:HD11	1:D:20:VAL:HG13	1.88	0.55
1:C:323:LYS:HE2	3:C:3791:HOH:O	2.05	0.55
1:A:227:ASP:O	1:A:238:ILE:HA	2.06	0.55
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.41	0.55
1:B:10:VAL:HG21	1:B:410:PRO:O	2.07	0.55
1:A:273:SER:HB3	3:A:1702:HOH:O	2.05	0.55
1:D:50:GLN:OE1	1:D:53:ARG:NH2	2.37	0.55
1:D:65:ARG:CG	1:D:65:ARG:NH1	2.64	0.55
1:C:323:LYS:CE	3:C:3791:HOH:O	2.54	0.55
1:C:101:LEU:HD12	1:C:102:GLY:N	2.21	0.55
1:D:292:THR:OG1	1:D:359:ASN:ND2	2.39	0.55
1:D:343:THR:CG2	1:D:344:GLY:N	2.70	0.55
1:B:309:ASP:OD2	1:B:311:SER:HB3	2.07	0.55
1:A:156:PRO:CG	1:A:187:GLN:NE2	2.70	0.55
1:B:132:LEU:HD11	1:B:154:LEU:HD11	1.88	0.55
1:B:350:ALA:HB3	1:B:377:TYR:OH	2.06	0.54
1:D:54:ASP:HA	3:D:4731:HOH:O	2.07	0.54
1:C:307:ARG:HH11	1:C:307:ARG:HG2	1.73	0.54
1:C:140:ILE:HG13	1:C:141:LEU:N	2.22	0.54
1:C:6:THR:O	1:C:6:THR:HG23	2.07	0.54
1:B:165:ARG:CD	1:B:405:HIS:O	2.52	0.54
1:A:199:HIS:HE1	1:A:201:GLU:HG3	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:OE2	1:A:296:GLU:N	2.41	0.54
1:C:17:LEU:HD21	1:C:20:VAL:CG1	2.38	0.54
1:A:199:HIS:CE1	1:A:201:GLU:HG3	2.42	0.54
1:D:343:THR:HG23	1:D:344:GLY:N	2.23	0.54
1:C:304:PHE:CE1	1:C:320:ARG:HG3	2.43	0.54
1:A:266:ILE:HD13	1:A:328:VAL:HG12	1.89	0.54
1:C:165:ARG:O	1:C:225:GLY:HA3	2.06	0.54
1:B:98:SER:HB2	3:B:2758:HOH:O	2.08	0.54
1:B:38:ASP:HB2	3:B:2577:HOH:O	2.07	0.54
1:A:355:TRP:CH2	1:A:357:ASP:HB2	2.43	0.53
1:C:7:LYS:HE2	1:C:206:GLU:OE1	2.08	0.53
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.43	0.53
1:A:148:LEU:HB3	3:A:1717:HOH:O	2.08	0.53
1:C:239:GLY:HA2	1:C:268:ALA:HB3	1.91	0.53
1:B:361:VAL:HG22	3:B:2761:HOH:O	2.08	0.53
1:A:106:GLU:HG2	3:A:1700:HOH:O	2.08	0.53
1:C:174:GLY:HA3	1:C:210:TRP:CE2	2.44	0.53
1:B:352:ARG:NH2	3:B:2667:HOH:O	2.41	0.53
1:C:353:GLU:HG2	3:C:3638:HOH:O	2.08	0.53
1:C:140:ILE:HG22	1:C:143:MET:CE	2.36	0.53
1:A:318:ILE:CD1	1:D:140:ILE:HD13	2.38	0.53
3:A:1681:HOH:O	1:D:97:ASP:HB3	2.08	0.53
1:B:304:PHE:CB	1:B:318:ILE:HD11	2.32	0.53
1:C:298:VAL:HA	1:C:301:ILE:CD1	2.39	0.53
1:A:254:GLN:NE2	1:A:314:TYR:O	2.42	0.53
1:D:325:PHE:HB3	3:D:4653:HOH:O	2.09	0.53
1:C:204:ASN:HB3	3:C:3716:HOH:O	2.10	0.52
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.91	0.52
1:B:33:THR:N	1:B:36:ASN:OD1	2.32	0.52
1:D:103:LEU:HD11	1:D:141:LEU:HD23	1.92	0.52
1:D:178:ASN:HB3	1:D:223:LEU:O	2.09	0.52
1:C:307:ARG:NH1	1:C:307:ARG:HG2	2.24	0.52
1:D:22:VAL:HA	1:D:164:THR:HG21	1.91	0.52
1:B:71:GLU:HB3	1:B:74:ASN:HD22	1.73	0.52
1:A:343:THR:HG22	1:A:378:THR:OG1	2.10	0.52
1:D:355:TRP:CH2	1:D:357:ASP:HB3	2.45	0.52
1:C:87:LYS:CE	3:C:3804:HOH:O	2.54	0.52
1:A:71:GLU:OE2	1:A:73:HIS:N	2.29	0.52
1:C:175:VAL:N	3:C:3784:HOH:O	2.43	0.51
1:A:359:ASN:O	1:A:360:ASN:CB	2.58	0.51
