Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BLB
Title	:	CLOSE PACKING OF AN OLIGOMERIC EYE LENS BETA-CRYSTALLIN INDUCES LOSS OF SYMMETRY AND ORDERING OF SEQUENCE EXTENSIONS
Authors	:	Nalini, V.; Bax, B.; Driessen, H.; Moss, D.S.; Lindley, P.F.; Slingsby, C.
Deposited on	:	1993-12-22
Resolution	:	3.30 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 (i)) were used in the production of this report:

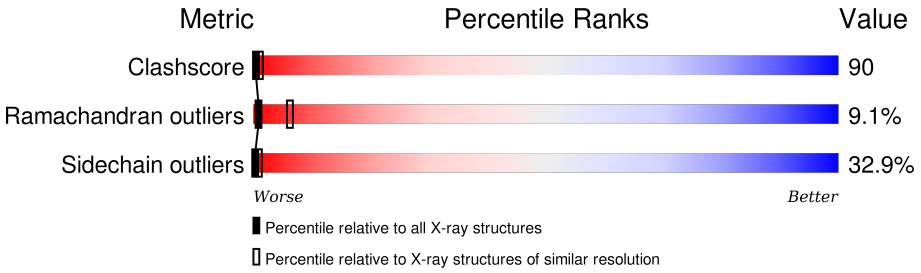
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	204	8% 43% 32% 7% 9%
1	B	204	15% 36% 29% 9% 11%
1	C	204	13% 47% 25% 7% 8%
1	D	204	16% 40% 23% 11% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5941 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 BETA B2-CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1492	942	261	285	4			
1	B	181	Total	C	N	O	S	0	0	0
			1464	924	256	280	4			
1	C	187	Total	C	N	O	S	0	0	0
			1505	950	264	287	4			
1	D	183	Total	C	N	O	S	0	0	0
			1480	934	259	283	4			

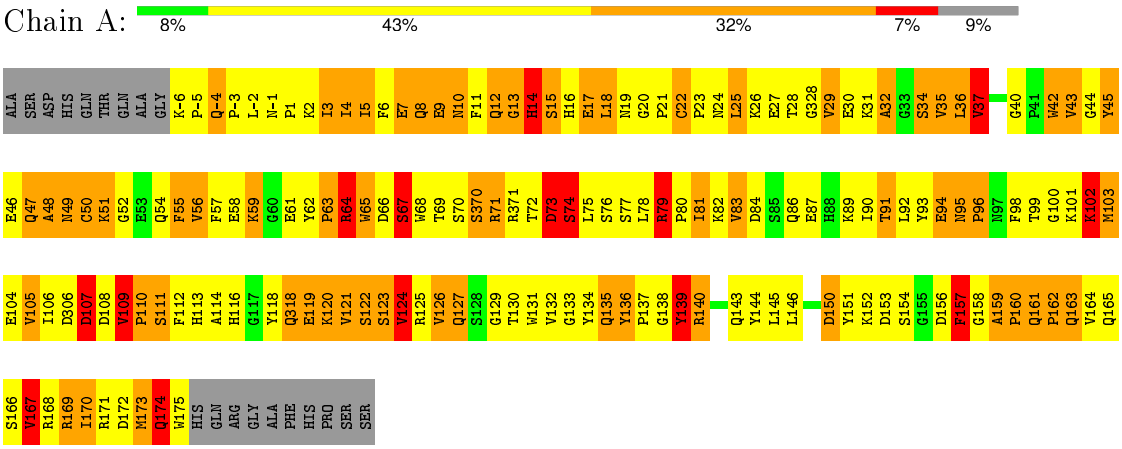
3 Residue-property plots (i)

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.

Note EDS was not executed.

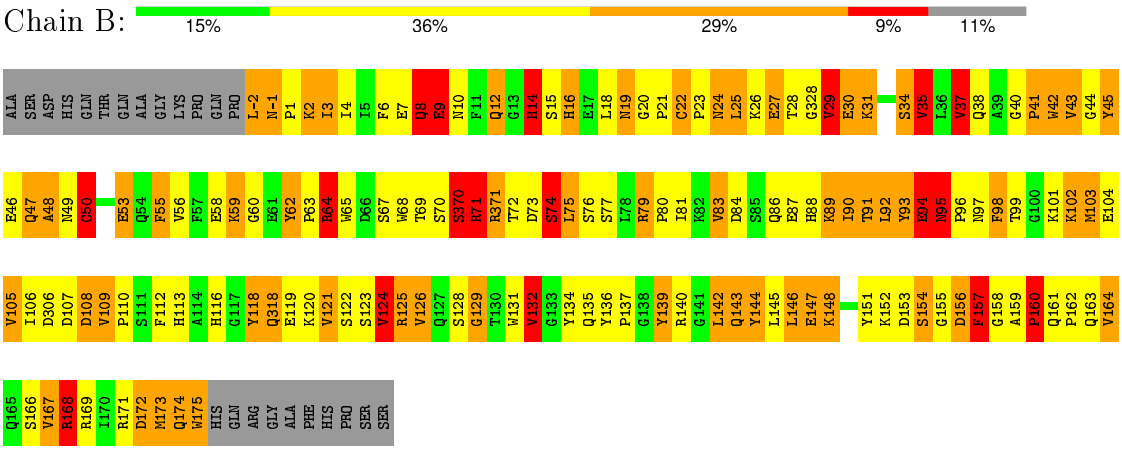
- Molecule 1: BETA B2-CRYSTALLIN

Chain A:



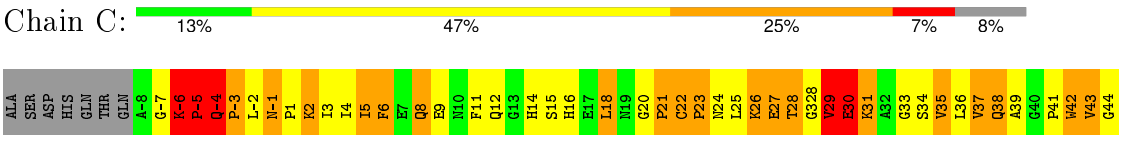
- Molecule 1: BETA B2-CRYSTALLIN

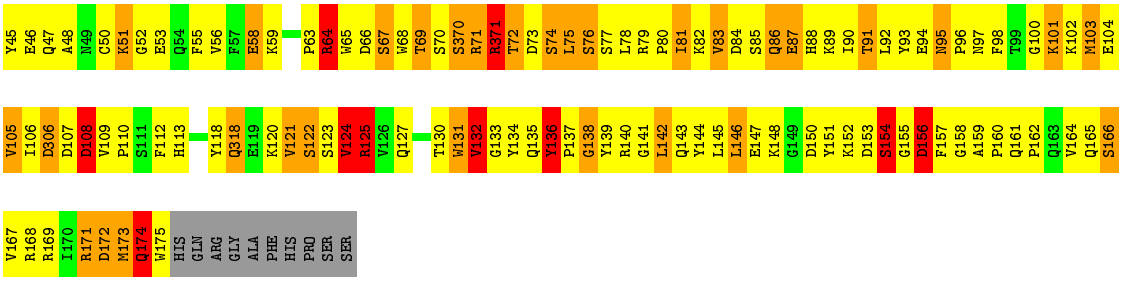
Chain B:



- Molecule 1: BETA B2-CRYSTALLIN

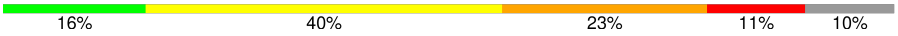
Chain C:

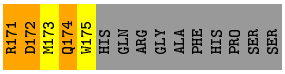




- Molecule 1: BETA B2-CRYSTALLIN

Chain D:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.71Å 165.90Å 78.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

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	1.31	6/1535 (0.4%)	1.83	34/2080 (1.6%)
1	B	1.30	6/1505 (0.4%)	1.77	38/2037 (1.9%)
1	C	1.28	6/1548 (0.4%)	1.80	29/2096 (1.4%)
1	D	1.30	7/1522 (0.5%)	1.80	39/2061 (1.9%)
All	All	1.30	25/6110 (0.4%)	1.80	140/8274 (1.7%)

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	2	5
1	B	1	7
1	C	3	5
1	D	5	7
All	All	11	24

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	GLN	CD-OE1	5.69	1.36	1.24
1	B	12	GLN	CD-OE1	5.58	1.36	1.24
1	D	42	TRP	NE1-CE2	-5.51	1.30	1.37
1	B	131	TRP	NE1-CE2	-5.49	1.30	1.37
1	B	74	SER	N-CA	5.48	1.57	1.46
1	A	318	GLN	CD-OE1	5.47	1.35	1.24
1	A	42	TRP	NE1-CE2	-5.43	1.30	1.37
1	C	318	GLN	CD-OE1	5.38	1.35	1.24
1	A	8	GLN	CD-OE1	5.35	1.35	1.24
1	C	131	TRP	NE1-CE2	-5.34	1.30	1.37
1	C	30	GLU	N-CA	5.33	1.57	1.46
1	B	86	GLN	CA-CB	-5.32	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	68	TRP	NE1-CE2	-5.26	1.30	1.37
1	D	163	GLN	CD-OE1	5.26	1.35	1.24
1	D	127	GLN	CD-OE1	5.23	1.35	1.24
1	A	15	SER	CA-CB	5.22	1.60	1.52
1	D	-4	GLN	CD-OE1	5.19	1.35	1.24
1	D	131	TRP	NE1-CE2	-5.18	1.30	1.37
1	A	12	GLN	CD-OE1	5.18	1.35	1.24
1	B	42	TRP	NE1-CE2	-5.15	1.30	1.37
1	C	-4	GLN	CD-OE1	5.13	1.35	1.24
1	A	161	GLN	CD-OE1	5.11	1.35	1.24
1	C	68	TRP	NE1-CE2	-5.08	1.30	1.37
1	D	95	ASN	CG-OD1	5.03	1.35	1.24
1	C	42	TRP	NE1-CE2	-5.02	1.31	1.37

