Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:43 PM JST

PDB ID	:	5I8I
Title	:	Crystal Structure of the K. lactis Urea Amidolyase
Authors	:	Zhao, J.; Xiang, S.
Deposited on	:	2016-02-19
Resolution	:	6.50 Å(reported)

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

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

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

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

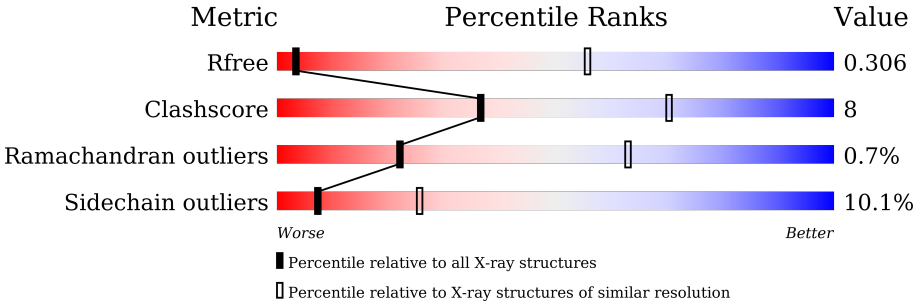
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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

Mol	Chain	Length	Quality of chain
1	A	1829	70% 18% • 9%
1	B	1829	69% 17% • 9%
1	C	1829	70% 17% • 9%
1	D	1829	70% 17% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 51722 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 Urea Amidolyase.

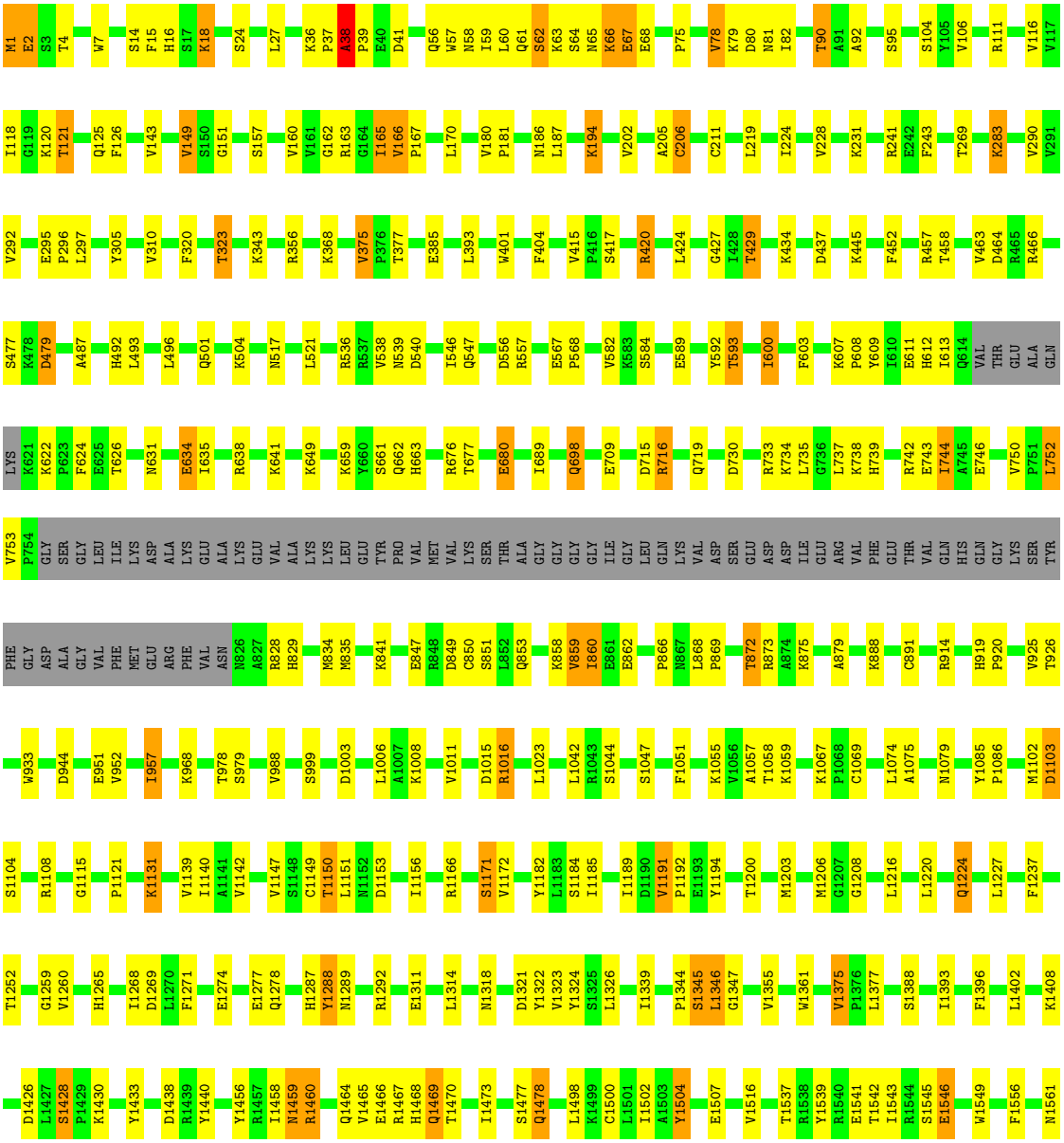
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1660	12939	8253	2183	2456	47	0	0	0
1	B	1658	12922	8243	2181	2452	46	0	0	0
1	C	1660	12939	8253	2183	2456	47	0	0	0
1	D	1658	12922	8243	2181	2452	46	0	0	0

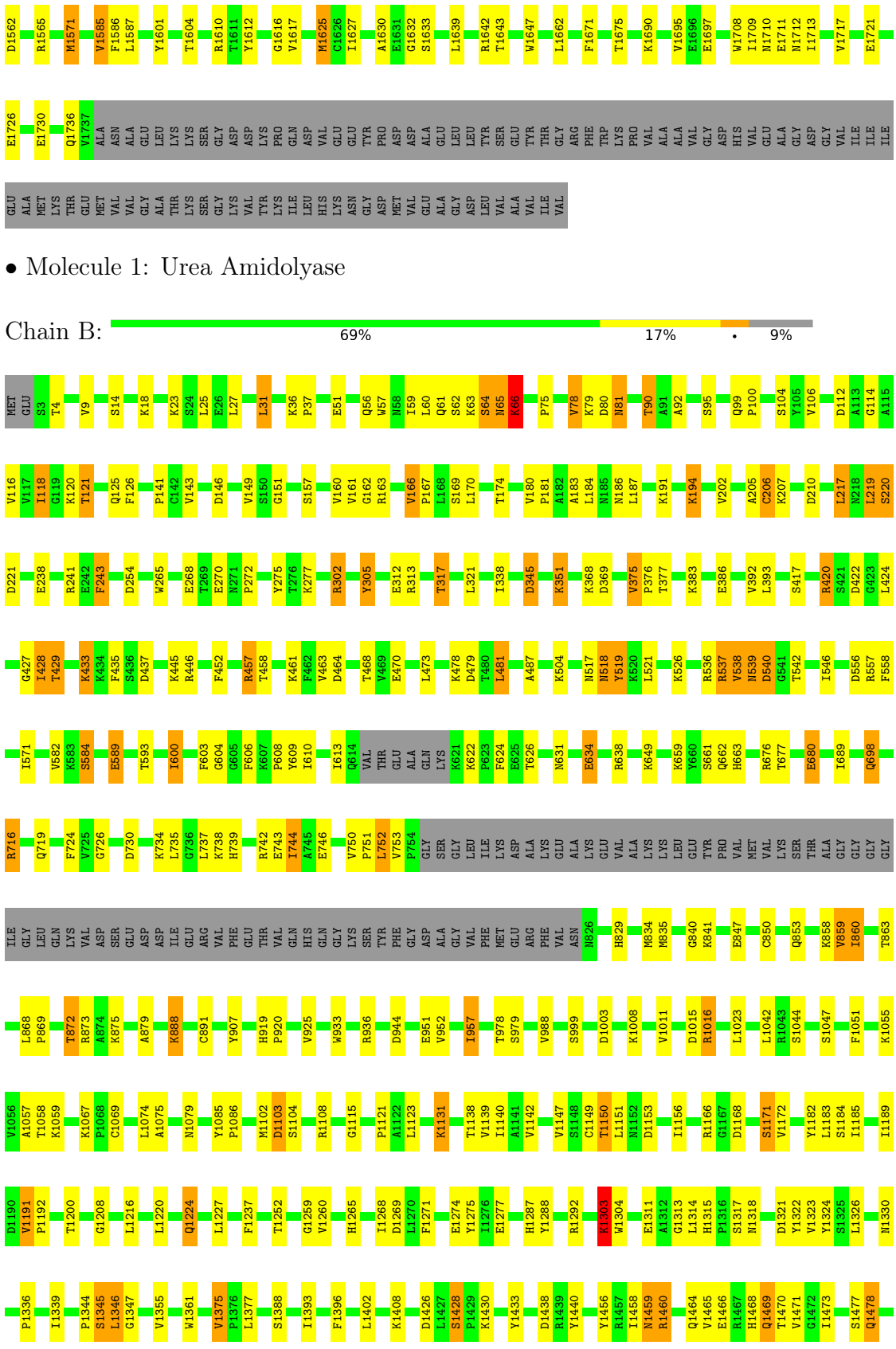
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Urea Amidolyase

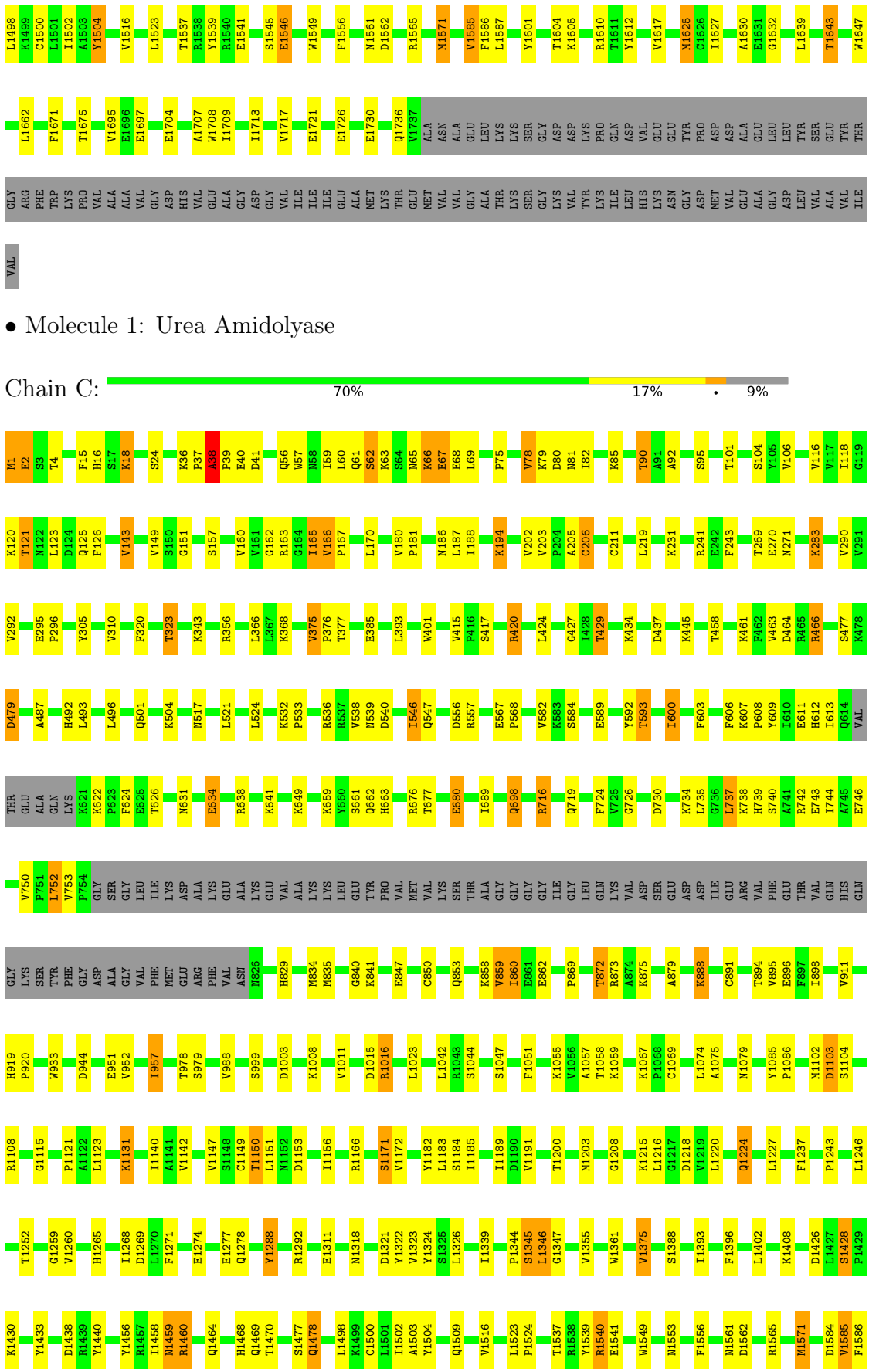
Chain A:





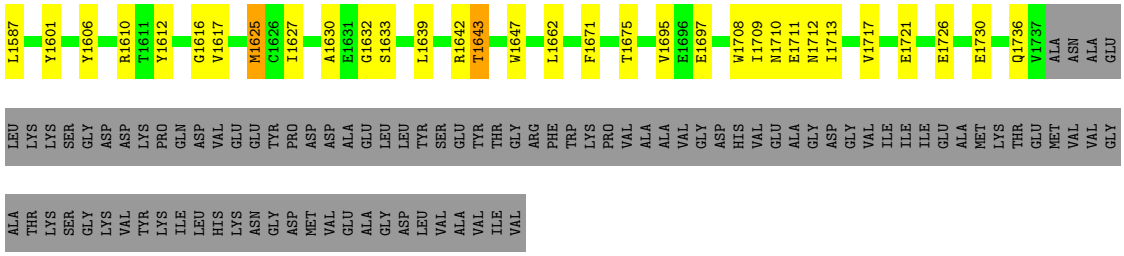
• Molecule 1: Urea Amidolyase

Chain B: 69% 17% • 9%



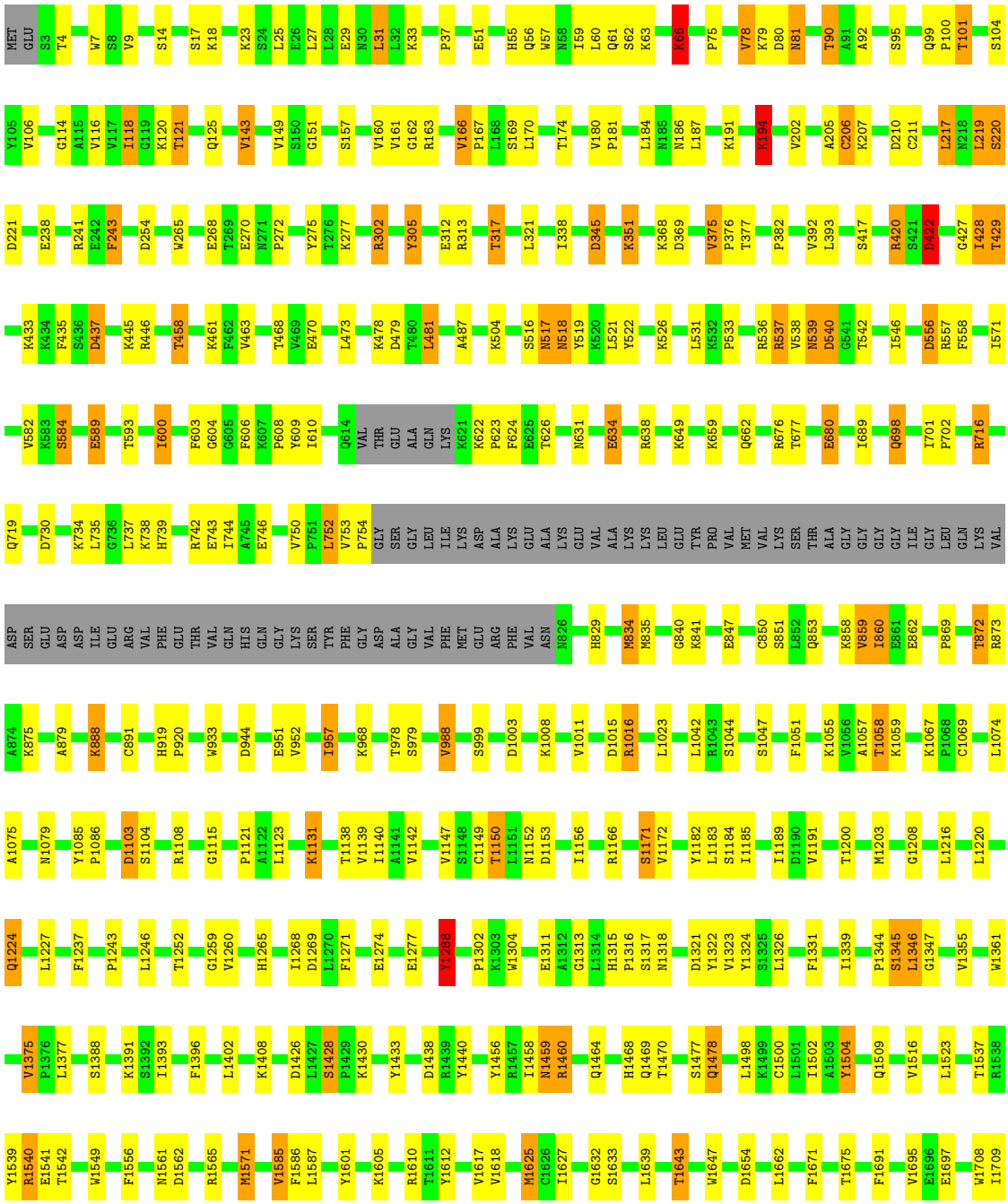
• Molecule 1: Urea Amidolyase

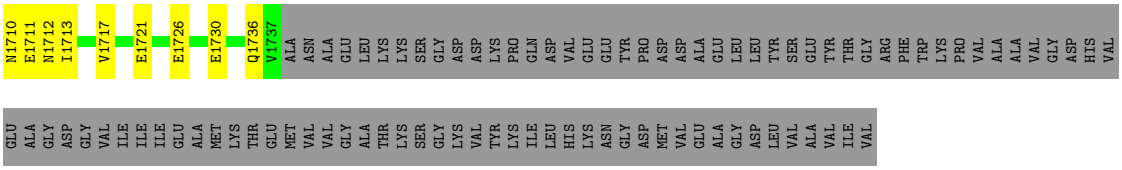
Chain C: 70% 17% • 9%



• Molecule 1: Urea Amidolyase

Chain D: 70% 17% • 9%




N1710
E1711
N1712
I1713
V1717
E1721
E1726
E1730
Q1736
V1737
ALA
ASN
ALA
GLU
LEU
LYS
LYS
SER
GLY
ASP
ASP
LYS
PRO
GLN
ASP
VAL
GLU
GLU
TYR
PRO
ASP
ASP
ALA
GLU
LEU
LEU
TYR
SER
GLU
TYR
THR
GLY
ARG
PHE
TRP
LYS
PRO
VAL
ALA
ALA
VAL
GLY
ASP
HIS
VAL

GLU
ALA
GLY
ASP
GLY
VAL
ILE
ILE
ILE
GLU
ALA
MET
LYS
THR
GLU
MET
VAL
VAL
VAL
GLY
ALA
THR
LYS
SER
GLY
LYS
VAL
TYR
LYS
ILE
LEU
HIS
LYS
ASN
GLY
ASP
MET
VAL
GLU
ALA
GLY
ASP
LEU
VAL
ALA
VAL
ILE
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.74Å 181.94Å 549.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.50 29.98 – 6.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.98-6.50) 96.0 (29.98-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.281 , 0.306	Depositor DCC
R_{free} test set	1017 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	216.1	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 238.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	51722	wwPDB-VP
Average B, all atoms (Å^2)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.40	1/13231 (0.0%)	0.70	4/17964 (0.0%)
1	B	0.51	2/13214 (0.0%)	0.86	23/17942 (0.1%)
1	C	0.39	1/13231 (0.0%)	0.69	5/17964 (0.0%)
1	D	0.49	3/13214 (0.0%)	0.83	21/17942 (0.1%)
All	All	0.45	7/52890 (0.0%)	0.77	53/71812 (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	2
1	B	0	2
1	C	0	3
1	D	0	6
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1546	GLU	CG-CD	-7.32	1.41	1.51
1	C	1288	TYR	CD2-CE2	6.77	1.49	1.39
1	B	1546	GLU	CG-CD	-5.72	1.43	1.51
1	D	17	SER	CA-CB	5.61	1.61	1.52
1	D	1288	TYR	CD2-CE2	5.39	1.47	1.39
1	D	392	VAL	CB-CG1	5.13	1.63	1.52
1	B	392	VAL	CB-CG1	5.11	1.63	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	556	ASP	N-CA-CB	-8.99	94.41	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	556	ASP	N-CA-CB	-8.84	94.69	110.60
1	A	1504	TYR	CB-CG-CD1	-8.11	116.14	121.00
1	D	1504	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	D	422	ASP	N-CA-CB	-7.68	96.78	110.60
1	D	194	LYS	CD-CE-NZ	-7.39	94.70	111.70
1	D	254	ASP	CB-CA-C	-7.35	95.71	110.40
1	B	558	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	B	254	ASP	CB-CA-C	-7.26	95.88	110.40
1	B	66	LYS	CD-CE-NZ	7.15	128.15	111.70
1	D	118	ILE	CG1-CB-CG2	-6.92	96.17	111.40
1	D	558	PHE	CB-CG-CD1	-6.80	116.04	120.80
1	B	305	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	B	118	ILE	CG1-CB-CG2	-6.72	96.62	111.40
1	B	194	LYS	CD-CE-NZ	-6.68	96.34	111.70
1	B	1504	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	1303	LYS	N-CA-C	-6.47	93.52	111.00
1	D	1504	TYR	CB-CG-CD2	6.44	124.87	121.00
1	A	1504	TYR	CB-CG-CD2	6.36	124.81	121.00
1	D	305	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	457	ARG	CG-CD-NE	6.28	124.99	111.80
1	D	31	LEU	CA-CB-CG	6.10	129.32	115.30
1	B	305	TYR	CB-CG-CD1	6.04	124.62	121.00
1	D	305	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	217	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	217	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	1288	TYR	CA-CB-CG	-5.89	102.21	113.40
1	D	66	LYS	CD-CE-NZ	5.88	125.22	111.70
1	B	217	LEU	CB-CG-CD2	5.82	120.89	111.00
1	C	38	ALA	C-N-CD	5.82	140.61	128.40
1	D	531	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	C	1540	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	D	481	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	519	TYR	N-CA-C	5.71	126.42	111.00
1	B	558	PHE	CB-CG-CD2	5.71	124.80	120.80
1	B	31	LEU	CA-CB-CG	5.69	128.39	115.30
1	D	217	LEU	CB-CG-CD2	5.68	120.66	111.00
1	A	38	ALA	C-N-CD	5.66	140.29	128.40
1	D	571	ILE	CG1-CB-CG2	-5.60	99.07	111.40
1	B	571	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	D	345	ASP	CB-CA-C	-5.56	99.28	110.40
1	B	481	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	64	SER	CB-CA-C	-5.38	99.89	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	558	PHE	CB-CG-CD2	5.37	124.56	120.80
1	B	345	ASP	CB-CA-C	-5.36	99.68	110.40
1	B	519	TYR	N-CA-CB	-5.28	101.10	110.60
1	B	464	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	1540	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	C	546	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	C	898	ILE	N-CA-C	-5.14	97.13	111.00
1	B	446	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	188	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	D	446	ARG	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1469	GLN	Mainchain
1	A	539	ASN	Peptide
1	B	1469	GLN	Mainchain
1	B	539	ASN	Peptide
1	C	1288	TYR	Mainchain
1	C	539	ASN	Peptide
1	C	896	GLU	Mainchain
1	D	101	THR	Mainchain
1	D	1288	TYR	Mainchain
1	D	382	PRO	Mainchain
1	D	422	ASP	Mainchain
1	D	517	ASN	Mainchain
1	D	539	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12939	0	12896	226	0
1	B	12922	0	12878	218	1
1	C	12939	0	12896	203	1
1	D	12922	0	12878	215	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51722	0	51548	813	1

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 8.

