



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:07 AM UTC

PDB ID : 3ER8 / pdb_00003er8
Title : Crystal structure of the heterodimeric vaccinia virus mRNA polyadenylate polymerase complex with two fragments of RNA
Authors : Li, C.; Li, H.; Zhou, S.; Poulos, T.L.; Gershon, P.D.
Deposited on : 2008-10-01
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

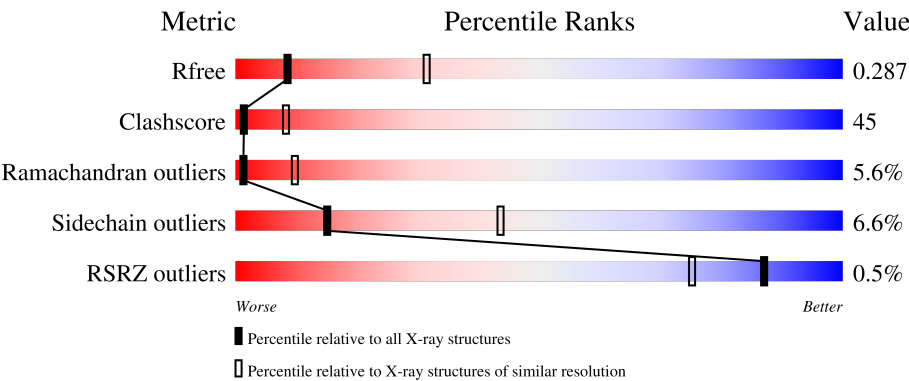
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.18 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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	43%46%8%.
1	B	297	44%46%7%.
2	C	479	% 26%56%10%.7%
2	D	479	28%54%10%.7%
3	E	5	20% 40%20%40%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	3	33% 67%
5	G	3	100%
5	H	3	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12289 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 Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2382	1552	394	424	12			
1	B	288	Total	C	N	O	S	0	0	0
			2382	1552	394	424	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	ARG	engineered mutation	UNP P07617
A	142	ALA	LYS	engineered mutation	UNP P07617
A	143	ALA	ARG	engineered mutation	UNP P07617
B	140	ALA	ARG	engineered mutation	UNP P07617
B	142	ALA	LYS	engineered mutation	UNP P07617
B	143	ALA	ARG	engineered mutation	UNP P07617

- Molecule 2 is a protein called Poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	445	Total	C	N	O	S	0	0	0
			3627	2318	605	680	24			
2	D	445	Total	C	N	O	S	0	0	0
			3627	2318	605	680	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	36	SER	LEU	engineered mutation	UNP P23371
D	36	SER	LEU	engineered mutation	UNP P23371

- Molecule 3 is DNA/RNA hybrid called RNA/DNA chimera 5'-D(CP*CP*)R(UP*UP*)D(C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			

- Molecule 4 is DNA/RNA hybrid called RNA/DNA chimera 5'-R(P*UP*UP*)D(C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	P	0	0	0
			59	27	7	22	3			

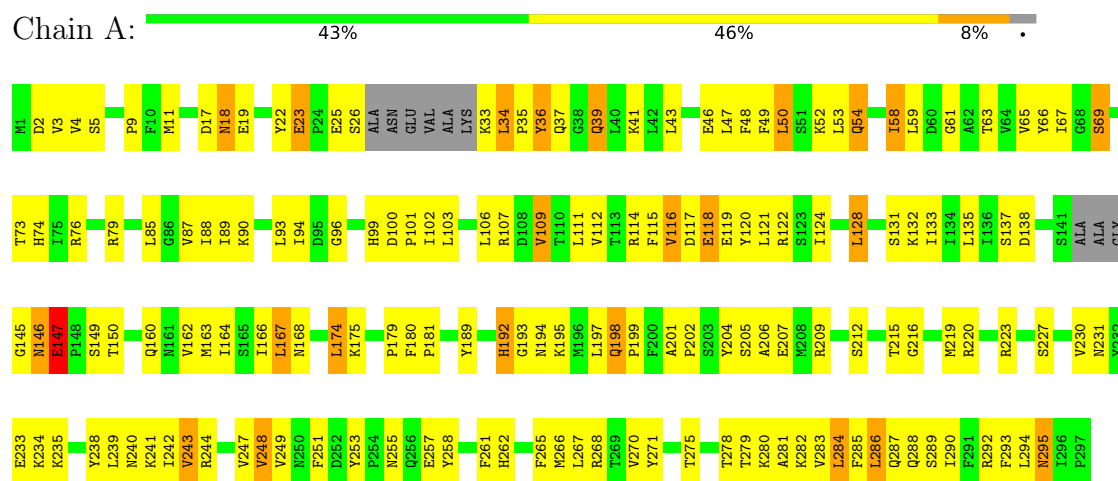
- Molecule 5 is DNA/RNA hybrid called RNA/DNA chimera 5'-D(P*CP*)R(UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	P	0	0	0
			59	27	7	22	3			
5	H	3	Total	C	N	O	P	0	0	0
			59	27	7	22	3			

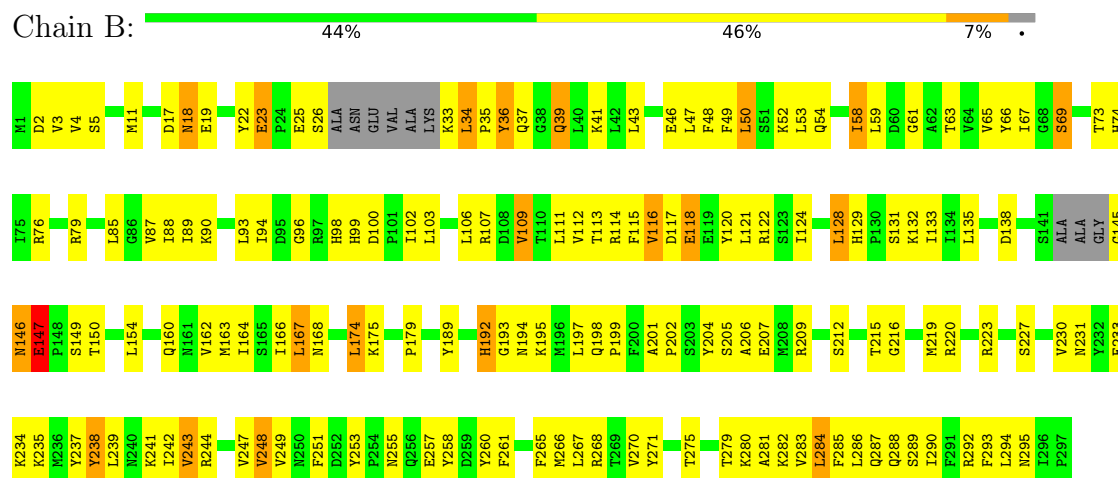
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase

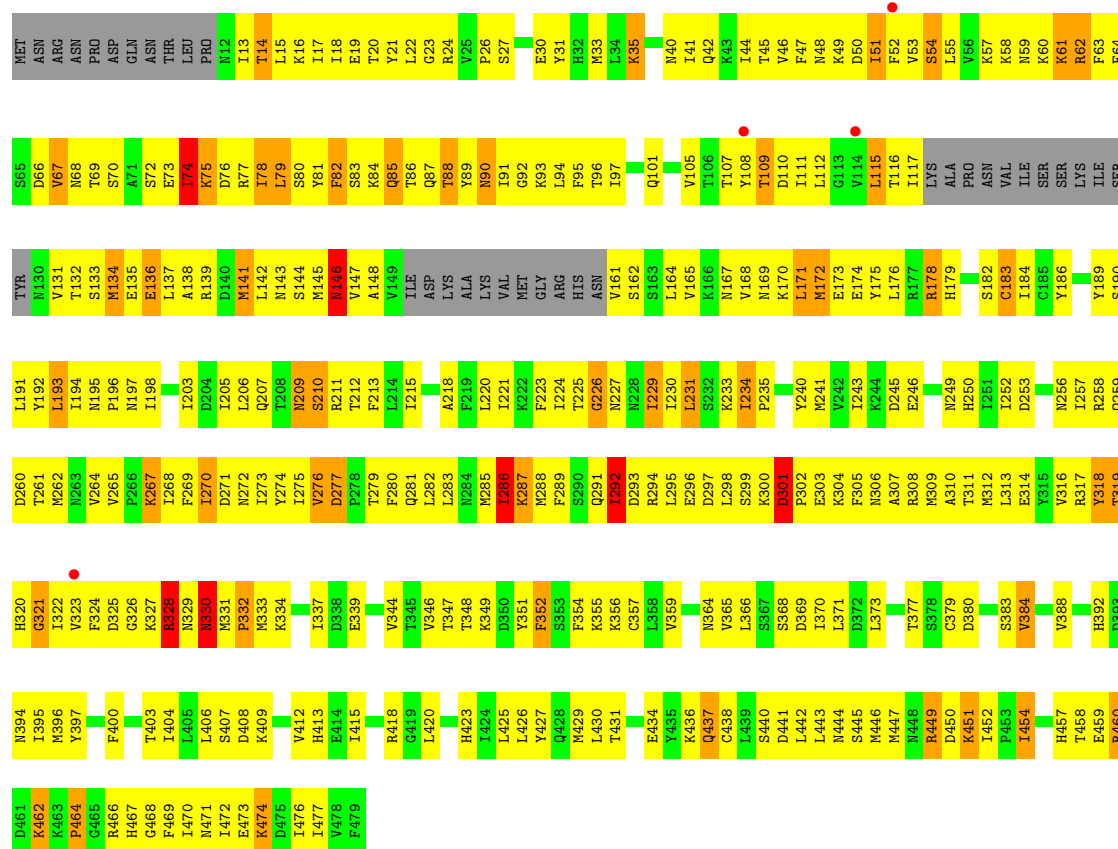


• Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



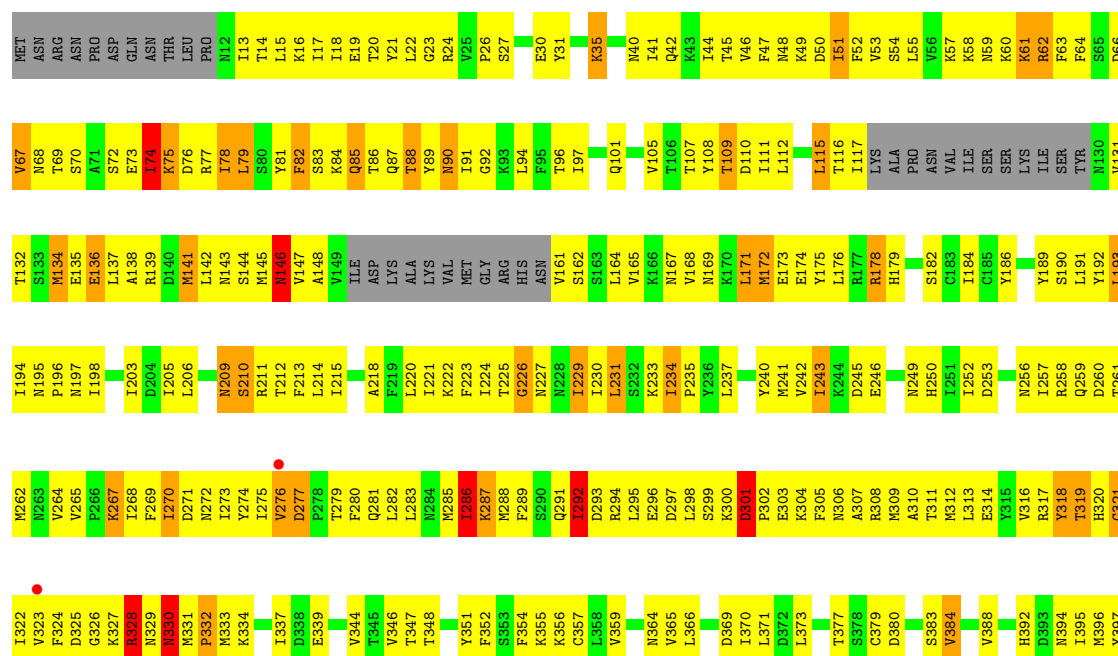
• Molecule 2: Poly(A) polymerase catalytic subunit

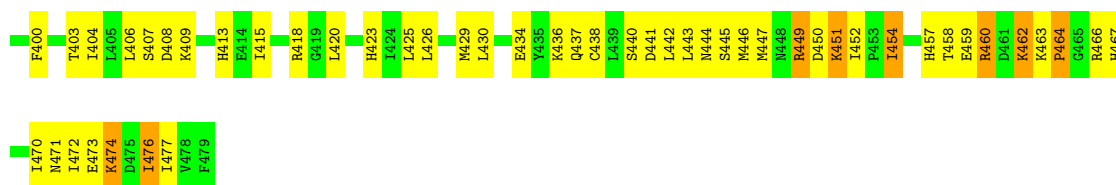




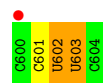
• Molecule 2: Poly(A) polymerase catalytic subunit

Chain D: 28% 54% 10% 7%





- Molecule 3: RNA/DNA chimera 5'-D(CP*CP*)R(UP*UP*)D(C)-3'



- Molecule 4: RNA/DNA chimera 5'-R(P*UP*UP*)D(C)-3'



- Molecule 5: RNA/DNA chimera 5'-D(P*CP*)R(UP*U)-3'



- Molecule 5: RNA/DNA chimera 5'-D(P*CP*)R(UP*U)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.61Å 77.24Å 106.85Å 74.88° 74.00° 63.69°	Depositor
Resolution (Å)	38.90 – 3.18 38.90 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.3 (38.90-3.18) 93.3 (38.90-3.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.285 0.244 , 0.287	Depositor DCC
R_{free} test set	1521 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12289	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/2444	1.08	18/3308 (0.5%)
1	B	0.62	0/2444	1.07	18/3308 (0.5%)
2	C	0.70	0/3686	1.06	22/4972 (0.4%)
2	D	0.68	0/3686	1.07	20/4972 (0.4%)
3	E	0.55	0/103	1.22	2/156 (1.3%)
4	F	0.82	0/64	0.78	0/96
5	G	0.90	0/64	1.13	0/96
5	H	0.92	0/64	1.31	1/96 (1.0%)
All	All	0.67	0/12555	1.07	81/17004 (0.5%)