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	GLY	C-N-CA	16.12	162.01	121.70
1	C	132	VAL	CA-CB-CG2	11.88	128.71	110.90
1	A	167	VAL	CA-CB-CG1	11.19	127.68	110.90
1	C	167	VAL	CA-CB-CG2	11.00	127.40	110.90
1	D	109	VAL	CA-CB-CG2	10.44	126.57	110.90
1	B	121	VAL	CA-CB-CG2	10.34	126.41	110.90
1	C	109	VAL	C-N-CD	-9.98	98.65	120.60
1	D	371	ARG	C-N-CA	9.01	144.22	121.70
1	C	371	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	C	103	MET	CG-SD-CE	8.72	114.15	100.20
1	B	157	PHE	C-N-CA	8.70	140.58	122.30
1	C	37	VAL	CA-CB-CG2	8.53	123.69	110.90
1	D	37	VAL	CA-CB-CG2	8.36	123.44	110.90
1	B	105	VAL	CA-CB-CG2	8.34	123.42	110.90
1	A	35	VAL	CA-CB-CG2	8.22	123.23	110.90
1	B	35	VAL	CA-CB-CG2	8.22	123.23	110.90
1	D	80	PRO	N-CA-CB	-8.22	93.44	103.30
1	A	109	VAL	CA-CB-CG2	8.18	123.17	110.90
1	C	105	VAL	CA-CB-CG2	7.99	122.89	110.90
1	C	136	TYR	C-N-CD	-7.93	103.14	120.60
1	C	121	VAL	CA-CB-CG2	7.92	122.78	110.90
1	A	140	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	D	105	VAL	CA-CB-CG2	7.80	122.59	110.90
1	B	172	ASP	C-N-CA	7.71	140.98	121.70
1	C	328	GLY	C-N-CA	7.53	140.52	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	103	MET	CG-SD-CE	7.52	112.23	100.20
1	C	43	VAL	CA-CB-CG2	7.51	122.16	110.90
1	C	35	VAL	CA-CB-CG2	7.50	122.14	110.90
1	B	124	VAL	CA-CB-CG2	7.43	122.05	110.90
1	B	126	VAL	CA-CB-CG2	7.34	121.91	110.90
1	B	144	TYR	CB-CG-CD2	-7.28	116.64	121.00
1	B	109	VAL	CA-CB-CG2	7.27	121.81	110.90
1	B	22	CYS	C-N-CD	-7.26	104.63	120.60
1	B	86	GLN	N-CA-CB	7.20	123.55	110.60
1	B	103	MET	CG-SD-CE	7.11	111.58	100.20
1	D	156	ASP	CB-CA-C	7.11	124.61	110.40
1	B	37	VAL	CA-CB-CG2	7.10	121.55	110.90
1	D	62	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	A	67	SER	N-CA-CB	7.07	121.10	110.50
1	C	-5	PRO	C-N-CA	6.94	139.04	121.70
1	C	125	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	50	CYS	CA-CB-SG	-6.76	101.83	114.00
1	A	121	VAL	CA-CB-CG2	6.75	121.03	110.90
1	D	97	ASN	N-CA-CB	6.67	122.61	110.60
1	A	37	VAL	CA-CB-CG2	6.63	120.84	110.90
1	B	160	PRO	N-CA-CB	-6.62	95.31	102.60
1	C	124	VAL	CA-CB-CG2	6.62	120.83	110.90
1	C	29	VAL	CA-CB-CG2	6.53	120.69	110.90
1	D	13	GLY	C-N-CA	6.50	137.94	121.70
1	A	-4	GLN	C-N-CD	-6.49	106.32	120.60
1	A	159	ALA	C-N-CD	-6.44	106.43	120.60
1	C	-4	GLN	C-N-CD	-6.44	106.44	120.60
1	D	29	VAL	CA-CB-CG2	6.41	120.51	110.90
1	C	66	ASP	C-N-CA	6.41	137.71	121.70
1	A	124	VAL	CA-CB-CG2	6.38	120.46	110.90
1	A	132	VAL	CA-CB-CG2	6.36	120.45	110.90
1	D	40	GLY	C-N-CD	-6.35	106.64	120.60
1	C	83	VAL	CA-CB-CG2	6.31	120.36	110.90
1	A	164	VAL	CA-CB-CG2	6.27	120.31	110.90
1	D	370	SER	C-N-CA	6.26	137.36	121.70
1	B	48	ALA	CB-CA-C	6.26	119.49	110.10
1	D	9	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	D	98	PHE	CB-CG-CD1	-6.26	116.42	120.80
1	D	156	ASP	N-CA-CB	6.24	121.84	110.60
1	B	22	CYS	N-CA-CB	6.19	121.75	110.60
1	D	126	VAL	CA-CB-CG2	6.19	120.18	110.90
1	B	83	VAL	CA-CB-CG2	6.16	120.14	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	70	SER	N-CA-CB	6.14	119.71	110.50
1	A	157	PHE	C-N-CA	6.11	135.12	122.30
1	D	173	MET	CG-SD-CE	6.08	109.93	100.20
1	B	144	TYR	CB-CG-CD1	6.08	124.65	121.00
1	B	29	VAL	CA-CB-CG2	6.02	119.93	110.90
1	D	56	VAL	CA-CB-CG2	6.01	119.92	110.90
1	A	81	ILE	N-CA-CB	6.00	124.61	110.80
1	B	93	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	D	7	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	B	132	VAL	CA-CB-CG2	5.92	119.77	110.90
1	B	94	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	107	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	173	MET	CG-SD-CE	5.89	109.62	100.20
1	C	109	VAL	CA-CB-CG2	5.88	119.72	110.90
1	B	86	GLN	CB-CA-C	5.87	122.14	110.40
1	D	161	GLN	N-CA-CB	5.86	121.14	110.60
1	D	164	VAL	CA-CB-CG2	5.85	119.68	110.90
1	D	83	VAL	CA-CB-CG2	5.85	119.67	110.90
1	C	174	GLN	N-CA-CB	5.83	121.09	110.60
1	D	12	GLN	C-N-CA	5.82	134.53	122.30
1	A	105	VAL	CA-CB-CG2	5.82	119.62	110.90
1	B	24	ASN	N-CA-CB	5.79	121.01	110.60
1	A	14	HIS	CA-CB-CG	-5.75	103.83	113.60
1	C	371	ARG	O-C-N	5.74	131.89	122.70
1	D	160	PRO	C-N-CA	5.74	136.04	121.70
1	D	35	VAL	CA-CB-CG2	5.72	119.48	110.90
1	A	126	VAL	CA-CB-CG2	5.70	119.45	110.90
1	D	63	PRO	N-CA-C	5.69	126.89	112.10
1	A	81	ILE	O-C-N	5.68	131.80	122.70
1	B	56	VAL	CA-CB-CG2	5.67	119.41	110.90
1	B	31	LYS	C-N-CA	5.64	135.80	121.70
1	B	41	PRO	N-CA-CB	-5.63	96.41	102.60
1	A	27	GLU	N-CA-CB	5.58	120.64	110.60
1	A	43	VAL	CA-CB-CG2	5.54	119.21	110.90
1	D	97	ASN	CB-CA-C	5.51	121.42	110.40
1	D	120	LYS	N-CA-CB	5.50	120.50	110.60
1	A	107	ASP	CA-CB-CG	5.49	125.49	113.40
1	D	121	VAL	CA-CB-CG2	5.49	119.14	110.90
1	D	124	VAL	CA-CB-CG2	5.45	119.07	110.90
1	C	108	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	29	VAL	C-N-CA	-5.40	108.20	121.70
1	D	66	ASP	CB-CG-OD1	5.39	123.15	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	56	VAL	CA-CB-CG2	5.37	118.96	110.90
1	B	31	LYS	O-C-N	5.37	131.28	122.70
1	A	79	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	108	ASP	C-N-CA	5.36	135.09	121.70
1	A	56	VAL	CA-CB-CG2	5.34	118.91	110.90
1	C	8	GLN	N-CA-CB	5.33	120.20	110.60
1	A	102	LYS	O-C-N	5.33	131.23	122.70
1	A	45	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	D	132	VAL	CA-CB-CG2	5.32	118.89	110.90
1	D	22	CYS	CA-CB-SG	-5.29	104.47	114.00
1	A	107	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	B	60	GLY	C-N-CA	5.26	134.86	121.70
1	A	17	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	D	172	ASP	C-N-CA	5.25	134.82	121.70
1	C	87	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	A	132	VAL	C-N-CA	5.20	133.22	122.30
1	D	371	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	50	CYS	N-CA-C	5.18	124.99	111.00
1	B	129	GLY	C-N-CA	5.17	134.63	121.70
1	B	164	VAL	CA-CB-CG2	5.17	118.66	110.90
1	C	38	GLN	O-C-N	-5.17	114.44	122.70
1	A	103	MET	CG-SD-CE	5.15	108.45	100.20
1	D	154	SER	O-C-N	5.15	131.96	123.20
1	A	63	PRO	N-CA-C	5.13	125.45	112.10
1	B	48	ALA	N-CA-CB	5.13	117.28	110.10
1	A	167	VAL	N-CA-CB	5.10	122.72	111.50
1	B	128	SER	O-C-N	-5.08	114.56	123.20
1	B	62	TYR	C-N-CD	-5.07	109.44	120.60
1	D	119	GLU	OE1-CD-OE2	-5.03	117.27	123.30
1	B	43	VAL	CA-CB-CG2	5.03	118.44	110.90
1	B	45	TYR	N-CA-CB	5.02	119.63	110.60

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	-6	LYS	CA
1	A	67	SER	CA
1	B	86	GLN	CA
1	C	-5	PRO	CA
1	C	37	VAL	CA
1	C	74	SER	CA
1	D	371	ARG	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	D	86	GLN	CA
1	D	97	ASN	CA
1	D	152	LYS	CA
1	D	156	ASP	CA

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Sidechain
1	A	168	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	71	ARG	Sidechain
1	A	79	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	140	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	371	ARG	Sidechain
1	B	64	ARG	Sidechain
1	B	79	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	140	ARG	Sidechain
1	C	171	ARG	Sidechain
1	C	371	ARG	Sidechain
1	C	64	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	140	ARG	Sidechain
1	D	171	ARG	Sidechain
1	D	371	ARG	Sidechain
1	D	64	ARG	Sidechain
1	D	71	ARG	Sidechain
1	D	79	ARG	Sidechain

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	1492	0	1416	270	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1464	0	1391	274	0
1	C	1505	0	1435	286	1
1	D	1480	0	1406	270	1
All	All	5941	0	5648	1041	3

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 90.