All (813) 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:59:ILE:O	1:B:62:SER:OG	1.78	1.01
1:B:79:LYS:HA	1:B:121:THR:HG22	1.45	0.97
1:C:1509:GLN:NE2	1:D:101:THR:O	1.97	0.97
1:D:79:LYS:HA	1:D:121:THR:HG22	1.45	0.95
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.47	0.94
1:C:79:LYS:HA	1:C:121:THR:HG22	1.51	0.93
1:A:1546:GLU:HB2	1:D:1288:TYR:CD1	2.06	0.91
1:A:63:LYS:HA	1:B:1468:HIS:O	1.70	0.91
1:A:1288:TYR:OH	1:D:1541:GLU:HB3	1.72	0.89
1:A:1468:HIS:HE1	1:B:59:ILE:HG23	1.39	0.88
1:C:1459:ASN:HD21	1:C:1460:ARG:HH11	1.21	0.87
1:A:79:LYS:HA	1:A:121:THR:HG22	1.55	0.86
1:D:59:ILE:O	1:D:62:SER:OG	1.94	0.84
1:A:1459:ASN:HD21	1:A:1460:ARG:HH11	1.22	0.84
1:D:1459:ASN:HD21	1:D:1460:ARG:HH11	1.22	0.83
1:D:79:LYS:HG2	1:D:81:ASN:HB2	1.60	0.82
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.59	0.82
1:B:79:LYS:HG2	1:B:81:ASN:HB2	1.61	0.82
1:B:1459:ASN:HD21	1:B:1460:ARG:HH11	1.23	0.81
1:C:59:ILE:HG23	1:D:1468:HIS:HE1	1.43	0.80
1:C:79:LYS:HG2	1:C:81:ASN:HB2	1.64	0.80
1:A:1468:HIS:O	1:B:63:LYS:HA	1.82	0.80
1:A:58:ASN:O	1:A:62:SER:OG	2.01	0.79
1:D:859:VAL:HG23	1:D:860:ILE:HD12	1.63	0.79
1:D:186:ASN:HD21	1:D:458:THR:HG22	1.45	0.79
1:C:59:ILE:HG23	1:D:1468:HIS:CE1	2.17	0.78
1:A:859:VAL:HG23	1:A:860:ILE:HD12	1.65	0.77
1:B:1585:VAL:HG13	1:B:1586:PHE:CD1	2.21	0.76
1:D:1585:VAL:HG13	1:D:1586:PHE:CD1	2.21	0.76
1:A:64:SER:HA	1:B:1471:VAL:HG23	1.68	0.76
1:B:859:VAL:HG23	1:B:860:ILE:HD12	1.68	0.76
1:C:1585:VAL:HG13	1:C:1586:PHE:CD1	2.20	0.76
1:C:859:VAL:HG23	1:C:860:ILE:HD12	1.65	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:VAL:HG13	1:A:1586:PHE:CD1	2.21	0.75
1:A:1546:GLU:HB2	1:D:1288:TYR:HD1	1.49	0.75
1:B:1016:ARG:NH2	1:B:1051:PHE:O	2.19	0.75
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.21	0.73
1:C:62:SER:O	1:D:1470:THR:HA	1.89	0.73
1:C:1016:ARG:NH2	1:C:1051:PHE:O	2.22	0.73
1:B:186:ASN:HD21	1:B:458:THR:HG22	1.54	0.72
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.71	0.72
1:C:1459:ASN:ND2	1:C:1460:ARG:HH11	1.87	0.72
1:C:493:LEU:HB2	1:C:496:LEU:HD12	1.70	0.72
1:D:1016:ARG:NH2	1:D:1051:PHE:O	2.23	0.72
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.87	0.71
1:B:275:TYR:HD1	1:B:428:ILE:HD11	1.55	0.71
1:C:1464:GLN:O	1:C:1468:HIS:HD2	1.73	0.71
1:D:1459:ASN:ND2	1:D:1460:ARG:HH11	1.88	0.71
1:A:1470:THR:HA	1:B:62:SER:O	1.91	0.71
1:A:1542:THR:O	1:D:1541:GLU:HG3	1.90	0.71
1:A:59:ILE:HG23	1:B:1468:HIS:HE1	1.56	0.71
1:B:1625:MET:HE1	1:B:1627:ILE:HG13	1.72	0.71
1:C:149:VAL:HG13	1:C:151:GLY:H	1.54	0.71
1:D:275:TYR:HD1	1:D:428:ILE:HD11	1.54	0.70
1:D:57:TRP:O	1:D:61:GLN:HG2	1.91	0.70
1:A:186:ASN:HD21	1:A:458:THR:HG22	1.57	0.70
1:A:1465:VAL:O	1:A:1469:GLN:N	2.25	0.69
1:B:1459:ASN:ND2	1:B:1460:ARG:HH11	1.90	0.69
1:C:186:ASN:HD21	1:C:458:THR:HG22	1.58	0.69
1:B:519:TYR:CE2	1:B:537:ARG:HB2	2.29	0.68
1:B:186:ASN:ND2	1:B:458:THR:HG22	2.08	0.67
1:D:1318:ASN:HD21	1:D:1605:LYS:H	1.43	0.67
1:C:1571:MET:HG2	1:C:1601:TYR:CE2	2.30	0.66
1:A:149:VAL:HG13	1:A:151:GLY:H	1.59	0.66
1:A:1287:HIS:CE1	1:A:1288:TYR:CE2	2.83	0.66
1:D:275:TYR:CD1	1:D:428:ILE:HD11	2.31	0.66
1:B:1313:GLY:HA3	1:B:1318:ASN:HD22	1.61	0.66
1:A:62:SER:O	1:B:1470:THR:HA	1.96	0.66
1:A:504:LYS:O	1:A:557:ARG:NH2	2.30	0.65
1:C:1625:MET:HE1	1:C:1627:ILE:HG13	1.77	0.65
1:B:90:THR:HG22	1:B:92:ALA:H	1.62	0.65
1:C:464:ASP:HA	1:C:466:ARG:HH21	1.62	0.65
1:D:186:ASN:ND2	1:D:458:THR:HG22	2.11	0.65
1:A:377:THR:HA	1:A:429:THR:HG22	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:TYR:CD1	1:B:428:ILE:HD11	2.32	0.65
1:C:63:LYS:HA	1:D:1468:HIS:O	1.97	0.64
1:C:377:THR:HA	1:C:429:THR:HG22	1.78	0.64
1:B:1318:ASN:HD21	1:B:1605:LYS:H	1.46	0.64
1:D:1428:SER:OG	1:D:1428:SER:O	2.13	0.64
1:C:504:LYS:O	1:C:557:ARG:NH2	2.30	0.64
1:C:1075:ALA:HB3	1:C:1131:LYS:HG2	1.80	0.64
1:A:464:ASP:HA	1:A:466:ARG:HH21	1.62	0.64
1:C:62:SER:HB3	1:D:1504:TYR:OH	1.99	0.63
1:B:626:THR:HG22	1:B:649:LYS:HB2	1.79	0.63
1:A:1468:HIS:ND1	1:B:62:SER:OG	2.31	0.63
1:D:1464:GLN:O	1:D:1468:HIS:HD2	1.81	0.63
1:D:121:THR:HG21	1:D:157:SER:OG	1.99	0.63
1:D:1625:MET:HE1	1:D:1627:ILE:HG13	1.79	0.63
1:A:1288:TYR:OH	1:D:1541:GLU:OE2	2.10	0.63
1:B:205:ALA:O	1:B:206:CYS:HB2	1.99	0.63
1:B:1150:THR:HG23	1:B:1153:ASP:H	1.64	0.63
1:B:220:SER:HB2	1:B:470:GLU:O	1.99	0.63
1:B:1466:GLU:C	1:B:1469:GLN:H	2.03	0.63
1:A:1428:SER:O	1:A:1428:SER:OG	2.17	0.62
1:D:205:ALA:O	1:D:206:CYS:HB2	1.99	0.62
1:C:1470:THR:HA	1:D:62:SER:O	1.99	0.62
1:B:121:THR:HG21	1:B:157:SER:OG	1.99	0.62
1:C:1537:THR:O	1:C:1541:GLU:HG2	2.00	0.62
1:A:163:ARG:HG3	1:A:165:ILE:HD13	1.82	0.62
1:C:1150:THR:HG23	1:C:1153:ASP:H	1.64	0.62
1:A:64:SER:N	1:B:1469:GLN:O	2.33	0.61
1:A:477:SER:OG	1:A:479:ASP:HB2	2.00	0.61
1:B:1075:ALA:HB3	1:B:1131:LYS:HG2	1.80	0.61
1:D:90:THR:HG22	1:D:92:ALA:H	1.64	0.61
1:A:1075:ALA:HB3	1:A:1131:LYS:HG2	1.82	0.61
1:C:162:GLY:HA2	1:C:187:LEU:HD21	1.83	0.61
1:D:220:SER:HB2	1:D:470:GLU:O	2.00	0.61
1:D:1150:THR:HG23	1:D:1153:ASP:H	1.65	0.61
1:A:205:ALA:O	1:A:206:CYS:HB2	2.00	0.61
1:B:1708:TRP:HE3	1:B:1709:ILE:HD12	1.63	0.61
1:C:101:THR:O	1:D:1509:GLN:NE2	2.33	0.61
1:C:205:ALA:O	1:C:206:CYS:HB2	2.00	0.61
1:D:1571:MET:HG2	1:D:1601:TYR:CE2	2.34	0.61
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.66	0.61
1:B:1339:ILE:HG23	1:B:1344:PRO:HD2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:HIS:CE1	1:B:1288:TYR:CE2	2.89	0.61
1:A:90:THR:HG22	1:A:92:ALA:H	1.64	0.61
1:D:1075:ALA:HB3	1:D:1131:LYS:HG2	1.82	0.61
1:B:377:THR:HA	1:B:429:THR:HG22	1.83	0.61
1:B:57:TRP:O	1:B:61:GLN:HG2	2.01	0.60
1:A:59:ILE:HG23	1:B:1468:HIS:CE1	2.37	0.60
1:A:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:D:1260:VAL:HG12	1:D:1355:VAL:HA	1.84	0.60
1:D:149:VAL:HG13	1:D:151:GLY:H	1.67	0.60
1:B:149:VAL:HG13	1:B:151:GLY:H	1.66	0.60
1:D:600:ILE:HD11	1:D:609:TYR:CE1	2.36	0.60
1:C:90:THR:HG22	1:C:92:ALA:H	1.66	0.60
1:C:1339:ILE:HG23	1:C:1344:PRO:HD2	1.83	0.60
1:D:1313:GLY:HA3	1:D:1318:ASN:HD22	1.67	0.60
1:B:1465:VAL:O	1:B:1469:GLN:N	2.35	0.60
1:A:1259:GLY:HA2	1:A:1375:VAL:HG12	1.84	0.59
1:B:1500:CYS:HB3	1:B:1504:TYR:CZ	2.36	0.59
1:D:1339:ILE:HG23	1:D:1344:PRO:HD2	1.83	0.59
1:C:1468:HIS:HE1	1:D:59:ILE:HG12	1.66	0.59
1:D:60:LEU:HD11	1:D:114:GLY:HA2	1.83	0.59
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.85	0.59
1:B:375:VAL:HG12	1:B:429:THR:HG23	1.84	0.59
1:B:478:LYS:O	1:B:481:LEU:HG	2.02	0.59
1:C:1428:SER:O	1:C:1428:SER:OG	2.18	0.59
1:D:375:VAL:HG12	1:D:429:THR:HG23	1.85	0.59
1:B:143:VAL:HG13	1:B:461:LYS:HB3	1.84	0.59
1:D:1708:TRP:HE3	1:D:1709:ILE:HD12	1.67	0.59
1:C:163:ARG:HG3	1:C:165:ILE:HD13	1.84	0.59
1:D:626:THR:HG22	1:D:649:LYS:HB2	1.85	0.59
1:D:377:THR:HA	1:D:429:THR:HG22	1.84	0.59
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.68	0.59
1:B:1260:VAL:HG12	1:B:1355:VAL:HA	1.83	0.59
1:D:519:TYR:CE2	1:D:537:ARG:HB2	2.37	0.59
1:A:186:ASN:ND2	1:A:458:THR:HG22	2.16	0.59
1:B:1428:SER:O	1:B:1428:SER:OG	2.18	0.59
1:C:1708:TRP:HE3	1:C:1709:ILE:HD12	1.66	0.59
1:C:626:THR:HG22	1:C:649:LYS:HB2	1.85	0.59
1:A:1469:GLN:HB3	1:B:64:SER:OG	2.02	0.58
1:B:1121:PRO:HG2	1:B:1189:ILE:H	1.68	0.58
1:C:186:ASN:ND2	1:C:458:THR:HG22	2.18	0.58
1:C:477:SER:OG	1:C:479:ASP:HB2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1121:PRO:HG2	1:D:1189:ILE:H	1.66	0.58
1:A:603:PHE:HB3	1:A:608:PRO:HB2	1.84	0.58
1:C:742:ARG:HH22	1:C:753:VAL:HB	1.69	0.58
1:D:1131:LYS:HB3	1:D:1171:SER:HB2	1.84	0.58
1:A:320:PHE:O	1:A:323:THR:HB	2.03	0.58
1:A:600:ILE:HD11	1:A:609:TYR:CZ	2.38	0.58
1:B:600:ILE:HD11	1:B:609:TYR:CE1	2.39	0.58
1:D:478:LYS:O	1:D:481:LEU:HG	2.03	0.58
1:A:1571:MET:HG2	1:A:1601:TYR:CE2	2.37	0.58
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.84	0.58
1:A:1260:VAL:HG12	1:A:1355:VAL:HA	1.85	0.58
1:D:317:THR:HG21	1:D:338:ILE:HG21	1.85	0.58
1:B:1131:LYS:HB3	1:B:1171:SER:HB2	1.85	0.58
1:C:56:GLN:O	1:C:59:ILE:HB	2.03	0.58
1:B:742:ARG:HH22	1:B:753:VAL:HB	1.67	0.58
1:C:1131:LYS:HB3	1:C:1171:SER:HB2	1.86	0.58
1:A:1339:ILE:HG23	1:A:1344:PRO:HD2	1.84	0.58
1:B:1259:GLY:HA2	1:B:1375:VAL:HG12	1.86	0.58
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.86	0.57
1:C:375:VAL:HG12	1:C:429:THR:HG23	1.85	0.57
1:C:1464:GLN:O	1:C:1468:HIS:CD2	2.55	0.57
1:D:853:GLN:HG2	1:D:858:LYS:HG2	1.86	0.57
1:C:600:ILE:HD11	1:C:609:TYR:CZ	2.39	0.57
1:D:1587:LEU:HB3	1:D:1647:TRP:CD2	2.39	0.57
1:A:1713:ILE:O	1:A:1717:VAL:HG23	2.05	0.57
1:C:603:PHE:HB3	1:C:608:PRO:HB2	1.86	0.57
1:D:1085:TYR:CD2	1:D:1108:ARG:HD3	2.39	0.57
1:A:1121:PRO:HG2	1:A:1189:ILE:H	1.70	0.57
1:B:603:PHE:HB3	1:B:608:PRO:HB2	1.86	0.57
1:C:1069:CYS:SG	1:C:1224:GLN:HB2	2.45	0.57
1:A:1466:GLU:C	1:A:1469:GLN:H	2.07	0.56
1:B:1587:LEU:HB3	1:B:1647:TRP:CD2	2.40	0.56
1:D:742:ARG:HH22	1:D:753:VAL:HB	1.70	0.56
1:C:1085:TYR:CD2	1:C:1108:ARG:HD3	2.40	0.56
1:C:1121:PRO:HG2	1:C:1189:ILE:H	1.71	0.56
1:D:752:LEU:H	1:D:752:LEU:HD12	1.70	0.56
1:D:1315:HIS:HD2	1:D:1317:SER:H	1.52	0.56
1:A:752:LEU:HD12	1:A:752:LEU:H	1.71	0.56
1:B:417:SER:OG	1:B:427:GLY:HA2	2.04	0.56
1:B:1069:CYS:SG	1:B:1224:GLN:HB2	2.46	0.56
1:A:61:GLN:O	1:A:66:LYS:NZ	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:TYR:CD2	1:A:1108:ARG:HD3	2.40	0.56
1:B:504:LYS:O	1:B:557:ARG:NH2	2.39	0.56
1:C:853:GLN:HG2	1:C:858:LYS:HG2	1.86	0.56