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLN	N-CA-C	-10.31	102.87	114.62
1	B	39	GLN	N-CA-C	-10.02	103.19	114.62
1	A	147	GLU	CA-C-N	-8.95	110.81	119.85
1	A	147	GLU	C-N-CA	-8.95	110.81	119.85
2	D	226	GLY	N-CA-C	-8.53	102.92	115.63
1	B	147	GLU	CA-C-N	-8.35	111.42	119.85
1	B	147	GLU	C-N-CA	-8.35	111.42	119.85
2	C	226	GLY	N-CA-C	-8.34	103.20	115.63
1	A	243	VAL	N-CA-C	8.19	118.19	110.74
1	B	227	SER	N-CA-C	-7.80	102.72	111.07
1	B	243	VAL	N-CA-C	7.79	117.83	110.74
2	C	259	GLN	N-CA-C	-7.75	102.83	111.28
3	E	603	U	C2'-C3'-O3'	7.50	120.75	109.50
2	C	212	THR	N-CA-C	-7.47	103.21	111.36
2	D	234	ILE	CA-C-N	7.32	126.58	118.97
2	D	234	ILE	C-N-CA	7.32	126.58	118.97
1	A	227	SER	N-CA-C	-7.29	103.27	111.07
2	D	212	THR	N-CA-C	-7.26	103.44	111.36
2	C	407	SER	N-CA-C	-7.14	102.53	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	259	GLN	N-CA-C	-6.94	103.71	111.28
2	D	407	SER	N-CA-C	-6.82	102.97	112.45
2	C	234	ILE	CA-C-N	6.72	125.96	118.97
2	C	234	ILE	C-N-CA	6.72	125.96	118.97
1	A	242	ILE	N-CA-C	6.66	117.53	111.81
2	C	141	MET	N-CA-C	6.65	118.18	111.07
2	D	141	MET	N-CA-C	6.60	118.13	111.07
1	B	242	ILE	N-CA-C	6.54	117.44	111.81
1	A	69	SER	N-CA-C	6.53	120.95	112.92
1	B	69	SER	N-CA-C	6.40	120.80	112.92
2	D	454	ILE	CB-CA-C	-6.36	105.43	112.68
2	D	85	GLN	N-CA-C	-6.33	105.03	112.89
2	C	85	GLN	N-CA-C	-6.32	105.05	112.89
3	E	602	U	C2'-C3'-O3'	6.24	118.85	109.50
2	D	476	ILE	N-CA-C	6.23	116.85	107.75
2	C	454	ILE	CB-CA-C	-6.20	105.61	112.68
1	B	47	LEU	N-CA-C	-6.00	104.66	111.14
2	C	75	LYS	N-CA-C	-5.99	107.79	114.62
1	A	47	LEU	N-CA-C	-5.99	104.67	111.14
1	B	206	ALA	N-CA-C	-5.95	105.99	113.72
1	A	192	HIS	N-CA-C	-5.88	100.91	110.20
1	B	192	HIS	N-CA-C	-5.85	100.96	110.20
2	C	67	VAL	N-CA-C	5.82	116.53	107.28
1	B	23	GLU	CA-C-N	5.80	127.09	119.84
1	B	23	GLU	C-N-CA	5.80	127.09	119.84
2	D	193	LEU	N-CA-C	-5.74	106.24	113.18
2	C	193	LEU	N-CA-C	-5.73	106.27	113.20
2	C	472	ILE	N-CA-C	5.73	116.37	110.36
2	D	287	LYS	N-CA-C	-5.72	106.14	113.01
1	A	17	ASP	N-CA-C	5.69	119.40	112.23
2	C	346	VAL	N-CA-C	5.68	116.76	108.58
2	C	287	LYS	N-CA-C	-5.66	106.22	113.01
5	H	902	U	C2'-C3'-O3'	5.66	117.99	109.50
1	A	206	ALA	N-CA-C	-5.65	106.38	113.72
1	A	240	ASN	N-CA-C	5.64	117.23	111.14
2	D	346	VAL	N-CA-C	5.64	116.70	108.58
1	B	116	VAL	N-CA-C	5.57	117.19	109.45
2	C	476	ILE	N-CA-C	5.51	115.80	107.75
2	D	172	MET	N-CA-C	5.51	118.21	111.82
1	A	73	THR	N-CA-C	-5.49	105.21	111.14
2	D	472	ILE	N-CA-C	5.45	116.08	110.36
1	B	128	LEU	N-CA-C	5.41	117.25	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	75	LYS	N-CA-C	-5.39	108.47	114.62
1	A	128	LEU	N-CA-C	5.39	117.23	111.36
1	B	73	THR	N-CA-C	-5.35	105.36	111.14
1	A	23	GLU	CA-C-N	5.32	126.49	119.84
1	A	23	GLU	C-N-CA	5.32	126.49	119.84
1	A	116	VAL	N-CA-C	5.31	116.83	109.45
1	B	17	ASP	N-CA-C	5.29	118.90	112.23
2	C	172	MET	N-CA-C	5.29	117.96	111.82
1	B	198	GLN	N-CA-C	5.27	117.84	109.40
2	D	67	VAL	N-CA-C	5.27	115.65	107.28
1	A	198	GLN	N-CA-C	5.22	117.75	109.40
2	C	138	ALA	N-CA-C	-5.22	105.77	111.82
2	D	138	ALA	N-CA-C	-5.20	105.78	111.82
1	B	238	TYR	N-CA-C	-5.19	105.27	111.03
2	C	14	THR	N-CA-C	-5.13	105.68	111.28
2	C	352	PHE	N-CA-C	5.12	117.60	109.50
2	D	352	PHE	N-CA-C	5.11	117.45	109.52
2	D	286	ILE	N-CA-C	-5.08	105.46	111.00
2	C	286	ILE	N-CA-C	-5.07	105.48	111.00
2	C	437	GLN	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2382	0	2389	155	0
1	B	2382	0	2389	153	0
2	C	3627	0	3689	416	0
2	D	3627	0	3689	398	0
3	E	94	0	55	14	0
4	F	59	0	32	8	0
5	G	59	0	32	4	0
5	H	59	0	32	3	0
All	All	12289	0	12307	1112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1112) 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)
3:E:603:U:H6	3:E:603:U:H5'	1.12	1.12
2:D:443:LEU:HA	2:D:446:MET:HE2	1.33	1.11
2:C:443:LEU:HA	2:C:446:MET:HE2	1.33	1.10
1:B:106:LEU:HB2	1:B:109:VAL:HG22	1.31	1.08
1:A:106:LEU:HB2	1:A:109:VAL:HG22	1.34	1.05
2:D:256:ASN:HD22	2:D:257:ILE:N	1.59	1.01
2:D:474:LYS:HE3	2:D:474:LYS:HA	1.42	1.00
2:C:256:ASN:HD22	2:C:257:ILE:N	1.60	0.99
2:C:291:GLN:HE21	2:C:293:ASP:H	1.07	0.97
2:C:474:LYS:HE3	2:C:474:LYS:HA	1.43	0.97
1:B:131:SER:HB3	2:C:466:ARG:HG2	1.47	0.96
1:A:131:SER:HB3	2:D:466:ARG:HG2	1.47	0.95
2:D:291:GLN:HE21	2:D:293:ASP:H	1.11	0.94
2:C:288:MET:HG2	2:C:294:ARG:HG3	1.48	0.94
2:D:148:ALA:HB2	2:D:295:LEU:HB3	1.49	0.94
3:E:603:U:H5'	3:E:603:U:C6	2.03	0.93
2:D:270:ILE:HG22	2:D:271:ASP:N	1.84	0.93
2:C:148:ALA:HB2	2:C:295:LEU:HB3	1.51	0.93
2:C:141:MET:HE2	2:C:446:MET:HB2	1.51	0.92
2:C:270:ILE:HG22	2:C:271:ASP:N	1.84	0.92
2:D:288:MET:HG2	2:D:294:ARG:HG3	1.50	0.91
2:C:178:ARG:HA	2:C:178:ARG:HH11	1.35	0.91
2:C:316:VAL:HG22	2:C:322:ILE:HG13	1.51	0.90
2:D:229:ILE:HD13	2:D:229:ILE:H	1.36	0.90
2:D:141:MET:HE2	2:D:446:MET:HB2	1.54	0.90
2:D:178:ARG:HA	2:D:178:ARG:HH11	1.37	0.89
2:D:283:LEU:HD23	2:D:426:LEU:HD23	1.55	0.89
2:D:73:GLU:HB3	2:D:77:ARG:NH1	1.87	0.88
2:C:418:ARG:NE	2:C:446:MET:HG2	1.88	0.88
2:C:73:GLU:HB3	2:C:77:ARG:NH1	1.86	0.88
5:G:801:U:O2'	5:G:802:U:H5''	1.71	0.88
2:C:229:ILE:HD13	2:C:229:ILE:H	1.39	0.87
2:C:13:ILE:O	2:C:17:ILE:HG12	1.75	0.87
1:B:106:LEU:HB2	1:B:109:VAL:CG2	2.05	0.86
2:C:283:LEU:HD23	2:C:426:LEU:HD23	1.58	0.86
2:D:231:LEU:HD22	2:D:241:MET:HE2	1.58	0.86
2:C:270:ILE:HG22	2:C:271:ASP:H	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ASN:HD22	2:C:198:ILE:HG12	1.39	0.85
2:D:21:TYR:CE2	2:D:85:GLN:HG2	2.10	0.85
2:D:316:VAL:HG22	2:D:322:ILE:HG13	1.55	0.85
2:D:270:ILE:HG22	2:D:271:ASP:H	1.39	0.85
2:C:60:LYS:HE2	2:C:67:VAL:HB	1.56	0.85
2:C:256:ASN:HD22	2:C:257:ILE:H	1.22	0.84
2:C:21:TYR:CE2	2:C:85:GLN:HG2	2.11	0.84
2:D:60:LYS:HE2	2:D:67:VAL:HB	1.56	0.84
2:D:256:ASN:HD22	2:D:257:ILE:H	1.21	0.84
2:C:53:VAL:HG11	2:C:75:LYS:HG2	1.60	0.84
2:D:146:ASN:HD21	2:D:302:PRO:HB3	1.41	0.84
2:D:333:MET:HE2	2:D:348:THR:HA	1.58	0.83
1:A:106:LEU:HB2	1:A:109:VAL:CG2	2.08	0.83
2:C:333:MET:HE2	2:C:348:THR:HA	1.59	0.83
2:D:418:ARG:NE	2:D:446:MET:HG2	1.92	0.83
1:A:168:ASN:HD22	1:B:223:ARG:CZ	1.91	0.83
2:D:195:ASN:HD22	2:D:198:ILE:HG12	1.41	0.83
2:C:231:LEU:HD22	2:C:241:MET:HE2	1.61	0.83
2:D:53:VAL:HG11	2:D:75:LYS:HG2	1.61	0.82
2:D:13:ILE:O	2:D:17:ILE:HG12	1.79	0.82
2:C:288:MET:HE3	2:C:294:ARG:HD2	1.59	0.81
2:C:146:ASN:HD21	2:C:302:PRO:HB3	1.45	0.81
5:G:800:DC:H2"	5:G:801:U:OP2	1.81	0.81
2:D:60:LYS:HA	2:D:64:PHE:HB2	1.63	0.80
2:C:473:GLU:HG3	2:C:474:LYS:N	1.97	0.80
2:D:84:LYS:HG3	2:D:97:ILE:HD13	1.63	0.79
2:C:90:ASN:HD22	2:C:91:ILE:N	1.82	0.78
2:C:60:LYS:HA	2:C:64:PHE:HB2	1.65	0.78
2:C:84:LYS:HG3	2:C:97:ILE:HD13	1.63	0.78
2:D:74:ILE:HG13	2:D:224:ILE:HA	1.66	0.78
2:D:225:THR:HG21	2:D:227:ASN:HB2	1.65	0.78
2:C:148:ALA:HA	2:C:454:ILE:CD1	2.14	0.77
2:C:184:ILE:CG2	2:C:206:LEU:HB2	2.15	0.77
2:C:344:VAL:HG11	2:C:420:LEU:HD11	1.66	0.77
2:C:74:ILE:HG13	2:C:224:ILE:HA	1.67	0.77
1:B:53:LEU:HD22	1:B:58:ILE:HG12	1.66	0.77
2:D:30:GLU:HG2	2:D:91:ILE:HD11	1.66	0.77
2:D:473:GLU:HG3	2:D:474:LYS:N	1.99	0.77
2:D:288:MET:HE3	2:D:294:ARG:HD2	1.65	0.77
2:D:90:ASN:HD22	2:D:91:ILE:N	1.83	0.77
2:D:289:PHE:CE1	2:D:309:MET:HE1	2.20	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:VAL:HG11	2:C:420:LEU:CD1	2.15	0.76
2:C:473:GLU:HG3	2:C:474:LYS:H	1.51	0.76
2:D:473:GLU:HG3	2:D:474:LYS:H	1.51	0.76
2:C:59:ASN:HD21	2:C:220:LEU:HD21	1.51	0.76
2:D:148:ALA:HA	2:D:454:ILE:CD1	2.16	0.76
2:D:184:ILE:CG2	2:D:206:LEU:HB2	2.16	0.76
1:B:23:GLU:HB3	1:B:25:GLU:OE1	1.86	0.75
2:C:289:PHE:CE1	2:C:309:MET:HE1	2.22	0.75
2:C:323:VAL:HG22	2:C:325:ASP:OD1	1.86	0.75
1:A:23:GLU:HB3	1:A:25:GLU:OE1	1.86	0.75
2:C:30:GLU:HG2	2:C:91:ILE:HD11	1.68	0.75
2:C:269:PHE:CZ	2:C:272:ASN:HA	2.22	0.74
2:D:323:VAL:HG22	2:D:325:ASP:OD1	1.87	0.74
1:A:53:LEU:HD22	1:A:58:ILE:HG12	1.68	0.74
2:C:225:THR:HG21	2:C:227:ASN:HB2	1.69	0.74
2:C:470:ILE:HG23	2:C:477:ILE:HG12	1.67	0.74
2:C:73:GLU:HB3	2:C:77:ARG:HH12	1.50	0.74
2:D:19:GLU:HG3	2:D:24:ARG:O	1.88	0.74
2:D:73:GLU:HB3	2:D:77:ARG:HH12	1.50	0.74
1:A:66:TYR:CD1	1:A:69:SER:HB3	2.23	0.74
2:C:19:GLU:HG3	2:C:24:ARG:O	1.88	0.74
2:D:331:MET:HG2	2:D:442:LEU:HA	1.70	0.74
2:D:344:VAL:HG11	2:D:420:LEU:HD11	1.69	0.74
1:A:121:LEU:HD13	1:A:163:MET:HA	1.70	0.73
2:D:470:ILE:HG23	2:D:477:ILE:HG12	1.69	0.73
2:D:59:ASN:HD21	2:D:220:LEU:HD21	1.53	0.73
2:D:344:VAL:HG11	2:D:420:LEU:CD1	2.18	0.73
2:C:195:ASN:ND2	2:C:198:ILE:HG12	2.03	0.73
1:B:66:TYR:CD1	1:B:69:SER:HB3	2.24	0.72
2:C:31:TYR:O	2:C:35:LYS:HB2	1.88	0.72
1:B:121:LEU:HD13	1:B:163:MET:HA	1.71	0.72
2:D:261:THR:O	2:D:265:VAL:HG23	1.88	0.72
2:C:229:ILE:O	2:C:230:ILE:HD13	1.90	0.72
2:C:300:LYS:O	2:C:301:ASP:HB2	1.88	0.72
2:C:162:SER:HB3	2:C:245:ASP:OD1	1.89	0.72
2:D:162:SER:HB3	2:D:245:ASP:OD1	1.89	0.72
2:C:331:MET:HB3	2:C:332:PRO:HD3	1.71	0.71
2:D:195:ASN:ND2	2:D:198:ILE:HG12	2.05	0.71
2:D:331:MET:HB3	2:D:332:PRO:HD3	1.72	0.71
2:D:90:ASN:ND2	2:D:92:GLY:H	1.89	0.71
2:C:69:THR:OG1	2:C:74:ILE:HD11	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:THR:O	2:C:265:VAL:HG23	1.89	0.71
2:D:69:THR:OG1	2:D:74:ILE:HD11	1.90	0.71
2:D:328:ARG:HA	2:D:328:ARG:NE	2.05	0.71
1:B:267:LEU:HB3	1:B:286:LEU:HD12	1.71	0.71
2:C:331:MET:HG2	2:C:442:LEU:HA	1.74	0.70
2:D:31:TYR:O	2:D:35:LYS:HB2	1.90	0.70
2:D:229:ILE:HD13	2:D:229:ILE:N	2.06	0.70
2:D:229:ILE:H	2:D:229:ILE:CD1	2.02	0.70
1:A:174:LEU:HD12	1:A:174:LEU:H	1.57	0.70
2:C:58:LYS:NZ	2:C:116:THR:HB	2.07	0.70
1:A:33:LYS:HG2	1:A:34:LEU:H	1.55	0.70
2:D:58:LYS:NZ	2:D:116:THR:HB	2.06	0.70
2:C:90:ASN:ND2	2:C:92:GLY:H	1.90	0.70
2:C:291:GLN:HE21	2:C:293:ASP:N	1.88	0.70
2:C:301:ASP:H	2:C:302:PRO:HD3	1.57	0.70
1:A:267:LEU:HB3	1:A:286:LEU:HD12	1.71	0.70
1:B:150:THR:HG23	1:B:179:PRO:HB3	1.74	0.70
2:C:328:ARG:HA	2:C:328:ARG:NE	2.07	0.70
2:C:148:ALA:HB3	2:C:299:SER:OG	1.91	0.69
2:C:17:ILE:HD12	2:C:42:GLN:HB2	1.74	0.69
2:D:240:TYR:HE1	2:D:253:ASP:HB2	1.56	0.69
1:A:100:ASP:OD1	1:A:102:ILE:HG12	1.91	0.69
2:D:269:PHE:CZ	2:D:272:ASN:HA	2.28	0.69
1:B:53:LEU:HB3	1:B:58:ILE:HG13	1.74	0.69
2:D:229:ILE:O	2:D:230:ILE:HD13	1.93	0.69
1:B:50:LEU:HD12	1:B:53:LEU:HD12	1.75	0.69
2:D:111:ILE:HG23	2:D:175:TYR:OH	1.93	0.69
2:D:301:ASP:H	2:D:302:PRO:HD3	1.58	0.69
1:A:150:THR:HG23	1:A:179:PRO:HB3	1.75	0.68
2:C:111:ILE:HG23	2:C:175:TYR:OH	1.93	0.68
2:C:92:GLY:HA3	5:H:901:U:H5"	1.75	0.68
1:A:53:LEU:HB3	1:A:58:ILE:HG13	1.75	0.68
2:C:413:HIS:CD2	2:C:415:ILE:H	2.12	0.68
2:C:229:ILE:HD13	2:C:229:ILE:N	2.09	0.68
2:D:300:LYS:O	2:D:301:ASP:HB2	1.92	0.68
