



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 3ERC / pdb_00003erc
Title : Crystal structure of the heterodimeric vaccinia virus mRNA polyadenylate polymerase with three fragments of RNA and 3'-deoxy ATP
Authors : Li, C.; Li, H.; Zhou, S.; Poulos, T.L.; Gershon, P.D.
Deposited on : 2008-10-01
Resolution : 3.21 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

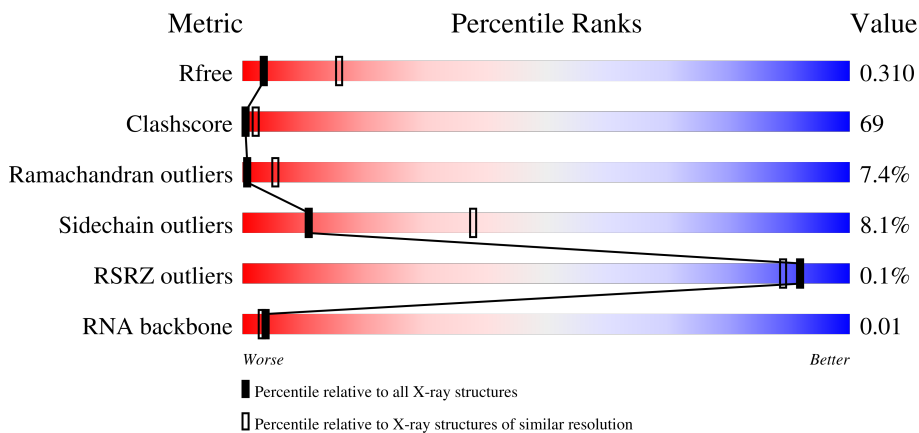
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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.





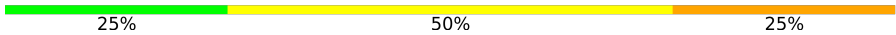
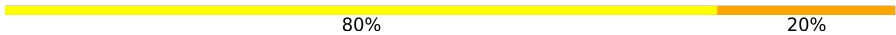
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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	
1	B	297	
2	C	479	
2	D	479	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	5	 40% 40% 20%
3	F	5	 40% 60%
4	G	4	 25% 50% 25%
5	I	5	 80% 20%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12480 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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 a RNA chain called RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*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			
3	F	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			

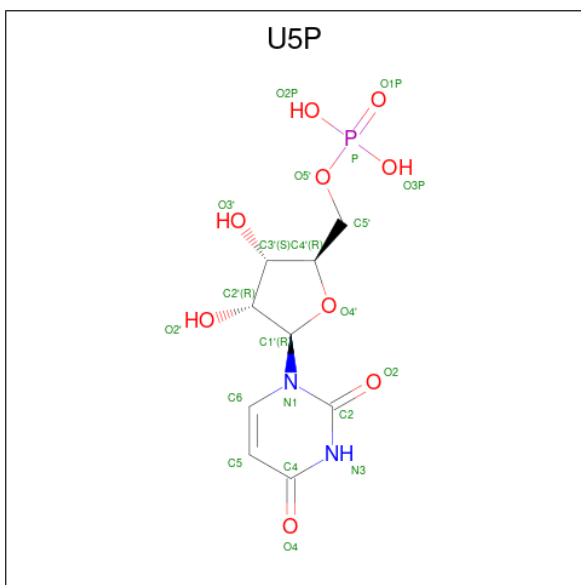
- Molecule 4 is a RNA chain called RNA/DNA chimera (5'-D(CP*)R(UP*UP*)-D(C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	G	4	Total	C	N	O	P	0	0	0
			75	36	10	26	3			

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

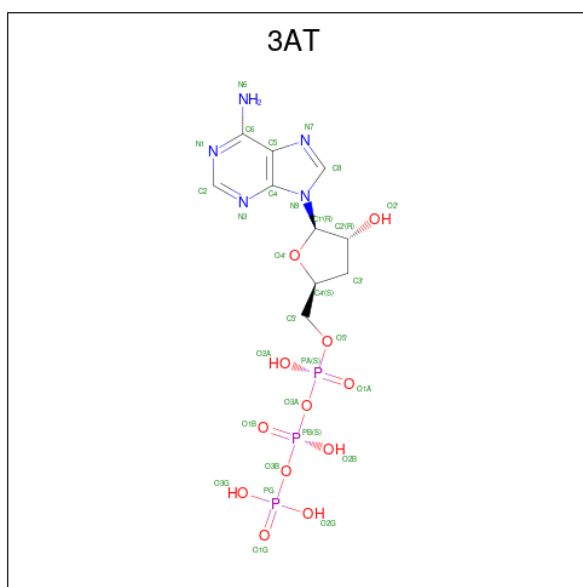
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	I	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			

- Molecule 6 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
6	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 7 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	Ca	0	0
			2	2		
8	D	2	Total	Ca	0	0
			2	2		