1:C:957:ILE:HG12	1:C:1023:LEU:HD22	1.86	0.56
1:A:1458:ILE:HG21	1:A:1478:GLN:HG2	1.88	0.56
1:D:265:TRP:CD2	1:D:272:PRO:HG3	2.41	0.56
1:C:320:PHE:O	1:C:323:THR:HB	2.06	0.56
1:B:853:GLN:HG2	1:B:858:LYS:HG2	1.88	0.56
1:C:1468:HIS:CE1	1:D:59:ILE:HG23	2.40	0.55
1:C:1587:LEU:HB3	1:C:1647:TRP:CD2	2.40	0.55
1:D:417:SER:OG	1:D:427:GLY:HA2	2.06	0.55
1:A:1587:LEU:HB3	1:A:1647:TRP:CD2	2.42	0.55
1:D:1713:ILE:O	1:D:1717:VAL:HG23	2.06	0.55
1:B:61:GLN:O	1:B:66:LYS:NZ	2.32	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.88	0.55
1:D:174:THR:OG1	1:D:210:ASP:OD1	2.24	0.55
1:C:57:TRP:O	1:C:61:GLN:HG2	2.06	0.55
1:A:626:THR:HG22	1:A:649:LYS:HB2	1.88	0.55
1:B:1464:GLN:O	1:B:1468:HIS:HD2	1.88	0.55
1:A:121:THR:HG21	1:A:157:SER:OG	2.06	0.55
1:A:375:VAL:HG12	1:A:429:THR:HG23	1.89	0.55
1:A:1500:CYS:HB3	1:A:1504:TYR:CZ	2.42	0.55
1:C:1571:MET:HG2	1:C:1601:TYR:HE2	1.70	0.55
1:B:80:ASP:OD1	1:B:90:THR:HB	2.07	0.55
1:C:1713:ILE:O	1:C:1717:VAL:HG23	2.06	0.55
1:B:1085:TYR:CD2	1:B:1108:ARG:HD3	2.42	0.54
1:B:1189:ILE:HG21	1:B:1220:LEU:HD23	1.89	0.54
1:A:57:TRP:O	1:A:61:GLN:HG2	2.07	0.54
1:B:1458:ILE:HG21	1:B:1478:GLN:HG2	1.89	0.54
1:C:1260:VAL:HG12	1:C:1355:VAL:HA	1.88	0.54
1:B:957:ILE:HG12	1:B:1023:LEU:HD22	1.89	0.54
1:D:504:LYS:O	1:D:557:ARG:NH2	2.39	0.54
1:A:1561:ASN:ND2	1:A:1601:TYR:HB3	2.21	0.54
1:D:80:ASP:OD1	1:D:90:THR:HB	2.07	0.54
1:A:65:ASN:O	1:A:68:GLU:HB2	2.07	0.54
1:B:847:GLU:OE2	1:B:873:ARG:NH1	2.41	0.54
1:C:1458:ILE:HG21	1:C:1478:GLN:HG2	1.90	0.54
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.90	0.54
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.38	0.54
1:C:607:LYS:HB2	1:C:608:PRO:CD	2.38	0.54
1:A:1069:CYS:SG	1:A:1224:GLN:HB2	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:HB	1:D:221:ASP:OD1	2.07	0.54
1:B:1561:ASN:ND2	1:B:1601:TYR:HB3	2.22	0.54
1:D:603:PHE:HB3	1:D:608:PRO:HB2	1.89	0.54
1:A:80:ASP:OD1	1:A:90:THR:HB	2.08	0.54
1:A:847:GLU:OE2	1:A:873:ARG:NH1	2.42	0.53
1:A:1200:THR:OG1	1:A:1208:GLY:HA3	2.09	0.53
1:A:1543:ILE:O	1:D:1542:THR:HA	2.08	0.53
1:B:487:ALA:HB3	1:B:584:SER:HB2	1.91	0.53
1:C:295:GLU:HB3	1:C:296:PRO:HD3	1.89	0.53
1:C:1710:ASN:C	1:C:1712:ASN:H	2.12	0.53
1:A:634:GLU:OE1	1:A:1008:LYS:HE2	2.09	0.53
1:D:1189:ILE:HG21	1:D:1220:LEU:HD23	1.90	0.53
1:A:62:SER:HB3	1:B:1504:TYR:CE2	2.44	0.53
1:A:624:PHE:HD1	1:A:698:GLN:HG3	1.74	0.53
1:C:592:TYR:OH	1:D:589:GLU:HG3	2.09	0.53
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.44	0.53
1:C:634:GLU:OE1	1:C:1008:LYS:HE2	2.09	0.53
1:D:957:ILE:HG12	1:D:1023:LEU:HD22	1.90	0.53
1:A:957:ILE:HG12	1:A:1023:LEU:HD22	1.90	0.53
1:B:1459:ASN:ND2	1:B:1460:ARG:HD2	2.24	0.53
1:C:1503:ALA:HB1	1:D:55:HIS:CD2	2.44	0.53
1:D:1259:GLY:HA2	1:D:1375:VAL:HG12	1.91	0.53
1:A:1149:CYS:HB2	1:A:1156:ILE:HG22	1.91	0.52
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.24	0.52
1:C:80:ASP:OD1	1:C:90:THR:HB	2.09	0.52
1:D:375:VAL:HG13	1:D:376:PRO:O	2.09	0.52
1:A:92:ALA:HB3	1:A:125:GLN:HA	1.90	0.52
1:A:163:ARG:HG3	1:A:165:ILE:CD1	2.39	0.52
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.91	0.52
1:D:56:GLN:O	1:D:59:ILE:HB	2.10	0.52
1:A:125:GLN:HG2	1:A:126:PHE:CD1	2.45	0.52
1:B:174:THR:OG1	1:B:210:ASP:OD1	2.27	0.52
1:C:600:ILE:HD11	1:C:609:TYR:CE1	2.45	0.52
1:C:375:VAL:CG1	1:C:401:TRP:HB3	2.40	0.52
1:D:634:GLU:OE1	1:D:1008:LYS:HE2	2.09	0.52
1:D:1459:ASN:ND2	1:D:1460:ARG:HD2	2.24	0.52
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.91	0.52
1:C:1459:ASN:ND2	1:C:1460:ARG:HD2	2.25	0.52
1:A:1710:ASN:C	1:A:1712:ASN:H	2.13	0.52
1:B:375:VAL:HG13	1:B:376:PRO:O	2.10	0.52
1:D:1571:MET:HG2	1:D:1601:TYR:HE2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:TYR:OH	1:B:589:GLU:HG3	2.10	0.52
1:A:1265:HIS:HE1	1:A:1322:TYR:CZ	2.28	0.52
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.91	0.52
1:B:919:HIS:ND1	1:B:920:PRO:HD3	2.25	0.52
1:C:829:HIS:CD2	1:C:850:CYS:HB2	2.45	0.52
1:C:835:MET:HG2	1:C:933:TRP:HE3	1.75	0.52
1:D:1200:THR:OG1	1:D:1208:GLY:HA3	2.09	0.52
1:D:1458:ILE:HG21	1:D:1478:GLN:HG2	1.91	0.52
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.74	0.52
1:A:1288:TYR:CZ	1:D:1541:GLU:HB3	2.45	0.52
1:A:75:PRO:O	1:A:166:VAL:HG22	2.11	0.51
1:A:589:GLU:O	1:A:593:THR:HB	2.09	0.51
1:B:9:VAL:HB	1:B:221:ASP:OD1	2.11	0.51
1:B:60:LEU:HD11	1:B:114:GLY:HA2	1.91	0.51
1:C:65:ASN:O	1:C:68:GLU:HB2	2.10	0.51
1:C:1189:ILE:HG21	1:C:1220:LEU:HD23	1.91	0.51
1:C:752:LEU:HD12	1:C:752:LEU:H	1.75	0.51
1:C:1259:GLY:HA2	1:C:1375:VAL:HG12	1.91	0.51
1:C:1469:GLN:HB2	1:D:63:LYS:HA	1.93	0.51
1:A:600:ILE:HD11	1:A:609:TYR:CE1	2.46	0.51
1:A:1288:TYR:CD1	1:A:1288:TYR:C	2.83	0.51
1:C:607:LYS:HB2	1:C:608:PRO:HD3	1.91	0.51
1:D:1498:LEU:O	1:D:1502:ILE:HG12	2.11	0.51
1:A:59:ILE:HD13	1:A:111:ARG:NH2	2.26	0.51
1:B:1315:HIS:HD2	1:B:1317:SER:H	1.58	0.51
1:B:1498:LEU:O	1:B:1502:ILE:HG12	2.11	0.51
1:C:92:ALA:HB3	1:C:125:GLN:HA	1.91	0.51
1:C:589:GLU:O	1:C:593:THR:HB	2.11	0.51
1:C:847:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
1:C:869:PRO:HD2	1:C:872:THR:CG2	2.41	0.51
1:D:487:ALA:HB3	1:D:584:SER:HB2	1.93	0.51
1:D:869:PRO:HD2	1:D:872:THR:CG2	2.41	0.51
1:B:351:LYS:HE3	1:B:351:LYS:O	2.11	0.51
1:D:1710:ASN:C	1:D:1712:ASN:H	2.13	0.51
1:A:63:LYS:O	1:A:66:LYS:NZ	2.34	0.51
1:B:1265:HIS:HE1	1:B:1322:TYR:CZ	2.28	0.51
1:D:829:HIS:CD2	1:D:850:CYS:HB2	2.47	0.50
1:C:125:GLN:HG2	1:C:126:PHE:CD1	2.47	0.50
1:C:62:SER:HB2	1:D:1468:HIS:HB3	1.93	0.50
1:D:1625:MET:HE3	1:D:1671:PHE:HZ	1.76	0.50
1:A:1470:THR:HB	1:A:1473:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1345:SER:OG	1:B:1346:LEU:N	2.44	0.50
1:B:1545:SER:C	1:B:1546:GLU:HG3	2.31	0.50
1:C:290:VAL:HG12	1:C:292:VAL:HG23	1.92	0.50
1:C:1149:CYS:HB2	1:C:1156:ILE:HG22	1.93	0.50
1:D:677:THR:OG1	1:D:680:GLU:HB2	2.12	0.50
1:A:1466:GLU:O	1:A:1469:GLN:HG3	2.12	0.50
1:D:143:VAL:HG13	1:D:461:LYS:HB3	1.94	0.50
1:A:1288:TYR:OH	1:D:1541:GLU:CB	2.54	0.50
1:B:610:ILE:O	1:B:610:ILE:HG22	2.12	0.50
1:B:1149:CYS:HB2	1:B:1156:ILE:HG22	1.93	0.50
1:C:1200:THR:OG1	1:C:1208:GLY:HA3	2.11	0.50
1:D:1140:ILE:HD11	1:D:1185:ILE:HD12	1.94	0.50
1:A:62:SER:HB2	1:B:1468:HIS:ND1	2.27	0.50
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.94	0.50
1:B:1625:MET:HE3	1:B:1671:PHE:HZ	1.77	0.50
1:D:219:LEU:HB3	1:D:473:LEU:HD21	1.94	0.50
1:A:1203:MET:HE1	1:A:1633:SER:HB3	1.94	0.49
1:B:317:THR:HG23	1:B:321:LEU:HD12	1.94	0.49
1:B:634:GLU:OE1	1:B:1008:LYS:HE2	2.13	0.49
1:A:194:LYS:HG2	1:A:211:CYS:SG	2.52	0.49
1:A:1287:HIS:CE1	1:A:1288:TYR:CZ	3.00	0.49
1:B:1625:MET:CE	1:B:1627:ILE:HG13	2.41	0.49
1:C:420:ARG:HG3	1:C:424:LEU:O	2.11	0.49
1:D:1324:TYR:CZ	1:D:1347:GLY:HA3	2.47	0.49
1:A:417:SER:OG	1:A:427:GLY:HA2	2.12	0.49
1:A:487:ALA:HB3	1:A:584:SER:HB2	1.93	0.49
1:A:1498:LEU:O	1:A:1502:ILE:HG12	2.13	0.49
1:B:1464:GLN:O	1:B:1468:HIS:CD2	2.65	0.49
1:C:1345:SER:OG	1:C:1346:LEU:N	2.45	0.49
1:A:611:GLU:C	1:A:613:ILE:H	2.15	0.49
1:C:163:ARG:HG3	1:C:165:ILE:CD1	2.41	0.49
1:C:1115:GLY:HA2	1:C:1237:PHE:HB2	1.93	0.49
1:D:835:MET:HG2	1:D:933:TRP:HE3	1.77	0.49
1:A:1203:MET:CE	1:A:1633:SER:HB3	2.42	0.49
1:C:1498:LEU:O	1:C:1502:ILE:HG12	2.13	0.49
1:D:847:GLU:OE2	1:D:873:ARG:NH1	2.46	0.49
1:D:1537:THR:O	1:D:1541:GLU:HG2	2.12	0.49
1:D:1625:MET:CE	1:D:1627:ILE:HG13	2.43	0.49
1:A:375:VAL:CG1	1:A:401:TRP:HB3	2.42	0.49
1:A:1464:GLN:O	1:A:1468:HIS:HD2	1.95	0.49
1:D:1269:ASP:OD2	1:D:1269:ASP:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1500:CYS:HB3	1:D:1504:TYR:CZ	2.48	0.49
1:A:1184:SER:C	1:A:1185:ILE:HD13	2.33	0.49
1:B:1200:THR:OG1	1:B:1208:GLY:HA3	2.13	0.49
1:A:1345:SER:OG	1:A:1346:LEU:N	2.46	0.49
1:B:162:GLY:HA2	1:B:187:LEU:HD21	1.95	0.49
1:B:452:PHE:CD1	1:B:457:ARG:HG3	2.48	0.49
1:B:677:THR:OG1	1:B:680:GLU:HB2	2.13	0.49
1:B:869:PRO:HD2	1:B:872:THR:CG2	2.43	0.49
1:C:1468:HIS:CE1	1:D:59:ILE:HG12	2.48	0.49
1:D:1274:GLU:HA	1:D:1277:GLU:HG3	1.95	0.49
1:A:1625:MET:CE	1:A:1627:ILE:HG13	2.42	0.49
1:D:317:THR:HG23	1:D:321:LEU:HD12	1.95	0.49
1:D:1265:HIS:HE1	1:D:1322:TYR:CZ	2.31	0.49
1:A:66:LYS:O	1:A:67:GLU:HB2	2.13	0.48
1:A:1617:VAL:HG11	1:A:1639:LEU:HD22	1.95	0.48
1:B:180:VAL:HB	1:B:181:PRO:HD3	1.95	0.48
1:A:75:PRO:HB2	1:A:118:ILE:CD1	2.43	0.48
1:B:1470:THR:HB	1:B:1473:ILE:HD12	1.96	0.48
1:B:1571:MET:HG2	1:B:1601:TYR:CE2	2.48	0.48
1:C:121:THR:HG21	1:C:157:SER:OG	2.12	0.48
1:C:1553:ASN:OD1	1:C:1606:TYR:OH	2.24	0.48
1:A:536:ARG:HD3	1:A:538:VAL:HG23	1.95	0.48
1:A:1537:THR:O	1:A:1541:GLU:HG2	2.14	0.48
1:B:420:ARG:HB2	1:B:422:ASP:HB2	1.95	0.48
1:D:539:ASN:O	1:D:540:ASP:O	2.31	0.48
1:A:290:VAL:HG12	1:A:292:VAL:HG23	1.95	0.48
1:B:1103:ASP:OD2	1:B:1361:TRP:HB2	2.14	0.48
1:C:536:ARG:HD3	1:C:538:VAL:HG23	1.94	0.48
1:C:1468:HIS:O	1:D:63:LYS:HA	2.13	0.48
1:D:92:ALA:HB3	1:D:125:GLN:HA	1.94	0.48
1:D:243:PHE:CZ	1:D:435:PHE:HA	2.49	0.48
1:A:1467:ARG:NH2	1:B:112:ASP:OD2	2.47	0.48
1:C:16:HIS:ND1	1:C:24:SER:HB2	2.28	0.48
1:C:1104:SER:O	1:C:1108:ARG:HG3	2.13	0.48
1:D:1069:CYS:SG	1:D:1224:GLN:HB2	2.53	0.48
1:B:99:GLN:NE2	1:B:100:PRO:HD2	2.28	0.48
1:C:1265:HIS:HE1	1:C:1322:TYR:CZ	2.31	0.48
1:D:7:TRP:O	1:D:167:PRO:HB3	2.14	0.48
1:D:1345:SER:OG	1:D:1346:LEU:N	2.47	0.48
1:A:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48