All (1041) 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:D:41:PRO:HB2	1:D:81:ILE:CD1	1.47	1.43
1:C:43:VAL:HG12	1:C:81:ILE:CD1	1.50	1.39
1:D:154:SER:HB2	1:D:159:ALA:CB	1.51	1.39
1:D:41:PRO:CB	1:D:81:ILE:HD11	1.55	1.36
1:D:154:SER:CB	1:D:159:ALA:HB3	1.61	1.31
1:C:86:GLN:NE2	1:C:86:GLN:O	1.64	1.30
1:C:94:GLU:C	1:C:95:ASN:HD22	1.32	1.29
1:B:151:TYR:CD2	1:B:157:PHE:HB3	1.65	1.28
1:A:7:GLU:CG	1:A:8:GLN:H	1.50	1.24
1:A:109:VAL:HG23	1:A:116:HIS:CE1	1.71	1.24
1:D:154:SER:HA	1:D:157:PHE:CZ	1.73	1.23
1:D:157:PHE:CE1	1:D:159:ALA:HB2	1.74	1.22
1:A:7:GLU:CD	1:A:8:GLN:H	1.42	1.21
1:D:69:THR:HB	1:D:371:ARG:N	1.55	1.21
1:D:69:THR:CG2	1:D:371:ARG:HA	1.69	1.21
1:B:157:PHE:HD1	1:B:157:PHE:O	1.24	1.20
1:A:24:ASN:O	1:A:25:LEU:HD23	1.03	1.20
1:D:7:GLU:O	1:D:33:GLY:HA3	1.42	1.16
1:C:43:VAL:HG12	1:C:81:ILE:HD11	1.26	1.15
1:B:2:LYS:NZ	1:B:38:GLN:OE1	1.77	1.15
1:B:144:TYR:O	1:B:146:LEU:HD13	1.46	1.14
1:A:10:ASN:HB3	1:A:12:GLN:NE2	1.60	1.14
1:A:72:THR:O	1:A:73:ASP:OD1	1.64	1.14
1:D:16:HIS:ND1	1:D:29:VAL:HG13	1.65	1.12
1:A:32:ALA:HB3	1:A:74:SER:HB3	1.11	1.11
1:D:94:GLU:HA	1:D:120:LYS:O	1.48	1.11
1:A:64:ARG:HG2	1:A:64:ARG:NH1	1.50	1.11
1:A:92:LEU:HD22	1:A:112:PHE:CE2	1.84	1.11
1:D:16:HIS:CE1	1:D:29:VAL:HG13	1.85	1.11
1:C:9:GLU:OE1	1:C:64:ARG:NH1	1.82	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:HE1	1:D:83:VAL:N	1.63	1.10
1:A:10:ASN:CB	1:A:12:GLN:HE21	1.63	1.09
1:A:64:ARG:CG	1:A:64:ARG:HH11	1.65	1.09
1:A:24:ASN:O	1:A:25:LEU:CD2	1.99	1.09
1:C:173:MET:CE	1:D:83:VAL:H	1.66	1.09
1:A:28:THR:HG22	1:A:29:VAL:H	1.06	1.09
1:C:43:VAL:HG12	1:C:81:ILE:HD13	1.24	1.09
1:D:69:THR:HG22	1:D:371:ARG:HA	1.12	1.09
1:C:175:TRP:HA	1:D:-1:ASN:HB3	1.35	1.08
1:C:136:TYR:HB3	1:C:137:PRO:HD2	1.32	1.08
1:B:157:PHE:CD1	1:B:157:PHE:O	2.07	1.07
1:A:7:GLU:HG2	1:A:8:GLN:N	1.68	1.07
1:C:94:GLU:HG3	1:C:95:ASN:ND2	1.70	1.06
1:B:18:LEU:HD12	1:B:19:ASN:H	1.18	1.06
1:C:94:GLU:C	1:C:95:ASN:ND2	2.09	1.05
1:D:41:PRO:CB	1:D:81:ILE:CD1	2.23	1.04
1:A:7:GLU:OE1	1:A:8:GLN:N	1.89	1.04
1:C:137:PRO:HD3	1:C:165:GLN:NE2	1.72	1.04
1:B:7:GLU:HA	1:B:14:HIS:NE2	1.72	1.04
1:A:10:ASN:HB3	1:A:12:GLN:HE21	0.92	1.04
1:C:173:MET:HE2	1:D:83:VAL:HB	1.35	1.04
1:B:151:TYR:HD2	1:B:157:PHE:HB3	0.90	1.03
1:A:32:ALA:HB2	1:A:75:LEU:HB2	1.36	1.03
1:D:135:GLN:HG2	1:D:142:LEU:H	1.23	1.02
1:A:65:TRP:CE3	1:A:72:THR:HB	1.95	1.01
1:B:92:LEU:HD13	1:B:124:VAL:HG22	1.37	1.01
1:B:18:LEU:HD12	1:B:19:ASN:N	1.75	1.01
1:B:58:GLU:O	1:B:59:LYS:HB2	1.58	1.00
1:C:121:VAL:HB	1:C:164:VAL:HG23	1.42	1.00
1:C:79:ARG:HG3	1:C:79:ARG:HH11	1.23	1.00
1:C:94:GLU:O	1:C:95:ASN:ND2	1.95	1.00
1:B:94:GLU:HG3	1:B:95:ASN:N	1.71	0.99
1:C:43:VAL:CG1	1:C:81:ILE:HD13	1.92	0.98
1:B:48:ALA:HB2	1:B:76:SER:HB3	1.45	0.98
1:D:154:SER:HB2	1:D:159:ALA:HB3	1.07	0.98
1:D:7:GLU:O	1:D:33:GLY:CA	2.10	0.98
1:A:92:LEU:HD22	1:A:112:PHE:HE2	1.14	0.98
1:D:157:PHE:HE1	1:D:159:ALA:HB2	1.20	0.97
1:A:7:GLU:CG	1:A:8:GLN:N	2.14	0.97
1:B:151:TYR:CD2	1:B:157:PHE:CB	2.46	0.97
1:A:106:ILE:O	1:A:107:ASP:N	1.96	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLN:CD	1:C:86:GLN:H	1.67	0.96
1:C:43:VAL:CG1	1:C:81:ILE:CD1	2.44	0.96
1:C:151:TYR:CD2	1:C:157:PHE:HB3	2.01	0.96
1:D:69:THR:CB	1:D:371:ARG:N	2.29	0.95
1:C:173:MET:HE1	1:D:83:VAL:H	0.80	0.95
1:D:145:LEU:C	1:D:146:LEU:HD12	1.86	0.95
1:A:109:VAL:HG23	1:A:116:HIS:ND1	1.81	0.95
1:A:90:ILE:HD11	1:A:146:LEU:HD23	1.49	0.95
1:A:7:GLU:HG2	1:A:8:GLN:H	1.26	0.95
1:A:18:LEU:HD21	1:A:22:CYS:HB2	1.45	0.95
1:D:8:GLN:OE1	1:D:14:HIS:NE2	2.00	0.94
1:A:28:THR:HG22	1:A:29:VAL:N	1.83	0.94
1:B:151:TYR:HD2	1:B:157:PHE:CB	1.80	0.94
1:C:132:VAL:O	1:C:134:TYR:CE1	2.21	0.93
1:D:14:HIS:N	1:D:14:HIS:ND1	2.14	0.93
1:C:370:SER:O	1:C:71:ARG:HB2	1.67	0.93
1:D:3:ILE:HG23	1:D:3:ILE:O	1.65	0.93
1:C:91:THR:HG23	1:C:104:GLU:HB2	1.51	0.93
1:B:42:TRP:O	1:B:81:ILE:HD11	1.69	0.92
1:C:30:GLU:OE1	1:C:31:LYS:HE3	1.68	0.92
1:C:146:LEU:HD13	1:C:146:LEU:N	1.83	0.92
1:C:18:LEU:HD21	1:C:22:CYS:HB2	1.51	0.92
1:C:79:ARG:HG3	1:C:79:ARG:NH1	1.80	0.92
1:C:51:LYS:HG2	1:C:52:GLY:N	1.81	0.92
1:D:154:SER:HB2	1:D:159:ALA:HB1	1.51	0.91
1:A:7:GLU:CD	1:A:8:GLN:N	2.19	0.91
1:B:55:PHE:HE2	1:B:72:THR:HG21	1.34	0.91
1:B:25:LEU:HG	1:B:29:VAL:HG23	1.53	0.91
1:B:8:GLN:O	1:B:9:GLU:O	1.87	0.91
1:B:109:VAL:O	1:B:109:VAL:HG12	1.70	0.91
1:D:-2:LEU:O	1:D:-1:ASN:C	2.07	0.91
1:C:173:MET:CE	1:D:83:VAL:HB	2.01	0.90
1:C:47:GLN:HG2	1:C:51:LYS:HD3	1.54	0.90
1:B:55:PHE:CE2	1:B:72:THR:HG21	2.06	0.90
1:A:130:THR:HG22	1:A:170:ILE:HB	1.54	0.89
1:C:136:TYR:HB3	1:C:137:PRO:CD	2.02	0.89
1:D:9:GLU:HG2	1:D:10:ASN:N	1.85	0.89
1:B:7:GLU:HG2	1:B:31:LYS:NZ	1.88	0.89
1:C:64:ARG:O	1:C:67:SER:HB2	1.73	0.89
1:A:10:ASN:CB	1:A:12:GLN:NE2	2.28	0.89
1:D:98:PHE:N	1:D:98:PHE:CD1	2.38	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLN:OE1	1:D:86:GLN:HA	1.73	0.89
1:B:34:SER:O	1:B:35:VAL:HG23	1.74	0.88
1:D:86:GLN:N	1:D:86:GLN:OE1	2.06	0.88
1:B:153:ASP:H	1:B:156:ASP:CB	1.87	0.88
1:A:18:LEU:HD11	1:A:22:CYS:SG	2.13	0.88
1:B:7:GLU:HG2	1:B:31:LYS:HZ2	1.38	0.88
1:C:18:LEU:HD21	1:C:22:CYS:CB	2.03	0.88
1:B:158:GLY:O	1:B:160:PRO:HD3	1.74	0.87
1:B:-2:LEU:CD2	1:B:-2:LEU:N	2.37	0.87
1:A:32:ALA:HB3	1:A:74:SER:CB	2.01	0.87
1:A:110:PRO:O	1:A:166:SER:HB3	1.75	0.86
1:B:-2:LEU:H3	1:B:-2:LEU:HD23	1.39	0.86
1:D:69:THR:CG2	1:D:371:ARG:CA	2.54	0.86
1:C:25:LEU:O	1:C:28:THR:HB	1.75	0.86
1:A:72:THR:C	1:A:73:ASP:OD1	2.13	0.86
1:D:-1:ASN:O	1:D:39:ALA:HB3	1.74	0.86
1:B:26:LYS:HE3	1:B:74:SER:HB2	1.56	0.86
1:A:32:ALA:CB	1:A:74:SER:HB3	2.04	0.86
1:C:22:CYS:SG	1:C:25:LEU:HD23	2.15	0.86
1:C:6:PHE:HD1	1:C:6:PHE:N	1.69	0.86
1:C:135:GLN:HB2	1:C:142:LEU:H	1.38	0.85
1:A:86:GLN:HB2	1:B:88:HIS:HE1	1.41	0.84
1:D:69:THR:HG22	1:D:371:ARG:CA	2.04	0.84
1:A:5:ILE:O	1:A:5:ILE:HG22	1.77	0.84
1:C:5:ILE:O	1:C:5:ILE:HD13	1.77	0.84
1:D:89:LYS:HB3	1:D:127:GLN:HG3	1.60	0.83
1:C:5:ILE:CD1	1:C:16:HIS:O	2.25	0.83
1:B:153:ASP:H	1:B:156:ASP:HB2	1.42	0.83
1:A:18:LEU:HD21	1:A:22:CYS:CB	2.09	0.83
1:A:145:LEU:O	1:A:146:LEU:HD12	1.76	0.83
1:D:69:THR:HB	1:D:371:ARG:H	1.41	0.83
1:B:7:GLU:HB2	1:B:14:HIS:CG	2.13	0.83
1:C:94:GLU:CG	1:C:95:ASN:ND2	2.40	0.83
1:A:7:GLU:OE2	1:A:14:HIS:N	2.11	0.83
1:D:16:HIS:ND1	1:D:29:VAL:CG1	2.41	0.83
1:C:6:PHE:CD1	1:C:6:PHE:N	2.40	0.82
1:D:167:VAL:CG1	1:D:167:VAL:O	2.27	0.82
1:A:7:GLU:HB3	1:A:14:HIS:O	1.79	0.82
1:C:86:GLN:CD	1:C:86:GLN:N	2.26	0.82
1:A:44:GLY:O	1:A:45:TYR:CG	2.32	0.82
1:B:8:GLN:HG2	1:B:31:LYS:HZ1	1.43	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:TRP:HA	1:B:68:TRP:CH2	2.14	0.81
1:A:40:GLY:H	1:B:174:GLN:HG3	1.44	0.81
1:C:47:GLN:HB3	1:C:51:LYS:O	1.80	0.81
1:B:27:GLU:OE1	1:B:27:GLU:C	2.19	0.81
1:B:103:MET:HB2	1:B:118:TYR:CD2	2.16	0.81
1:A:5:ILE:HD11	1:A:75:LEU:HD13	1.63	0.81
1:C:53:GLU:OE2	1:C:55:PHE:HE1	1.64	0.81
1:B:44:GLY:O	1:B:45:TYR:CD1	2.34	0.81
1:B:49:ASN:C	1:B:50:CYS:SG	2.59	0.81
1:B:135:GLN:HG2	1:B:136:TYR:CE1	2.16	0.80
1:D:69:THR:CB	1:D:371:ARG:H	1.91	0.80
1:D:98:PHE:HD1	1:D:98:PHE:N	1.75	0.80
1:D:167:VAL:HG13	1:D:167:VAL:O	1.80	0.80
1:C:5:ILE:H	1:C:5:ILE:CD1	1.94	0.79
1:C:95:ASN:N	1:C:95:ASN:HD22	1.80	0.79
1:A:-1:ASN:HB2	1:A:1:PRO:CD	2.12	0.79
1:A:18:LEU:HD11	1:A:22:CYS:CB	2.13	0.79
1:A:47:GLN:HB2	1:A:51:LYS:O	1.83	0.78
1:B:72:THR:HG22	1:B:73:ASP:H	1.48	0.78
1:A:28:THR:HG21	1:A:29:VAL:HG12	1.65	0.78
1:A:37:VAL:HG12	1:A:59:LYS:HA	1.65	0.78
1:A:7:GLU:OE2	1:A:13:GLY:HA3	1.83	0.78
1:D:23:PRO:O	1:D:24:ASN:HB2	1.83	0.78
1:D:26:LYS:HD3	1:D:29:VAL:O	1.84	0.78
1:A:109:VAL:CG2	1:A:116:HIS:ND1	2.47	0.78
1:B:69:THR:C	1:B:370:SER:H	1.83	0.78
1:C:58:GLU:OE2	1:D:168:ARG:NH2	2.17	0.77
1:C:125:ARG:HG2	1:C:125:ARG:HH11	1.48	0.77
1:A:44:GLY:O	1:A:45:TYR:CD1	2.37	0.77
1:B:152:LYS:N	1:B:156:ASP:OD2	2.18	0.77
1:D:69:THR:HB	1:D:71:ARG:C	2.04	0.77
1:D:86:GLN:OE1	1:D:86:GLN:CA	2.33	0.77
1:D:41:PRO:CG	1:D:81:ILE:CD1	2.62	0.77
1:D:159:ALA:O	1:D:162:PRO:HD3	1.85	0.77
1:D:98:PHE:HD1	1:D:98:PHE:H	1.33	0.77
1:C:136:TYR:CB	1:C:137:PRO:CD	2.60	0.76
1:D:42:TRP:CE3	1:D:80:PRO:HD3	2.20	0.76
1:B:144:TYR:CE2	1:B:157:PHE:HE1	2.04	0.76
1:A:4:ILE:O	1:A:6:PHE:CD1	2.38	0.76
1:D:132:VAL:CG2	1:D:170:ILE:HD11	2.16	0.76
1:C:175:TRP:HA	1:D:-1:ASN:CB	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:CE	1:D:83:VAL:N	2.34	0.76
1:C:4:ILE:HG22	1:C:6:PHE:CE1	2.21	0.76
1:B:144:TYR:O	1:B:145:LEU:C	2.22	0.76
1:D:3:ILE:O	1:D:3:ILE:CG2	2.34	0.76
1:B:8:GLN:CG	1:B:31:LYS:HZ1	1.98	0.75
1:A:4:ILE:O	1:A:6:PHE:HD1	1.69	0.75
1:B:-2:LEU:HD23	1:B:-2:LEU:N	2.01	0.75
1:C:5:ILE:C	1:C:6:PHE:HD1	1.89	0.75
1:C:86:GLN:NE2	1:C:86:GLN:C	2.39	0.75
1:C:44:GLY:HA2	1:C:78:LEU:HD23	1.68	0.75
1:B:93:TYR:HB2	1:B:123:SER:HB2	1.67	0.75
1:A:109:VAL:CG2	1:A:116:HIS:CE1	2.63	0.74
1:C:37:VAL:HG12	1:C:59:LYS:HA	1.67	0.74
1:D:154:SER:CA	1:D:157:PHE:CZ	2.64	0.74
1:A:65:TRP:CZ3	1:A:72:THR:HB	2.22	0.74
1:B:98:PHE:CD1	1:B:98:PHE:N	2.53	0.74
1:D:146:LEU:N	1:D:146:LEU:HD12	2.01	0.74
1:A:7:GLU:HG3	1:A:14:HIS:HB3	1.69	0.74
1:C:50:CYS:SG	1:C:79:ARG:HD3	2.28	0.74
1:C:91:THR:HG23	1:C:104:GLU:CB	2.18	0.73
1:D:5:ILE:CG1	1:D:5:ILE:O	2.34	0.73
1:D:155:GLY:O	1:D:156:ASP:C	2.23	0.73
1:D:96:PRO:HA	1:D:123:SER:OG	1.88	0.73
1:B:46:GLU:O	1:B:73:ASP:HB2	1.88	0.73
1:A:-1:ASN:HB2	1:A:1:PRO:HD2	1.68	0.73
1:D:154:SER:HA	1:D:157:PHE:CE2	2.22	0.73
1:C:70:SER:HB3	1:D:140:ARG:HG2	1.69	0.73
1:D:88:HIS:HA	1:D:128:SER:OG	1.88	0.73
1:A:136:TYR:C	1:A:165:GLN:HB2	2.08	0.73
1:B:109:VAL:HG11	1:B:112:PHE:CE1	2.22	0.73
1:D:153:ASP:OD2	1:D:155:GLY:HA3	1.87	0.73
1:A:5:ILE:HD11	1:A:75:LEU:CD1	2.18	0.73
1:B:88:HIS:CD2	1:B:169:ARG:CZ	2.72	0.73
1:B:27:GLU:OE1	1:B:28:THR:N	2.22	0.73
1:B:92:LEU:CD1	1:B:124:VAL:HG22	2.15	0.73
1:A:98:PHE:CD1	1:A:123:SER:HB3	2.23	0.72
1:B:7:GLU:HA	1:B:14:HIS:CD2	2.23	0.72
1:C:136:TYR:HA	1:C:165:GLN:HE21	1.54	0.72
1:B:37:VAL:HB	1:B:59:LYS:HA	1.69	0.72
1:C:5:ILE:H	1:C:5:ILE:HD13	1.52	0.72
1:A:93:TYR:CE2	1:A:98:PHE:HB3	2.25	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:CG	1:B:31:LYS:HZ2	2.02	0.72
1:B:143:GLN:O	1:B:144:TYR:HD1	1.73	0.72
1:D:-2:LEU:O	1:D:1:PRO:O	2.07	0.72
1:C:94:GLU:HG2	1:C:101:LYS:N	2.05	0.72
1:C:47:GLN:HG2	1:C:51:LYS:CD	2.18	0.72
1:B:3:ILE:CG2	1:B:18:LEU:HB3	2.20	0.72
1:C:-4:GLN:O	1:C:-3:PRO:O	2.07	0.72
1:D:69:THR:CG2	1:D:371:ARG:N	2.53	0.71
1:C:121:VAL:CB	1:C:164:VAL:HG23	2.18	0.71
1:D:53:GLU:HB3	1:D:55:PHE:HE1	1.53	0.71
1:A:59:LYS:HD2	1:B:174:GLN:NE2	2.03	0.71
1:A:9:GLU:HA	1:A:34:SER:OG	1.90	0.71
1:A:18:LEU:HD11	1:A:22:CYS:HB3	1.71	0.71
1:D:24:ASN:OD1	1:D:26:LYS:N	2.24	0.71
1:A:175:TRP:HD1	1:B:40:GLY:O	1.72	0.71
1:B:137:PRO:HA	1:B:166:SER:OG	1.91	0.71
1:A:40:GLY:N	1:B:174:GLN:HG3	2.05	0.71
1:A:90:ILE:HD11	1:A:146:LEU:CD2	2.20	0.71
1:D:144:TYR:O	1:D:146:LEU:CD1	2.38	0.70
1:A:3:ILE:O	1:A:3:ILE:HG23	1.91	0.70
1:D:-2:LEU:O	1:D:1:PRO:C	2.29	0.70
1:B:26:LYS:HE2	1:B:74:SER:O	1.91	0.70
1:C:146:LEU:CD1	1:C:146:LEU:N	2.54	0.70
1:D:155:GLY:O	1:D:158:GLY:N	2.24	0.70
1:D:112:PHE:N	1:D:165:GLN:O	2.21	0.70