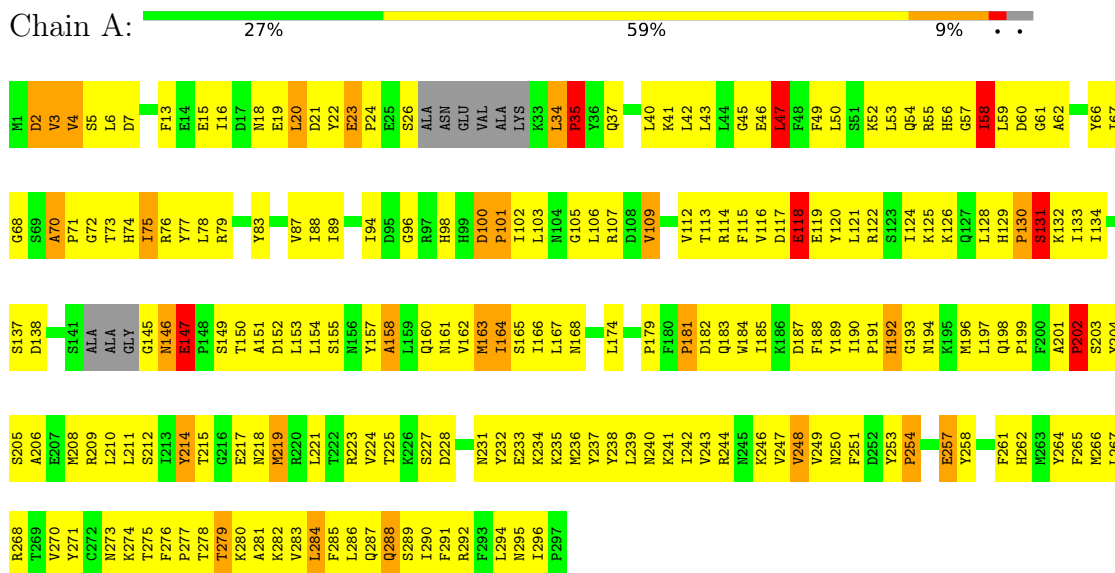
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	O	0	0
			1	1		