1:A:1324:TYR:CZ	1:A:1347:GLY:HA3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:SER:C	1:B:1185:ILE:HD13	2.34	0.48
1:C:624:PHE:HD1	1:C:698:GLN:HG3	1.79	0.48
1:D:610:ILE:O	1:D:610:ILE:HG22	2.14	0.48
1:A:1115:GLY:HA2	1:A:1237:PHE:HB2	1.94	0.48
1:D:162:GLY:HA2	1:D:187:LEU:HD21	1.96	0.48
1:A:1587:LEU:HD12	1:A:1630:ALA:HB2	1.96	0.48
1:B:219:LEU:HB3	1:B:473:LEU:HD21	1.95	0.48
1:B:539:ASN:O	1:B:540:ASP:O	2.32	0.48
1:D:1149:CYS:HB2	1:D:1156:ILE:HG22	1.96	0.48
1:D:1561:ASN:ND2	1:D:1601:TYR:HB3	2.28	0.48
1:A:634:GLU:CD	1:A:1008:LYS:HE2	2.35	0.47
1:A:1269:ASP:OD2	1:A:1269:ASP:N	2.46	0.47
1:C:377:THR:HA	1:C:429:THR:CG2	2.44	0.47
1:C:1184:SER:C	1:C:1185:ILE:HD13	2.34	0.47
1:A:1545:SER:C	1:A:1546:GLU:HG3	2.34	0.47
1:C:1324:TYR:CZ	1:C:1347:GLY:HA3	2.49	0.47
1:A:420:ARG:HG3	1:A:424:LEU:O	2.13	0.47
1:A:492:HIS:NE2	1:A:501:GLN:OE1	2.41	0.47
1:A:1542:THR:HB	1:D:1541:GLU:OE1	2.14	0.47
1:B:1585:VAL:HG13	1:B:1586:PHE:HD1	1.75	0.47
1:D:919:HIS:ND1	1:D:920:PRO:HD3	2.29	0.47
1:D:1459:ASN:HD22	1:D:1460:ARG:HD2	1.80	0.47
1:C:85:LYS:HD3	1:D:1509:GLN:NE2	2.28	0.47
1:C:677:THR:OG1	1:C:680:GLU:HB2	2.14	0.47
1:D:351:LYS:O	1:D:351:LYS:HE3	2.14	0.47
1:A:1142:VAL:HA	1:A:1182:TYR:O	2.15	0.47
1:C:492:HIS:NE2	1:C:501:GLN:OE1	2.45	0.47
1:C:1587:LEU:HD12	1:C:1630:ALA:HB2	1.96	0.47
1:C:1625:MET:CE	1:C:1627:ILE:HG13	2.44	0.47
1:C:1708:TRP:CE3	1:C:1709:ILE:HD12	2.49	0.47
1:D:1103:ASP:OD2	1:D:1361:TRP:HB2	2.14	0.47
1:D:1464:GLN:O	1:D:1468:HIS:CD2	2.64	0.47
1:A:1059:LYS:HA	1:A:1059:LYS:HD2	1.75	0.47
1:B:546:ILE:N	1:B:546:ILE:HD12	2.30	0.47
1:B:1708:TRP:CE3	1:B:1709:ILE:HD12	2.48	0.47
1:C:919:HIS:ND1	1:C:920:PRO:HD3	2.29	0.47
1:D:78:VAL:HG22	1:D:120:LYS:HE3	1.96	0.47
1:D:1115:GLY:HA2	1:D:1237:PHE:HB2	1.96	0.47
1:A:862:GLU:OE1	1:A:1016:ARG:NH1	2.47	0.47
1:B:1587:LEU:HD12	1:B:1630:ALA:HB2	1.97	0.47
1:C:634:GLU:CD	1:C:1008:LYS:HE2	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1585:VAL:HG13	1:C:1586:PHE:HD1	1.75	0.47
1:D:99:GLN:NE2	1:D:100:PRO:HD2	2.29	0.47
1:D:1184:SER:C	1:D:1185:ILE:HD13	2.35	0.47
1:B:1259:GLY:HA3	1:B:1377:LEU:HD22	1.97	0.47
1:C:417:SER:OG	1:C:427:GLY:HA2	2.15	0.47
1:C:1561:ASN:ND2	1:C:1601:TYR:HB3	2.30	0.47
1:D:546:ILE:N	1:D:546:ILE:HD12	2.29	0.47
1:D:622:LYS:HB2	1:D:622:LYS:HE3	1.67	0.47
1:A:1459:ASN:HD22	1:A:1460:ARG:HD2	1.80	0.47
1:B:302:ARG:HE	1:B:302:ARG:HB3	1.47	0.47
1:B:1269:ASP:OD2	1:B:1269:ASP:N	2.47	0.47
1:A:78:VAL:HG22	1:A:120:LYS:HE3	1.96	0.46
1:A:521:LEU:HB2	1:A:546:ILE:HG12	1.97	0.46
1:A:1140:ILE:HD11	1:A:1185:ILE:HD12	1.96	0.46
1:A:1288:TYR:CD1	1:A:1289:ASN:N	2.84	0.46
1:B:14:SER:O	1:B:18:LYS:HG2	2.15	0.46
1:B:1275:TYR:HB2	1:B:1303:LYS:HG3	1.98	0.46
1:B:1713:ILE:O	1:B:1717:VAL:HG23	2.15	0.46
1:C:1:MET:HB2	1:C:2:GLU:H	1.60	0.46
1:C:61:GLN:O	1:C:66:LYS:NZ	2.40	0.46
1:A:38:ALA:HB1	1:A:39:PRO:HD3	1.97	0.46
1:A:377:THR:HA	1:A:429:THR:CG2	2.43	0.46
1:A:829:HIS:CD2	1:A:850:CYS:HB2	2.50	0.46
1:B:377:THR:HA	1:B:429:THR:CG2	2.45	0.46
1:B:518:ASN:O	1:B:538:VAL:HG23	2.15	0.46
1:B:1459:ASN:HD22	1:B:1460:ARG:HD2	1.80	0.46
1:C:38:ALA:HB1	1:C:39:PRO:HD3	1.97	0.46
1:C:750:VAL:HG22	1:C:879:ALA:HB1	1.97	0.46
1:D:1315:HIS:CD2	1:D:1317:SER:H	2.32	0.46
1:B:92:ALA:HB3	1:B:125:GLN:HA	1.96	0.46
1:D:207:LYS:NZ	1:D:238:GLU:OE2	2.46	0.46
1:B:206:CYS:HA	1:B:312:GLU:CB	2.46	0.46
1:C:1617:VAL:HG11	1:C:1639:LEU:HD22	1.96	0.46
1:D:716:ARG:HH11	1:D:716:ARG:HG3	1.81	0.46
1:B:56:GLN:O	1:B:59:ILE:HB	2.15	0.46
1:B:1537:THR:O	1:B:1541:GLU:HG2	2.16	0.46
1:D:377:THR:HA	1:D:429:THR:CG2	2.46	0.46
1:A:1469:GLN:O	1:B:64:SER:HB3	2.16	0.46
1:B:742:ARG:HD3	1:B:752:LEU:HD23	1.97	0.46
1:B:1104:SER:O	1:B:1108:ARG:HG3	2.16	0.46
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1123:LEU:HD12	1:C:1183:LEU:HD23	1.98	0.46
1:C:1625:MET:HE3	1:C:1671:PHE:HZ	1.80	0.46
1:D:600:ILE:HD11	1:D:609:TYR:CZ	2.51	0.46
1:D:1085:TYR:CD1	1:D:1086:PRO:HA	2.51	0.46
1:D:1203:MET:HE1	1:D:1633:SER:HB3	1.98	0.46
1:A:677:THR:OG1	1:A:680:GLU:HB2	2.16	0.46
1:A:869:PRO:HD2	1:A:872:THR:CG2	2.45	0.46
1:A:1504:TYR:OH	1:B:62:SER:HB2	2.15	0.46
1:B:161:VAL:HG12	1:B:187:LEU:HD22	1.98	0.46
1:B:1274:GLU:HA	1:B:1277:GLU:HG3	1.98	0.46
1:D:75:PRO:O	1:D:167:PRO:HD2	2.15	0.46
1:D:1104:SER:O	1:D:1108:ARG:HG3	2.16	0.46
1:B:125:GLN:HG2	1:B:126:PHE:CD1	2.52	0.45
1:B:624:PHE:HD1	1:B:698:GLN:HG3	1.81	0.45
1:B:1085:TYR:CD1	1:B:1086:PRO:HA	2.52	0.45
1:B:1500:CYS:HB3	1:B:1504:TYR:OH	2.15	0.45
1:D:302:ARG:HE	1:D:302:ARG:HB3	1.48	0.45
1:D:624:PHE:HD1	1:D:698:GLN:HG3	1.81	0.45
1:A:1625:MET:HE3	1:A:1671:PHE:HZ	1.82	0.45
1:B:1268:ILE:HA	1:B:1271:PHE:O	2.16	0.45
1:D:1103:ASP:HA	1:D:1361:TRP:HA	1.98	0.45
1:A:1139:VAL:O	1:A:1140:ILE:HD12	2.17	0.45
1:A:1708:TRP:CE3	1:A:1709:ILE:HD12	2.50	0.45
1:B:1115:GLY:HA2	1:B:1237:PHE:HB2	1.99	0.45
1:B:1539:TYR:CD1	1:B:1610:ARG:HG2	2.52	0.45
1:C:611:GLU:C	1:C:613:ILE:H	2.20	0.45
1:D:180:VAL:HB	1:D:181:PRO:HD3	1.99	0.45
1:B:744:ILE:H	1:B:744:ILE:HG12	1.56	0.45
1:D:420:ARG:H	1:D:420:ARG:HG2	1.36	0.45
1:D:634:GLU:CD	1:D:1008:LYS:HE2	2.37	0.45
1:A:56:GLN:O	1:A:59:ILE:HB	2.16	0.45
1:A:1085:TYR:CD1	1:A:1086:PRO:HA	2.51	0.45
1:B:829:HIS:CD2	1:B:850:CYS:HB2	2.51	0.45
1:C:1057:ALA:C	1:C:1059:LYS:H	2.20	0.45
1:A:1057:ALA:C	1:A:1059:LYS:H	2.20	0.45
1:B:1625:MET:HE3	1:B:1671:PHE:CZ	2.51	0.45
1:C:1085:TYR:CD1	1:C:1086:PRO:HA	2.52	0.45
1:C:1142:VAL:HA	1:C:1182:TYR:O	2.17	0.45
1:A:36:LYS:O	1:A:41:ASP:HB3	2.16	0.45
1:A:1468:HIS:O	1:A:1469:GLN:C	2.53	0.45
1:A:1542:THR:O	1:D:1541:GLU:CG	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:MET:HG2	1:A:1601:TYR:HE2	1.79	0.45
1:B:1140:ILE:HD11	1:B:1185:ILE:HD12	1.98	0.45
1:B:1704:GLU:O	1:B:1707:ALA:HB3	2.17	0.45
1:A:1433:TYR:CE1	1:A:1502:ILE:HD13	2.52	0.45
1:D:522:TYR:O	1:D:533:PRO:HA	2.17	0.45
1:D:546:ILE:HA	1:D:604:GLY:O	2.16	0.45
1:D:1203:MET:CE	1:D:1633:SER:HB3	2.46	0.45
1:C:66:LYS:O	1:C:67:GLU:HB2	2.16	0.45
1:A:75:PRO:O	1:A:167:PRO:HD2	2.17	0.45
1:A:1274:GLU:HA	1:A:1277:GLU:HG3	1.99	0.45
1:B:521:LEU:HD23	1:B:600:ILE:CG2	2.47	0.45
1:B:1102:MET:HE1	1:B:1292:ARG:HA	1.99	0.45
1:C:194:LYS:HG2	1:C:211:CYS:SG	2.57	0.45
1:A:1259:GLY:HA3	1:A:1377:LEU:HD22	2.00	0.44
1:B:65:ASN:O	1:B:66:LYS:C	2.54	0.44
1:B:143:VAL:CG1	1:B:461:LYS:HB3	2.46	0.44
1:B:622:LYS:HB2	1:B:622:LYS:HE3	1.63	0.44
1:A:1103:ASP:OD2	1:A:1361:TRP:HB2	2.18	0.44
1:B:433:LYS:H	1:B:433:LYS:HG2	1.62	0.44
1:C:271:ASN:OD1	1:C:420:ARG:HD2	2.16	0.44
1:C:641:LYS:HB3	1:C:641:LYS:HE3	1.58	0.44
1:A:75:PRO:HB2	1:A:118:ILE:HD11	1.99	0.44
1:A:828:ARG:NH2	1:A:866:PRO:O	2.43	0.44
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.17	0.44
1:B:1612:TYR:CD1	1:B:1632:GLY:HA2	2.52	0.44
1:D:606:PHE:CZ	1:D:610:ILE:HD11	2.52	0.44
1:D:1539:TYR:CD1	1:D:1610:ARG:HG2	2.52	0.44
1:D:1625:MET:HE3	1:D:1671:PHE:CZ	2.51	0.44
1:A:38:ALA:HB1	1:A:39:PRO:CD	2.48	0.44
1:C:66:LYS:H	1:C:66:LYS:HG3	1.55	0.44
1:C:75:PRO:O	1:C:166:VAL:HG22	2.18	0.44
1:B:1057:ALA:C	1:B:1059:LYS:H	2.20	0.44
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.57	0.44
1:B:141:PRO:HB2	1:B:146:ASP:HA	1.99	0.44
1:C:1274:GLU:HA	1:C:1277:GLU:HG3	1.99	0.44
1:C:1612:TYR:CD1	1:C:1632:GLY:HA2	2.52	0.44
1:D:75:PRO:O	1:D:166:VAL:HG22	2.17	0.44
1:A:283:LYS:HB2	1:A:283:LYS:HE2	1.67	0.44
1:B:634:GLU:CD	1:B:1008:LYS:HE2	2.38	0.44
1:C:36:LYS:O	1:C:41:ASP:HB3	2.17	0.44
1:C:556:ASP:OD2	1:C:557:ARG:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:ASP:OD2	1:C:1361:TRP:HB2	2.18	0.44
1:C:1433:TYR:CE1	1:C:1502:ILE:HD13	2.52	0.44
1:D:1710:ASN:O	1:D:1712:ASN:N	2.51	0.44
1:A:835:MET:HG2	1:A:933:TRP:CE3	2.53	0.44
1:B:75:PRO:O	1:B:167:PRO:HD2	2.17	0.44
1:B:268:GLU:OE2	1:B:270:GLU:HB2	2.18	0.44
1:B:1549:TRP:HA	1:B:1556:PHE:HB2	2.00	0.44
1:C:894:THR:HG22	1:C:895:VAL:N	2.33	0.44
1:C:1459:ASN:HD22	1:C:1460:ARG:HD2	1.81	0.44
1:D:1057:ALA:C	1:D:1059:LYS:H	2.22	0.44
1:A:375:VAL:HG13	1:A:401:TRP:HB3	1.99	0.44
1:A:556:ASP:OD2	1:A:557:ARG:HG2	2.18	0.44
1:A:1318:ASN:N	1:A:1318:ASN:HD22	2.16	0.44
1:C:38:ALA:HB1	1:C:39:PRO:CD	2.48	0.44
1:C:375:VAL:HG13	1:C:401:TRP:HB3	1.98	0.44
1:C:1215:LYS:N	1:C:1218:ASP:OD2	2.41	0.44
1:D:14:SER:O	1:D:18:LYS:HG2	2.17	0.44
1:B:546:ILE:HA	1:B:604:GLY:O	2.18	0.43
1:B:716:ARG:HG3	1:B:716:ARG:HH11	1.83	0.43
1:A:849:ASP:OD1	1:A:851:SER:OG	2.29	0.43
1:A:1468:HIS:O	1:B:62:SER:O	2.35	0.43
1:B:78:VAL:O	1:B:120:LYS:HA	2.18	0.43
1:B:661:SER:OG	1:B:663:HIS:ND1	2.51	0.43
1:B:1323:VAL:HG21	1:B:1477:SER:HB3	2.00	0.43
1:C:78:VAL:HG22	1:C:120:LYS:HE3	2.00	0.43
1:C:567:GLU:HG2	1:C:568:PRO:HA	1.99	0.43
1:C:1203:MET:HE1	1:C:1633:SER:HB3	1.99	0.43
1:C:1318:ASN:N	1:C:1318:ASN:HD22	2.16	0.43
1:D:29:GLU:O	1:D:33:LYS:HG3	2.18	0.43
1:D:862:GLU:OE1	1:D:1016:ARG:NH1	2.51	0.43
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.53	0.43
1:B:1103:ASP:HA	1:B:1361:TRP:HA	2.00	0.43
1:C:283:LYS:HE2	1:C:283:LYS:HB2	1.68	0.43
1:C:1140:ILE:HD11	1:C:1185:ILE:HD12	1.99	0.43
1:A:1104:SER:O	1:A:1108:ARG:HG3	2.18	0.43
1:B:78:VAL:HG22	1:B:120:LYS:HE3	2.00	0.43
1:B:1324:TYR:CZ	1:B:1347:GLY:HA3	2.53	0.43
1:B:1330:ASN:O	1:B:1336:PRO:HA	2.19	0.43
1:B:1571:MET:HG2	1:B:1601:TYR:HE2	1.83	0.43
1:C:521:LEU:HB2	1:C:546:ILE:HG12	2.00	0.43
1:D:834:MET:HG2	1:D:835:MET:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.43
1:B:1617:VAL:HG11	1:B:1639:LEU:HD22	2.01	0.43