2:C:21:TYR:CG	2:C:41:ILE:HG23	2.29	0.68
2:C:316:VAL:HG22	2:C:322:ILE:CG1	2.23	0.68
2:C:229:ILE:H	2:C:229:ILE:CD1	2.05	0.68
2:C:240:TYR:HE1	2:C:253:ASP:HB2	1.57	0.68
2:D:413:HIS:CD2	2:D:415:ILE:H	2.12	0.68
1:B:160:GLN:O	1:B:164:ILE:HG12	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LYS:HZ3	2:D:116:THR:HB	1.59	0.67
2:C:131:VAL:CG1	2:C:311:THR:HA	2.24	0.67
1:A:50:LEU:HD12	1:A:53:LEU:HD12	1.77	0.67
2:C:184:ILE:HG22	2:C:206:LEU:HB2	1.76	0.67
2:D:134:MET:HE3	2:D:134:MET:HA	1.75	0.67
1:B:33:LYS:HG2	1:B:34:LEU:H	1.58	0.67
1:B:174:LEU:H	1:B:174:LEU:HD12	1.60	0.67
2:D:474:LYS:HE3	2:D:474:LYS:CA	2.21	0.67
2:C:327:LYS:HE2	2:C:327:LYS:O	1.93	0.67
2:C:21:TYR:CD1	2:C:41:ILE:HG23	2.29	0.67
2:D:327:LYS:O	2:D:327:LYS:HE2	1.93	0.67
1:A:195:LYS:HD2	1:A:195:LYS:N	2.09	0.66
2:C:176:LEU:HD13	2:C:273:ILE:HD12	1.78	0.66
2:D:21:TYR:CG	2:D:41:ILE:HG23	2.31	0.66
2:D:288:MET:HE1	2:D:305:PHE:CE2	2.30	0.66
2:D:195:ASN:C	2:D:197:ASN:H	2.04	0.66
2:D:286:ILE:HD12	2:D:286:ILE:N	2.11	0.66
1:A:53:LEU:HD13	1:A:58:ILE:HD11	1.78	0.66
2:C:291:GLN:NE2	2:C:293:ASP:H	1.89	0.66
2:D:17:ILE:HD12	2:D:42:GLN:HB2	1.78	0.66
1:B:53:LEU:HD13	1:B:58:ILE:HD11	1.78	0.66
2:C:134:MET:HA	2:C:134:MET:HE3	1.77	0.66
2:C:164:LEU:HA	2:C:167:ASN:HB3	1.78	0.66
2:D:60:LYS:O	2:D:64:PHE:C	2.39	0.66
2:C:148:ALA:HA	2:C:454:ILE:HD11	1.78	0.65
2:D:148:ALA:HB3	2:D:299:SER:OG	1.96	0.65
1:A:25:GLU:CD	1:A:25:GLU:H	2.03	0.65
2:D:146:ASN:ND2	2:D:302:PRO:HB3	2.11	0.65
1:A:231:ASN:HD21	1:A:235:LYS:HE3	1.60	0.65
1:A:118:GLU:HG2	1:A:122:ARG:NH1	2.10	0.65
1:A:174:LEU:HD12	1:A:174:LEU:N	2.11	0.65
1:B:100:ASP:OD1	1:B:102:ILE:HG12	1.95	0.65
2:D:30:GLU:HG2	2:D:91:ILE:CD1	2.26	0.65
2:D:148:ALA:HA	2:D:454:ILE:HD11	1.79	0.65
1:A:160:GLN:O	1:A:164:ILE:HG12	1.97	0.65
2:C:474:LYS:HE3	2:C:474:LYS:CA	2.24	0.65
2:D:21:TYR:CD1	2:D:41:ILE:HG23	2.31	0.65
2:D:184:ILE:HG22	2:D:206:LEU:HB2	1.78	0.65
2:D:331:MET:HG2	2:D:442:LEU:CA	2.27	0.65
2:C:288:MET:HE1	2:C:305:PHE:CE2	2.32	0.64
2:D:27:SER:OG	2:D:30:GLU:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:OH	1:A:241:LYS:HD2	1.98	0.64
1:B:174:LEU:HD12	1:B:174:LEU:N	2.12	0.64
2:D:139:ARG:HH11	2:D:139:ARG:HG2	1.63	0.64
1:B:195:LYS:N	1:B:195:LYS:HD2	2.12	0.64
2:C:331:MET:CE	2:C:441:ASP:HB2	2.28	0.64
2:C:195:ASN:C	2:C:197:ASN:H	2.06	0.64
2:D:58:LYS:HD2	3:E:601:DC:C2	2.33	0.64
1:B:26:SER:HB3	1:B:204:TYR:CE2	2.33	0.64
2:C:146:ASN:ND2	2:C:302:PRO:HB3	2.13	0.64
1:A:118:GLU:HG2	1:A:122:ARG:HH12	1.62	0.63
2:C:74:ILE:N	2:C:74:ILE:HD12	2.12	0.63
2:D:225:THR:CG2	2:D:227:ASN:HB2	2.28	0.63
1:B:231:ASN:HD21	1:B:235:LYS:HE3	1.63	0.63
2:C:161:VAL:HA	2:C:165:VAL:HG21	1.79	0.63
2:D:210:SER:HA	2:D:213:PHE:HB3	1.81	0.63
2:C:331:MET:HG2	2:C:442:LEU:CA	2.29	0.63
2:C:285:MET:O	2:C:288:MET:HB3	1.98	0.63
2:D:131:VAL:CG1	2:D:311:THR:HA	2.29	0.63
2:D:331:MET:CE	2:D:441:ASP:HB2	2.29	0.63
1:B:204:TYR:OH	1:B:241:LYS:HD2	1.99	0.63
2:D:198:ILE:HD12	2:D:308:ARG:HD3	1.80	0.63
2:C:245:ASP:OD1	2:C:249:ASN:HB2	1.99	0.62
2:D:161:VAL:HA	2:D:165:VAL:HG21	1.79	0.62
2:D:164:LEU:HA	2:D:167:ASN:HB3	1.81	0.62
2:C:210:SER:HA	2:C:213:PHE:HB3	1.82	0.62
2:C:27:SER:OG	2:C:30:GLU:HG3	2.00	0.62
2:C:58:LYS:C	2:C:61:LYS:HZ2	2.08	0.62
2:C:234:ILE:HD12	2:C:240:TYR:HE2	1.65	0.62
2:C:30:GLU:HG2	2:C:91:ILE:CD1	2.29	0.62
1:A:138:ASP:OD1	1:A:209:ARG:NH2	2.25	0.62
1:B:118:GLU:HG2	1:B:122:ARG:NH1	2.14	0.62
2:C:73:GLU:C	2:C:75:LYS:H	2.06	0.62
2:C:90:ASN:HD22	2:C:90:ASN:C	2.07	0.62
2:C:141:MET:HE3	2:C:447:MET:CG	2.30	0.62
2:C:286:ILE:N	2:C:286:ILE:HD12	2.15	0.62
2:D:141:MET:HE3	2:D:447:MET:HG2	1.82	0.62
2:D:331:MET:HE3	2:D:441:ASP:HB2	1.81	0.62
1:B:4:VAL:HG22	1:B:5:SER:N	2.14	0.61
1:B:25:GLU:H	1:B:25:GLU:CD	2.07	0.61
2:D:90:ASN:HD22	2:D:90:ASN:C	2.06	0.61
2:D:74:ILE:HD12	2:D:74:ILE:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:VAL:HG22	2:D:322:ILE:CG1	2.27	0.61
1:A:163:MET:O	1:A:167:LEU:HB2	2.01	0.61
1:A:175:LYS:NZ	1:A:207:GLU:OE2	2.23	0.61
1:B:79:ARG:C	1:B:79:ARG:HD3	2.26	0.61
1:B:118:GLU:HG2	1:B:122:ARG:HH12	1.65	0.61
2:C:288:MET:CG	2:C:294:ARG:HG3	2.27	0.61
2:D:47:PHE:CD1	2:D:105:VAL:HG13	2.35	0.61
2:D:73:GLU:C	2:D:75:LYS:H	2.06	0.61
2:D:40:ASN:O	2:D:44:ILE:HG13	2.00	0.61
2:D:53:VAL:HG12	2:D:57:LYS:HE3	1.81	0.61
2:D:331:MET:HB2	2:D:441:ASP:HB3	1.83	0.61
2:C:142:LEU:HD11	2:C:306:ASN:N	2.15	0.61
2:C:198:ILE:HD12	2:C:308:ARG:HD3	1.82	0.61
2:D:134:MET:HG3	2:D:137:LEU:HD23	1.83	0.61
1:A:26:SER:HB3	1:A:204:TYR:CE2	2.36	0.61
1:B:88:ILE:HD11	2:C:211:ARG:HD3	1.83	0.61
2:D:333:MET:CE	2:D:348:THR:HA	2.30	0.61
1:A:106:LEU:O	5:G:800:DC:N4	2.34	0.61
2:C:148:ALA:HA	2:C:454:ILE:HD12	1.81	0.61
2:C:331:MET:HG2	2:C:442:LEU:N	2.16	0.61
1:A:294:LEU:O	1:A:295:ASN:HB2	1.99	0.60
2:C:331:MET:HE3	2:C:441:ASP:HB2	1.83	0.60
2:D:74:ILE:HG22	2:D:74:ILE:O	2.01	0.60
2:D:141:MET:HE3	2:D:447:MET:CG	2.31	0.60
2:D:328:ARG:HB3	2:D:444:ASN:HB2	1.82	0.60
2:C:53:VAL:HG12	2:C:57:LYS:HE3	1.82	0.60
2:D:291:GLN:NE2	2:D:293:ASP:H	1.93	0.60
2:C:22:LEU:O	2:C:86:THR:HA	2.01	0.60
2:C:134:MET:HG3	2:C:137:LEU:HD23	1.83	0.60
2:D:148:ALA:HA	2:D:454:ILE:HD12	1.82	0.60
2:D:22:LEU:O	2:D:86:THR:HA	2.01	0.60
2:D:143:ASN:O	2:D:451:LYS:HE2	2.02	0.60
2:C:61:LYS:HZ3	2:C:62:ARG:HB2	1.66	0.60
1:B:160:GLN:HB3	1:B:174:LEU:HD23	1.82	0.60
2:C:233:LYS:HG3	2:C:240:TYR:O	2.02	0.60
2:C:331:MET:HB2	2:C:441:ASP:HB3	1.84	0.60
2:D:145:MET:HB3	2:D:415:ILE:HD11	1.83	0.60
2:C:141:MET:HE3	2:C:447:MET:HG2	1.84	0.60
1:B:26:SER:HB3	1:B:204:TYR:CD2	2.36	0.60
2:C:23:GLY:HA3	2:C:86:THR:HG22	1.82	0.60
2:D:285:MET:O	2:D:288:MET:HB3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:MET:O	2:D:333:MET:N	2.35	0.60
2:C:44:ILE:O	2:C:49:LYS:HE3	2.02	0.59
2:C:109:THR:HG23	4:F:702:U:O2'	2.03	0.59
2:D:44:ILE:O	2:D:49:LYS:HE3	2.02	0.59
2:D:147:VAL:HG12	2:D:451:LYS:HB3	1.84	0.59
2:D:234:ILE:HD12	2:D:240:TYR:HE2	1.67	0.59
1:B:59:LEU:HD11	1:B:89:ILE:HD13	1.84	0.59
2:C:331:MET:O	2:C:333:MET:N	2.35	0.59
2:D:142:LEU:HD11	2:D:306:ASN:N	2.17	0.59
1:B:46:GLU:OE2	1:B:66:TYR:OH	2.21	0.59
1:B:219:MET:HE3	1:B:220:ARG:O	2.02	0.59
2:C:74:ILE:HG22	2:C:74:ILE:O	2.02	0.59
2:C:301:ASP:N	2:C:302:PRO:HD3	2.17	0.59
2:D:474:LYS:HA	2:D:474:LYS:CE	2.24	0.59
2:C:139:ARG:HG2	2:C:139:ARG:HH11	1.68	0.59
1:A:160:GLN:HB3	1:A:174:LEU:HD23	1.82	0.59
2:D:191:LEU:HB2	2:D:198:ILE:HG21	1.84	0.59
2:D:198:ILE:HD11	2:D:311:THR:OG1	2.02	0.59
2:D:331:MET:HG2	2:D:442:LEU:N	2.17	0.59
1:A:26:SER:HB3	1:A:204:TYR:CD2	2.37	0.59
1:B:147:GLU:OE1	1:B:147:GLU:HA	2.01	0.59
2:D:84:LYS:CG	2:D:97:ILE:HD13	2.33	0.59
2:D:333:MET:HB3	2:D:347:THR:O	2.03	0.59
1:A:59:LEU:HD11	1:A:89:ILE:HD13	1.85	0.59
1:A:219:MET:HE3	1:A:220:ARG:O	2.02	0.59
2:C:131:VAL:HA	2:C:314:GLU:HG2	1.84	0.59
2:D:184:ILE:HB	2:D:262:MET:HE1	1.85	0.59
3:E:602:U:H4'	3:E:603:U:H5''	1.84	0.59
1:A:121:LEU:C	1:A:166:ILE:HG21	2.27	0.59
1:B:163:MET:O	1:B:167:LEU:HB2	2.03	0.59
2:C:60:LYS:O	2:C:64:PHE:C	2.46	0.59
2:C:134:MET:CG	2:C:137:LEU:HD23	2.32	0.59
2:C:225:THR:CG2	2:C:227:ASN:HB2	2.33	0.59
2:C:333:MET:CE	2:C:348:THR:HA	2.32	0.59
2:D:61:LYS:HZ3	2:D:62:ARG:HB2	1.67	0.59
2:D:288:MET:CG	2:D:294:ARG:HG3	2.30	0.59
2:D:291:GLN:HE21	2:D:293:ASP:N	1.92	0.59
1:A:88:ILE:HD11	2:D:211:ARG:HD3	1.85	0.58
1:B:121:LEU:C	1:B:166:ILE:HG21	2.28	0.58
2:C:109:THR:HG22	2:C:110:ASP:N	2.18	0.58
2:C:198:ILE:CD1	2:C:308:ARG:HH11	2.15	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:MET:HB3	2:C:347:THR:O	2.03	0.58
2:D:179:HIS:HB3	2:D:182:SER:OG	2.03	0.58
2:C:147:VAL:HG12	2:C:451:LYS:HB3	1.85	0.58
2:C:258:ARG:NH2	2:C:380:ASP:O	2.36	0.58
2:D:245:ASP:OD1	2:D:249:ASN:HB2	2.04	0.58
2:D:258:ARG:NH2	2:D:380:ASP:O	2.36	0.58
2:D:283:LEU:HD21	2:D:425:LEU:HB2	1.85	0.58
2:D:406:LEU:HA	2:D:413:HIS:H	1.68	0.58
1:A:79:ARG:HD3	1:A:79:ARG:C	2.29	0.58
2:D:176:LEU:HD13	2:D:273:ILE:HD12	1.86	0.58
2:D:186:TYR:HA	2:D:190:SER:HB2	1.86	0.58
1:A:4:VAL:HG22	1:A:5:SER:N	2.18	0.58
2:C:47:PHE:CD1	2:C:105:VAL:HG13	2.37	0.58
2:C:328:ARG:HB3	2:C:444:ASN:HB2	1.85	0.58
2:D:135:GLU:O	2:D:139:ARG:HB2	2.04	0.58
2:D:301:ASP:N	2:D:302:PRO:HD3	2.18	0.58
1:A:33:LYS:O	1:A:34:LEU:O	2.21	0.58
2:C:176:LEU:HB3	2:C:273:ILE:HB	1.85	0.58
2:C:406:LEU:HA	2:C:413:HIS:H	1.68	0.58
1:A:61:GLY:HA2	1:A:88:ILE:O	2.04	0.58
1:A:192:HIS:O	1:A:212:SER:HB3	2.04	0.58
2:D:145:MET:CB	2:D:415:ILE:HD11	2.32	0.58
2:D:233:LYS:HG3	2:D:240:TYR:O	2.04	0.58
2:D:325:ASP:N	2:D:447:MET:HE1	2.19	0.58
1:A:162:VAL:O	1:A:166:ILE:HG12	2.04	0.58
2:C:198:ILE:HD11	2:C:311:THR:OG1	2.04	0.58
1:B:294:LEU:O	1:B:295:ASN:HB2	2.03	0.57
2:C:164:LEU:HD23	2:C:167:ASN:HD22	1.68	0.57
2:C:325:ASP:N	2:C:447:MET:HE1	2.20	0.57
2:D:404:ILE:O	2:D:457:HIS:HA	2.04	0.57
1:A:107:ARG:CZ	2:D:477:ILE:HG21	2.34	0.57
2:C:189:TYR:CE2	2:C:193:LEU:HD21	2.39	0.57
2:C:164:LEU:CD2	2:C:167:ASN:HD22	2.16	0.57
2:C:186:TYR:HA	2:C:190:SER:HB2	1.87	0.57
2:C:59:ASN:ND2	2:C:220:LEU:HD21	2.17	0.57
2:C:90:ASN:ND2	2:C:90:ASN:C	2.60	0.57
2:D:283:LEU:HD22	2:D:429:MET:CE	2.34	0.57
1:A:39:GLN:HB3	1:A:294:LEU:HD22	1.87	0.57
2:C:234:ILE:HD12	2:C:240:TYR:CE2	2.39	0.57
2:D:109:THR:HG22	2:D:110:ASP:N	2.19	0.57
2:D:131:VAL:HA	2:D:314:GLU:HG2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:O	1:A:43:LEU:HD12	2.05	0.57
2:C:40:ASN:O	2:C:44:ILE:HG13	2.04	0.57
2:C:143:ASN:O	2:C:451:LYS:HE2	2.05	0.57
2:C:57:LYS:C	2:C:59:ASN:H	2.13	0.57
2:C:179:HIS:HB3	2:C:182:SER:OG	2.05	0.57
1:B:286:LEU:O	1:B:287:GLN:C	2.48	0.57
2:C:134:MET:HG3	2:C:137:LEU:HB3	1.87	0.57
2:D:22:LEU:HD23	2:D:85:GLN:HB3	1.85	0.57
1:A:46:GLU:OE2	1:A:66:TYR:OH	2.23	0.57
2:C:24:ARG:HD3	2:C:89:TYR:CE2	2.40	0.57
2:C:135:GLU:O	2:C:139:ARG:HB2	2.05	0.57
2:C:132:THR:HA	2:C:135:GLU:HG3	1.86	0.56
2:C:184:ILE:HB	2:C:262:MET:HE1	1.87	0.56
2:C:325:ASP:OD2	2:C:327:LYS:HE2	2.03	0.56
2:D:23:GLY:HA3	2:D:86:THR:HG22	1.86	0.56
2:C:44:ILE:HG12	2:C:105:VAL:HG21	1.87	0.56
2:C:58:LYS:HZ3	2:C:116:THR:HB	1.69	0.56
2:C:191:LEU:HB2	2:C:198:ILE:HG21	1.86	0.56
2:C:198:ILE:HD13	2:C:308:ARG:NH1	2.20	0.56
2:C:288:MET:HE3	2:C:294:ARG:CD	2.33	0.56
2:C:474:LYS:HA	2:C:474:LYS:CE	2.27	0.56
2:C:283:LEU:HD21	2:C:425:LEU:HB2	1.87	0.56
1:A:147:GLU:HA	1:A:147:GLU:OE1	2.05	0.56
1:A:265:PHE:HA	1:A:268:ARG:HD3	1.86	0.56
2:D:90:ASN:ND2	2:D:90:ASN:C	2.62	0.56
2:D:234:ILE:HD12	2:D:240:TYR:CE2	2.41	0.56
1:B:3:VAL:HB	1:B:249:VAL:HG13	1.86	0.56
1:B:43:LEU:HD12	1:B:43:LEU:O	2.06	0.56
1:B:192:HIS:O	1:B:212:SER:HB3	2.06	0.56