1:C:43:ASP:OD2	1:C:401:ARG:NE	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TRP:CZ3	1:B:357:ASP:HB2	2.45	0.51
1:B:259:LYS:CD	1:B:259:LYS:N	2.73	0.51
1:B:199:HIS:CE1	1:B:201:GLU:HB2	2.46	0.51
1:A:344:GLY:HA2	3:A:1670:HOH:O	2.10	0.51
1:A:146:GLU:HG3	3:A:1623:HOH:O	2.11	0.51
1:D:231:ILE:HD12	1:D:231:ILE:C	2.30	0.51
1:C:240:MET:CG	1:C:241:GLY:N	2.71	0.51
1:B:344:GLY:C	3:B:2668:HOH:O	2.48	0.51
1:D:276:ALA:HB2	3:D:4575:HOH:O	2.10	0.51
1:A:353:GLU:HG2	3:A:1640:HOH:O	2.09	0.51
1:D:312:SER:HB3	1:D:314:TYR:CD1	2.46	0.51
1:C:158:LEU:HD21	1:C:187:GLN:HB2	1.93	0.51
1:D:299:LYS:HD2	1:D:300:GLU:HG2	1.93	0.51
1:D:242:GLU:HB2	3:D:4722:HOH:O	2.10	0.51
1:C:84:GLU:HB2	3:C:3705:HOH:O	2.10	0.51
1:D:352:ARG:HB2	1:D:352:ARG:CZ	2.41	0.51
1:A:181:TYR:HD2	1:A:243:ARG:HD3	1.75	0.50
1:A:240:MET:HE2	1:A:246:ARG:HA	1.92	0.50
1:B:305:SER:O	1:B:318:ILE:HD12	2.11	0.50
1:D:145:ARG:NH2	1:D:146:GLU:HB2	2.27	0.50
1:B:361:VAL:HB	1:B:369:VAL:CG1	2.39	0.50
1:B:363:CYS:HB2	1:B:413:ARG:NH2	2.26	0.50
1:A:374:ARG:NH2	1:B:396:GLU:OE2	2.45	0.50
1:B:31:ARG:HH11	1:B:31:ARG:HG2	1.76	0.50
1:C:33:THR:CG2	1:C:35:SER:H	2.08	0.50
1:B:165:ARG:HD2	1:B:408:THR:O	2.10	0.50
1:C:293:VAL:HG13	1:C:298:VAL:CG2	2.41	0.50
1:C:8:LEU:HD22	1:C:411:ILE:HG22	1.94	0.50
1:A:264:ARG:HD3	1:A:307:ARG:CZ	2.42	0.50
1:B:217:ASP:HA	3:B:2682:HOH:O	2.11	0.50
1:C:227:ASP:O	1:C:238:ILE:HA	2.12	0.50
1:A:286:CYS:SG	1:A:292:THR:HG23	2.52	0.49
1:B:60:THR:HG23	3:B:2772:HOH:O	2.11	0.49
1:D:274:ARG:C	1:D:276:ALA:H	2.15	0.49
1:A:318:ILE:HG22	1:A:319:ARG:H	1.76	0.49
1:D:284:SER:OG	1:D:292:THR:OG1	2.27	0.49
1:B:45:VAL:HG13	3:B:2510:HOH:O	2.13	0.49
1:B:305:SER:C	1:B:318:ILE:HD12	2.32	0.49
1:A:140:ILE:HG13	1:A:141:LEU:N	2.27	0.49
1:D:101:LEU:HG	3:D:4742:HOH:O	2.13	0.49
1:A:130:ASP:OD1	1:A:145:ARG:NH1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:SER:HB3	1:D:395:SER:OG	2.12	0.49
1:A:318:ILE:HD11	3:D:4519:HOH:O	2.12	0.49
1:C:380:THR:HG22	3:C:3772:HOH:O	2.12	0.49
1:A:283:PHE:HD1	1:A:293:VAL:HG12	1.77	0.49
1:B:403:GLY:O	1:B:407:MET:HG3	2.12	0.49
1:B:306:LEU:HD13	1:B:318:ILE:HB	1.94	0.49
1:A:148:LEU:CB	3:A:1717:HOH:O	2.61	0.49
1:A:148:LEU:HD11	1:D:302:VAL:HB	1.94	0.49
1:D:87:LYS:CE	3:D:4672:HOH:O	2.61	0.49
1:C:187:GLN:NE2	1:C:187:GLN:HA	2.27	0.49
1:C:290:LEU:HD23	1:C:339:ARG:O	2.13	0.49
1:C:240:MET:HB2	1:C:249:ILE:CD1	2.43	0.49
1:A:301:ILE:HD13	1:A:325:PHE:CD1	2.47	0.49
1:C:7:LYS:HE2	1:C:206:GLU:CD	2.33	0.49
1:B:320:ARG:HG2	1:B:320:ARG:NH1	2.28	0.49
1:A:301:ILE:HG12	1:A:302:VAL:N	2.28	0.49
1:D:22:VAL:CA	1:D:164:THR:HG21	2.42	0.49
1:A:237:LEU:HD21	1:A:329:VAL:HG22	1.95	0.49
1:C:115:GLU:H	1:C:118:LYS:HE3	1.77	0.48
1:B:370:VAL:HA	1:B:390:ILE:O	2.13	0.48
1:A:80:ILE:HD11	1:A:116:PRO:HB3	1.94	0.48
1:A:359:ASN:HA	3:A:1646:HOH:O	2.13	0.48