1:D:988:VAL:HA	1:D:1008:LYS:O	2.18	0.43
1:D:1323:VAL:HG21	1:D:1477:SER:HB3	2.01	0.43
1:A:715:ASP:OD2	1:A:733:ARG:NH2	2.45	0.43
1:B:75:PRO:O	1:B:166:VAL:HG22	2.19	0.43
1:B:519:TYR:HB2	1:B:546:ILE:HD13	1.99	0.43
1:B:1139:VAL:O	1:B:1140:ILE:HD12	2.18	0.43
1:C:487:ALA:HB3	1:C:584:SER:HB2	1.99	0.43
1:C:1268:ILE:HA	1:C:1271:PHE:O	2.18	0.43
1:D:161:VAL:HG12	1:D:187:LEU:HD22	2.00	0.43
1:D:1059:LYS:HA	1:D:1059:LYS:HD2	1.77	0.43
1:A:1464:GLN:O	1:A:1468:HIS:CD2	2.71	0.43
1:C:1102:MET:HE1	1:C:1292:ARG:HA	2.01	0.43
1:C:1549:TRP:HA	1:C:1556:PHE:HB2	2.01	0.43
1:D:521:LEU:HD11	1:D:533:PRO:HB2	2.01	0.43
1:D:1549:TRP:HA	1:D:1556:PHE:HB2	2.01	0.43
1:A:716:ARG:HG3	1:A:716:ARG:HH11	1.84	0.43
1:C:63:LYS:O	1:C:66:LYS:NZ	2.42	0.43
1:C:1540:ARG:HH11	1:C:1540:ARG:HD2	1.66	0.43
1:D:1142:VAL:HA	1:D:1182:TYR:O	2.19	0.43
1:D:1617:VAL:HG11	1:D:1639:LEU:HD22	2.00	0.43
1:A:7:TRP:O	1:A:167:PRO:HB3	2.19	0.43
1:A:1690:LYS:HA	1:A:1690:LYS:HD3	1.82	0.43
1:B:36:LYS:HA	1:B:36:LYS:HD3	1.72	0.43
1:B:1123:LEU:HD12	1:B:1183:LEU:HD23	2.01	0.43
1:B:1523:LEU:HB3	1:B:1643:THR:HG21	2.01	0.43
1:C:840:GLY:N	1:C:888:LYS:HG3	2.33	0.43
1:C:1203:MET:CE	1:C:1633:SER:HB3	2.49	0.43
1:C:1243:PRO:HB2	1:C:1246:LEU:HG	2.01	0.43
1:D:268:GLU:OE2	1:D:270:GLU:HB2	2.18	0.43
1:D:437:ASP:OD1	1:D:437:ASP:N	2.52	0.43
1:D:1730:GLU:OE2	1:D:1730:GLU:HA	2.19	0.43
1:B:600:ILE:HD11	1:B:609:TYR:CZ	2.54	0.42
1:B:750:VAL:HG22	1:B:879:ALA:HB1	2.00	0.42
1:C:75:PRO:HB2	1:C:118:ILE:CD1	2.48	0.42
1:C:957:ILE:CG1	1:C:1023:LEU:HD22	2.49	0.42
1:C:1710:ASN:O	1:C:1712:ASN:N	2.52	0.42
1:A:567:GLU:HG2	1:A:568:PRO:HA	2.00	0.42
1:C:1274:GLU:O	1:C:1278:GLN:HG3	2.19	0.42
1:D:143:VAL:CG2	1:D:163:ARG:HG3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:HB3	1:D:557:ARG:HG2	2.01	0.42
1:D:716:ARG:HG3	1:D:716:ARG:NH1	2.34	0.42
1:D:1259:GLY:HA3	1:D:1377:LEU:HD22	2.01	0.42
1:A:66:LYS:O	1:A:67:GLU:CB	2.67	0.42
1:A:661:SER:OG	1:A:663:HIS:ND1	2.52	0.42
1:A:1323:VAL:HG21	1:A:1477:SER:HB3	2.00	0.42
1:C:661:SER:OG	1:C:663:HIS:ND1	2.51	0.42
1:C:835:MET:HG2	1:C:933:TRP:CE3	2.54	0.42
1:C:1585:VAL:HG13	1:C:1586:PHE:CE1	2.54	0.42
1:D:157:SER:HB3	1:D:169:SER:OG	2.18	0.42
1:A:1507:GLU:OE2	1:B:59:ILE:HG12	2.20	0.42
1:B:1102:MET:CE	1:B:1292:ARG:HA	2.50	0.42
1:C:15:PHE:HA	1:C:18:LYS:HE2	2.01	0.42
1:A:1103:ASP:HA	1:A:1361:TRP:HA	2.01	0.42
1:B:1304:TRP:CH2	1:B:1317:SER:HB3	2.54	0.42
1:C:716:ARG:HG3	1:C:716:ARG:HH11	1.85	0.42
1:D:66:LYS:H	1:D:66:LYS:HG3	1.59	0.42
1:D:1123:LEU:HD12	1:D:1183:LEU:HD23	2.00	0.42
1:A:81:ASN:HB3	1:A:82:ILE:HG13	2.01	0.42
1:A:744:ILE:H	1:A:744:ILE:HG12	1.55	0.42
1:A:1616:GLY:C	1:A:1642:ARG:HG3	2.40	0.42
1:B:1456:TYR:CZ	1:B:1460:ARG:HD3	2.54	0.42
1:C:180:VAL:HB	1:C:181:PRO:HD3	2.01	0.42
1:C:1346:LEU:HD13	1:C:1584:ASP:HB2	2.01	0.42
1:D:1243:PRO:HB2	1:D:1246:LEU:HG	2.02	0.42
1:D:1585:VAL:HG13	1:D:1586:PHE:HD1	1.77	0.42
1:D:1708:TRP:CE3	1:D:1709:ILE:HD12	2.50	0.42
1:A:1456:TYR:CZ	1:A:1460:ARG:HD3	2.55	0.42
1:B:420:ARG:H	1:B:420:ARG:HG2	1.31	0.42
1:B:609:TYR:CZ	1:B:613:ILE:HD11	2.55	0.42
1:B:1184:SER:O	1:B:1185:ILE:HD13	2.20	0.42
1:B:1585:VAL:HG13	1:B:1586:PHE:CE1	2.55	0.42
1:D:1433:TYR:CE1	1:D:1502:ILE:HD13	2.55	0.42
1:B:936:ARG:HE	1:B:936:ARG:HB3	1.64	0.42
1:A:15:PHE:CZ	1:A:27:LEU:HD22	2.55	0.42
1:A:297:LEU:HD22	1:A:404:PHE:CD1	2.55	0.42
1:A:709:GLU:HG3	1:A:914:ARG:HD3	2.02	0.42
1:A:968:LYS:HA	1:A:968:LYS:HD2	1.87	0.42
1:B:1138:THR:OG1	1:B:1139:VAL:N	2.52	0.42
1:B:1142:VAL:HA	1:B:1182:TYR:O	2.20	0.42
1:C:1456:TYR:CZ	1:C:1460:ARG:HD3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:LYS:HA	1:D:623:PRO:HD2	1.80	0.42
1:A:224:ILE:O	1:A:228:VAL:HG23	2.20	0.42
1:A:868:LEU:HA	1:A:869:PRO:HD3	1.89	0.42
1:B:860:ILE:HG23	1:B:957:ILE:CD1	2.50	0.42
1:C:724:PHE:CE2	1:C:726:GLY:HA3	2.55	0.42
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.86	0.42
1:D:1268:ILE:HA	1:D:1271:PHE:O	2.19	0.42
1:B:207:LYS:NZ	1:B:238:GLU:OE2	2.47	0.41
1:B:420:ARG:HG2	1:B:424:LEU:O	2.20	0.41
1:B:863:THR:HG23	1:B:925:VAL:HG11	2.01	0.41
1:C:1730:GLU:HA	1:C:1730:GLU:OE2	2.20	0.41
1:D:265:TRP:CG	1:D:272:PRO:HG3	2.54	0.41
1:D:1184:SER:O	1:D:1185:ILE:HD13	2.19	0.41
1:D:1456:TYR:CZ	1:D:1460:ARG:HD3	2.55	0.41
1:A:1191:VAL:HG22	1:A:1192:PRO:HD2	2.01	0.41
1:A:1625:MET:HE3	1:A:1671:PHE:CZ	2.55	0.41
1:B:1314:LEU:HD23	1:B:1314:LEU:HA	1.88	0.41
1:C:862:GLU:OE1	1:C:1016:ARG:NH1	2.53	0.41
1:D:1654:ASP:HB3	1:D:1691:PHE:O	2.20	0.41
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.67	0.41
1:A:1102:MET:CE	1:A:1292:ARG:HA	2.50	0.41
1:D:194:LYS:HG2	1:D:211:CYS:SG	2.60	0.41
1:D:420:ARG:C	1:D:422:ASP:N	2.73	0.41
1:A:1539:TYR:CD1	1:A:1610:ARG:HG2	2.55	0.41
1:A:1549:TRP:HA	1:A:1556:PHE:HB2	2.02	0.41
1:A:1612:TYR:CD1	1:A:1632:GLY:HA2	2.55	0.41
1:B:243:PHE:CZ	1:B:435:PHE:HA	2.55	0.41
1:B:835:MET:HG2	1:B:933:TRP:HE3	1.85	0.41
1:C:533:PRO:HD3	1:C:606:PHE:CZ	2.55	0.41
1:C:1523:LEU:HB3	1:C:1643:THR:HG21	2.03	0.41
1:C:1616:GLY:C	1:C:1642:ARG:HG3	2.40	0.41
1:C:1625:MET:HE3	1:C:1671:PHE:CZ	2.55	0.41
1:D:78:VAL:O	1:D:120:LYS:HA	2.21	0.41
1:A:180:VAL:HB	1:A:181:PRO:HD3	2.03	0.41
1:A:860:ILE:HG23	1:A:957:ILE:CD1	2.51	0.41
1:A:1268:ILE:HA	1:A:1271:PHE:O	2.19	0.41
1:B:183:ALA:HB2	1:B:377:THR:HG21	2.03	0.41
1:B:1433:TYR:CE1	1:B:1502:ILE:HD13	2.56	0.41
1:D:51:GLU:H	1:D:51:GLU:CD	2.24	0.41
1:A:79:LYS:C	1:A:81:ASN:H	2.24	0.41
1:B:600:ILE:O	1:B:600:ILE:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:GLY:N	1:B:888:LYS:HG3	2.36	0.41
1:B:1523:LEU:HB3	1:B:1643:THR:CG2	2.50	0.41
1:C:15:PHE:HE2	1:C:24:SER:HA	1.85	0.41
1:C:270:GLU:HB3	1:C:420:ARG:HB3	2.03	0.41
1:C:1500:CYS:HB3	1:C:1504:TYR:CZ	2.55	0.41
1:D:206:CYS:HA	1:D:312:GLU:CB	2.50	0.41
1:D:1618:VAL:HG13	1:D:1625:MET:HE2	2.02	0.41
1:A:14:SER:O	1:A:18:LYS:HG3	2.21	0.41
1:A:1151:LEU:HB3	1:A:1156:ILE:HD13	2.02	0.41
1:A:1288:TYR:CD2	1:D:1540:ARG:NH1	2.88	0.41
1:A:1556:PHE:CZ	1:A:1604:THR:HG22	2.55	0.41
1:B:383:LYS:HB2	1:B:386:GLU:OE1	2.20	0.41
1:B:606:PHE:CZ	1:B:610:ILE:HD11	2.56	0.41
1:B:1556:PHE:CZ	1:B:1604:THR:HG22	2.56	0.41
1:C:1103:ASP:HA	1:C:1361:TRP:HA	2.02	0.41
1:C:1459:ASN:HD21	1:C:1460:ARG:NH1	2.03	0.41
1:D:840:GLY:N	1:D:888:LYS:HG3	2.36	0.41
1:D:1612:TYR:CD1	1:D:1632:GLY:HA2	2.56	0.41
1:A:16:HIS:ND1	1:A:24:SER:HB2	2.36	0.41
1:A:635:ILE:HD12	1:A:635:ILE:HA	1.88	0.41
1:B:1466:GLU:O	1:B:1469:GLN:N	2.52	0.41
1:D:1152:ASN:O	1:D:1153:ASP:HB2	2.20	0.41
1:D:1304:TRP:CG	1:D:1316:PRO:HB2	2.56	0.41
1:A:1274:GLU:O	1:A:1278:GLN:HG3	2.20	0.41
1:A:1314:LEU:HD23	1:A:1314:LEU:HA	1.88	0.41
1:B:51:GLU:CD	1:B:51:GLU:H	2.24	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.89	0.41
1:B:868:LEU:HA	1:B:869:PRO:HD3	1.90	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.90	0.41
1:C:81:ASN:HB3	1:C:82:ILE:HG13	2.02	0.41
1:C:143:VAL:HG13	1:C:461:LYS:HB3	2.02	0.41
1:C:296:PRO:HG2	1:C:366:LEU:HD22	2.03	0.41
1:C:1184:SER:O	1:C:1185:ILE:HD13	2.20	0.41
1:C:1323:VAL:HG21	1:C:1477:SER:HB3	2.02	0.41
1:C:1539:TYR:CD1	1:C:1610:ARG:HG2	2.56	0.41
1:D:516:SER:O	1:D:518:ASN:N	2.52	0.41
1:D:701:ILE:HA	1:D:702:PRO:HD3	1.92	0.41
1:D:750:VAL:HG22	1:D:879:ALA:HB1	2.02	0.41
1:D:753:VAL:HA	1:D:754:PRO:HD3	1.95	0.41
1:D:968:LYS:HA	1:D:968:LYS:HD2	1.90	0.41
1:B:751:PRO:O	1:B:907:TYR:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1468:HIS:O	1:B:1469:GLN:HB2	2.20	0.41
1:B:1561:ASN:HD21	1:B:1601:TYR:HB3	1.86	0.41
1:C:81:ASN:O	1:C:203:VAL:HG13	2.21	0.41
1:C:85:LYS:HD3	1:D:1509:GLN:HE22	1.85	0.41
1:C:860:ILE:HG23	1:C:957:ILE:CD1	2.50	0.41
1:C:1269:ASP:OD2	1:C:1269:ASP:N	2.47	0.41
1:D:851:SER:O	1:D:1058:THR:HA	2.21	0.41
1:D:1139:VAL:O	1:D:1140:ILE:HD12	2.20	0.41
1:A:1:MET:HB2	1:A:2:GLU:H	1.59	0.40
1:A:1469:GLN:CB	1:B:64:SER:H	2.34	0.40
1:C:90:THR:HG22	1:C:92:ALA:N	2.32	0.40
1:C:524:LEU:HB2	1:C:532:LYS:O	2.20	0.40
1:C:737:LEU:HB2	1:C:740:SER:OG	2.21	0.40
1:C:1524:PRO:O	1:C:1643:THR:HG23	2.22	0.40
1:D:1138:THR:OG1	1:D:1139:VAL:N	2.54	0.40
1:A:78:VAL:HG23	1:A:82:ILE:HB	2.02	0.40
1:A:1194:TYR:CE2	1:A:1206:MET:HG2	2.56	0.40
1:B:724:PHE:CE2	1:B:726:GLY:HA3	2.56	0.40
1:B:1151:LEU:HB3	1:B:1156:ILE:HD13	2.04	0.40
1:C:894:THR:O	1:C:911:VAL:HG13	2.21	0.40
1:C:1151:LEU:HB3	1:C:1156:ILE:HD13	2.02	0.40
1:D:1523:LEU:HB3	1:D:1643:THR:HG21	2.03	0.40
1:A:1006:LEU:HD23	1:A:1006:LEU:HA	1.96	0.40
1:A:1085:TYR:CE2	1:A:1108:ARG:HD3	2.56	0.40
1:A:1730:GLU:HA	1:A:1730:GLU:OE2	2.21	0.40
1:B:1191:VAL:HG22	1:B:1192:PRO:HD2	2.04	0.40
1:C:75:PRO:O	1:C:167:PRO:HD2	2.21	0.40
1:C:375:VAL:HG13	1:C:376:PRO:O	2.21	0.40
1:D:1085:TYR:CE2	1:D:1108:ARG:HD3	2.56	0.40
1:D:1302:PRO:HG3	1:D:1331:PHE:CE2	2.56	0.40
1:D:1391:LYS:HA	1:D:1391:LYS:HD2	1.93	0.40
1:D:1459:ASN:HD21	1:D:1460:ARG:NH1	2.04	0.40
1:A:925:VAL:HG23	1:A:926:THR:HG23	2.04	0.40
1:B:1730:GLU:OE2	1:B:1730:GLU:HA	2.20	0.40
1:C:36:LYS:HD3	1:C:40:GLU:CD	2.42	0.40
1:C:622:LYS:HB2	1:C:622:LYS:HE3	1.71	0.40
1:B:157:SER:HB3	1:B:169:SER:OG	2.21	0.40
1:B:519:TYR:CB	1:B:546:ILE:HD13	2.52	0.40
1:B:1151:LEU:HD11	1:B:1168:ASP:HB3	2.04	0.40
1:C:1059:LYS:HA	1:C:1059:LYS:HD2	1.75	0.40
1:D:860:ILE:HG23	1:D:957:ILE:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1468:HIS:O	1:D:1469:GLN:C	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:TYR:OH	1:C:1541:GLU:OE2[2_455]	1.97	0.23