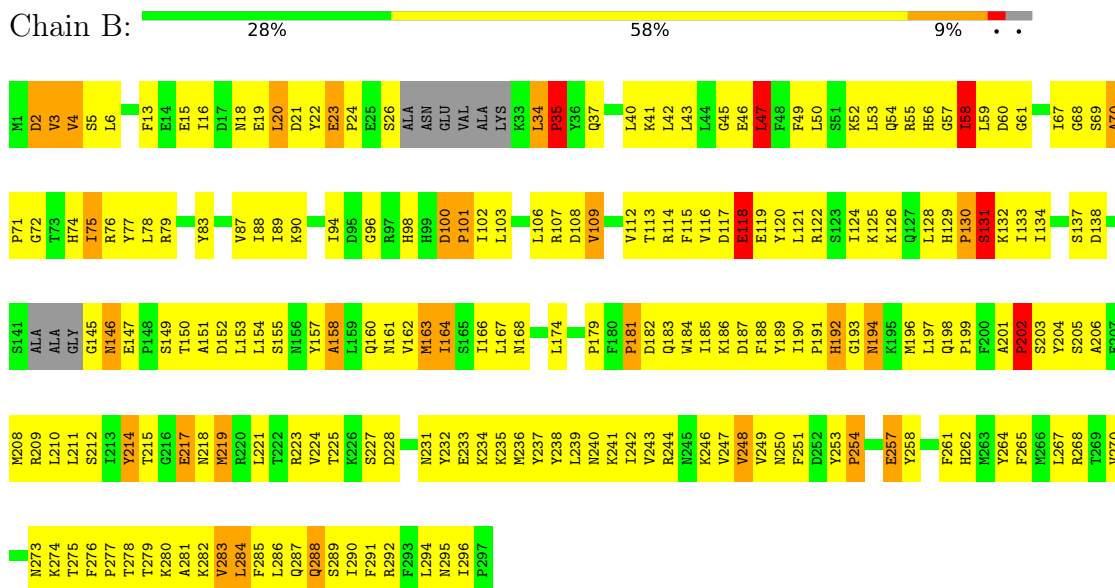
3 Residue-property plots

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

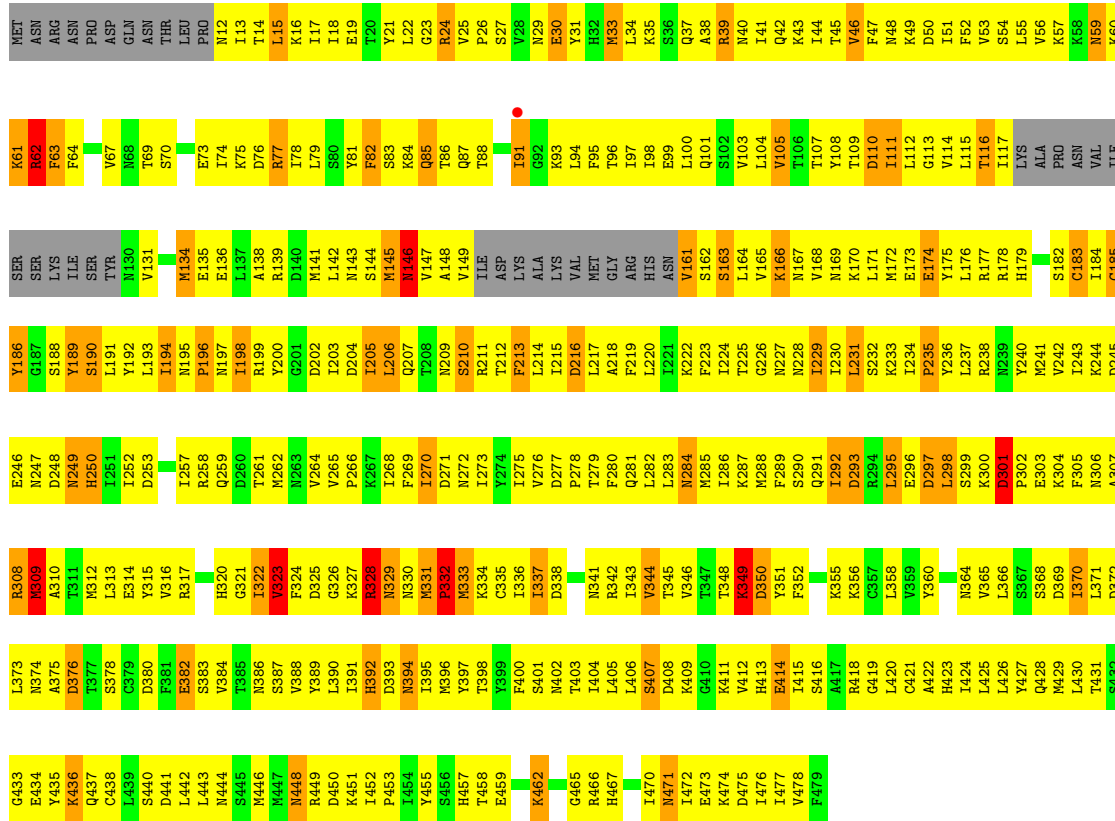


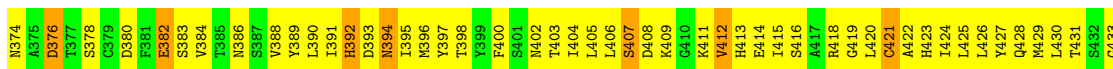
- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



• Molecule 2: Poly(A) polymerase catalytic subunit

Chain C: 15% 62% 14% 7%





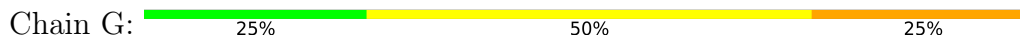
- Molecule 3: RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*C)-3')



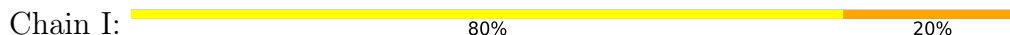
- Molecule 3: RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*C)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.92Å 77.15Å 108.03Å 89.52° 73.45° 63.76°	Depositor
Resolution (Å)	38.55 – 3.21 38.55 – 3.21	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.55-3.21) 93.8 (38.55-3.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.309 0.247 , 0.310	Depositor DCC
R_{free} test set	1453 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.056 for h,h-k,h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U5P, 3AT, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/2444	1.05	23/3308 (0.7%)
1	B	0.63	0/2444	1.05	20/3308 (0.6%)
2	C	0.55	1/3686 (0.0%)	1.07	26/4972 (0.5%)
2	D	0.55	0/3686	1.07	26/4972 (0.5%)
3	E	0.62	0/103	0.80	0/156
3	F	0.50	0/103	0.80	0/156
4	G	0.52	0/82	0.57	0/124
5	I	0.50	0/103	0.58	0/156
All	All	0.58	1/12651 (0.0%)	1.05	95/17152 (0.6%)