1:B:271:PRO:HD3	1:C:148:LEU:CD2	2.43	0.48
1:D:86:LEU:O	1:D:90:LEU:HG	2.13	0.48
1:B:288:ARG:NH1	1:B:288:ARG:HG3	2.28	0.48
1:C:166:ASP:HA	1:C:225:GLY:HA3	1.95	0.48
1:D:400:GLY:O	1:D:401:ARG:HB2	2.14	0.48
1:A:16:LYS:HE2	1:A:365:GLU:HG2	1.95	0.48
1:D:18:ARG:CG	1:D:18:ARG:HH11	2.25	0.48
1:A:295:PRO:CG	1:A:342:GLU:HB3	2.42	0.48
1:C:106:GLU:HG2	3:C:3509:HOH:O	2.14	0.48
1:D:175:VAL:HG22	1:D:176:THR:N	2.28	0.48
1:C:78:GLU:OE1	1:C:199:HIS:HE1	1.96	0.48
1:A:178:ASN:HB2	1:A:180:MET:HE1	1.95	0.48
1:A:145:ARG:HG2	1:A:146:GLU:N	2.28	0.48
1:A:17:LEU:HD21	1:A:20:VAL:HG13	1.95	0.48
1:A:257:PHE:CD2	1:A:316:MET:HG2	2.49	0.48
1:D:12:SER:HA	1:D:230:PRO:O	2.14	0.48
1:C:288:ARG:NH1	1:C:416:ILE:HG23	2.29	0.48
1:A:178:ASN:HA	1:A:179:PRO:HD3	1.69	0.48
1:C:187:GLN:HE21	1:C:187:GLN:CA	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ILE:HG21	1:B:249:ILE:HG12	1.95	0.48
1:B:350:ALA:C	1:B:351:GLU:HG3	2.31	0.48
1:D:46:ILE:HG22	1:D:399:ARG:HD2	1.96	0.48
1:A:107:LEU:C	1:A:107:LEU:HD13	2.34	0.48
1:B:358:GLY:HA3	1:B:378:THR:HG21	1.96	0.47
1:C:17:LEU:HD13	1:C:413:ARG:NH2	2.29	0.47
1:D:330:ALA:O	1:D:335:LEU:HB2	2.14	0.47
1:B:400:GLY:O	2:B:2500:ARG:N	2.47	0.47
1:C:174:GLY:HA3	1:C:210:TRP:NE1	2.29	0.47
1:B:165:ARG:NH2	3:B:2522:HOH:O	2.46	0.47
1:A:29:HIS:HE1	3:A:1653:HOH:O	1.98	0.47
1:A:193:THR:HG21	1:A:214:PRO:HG3	1.96	0.47
1:B:254:GLN:NE2	1:C:101:LEU:HD22	2.28	0.47
1:C:248:ALA:O	1:C:252:VAL:HG23	2.14	0.47
1:B:170:TRP:N	1:B:170:TRP:CD1	2.82	0.47
1:C:336:LYS:HE2	1:C:336:LYS:HB3	1.79	0.47
1:D:78:GLU:HA	1:D:81:GLN:HG3	1.96	0.47
1:B:47:TRP:CD2	1:B:50:GLN:HB2	2.50	0.47
1:D:222:THR:O	1:D:244:SER:HA	2.15	0.47
1:C:354:GLN:HE22	1:D:47:TRP:CA	2.15	0.47
1:D:107:LEU:HD11	1:D:155:LEU:CD1	2.44	0.47
1:C:380:THR:HG23	3:C:3564:HOH:O	2.15	0.47
1:A:46:ILE:HG22	1:A:399:ARG:HD2	1.97	0.47
1:A:45:VAL:HG12	1:A:46:ILE:N	2.30	0.47
1:C:180:MET:HA	1:C:180:MET:CE	2.45	0.47
1:A:129:ALA:HB3	3:A:1647:HOH:O	2.15	0.47
1:A:80:ILE:C	1:A:80:ILE:HD12	2.35	0.47
1:A:202:PHE:O	1:A:205:ALA:HB3	2.15	0.47
1:C:62:MET:CG	1:C:67:ILE:HD12	2.45	0.47
1:D:287:ASP:HB3	1:D:290:LEU:HB2	1.96	0.47
1:D:293:VAL:O	1:D:295:PRO:HD3	2.14	0.47
1:C:62:MET:HG3	1:C:67:ILE:HD12	1.96	0.47
1:D:11:HIS:HB2	1:D:415:PRO:HD3	1.97	0.46
1:A:231:ILE:HD12	1:A:333:LEU:HD23	1.96	0.46
1:A:275:ALA:HB3	3:A:1619:HOH:O	2.16	0.46
1:B:167:THR:HG23	3:B:2519:HOH:O	2.15	0.46
1:A:88:TRP:O	1:A:92:ARG:HD2	2.14	0.46
1:B:288:ARG:CG	1:B:288:ARG:NH1	2.78	0.46
1:A:221:SER:OG	1:A:247:GLN:HB3	2.15	0.46
1:C:175:VAL:CG1	3:C:3784:HOH:O	2.60	0.46
1:B:98:SER:CA	3:B:2758:HOH:O	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HD2	1:B:157:PRO:HB3	1.98	0.46
1:B:97:ASP:O	1:C:220:SER:HB2	2.15	0.46
1:D:380:THR:O	1:D:384:LYS:HG2	2.16	0.46