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	1654/1829 (90%)	1540 (93%)	101 (6%)	13 (1%)	19	60
1	B	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22	63
1	C	1654/1829 (90%)	1539 (93%)	102 (6%)	13 (1%)	19	60
1	D	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22	63
All	All	6612/7316 (90%)	6167 (93%)	397 (6%)	48 (1%)	22	63

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	1166	ARG
1	A	1711	GLU
1	B	1166	ARG
1	C	38	ALA
1	C	1166	ARG
1	C	1711	GLU
1	D	1166	ARG
1	D	1711	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	CYS
1	A	479	ASP
1	A	1438	ASP
1	B	206	CYS
1	B	479	ASP
1	B	540	ASP
1	B	1438	ASP
1	C	206	CYS
1	C	479	ASP
1	C	1438	ASP
1	D	206	CYS
1	D	479	ASP
1	D	540	ASP
1	D	1438	ASP
1	A	891	CYS
1	B	104	SER
1	B	891	CYS
1	C	891	CYS
1	D	104	SER
1	D	891	CYS
1	A	104	SER
1	A	517	ASN
1	A	612	HIS
1	C	104	SER
1	C	517	ASN
1	C	612	HIS
1	A	1003	ASP
1	A	1058	THR
1	B	65	ASN
1	B	1003	ASP
1	C	1003	ASP
1	C	1058	THR
1	D	1003	ASP
1	D	1058	THR
1	B	1058	THR
1	A	37	PRO
1	C	37	PRO
1	B	37	PRO
1	D	37	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	1413/1547 (91%)	1275 (90%)	138 (10%)	8 27
1	B	1411/1547 (91%)	1264 (90%)	147 (10%)	7 25
1	C	1413/1547 (91%)	1274 (90%)	139 (10%)	8 27
1	D	1411/1547 (91%)	1263 (90%)	148 (10%)	7 24
All	All	5648/6188 (91%)	5076 (90%)	572 (10%)	7 25