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
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	323	VAL	CA-CB	5.04	1.61	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	226	GLY	N-CA-C	-9.85	101.55	115.43
2	D	226	GLY	N-CA-C	-9.79	101.63	115.43
2	C	164	LEU	N-CA-C	-9.73	100.51	112.38
2	D	164	LEU	N-CA-C	-9.55	100.73	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	296	GLU	N-CA-C	-9.07	102.14	113.02
2	D	296	GLU	N-CA-C	-9.02	102.20	113.02
1	B	83	TYR	N-CA-C	-8.43	101.78	110.97
1	A	83	TYR	N-CA-C	-8.30	101.92	110.97
2	D	290	SER	N-CA-C	-8.12	102.93	112.92
2	C	290	SER	N-CA-C	-7.97	103.12	112.92
1	B	116	VAL	N-CA-C	7.63	119.94	109.80
2	C	194	ILE	N-CA-C	-7.62	106.47	113.71
2	D	194	ILE	N-CA-C	-7.48	106.60	113.71
1	A	116	VAL	N-CA-C	7.47	119.74	109.80
2	D	337	ILE	N-CA-C	7.34	117.20	106.55
2	C	337	ILE	N-CA-C	7.28	117.10	106.55
2	C	63	PHE	N-CA-C	-7.25	105.36	114.56
2	D	63	PHE	N-CA-C	-7.05	105.61	114.56
2	D	111	ILE	N-CA-C	6.91	118.54	111.00
2	D	259	GLN	N-CA-C	-6.82	103.84	111.28
1	A	163	MET	N-CA-C	-6.81	102.71	111.02
1	B	163	MET	N-CA-C	-6.79	102.73	111.02
2	C	259	GLN	N-CA-C	-6.79	103.87	111.28
1	A	227	SER	N-CA-C	-6.64	104.04	111.28
2	C	111	ILE	N-CA-C	6.54	118.13	111.00
1	B	227	SER	N-CA-C	-6.37	104.34	111.28
2	C	205	ILE	N-CA-C	6.37	117.88	108.65
2	D	337	ILE	CB-CA-C	-6.35	105.44	112.68
1	A	47	LEU	N-CA-C	-6.33	104.38	111.28
2	D	407	SER	N-CA-C	-6.31	105.58	113.28
2	D	23	GLY	N-CA-C	-6.25	104.36	113.48
2	D	205	ILE	N-CA-C	6.19	117.62	108.65
1	B	47	LEU	N-CA-C	-6.16	104.57	111.28
2	C	407	SER	N-CA-C	-6.15	105.78	113.28
2	C	337	ILE	CB-CA-C	-6.11	105.71	112.68
2	D	328	ARG	N-CA-C	6.11	118.00	107.93
2	D	297	ASP	N-CA-C	-6.10	106.45	114.31
2	C	328	ARG	N-CA-C	5.93	117.72	107.93
2	C	297	ASP	N-CA-C	-5.93	106.67	114.31
1	A	131	SER	N-CA-C	-5.92	101.89	110.24
1	B	23	GLU	CA-C-N	5.90	127.21	119.84
1	B	23	GLU	C-N-CA	5.90	127.21	119.84
1	B	133	ILE	N-CA-C	5.86	117.44	108.71
1	A	23	GLU	CA-C-N	5.73	127.01	119.84
1	A	23	GLU	C-N-CA	5.73	127.01	119.84
1	A	133	ILE	N-CA-C	5.69	116.78	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	SER	N-CA-C	-5.64	102.28	110.24
1	B	158	ALA	N-CA-C	-5.62	105.06	111.07
2	C	414	GLU	N-CA-C	5.60	118.11	111.33
1	B	192	HIS	N-CA-C	-5.53	103.19	110.43
1	A	147	GLU	CA-C-N	5.52	126.74	119.84
1	A	147	GLU	C-N-CA	5.52	126.74	119.84
2	C	392	HIS	N-CA-C	-5.49	102.76	110.50
2	D	392	HIS	N-CA-C	-5.46	102.80	110.50
2	D	478	VAL	N-CA-C	5.46	115.75	108.27
2	D	338	ASP	N-CA-C	-5.45	101.84	109.96
2	C	338	ASP	N-CA-C	-5.45	101.84	109.96
1	A	158	ALA	N-CA-C	-5.44	105.25	111.07
1	B	219	MET	N-CA-C	-5.43	103.36	110.53
2	D	295	LEU	N-CA-C	-5.39	106.87	113.50
1	B	100	ASP	CA-C-N	5.35	126.52	119.84
1	B	100	ASP	C-N-CA	5.35	126.52	119.84
2	C	295	LEU	N-CA-C	-5.32	106.96	113.50
2	D	329	ASN	N-CA-C	5.30	117.67	110.35
2	D	185	CYS	N-CA-C	5.30	117.92	109.81
2	C	105	VAL	N-CA-C	5.28	120.31	109.34
1	A	68	GLY	N-CA-C	-5.26	107.31	115.67
1	A	100	ASP	CA-C-N	5.24	126.39	119.84
1	A	100	ASP	C-N-CA	5.24	126.39	119.84
1	A	15	GLU	N-CA-C	5.24	119.67	113.28
1	A	219	MET	N-CA-C	-5.24	103.61	110.53
1	A	279	THR	N-CA-C	-5.23	105.02	111.40
2	D	105	VAL	N-CA-C	5.22	120.20	109.34
2	D	284	ASN	N-CA-C	-5.22	105.71	111.71
2	C	185	CYS	N-CA-C	5.20	117.77	109.81
1	B	15	GLU	N-CA-C	5.19	119.62	113.28
2	D	322	ILE	N-CA-C	5.19	115.69	108.84
2	D	206	LEU	N-CA-C	-5.18	100.00	108.76
1	A	214	TYR	N-CA-C	5.17	118.50	110.17
2	C	478	VAL	N-CA-C	5.17	115.36	108.27
1	A	7	ASP	N-CA-C	-5.16	107.11	113.41
1	B	214	TYR	N-CA-C	5.14	118.44	110.17
1	A	192	HIS	N-CA-C	-5.12	103.73	110.43
2	D	412	VAL	CB-CA-C	-5.12	106.38	111.80
2	C	146	ASN	N-CA-C	5.11	121.67	110.80
2	C	322	ILE	N-CA-C	5.08	115.55	108.84
2	C	329	ASN	N-CA-C	5.07	117.35	110.35
1	B	90	LYS	N-CA-C	-5.07	101.44	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	298	LEU	N-CA-C	-5.07	105.45	111.69
1	B	34	LEU	CA-C-N	5.05	126.16	119.84
1	B	34	LEU	C-N-CA	5.05	126.16	119.84
1	B	68	GLY	N-CA-C	-5.05	107.65	115.67
2	C	284	ASN	N-CA-C	-5.04	105.91	111.71
1	A	34	LEU	CA-C-N	5.01	126.10	119.84
1	A	34	LEU	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	455	TYR	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	2382	0	2389	243	0
1	B	2382	0	2389	251	0
2	C	3627	0	3689	618	0
2	D	3627	0	3689	630	0
3	E	94	0	55	7	0
3	F	94	0	55	14	0
4	G	75	0	44	5	0
5	I	94	0	55	11	0
6	C	20	0	11	3	0
6	D	20	0	11	3	0
7	C	30	0	12	3	0
7	D	30	0	12	4	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	C	1	0	0	2	0
All	All	12480	0	12411	1716	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 69.