1:B:39:GLN:HB3	1:B:294:LEU:HD22	1.88	0.56
2:C:288:MET:HE1	2:C:305:PHE:CZ	2.40	0.56
2:D:44:ILE:HG12	2:D:105:VAL:HG21	1.86	0.56
2:D:57:LYS:C	2:D:59:ASN:H	2.14	0.56
1:A:33:LYS:O	1:A:34:LEU:C	2.48	0.56
1:A:4:VAL:O	1:A:249:VAL:HG22	2.04	0.56
2:D:198:ILE:CD1	2:D:308:ARG:HH11	2.18	0.56
1:B:33:LYS:O	1:B:34:LEU:O	2.24	0.55
2:D:19:GLU:HB2	2:D:26:PRO:HD3	1.89	0.55
1:B:107:ARG:CZ	2:C:477:ILE:HG21	2.36	0.55
2:C:76:ASP:O	2:C:77:ARG:C	2.48	0.55
2:D:176:LEU:HB3	2:D:273:ILE:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ILE:HD13	2:D:308:ARG:NH1	2.21	0.55
2:C:143:ASN:HA	2:C:146:ASN:HB2	1.88	0.55
2:D:444:ASN:ND2	2:D:447:MET:HE2	2.21	0.55
1:A:112:VAL:CG1	1:A:114:ARG:HG2	2.37	0.55
2:D:51:ILE:HD12	3:E:603:U:C4	2.41	0.55
2:D:134:MET:CG	2:D:137:LEU:HD23	2.36	0.55
2:D:288:MET:HE1	2:D:305:PHE:CZ	2.41	0.55
1:B:61:GLY:HA2	1:B:88:ILE:O	2.07	0.55
2:D:132:THR:HA	2:D:135:GLU:HG3	1.88	0.55
2:D:298:LEU:HD13	2:D:305:PHE:CD1	2.42	0.55
1:B:87:VAL:HG12	1:B:89:ILE:HG13	1.88	0.55
2:C:51:ILE:HG23	4:F:703:U:N3	2.21	0.55
2:C:325:ASP:O	2:C:327:LYS:N	2.40	0.55
2:C:227:ASN:OD1	2:C:246:GLU:HG3	2.05	0.55
2:C:449:ARG:NH1	2:C:449:ARG:HB3	2.22	0.55
2:D:134:MET:O	2:D:137:LEU:HB3	2.06	0.55
2:D:51:ILE:HG23	3:E:603:U:C4	2.42	0.55
2:D:76:ASP:O	2:D:77:ARG:C	2.49	0.55
1:A:109:VAL:HG23	1:A:109:VAL:O	2.06	0.54
1:A:114:ARG:HD3	1:A:120:TYR:CE1	2.42	0.54
2:D:44:ILE:O	2:D:47:PHE:HB3	2.06	0.54
1:B:138:ASP:OD1	1:B:209:ARG:NH2	2.26	0.54
2:C:108:TYR:CE1	2:C:112:LEU:HB2	2.42	0.54
2:C:320:HIS:O	2:C:321:GLY:C	2.50	0.54
2:D:63:PHE:CD2	2:D:171:LEU:HA	2.42	0.54
2:D:331:MET:CG	2:D:442:LEU:HA	2.36	0.54
1:B:162:VAL:O	1:B:166:ILE:HG12	2.07	0.54
2:C:145:MET:CB	2:C:415:ILE:HD11	2.36	0.54
2:C:276:VAL:O	2:C:281:GLN:HG3	2.06	0.54
1:B:265:PHE:HA	1:B:268:ARG:HD3	1.88	0.54
2:C:44:ILE:O	2:C:47:PHE:HB3	2.07	0.54
2:C:404:ILE:O	2:C:457:HIS:HA	2.08	0.54
1:A:3:VAL:HB	1:A:249:VAL:HG13	1.88	0.54
1:A:286:LEU:O	1:A:287:GLN:C	2.51	0.54
1:B:106:LEU:HD12	1:B:109:VAL:HG11	1.90	0.54
2:D:58:LYS:C	2:D:61:LYS:HZ2	2.16	0.54
2:D:324:PHE:C	2:D:447:MET:HE1	2.31	0.54
2:D:240:TYR:CE1	2:D:253:ASP:HB2	2.41	0.54
2:D:134:MET:HG3	2:D:137:LEU:HB3	1.90	0.54
2:C:63:PHE:CD2	2:C:171:LEU:HA	2.43	0.54
2:C:145:MET:HB3	2:C:415:ILE:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:LEU:HD22	2:C:429:MET:CE	2.37	0.54
5:H:900:DC:H4'	5:H:901:U:H5''	1.90	0.54
1:A:87:VAL:HG12	1:A:89:ILE:HG13	1.90	0.54
1:A:223:ARG:HD2	1:B:168:ASN:ND2	2.23	0.54
2:C:174:GLU:O	2:C:178:ARG:HG2	2.08	0.54
2:D:24:ARG:HD3	2:D:89:TYR:CE2	2.43	0.54
2:D:59:ASN:ND2	2:D:220:LEU:HD21	2.21	0.54
1:B:4:VAL:O	1:B:249:VAL:HG22	2.06	0.54
2:C:116:THR:O	2:C:117:ILE:HG13	2.08	0.54
2:D:116:THR:O	2:D:117:ILE:HG13	2.08	0.54
1:B:286:LEU:O	1:B:289:SER:N	2.37	0.53
2:C:51:ILE:HD13	2:C:51:ILE:O	2.08	0.53
2:C:331:MET:CG	2:C:442:LEU:HA	2.37	0.53
1:A:286:LEU:O	1:A:289:SER:N	2.38	0.53
1:B:114:ARG:HD3	1:B:120:TYR:CE1	2.43	0.53
2:C:20:THR:HG22	2:C:20:THR:O	2.08	0.53
2:C:331:MET:HG2	2:C:441:ASP:C	2.32	0.53
2:D:141:MET:O	2:D:144:SER:HB2	2.08	0.53
2:D:164:LEU:CD2	2:D:167:ASN:HD22	2.21	0.53
1:B:109:VAL:O	1:B:109:VAL:HG23	2.07	0.53
2:D:147:VAL:CG1	2:D:451:LYS:HB3	2.39	0.53
2:C:51:ILE:HG23	4:F:703:U:H3	1.73	0.53
2:C:84:LYS:CG	2:C:97:ILE:HD13	2.34	0.53
2:C:356:LYS:HE3	2:C:395:ILE:HD12	1.90	0.53
2:D:280:PHE:HD1	2:D:429:MET:SD	2.31	0.53
1:A:106:LEU:HD12	1:A:109:VAL:HG11	1.91	0.53
2:C:22:LEU:HD23	2:C:85:GLN:HB3	1.89	0.53
2:C:189:TYR:CZ	2:C:193:LEU:HD21	2.44	0.53
2:D:449:ARG:HB3	2:D:449:ARG:NH1	2.23	0.53
1:B:33:LYS:O	1:B:34:LEU:C	2.51	0.53
2:C:240:TYR:CE1	2:C:253:ASP:HB2	2.42	0.53
2:D:13:ILE:HA	2:D:16:LYS:HZ3	1.74	0.53
2:D:112:LEU:HD13	2:D:220:LEU:HD22	1.89	0.53
2:C:366:LEU:O	2:C:370:ILE:HG13	2.08	0.53
2:C:267:LYS:HD3	2:C:274:TYR:CD2	2.43	0.53
2:C:434:GLU:HA	2:C:434:GLU:OE1	2.08	0.53
2:D:20:THR:O	2:D:20:THR:HG22	2.09	0.53
2:C:283:LEU:HD21	2:C:425:LEU:CB	2.38	0.53
2:C:286:ILE:HG12	2:C:442:LEU:HD21	1.91	0.53
2:C:357:CYS:HA	2:C:396:MET:O	2.09	0.53
2:D:164:LEU:HD23	2:D:167:ASN:HD22	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:TYR:CD1	2:D:397:TYR:N	2.77	0.53
2:D:283:LEU:HD21	2:D:425:LEU:CB	2.38	0.53
2:D:286:ILE:HG12	2:D:442:LEU:HD21	1.91	0.53
1:A:168:ASN:HD22	1:B:223:ARG:NE	2.07	0.52
2:C:136:GLU:CD	2:C:136:GLU:H	2.15	0.52
2:C:168:VAL:O	2:C:171:LEU:N	2.42	0.52
1:B:112:VAL:CG1	1:B:114:ARG:HG2	2.39	0.52
2:C:134:MET:O	2:C:137:LEU:HB3	2.09	0.52
2:C:198:ILE:HD12	2:C:308:ARG:HH11	1.74	0.52
2:C:324:PHE:C	2:C:447:MET:HE1	2.33	0.52
2:D:143:ASN:HA	2:D:146:ASN:HB2	1.90	0.52
1:A:124:ILE:O	1:A:128:LEU:HD13	2.09	0.52
2:C:444:ASN:ND2	2:C:447:MET:HE2	2.24	0.52
2:D:168:VAL:O	2:D:171:LEU:N	2.43	0.52
2:D:331:MET:HE3	2:D:438:CYS:O	2.09	0.52
2:D:331:MET:HG2	2:D:441:ASP:C	2.34	0.52
1:B:35:PRO:O	1:B:36:TYR:HB2	2.09	0.52
2:C:19:GLU:HB2	2:C:26:PRO:HD3	1.92	0.52
2:C:317:ARG:HG2	2:C:317:ARG:HH11	1.73	0.52
2:D:189:TYR:CE2	2:D:193:LEU:HD21	2.45	0.52
2:D:276:VAL:O	2:D:281:GLN:HG3	2.08	0.52
2:C:198:ILE:CD1	2:C:308:ARG:NH1	2.73	0.52
1:A:168:ASN:ND2	1:B:223:ARG:CZ	2.69	0.52
2:C:112:LEU:HD13	2:C:220:LEU:HD22	1.91	0.52
1:A:22:TYR:HB2	1:A:233:GLU:HG2	1.92	0.52
2:C:298:LEU:HD13	2:C:305:PHE:CD1	2.45	0.52
2:D:267:LYS:HD3	2:D:274:TYR:CD2	2.44	0.52
1:B:280:LYS:O	1:B:284:LEU:HB2	2.10	0.52
2:C:110:ASP:O	2:C:179:HIS:HE1	1.92	0.52
2:C:141:MET:O	2:C:144:SER:HB2	2.10	0.52
2:C:178:ARG:HH11	2:C:178:ARG:CA	2.17	0.52
1:B:43:LEU:HD23	1:B:290:ILE:HG23	1.92	0.52
2:C:60:LYS:HD3	2:C:60:LYS:C	2.35	0.52
2:D:108:TYR:CE1	2:D:112:LEU:HB2	2.45	0.52
2:D:136:GLU:H	2:D:136:GLU:CD	2.16	0.52
2:D:221:ILE:O	2:D:225:THR:HB	2.10	0.52
2:D:434:GLU:OE1	2:D:434:GLU:HA	2.09	0.52
2:C:178:ARG:HA	2:C:178:ARG:NH1	2.15	0.51
2:D:270:ILE:CG2	2:D:271:ASP:N	2.55	0.51
2:C:49:LYS:HZ3	2:C:82:PHE:HD2	1.58	0.51
2:C:397:TYR:CD1	2:C:397:TYR:N	2.78	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:PHE:CE2	2:D:298:LEU:HD22	2.45	0.51
2:C:276:VAL:O	2:C:277:ASP:C	2.53	0.51
2:C:289:PHE:CE2	2:C:298:LEU:HD22	2.45	0.51
2:D:289:PHE:HE1	2:D:309:MET:HE1	1.71	0.51
2:D:325:ASP:OD2	2:D:327:LYS:HE2	2.09	0.51
2:C:51:ILE:HD13	2:C:51:ILE:C	2.36	0.51
2:C:351:TYR:HD2	2:C:438:CYS:HG	1.58	0.51
2:D:61:LYS:HZ3	2:D:62:ARG:CB	2.24	0.51
1:A:35:PRO:O	1:A:36:TYR:HB2	2.10	0.51
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.76	0.51
1:B:18:ASN:HB2	1:B:238:TYR:CZ	2.46	0.51
2:C:331:MET:HE3	2:C:438:CYS:O	2.11	0.51
2:D:227:ASN:OD1	2:D:246:GLU:HG3	2.09	0.51
1:B:76:ARG:HD2	1:B:76:ARG:O	2.11	0.51
2:D:195:ASN:O	2:D:197:ASN:N	2.44	0.51
2:D:198:ILE:CD1	2:D:308:ARG:NH1	2.74	0.51
2:D:288:MET:HE3	2:D:294:ARG:CD	2.38	0.51
1:A:18:ASN:HB2	1:A:238:TYR:CZ	2.46	0.51
1:A:112:VAL:HG12	1:A:114:ARG:HG2	1.91	0.51
2:C:74:ILE:N	2:C:74:ILE:CD1	2.73	0.51
2:C:318:TYR:O	2:C:321:GLY:N	2.44	0.51
2:C:344:VAL:HG11	2:C:420:LEU:HD13	1.91	0.51
1:A:289:SER:O	1:A:292:ARG:HB3	2.10	0.51
2:D:317:ARG:HH11	2:D:317:ARG:HG2	1.75	0.51
2:D:318:TYR:O	2:D:321:GLY:N	2.43	0.51
2:C:147:VAL:CG1	2:C:451:LYS:HB3	2.41	0.50
2:C:379:CYS:C	2:C:388:VAL:HG23	2.36	0.50
2:C:450:ASP:O	2:C:452:ILE:N	2.45	0.50
2:D:60:LYS:HD3	2:D:60:LYS:C	2.36	0.50
1:A:99:HIS:HB3	1:A:103:LEU:HD12	1.94	0.50
1:B:124:ILE:O	1:B:128:LEU:HD13	2.10	0.50
2:C:218:ALA:O	2:C:229:ILE:HD11	2.11	0.50
2:D:320:HIS:O	2:D:321:GLY:C	2.54	0.50
1:B:93:LEU:HD12	1:B:111:LEU:HD21	1.92	0.50
2:C:90:ASN:HD21	2:C:92:GLY:H	1.58	0.50
2:C:462:LYS:HB2	2:C:462:LYS:NZ	2.25	0.50
2:D:462:LYS:HB2	2:D:462:LYS:NZ	2.26	0.50
3:E:602:U:H4'	3:E:603:U:C5'	2.40	0.50
1:B:22:TYR:HB2	1:B:233:GLU:HG2	1.93	0.50
2:C:221:ILE:O	2:C:225:THR:HB	2.11	0.50
2:D:112:LEU:O	2:D:115:LEU:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:366:LEU:O	2:D:370:ILE:HG13	2.11	0.50
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.77	0.50
2:D:450:ASP:O	2:D:452:ILE:N	2.45	0.50
2:C:13:ILE:HA	2:C:16:LYS:HZ3	1.76	0.50
2:C:75:LYS:CE	2:C:79:LEU:HD11	2.42	0.50
2:C:195:ASN:HD22	2:C:198:ILE:CG1	2.17	0.50
1:A:100:ASP:CG	1:A:102:ILE:HG12	2.36	0.50
2:C:322:ILE:HG21	2:C:443:LEU:CD1	2.42	0.50
2:D:178:ARG:HA	2:D:178:ARG:NH1	2.16	0.50
2:D:51:ILE:HD13	2:D:51:ILE:O	2.11	0.50
2:D:325:ASP:O	2:D:327:LYS:N	2.45	0.50
2:C:280:PHE:HD1	2:C:429:MET:SD	2.35	0.50
2:C:292:ILE:HG13	2:C:457:HIS:ND1	2.26	0.50
2:D:276:VAL:O	2:D:277:ASP:C	2.54	0.50
2:D:406:LEU:C	2:D:413:HIS:HB2	2.37	0.50
2:D:471:ASN:OD1	2:D:473:GLU:HG2	2.12	0.50
2:C:112:LEU:O	2:C:115:LEU:HB2	2.12	0.49
2:D:444:ASN:HD22	2:D:447:MET:HE2	1.76	0.49
1:A:37:GLN:C	1:A:39:GLN:H	2.20	0.49
2:C:44:ILE:HD13	2:C:101:GLN:HE21	1.76	0.49
5:H:900:DC:H4'	5:H:901:U:C5'	2.41	0.49
1:A:280:LYS:O	1:A:284:LEU:HB2	2.12	0.49
2:C:207:GLN:NE2	2:C:213:PHE:CD2	2.71	0.49
2:D:110:ASP:O	2:D:179:HIS:HE1	1.95	0.49
2:D:256:ASN:HD22	2:D:256:ASN:C	2.16	0.49
2:C:148:ALA:HB1	2:C:296:GLU:HG2	1.94	0.49
2:C:270:ILE:CG2	2:C:271:ASP:N	2.54	0.49
2:D:47:PHE:CD2	2:D:105:VAL:HG22	2.48	0.49
2:D:51:ILE:HD13	2:D:51:ILE:C	2.38	0.49
1:B:289:SER:O	1:B:292:ARG:HB3	2.11	0.49
2:C:325:ASP:C	2:C:327:LYS:N	2.70	0.49
2:C:420:LEU:O	2:C:423:HIS:HB3	2.13	0.49
2:D:252:ILE:HD12	2:D:253:ASP:H	1.77	0.49
3:E:603:U:H6	3:E:603:U:C5'	2.03	0.49
1:A:293:PHE:C	1:A:293:PHE:CD2	2.91	0.49
1:B:99:HIS:HB3	1:B:103:LEU:HD12	1.95	0.49
2:D:90:ASN:HD21	2:D:92:GLY:H	1.59	0.49
2:D:337:ILE:HD12	2:D:404:ILE:HG21	1.93	0.49
1:A:215:THR:HG23	2:D:364:ASN:ND2	2.27	0.49
1:A:223:ARG:CD	1:B:168:ASN:ND2	2.75	0.49
1:A:253:TYR:OH	1:A:287:GLN:NE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:PHE:CG	2:D:105:VAL:HG13	2.47	0.49
1:B:18:ASN:O	1:B:235:LYS:HG2	2.13	0.49
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.77	0.49
2:C:47:PHE:CG	2:C:105:VAL:HG13	2.47	0.49
1:A:202:PRO:HB2	1:A:205:SER:HB2	1.94	0.49
2:D:148:ALA:HB1	2:D:296:GLU:HG2	1.94	0.49
2:D:344:VAL:HG11	2:D:420:LEU:HD13	1.93	0.49
1:A:109:VAL:CG2	1:A:109:VAL:O	2.60	0.48
2:C:51:ILE:HD12	4:F:703:U:C4	2.48	0.48
2:C:194:ILE:HD11	2:C:270:ILE:HD11	1.95	0.48
2:C:406:LEU:C	2:C:413:HIS:HB2	2.38	0.48
2:D:145:MET:HB3	2:D:415:ILE:CD1	2.42	0.48
2:D:189:TYR:CZ	2:D:193:LEU:HD21	2.48	0.48
2:D:292:ILE:O	2:D:295:LEU:HB2	2.12	0.48
2:D:292:ILE:HG13	2:D:457:HIS:ND1	2.27	0.48
2:C:51:ILE:CG2	4:F:703:U:N3	2.76	0.48
2:C:137:LEU:HG	2:C:313:LEU:HD13	1.96	0.48
2:C:195:ASN:O	2:C:197:ASN:N	2.46	0.48
2:C:444:ASN:HD22	2:C:447:MET:HE2	1.77	0.48
2:C:471:ASN:OD1	2:C:473:GLU:HG2	2.13	0.48
2:D:51:ILE:HD13	2:D:55:LEU:HG	1.95	0.48
2:D:194:ILE:HD11	2:D:270:ILE:HD11	1.95	0.48