1:C:9:GLU:HA	1:C:33:GLY:O	1.90	0.70
1:D:5:ILE:HG12	1:D:5:ILE:O	1.91	0.70
1:D:-2:LEU:HA	1:D:19:ASN:HD22	1.56	0.70
1:C:370:SER:O	1:C:71:ARG:CB	2.33	0.70
1:B:-2:LEU:HD22	1:B:-2:LEU:H1	1.57	0.70
1:B:94:GLU:CG	1:B:95:ASN:N	2.48	0.70
1:A:154:SER:HA	1:A:157:PHE:CD1	2.25	0.70
1:C:-7:GLY:C	1:C:-6:LYS:HG2	2.11	0.70
1:B:65:TRP:HA	1:B:68:TRP:CZ3	2.27	0.70
1:D:22:CYS:SG	1:D:25:LEU:HD23	2.32	0.69
1:D:28:THR:C	1:D:29:VAL:H	1.93	0.69
1:D:95:ASN:HD22	1:D:95:ASN:C	1.95	0.69
1:D:154:SER:CA	1:D:159:ALA:HB3	2.21	0.69
1:A:25:LEU:O	1:A:28:THR:HB	1.92	0.69
1:C:173:MET:HE2	1:D:83:VAL:CB	2.18	0.69
1:B:144:TYR:CD2	1:B:157:PHE:CE1	2.80	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:NE2	1:B:59:LYS:HD2	2.07	0.69
1:B:8:GLN:HB3	1:B:31:LYS:NZ	2.07	0.69
1:B:135:GLN:HG2	1:B:136:TYR:CZ	2.28	0.69
1:D:135:GLN:HG2	1:D:142:LEU:N	2.03	0.69
1:C:153:ASP:O	1:C:156:ASP:HB2	1.92	0.69
1:C:91:THR:CG2	1:C:104:GLU:HB2	2.22	0.69
1:A:59:LYS:HD2	1:B:174:GLN:HE22	1.56	0.69
1:B:18:LEU:HD21	1:B:20:GLY:O	1.93	0.69
1:B:7:GLU:CA	1:B:14:HIS:CD2	2.76	0.69
1:C:91:THR:HG23	1:C:104:GLU:HA	1.74	0.69
1:B:98:PHE:HD1	1:B:98:PHE:N	1.89	0.69
1:D:88:HIS:O	1:D:131:TRP:HZ2	1.75	0.69
1:D:7:GLU:HA	1:D:31:LYS:O	1.91	0.69
1:C:5:ILE:O	1:C:5:ILE:CD1	2.40	0.69
1:C:108:ASP:HB3	1:C:168:ARG:HA	1.75	0.69
1:A:7:GLU:OE1	1:A:12:GLN:O	2.09	0.68
1:A:8:GLN:HB2	1:A:12:GLN:O	1.92	0.68
1:D:-2:LEU:CD1	1:D:2:LYS:HB2	2.23	0.68
1:C:136:TYR:CB	1:C:137:PRO:HD2	2.14	0.68
1:C:20:GLY:O	1:C:21:PRO:O	2.11	0.68
1:D:41:PRO:HD2	1:D:81:ILE:HD12	1.74	0.68
1:C:45:TYR:HB2	1:C:77:SER:HB2	1.75	0.68
1:C:53:GLU:CD	1:C:55:PHE:HE1	1.96	0.68
1:C:44:GLY:CA	1:C:78:LEU:HD23	2.24	0.68
1:A:124:VAL:HG23	1:A:151:TYR:HB2	1.76	0.68
1:A:136:TYR:HA	1:A:165:GLN:HG3	1.73	0.68
1:C:132:VAL:O	1:C:134:TYR:HE1	1.72	0.68
1:C:92:LEU:HD22	1:C:112:PHE:CZ	2.29	0.68
1:A:130:THR:CG2	1:A:170:ILE:HB	2.22	0.68
1:C:89:LYS:HD2	1:C:127:GLN:HE21	1.59	0.67
1:D:161:GLN:O	1:D:163:GLN:N	2.26	0.67
1:D:28:THR:O	1:D:29:VAL:N	2.27	0.67
1:C:70:SER:HA	1:C:71:ARG:NH2	2.10	0.67
1:D:154:SER:CB	1:D:159:ALA:CB	2.36	0.67
1:C:79:ARG:CG	1:C:79:ARG:NH1	2.52	0.67
1:D:8:GLN:HB3	1:D:12:GLN:HB3	1.75	0.67
1:A:84:ASP:OD2	1:A:86:GLN:NE2	2.27	0.67
1:A:86:GLN:HB2	1:B:88:HIS:CE1	2.26	0.67
1:C:125:ARG:HG2	1:C:125:ARG:NH1	2.06	0.67
1:A:90:ILE:HD12	1:A:126:VAL:HG22	1.77	0.67
1:B:142:LEU:HB3	1:B:144:TYR:HE1	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PRO:O	1:B:48:ALA:HB1	1.95	0.67
1:A:154:SER:HA	1:A:157:PHE:HD1	1.60	0.67
1:C:90:ILE:CG2	1:C:90:ILE:O	2.43	0.67
1:C:151:TYR:CE2	1:C:157:PHE:HB3	2.31	0.67
1:B:91:THR:HG23	1:B:104:GLU:HG3	1.75	0.67
1:C:137:PRO:HD3	1:C:165:GLN:HE21	1.58	0.66
1:C:135:GLN:HB2	1:C:142:LEU:N	2.07	0.66
1:B:3:ILE:HG22	1:B:18:LEU:HB3	1.77	0.66
1:C:106:ILE:O	1:C:107:ASP:N	2.23	0.66
1:B:-2:LEU:H1	1:B:-2:LEU:CD2	2.08	0.66
1:B:91:THR:CG2	1:B:104:GLU:HG3	2.25	0.66
1:D:119:GLU:H	1:D:119:GLU:CD	1.98	0.66
1:A:44:GLY:O	1:A:45:TYR:CD2	2.48	0.66
1:C:22:CYS:SG	1:C:22:CYS:O	2.53	0.66
1:B:155:GLY:C	1:B:157:PHE:H	1.99	0.66
1:A:83:VAL:HG13	1:B:173:MET:SD	2.35	0.66
1:B:47:GLN:O	1:B:76:SER:HB2	1.96	0.66
1:B:109:VAL:HG11	1:B:112:PHE:CD1	2.29	0.66
1:D:-2:LEU:HD12	1:D:19:ASN:ND2	2.11	0.66
1:A:7:GLU:CG	1:A:14:HIS:HB3	2.27	0.65
1:A:32:ALA:CB	1:A:75:LEU:HB2	2.19	0.65
1:A:28:THR:CG2	1:A:29:VAL:HG12	2.26	0.65
1:D:25:LEU:O	1:D:29:VAL:HG23	1.97	0.65
1:C:36:LEU:HD23	1:C:36:LEU:C	2.17	0.65
1:B:109:VAL:O	1:B:109:VAL:CG1	2.42	0.65
1:B:144:TYR:O	1:B:146:LEU:CD1	2.34	0.65
1:A:95:ASN:HD21	1:A:99:THR:HB	1.61	0.65
1:A:49:ASN:O	1:A:50:CYS:HB2	1.95	0.65
1:D:26:LYS:HZ2	1:D:30:GLU:C	2.00	0.65
1:D:69:THR:CG2	1:D:371:ARG:H	2.10	0.65
1:B:34:SER:O	1:B:35:VAL:CG2	2.44	0.65
1:C:5:ILE:N	1:C:5:ILE:HD13	2.11	0.65
1:B:26:LYS:CE	1:B:74:SER:HB2	2.28	0.64
1:A:120:LYS:HZ1	1:A:162:PRO:HG2	1.62	0.64
1:A:92:LEU:HD22	1:A:112:PHE:CZ	2.30	0.64
1:B:21:PRO:O	1:B:22:CYS:HB2	1.97	0.64
1:A:-6:LYS:CB	1:A:-5:PRO:CD	2.75	0.64
1:B:26:LYS:HG2	1:B:76:SER:HA	1.78	0.64
1:A:64:ARG:O	1:A:66:ASP:N	2.31	0.64
1:D:-2:LEU:HD11	1:D:2:LYS:HB2	1.80	0.64
1:B:-1:ASN:HB2	1:B:1:PRO:HD2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:TRP:CH2	1:D:169:ARG:HD3	2.33	0.64
1:B:153:ASP:OD1	1:B:154:SER:N	2.30	0.64
1:D:42:TRP:CZ3	1:D:80:PRO:HD3	2.32	0.64
1:C:92:LEU:HD22	1:C:112:PHE:HZ	1.60	0.64
1:B:157:PHE:CD1	1:B:157:PHE:C	2.71	0.63
1:A:7:GLU:OE2	1:A:13:GLY:CA	2.46	0.63
1:C:137:PRO:O	1:C:138:GLY:C	2.36	0.63
1:B:157:PHE:CE1	1:B:159:ALA:HB2	2.33	0.63
1:B:144:TYR:CE2	1:B:159:ALA:HB2	2.33	0.63
1:B:49:ASN:HD22	1:B:49:ASN:N	1.96	0.63
1:C:96:PRO:O	1:C:97:ASN:HB2	1.99	0.63
1:A:6:PHE:CD2	1:A:11:PHE:HA	2.32	0.63
1:D:136:TYR:HB3	1:D:137:PRO:HD2	1.79	0.63
1:A:120:LYS:NZ	1:A:162:PRO:HG2	2.12	0.63
1:D:132:VAL:HG23	1:D:170:ILE:HG12	1.80	0.63
1:D:159:ALA:HB1	1:D:162:PRO:HA	1.80	0.63
1:B:143:GLN:C	1:B:144:TYR:HD1	2.02	0.63
1:D:26:LYS:CD	1:D:29:VAL:O	2.47	0.63
1:B:8:GLN:CG	1:B:31:LYS:NZ	2.62	0.63
1:B:8:GLN:CB	1:B:31:LYS:NZ	2.62	0.63
1:C:151:TYR:CD1	1:C:151:TYR:N	2.67	0.63
1:A:21:PRO:HD3	1:A:80:PRO:HD3	1.80	0.63
1:C:69:THR:HG22	1:C:71:ARG:H	1.63	0.63
1:B:158:GLY:O	1:B:160:PRO:CD	2.45	0.63
1:B:155:GLY:O	1:B:157:PHE:N	2.31	0.62
1:C:86:GLN:OE1	1:D:88:HIS:NE2	2.32	0.62
1:C:173:MET:CE	1:D:83:VAL:CB	2.76	0.62
1:C:18:LEU:CD2	1:C:22:CYS:HB2	2.27	0.62
1:D:92:LEU:HD13	1:D:112:PHE:CZ	2.34	0.62
1:A:10:ASN:O	1:A:11:PHE:HB2	1.99	0.62
1:D:8:GLN:OE1	1:D:14:HIS:CE1	2.52	0.62
1:C:-1:ASN:O	1:C:-1:ASN:ND2	2.32	0.62
1:D:155:GLY:O	1:D:157:PHE:N	2.32	0.62
1:A:50:CYS:HB2	1:A:51:LYS:HZ1	1.64	0.62
1:A:92:LEU:CD2	1:A:112:PHE:CE2	2.74	0.62
1:C:90:ILE:HG23	1:C:90:ILE:O	1.98	0.62
1:A:135:GLN:HG2	1:A:136:TYR:CE1	2.34	0.62
1:A:136:TYR:O	1:A:165:GLN:HB2	1.99	0.62
1:B:18:LEU:CD1	1:B:19:ASN:N	2.58	0.62
1:A:92:LEU:HD23	1:A:121:VAL:HG11	1.81	0.62
1:A:63:PRO:O	1:A:64:ARG:HB3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:N	1:C:125:ARG:O	2.28	0.62
1:C:-1:ASN:N	1:C:-1:ASN:HD22	1.97	0.61
1:D:41:PRO:CD	1:D:81:ILE:HD12	2.30	0.61
1:B:45:TYR:N	1:B:55:PHE:CE1	2.68	0.61
1:D:157:PHE:CE1	1:D:159:ALA:CB	2.68	0.61
1:B:72:THR:HG22	1:B:73:ASP:N	2.14	0.61
1:D:9:GLU:CG	1:D:10:ASN:N	2.61	0.61
1:B:69:THR:O	1:B:370:SER:N	2.28	0.61
1:A:-6:LYS:CB	1:A:-5:PRO:HD3	2.31	0.61
1:A:56:VAL:N	1:B:143:GLN:OE1	2.23	0.61
1:A:61:GLU:C	1:A:63:PRO:HD3	2.20	0.61
1:D:65:TRP:CE3	1:D:69:THR:HG21	2.35	0.61
1:D:-2:LEU:HD12	1:D:19:ASN:HD21	1.65	0.61
1:A:169:ARG:NH2	1:A:171:ARG:HE	1.98	0.61
1:D:-3:PRO:O	1:D:-2:LEU:C	2.39	0.61
1:B:41:PRO:HG2	1:B:81:ILE:HB	1.83	0.61
1:C:69:THR:CG2	1:C:71:ARG:H	2.13	0.61
1:C:25:LEU:HA	1:C:28:THR:HB	1.82	0.61
1:D:41:PRO:C	1:D:81:ILE:HD11	2.21	0.61
1:C:14:HIS:ND1	1:C:29:VAL:HG13	2.15	0.61
1:D:-2:LEU:O	1:D:1:PRO:N	2.33	0.61
1:C:6:PHE:HA	1:C:15:SER:HA	1.82	0.61
1:C:25:LEU:C	1:C:28:THR:HB	2.20	0.61
1:A:129:GLY:HA2	1:B:84:ASP:O	2.01	0.60
1:A:40:GLY:H	1:B:174:GLN:CG	2.13	0.60
1:D:47:GLN:HG2	1:D:51:LYS:O	2.01	0.60
1:A:64:ARG:HH11	1:A:64:ARG:HG2	0.70	0.60
1:B:9:GLU:HG2	1:B:64:ARG:HG3	1.84	0.60
1:D:41:PRO:CA	1:D:81:ILE:HD11	2.30	0.60
1:D:41:PRO:HB2	1:D:81:ILE:HD11	0.67	0.60
1:A:72:THR:O	1:A:73:ASP:CG	2.39	0.60
1:A:25:LEU:O	1:A:29:VAL:O	2.19	0.60
1:D:26:LYS:NZ	1:D:30:GLU:C	2.55	0.60
1:C:137:PRO:CD	1:C:165:GLN:NE2	2.58	0.60
1:B:44:GLY:C	1:B:45:TYR:CD1	2.75	0.60
1:C:121:VAL:HB	1:C:164:VAL:CG2	2.27	0.60
1:D:45:TYR:CE2	1:D:50:CYS:HB3	2.37	0.60
1:D:-2:LEU:HA	1:D:19:ASN:ND2	2.16	0.60
1:D:-2:LEU:C	1:D:1:PRO:HD2	2.22	0.60
1:D:89:LYS:CB	1:D:127:GLN:HG3	2.29	0.60
1:B:-1:ASN:CB	1:B:1:PRO:CD	2.79	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:O	1:A:170:ILE:N	2.31	0.60
1:D:9:GLU:HG2	1:D:10:ASN:HB2	1.83	0.60
1:B:92:LEU:HD13	1:B:124:VAL:CG2	2.22	0.59
1:D:109:VAL:O	1:D:166:SER:HB2	2.02	0.59
1:D:88:HIS:N	1:D:88:HIS:ND1	2.50	0.59
1:A:2:LYS:O	1:A:3:ILE:HB	2.01	0.59
1:C:6:PHE:CD1	1:C:15:SER:HB2	2.36	0.59
1:B:93:TYR:CE1	1:B:102:LYS:HB2	2.37	0.59
1:C:-6:LYS:CG	1:C:-5:PRO:HD3	2.33	0.59
1:A:18:LEU:CD1	1:A:22:CYS:HB3	2.33	0.59
1:B:58:GLU:O	1:B:59:LYS:CB	2.30	0.59
1:C:70:SER:HB3	1:D:140:ARG:CG	2.31	0.59
1:C:-6:LYS:HG3	1:C:-5:PRO:HD3	1.83	0.59
1:D:306:ASP:O	1:D:171:ARG:NH2	2.35	0.59
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.83	0.59
1:B:153:ASP:H	1:B:156:ASP:HB3	1.65	0.59
1:C:53:GLU:OE2	1:C:55:PHE:CE1	2.53	0.59
1:B:25:LEU:HD12	1:B:29:VAL:HG21	1.85	0.59
1:B:69:THR:C	1:B:370:SER:N	2.55	0.59
1:D:106:ILE:O	1:D:106:ILE:HG23	2.02	0.59
1:D:153:ASP:C	1:D:155:GLY:N	2.50	0.59
1:A:69:THR:HG22	1:A:370:SER:HB2	1.83	0.59
1:D:134:TYR:CD2	1:D:139:TYR:C	2.76	0.59
1:B:145:LEU:C	1:B:146:LEU:HD13	2.23	0.59
1:A:29:VAL:HG13	1:A:30:GLU:N	2.16	0.59
1:B:103:MET:SD	1:B:112:PHE:CD1	2.96	0.59
1:B:42:TRP:O	1:B:81:ILE:CD1	2.50	0.58
1:B:4:ILE:HA	1:B:16:HIS:O	2.03	0.58
1:C:161:GLN:NE2	1:C:161:GLN:HA	2.17	0.58
1:C:5:ILE:HD12	1:C:16:HIS:O	2.02	0.58
1:A:161:GLN:O	1:A:163:GLN:N	2.35	0.58
1:C:110:PRO:HG3	1:C:139:TYR:OH	2.02	0.58
1:C:4:ILE:HG22	1:C:6:PHE:HE1	1.64	0.58
1:A:5:ILE:HG12	1:A:35:VAL:HG22	1.85	0.58
1:A:92:LEU:CD2	1:A:112:PHE:CZ	2.87	0.58
1:C:84:ASP:O	1:C:84:ASP:CG	2.40	0.58
1:C:92:LEU:HD12	1:C:92:LEU:N	2.17	0.58
1:C:135:GLN:HB3	1:C:141:GLY:HA3	1.86	0.58
1:C:5:ILE:O	1:C:5:ILE:CG1	2.52	0.58
1:A:-1:ASN:CB	1:A:1:PRO:CD	2.75	0.58
1:D:154:SER:C	1:D:159:ALA:HB3	2.23	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:HG11	1:C:164:VAL:HG21	1.86	0.57
1:A:129:GLY:CA	1:B:84:ASP:HB3	2.33	0.57
1:B:113:HIS:CD2	1:B:318:GLN:HA	2.39	0.57
1:C:370:SER:OG	1:C:71:ARG:N	2.35	0.57
1:C:46:GLU:OE2	1:C:73:ASP:HB3	2.04	0.57
1:D:6:PHE:CD2	1:D:11:PHE:O	2.57	0.57
1:C:86:GLN:OE1	1:D:88:HIS:CE1	2.58	0.57
1:B:153:ASP:N	1:B:156:ASP:HB2	2.18	0.57
1:B:14:HIS:NE2	1:B:31:LYS:O	2.33	0.57
1:B:95:ASN:HB3	1:B:99:THR:HB	1.87	0.57
1:B:144:TYR:CE2	1:B:157:PHE:CE1	2.91	0.57
1:C:79:ARG:HH11	1:C:79:ARG:CG	1.98	0.57
1:A:47:GLN:O	1:A:48:ALA:O	2.23	0.57
1:C:47:GLN:HB3	1:C:51:LYS:C	2.24	0.57
1:C:89:LYS:HD2	1:C:127:GLN:NE2	2.19	0.57
1:D:145:LEU:CA	1:D:146:LEU:HD12	2.34	0.57
1:C:94:GLU:CD	1:C:95:ASN:HD21	2.08	0.57
1:A:58:GLU:O	1:A:59:LYS:C	2.41	0.57
1:D:94:GLU:HG2	1:D:95:ASN:N	2.12	0.57
1:B:102:LYS:HG2	1:B:103:MET:N	2.04	0.57
1:A:43:VAL:HG11	1:B:145:LEU:HD12	1.87	0.56
1:C:94:GLU:HG3	1:C:95:ASN:HD22	1.48	0.56
1:C:46:GLU:O	1:C:76:SER:HB3	2.05	0.56
1:C:-1:ASN:N	1:C:-1:ASN:ND2	2.51	0.56
1:C:91:THR:CG2	1:C:104:GLU:CB	2.82	0.56
1:A:111:SER:OG	1:A:114:ALA:N	2.39	0.56
1:A:134:TYR:CD1	1:A:139:TYR:HB3	2.40	0.56
1:D:28:THR:C	1:D:29:VAL:N	2.58	0.56
1:D:26:LYS:NZ	1:D:30:GLU:O	2.36	0.56
1:B:4:ILE:HG23	1:B:16:HIS:O	2.05	0.56
1:D:152:LYS:HA	1:D:156:ASP:HB2	1.87	0.56
1:D:93:TYR:O	1:D:121:VAL:HA	2.06	0.56
1:C:86:GLN:NE2	1:C:86:GLN:CA	2.69	0.56
1:B:134:TYR:CE2	1:B:139:TYR:HB3	2.41	0.56
1:D:53:GLU:HB3	1:D:55:PHE:CE1	2.38	0.56
1:A:131:TRP:CZ3	1:A:169:ARG:HB2	2.41	0.56
1:A:133:GLY:HA2	1:A:167:VAL:HG23	1.87	0.56
1:A:57:PHE:HZ	1:A:75:LEU:HD21	1.71	0.56
1:C:25:LEU:CA	1:C:28:THR:HB	2.36	0.55
1:D:159:ALA:O	1:D:160:PRO:C	2.44	0.55