All (1716) 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)
2:C:168:VAL:HA	2:C:171:LEU:HD12	1.23	1.11
2:D:168:VAL:HA	2:D:171:LEU:HD12	1.22	1.10
2:D:333:MET:HE3	2:D:348:THR:HA	1.33	1.09
2:C:333:MET:HE3	2:C:348:THR:HA	1.34	1.09
2:C:86:THR:HB	2:C:87:GLN:HE22	1.20	1.06
2:C:91:ILE:HD13	2:C:91:ILE:H	1.21	1.06
2:C:328:ARG:HA	2:C:328:ARG:HH11	1.22	1.04
2:C:331:MET:HB3	2:C:332:PRO:HD2	1.40	1.03
2:D:91:ILE:H	2:D:91:ILE:HD13	1.23	1.03
2:D:86:THR:HB	2:D:87:GLN:HE22	1.24	1.03
2:C:231:LEU:HD22	2:C:241:MET:HE2	1.41	1.02
2:D:328:ARG:HA	2:D:328:ARG:HH11	1.25	1.02
2:D:331:MET:HB3	2:D:332:PRO:HD2	1.42	1.01
2:C:344:VAL:HG12	2:C:345:THR:H	1.22	1.01
2:C:143:ASN:HA	2:C:146:ASN:HD22	1.22	1.00
2:D:344:VAL:HG12	2:D:345:THR:H	1.24	1.00
1:A:52:LYS:HE2	2:D:376:ASP:HB3	1.44	1.00
2:D:231:LEU:HD22	2:D:241:MET:HE2	1.44	0.99
2:D:143:ASN:HA	2:D:146:ASN:HD22	1.25	0.98
1:A:19:GLU:HB3	1:A:234:LYS:HB3	1.45	0.98
1:B:52:LYS:HE2	2:C:376:ASP:HB3	1.39	0.98
2:C:218:ALA:HB1	2:C:472:ILE:HD11	1.46	0.97
2:D:218:ALA:HB1	2:D:472:ILE:HD11	1.47	0.97
1:B:19:GLU:HB3	1:B:234:LYS:HB3	1.47	0.96
2:D:443:LEU:HA	2:D:446:MET:HE3	1.48	0.93
2:C:443:LEU:HA	2:C:446:MET:HE3	1.49	0.92
2:C:142:LEU:HA	2:C:145:MET:HE3	1.50	0.92
2:C:74:ILE:HA	2:C:77:ARG:HH11	1.35	0.91
2:C:300:LYS:C	2:C:302:PRO:HD3	1.96	0.90
2:D:74:ILE:HA	2:D:77:ARG:HH11	1.36	0.90
1:B:137:SER:HB3	1:B:174:LEU:HD23	1.53	0.90
2:C:415:ILE:HA	2:C:418:ARG:HD3	1.52	0.90
2:D:227:ASN:HD21	2:D:246:GLU:HB2	1.36	0.90
2:C:85:GLN:NE2	2:C:85:GLN:H	1.70	0.90
2:D:142:LEU:HA	2:D:145:MET:HE3	1.53	0.89
1:A:106:LEU:HB2	1:A:109:VAL:HG22	1.53	0.89
1:A:137:SER:HB3	1:A:174:LEU:HD23	1.52	0.89
2:D:300:LYS:C	2:D:302:PRO:HD3	1.97	0.89
2:C:227:ASN:HD21	2:C:246:GLU:HB2	1.37	0.89
1:B:131:SER:HA	2:C:466:ARG:H	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:ILE:HA	2:D:418:ARG:HD3	1.52	0.88
2:D:229:ILE:HD13	2:D:229:ILE:H	1.38	0.88
2:C:40:ASN:O	2:C:44:ILE:HG13	1.73	0.88
2:D:85:GLN:NE2	2:D:85:GLN:H	1.72	0.88
3:F:606:DC:H1'	3:F:607:U:O4'	1.74	0.87
2:C:337:ILE:HD11	2:C:412:VAL:HG13	1.56	0.87
2:C:86:THR:HB	2:C:87:GLN:NE2	1.90	0.87
3:E:602:U:HO2'	3:E:603:U:H6	0.92	0.87
1:B:106:LEU:HB2	1:B:109:VAL:HG22	1.56	0.87
2:D:40:ASN:O	2:D:44:ILE:HG13	1.75	0.87
2:C:282:LEU:HD22	2:C:312:MET:HB3	1.56	0.86
2:D:337:ILE:HD11	2:D:412:VAL:HG13	1.56	0.86