1:B:251:PHE:CE2	1:B:253:TYR:HB3	2.48	0.48
2:C:252:ILE:HD12	2:C:253:ASP:H	1.78	0.48
2:D:198:ILE:HD12	2:D:308:ARG:HH11	1.78	0.48
2:D:273:ILE:HG13	2:D:273:ILE:O	2.13	0.48
2:D:357:CYS:HA	2:D:396:MET:O	2.13	0.48
1:B:67:ILE:HD12	1:B:135:LEU:HD11	1.95	0.48
1:B:293:PHE:C	1:B:293:PHE:CD2	2.92	0.48
2:D:270:ILE:O	2:D:272:ASN:N	2.44	0.48
2:D:420:LEU:O	2:D:423:HIS:HB3	2.14	0.48
2:C:289:PHE:HE1	2:C:309:MET:HE1	1.76	0.48
2:D:75:LYS:CE	2:D:79:LEU:HD11	2.43	0.48
2:D:379:CYS:C	2:D:388:VAL:HG23	2.38	0.48
1:B:37:GLN:C	1:B:39:GLN:H	2.22	0.48
2:C:256:ASN:HD22	2:C:256:ASN:C	2.18	0.48
2:D:291:GLN:O	2:D:292:ILE:C	2.56	0.48
1:B:255:ASN:OD1	1:B:260:TYR:CD1	2.67	0.48
2:C:90:ASN:ND2	2:C:91:ILE:N	2.57	0.48
2:C:418:ARG:CD	2:C:446:MET:HG2	2.43	0.48
2:D:174:GLU:O	2:D:178:ARG:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HG2	1:A:34:LEU:N	2.26	0.48
1:A:253:TYR:HE2	1:A:287:GLN:HE22	1.62	0.48
1:B:112:VAL:HG12	1:B:114:ARG:HG2	1.94	0.48
2:C:75:LYS:HE3	2:C:79:LEU:HD11	1.95	0.48
1:B:109:VAL:CG2	1:B:109:VAL:O	2.61	0.48
2:C:293:ASP:O	2:C:296:GLU:N	2.47	0.48
2:C:413:HIS:HE1	2:C:452:ILE:O	1.97	0.48
2:D:50:ASP:O	2:D:53:VAL:N	2.46	0.48
2:D:195:ASN:HD22	2:D:198:ILE:CG1	2.20	0.48
2:D:418:ARG:CD	2:D:446:MET:HG2	2.44	0.48
2:C:229:ILE:C	2:C:230:ILE:HD13	2.39	0.47
2:D:74:ILE:N	2:D:74:ILE:CD1	2.76	0.47
2:D:286:ILE:N	2:D:286:ILE:CD1	2.76	0.47
1:B:100:ASP:CG	1:B:102:ILE:HG12	2.38	0.47
1:B:202:PRO:HB2	1:B:205:SER:HB2	1.94	0.47
2:D:14:THR:O	2:D:18:ILE:HG13	2.13	0.47
1:B:85:LEU:HD11	1:B:271:TYR:O	2.14	0.47
1:B:265:PHE:HA	1:B:268:ARG:CD	2.44	0.47
1:A:244:ARG:HA	1:A:258:TYR:CD2	2.49	0.47
1:A:265:PHE:HA	1:A:268:ARG:CD	2.44	0.47
2:D:137:LEU:HG	2:D:313:LEU:HD13	1.97	0.47
2:D:322:ILE:HG21	2:D:443:LEU:CD1	2.45	0.47
1:A:168:ASN:ND2	1:B:223:ARG:HD2	2.29	0.47
1:A:195:LYS:N	1:A:195:LYS:CD	2.77	0.47
2:C:298:LEU:HD13	2:C:305:PHE:HD1	1.79	0.47
1:A:93:LEU:HD12	1:A:111:LEU:HD21	1.95	0.47
2:C:61:LYS:HZ3	2:C:62:ARG:CB	2.27	0.47
2:C:134:MET:HE2	2:C:137:LEU:HB2	1.96	0.47
2:C:373:LEU:HB3	2:C:392:HIS:CD2	2.49	0.47
2:D:356:LYS:HE3	2:D:395:ILE:HD12	1.96	0.47
2:C:46:VAL:HG12	2:C:46:VAL:O	2.14	0.47
2:C:58:LYS:C	2:C:61:LYS:NZ	2.73	0.47
2:C:58:LYS:O	2:C:116:THR:HG21	2.15	0.47
2:C:194:ILE:CD1	2:C:270:ILE:HD11	2.44	0.47
2:C:292:ILE:O	2:C:295:LEU:HB2	2.13	0.47
2:C:337:ILE:HD12	2:C:404:ILE:HG21	1.95	0.47
2:C:383:SER:O	2:C:384:VAL:C	2.58	0.47
2:D:49:LYS:HZ3	2:D:82:PHE:HD2	1.62	0.47
2:D:49:LYS:HE2	2:D:82:PHE:HD2	1.80	0.47
2:D:84:LYS:O	2:D:88:THR:HB	2.15	0.47
2:D:298:LEU:HD13	2:D:305:PHE:HD1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:304:LYS:HD3	2:D:305:PHE:CE1	2.50	0.47
2:D:307:ALA:HB1	2:D:308:ARG:NH1	2.30	0.47
2:D:325:ASP:C	2:D:327:LYS:N	2.73	0.47
1:A:43:LEU:HD23	1:A:290:ILE:HG23	1.96	0.47
1:A:168:ASN:ND2	1:B:223:ARG:CD	2.77	0.47
2:C:162:SER:N	2:C:165:VAL:HG23	2.30	0.47
2:C:291:GLN:O	2:C:292:ILE:C	2.57	0.47
2:D:19:GLU:HB2	2:D:26:PRO:CD	2.44	0.47
1:B:189:TYR:CE2	1:B:223:ARG:HB2	2.50	0.47
2:D:194:ILE:CD1	2:D:270:ILE:HD11	2.44	0.47
2:D:277:ASP:OD1	2:D:279:THR:N	2.43	0.47
2:D:413:HIS:HE1	2:D:452:ILE:O	1.98	0.47
1:B:201:ALA:O	1:B:202:PRO:C	2.58	0.47
2:D:75:LYS:HE3	2:D:79:LEU:HD11	1.96	0.47
2:D:293:ASP:O	2:D:296:GLU:N	2.48	0.47
3:E:602:U:C4'	3:E:603:U:OP2	2.63	0.47
2:C:250:HIS:C	2:C:250:HIS:CD2	2.93	0.46
1:B:285:PHE:O	1:B:288:GLN:HB3	2.15	0.46
2:D:58:LYS:HD2	3:E:601:DC:N3	2.30	0.46
2:D:250:HIS:C	2:D:250:HIS:CD2	2.94	0.46
1:B:43:LEU:HB2	1:B:74:HIS:HB2	1.97	0.46
1:B:230:VAL:O	1:B:234:LYS:HG2	2.16	0.46
2:C:145:MET:HG2	2:C:415:ILE:HG12	1.98	0.46
2:C:288:MET:CE	2:C:294:ARG:HD2	2.40	0.46
1:A:201:ALA:O	1:A:202:PRO:C	2.59	0.46
2:C:47:PHE:CD2	2:C:105:VAL:HG22	2.51	0.46
2:C:231:LEU:CD2	2:C:241:MET:HE2	2.40	0.46
2:C:270:ILE:O	2:C:272:ASN:N	2.45	0.46
1:A:96:GLY:HA3	1:A:115:PHE:CE1	2.51	0.46
1:A:168:ASN:ND2	1:B:223:ARG:NE	2.64	0.46
1:B:239:LEU:HA	1:B:243:VAL:CG2	2.46	0.46
2:C:141:MET:CE	2:C:443:LEU:O	2.63	0.46
2:D:192:TYR:CD2	2:D:193:LEU:HD22	2.50	0.46
2:D:218:ALA:O	2:D:229:ILE:HD11	2.15	0.46
1:B:49:PHE:CD2	1:B:50:LEU:HD13	2.51	0.46
1:B:267:LEU:HA	1:B:270:VAL:HG23	1.98	0.46
2:C:172:MET:HE2	2:C:205:ILE:HD13	1.98	0.46
2:D:50:ASP:C	2:D:52:PHE:N	2.64	0.46
1:A:48:PHE:HB2	1:A:266:MET:HE2	1.98	0.46
2:C:17:ILE:HD12	2:C:42:GLN:CB	2.44	0.46
2:C:49:LYS:HE2	2:C:82:PHE:HD2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:ASP:O	2:C:53:VAL:N	2.48	0.46
2:C:50:ASP:C	2:C:52:PHE:N	2.65	0.46
2:C:275:ILE:O	2:C:275:ILE:HG13	2.15	0.46
2:D:78:ILE:HG12	2:D:223:PHE:CD1	2.51	0.46
2:D:289:PHE:HE1	2:D:309:MET:CE	2.28	0.46
1:A:251:PHE:CE2	1:A:253:TYR:HB3	2.50	0.46
1:B:59:LEU:O	1:B:59:LEU:HG	2.16	0.46
1:B:94:ILE:HG23	1:B:112:VAL:HB	1.97	0.46
2:C:277:ASP:OD1	2:C:279:THR:N	2.44	0.46
2:D:169:ASN:O	2:D:173:GLU:HG3	2.16	0.46
1:A:63:THR:HG23	1:A:90:LYS:HG3	1.97	0.46
1:A:94:ILE:HG23	1:A:112:VAL:HB	1.97	0.46
1:A:189:TYR:CE2	1:A:223:ARG:HB2	2.51	0.46
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.80	0.46
1:B:52:LYS:HD3	2:C:371:LEU:HD13	1.98	0.46
1:B:215:THR:HG23	2:C:364:ASN:ND2	2.31	0.46
2:C:51:ILE:HD13	2:C:55:LEU:HG	1.98	0.46
2:C:331:MET:HE2	2:C:441:ASP:HB2	1.96	0.46
2:D:44:ILE:HD13	2:D:101:GLN:HE21	1.80	0.46
2:D:322:ILE:HB	2:D:324:PHE:HE1	1.81	0.46
1:A:43:LEU:HB2	1:A:74:HIS:HB2	1.98	0.45
2:D:366:LEU:HD11	2:D:370:ILE:HD11	1.98	0.45
2:D:426:LEU:O	2:D:430:LEU:HG	2.16	0.45
1:A:18:ASN:O	1:A:235:LYS:HG2	2.16	0.45
1:A:67:ILE:HD12	1:A:135:LEU:HD11	1.98	0.45
1:A:285:PHE:O	1:A:288:GLN:HB3	2.15	0.45
1:B:3:VAL:HB	1:B:249:VAL:CG1	2.46	0.45
2:D:51:ILE:HD12	3:E:603:U:C5	2.52	0.45
2:D:53:VAL:CG1	2:D:57:LYS:HE3	2.47	0.45
2:D:214:LEU:HD22	2:D:243:ILE:HD11	1.96	0.45
1:B:253:TYR:OH	1:B:287:GLN:NE2	2.49	0.45
2:C:169:ASN:O	2:C:173:GLU:HG3	2.17	0.45
2:C:192:TYR:CD2	2:C:193:LEU:HD22	2.51	0.45
2:C:319:THR:HG22	2:C:320:HIS:CD2	2.52	0.45
2:C:328:ARG:HB3	2:C:444:ASN:CB	2.45	0.45
2:D:19:GLU:CB	2:D:26:PRO:HD3	2.46	0.45
2:D:58:LYS:O	2:D:116:THR:HG21	2.17	0.45
2:D:229:ILE:C	2:D:230:ILE:HD13	2.42	0.45
2:D:351:TYR:HD2	2:D:438:CYS:HG	1.65	0.45
2:C:273:ILE:O	2:C:273:ILE:HG13	2.16	0.45
2:D:59:ASN:HD22	2:D:220:LEU:HD11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:383:SER:O	2:D:384:VAL:C	2.60	0.45
1:A:122:ARG:HG2	1:A:166:ILE:HG23	1.98	0.45
1:B:63:THR:HG23	1:B:90:LYS:HG3	1.97	0.45
1:B:244:ARG:HA	1:B:258:TYR:CD2	2.51	0.45
1:B:258:TYR:O	1:B:261:PHE:HB3	2.16	0.45
2:D:107:THR:O	2:D:108:TYR:C	2.60	0.45
2:D:145:MET:HG2	2:D:415:ILE:HG12	1.99	0.45
1:A:49:PHE:CD2	1:A:50:LEU:HD13	2.52	0.45
2:C:96:THR:HG23	2:C:477:ILE:HG13	1.98	0.45
2:D:282:LEU:HD13	2:D:312:MET:HE3	1.97	0.45
1:A:76:ARG:HD2	1:A:76:ARG:O	2.17	0.45
1:B:195:LYS:N	1:B:195:LYS:CD	2.79	0.45
2:C:78:ILE:O	2:C:79:LEU:C	2.59	0.45
2:C:78:ILE:HG12	2:C:223:PHE:CD1	2.51	0.45
2:C:331:MET:HB3	2:C:445:SER:OG	2.17	0.45
2:D:191:LEU:O	2:D:194:ILE:HB	2.17	0.45
2:D:373:LEU:HB3	2:D:392:HIS:CD2	2.51	0.45
1:B:175:LYS:NZ	1:B:207:GLU:OE2	2.25	0.45
1:B:282:LYS:O	1:B:283:VAL:C	2.59	0.45
2:C:75:LYS:O	2:C:75:LYS:HD3	2.16	0.45
2:C:141:MET:HE3	2:C:447:MET:HG3	1.99	0.45
2:D:24:ARG:HD3	2:D:89:TYR:HE2	1.82	0.45
1:B:33:LYS:HG2	1:B:34:LEU:N	2.28	0.45
1:B:117:ASP:O	1:B:118:GLU:C	2.59	0.45
2:C:304:LYS:HD3	2:C:305:PHE:CE1	2.52	0.45
1:A:3:VAL:HB	1:A:249:VAL:CG1	2.47	0.44
1:A:258:TYR:O	1:A:261:PHE:HB3	2.17	0.44
1:B:96:GLY:HA3	1:B:115:PHE:CE1	2.52	0.44
2:C:14:THR:O	2:C:18:ILE:HG13	2.16	0.44
2:C:44:ILE:HG21	2:C:101:GLN:NE2	2.32	0.44
1:A:52:LYS:HD3	2:D:371:LEU:HD13	1.99	0.44
1:A:53:LEU:O	1:A:54:GLN:C	2.59	0.44
1:A:121:LEU:CD1	1:A:163:MET:HA	2.45	0.44
1:B:150:THR:O	1:B:154:LEU:HG	2.16	0.44
1:B:253:TYR:HE2	1:B:287:GLN:HE22	1.65	0.44
2:C:316:VAL:CG2	2:C:322:ILE:HG13	2.36	0.44
2:D:70:SER:C	2:D:72:SER:H	2.25	0.44
1:A:66:TYR:CG	1:A:69:SER:HB3	2.52	0.44
1:B:93:LEU:HB2	1:B:111:LEU:CD2	2.47	0.44
2:C:53:VAL:HG13	2:C:75:LYS:HA	1.99	0.44
2:D:476:ILE:HD13	5:G:802:U:H4'	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HA	1:A:243:VAL:CG2	2.48	0.44
2:C:24:ARG:HD3	2:C:89:TYR:HE2	1.79	0.44
2:C:59:ASN:HD22	2:C:220:LEU:HD11	1.82	0.44
2:C:318:TYR:C	2:C:318:TYR:CD1	2.95	0.44
2:D:44:ILE:HG21	2:D:101:GLN:NE2	2.33	0.44
2:D:58:LYS:C	2:D:61:LYS:NZ	2.76	0.44
2:D:172:MET:HE2	2:D:205:ILE:HD13	2.00	0.44
1:A:282:LYS:O	1:A:283:VAL:C	2.60	0.44
2:C:53:VAL:O	2:C:57:LYS:HG3	2.18	0.44
2:C:437:GLN:O	2:C:440:SER:HB3	2.18	0.44
2:D:437:GLN:O	2:D:440:SER:HB3	2.18	0.44
2:C:49:LYS:CE	2:C:82:PHE:HD2	2.30	0.44
2:D:53:VAL:HG13	2:D:75:LYS:HA	2.00	0.44
2:D:75:LYS:O	2:D:75:LYS:HD3	2.17	0.44
2:D:94:LEU:O	2:D:97:ILE:N	2.48	0.44
2:D:169:ASN:OD1	2:D:203:ILE:HG13	2.17	0.44
1:B:59:LEU:HG	1:B:89:ILE:HD11	2.00	0.44
1:B:122:ARG:HG2	1:B:166:ILE:HG23	1.99	0.44
1:B:167:LEU:O	1:B:168:ASN:C	2.61	0.44
2:C:21:TYR:CG	2:C:41:ILE:CG2	2.99	0.44
2:C:174:GLU:OE1	2:C:178:ARG:HD3	2.18	0.44
2:C:203:ILE:O	2:C:252:ILE:HD11	2.17	0.44
2:D:78:ILE:O	2:D:79:LEU:C	2.60	0.44
2:D:230:ILE:HD12	2:D:471:ASN:ND2	2.31	0.44
2:D:328:ARG:HB3	2:D:444:ASN:CB	2.45	0.44
1:A:58:ILE:HD12	1:A:58:ILE:O	2.18	0.44
1:A:278:THR:O	1:A:281:ALA:HB3	2.18	0.44
2:C:286:ILE:N	2:C:286:ILE:CD1	2.79	0.44
2:C:354:PHE:HB2	2:C:394:ASN:O	2.18	0.44
1:B:248:VAL:HG21	1:B:261:PHE:CD2	2.53	0.44
2:C:48:ASN:HB3	4:F:703:U:O2	2.18	0.44
2:C:115:LEU:CD1	2:C:171:LEU:CD2	2.96	0.44
2:C:322:ILE:HB	2:C:324:PHE:HE1	1.83	0.44
2:D:235:PRO:HD2	2:D:467:HIS:ND1	2.32	0.44
1:B:279:THR:O	1:B:282:LYS:N	2.50	0.43
2:C:53:VAL:CG1	2:C:57:LYS:HE3	2.48	0.43
2:C:366:LEU:HD11	2:C:370:ILE:HD11	2.00	0.43
2:D:59:ASN:ND2	2:D:220:LEU:HD11	2.33	0.43
2:D:73:GLU:CB	2:D:77:ARG:HH12	2.24	0.43
2:D:74:ILE:CG1	2:D:224:ILE:HA	2.42	0.43
2:C:70:SER:C	2:C:72:SER:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:ARG:HG2	2:C:317:ARG:NH1	2.32	0.43
2:D:319:THR:HG22	2:D:320:HIS:CD2	2.54	0.43
1:A:248:VAL:HG21	1:A:261:PHE:CD2	2.53	0.43
1:B:58:ILE:HD12	1:B:58:ILE:O	2.18	0.43
2:C:77:ARG:NE	2:C:226:GLY:HA2	2.33	0.43
2:C:107:THR:O	2:C:108:TYR:C	2.62	0.43
2:C:145:MET:HB3	2:C:415:ILE:CD1	2.47	0.43
2:C:307:ALA:HB1	2:C:308:ARG:NH1	2.33	0.43
2:C:459:GLU:O	2:C:460:ARG:C	2.61	0.43
2:C:468:GLY:O	2:C:469:PHE:HB3	2.18	0.43
2:D:51:ILE:O	2:D:54:SER:HB2	2.17	0.43
2:D:53:VAL:O	2:D:57:LYS:HG3	2.19	0.43
1:A:117:ASP:O	1:A:118:GLU:C	2.60	0.43
1:A:192:HIS:O	1:A:212:SER:CB	2.66	0.43
1:A:253:TYR:OH	1:A:284:LEU:HA	2.17	0.43
2:C:133:SER:O	2:C:134:MET:HE3	2.19	0.43
2:C:276:VAL:O	2:C:281:GLN:NE2	2.39	0.43
2:C:325:ASP:C	2:C:327:LYS:H	2.26	0.43