1:D:78:LEU:O	1:D:79:ARG:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:HE2	1:D:83:VAL:CA	2.37	0.55
1:B:175:TRP:N	1:B:175:TRP:CD1	2.74	0.55
1:A:3:ILE:HG13	1:A:37:VAL:HG22	1.88	0.55
1:A:45:TYR:HB2	1:A:77:SER:HB2	1.89	0.55
1:A:59:LYS:HB2	1:B:174:GLN:HE22	1.71	0.55
1:B:121:VAL:O	1:B:162:PRO:CB	2.55	0.55
1:A:80:PRO:HG2	1:A:82:LYS:HE3	1.88	0.55
1:C:-6:LYS:CB	1:C:-5:PRO:HD3	2.36	0.55
1:D:71:ARG:O	1:D:371:ARG:HB2	2.06	0.55
1:A:157:PHE:CG	1:A:157:PHE:O	2.59	0.55
1:D:159:ALA:O	1:D:162:PRO:CD	2.54	0.55
1:D:-2:LEU:CD1	1:D:19:ASN:HD21	2.19	0.55
1:B:103:MET:HE3	1:B:116:HIS:HB2	1.89	0.55
1:A:24:ASN:C	1:A:25:LEU:HD23	2.12	0.55
1:A:44:GLY:O	1:A:45:TYR:CE1	2.59	0.55
1:C:175:TRP:HB2	1:D:1:PRO:N	2.22	0.55
1:D:112:PHE:CE2	1:D:164:VAL:HG12	2.42	0.55
1:A:16:HIS:CE1	1:A:17:GLU:O	2.60	0.55
1:A:61:GLU:O	1:A:63:PRO:HD3	2.06	0.55
1:D:-1:ASN:HB2	1:D:1:PRO:HD3	1.89	0.55
1:B:26:LYS:O	1:B:30:GLU:HG3	2.07	0.55
1:D:112:PHE:HB2	1:D:165:GLN:HA	1.89	0.55
1:D:153:ASP:O	1:D:154:SER:C	2.44	0.55
1:B:14:HIS:HB2	1:B:16:HIS:HE1	1.72	0.55
1:A:94:GLU:HG3	1:A:119:GLU:HG3	1.87	0.55
1:B:134:TYR:CD2	1:B:139:TYR:HB3	2.42	0.54
1:C:132:VAL:O	1:C:134:TYR:CD1	2.60	0.54
1:C:22:CYS:SG	1:C:25:LEU:CD2	2.94	0.54
1:B:103:MET:HB2	1:B:118:TYR:CE2	2.42	0.54
1:D:132:VAL:HG22	1:D:170:ILE:HD11	1.86	0.54
1:A:90:ILE:CD1	1:A:126:VAL:HG22	2.37	0.54
1:C:1:PRO:HD3	1:D:175:TRP:CZ3	2.42	0.54
1:D:146:LEU:N	1:D:146:LEU:CD1	2.70	0.54
1:D:69:THR:HG21	1:D:371:ARG:HA	1.75	0.54
1:A:3:ILE:HG22	1:A:18:LEU:O	2.08	0.54
1:C:92:LEU:CD1	1:C:92:LEU:N	2.70	0.54
1:A:-1:ASN:HB2	1:A:1:PRO:HD3	1.90	0.54
1:D:154:SER:OG	1:D:159:ALA:HB3	2.06	0.54
1:C:118:TYR:HE2	1:C:120:LYS:O	1.90	0.54
1:C:152:LYS:N	1:C:156:ASP:OD2	2.41	0.54
1:C:47:GLN:HB2	1:C:52:GLY:HA3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:CG2	1:D:170:ILE:CD1	2.86	0.54
1:C:11:PHE:CE2	1:C:63:PRO:HB3	2.42	0.54
1:C:157:PHE:O	1:C:157:PHE:CD1	2.61	0.54
1:A:84:ASP:OD1	1:B:129:GLY:N	2.38	0.54
1:D:26:LYS:HD2	1:D:30:GLU:HA	1.89	0.54
1:B:112:PHE:HB3	1:B:118:TYR:HB3	1.90	0.54
1:C:141:GLY:O	1:D:70:SER:HB3	2.07	0.54
1:C:143:GLN:NE2	1:D:55:PHE:HA	2.22	0.54
1:C:9:GLU:OE1	1:C:64:ARG:CZ	2.53	0.54
1:B:98:PHE:H	1:B:98:PHE:HD1	1.55	0.54
1:B:15:SER:C	1:B:16:HIS:ND1	2.62	0.53
1:C:69:THR:O	1:C:71:ARG:HG3	2.08	0.53
1:B:91:THR:HA	1:B:103:MET:O	2.08	0.53
1:D:111:SER:HB2	1:D:114:ALA:H	1.72	0.53
1:A:18:LEU:HD22	1:A:20:GLY:O	2.09	0.53
1:C:153:ASP:O	1:C:156:ASP:N	2.41	0.53
1:A:99:THR:HG22	1:A:100:GLY:N	2.22	0.53
1:D:153:ASP:OD2	1:D:155:GLY:CA	2.55	0.53
1:A:11:PHE:CE2	1:A:61:GLU:HB3	2.44	0.53
1:A:153:ASP:O	1:A:156:ASP:OD1	2.27	0.53
1:B:25:LEU:HG	1:B:29:VAL:CG2	2.35	0.53
1:C:3:ILE:HG23	1:C:3:ILE:O	2.09	0.53
1:A:21:PRO:HD3	1:A:80:PRO:CD	2.39	0.53
1:B:155:GLY:C	1:B:157:PHE:N	2.62	0.53
1:B:18:LEU:HG	1:B:42:TRP:CH2	2.44	0.53
1:D:41:PRO:C	1:D:81:ILE:CD1	2.77	0.53
1:B:7:GLU:HG2	1:B:8:GLN:HG3	1.91	0.53
1:C:121:VAL:CB	1:C:164:VAL:CG2	2.86	0.53
1:A:22:CYS:O	1:A:22:CYS:SG	2.67	0.53
1:A:3:ILE:O	1:A:3:ILE:CG2	2.56	0.53
1:C:133:GLY:C	1:C:134:TYR:CD1	2.82	0.53
1:D:144:TYR:O	1:D:146:LEU:HD11	2.09	0.52
1:B:144:TYR:HD2	1:B:157:PHE:CE1	2.27	0.52
1:A:4:ILE:HB	1:A:6:PHE:HE1	1.74	0.52
1:D:95:ASN:ND2	1:D:96:PRO:O	2.42	0.52
1:D:8:GLN:HB2	1:D:14:HIS:CE1	2.43	0.52
1:B:88:HIS:HD2	1:B:169:ARG:CZ	2.19	0.52
1:A:2:LYS:NZ	1:A:17:GLU:OE1	2.42	0.52
1:A:94:GLU:O	1:A:122:SER:OG	2.27	0.52
1:C:94:GLU:CG	1:C:95:ASN:HD21	2.19	0.52
1:A:98:PHE:HD1	1:A:123:SER:HB3	1.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:CD	1:C:31:LYS:HE3	2.28	0.52
1:D:88:HIS:O	1:D:131:TRP:CZ2	2.59	0.52
1:D:41:PRO:CG	1:D:81:ILE:HD12	2.39	0.52
1:B:142:LEU:HB3	1:B:144:TYR:CE1	2.43	0.52
1:D:95:ASN:ND2	1:D:95:ASN:C	2.60	0.52
1:B:58:GLU:N	1:B:62:TYR:OH	2.42	0.52
1:A:91:THR:HG23	1:A:104:GLU:HA	1.92	0.52
1:D:65:TRP:CZ3	1:D:69:THR:HG21	2.44	0.52
1:B:26:LYS:HA	1:B:29:VAL:O	2.09	0.52
1:B:88:HIS:CD2	1:B:169:ARG:NH1	2.78	0.52
1:C:84:ASP:O	1:D:129:GLY:HA2	2.10	0.52
1:B:46:GLU:HB2	1:B:72:THR:HG23	1.91	0.52
1:C:130:THR:O	1:C:169:ARG:HG3	2.10	0.52
1:D:88:HIS:CD2	1:D:169:ARG:NH1	2.78	0.52
1:A:50:CYS:HB2	1:A:51:LYS:NZ	2.24	0.52
1:B:-1:ASN:HB2	1:B:1:PRO:CD	2.39	0.52
1:A:94:GLU:HG3	1:A:101:LYS:HB3	1.91	0.52
1:A:44:GLY:C	1:A:45:TYR:CG	2.82	0.52
1:B:8:GLN:CB	1:B:31:LYS:HZ3	2.23	0.52
1:D:55:PHE:HE2	1:D:75:LEU:HD13	1.75	0.52
1:D:131:TRP:CZ3	1:D:169:ARG:HB2	2.45	0.52
1:D:-2:LEU:HD12	1:D:2:LYS:HB2	1.91	0.52
1:C:25:LEU:CD2	1:C:28:THR:OG1	2.58	0.52
1:A:99:THR:CG2	1:A:100:GLY:N	2.72	0.52
1:D:34:SER:HB3	1:D:63:PRO:O	2.10	0.52
1:B:135:GLN:HB2	1:B:142:LEU:H	1.74	0.51
1:C:48:ALA:HA	1:C:76:SER:OG	2.09	0.51
1:C:11:PHE:C	1:C:12:GLN:NE2	2.64	0.51
1:B:16:HIS:ND1	1:B:16:HIS:N	2.58	0.51
1:A:129:GLY:HA2	1:B:84:ASP:HB3	1.92	0.51
1:A:7:GLU:OE2	1:A:13:GLY:C	2.49	0.51
1:B:2:LYS:HD3	1:B:38:GLN:OE1	2.10	0.51
1:A:135:GLN:HG2	1:A:136:TYR:CD1	2.45	0.51
1:B:3:ILE:HD12	1:B:37:VAL:HG13	1.93	0.51
1:A:89:LYS:HE2	1:A:127:GLN:NE2	2.25	0.51
1:A:95:ASN:O	1:A:96:PRO:O	2.28	0.51
1:C:94:GLU:HG2	1:C:101:LYS:H	1.75	0.51
1:C:173:MET:CE	1:D:83:VAL:CA	2.88	0.51
1:C:133:GLY:H	1:C:146:LEU:HD22	1.76	0.51
1:C:92:LEU:O	1:C:102:LYS:HA	2.10	0.51
1:D:9:GLU:O	1:D:10:ASN:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:O	1:A:139:TYR:C	2.48	0.51
1:D:15:SER:O	1:D:16:HIS:CD2	2.64	0.51
1:C:27:GLU:O	1:C:27:GLU:HG2	2.10	0.51
1:C:-1:ASN:C	1:C:-1:ASN:HD22	2.06	0.51
1:A:56:VAL:HG13	1:A:81:ILE:HD11	1.92	0.51
1:B:154:SER:OG	1:B:162:PRO:HB3	2.09	0.51
1:A:59:LYS:HB2	1:B:174:GLN:NE2	2.25	0.51
1:B:6:PHE:HA	1:B:14:HIS:O	2.10	0.51
1:B:46:GLU:HG3	1:B:73:ASP:HB2	1.92	0.51
1:C:175:TRP:CA	1:D:-1:ASN:HB3	2.24	0.51
1:C:124:VAL:HG13	1:C:151:TYR:HB2	1.93	0.51
1:C:25:LEU:HD11	1:C:78:LEU:CD1	2.41	0.51
1:C:36:LEU:HD23	1:C:37:VAL:N	2.26	0.51
1:D:132:VAL:HG21	1:D:170:ILE:HD11	1.92	0.50
1:A:370:SER:OG	1:B:142:LEU:CD2	2.59	0.50
1:D:65:TRP:CD1	1:D:66:ASP:N	2.79	0.50
1:D:48:ALA:N	1:D:76:SER:OG	2.43	0.50
1:C:-1:ASN:ND2	1:C:-1:ASN:C	2.65	0.50
1:A:93:TYR:OH	1:A:125:ARG:NH1	2.44	0.50
1:D:135:GLN:CG	1:D:142:LEU:H	2.08	0.50
1:A:-1:ASN:OD1	1:A:-1:ASN:N	2.43	0.50
1:A:92:LEU:HA	1:A:124:VAL:CG1	2.41	0.50
1:B:95:ASN:CB	1:B:99:THR:HB	2.41	0.50
1:A:175:TRP:CD1	1:B:40:GLY:O	2.60	0.50
1:B:53:GLU:OE2	1:B:72:THR:OG1	2.28	0.50
1:B:93:TYR:HE1	1:B:102:LYS:HB2	1.76	0.50
1:C:-1:ASN:H	1:C:-1:ASN:HD22	1.59	0.50
1:A:65:TRP:HA	1:A:68:TRP:CH2	2.47	0.50
1:B:43:VAL:HG22	1:B:81:ILE:HD11	1.94	0.50
1:C:143:GLN:HE22	1:D:55:PHE:HB3	1.76	0.50
1:B:96:PRO:O	1:B:97:ASN:C	2.50	0.50
1:B:7:GLU:HA	1:B:14:HIS:CE1	2.46	0.50
1:A:126:VAL:HG12	1:A:126:VAL:O	2.12	0.50
1:C:91:THR:HG23	1:C:104:GLU:CA	2.40	0.50
1:C:47:GLN:CB	1:C:52:GLY:HA3	2.42	0.50
1:C:51:LYS:HG2	1:C:52:GLY:H	1.69	0.50
1:A:62:TYR:N	1:A:63:PRO:HD3	2.25	0.50
1:B:119:GLU:OE2	1:B:119:GLU:N	2.44	0.50
1:C:145:LEU:HD22	1:D:43:VAL:HG21	1.94	0.50
1:B:93:TYR:HE2	1:B:125:ARG:HH21	1.59	0.50
1:C:65:TRP:HE3	1:C:72:THR:HG21	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:THR:HG21	1:D:371:ARG:H	1.77	0.49
1:B:8:GLN:O	1:B:9:GLU:C	2.49	0.49
1:D:67:SER:O	1:D:68:TRP:HB3	2.11	0.49
1:D:144:TYR:O	1:D:146:LEU:HD12	2.12	0.49
1:B:157:PHE:HE1	1:B:159:ALA:HB2	1.74	0.49
1:A:125:ARG:HG2	1:A:150:ASP:CG	2.32	0.49
1:B:-1:ASN:CB	1:B:1:PRO:HD2	2.41	0.49
1:A:48:ALA:C	1:A:50:CYS:H	2.15	0.49
1:A:48:ALA:C	1:A:50:CYS:N	2.65	0.49
1:D:98:PHE:CE1	1:D:123:SER:HB3	2.47	0.49
1:C:95:ASN:HB3	1:C:96:PRO:CD	2.42	0.49
1:A:20:GLY:O	1:A:21:PRO:C	2.50	0.49
1:A:32:ALA:HB2	1:A:75:LEU:CB	2.24	0.49
1:B:92:LEU:N	1:B:92:LEU:HD22	2.28	0.49
1:C:157:PHE:O	1:C:157:PHE:HD1	1.95	0.49
1:B:88:HIS:HD2	1:B:169:ARG:NE	2.11	0.49
1:A:9:GLU:O	1:A:10:ASN:CB	2.61	0.49
1:A:110:PRO:O	1:A:166:SER:CB	2.55	0.49
1:C:174:GLN:NE2	1:D:59:LYS:HB2	2.26	0.49
1:B:43:VAL:CG2	1:B:81:ILE:HG12	2.43	0.49
1:C:18:LEU:CD2	1:C:22:CYS:CB	2.86	0.49
1:A:6:PHE:CG	1:A:15:SER:HB3	2.47	0.49
1:B:43:VAL:HG23	1:B:81:ILE:HG12	1.95	0.49
1:A:86:GLN:CB	1:B:88:HIS:HE1	2.18	0.49
1:D:41:PRO:HG2	1:D:81:ILE:CD1	2.40	0.49
1:A:3:ILE:HG13	1:A:37:VAL:CG2	2.42	0.49
1:A:98:PHE:H	1:A:123:SER:CB	2.24	0.49
1:A:130:THR:O	1:A:169:ARG:HG3	2.12	0.49
1:A:94:GLU:HB2	1:A:101:LYS:O	2.12	0.49
1:B:144:TYR:HE2	1:B:157:PHE:HE1	1.56	0.49
1:A:11:PHE:HE2	1:A:61:GLU:HB3	1.78	0.49
1:B:46:GLU:HG3	1:B:73:ASP:CB	2.42	0.49
1:B:135:GLN:HG2	1:B:136:TYR:CD1	2.48	0.49
1:B:45:TYR:O	1:B:55:PHE:CZ	2.66	0.49
1:B:103:MET:SD	1:B:112:PHE:CE1	3.06	0.49
1:C:38:GLN:O	1:C:39:ALA:HB2	2.13	0.49
1:C:43:VAL:CG1	1:C:81:ILE:HD11	2.18	0.48
1:C:2:LYS:HB2	1:C:39:ALA:HB3	1.95	0.48
1:B:126:VAL:HG12	1:B:148:LYS:HA	1.95	0.48
1:B:7:GLU:HB2	1:B:14:HIS:CD2	2.48	0.48
1:B:144:TYR:HE2	1:B:159:ALA:HB2	1.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASP:O	1:C:173:MET:HG2	2.14	0.48
1:D:-1:ASN:HB2	1:D:1:PRO:CD	2.43	0.48
1:D:13:GLY:HA3	1:D:14:HIS:ND1	2.27	0.48
1:C:69:THR:C	1:C:370:SER:H	2.15	0.48
1:B:45:TYR:N	1:B:55:PHE:HE1	2.08	0.48
1:B:55:PHE:CZ	1:B:72:THR:HG21	2.45	0.48
1:D:87:GLU:CD	1:D:106:ILE:HD11	2.33	0.48
1:C:137:PRO:O	1:C:139:TYR:N	2.47	0.48
1:B:18:LEU:CD1	1:B:20:GLY:H	2.27	0.48
1:C:5:ILE:O	1:C:5:ILE:HG12	2.13	0.48
1:A:120:LYS:NZ	1:A:162:PRO:CB	2.77	0.48
1:C:94:GLU:HB3	1:C:118:TYR:OH	2.14	0.48
1:B:1:PRO:CG	1:B:80:PRO:HB3	2.44	0.48
1:C:25:LEU:HD11	1:C:78:LEU:HD12	1.94	0.48
1:B:46:GLU:HG3	1:B:73:ASP:N	2.29	0.48
1:D:137:PRO:HD3	1:D:165:GLN:CD	2.34	0.48
1:A:64:ARG:CG	1:A:64:ARG:NH1	2.36	0.48
1:B:1:PRO:O	1:B:19:ASN:HA	2.14	0.48
1:A:83:VAL:CG1	1:B:173:MET:SD	3.00	0.48
1:D:24:ASN:C	1:D:24:ASN:OD1	2.51	0.48
1:A:98:PHE:HE1	1:A:151:TYR:O	1.96	0.48
1:C:9:GLU:HB3	1:C:64:ARG:HH11	1.79	0.48
1:C:5:ILE:H	1:C:5:ILE:HD12	1.77	0.48
1:D:125:ARG:O	1:D:125:ARG:HG3	2.10	0.48
1:B:143:GLN:C	1:B:144:TYR:CD1	2.86	0.47
1:D:26:LYS:HA	1:D:29:VAL:O	2.14	0.47
1:C:136:TYR:C	1:C:165:GLN:HB2	2.34	0.47
1:A:23:PRO:O	1:A:24:ASN:HB2	2.13	0.47
1:A:55:PHE:CD1	1:A:55:PHE:N	2.82	0.47
1:C:145:LEU:C	1:C:146:LEU:HD13	2.35	0.47
1:C:159:ALA:HB1	1:C:161:GLN:O	2.14	0.47
1:C:91:THR:C	1:C:92:LEU:HD12	2.34	0.47
1:C:6:PHE:HA	1:C:14:HIS:O	2.14	0.47
1:D:102:LYS:CG	1:D:102:LYS:O	2.62	0.47
1:D:145:LEU:C	1:D:146:LEU:CD1	2.73	0.47
1:D:95:ASN:HD21	1:D:99:THR:CB	2.26	0.47
1:B:55:PHE:HE2	1:B:72:THR:CG2	2.18	0.47
1:B:65:TRP:HA	1:B:68:TRP:CZ2	2.50	0.47
1:C:-1:ASN:HA	1:D:175:TRP:CE3	2.49	0.47
1:B:121:VAL:HG21	1:B:164:VAL:HB	1.95	0.47
1:D:72:THR:HB	1:D:73:ASP:H	1.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:HB1	1:D:162:PRO:CA	2.43	0.47
1:A:131:TRP:CZ2	1:A:169:ARG:HD3	2.49	0.47
1:A:36:LEU:HD23	1:A:37:VAL:N	2.30	0.47
1:C:-6:LYS:N	1:C:-5:PRO:CD	2.77	0.47
1:B:147:GLU:O	1:B:148:LYS:C	2.52	0.47
1:D:23:PRO:O	1:D:48:ALA:HB1	2.15	0.47
1:C:136:TYR:O	1:C:165:GLN:HB2	2.14	0.47
1:C:46:GLU:CD	1:C:73:ASP:HB3	2.35	0.47
1:C:106:ILE:O	1:C:306:ASP:HB2	2.14	0.47
1:A:59:LYS:CD	1:B:174:GLN:HE22	2.23	0.47
1:A:136:TYR:HB3	1:A:137:PRO:HD2	1.97	0.47
1:C:25:LEU:HA	1:C:28:THR:CB	2.45	0.47
1:A:65:TRP:CG	1:A:66:ASP:N	2.83	0.47
1:A:59:LYS:HB2	1:B:174:GLN:OE1	2.14	0.47