2:D:282:LEU:HD22	2:D:312:MET:HB3	1.56	0.86
1:A:206:ALA:HA	1:A:236:MET:HE3	1.58	0.86
2:C:229:ILE:H	2:C:229:ILE:HD13	1.40	0.86
2:D:141:MET:HE2	2:D:446:MET:HB2	1.55	0.86
1:B:34:LEU:HB3	1:B:35:PRO:HD2	1.58	0.85
2:C:141:MET:HE2	2:C:446:MET:HB2	1.57	0.85
2:C:331:MET:CB	2:C:332:PRO:HD2	2.06	0.84
2:C:328:ARG:HD3	2:C:328:ARG:C	2.02	0.83
2:C:301:ASP:HB3	2:C:304:LYS:HB3	1.58	0.83
2:D:88:THR:HG22	2:D:94:LEU:HG	1.58	0.83
1:B:88:ILE:HD11	2:C:211:ARG:HD2	1.58	0.83
2:D:86:THR:HB	2:D:87:GLN:NE2	1.94	0.83
1:B:206:ALA:HA	1:B:236:MET:HE3	1.61	0.83
1:A:34:LEU:HB3	1:A:35:PRO:HD2	1.60	0.82
3:F:606:DC:H1'	3:F:607:U:C4'	2.09	0.82
2:D:301:ASP:HB3	2:D:304:LYS:HB3	1.59	0.82
2:D:331:MET:CB	2:D:332:PRO:HD2	2.08	0.82
1:A:219:MET:HE2	1:B:221:LEU:HD13	1.61	0.82
1:A:42:LEU:O	1:A:46:GLU:HG3	1.80	0.82
3:E:601:DC:H1'	3:E:602:U:O5'	1.78	0.82
2:C:88:THR:HG22	2:C:94:LEU:HG	1.60	0.81
2:D:64:PHE:CZ	2:D:171:LEU:HD11	2.15	0.81
2:D:328:ARG:C	2:D:328:ARG:HD3	2.05	0.81
1:B:42:LEU:O	1:B:46:GLU:HG3	1.81	0.81
2:C:334:LYS:HG2	2:C:336:ILE:HD11	1.63	0.81
2:D:64:PHE:HZ	2:D:171:LEU:HD11	1.45	0.81
3:F:606:DC:H2''	3:F:607:U:H5''	1.62	0.80
2:C:64:PHE:CZ	2:C:171:LEU:HD11	2.16	0.80
2:C:60:LYS:HE2	2:C:67:VAL:HB	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:MET:HE2	2:D:313:LEU:HG	1.62	0.80
2:D:334:LYS:HG2	2:D:336:ILE:HD11	1.64	0.79
2:C:64:PHE:HZ	2:C:171:LEU:HD11	1.46	0.79
2:D:59:ASN:HD22	2:D:59:ASN:C	1.89	0.79
2:D:437:GLN:H	2:D:437:GLN:CD	1.90	0.79
2:D:308:ARG:HG2	2:D:308:ARG:HH11	1.47	0.79
1:B:231:ASN:HD21	1:B:235:LYS:HD2	1.47	0.79
2:C:328:ARG:HD3	2:C:329:ASN:N	1.97	0.78
2:D:228:ASN:HB3	2:D:473:GLU:CD	2.07	0.78
2:D:166:LYS:HA	2:D:166:LYS:HE2	1.65	0.78
2:C:308:ARG:HG2	2:C:308:ARG:HH11	1.48	0.78
2:D:60:LYS:HE2	2:D:67:VAL:HB	1.66	0.78
2:C:344:VAL:HG12	2:C:345:THR:N	1.99	0.78
2:D:245:ASP:HB3	2:D:249:ASN:H	1.49	0.78
1:B:34:LEU:HB3	1:B:35:PRO:CD	2.14	0.77
2:D:74:ILE:HD13	2:D:77:ARG:NH1	2.00	0.77
2:D:73:GLU:HG2	2:D:77:ARG:HH12	1.49	0.77
2:C:166:LYS:HE2	2:C:166:LYS:HA	1.66	0.77
1:A:231:ASN:HD21	1:A:235:LYS:HD2	1.48	0.77
1:A:219:MET:HE3	1:A:221:LEU:HD11	1.65	0.77
2:C:228:ASN:HB3	2:C:473:GLU:CD	2.09	0.77
2:C:74:ILE:HD13	2:C:77:ARG:NH1	2.00	0.77
2:C:309:MET:HE2	2:C:313:LEU:HG	1.66	0.77
2:D:266:PRO:HD3	2:D:430:LEU:HD23	1.66	0.77