1:C:240:MET:HE3	1:C:267:VAL:HG11	1.94	0.46
1:B:103:LEU:HD13	1:B:154:LEU:HD21	1.97	0.46
1:D:87:LYS:O	1:D:91:ASP:HB2	2.15	0.46
1:A:356:ASP:OD1	1:A:356:ASP:C	2.54	0.46
1:B:304:PHE:CE1	1:C:143:MET:HE2	2.39	0.46
1:D:370:VAL:HA	1:D:390:ILE:O	2.16	0.46
1:D:167:THR:HA	1:D:180:MET:HE2	1.97	0.46
1:C:33:THR:HG23	1:C:34:PRO:CD	2.46	0.46
1:C:299:LYS:NZ	1:C:299:LYS:HB3	2.31	0.46
1:A:94:ILE:HG23	3:A:1721:HOH:O	2.13	0.46
1:C:416:ILE:HG22	1:C:417:ASP:N	2.31	0.46
1:A:99:VAL:HG13	1:A:154:LEU:HD12	1.98	0.46
1:B:398:GLY:C	1:B:400:GLY:H	2.19	0.46
1:D:208:GLU:OE1	1:D:259:LYS:HE3	2.15	0.46
1:D:165:ARG:O	1:D:225:GLY:HA3	2.16	0.45
1:B:71:GLU:HB3	1:B:74:ASN:ND2	2.30	0.45
1:B:9:GLY:HA2	1:B:172:TYR:O	2.16	0.45
1:A:240:MET:HG2	1:A:241:GLY:N	2.30	0.45
1:A:80:ILE:HD11	1:A:116:PRO:CB	2.46	0.45
1:D:344:GLY:N	1:D:356:ASP:O	2.46	0.45
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.46	0.45
1:C:229:MET:HB2	1:C:237:LEU:HB2	1.98	0.45
1:D:277:MET:CG	3:D:4727:HOH:O	2.64	0.45
1:A:139:ASN:HB3	3:A:1631:HOH:O	2.15	0.45
1:A:14:ALA:HB3	1:A:416:ILE:HD11	1.98	0.45
1:B:272:LYS:HD2	1:B:272:LYS:HA	1.61	0.45
1:C:331:GLU:CG	3:C:3728:HOH:O	2.60	0.45
1:C:61:LYS:HD3	1:C:390:ILE:CG2	2.45	0.45
1:A:354:GLN:HE22	1:B:47:TRP:HA	1.80	0.45
1:C:24:SER:HA	1:C:55:HIS:CD2	2.51	0.45
1:D:28:ALA:HB2	1:D:125:GLY:HA2	1.98	0.45
1:A:180:MET:HG3	1:A:185:ARG:O	2.16	0.45
1:D:398:GLY:C	1:D:400:GLY:N	2.70	0.45
1:C:33:THR:CG2	1:C:34:PRO:N	2.79	0.45
1:B:217:ASP:OD1	1:B:217:ASP:O	2.34	0.45
1:C:7:LYS:HG2	1:C:206:GLU:CG	2.46	0.45
1:A:242:GLU:OE1	1:A:272:LYS:HD3	2.17	0.45
1:C:154:LEU:N	1:C:154:LEU:HD22	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:CG2	1:A:319:ARG:N	2.79	0.45
1:D:180:MET:HE3	1:D:224:GLU:HG2	1.98	0.45
1:D:381:LEU:N	1:D:381:LEU:HD23	2.32	0.45
1:A:156:PRO:CD	1:A:187:GLN:HE22	2.30	0.45
1:A:355:TRP:HH2	3:B:2764:HOH:O	1.99	0.45
1:B:320:ARG:HG2	1:B:320:ARG:HH11	1.83	0.45
1:A:290:LEU:HD22	1:A:291:VAL:N	2.31	0.44
1:D:231:ILE:HD13	1:D:333:LEU:HD23	1.96	0.44
1:A:145:ARG:NH1	3:A:1647:HOH:O	2.49	0.44
1:A:156:PRO:HG3	1:A:187:GLN:HE22	1.80	0.44
1:B:71:GLU:HG3	1:B:74:ASN:H	1.82	0.44
1:B:11:HIS:HB2	1:B:415:PRO:HB3	1.99	0.44
1:C:200:PRO:HA	3:C:3704:HOH:O	2.16	0.44
1:D:8:LEU:HA	1:D:412:VAL:HG22	1.98	0.44
1:C:280:ASP:HA	1:C:283:PHE:O	2.18	0.44
1:B:108:ARG:O	1:B:112:GLU:HG3	2.18	0.44
1:D:256:LEU:HB2	3:D:4747:HOH:O	2.18	0.44
1:A:374:ARG:NH2	1:B:399:ARG:CZ	2.80	0.44
1:C:199:HIS:HD2	1:C:201:GLU:N	1.94	0.44
1:D:246:ARG:HG3	1:D:247:GLN:N	2.33	0.44
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.31	0.44
1:B:183:PRO:HA	1:B:186:ARG:HG2	2.00	0.44
1:A:275:ALA:CB	3:A:1619:HOH:O	2.65	0.44
1:B:180:MET:O	1:B:186:ARG:NE	2.50	0.44
1:B:148:LEU:HD11	1:C:302:VAL:HB	2.00	0.44
1:D:177:LEU:N	1:D:177:LEU:HD23	2.32	0.44