2:D:96:THR:HG23	2:D:477:ILE:HG13	1.99	0.43
1:B:34:LEU:HD11	1:B:260:TYR:OH	2.18	0.43
2:C:73:GLU:C	2:C:75:LYS:N	2.75	0.43
2:C:84:LYS:O	2:C:88:THR:HB	2.19	0.43
2:D:174:GLU:OE1	2:D:178:ARG:HD3	2.19	0.43
2:D:473:GLU:CG	2:D:474:LYS:H	2.25	0.43
1:B:4:VAL:CG2	1:B:5:SER:N	2.81	0.43
1:B:121:LEU:CD1	1:B:163:MET:HA	2.46	0.43
2:C:288:MET:SD	2:C:294:ARG:NE	2.91	0.43
2:C:473:GLU:CG	2:C:474:LYS:H	2.26	0.43
2:D:46:VAL:O	2:D:46:VAL:HG12	2.18	0.43
2:D:49:LYS:CE	2:D:82:PHE:HD2	2.31	0.43
1:A:267:LEU:HA	1:A:270:VAL:HG23	2.01	0.43
1:B:48:PHE:HB2	1:B:266:MET:HE2	2.01	0.43
2:C:19:GLU:HB2	2:C:26:PRO:CD	2.48	0.43
2:C:395:ILE:HB	2:C:397:TYR:CE1	2.54	0.43
2:D:77:ARG:NE	2:D:226:GLY:HA2	2.34	0.43
3:E:603:U:C6	3:E:603:U:C5'	2.90	0.43
1:A:46:GLU:CD	1:A:66:TYR:OH	2.62	0.43
1:B:257:GLU:OE2	1:B:257:GLU:N	2.51	0.43
2:C:61:LYS:HD2	2:C:61:LYS:C	2.43	0.43
2:C:137:LEU:HD21	2:C:324:PHE:CD2	2.54	0.43
2:C:168:VAL:O	2:C:169:ASN:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:264:VAL:HB	2:C:430:LEU:O	2.18	0.43
2:D:316:VAL:HG13	2:D:317:ARG:N	2.34	0.43
1:A:54:GLN:HB2	1:A:59:LEU:HD23	2.01	0.43
1:A:93:LEU:HB2	1:A:111:LEU:CD2	2.48	0.43
1:A:257:GLU:OE2	1:A:257:GLU:N	2.51	0.43
1:B:41:LYS:HE2	1:B:41:LYS:HB3	1.78	0.43
2:C:57:LYS:C	2:C:59:ASN:N	2.76	0.43
2:C:289:PHE:HE1	2:C:309:MET:CE	2.31	0.43
2:D:75:LYS:HD3	2:D:75:LYS:C	2.44	0.43
2:D:203:ILE:O	2:D:252:ILE:HD11	2.18	0.43
1:A:118:GLU:O	1:A:119:GLU:C	2.61	0.43
1:B:132:LYS:HD3	2:C:464:PRO:HB2	2.00	0.43
1:B:145:GLY:O	1:B:146:ASN:HB2	2.19	0.43
2:C:45:THR:C	2:C:47:PHE:H	2.27	0.43
1:A:253:TYR:CE1	1:A:284:LEU:HG	2.54	0.42
2:C:268:ILE:CG1	2:C:277:ASP:HA	2.49	0.42
2:C:292:ILE:CG2	2:C:293:ASP:N	2.81	0.42
2:C:296:GLU:O	2:C:299:SER:HB2	2.18	0.42
2:D:45:THR:C	2:D:47:PHE:H	2.28	0.42
2:D:287:LYS:O	2:D:287:LYS:HG2	2.17	0.42
1:A:59:LEU:HG	1:A:89:ILE:HD11	2.02	0.42
1:A:255:ASN:OD1	1:A:257:GLU:OE2	2.36	0.42
1:B:65:VAL:HG23	1:B:133:ILE:HG23	2.00	0.42
2:C:19:GLU:CB	2:C:26:PRO:HD3	2.49	0.42
2:C:322:ILE:HG21	2:C:443:LEU:HD12	1.99	0.42
2:D:105:VAL:O	2:D:105:VAL:HG12	2.17	0.42
2:D:471:ASN:OD1	2:D:473:GLU:CG	2.68	0.42
1:A:239:LEU:O	1:A:243:VAL:HB	2.19	0.42
2:C:75:LYS:HD3	2:C:75:LYS:C	2.44	0.42
2:C:191:LEU:O	2:C:194:ILE:HB	2.19	0.42
2:C:310:ALA:C	2:C:312:MET:N	2.75	0.42
2:D:134:MET:HE2	2:D:137:LEU:HB2	2.01	0.42
2:D:242:VAL:HG23	2:D:252:ILE:O	2.19	0.42
2:D:268:ILE:CG1	2:D:277:ASP:HA	2.49	0.42
1:A:137:SER:OG	1:A:160:GLN:HG2	2.19	0.42
1:B:18:ASN:HB2	1:B:238:TYR:CE2	2.54	0.42
2:C:109:THR:CG2	4:F:702:U:O2'	2.66	0.42
2:D:57:LYS:C	2:D:59:ASN:N	2.77	0.42
2:D:73:GLU:C	2:D:75:LYS:N	2.75	0.42
2:D:275:ILE:O	2:D:275:ILE:HG13	2.19	0.42
2:D:366:LEU:HD12	2:D:370:ILE:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG23	1:A:133:ILE:HG23	2.00	0.42
2:C:94:LEU:O	2:C:97:ILE:N	2.50	0.42
2:C:235:PRO:HD2	2:C:467:HIS:ND1	2.34	0.42
2:D:55:LEU:HD22	3:E:602:U:C5	2.54	0.42
2:D:162:SER:O	2:D:165:VAL:HB	2.20	0.42
2:D:262:MET:HE3	2:D:267:LYS:HZ2	1.85	0.42
2:D:354:PHE:HB2	2:D:394:ASN:O	2.20	0.42
1:A:198:GLN:HA	1:A:199:PRO:HD3	1.73	0.42
1:A:285:PHE:O	1:A:286:LEU:C	2.63	0.42
1:B:53:LEU:O	1:B:54:GLN:C	2.61	0.42
2:C:78:ILE:O	2:C:80:SER:N	2.53	0.42
2:C:96:THR:HG23	2:C:477:ILE:HD12	2.02	0.42
2:C:327:LYS:O	2:C:328:ARG:HB2	2.18	0.42
2:C:366:LEU:HD12	2:C:370:ILE:HG13	2.02	0.42
2:D:21:TYR:CG	2:D:41:ILE:CG2	3.01	0.42
2:D:137:LEU:HD21	2:D:324:PHE:CD2	2.55	0.42
2:D:209:ASN:O	2:D:211:ARG:N	2.52	0.42
2:D:325:ASP:C	2:D:327:LYS:H	2.27	0.42
2:D:331:MET:HE2	2:D:441:ASP:HB2	2.00	0.42
1:B:46:GLU:CD	1:B:66:TYR:OH	2.62	0.42
1:B:122:ARG:N	1:B:166:ILE:HG21	2.34	0.42
2:C:211:ARG:O	2:C:215:ILE:HG13	2.19	0.42
2:D:61:LYS:HD2	2:D:61:LYS:C	2.44	0.42
2:D:189:TYR:O	2:D:193:LEU:HD23	2.19	0.42
2:D:310:ALA:C	2:D:312:MET:N	2.76	0.42
2:D:365:VAL:HG12	2:D:369:ASP:OD2	2.20	0.42
1:A:19:GLU:HB2	1:A:234:LYS:HB3	2.02	0.42
1:A:25:GLU:CD	1:A:25:GLU:N	2.74	0.42
2:C:74:ILE:CD1	2:C:74:ILE:H	2.33	0.42
2:C:78:ILE:O	2:C:81:TYR:N	2.53	0.42
2:C:209:ASN:O	2:C:211:ARG:N	2.53	0.42
2:D:264:VAL:HB	2:D:430:LEU:O	2.19	0.42
2:D:331:MET:HB3	2:D:445:SER:OG	2.20	0.42
2:D:463:LYS:HA	2:D:464:PRO:HD3	1.89	0.42
1:A:58:ILE:HD12	1:A:58:ILE:C	2.44	0.42
1:B:121:LEU:CB	1:B:166:ILE:HG21	2.50	0.42
2:C:473:GLU:CG	2:C:474:LYS:N	2.74	0.42
2:D:53:VAL:HG11	2:D:75:LYS:CG	2.43	0.42
2:D:268:ILE:HG12	2:D:277:ASP:HA	2.02	0.42
2:D:317:ARG:HG2	2:D:317:ARG:NH1	2.34	0.42
1:A:145:GLY:O	1:A:146:ASN:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HD12	1:B:58:ILE:C	2.45	0.42
1:B:66:TYR:CG	1:B:69:SER:HB3	2.55	0.42
2:C:49:LYS:NZ	2:C:82:PHE:HD2	2.18	0.42
2:C:268:ILE:HG12	2:C:277:ASP:HA	2.02	0.42
2:C:270:ILE:CG2	2:C:271:ASP:H	2.05	0.42
2:C:301:ASP:C	2:C:303:GLU:H	2.27	0.42
2:C:301:ASP:C	2:C:303:GLU:N	2.77	0.42
2:C:395:ILE:HB	2:C:397:TYR:HE1	1.85	0.42
2:C:403:THR:HG22	2:C:458:THR:O	2.20	0.42
1:A:9:PRO:HD2	1:A:265:PHE:CD2	2.54	0.41
1:A:41:LYS:HE2	1:A:41:LYS:HB3	1.79	0.41
1:A:121:LEU:CB	1:A:166:ILE:HG21	2.50	0.41
1:A:230:VAL:O	1:A:234:LYS:HG2	2.20	0.41
1:B:199:PRO:HG2	1:B:266:MET:SD	2.60	0.41
2:C:135:GLU:HB3	2:C:139:ARG:NH2	2.35	0.41
2:C:147:VAL:HG23	2:C:454:ILE:HG13	2.02	0.41
2:C:230:ILE:HD12	2:C:471:ASN:ND2	2.34	0.41
2:C:318:TYR:O	2:C:320:HIS:N	2.53	0.41
2:C:427:TYR:CE1	2:C:431:THR:HG21	2.55	0.41
2:C:449:ARG:HB3	2:C:449:ARG:HH11	1.83	0.41
2:D:135:GLU:HB3	2:D:139:ARG:NH2	2.35	0.41
2:D:459:GLU:O	2:D:460:ARG:C	2.63	0.41
1:A:59:LEU:HG	1:A:59:LEU:O	2.21	0.41
1:B:248:VAL:HG21	1:B:261:PHE:CG	2.55	0.41
2:C:316:VAL:HG13	2:C:317:ARG:N	2.36	0.41
2:D:61:LYS:NZ	2:D:62:ARG:HG3	2.36	0.41
2:D:115:LEU:CD1	2:D:171:LEU:CD2	2.98	0.41
2:D:256:ASN:ND2	2:D:257:ILE:H	2.02	0.41
2:D:395:ILE:HB	2:D:397:TYR:CE1	2.55	0.41
1:A:193:GLY:HA3	1:A:212:SER:HB3	2.02	0.41
1:A:292:ARG:HG3	1:A:292:ARG:NH1	2.34	0.41
1:B:279:THR:O	1:B:280:LYS:C	2.60	0.41
2:C:143:ASN:HA	2:C:146:ASN:HD22	1.85	0.41
2:C:301:ASP:O	2:C:303:GLU:N	2.53	0.41
2:D:143:ASN:HA	2:D:146:ASN:HD22	1.85	0.41
2:D:211:ARG:O	2:D:215:ILE:HG13	2.20	0.41
2:D:292:ILE:CG2	2:D:293:ASP:N	2.82	0.41
2:D:473:GLU:CG	2:D:474:LYS:N	2.75	0.41
2:D:318:TYR:O	2:D:320:HIS:N	2.53	0.41
2:D:322:ILE:HB	2:D:324:PHE:CE1	2.55	0.41
2:D:329:ASN:HB2	2:D:330:ASN:H	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG21	1:A:261:PHE:CG	2.56	0.41
1:B:11:MET:HE1	1:B:266:MET:HG2	2.02	0.41
1:B:98:HIS:CE1	1:B:113:THR:HG21	2.55	0.41
1:B:192:HIS:O	1:B:212:SER:CB	2.68	0.41
2:C:162:SER:N	2:C:165:VAL:CG2	2.83	0.41
2:C:347:THR:CG2	2:C:349:LYS:HG2	2.50	0.41
2:C:462:LYS:HB2	2:C:462:LYS:HZ3	1.85	0.41
2:D:48:ASN:N	3:E:603:U:O2	2.54	0.41
2:D:49:LYS:HG3	2:D:82:PHE:CD2	2.55	0.41
2:D:77:ARG:HE	2:D:226:GLY:HA2	1.85	0.41
1:A:18:ASN:HB2	1:A:238:TYR:CE2	2.55	0.41
1:B:193:GLY:HA3	1:B:212:SER:HB3	2.02	0.41
2:C:90:ASN:OD1	2:C:93:LYS:HG3	2.21	0.41
2:C:233:LYS:HB2	2:C:241:MET:HG2	2.02	0.41
2:C:256:ASN:ND2	2:C:257:ILE:H	2.03	0.41
2:C:352:PHE:HE2	2:C:434:GLU:O	2.04	0.41
2:D:17:ILE:HD12	2:D:42:GLN:CB	2.47	0.41
2:D:164:LEU:O	2:D:165:VAL:C	2.64	0.41
2:D:286:ILE:CD1	2:D:286:ILE:H	2.33	0.41
2:C:74:ILE:CG1	2:C:224:ILE:HA	2.46	0.41
2:C:81:TYR:O	2:C:83:SER:N	2.54	0.41
2:C:183:CYS:SG	2:C:205:ILE:HD12	2.60	0.41
2:C:301:ASP:N	2:C:302:PRO:CD	2.84	0.41
1:A:279:THR:O	1:A:280:LYS:C	2.61	0.41
2:C:141:MET:HE1	2:C:443:LEU:O	2.21	0.41
2:C:356:LYS:HG3	2:C:395:ILE:HD12	2.02	0.41
2:D:90:ASN:ND2	2:D:91:ILE:N	2.60	0.41
1:A:4:VAL:CG2	1:A:5:SER:N	2.83	0.41
1:A:101:PRO:C	1:A:103:LEU:H	2.29	0.41
1:A:180:PHE:O	1:A:181:PRO:C	2.64	0.41
1:B:88:ILE:C	1:B:89:ILE:HG13	2.46	0.41
1:B:93:LEU:HB2	1:B:111:LEU:HD23	2.02	0.41
1:B:128:LEU:O	1:B:129:HIS:C	2.64	0.41
1:B:279:THR:C	1:B:281:ALA:N	2.78	0.41
1:B:285:PHE:O	1:B:286:LEU:C	2.64	0.41
2:C:51:ILE:O	2:C:54:SER:HB2	2.20	0.41
2:C:115:LEU:HD13	2:C:171:LEU:CD2	2.50	0.41
2:C:169:ASN:OD1	2:C:203:ILE:HG13	2.20	0.41
2:C:359:VAL:CG1	2:C:400:PHE:HB2	2.51	0.41
2:D:16:LYS:O	2:D:17:ILE:C	2.63	0.41
2:D:78:ILE:HG22	2:D:79:LEU:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:TYR:O	2:D:83:SER:N	2.54	0.41
2:D:354:PHE:CZ	2:D:396:MET:HE3	2.56	0.41
1:A:132:LYS:HD3	2:D:464:PRO:HB2	2.02	0.41
1:B:19:GLU:HB2	1:B:234:LYS:HB3	2.03	0.41
1:B:54:GLN:HB2	1:B:59:LEU:HD23	2.03	0.41
2:C:164:LEU:HD23	2:C:167:ASN:ND2	2.34	0.41
2:C:329:ASN:HB2	2:C:330:ASN:H	1.72	0.41
2:D:359:VAL:CG1	2:D:400:PHE:HB2	2.51	0.41
1:A:11:MET:HE1	1:A:266:MET:HG2	2.03	0.40
1:A:85:LEU:HD11	1:A:271:TYR:O	2.21	0.40
1:B:237:TYR:OH	1:B:241:LYS:HD3	2.21	0.40
2:C:51:ILE:CG2	4:F:703:U:H3	2.32	0.40
2:C:287:LYS:O	2:C:287:LYS:HG2	2.20	0.40
2:D:262:MET:HE3	2:D:267:LYS:NZ	2.36	0.40
2:C:193:LEU:HB3	2:C:270:ILE:HG21	2.03	0.40
2:C:294:ARG:HA	2:C:297:ASP:OD2	2.21	0.40
2:C:331:MET:HE2	2:C:441:ASP:CB	2.51	0.40
2:C:364:ASN:OD1	2:C:365:VAL:N	2.54	0.40
2:C:365:VAL:HG12	2:C:369:ASP:OD2	2.21	0.40
2:C:426:LEU:O	2:C:430:LEU:HG	2.21	0.40
2:D:96:THR:HG23	2:D:477:ILE:HD12	2.03	0.40
2:D:141:MET:HE3	2:D:447:MET:HG3	2.03	0.40
2:D:168:VAL:O	2:D:169:ASN:C	2.64	0.40
2:D:214:LEU:HD11	2:D:241:MET:O	2.21	0.40
2:D:234:ILE:HG21	2:D:237:LEU:HD23	2.03	0.40
2:D:308:ARG:O	2:D:312:MET:HG3	2.21	0.40
1:A:167:LEU:O	1:A:168:ASN:C	2.61	0.40
1:A:199:PRO:HG3	1:A:262:HIS:CE1	2.56	0.40
2:C:96:THR:HG23	2:C:477:ILE:CD1	2.51	0.40
2:C:168:VAL:C	2:C:170:LYS:N	2.79	0.40
2:C:301:ASP:H	2:C:302:PRO:CD	2.31	0.40
2:D:142:LEU:HD22	2:D:298:LEU:HD21	2.03	0.40
2:D:145:MET:O	2:D:147:VAL:HG22	2.21	0.40
2:D:283:LEU:HD22	2:D:429:MET:HE3	2.02	0.40
2:D:301:ASP:N	2:D:302:PRO:CD	2.84	0.40
1:A:279:THR:O	1:A:282:LYS:N	2.55	0.40
1:B:239:LEU:O	1:B:243:VAL:HB	2.21	0.40
1:B:253:TYR:OH	1:B:284:LEU:HA	2.20	0.40
2:C:33:MET:HB3	2:C:95:PHE:CZ	2.56	0.40
2:C:33:MET:HB3	2:C:95:PHE:HZ	1.87	0.40
2:C:162:SER:O	2:C:165:VAL:HB	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:LYS:O	2:D:226:GLY:N	2.55	0.40
2:D:322:ILE:HG21	2:D:443:LEU:HD12	2.02	0.40
2:D:403:THR:HG22	2:D:458:THR:O	2.22	0.40
1:A:223:ARG:CD	1:B:168:ASN:HD22	2.35	0.40
2:C:282:LEU:HD13	2:C:312:MET:HE3	2.02	0.40
2:C:365:VAL:O	2:C:368:SER:N	2.50	0.40
2:D:294:ARG:HA	2:D:297:ASP:OD2	2.21	0.40
2:D:301:ASP:C	2:D:303:GLU:N	2.79	0.40
2:D:449:ARG:HB3	2:D:449:ARG:HH11	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/297 (95%)	244 (86%)	30 (11%)	8 (3%)	4	22
1	B	282/297 (95%)	244 (86%)	33 (12%)	5 (2%)	6	31
2	C	439/479 (92%)	330 (75%)	74 (17%)	35 (8%)	1	4
2	D	439/479 (92%)	329 (75%)	77 (18%)	33 (8%)	1	5
All	All	1442/1552 (93%)	1147 (80%)	214 (15%)	81 (6%)	1	10