1:B:219:MET:HE3	1:B:221:LEU:HD11	1.65	0.77
2:C:192:TYR:HB2	2:C:198:ILE:HG22	1.67	0.76
4:G:500:DC:H2''	4:G:501:U:OP2	1.84	0.76
2:C:22:LEU:HD22	2:C:24:ARG:NH2	1.99	0.76
2:C:93:LYS:O	2:C:97:ILE:HG13	1.85	0.76
2:D:22:LEU:HD22	2:D:24:ARG:NH2	1.99	0.76
2:D:328:ARG:HD3	2:D:329:ASN:N	1.99	0.76
1:A:34:LEU:HB3	1:A:35:PRO:CD	2.15	0.76
2:C:131:VAL:HA	2:C:314:GLU:HG2	1.65	0.76
2:C:139:ARG:HG3	2:C:306:ASN:HD21	1.49	0.76
2:D:93:LYS:O	2:D:97:ILE:HG13	1.86	0.76
2:D:53:VAL:HG11	2:D:75:LYS:HG3	1.66	0.76
2:D:162:SER:O	2:D:165:VAL:HG23	1.86	0.75
2:C:53:VAL:HG11	2:C:75:LYS:HG3	1.68	0.75
3:E:602:U:O2'	3:E:603:U:H6	1.69	0.75
2:C:266:PRO:HD3	2:C:430:LEU:HD23	1.68	0.75
2:C:245:ASP:HB3	2:C:249:ASN:H	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:VAL:HG12	2:D:345:THR:N	2.02	0.75
2:C:437:GLN:CD	2:C:437:GLN:H	1.94	0.75
1:B:280:LYS:O	1:B:284:LEU:HB2	1.87	0.75
2:C:59:ASN:C	2:C:59:ASN:HD22	1.94	0.75
2:C:60:LYS:HD3	2:C:64:PHE:O	1.87	0.75
2:C:73:GLU:HG2	2:C:77:ARG:HH12	1.51	0.75
2:C:91:ILE:HA	2:C:94:LEU:HD12	1.68	0.75
2:D:139:ARG:HG3	2:D:306:ASN:HD21	1.51	0.74
2:D:323:VAL:HG12	2:D:440:SER:OG	1.86	0.74
2:C:349:LYS:HE3	2:C:350:ASP:OD1	1.86	0.74
2:C:282:LEU:O	2:C:285:MET:HB3	1.88	0.74
2:D:408:ASP:HB3	2:D:411:LYS:CG	2.17	0.74
2:C:162:SER:O	2:C:165:VAL:HG23	1.87	0.74
1:A:131:SER:HA	2:D:466:ARG:H	1.52	0.74
2:C:199:ARG:HH12	2:C:304:LYS:HA	1.52	0.74
2:C:323:VAL:HG12	2:C:440:SER:OG	1.87	0.74
2:D:192:TYR:HB2	2:D:198:ILE:HG22	1.70	0.74
1:B:121:LEU:HD13	1:B:163:MET:HA	1.69	0.74
2:C:231:LEU:HG	2:C:243:ILE:HG12	1.70	0.74
2:D:282:LEU:O	2:D:285:MET:HB3	1.88	0.74
1:B:52:LYS:CE	2:C:376:ASP:HB3	2.17	0.74
2:D:195:ASN:HD22	2:D:198:ILE:HG12	1.53	0.74
2:D:53:VAL:HA	2:D:78:ILE:HD12	1.70	0.73
2:D:174:GLU:OE1	2:D:178:ARG:HD3	1.88	0.73
2:C:269:PHE:CZ	2:C:272:ASN:HA	2.22	0.73
1:A:280:LYS:O	1:A:284:LEU:HB2	1.89	0.73
1:B:193:GLY:HA3	1:B:212:SER:HB3	1.71	0.73
1:B:253:TYR:HE2	1:B:287:GLN:HE22	1.35	0.73
2:C:349:LYS:HG3	2:C:350:ASP:N	2.03	0.73
2:D:424:ILE:O	2:D:427:TYR:HB3	1.89	0.73
2:C:424:ILE:O	2:C:427:TYR:HB3	1.89	0.73
2:C:53:VAL:HA	2:C:78:ILE:HD12	1.71	0.73
2:C:195:ASN:HD22	2:C:198:ILE:HG12	1.54	0.73
2:D:131:VAL:HA	2:D:314:GLU:HG2	1.68	0.73
2:C:409:LYS:HE2	2:C:455:TYR:OH	1.89	0.73
1:A:26:SER:HB3	1:A:204:TYR:CD2	2.24	0.72
2:C:170:LYS:HD2	2:C:173:GLU:OE2	1.88	0.72