1:D:95:ASN:ND2	1:D:99:THR:OG1	2.25	0.47
1:C:14:HIS:ND1	1:C:29:VAL:CG1	2.77	0.47
1:C:72:THR:O	1:C:72:THR:HG23	2.15	0.47
1:C:2:LYS:CB	1:C:39:ALA:HB3	2.45	0.47
1:C:9:GLU:HA	1:C:34:SER:OG	2.15	0.47
1:B:7:GLU:O	1:B:31:LYS:HD2	2.15	0.47
1:B:25:LEU:O	1:B:29:VAL:HG23	2.15	0.47
1:C:36:LEU:CD2	1:C:36:LEU:C	2.83	0.47
1:C:90:ILE:HG22	1:C:105:VAL:HB	1.97	0.47
1:A:101:LYS:HG3	1:A:118:TYR:CE1	2.50	0.47
1:C:98:PHE:CE1	1:C:123:SER:HB3	2.50	0.47
1:D:144:TYR:CZ	1:D:158:GLY:O	2.68	0.46
1:A:135:GLN:CG	1:A:136:TYR:CE1	2.98	0.46
1:B:18:LEU:HD11	1:B:20:GLY:H	1.80	0.46
1:B:8:GLN:HB3	1:B:31:LYS:HZ3	1.79	0.46
1:C:88:HIS:O	1:C:131:TRP:HZ2	1.97	0.46
1:C:43:VAL:HG11	1:D:145:LEU:HD22	1.97	0.46
1:A:137:PRO:HD3	1:A:165:GLN:CD	2.35	0.46
1:C:75:LEU:HD12	1:C:76:SER:H	1.80	0.46
1:B:27:GLU:C	1:B:328:GLY:H	2.19	0.46
1:C:88:HIS:CD2	1:C:169:ARG:NH1	2.83	0.46
1:A:48:ALA:CA	1:A:76:SER:HB2	2.45	0.46
1:B:25:LEU:CD1	1:B:29:VAL:HG21	2.45	0.46
1:B:370:SER:O	1:B:71:ARG:HB2	2.16	0.46
1:A:120:LYS:NZ	1:A:162:PRO:HB2	2.29	0.46
1:D:154:SER:O	1:D:157:PHE:CD1	2.69	0.46
1:D:15:SER:O	1:D:16:HIS:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:HB3	1:B:31:LYS:HZ1	1.80	0.46
1:B:46:GLU:HA	1:B:72:THR:HG22	1.97	0.46
1:C:-6:LYS:H	1:C:-5:PRO:CD	2.28	0.46
1:B:46:GLU:CG	1:B:73:ASP:OD2	2.63	0.46
1:B:27:GLU:O	1:B:328:GLY:N	2.48	0.46
1:D:46:GLU:HB2	1:D:53:GLU:HB2	1.96	0.46
1:B:26:LYS:CG	1:B:76:SER:HA	2.44	0.46
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.53	0.46
1:B:24:ASN:OD1	1:B:26:LYS:HB2	2.16	0.46
1:C:22:CYS:O	1:C:23:PRO:C	2.53	0.46
1:A:133:GLY:CA	1:A:167:VAL:HG23	2.46	0.46
1:B:95:ASN:O	1:B:122:SER:HB2	2.15	0.46
1:A:131:TRP:CE3	1:A:169:ARG:HB2	2.51	0.46
1:D:9:GLU:O	1:D:10:ASN:CB	2.63	0.46
1:C:42:TRP:CH2	1:C:80:PRO:HG3	2.51	0.46
1:A:144:TYR:CZ	1:A:159:ALA:HB2	2.50	0.46
1:D:169:ARG:O	1:D:170:ILE:C	2.52	0.46
1:A:10:ASN:HB2	1:A:12:GLN:NE2	2.27	0.46
1:A:28:THR:HG21	1:A:29:VAL:CG1	2.40	0.46
1:B:19:ASN:N	1:B:19:ASN:OD1	2.49	0.46
1:B:9:GLU:HG2	1:B:64:ARG:CG	2.46	0.46
1:C:121:VAL:CG2	1:C:164:VAL:HG23	2.45	0.46
1:D:102:LYS:HG3	1:D:102:LYS:O	2.15	0.46
1:C:134:TYR:OH	1:C:168:ARG:NE	2.30	0.45
1:C:26:LYS:N	1:C:26:LYS:HD3	2.31	0.45
1:C:-1:ASN:HB2	1:C:1:PRO:HD2	1.98	0.45
1:B:103:MET:CE	1:B:112:PHE:CD1	2.99	0.45
1:C:3:ILE:HD12	1:C:37:VAL:HG22	1.97	0.45
1:B:132:VAL:O	1:B:132:VAL:HG22	2.16	0.45
1:A:48:ALA:N	1:A:76:SER:HB2	2.31	0.45
1:C:174:GLN:O	1:D:39:ALA:HB1	2.15	0.45
1:A:145:LEU:C	1:A:146:LEU:HD12	2.35	0.45
1:D:3:ILE:HB	1:D:42:TRP:CE2	2.51	0.45
1:C:41:PRO:HB2	1:C:81:ILE:HG13	1.97	0.45
1:C:59:LYS:HB2	1:D:174:GLN:OE1	2.16	0.45
1:D:-1:ASN:N	1:D:-1:ASN:OD1	2.48	0.45
1:D:142:LEU:HD12	1:D:142:LEU:HA	1.56	0.45
1:C:46:GLU:HB2	1:C:55:PHE:CZ	2.52	0.45
1:A:86:GLN:H	1:B:88:HIS:CE1	2.34	0.45
1:A:136:TYR:HB3	1:A:137:PRO:CD	2.47	0.45
1:B:4:ILE:CG2	1:B:16:HIS:O	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-4:GLN:O	1:C:-3:PRO:C	2.55	0.45
1:B:106:ILE:HG22	1:B:106:ILE:O	2.16	0.45
1:D:152:LYS:HA	1:D:156:ASP:CB	2.46	0.45
1:D:-1:ASN:O	1:D:39:ALA:CB	2.55	0.45
1:D:131:TRP:CZ3	1:D:169:ARG:HD3	2.51	0.45
1:C:174:GLN:N	1:C:174:GLN:CD	2.71	0.45
1:B:18:LEU:HG	1:B:42:TRP:HH2	1.80	0.45
1:C:135:GLN:CB	1:C:142:LEU:H	2.19	0.45
1:C:-4:GLN:HA	1:C:-3:PRO:HD3	1.59	0.45
1:D:45:TYR:CD2	1:D:50:CYS:HA	2.52	0.45
1:D:6:PHE:N	1:D:6:PHE:CD1	2.84	0.45
1:A:94:GLU:HG2	1:A:119:GLU:HB2	1.98	0.45
1:D:132:VAL:HG23	1:D:170:ILE:CG1	2.47	0.45
1:C:120:LYS:HB2	1:C:162:PRO:O	2.17	0.45
1:A:48:ALA:O	1:A:50:CYS:N	2.51	0.45
1:B:7:GLU:N	1:B:14:HIS:CD2	2.85	0.45
1:B:53:GLU:HG2	1:B:53:GLU:O	2.16	0.45
1:A:1:PRO:HB2	1:A:42:TRP:CZ2	2.52	0.45
1:D:49:ASN:O	1:D:51:LYS:HG3	2.17	0.45
1:D:69:THR:HB	1:D:71:ARG:CA	2.47	0.44
1:C:144:TYR:O	1:C:146:LEU:HD13	2.17	0.44
1:B:144:TYR:CD2	1:B:157:PHE:CD1	3.05	0.44
1:A:18:LEU:CD2	1:A:22:CYS:CB	2.88	0.44
1:A:125:ARG:HA	1:A:150:ASP:HA	2.00	0.44
1:A:105:VAL:C	1:A:106:ILE:HG13	2.37	0.44
1:C:157:PHE:CE1	1:C:159:ALA:HB2	2.52	0.44
1:D:169:ARG:HG2	1:D:169:ARG:NH1	2.31	0.44
1:C:94:GLU:CG	1:C:100:GLY:HA3	2.48	0.44
1:B:6:PHE:HB2	1:B:34:SER:HB2	1.99	0.44
1:C:135:GLN:HE22	1:C:142:LEU:HD13	1.81	0.44
1:B:89:LYS:HG3	1:B:106:ILE:HG12	1.99	0.44
1:B:108:ASP:OD1	1:B:168:ARG:HA	2.17	0.44
1:D:154:SER:CB	1:D:162:PRO:HD3	2.47	0.44
1:C:86:GLN:N	1:C:86:GLN:OE1	2.36	0.44
1:D:108:ASP:HB3	1:D:139:TYR:OH	2.17	0.44
1:D:23:PRO:O	1:D:24:ASN:CB	2.52	0.44
1:D:-2:LEU:O	1:D:-1:ASN:O	2.35	0.44
1:A:10:ASN:HB2	1:A:12:GLN:HE21	1.70	0.44
1:D:95:ASN:OD1	1:D:99:THR:HB	2.18	0.44
1:C:5:ILE:HD11	1:C:16:HIS:O	2.15	0.44
1:A:120:LYS:NZ	1:A:162:PRO:CG	2.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG22	1:B:134:TYR:CE2	2.53	0.44
1:A:4:ILE:O	1:A:6:PHE:CE1	2.71	0.44
1:D:-2:LEU:HD11	1:D:2:LYS:HD2	1.99	0.44
1:D:65:TRP:CG	1:D:66:ASP:N	2.86	0.44
1:A:130:THR:HB	1:B:83:VAL:HG13	1.99	0.44
1:A:49:ASN:O	1:A:51:LYS:HE2	2.18	0.44
1:C:134:TYR:HD1	1:C:166:SER:O	2.01	0.44
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.32	0.44
1:B:22:CYS:HA	1:B:23:PRO:HD3	1.11	0.44
1:C:25:LEU:HD23	1:C:28:THR:OG1	2.18	0.44
1:B:121:VAL:O	1:B:162:PRO:HB3	2.18	0.43
1:A:45:TYR:CE1	1:A:54:GLN:HB3	2.53	0.43
1:C:-6:LYS:H	1:C:-5:PRO:HD2	1.83	0.43
1:D:50:CYS:O	1:D:51:LYS:HG2	2.18	0.43
1:A:109:VAL:HA	1:A:110:PRO:HD2	1.85	0.43
1:A:102:LYS:HB3	1:A:102:LYS:HE2	1.12	0.43
1:A:8:GLN:CB	1:A:12:GLN:O	2.64	0.43
1:B:8:GLN:C	1:B:9:GLU:O	2.54	0.43
1:C:93:TYR:CE1	1:C:102:LYS:HE3	2.53	0.43
1:C:22:CYS:O	1:C:24:ASN:N	2.52	0.43
1:A:370:SER:C	1:A:371:ARG:N	2.69	0.43
1:B:153:ASP:CG	1:B:154:SER:N	2.71	0.43
1:D:46:GLU:HB3	1:D:53:GLU:N	2.34	0.43
1:D:41:PRO:HG2	1:D:81:ILE:HD13	2.00	0.43
1:B:1:PRO:HG2	1:B:80:PRO:HB3	2.00	0.43
1:C:121:VAL:HG21	1:C:164:VAL:CG2	2.48	0.43
1:B:26:LYS:HG2	1:B:75:LEU:O	2.18	0.43
1:B:90:ILE:HG22	1:B:105:VAL:HB	1.99	0.43
1:B:7:GLU:HA	1:B:14:HIS:HE2	1.75	0.43
1:B:27:GLU:C	1:B:328:GLY:N	2.72	0.43
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.66	0.43
1:A:40:GLY:O	1:B:174:GLN:HG3	2.19	0.43
1:B:6:PHE:C	1:B:14:HIS:CD2	2.92	0.43
1:C:158:GLY:O	1:C:160:PRO:HD3	2.19	0.43
1:A:112:PHE:N	1:A:165:GLN:O	2.48	0.43
1:B:69:THR:HG23	1:B:69:THR:O	2.19	0.43
1:D:92:LEU:HD13	1:D:112:PHE:HZ	1.80	0.43
1:C:1:PRO:HB3	1:C:80:PRO:HB3	2.00	0.43
1:A:72:THR:OG1	1:A:73:ASP:N	2.52	0.43
1:B:8:GLN:CB	1:B:31:LYS:HZ1	2.25	0.43
1:B:26:LYS:HD3	1:B:30:GLU:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG12	1:A:106:ILE:N	2.33	0.43
1:C:24:ASN:O	1:C:27:GLU:HB3	2.18	0.43
1:B:90:ILE:CD1	1:B:167:VAL:HG21	2.49	0.43
1:D:-3:PRO:C	1:D:-1:ASN:N	2.72	0.43
1:C:110:PRO:O	1:C:138:GLY:N	2.48	0.43
1:B:49:ASN:N	1:B:49:ASN:ND2	2.65	0.43
1:B:112:PHE:O	1:B:116:HIS:N	2.48	0.43
1:C:1:PRO:HD3	1:D:175:TRP:CE3	2.53	0.43
1:C:95:ASN:N	1:C:95:ASN:ND2	2.50	0.42
1:A:18:LEU:HD21	1:A:22:CYS:HB3	1.98	0.42
1:B:95:ASN:HB2	1:B:99:THR:O	2.19	0.42
1:D:6:PHE:H	1:D:6:PHE:HD1	1.65	0.42
1:D:122:SER:O	1:D:157:PHE:HE2	2.01	0.42
1:C:83:VAL:O	1:C:83:VAL:HG12	2.19	0.42
1:D:132:VAL:HG12	1:D:134:TYR:CE1	2.55	0.42
1:C:45:TYR:O	1:C:75:LEU:HD12	2.19	0.42
1:B:101:LYS:HE3	1:B:119:GLU:OE1	2.20	0.42
1:D:41:PRO:O	1:D:81:ILE:CD1	2.68	0.42
1:A:3:ILE:CG1	1:A:37:VAL:HG22	2.49	0.42
1:A:44:GLY:O	1:A:45:TYR:CE2	2.71	0.42
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.87	0.42
1:D:45:TYR:CD2	1:D:50:CYS:HB3	2.54	0.42
1:B:151:TYR:CD1	1:B:151:TYR:N	2.88	0.42
1:A:123:SER:O	1:A:124:VAL:HG13	2.18	0.42
1:C:91:THR:CG2	1:C:104:GLU:HA	2.45	0.42
1:C:16:HIS:CE1	1:C:18:LEU:HD12	2.54	0.42
1:C:44:GLY:HA3	1:C:78:LEU:HD23	2.01	0.42
1:A:92:LEU:HA	1:A:124:VAL:HG13	2.02	0.42
1:B:26:LYS:HE2	1:B:74:SER:C	2.39	0.42
1:C:144:TYR:CE1	1:C:159:ALA:HA	2.54	0.42
1:A:46:GLU:HG2	1:A:52:GLY:HA3	2.01	0.42
1:A:125:ARG:HG2	1:A:150:ASP:OD1	2.20	0.42
1:C:153:ASP:O	1:C:155:GLY:N	2.52	0.42
1:D:97:ASN:HD21	1:D:152:LYS:HE2	1.85	0.42
1:D:95:ASN:HD22	1:D:96:PRO:N	2.18	0.42
1:A:144:TYR:HE1	1:A:158:GLY:O	2.03	0.42
1:A:173:MET:HE2	1:A:173:MET:HB2	2.00	0.42
1:D:110:PRO:HA	1:D:166:SER:HB2	2.01	0.42
1:B:134:TYR:O	1:B:164:VAL:HA	2.20	0.42
1:A:46:GLU:C	1:A:76:SER:OG	2.58	0.42
1:D:25:LEU:HD11	1:D:78:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLY:O	1:C:34:SER:OG	2.37	0.42
1:C:153:ASP:O	1:C:154:SER:C	2.58	0.42
1:C:25:LEU:HD22	1:C:28:THR:OG1	2.20	0.42
1:D:49:ASN:O	1:D:51:LYS:CG	2.68	0.42
1:C:65:TRP:N	1:C:65:TRP:CD1	2.87	0.42
1:D:93:TYR:CE1	1:D:102:LYS:HB3	2.54	0.42
1:C:53:GLU:CD	1:C:55:PHE:CE1	2.85	0.41
1:B:154:SER:O	1:B:159:ALA:HB3	2.19	0.41
1:A:92:LEU:HA	1:A:124:VAL:HG12	2.01	0.41
1:C:159:ALA:HA	1:C:160:PRO:HD3	1.69	0.41
1:A:90:ILE:O	1:A:90:ILE:CG2	2.68	0.41
1:D:147:GLU:O	1:D:148:LYS:C	2.57	0.41
1:D:71:ARG:O	1:D:371:ARG:CB	2.66	0.41
1:A:16:HIS:HE1	1:A:18:LEU:HG	1.86	0.41
1:A:36:LEU:HD23	1:A:37:VAL:H	1.84	0.41
1:A:47:GLN:C	1:A:48:ALA:O	2.57	0.41
1:A:32:ALA:CB	1:A:75:LEU:H	2.33	0.41
1:A:28:THR:HG22	1:A:328:GLY:N	2.36	0.41
1:A:49:ASN:O	1:A:50:CYS:CB	2.67	0.41
1:A:54:GLN:C	1:A:55:PHE:CG	2.94	0.41
1:B:109:VAL:HA	1:B:110:PRO:HD2	1.90	0.41
1:C:2:LYS:O	1:C:39:ALA:N	2.54	0.41
1:A:6:PHE:HB3	1:A:7:GLU:H	1.50	0.41
1:C:122:SER:O	1:C:153:ASP:HA	2.21	0.41
1:C:35:VAL:CG1	1:C:36:LEU:N	2.82	0.41
1:D:55:PHE:CE2	1:D:75:LEU:HD13	2.55	0.41
1:A:159:ALA:HA	1:A:160:PRO:HD2	1.88	0.41
1:B:146:LEU:HD13	1:B:146:LEU:N	2.35	0.41
1:D:7:GLU:HG2	1:D:31:LYS:O	2.20	0.41
1:B:45:TYR:CE2	1:B:50:CYS:O	2.74	0.41
1:A:18:LEU:CD2	1:A:22:CYS:HB3	2.50	0.41
1:A:135:GLN:O	1:A:165:GLN:HG3	2.21	0.41
1:A:93:TYR:CE1	1:A:102:LYS:CE	3.03	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.75	0.41
1:C:44:GLY:N	1:C:55:PHE:O	2.53	0.41
1:C:-1:ASN:O	1:C:1:PRO:C	2.58	0.41
1:D:161:GLN:HA	1:D:162:PRO:HD2	1.82	0.41
1:D:26:LYS:HD3	1:D:26:LYS:HA	1.09	0.41
1:D:47:GLN:CG	1:D:51:LYS:O	2.69	0.41
1:D:6:PHE:HD2	1:D:11:PHE:O	2.00	0.41
1:A:36:LEU:CD2	1:A:37:VAL:N	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:CG2	1:C:164:VAL:CG2	2.99	0.41
1:C:132:VAL:HG21	1:D:56:VAL:HG21	2.03	0.41
1:C:93:TYR:HE2	1:C:125:ARG:HB2	1.86	0.41
1:A:69:THR:HG22	1:A:370:SER:CB	2.51	0.41
1:C:37:VAL:CG1	1:C:59:LYS:HA	2.43	0.41
1:C:65:TRP:CE3	1:C:72:THR:HG21	2.54	0.41
1:B:87:GLU:OE1	1:B:106:ILE:HD13	2.21	0.41
1:B:161:GLN:OE1	1:B:163:GLN:HB2	2.21	0.41
1:B:121:VAL:O	1:B:162:PRO:HB2	2.20	0.40
1:A:54:GLN:H	1:A:54:GLN:HG2	1.38	0.40
1:D:114:ALA:C	1:D:117:GLY:H	2.24	0.40
1:B:119:GLU:N	1:B:119:GLU:CD	2.74	0.40
1:D:131:TRP:CH2	1:D:169:ARG:CD	3.04	0.40
1:A:64:ARG:NH1	1:A:66:ASP:OD2	2.54	0.40
1:C:151:TYR:HB3	1:C:156:ASP:HB3	2.03	0.40
1:D:9:GLU:HG2	1:D:10:ASN:CB	2.48	0.40
1:B:90:ILE:HD12	1:B:167:VAL:HG21	2.03	0.40
1:D:108:ASP:O	1:D:109:VAL:HG13	2.21	0.40
1:D:132:VAL:CG2	1:D:170:ILE:CG1	2.99	0.40
1:A:22:CYS:HA	1:A:23:PRO:HD3	1.77	0.40
1:D:98:PHE:HE1	1:D:123:SER:HB3	1.86	0.40
1:C:102:LYS:HB3	1:C:102:LYS:HE3	1.86	0.40
1:A:-4:GLN:HA	1:A:-3:PRO:HD3	1.72	0.40
1:A:24:ASN:ND2	1:A:48:ALA:HB1	2.36	0.40
1:A:50:CYS:N	1:A:77:SER:OG	2.52	0.40
1:B:45:TYR:O	1:B:55:PHE:HZ	2.04	0.40
1:C:89:LYS:HB3	1:C:127:GLN:HB3	2.04	0.40