1:C:298:VAL:HA	1:C:301:ILE:HD12	2.00	0.44
1:A:73:HIS:CD2	1:A:124:ILE:HD12	2.53	0.44
1:D:374:ARG:CZ	3:D:4738:HOH:O	2.66	0.44
1:D:75:LEU:HD23	3:D:4640:HOH:O	2.18	0.44
1:B:187:GLN:HG3	3:B:2604:HOH:O	2.17	0.44
1:A:382:LEU:HA	1:A:382:LEU:HD12	1.89	0.44
1:B:242:GLU:HB2	3:B:2562:HOH:O	2.18	0.43
1:B:350:ALA:CB	1:B:377:TYR:OH	2.65	0.43
1:B:343:THR:HG22	1:B:378:THR:OG1	2.17	0.43
1:C:306:LEU:HA	1:C:317:ASN:O	2.18	0.43
1:D:213:ASP:OD1	1:D:213:ASP:C	2.55	0.43
1:B:257:PHE:CG	1:B:308:PRO:HG3	2.52	0.43
1:A:240:MET:CG	1:A:241:GLY:N	2.80	0.43
1:B:150:HIS:CE1	1:C:241:GLY:HA3	2.53	0.43
1:C:87:LYS:NZ	3:C:3804:HOH:O	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:HB3	1:A:142:LYS:HZ2	1.83	0.43
1:B:309:ASP:O	1:B:315:GLY:HA2	2.18	0.43
1:B:98:SER:HA	3:B:2758:HOH:O	2.18	0.43
1:A:170:TRP:CE2	1:A:411:ILE:HG23	2.53	0.43
1:D:302:VAL:HA	1:D:303:PRO:HD3	1.78	0.43
1:D:264:ARG:CZ	1:D:266:ILE:HD11	2.48	0.43
1:C:167:THR:HG21	3:C:3644:HOH:O	2.17	0.43
1:D:273:SER:OG	1:D:273:SER:O	2.31	0.43
1:B:281:THR:O	1:B:281:THR:CG2	2.65	0.43
1:A:414:ASP:HA	1:A:415:PRO:HD3	1.81	0.43
1:C:298:VAL:HG13	1:C:301:ILE:HD12	2.01	0.43
1:B:41:LEU:HD13	2:B:2500:ARG:OXT	2.19	0.43
1:A:213:ASP:OD1	1:A:215:ASP:HB2	2.19	0.43
1:A:55:HIS:O	1:A:58:PHE:HB3	2.19	0.43
1:A:21:MET:HE1	3:A:1615:HOH:O	2.18	0.43
1:B:20:VAL:HG12	1:B:410:PRO:HA	1.99	0.43
1:A:99:VAL:CG1	1:A:154:LEU:HD12	2.48	0.43
1:B:98:SER:CB	3:B:2758:HOH:O	2.66	0.43
1:D:309:ASP:N	1:D:316:MET:HA	2.33	0.43
1:C:361:VAL:HG21	1:C:369:VAL:HG21	1.99	0.43
1:C:140:ILE:HA	1:C:143:MET:HB2	2.00	0.43
1:A:356:ASP:HB2	3:A:1621:HOH:O	2.18	0.43
1:B:80:ILE:HD12	1:B:120:ALA:HB2	1.99	0.43
1:C:17:LEU:HD13	1:C:413:ARG:CZ	2.49	0.43
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.94	0.43
1:A:240:MET:CB	3:A:1703:HOH:O	2.60	0.43
1:A:292:THR:HA	1:A:341:VAL:O	2.18	0.43
1:A:413:ARG:NH1	3:A:1522:HOH:O	2.37	0.43
1:C:341:VAL:HG21	1:C:382:LEU:CD1	2.49	0.43
1:D:314:TYR:N	1:D:314:TYR:HD1	2.16	0.43
1:C:312:SER:HA	1:C:313:PRO:HD3	1.75	0.43
1:B:178:ASN:OD1	1:B:223:LEU:HD13	2.18	0.43
1:D:362:VAL:HG13	1:D:362:VAL:O	2.17	0.43
1:A:397:LEU:HA	1:A:397:LEU:HD12	1.85	0.43
1:A:157:PRO:O	3:A:1709:HOH:O	2.21	0.43
1:D:80:ILE:HG23	1:D:86:LEU:HD23	2.00	0.43
1:A:140:ILE:O	1:A:143:MET:HB3	2.19	0.43
1:B:259:LYS:HD3	1:B:259:LYS:N	2.34	0.43
1:A:213:ASP:HA	1:A:214:PRO:HD2	1.74	0.43
1:D:180:MET:HG2	1:D:185:ARG:HB3	2.01	0.43
1:B:351:GLU:HA	3:B:2665:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:GLY:O	1:C:401:ARG:HB2	2.19	0.42
1:A:337:LYS:HE2	3:A:1711:HOH:O	2.19	0.42
1:C:364:LEU:HD11	1:C:370:VAL:CG2	2.49	0.42
1:D:167:THR:HG22	1:D:168:THR:HG23	2.00	0.42
1:D:309:ASP:H	1:D:316:MET:HA	1.84	0.42
1:C:355:TRP:CZ3	1:C:357:ASP:HB2	2.54	0.42