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	146	ASN
1	B	2	ASP
2	C	78	ILE
2	C	146	ASN
2	C	301	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	319	THR
2	C	328	ARG
2	C	334	LYS
2	C	451	LYS
2	D	78	ILE
2	D	146	ASN
2	D	301	ASP
2	D	319	THR
2	D	334	LYS
2	D	451	LYS
1	A	34	LEU
1	B	34	LEU
1	B	146	ASN
2	C	66	ASP
2	C	82	PHE
2	C	115	LEU
2	C	209	ASN
2	C	210	SER
2	C	321	GLY
2	C	326	GLY
2	C	355	LYS
2	C	409	LYS
2	C	436	LYS
2	D	66	ASP
2	D	82	PHE
2	D	115	LEU
2	D	209	ASN
2	D	210	SER
2	D	321	GLY
2	D	326	GLY
2	D	328	ARG
2	D	330	ASN
2	D	355	LYS
2	D	436	LYS
2	C	74	ILE
2	C	79	LEU
2	C	196	PRO
2	C	270	ILE
2	C	330	ASN
2	C	339	GLU
2	C	460	ARG
2	D	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	79	LEU
2	D	196	PRO
2	D	270	ILE
2	D	339	GLU
2	D	409	LYS
2	C	276	VAL
2	C	318	TYR
2	C	384	VAL
2	C	464	PRO
2	D	318	TYR
2	D	460	ARG
2	D	464	PRO
1	A	36	TYR
1	A	54	GLN
1	A	295	ASN
1	B	36	TYR
1	B	216	GLY
2	C	68	ASN
2	C	183	CYS
2	C	332	PRO
2	D	276	VAL
2	D	292	ILE
2	D	332	PRO
2	D	384	VAL
1	A	286	LEU
2	C	35	LYS
2	C	292	ILE
2	D	35	LYS
2	D	68	ASN
1	A	216	GLY
2	C	277	ASP
2	D	277	ASP
2	C	412	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/270 (98%)	250 (94%)	16 (6%)	17	46
1	B	266/270 (98%)	250 (94%)	16 (6%)	17	46
2	C	422/453 (93%)	392 (93%)	30 (7%)	13	41
2	D	422/453 (93%)	393 (93%)	29 (7%)	14	42
All	All	1376/1446 (95%)	1285 (93%)	91 (7%)	15	43