All (3) 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:A:19:ASN:ND2	1:D:-4:GLN:O[1_554]	1.99	0.21
1:A:67:SER:OG	1:A:136:TYR:CD2[3_555]	2.02	0.18
1:C:371:ARG:CD	1:C:371:ARG:CD[4_555]	2.03	0.17

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	183/204 (90%)	144 (79%)	21 (12%)	18 (10%)	1 5
1	B	179/204 (88%)	130 (73%)	34 (19%)	15 (8%)	1 7
1	C	185/204 (91%)	137 (74%)	31 (17%)	17 (9%)	1 6
1	D	181/204 (89%)	136 (75%)	29 (16%)	16 (9%)	1 7
All	All	728/816 (89%)	547 (75%)	115 (16%)	66 (9%)	1 6

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	48	ALA
1	A	65	TRP
1	A	73	ASP
1	A	96	PRO
1	A	306	ASP
1	A	160	PRO
1	B	9	GLU
1	B	71	ARG
1	B	156	ASP
1	C	-5	PRO
1	C	-4	GLN
1	C	-3	PRO
1	C	21	PRO
1	C	29	VAL
1	D	14	HIS
1	D	70	SER
1	D	119	GLU
1	D	152	LYS
1	A	14	HIS
1	A	32	ALA
1	B	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	LEU
1	C	-6	LYS
1	C	64	ARG
1	C	71	ARG
1	C	154	SER
1	C	156	ASP
1	D	-1	ASN
1	D	9	GLU
1	D	328	GLY
1	D	65	TRP
1	D	156	ASP
1	D	162	PRO
1	D	167	VAL
1	A	59	LYS
1	A	110	PRO
1	A	139	TYR
1	A	174	GLN
1	B	14	HIS
1	B	63	PRO
1	B	70	SER
1	B	370	SER
1	B	148	LYS
1	C	74	SER
1	D	67	SER
1	D	71	ARG
1	A	64	ARG
1	A	74	SER
1	B	10	ASN
1	C	138	GLY
1	D	68	TRP
1	A	67	SER
1	B	306	ASP
1	C	306	ASP
1	C	136	TYR
1	C	148	LYS
1	D	50	CYS
1	B	124	VAL
1	D	137	PRO
1	A	162	PRO
1	B	35	VAL
1	C	23	PRO
1	B	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	22	CYS
1	A	136	TYR