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	4	THR
1	A	18	LYS
1	A	60	LEU
1	A	62	SER
1	A	66	LYS
1	A	67	GLU
1	A	78	VAL
1	A	90	THR
1	A	95	SER
1	A	106	VAL
1	A	116	VAL
1	A	121	THR
1	A	143	VAL
1	A	149	VAL
1	A	160	VAL
1	A	165	ILE
1	A	166	VAL
1	A	170	LEU
1	A	194	LYS
1	A	202	VAL
1	A	219	LEU
1	A	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	ARG
1	A	243	PHE
1	A	269	THR
1	A	283	LYS
1	A	305	TYR
1	A	310	VAL
1	A	323	THR
1	A	343	LYS
1	A	356	ARG
1	A	368	LYS
1	A	375	VAL
1	A	385	GLU
1	A	393	LEU
1	A	415	VAL
1	A	420	ARG
1	A	429	THR
1	A	434	LYS
1	A	437	ASP
1	A	445	LYS
1	A	463	VAL
1	A	540	ASP
1	A	547	GLN
1	A	582	VAL
1	A	593	THR
1	A	600	ILE
1	A	631	ASN
1	A	634	GLU
1	A	638	ARG
1	A	659	LYS
1	A	662	GLN
1	A	676	ARG
1	A	680	GLU
1	A	689	ILE
1	A	698	GLN
1	A	716	ARG
1	A	719	GLN
1	A	730	ASP
1	A	734	LYS
1	A	735	LEU
1	A	737	LEU
1	A	738	LYS
1	A	739	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	743	GLU
1	A	744	ILE
1	A	746	GLU
1	A	752	LEU
1	A	834	MET
1	A	841	LYS
1	A	859	VAL
1	A	860	ILE
1	A	872	THR
1	A	875	LYS
1	A	888	LYS
1	A	944	ASP
1	A	951	GLU
1	A	952	VAL
1	A	957	ILE
1	A	978	THR
1	A	979	SER
1	A	988	VAL
1	A	999	SER
1	A	1011	VAL
1	A	1015	ASP
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1047	SER
1	A	1055	LYS
1	A	1067	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP
1	A	1131	LYS
1	A	1147	VAL
1	A	1150	THR
1	A	1171	SER
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1321	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1326	LEU
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
1	A	1388	SER
1	A	1393	ILE
1	A	1396	PHE
1	A	1402	LEU
1	A	1408	LYS
1	A	1426	ASP
1	A	1428	SER
1	A	1430	LYS
1	A	1440	TYR
1	A	1459	ASN
1	A	1460	ARG
1	A	1478	GLN
1	A	1516	VAL
1	A	1562	ASP
1	A	1565	ARG
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1643	THR
1	A	1662	LEU
1	A	1675	THR
1	A	1695	VAL
1	A	1697	GLU
1	A	1721	GLU
1	A	1726	GLU
1	A	1736	GLN
1	B	4	THR
1	B	23	LYS
1	B	25	LEU
1	B	27	LEU
1	B	31	LEU
1	B	66	LYS
1	B	78	VAL
1	B	81	ASN
1	B	90	THR
1	B	95	SER
1	B	106	VAL
1	B	116	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	118	ILE
1	B	121	THR
1	B	160	VAL
1	B	166	VAL
1	B	170	LEU
1	B	184	LEU
1	B	191	LYS
1	B	194	LYS
1	B	202	VAL
1	B	217	LEU
1	B	219	LEU
1	B	220	SER
1	B	241	ARG
1	B	243	PHE
1	B	277	LYS
1	B	302	ARG
1	B	305	TYR
1	B	313	ARG
1	B	317	THR
1	B	345	ASP
1	B	351	LYS
1	B	368	LYS
1	B	369	ASP
1	B	375	VAL
1	B	393	LEU
1	B	420	ARG
1	B	428	ILE
1	B	429	THR
1	B	433	LYS
1	B	437	ASP
1	B	445	LYS
1	B	463	VAL
1	B	468	THR
1	B	517	ASN
1	B	518	ASN
1	B	526	LYS
1	B	536	ARG
1	B	537	ARG
1	B	538	VAL
1	B	542	THR
1	B	582	VAL
1	B	584	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	589	GLU
1	B	593	THR
1	B	600	ILE
1	B	631	ASN
1	B	634	GLU
1	B	638	ARG
1	B	659	LYS
1	B	662	GLN
1	B	676	ARG
1	B	680	GLU
1	B	689	ILE
1	B	698	GLN
1	B	716	ARG
1	B	719	GLN
1	B	730	ASP
1	B	734	LYS
1	B	735	LEU
1	B	737	LEU
1	B	738	LYS
1	B	739	HIS
1	B	743	GLU
1	B	744	ILE
1	B	746	GLU
1	B	752	LEU
1	B	834	MET
1	B	841	LYS
1	B	859	VAL
1	B	860	ILE
1	B	872	THR
1	B	875	LYS
1	B	888	LYS
1	B	944	ASP
1	B	951	GLU
1	B	952	VAL
1	B	957	ILE
1	B	978	THR
1	B	979	SER
1	B	988	VAL
1	B	999	SER
1	B	1011	VAL
1	B	1015	ASP
1	B	1016	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1042	LEU
1	B	1044	SER
1	B	1047	SER
1	B	1055	LYS
1	B	1067	LYS
1	B	1074	LEU
1	B	1079	ASN
1	B	1103	ASP
1	B	1131	LYS
1	B	1147	VAL
1	B	1150	THR
1	B	1171	SER
1	B	1172	VAL
1	B	1191	VAL
1	B	1216	LEU
1	B	1224	GLN
1	B	1227	LEU
1	B	1252	THR
1	B	1303	LYS
1	B	1311	GLU
1	B	1321	ASP
1	B	1326	LEU
1	B	1345	SER
1	B	1346	LEU
1	B	1375	VAL
1	B	1388	SER
1	B	1393	ILE
1	B	1396	PHE
1	B	1402	LEU
1	B	1408	LYS
1	B	1426	ASP
1	B	1428	SER
1	B	1430	LYS
1	B	1440	TYR
1	B	1459	ASN
1	B	1460	ARG
1	B	1478	GLN
1	B	1516	VAL
1	B	1562	ASP
1	B	1565	ARG
1	B	1571	MET
1	B	1585	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1625	MET
1	B	1643	THR
1	B	1662	LEU
1	B	1675	THR
1	B	1695	VAL
1	B	1697	GLU
1	B	1721	GLU
1	B	1726	GLU
1	B	1736	GLN
1	C	1	MET
1	C	2	GLU
1	C	4	THR
1	C	18	LYS
1	C	60	LEU
1	C	62	SER
1	C	66	LYS
1	C	67	GLU
1	C	78	VAL
1	C	90	THR
1	C	95	SER
1	C	106	VAL
1	C	116	VAL
1	C	121	THR
1	C	123	LEU
1	C	143	VAL
1	C	160	VAL
1	C	165	ILE
1	C	166	VAL
1	C	170	LEU
1	C	194	LYS
1	C	202	VAL
1	C	219	LEU
1	C	231	LYS
1	C	241	ARG
1	C	243	PHE
1	C	269	THR
1	C	283	LYS
1	C	305	TYR
1	C	310	VAL
1	C	323	THR
1	C	343	LYS
1	C	356	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	368	LYS
1	C	375	VAL
1	C	385	GLU
1	C	393	LEU
1	C	415	VAL
1	C	420	ARG
1	C	429	THR
1	C	434	LYS
1	C	437	ASP
1	C	445	LYS
1	C	463	VAL
1	C	466	ARG
1	C	540	ASP
1	C	547	GLN
1	C	582	VAL
1	C	593	THR
1	C	600	ILE
1	C	631	ASN
1	C	634	GLU
1	C	638	ARG
1	C	659	LYS
1	C	662	GLN
1	C	676	ARG
1	C	680	GLU
1	C	689	ILE
1	C	698	GLN
1	C	716	ARG
1	C	719	GLN
1	C	730	ASP
1	C	734	LYS
1	C	735	LEU
1	C	737	LEU
1	C	738	LYS
1	C	739	HIS
1	C	743	GLU
1	C	744	ILE
1	C	746	GLU
1	C	752	LEU
1	C	834	MET
1	C	841	LYS
1	C	859	VAL
1	C	860	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	872	THR
1	C	875	LYS
1	C	888	LYS
1	C	944	ASP
1	C	951	GLU
1	C	952	VAL
1	C	957	ILE
1	C	978	THR
1	C	979	SER
1	C	988	VAL
1	C	999	SER
1	C	1011	VAL
1	C	1015	ASP
1	C	1016	ARG
1	C	1042	LEU
1	C	1044	SER
1	C	1047	SER
1	C	1055	LYS
1	C	1067	LYS
1	C	1074	LEU
1	C	1079	ASN
1	C	1103	ASP
1	C	1131	LYS
1	C	1147	VAL
1	C	1150	THR
1	C	1171	SER
1	C	1172	VAL
1	C	1191	VAL
1	C	1216	LEU
1	C	1224	GLN
1	C	1227	LEU
1	C	1252	THR
1	C	1311	GLU
1	C	1321	ASP
1	C	1326	LEU
1	C	1345	SER
1	C	1346	LEU
1	C	1375	VAL
1	C	1388	SER
1	C	1393	ILE
1	C	1396	PHE
1	C	1402	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1408	LYS
1	C	1426	ASP
1	C	1428	SER
1	C	1430	LYS
1	C	1440	TYR
1	C	1459	ASN
1	C	1460	ARG
1	C	1478	GLN
1	C	1516	VAL
1	C	1562	ASP
1	C	1565	ARG
1	C	1571	MET
1	C	1585	VAL
1	C	1625	MET
1	C	1643	THR
1	C	1662	LEU
1	C	1675	THR
1	C	1695	VAL
1	C	1697	GLU
1	C	1721	GLU
1	C	1726	GLU
1	C	1736	GLN
1	D	4	THR
1	D	23	LYS
1	D	25	LEU
1	D	27	LEU
1	D	31	LEU
1	D	66	LYS
1	D	78	VAL
1	D	81	ASN
1	D	90	THR
1	D	95	SER
1	D	106	VAL
1	D	116	VAL
1	D	118	ILE
1	D	121	THR
1	D	143	VAL
1	D	160	VAL
1	D	166	VAL
1	D	170	LEU
1	D	184	LEU
1	D	191	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	194	LYS
1	D	202	VAL
1	D	217	LEU
1	D	219	LEU
1	D	220	SER
1	D	241	ARG
1	D	243	PHE
1	D	277	LYS
1	D	302	ARG
1	D	305	TYR
1	D	313	ARG
1	D	317	THR
1	D	345	ASP
1	D	351	LYS
1	D	368	LYS
1	D	369	ASP
1	D	375	VAL
1	D	393	LEU
1	D	420	ARG
1	D	428	ILE
1	D	429	THR
1	D	433	LYS
1	D	437	ASP
1	D	445	LYS
1	D	458	THR
1	D	463	VAL
1	D	468	THR
1	D	517	ASN
1	D	518	ASN
1	D	526	LYS
1	D	536	ARG
1	D	537	ARG
1	D	538	VAL
1	D	542	THR
1	D	582	VAL
1	D	584	SER
1	D	589	GLU
1	D	593	THR
1	D	600	ILE
1	D	631	ASN
1	D	634	GLU
1	D	638	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	659	LYS
1	D	662	GLN
1	D	676	ARG
1	D	680	GLU
1	D	689	ILE
1	D	698	GLN
1	D	716	ARG
1	D	719	GLN
1	D	730	ASP
1	D	734	LYS
1	D	735	LEU
1	D	737	LEU
1	D	738	LYS
1	D	739	HIS
1	D	743	GLU
1	D	744	ILE
1	D	746	GLU
1	D	752	LEU
1	D	834	MET
1	D	841	LYS
1	D	859	VAL
1	D	860	ILE
1	D	872	THR
1	D	875	LYS
1	D	888	LYS
1	D	944	ASP
1	D	951	GLU
1	D	952	VAL
1	D	957	ILE
1	D	978	THR
1	D	979	SER
1	D	988	VAL
1	D	999	SER
1	D	1011	VAL
1	D	1015	ASP
1	D	1016	ARG
1	D	1042	LEU
1	D	1044	SER
1	D	1047	SER
1	D	1055	LYS
1	D	1067	LYS
1	D	1074	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1079	ASN
1	D	1103	ASP
1	D	1131	LYS
1	D	1147	VAL
1	D	1150	THR
1	D	1171	SER
1	D	1172	VAL
1	D	1191	VAL
1	D	1216	LEU
1	D	1224	GLN
1	D	1227	LEU
1	D	1252	THR
1	D	1311	GLU
1	D	1321	ASP
1	D	1326	LEU
1	D	1345	SER
1	D	1346	LEU
1	D	1375	VAL
1	D	1388	SER
1	D	1393	ILE
1	D	1396	PHE
1	D	1402	LEU
1	D	1408	LYS
1	D	1426	ASP
1	D	1428	SER
1	D	1430	LYS
1	D	1440	TYR
1	D	1459	ASN
1	D	1460	ARG
1	D	1478	GLN
1	D	1516	VAL
1	D	1562	ASP
1	D	1565	ARG
1	D	1571	MET
1	D	1585	VAL
1	D	1625	MET
1	D	1643	THR
1	D	1662	LEU
1	D	1675	THR
1	D	1695	VAL
1	D	1697	GLU
1	D	1721	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1726	GLU
1	D	1736	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	81	ASN
1	A	186	ASN
1	A	829	HIS
1	A	1459	ASN
1	B	99	GLN
1	B	186	ASN
1	B	539	ASN
1	B	829	HIS
1	B	1315	HIS
1	B	1318	ASN
1	B	1459	ASN
1	C	55	HIS
1	C	58	ASN
1	C	65	ASN
1	C	81	ASN
1	C	186	ASN
1	C	829	HIS
1	C	1459	ASN
1	C	1468	HIS
1	C	1509	GLN
1	D	99	GLN
1	D	186	ASN
1	D	539	ASN
1	D	829	HIS
1	D	1315	HIS
1	D	1318	ASN
1	D	1459	ASN
1	D	1468	HIS
1	D	1509	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.