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	50	LEU
1	A	58	ILE
1	A	109	VAL
1	A	116	VAL
1	A	118	GLU
1	A	147	GLU
1	A	149	SER
1	A	167	LEU
1	A	174	LEU
1	A	194	ASN
1	A	197	LEU
1	A	247	VAL
1	A	248	VAL
1	A	275	THR
1	A	284	LEU
1	B	18	ASN
1	B	50	LEU
1	B	58	ILE
1	B	109	VAL
1	B	116	VAL
1	B	118	GLU
1	B	147	GLU
1	B	149	SER
1	B	167	LEU
1	B	174	LEU
1	B	194	ASN
1	B	197	LEU
1	B	247	VAL
1	B	248	VAL
1	B	275	THR
1	B	284	LEU
2	C	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	51	ILE
2	C	54	SER
2	C	61	LYS
2	C	62	ARG
2	C	74	ILE
2	C	87	GLN
2	C	88	THR
2	C	90	ASN
2	C	109	THR
2	C	134	MET
2	C	136	GLU
2	C	146	ASN
2	C	171	LEU
2	C	178	ARG
2	C	229	ILE
2	C	231	LEU
2	C	243	ILE
2	C	260	ASP
2	C	267	LYS
2	C	286	ILE
2	C	292	ILE
2	C	301	ASP
2	C	328	ARG
2	C	330	ASN
2	C	377	THR
2	C	408	ASP
2	C	449	ARG
2	C	462	LYS
2	C	474	LYS
2	D	15	LEU
2	D	51	ILE
2	D	61	LYS
2	D	62	ARG
2	D	74	ILE
2	D	87	GLN
2	D	88	THR
2	D	90	ASN
2	D	109	THR
2	D	134	MET
2	D	136	GLU
2	D	146	ASN
2	D	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	178	ARG
2	D	229	ILE
2	D	231	LEU
2	D	243	ILE
2	D	260	ASP
2	D	267	LYS
2	D	286	ILE
2	D	292	ILE
2	D	301	ASP
2	D	328	ARG
2	D	330	ASN
2	D	377	THR
2	D	408	ASP
2	D	449	ARG
2	D	462	LYS
2	D	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	39	GLN
1	A	54	GLN
1	A	84	ASN
1	A	98	HIS
1	A	127	GLN
1	A	146	ASN
1	A	156	ASN
1	A	160	GLN
1	A	168	ASN
1	A	183	GLN
1	A	194	ASN
1	A	198	GLN
1	A	231	ASN
1	A	287	GLN
1	A	288	GLN
1	B	18	ASN
1	B	37	GLN
1	B	39	GLN
1	B	54	GLN
1	B	84	ASN
1	B	98	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	127	GLN
1	B	146	ASN
1	B	168	ASN
1	B	183	GLN
1	B	194	ASN
1	B	198	GLN
1	B	231	ASN
1	B	287	GLN
1	B	288	GLN
2	C	42	GLN
2	C	59	ASN
2	C	85	GLN
2	C	90	ASN
2	C	101	GLN
2	C	146	ASN
2	C	167	ASN
2	C	179	HIS
2	C	180	ASN
2	C	247	ASN
2	C	250	HIS
2	C	256	ASN
2	C	291	GLN
2	C	320	HIS
2	C	392	HIS
2	C	394	ASN
2	C	413	HIS
2	C	448	ASN
2	D	29	ASN
2	D	42	GLN
2	D	59	ASN
2	D	85	GLN
2	D	90	ASN
2	D	101	GLN
2	D	146	ASN
2	D	167	ASN
2	D	179	HIS
2	D	180	ASN
2	D	247	ASN
2	D	250	HIS
2	D	256	ASN
2	D	291	GLN
2	D	320	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	392	HIS
2	D	394	ASN
2	D	413	HIS
2	D	448	ASN

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 oligosaccharides 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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	288/297 (96%)	-0.22	0	100	100	36, 61, 94, 135	0
1	B	288/297 (96%)	-0.21	0	100	100	38, 62, 95, 147	0
2	C	445/479 (92%)	0.16	4 (0%)	81	64	46, 93, 130, 149	0
2	D	445/479 (92%)	0.11	2 (0%)	88	78	43, 88, 122, 156	0
3	E	5/5 (100%)	1.01	1 (20%)	3	2	74, 92, 107, 119	0
4	F	3/3 (100%)	0.30	0	100	100	87, 87, 110, 112	0
5	G	3/3 (100%)	0.71	0	100	100	115, 115, 118, 123	0
5	H	3/3 (100%)	0.59	0	100	100	106, 106, 112, 124	0
All	All	1480/1566 (94%)	0.00	7 (0%)	87	75	36, 79, 123, 156	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	323	VAL	3.1
2	D	276	VAL	2.8
3	E	600	DC	2.5
2	C	52	PHE	2.4
2	D	323	VAL	2.2
2	C	108	TYR	2.2
2	C	114	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.