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	162/177 (92%)	104 (64%)	58 (36%)	0 1
1	B	159/177 (90%)	104 (65%)	55 (35%)	0 1
1	C	163/177 (92%)	111 (68%)	52 (32%)	0 1
1	D	161/177 (91%)	114 (71%)	47 (29%)	0 1
All	All	645/708 (91%)	433 (67%)	212 (33%)	0 1

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	LEU
1	A	4	ILE
1	A	5	ILE
1	A	7	GLU
1	A	9	GLU
1	A	10	ASN
1	A	18	LEU
1	A	22	CYS
1	A	25	LEU
1	A	26	LYS
1	A	29	VAL
1	A	31	LYS
1	A	34	SER
1	A	36	LEU
1	A	37	VAL
1	A	47	GLN
1	A	49	ASN
1	A	51	LYS
1	A	55	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	ARG
1	A	67	SER
1	A	70	SER
1	A	370	SER
1	A	71	ARG
1	A	73	ASP
1	A	74	SER
1	A	79	ARG
1	A	83	VAL
1	A	87	GLU
1	A	91	THR
1	A	94	GLU
1	A	95	ASN
1	A	102	LYS
1	A	103	MET
1	A	107	ASP
1	A	108	ASP
1	A	109	VAL
1	A	111	SER
1	A	113	HIS
1	A	318	GLN
1	A	119	GLU
1	A	120	LYS
1	A	122	SER
1	A	123	SER
1	A	124	VAL
1	A	127	GLN
1	A	135	GLN
1	A	139	TYR
1	A	143	GLN
1	A	150	ASP
1	A	152	LYS
1	A	157	PHE
1	A	163	GLN
1	A	167	VAL
1	A	170	ILE
1	A	172	ASP
1	A	173	MET
1	A	174	GLN
1	B	-2	LEU
1	B	-1	ASN
1	B	2	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3	ILE
1	B	8	GLN
1	B	9	GLU
1	B	12	GLN
1	B	14	HIS
1	B	16	HIS
1	B	19	ASN
1	B	25	LEU
1	B	27	GLU
1	B	29	VAL
1	B	30	GLU
1	B	34	SER
1	B	37	VAL
1	B	47	GLN
1	B	50	CYS
1	B	53	GLU
1	B	55	PHE
1	B	64	ARG
1	B	67	SER
1	B	370	SER
1	B	71	ARG
1	B	371	ARG
1	B	74	SER
1	B	77	SER
1	B	79	ARG
1	B	89	LYS
1	B	90	ILE
1	B	91	THR
1	B	92	LEU
1	B	94	GLU
1	B	95	ASN
1	B	98	PHE
1	B	102	LYS
1	B	107	ASP
1	B	118	TYR
1	B	318	GLN
1	B	120	LYS
1	B	132	VAL
1	B	139	TYR
1	B	142	LEU
1	B	143	GLN
1	B	146	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	147	GLU
1	B	154	SER
1	B	157	PHE
1	B	160	PRO
1	B	167	VAL
1	B	168	ARG
1	B	172	ASP
1	B	173	MET
1	B	174	GLN
1	B	175	TRP
1	C	-6	LYS
1	C	-4	GLN
1	C	-2	LEU
1	C	-1	ASN
1	C	2	LYS
1	C	5	ILE
1	C	6	PHE
1	C	8	GLN
1	C	18	LEU
1	C	26	LYS
1	C	27	GLU
1	C	28	THR
1	C	29	VAL
1	C	30	GLU
1	C	31	LYS
1	C	51	LYS
1	C	58	GLU
1	C	64	ARG
1	C	67	SER
1	C	69	THR
1	C	370	SER
1	C	371	ARG
1	C	72	THR
1	C	74	SER
1	C	75	LEU
1	C	76	SER
1	C	81	ILE
1	C	82	LYS
1	C	85	SER
1	C	86	GLN
1	C	87	GLU
1	C	91	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	ASN
1	C	101	LYS
1	C	103	MET
1	C	108	ASP
1	C	113	HIS
1	C	318	GLN
1	C	122	SER
1	C	124	VAL
1	C	125	ARG
1	C	132	VAL
1	C	142	LEU
1	C	146	LEU
1	C	147	GLU
1	C	150	ASP
1	C	154	SER
1	C	156	ASP
1	C	166	SER
1	C	171	ARG
1	C	172	ASP
1	C	174	GLN
1	D	2	LYS
1	D	5	ILE
1	D	6	PHE
1	D	10	ASN
1	D	12	GLN
1	D	14	HIS
1	D	26	LYS
1	D	28	THR
1	D	29	VAL
1	D	36	LEU
1	D	38	GLN
1	D	50	CYS
1	D	55	PHE
1	D	65	TRP
1	D	67	SER
1	D	69	THR
1	D	71	ARG
1	D	371	ARG
1	D	72	THR
1	D	76	SER
1	D	77	SER
1	D	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	79	ARG
1	D	81	ILE
1	D	82	LYS
1	D	86	GLN
1	D	88	HIS
1	D	89	LYS
1	D	90	ILE
1	D	91	THR
1	D	94	GLU
1	D	95	ASN
1	D	98	PHE
1	D	99	THR
1	D	120	LYS
1	D	121	VAL
1	D	122	SER
1	D	124	VAL
1	D	125	ARG
1	D	127	GLN
1	D	140	ARG
1	D	142	LEU
1	D	143	GLN
1	D	161	GLN
1	D	170	ILE
1	D	172	ASP
1	D	174	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	16	HIS
1	A	95	ASN
1	A	127	GLN
1	B	8	GLN
1	B	12	GLN
1	B	47	GLN
1	B	49	ASN
1	B	88	HIS
1	B	113	HIS
1	B	318	GLN
1	B	165	GLN
1	B	174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	-4	GLN
1	C	-1	ASN
1	C	10	ASN
1	C	95	ASN
1	C	113	HIS
1	C	127	GLN
1	C	135	GLN
1	C	143	GLN
1	C	165	GLN
1	D	19	ASN
1	D	95	ASN
1	D	135	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.