1:D:18:ARG:HB2	1:D:412:VAL:HG12	2.02	0.42
1:A:309:ASP:HB2	1:A:317:ASN:ND2	2.34	0.42
1:D:144:TYR:O	1:D:148:LEU:HB2	2.19	0.42
1:C:187:GLN:NE2	1:C:187:GLN:CA	2.82	0.42
1:B:38:ASP:HB3	3:B:2572:HOH:O	2.20	0.42
1:C:13:GLU:HG3	1:C:229:MET:HE2	2.00	0.42
1:B:72:MET:HE3	1:B:164:THR:HG22	2.00	0.42
1:B:101:LEU:CD1	1:B:101:LEU:N	2.71	0.42
1:A:156:PRO:CG	1:A:187:GLN:HE22	2.32	0.42
1:B:223:LEU:HD22	1:B:224:GLU:N	2.35	0.42
1:D:148:LEU:HD13	1:D:150:HIS:CE1	2.54	0.42
1:C:62:MET:HB3	1:C:69:VAL:HG21	2.00	0.42
1:C:82:ASN:C	1:C:82:ASN:OD1	2.57	0.42
1:B:119:LEU:HD23	1:B:123:LEU:HG	2.00	0.42
1:A:272:LYS:HD2	1:A:273:SER:H	1.85	0.42
1:A:352:ARG:N	3:A:1710:HOH:O	2.52	0.42
1:B:370:VAL:HG22	1:B:390:ILE:HB	2.01	0.42
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.84	0.42
1:D:76:LEU:HD22	1:D:80:ILE:CD1	2.42	0.42
1:C:65:ARG:HH11	1:C:65:ARG:HG3	1.84	0.42
1:B:57:ASP:OD1	1:B:61:LYS:HE3	2.20	0.42
1:D:152:SER:CB	3:D:4734:HOH:O	2.67	0.42
1:D:160:ASN:C	1:D:162:GLN:N	2.71	0.42
1:A:238:ILE:CG2	1:A:249:ILE:HG12	2.43	0.42
1:D:212:GLY:O	1:D:213:ASP:HB2	2.20	0.42
1:D:27:LEU:HA	1:D:30:GLN:NE2	2.34	0.42
1:C:47:TRP:CD2	1:C:50:GLN:HB2	2.54	0.42
1:A:63:ARG:CA	3:A:1504:HOH:O	2.68	0.42
1:D:374:ARG:NE	3:D:4738:HOH:O	2.52	0.42
1:A:257:PHE:HD2	1:A:316:MET:HG2	1.85	0.42
1:A:76:LEU:O	1:A:79:THR:HB	2.20	0.42
1:D:9:GLY:HA2	1:D:172:TYR:O	2.20	0.42
1:D:372:TYR:CG	1:D:394:ALA:HB2	2.55	0.41
1:D:323:LYS:HG2	1:D:327:GLU:CB	2.38	0.41
1:C:18:ARG:NH1	3:C:3642:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ASN:HB2	3:C:3785:HOH:O	2.18	0.41
1:D:165:ARG:HB2	1:D:408:THR:O	2.20	0.41
1:D:53:ARG:NH2	3:D:4501:HOH:O	2.46	0.41
1:D:152:SER:HB2	3:D:4734:HOH:O	2.18	0.41
1:D:119:LEU:HD12	1:D:123:LEU:HG	2.02	0.41
1:C:279:LEU:CA	3:C:3786:HOH:O	2.59	0.41
1:D:208:GLU:HG2	1:D:210:TRP:CZ3	2.55	0.41
1:A:320:ARG:NH2	1:A:322:GLU:OE1	2.53	0.41
1:B:305:SER:O	1:B:318:ILE:HA	2.21	0.41
1:A:359:ASN:O	1:A:360:ASN:HB2	2.19	0.41
1:B:86:LEU:HA	1:B:86:LEU:HD23	1.72	0.41
1:A:239:GLY:HA2	1:A:268:ALA:HB3	2.01	0.41
1:C:213:ASP:OD1	1:C:215:ASP:HB2	2.21	0.41
1:D:312:SER:HB3	1:D:314:TYR:CE1	2.56	0.41
1:C:158:LEU:CD2	1:C:187:GLN:HB2	2.51	0.41
1:C:58:PHE:CE1	1:C:370:VAL:HG11	2.56	0.41
1:D:343:THR:HG23	1:D:344:GLY:H	1.86	0.41
1:B:63:ARG:C	1:B:65:ARG:N	2.73	0.41
1:D:291:VAL:HG22	1:D:340:VAL:HG12	2.03	0.41
1:B:272:LYS:HD2	1:B:273:SER:H	1.85	0.41
1:D:145:ARG:HH21	1:D:146:GLU:HB2	1.86	0.41
1:D:317:ASN:O	3:D:4741:HOH:O	2.22	0.41
1:A:274:ARG:NH1	1:A:274:ARG:HG2	2.32	0.41
1:A:324:THR:O	1:A:327:GLU:N	2.54	0.41
1:A:193:THR:O	1:A:197:LYS:HB2	2.21	0.41
1:B:147:TYR:HB3	1:C:302:VAL:HG21	2.01	0.41
1:A:11:HIS:O	1:A:12:SER:HB3	2.21	0.41
1:C:64:GLU:CG	3:C:3618:HOH:O	2.69	0.41
1:A:318:ILE:HB	1:D:140:ILE:HD13	2.03	0.41
1:D:253:ALA:HA	3:D:4747:HOH:O	2.21	0.41
1:D:268:ALA:HB2	1:D:325:PHE:CE1	2.55	0.41
1:D:295:PRO:O	1:D:299:LYS:HG3	2.21	0.40
1:D:303:PRO:HB2	1:D:321:GLU:HB2	2.03	0.40
1:A:146:GLU:CG	3:A:1623:HOH:O	2.69	0.40
1:A:336:LYS:NZ	3:A:1629:HOH:O	2.49	0.40
1:C:86:LEU:HD22	1:C:90:LEU:HG	2.03	0.40
1:B:216:LYS:HG2	1:B:217:ASP:N	2.37	0.40
1:D:307:ARG:HH11	1:D:307:ARG:HG2	1.86	0.40
1:C:180:MET:HB2	1:C:186:ARG:HG2	2.03	0.40
1:D:166:ASP:C	1:D:180:MET:HE2	2.41	0.40
1:D:84:GLU:HG2	1:D:198:PHE:HE1	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:MET:CE	1:D:283:PHE:HD2	2.34	0.40
1:A:115:GLU:H	1:A:115:GLU:HG2	1.66	0.40
1:C:293:VAL:CG1	1:C:294:PHE:N	2.83	0.40
1:D:46:ILE:HG22	1:D:399:ARG:CD	2.50	0.40
1:C:299:LYS:CE	3:C:3729:HOH:O	2.68	0.40
1:D:213:ASP:C	1:D:215:ASP:H	2.24	0.40
1:B:67:ILE:H	1:B:67:ILE:HG13	1.72	0.40
1:A:33:THR:HG22	1:A:36:ASN:OD1	2.21	0.40
1:A:55:HIS:O	1:A:59:VAL:HG23	2.21	0.40
1:A:9:GLY:O	1:A:412:VAL:HA	2.21	0.40
1:A:94:ILE:C	3:A:1721:HOH:O	2.58	0.40
1:D:206:GLU:HA	3:D:4584:HOH:O	2.22	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	401/418 (96%)	366 (91%)	27 (7%)	8 (2%)	9	7
1	B	399/418 (96%)	367 (92%)	30 (8%)	2 (0%)	34	41
1	C	396/418 (95%)	368 (93%)	26 (7%)	2 (0%)	34	41
1	D	402/418 (96%)	363 (90%)	32 (8%)	7 (2%)	11	10
All	All	1598/1672 (96%)	1464 (92%)	115 (7%)	19 (1%)	16	16

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	GLU
1	B	352	ARG
1	A	273	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	353	GLU
1	B	351	GLU
1	D	273	SER
1	D	275	ALA
1	D	296	GLU
1	D	360	ASN
1	A	12	SER
1	A	172	TYR
1	A	360	ASN
1	D	213	ASP
1	D	277	MET
1	A	207	PHE
1	D	101	LEU
1	C	416	ILE
1	C	295	PRO
1	A	230	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/354 (97%)	314 (91%)	30 (9%)	13	15
1	B	344/354 (97%)	312 (91%)	32 (9%)	11	13
1	C	342/354 (97%)	313 (92%)	29 (8%)	13	16
1	D	344/354 (97%)	310 (90%)	34 (10%)	10	11
All	All	1374/1416 (97%)	1249 (91%)	125 (9%)	12	13

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	20	VAL
1	A	39	GLU
1	A	40	LEU
1	A	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	SER
1	A	113	SER
1	A	115	GLU
1	A	119	LEU
1	A	130	ASP
1	A	131	ASP
1	A	145	ARG
1	A	155	LEU
1	A	197	LYS
1	A	208	GLU
1	A	223	LEU
1	A	233	ASN
1	A	242	GLU
1	A	273	SER
1	A	290	LEU
1	A	301	ILE
1	A	319	ARG
1	A	323	LYS
1	A	333	LEU
1	A	352	ARG
1	A	356	ASP
1	A	360	ASN
1	A	369	VAL
1	A	382	LEU
1	A	397	LEU
1	B	20	VAL
1	B	38	ASP
1	B	40	LEU
1	B	64	GLU
1	B	76	LEU
1	B	86	LEU
1	B	101	LEU
1	B	107	LEU
1	B	113	SER
1	B	141	LEU
1	B	167	THR
1	B	208	GLU
1	B	217	ASP
1	B	223	LEU
1	B	247	GLN
1	B	259	LYS
1	B	271	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	272	LYS
1	B	274	ARG
1	B	307	ARG
1	B	317	ASN
1	B	319	ARG
1	B	331	GLU
1	B	337	LYS
1	B	351	GLU
1	B	355	TRP
1	B	356	ASP
1	B	360	ASN
1	B	369	VAL
1	B	382	LEU
1	B	397	LEU
1	B	416	ILE
1	C	38	ASP
1	C	40	LEU
1	C	62	MET
1	C	64	GLU
1	C	65	ARG
1	C	76	LEU
1	C	86	LEU
1	C	101	LEU
1	C	107	LEU
1	C	119	LEU
1	C	130	ASP
1	C	141	LEU
1	C	143	MET
1	C	155	LEU
1	C	167	THR
1	C	180	MET
1	C	223	LEU
1	C	259	LYS
1	C	290	LEU
1	C	299	LYS
1	C	323	LYS
1	C	336	LYS
1	C	337	LYS
1	C	353	GLU
1	C	356	ASP
1	C	369	VAL
1	C	374	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	382	LEU
1	C	397	LEU
1	D	20	VAL
1	D	40	LEU
1	D	63	ARG
1	D	74	ASN
1	D	76	LEU
1	D	86	LEU
1	D	107	LEU
1	D	113	SER
1	D	115	GLU
1	D	116	PRO
1	D	119	LEU
1	D	130	ASP
1	D	165	ARG
1	D	180	MET
1	D	214	PRO
1	D	223	LEU
1	D	264	ARG
1	D	273	SER
1	D	274	ARG
1	D	277	MET
1	D	290	LEU
1	D	293	VAL
1	D	299	LYS
1	D	311	SER
1	D	312	SER
1	D	313	PRO
1	D	314	TYR
1	D	323	LYS
1	D	331	GLU
1	D	343	THR
1	D	357	ASP
1	D	381	LEU
1	D	397	LEU
1	D	415	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	ASN
1	B	254	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	359	ASN
1	C	55	HIS
1	C	187	GLN
1	C	199	HIS
1	C	204	ASN
1	C	354	GLN
1	D	29	HIS
1	D	30	GLN
1	D	199	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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ARG	A	1500	-	5,11,11	0.52	0	3,13,13	0.69	0
2	ARG	B	2500	-	5,11,11	0.30	0	3,13,13	0.79	0
2	ARG	C	3500	-	5,11,11	0.46	0	3,13,13	0.60	0
2	ARG	D	4500	-	5,11,11	0.50	0	3,13,13	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	1500	-	-	0/5/11/11	0/0/0/0
2	ARG	B	2500	-	-	0/5/11/11	0/0/0/0
2	ARG	C	3500	-	-	0/5/11/11	0/0/0/0
2	ARG	D	4500	-	-	0/5/11/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2500	ARG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	405/418 (96%)	-0.25	6 (1%)	76	81	21, 38, 63, 78	0
1	B	405/418 (96%)	-0.42	7 (1%)	73	79	18, 30, 54, 78	0
1	C	402/418 (96%)	-0.49	2 (0%)	91	94	18, 30, 54, 74	0
1	D	406/418 (97%)	-0.33	9 (2%)	65	73	20, 36, 62, 79	0
All	All	1618/1672 (96%)	-0.37	24 (1%)	76	81	18, 33, 60, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	5.2
1	A	6	THR	4.9
1	D	274	ARG	4.7
1	B	349	ALA	4.2
1	D	311	SER	4.2
1	A	275	ALA	4.1
1	B	273	SER	4.1
1	A	274	ARG	4.0
1	B	274	ARG	3.8
1	B	6	THR	3.0
1	C	6	THR	2.9
1	D	314	TYR	2.9
1	B	351	GLU	2.8
1	A	344	GLY	2.6
1	D	6	THR	2.6
1	A	311	SER	2.5
1	D	277	MET	2.5
1	C	117	ARG	2.4
1	D	313	PRO	2.2
1	A	319	ARG	2.2
1	D	417	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	313	PRO	2.2
1	D	310	PRO	2.1
1	D	275	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ARG	D	4500	12/12	0.97	0.10	0.55	16,28,37,38	0
2	ARG	A	1500	12/12	0.98	0.10	0.09	16,28,39,46	0
2	ARG	C	3500	12/12	0.97	0.09	-0.18	16,21,29,33	0
2	ARG	B	2500	12/12	0.98	0.07	-1.20	16,23,26,32	0

6.5 Other polymers (i)

There are no such residues in this entry.