2:C:408:ASP:HB3	2:C:411:LYS:CG	2.19	0.72
1:A:121:LEU:HD13	1:A:163:MET:HA	1.70	0.72
1:A:193:GLY:HA3	1:A:212:SER:HB3	1.72	0.72
1:A:253:TYR:HE2	1:A:287:GLN:HE22	1.35	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HB2	1:A:109:VAL:CG2	2.19	0.72
1:B:202:PRO:HB2	1:B:205:SER:HB2	1.71	0.72
1:B:26:SER:HB3	1:B:204:TYR:CD2	2.25	0.72
1:A:70:ALA:HA	1:A:71:PRO:C	2.14	0.72
2:D:170:LYS:HD2	2:D:173:GLU:OE2	1.89	0.72
2:D:227:ASN:HD21	2:D:246:GLU:CB	2.02	0.72
2:C:169:ASN:OD1	2:C:203:ILE:HG13	1.90	0.71
2:D:60:LYS:HD3	2:D:64:PHE:O	1.90	0.71
2:C:172:MET:HB2	2:C:203:ILE:HD12	1.70	0.71
2:D:169:ASN:OD1	2:D:203:ILE:HG13	1.90	0.71
2:D:409:LYS:HE2	2:D:455:TYR:OH	1.90	0.71
1:B:253:TYR:OH	1:B:284:LEU:HA	1.91	0.71
2:D:269:PHE:CZ	2:D:272:ASN:HA	2.25	0.71
1:A:253:TYR:OH	1:A:284:LEU:HA	1.91	0.71
2:C:358:LEU:HD12	2:C:397:TYR:CE2	2.26	0.71
1:B:70:ALA:HA	1:B:71:PRO:C	2.15	0.70
2:D:172:MET:HB2	2:D:203:ILE:HD12	1.70	0.70
1:A:124:ILE:O	1:A:128:LEU:HD13	1.92	0.70
1:A:239:LEU:HA	1:A:243:VAL:CG2	2.21	0.70
1:B:53:LEU:HD22	1:B:58:ILE:HG12	1.74	0.70
2:C:227:ASN:HD21	2:C:246:GLU:CB	2.04	0.70
2:D:166:LYS:HE2	2:D:166:LYS:CA	2.21	0.70
2:C:303:GLU:HA	2:C:306:ASN:HB2	1.74	0.70
1:B:122:ARG:O	1:B:126:LYS:HG3	1.91	0.70
2:C:166:LYS:HE2	2:C:166:LYS:CA	2.21	0.70
1:A:53:LEU:HD22	1:A:58:ILE:HG12	1.73	0.70
2:C:74:ILE:HA	2:C:77:ARG:NH1	2.06	0.70
2:D:199:ARG:HH12	2:D:304:LYS:HA	1.55	0.70
2:D:349:LYS:HG3	2:D:350:ASP:N	2.06	0.70
1:A:279:THR:HG22	1:A:283:VAL:HG23	1.74	0.70
2:D:303:GLU:HA	2:D:306:ASN:HB2	1.74	0.70
2:C:61:LYS:HB2	2:C:61:LYS:NZ	2.07	0.70
2:C:240:TYR:CE1	2:C:253:ASP:HB2	2.26	0.70
2:D:462:LYS:H	2:D:462:LYS:HD2	1.55	0.70
2:D:91:ILE:HA	2:D:94:LEU:HD12	1.74	0.69
2:C:174:GLU:OE1	2:C:178:ARG:HD3	1.92	0.69
2:C:174:GLU:O	2:C:178:ARG:HG2	1.92	0.69
2:C:269:PHE:CE1	2:C:272:ASN:HA	2.26	0.69
2:D:61:LYS:HB2	2:D:61:LYS:NZ	2.07	0.69
1:B:106:LEU:HB2	1:B:109:VAL:CG2	2.22	0.69
2:D:358:LEU:HD12	2:D:397:TYR:CE2	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ILE:HA	2:D:77:ARG:NH1	2.07	0.69
2:D:473:GLU:HG3	2:D:474:LYS:H	1.57	0.69
2:C:389:TYR:HB3	2:C:396:MET:HE2	1.73	0.69
2:D:389:TYR:HB3	2:D:396:MET:HE2	1.74	0.69
2:C:282:LEU:HD12	2:C:285:MET:HB3	1.74	0.69
1:A:53:LEU:HB3	1:A:58:ILE:HG13	1.75	0.69
2:C:462:LYS:HD2	2:C:462:LYS:H	1.56	0.69
1:B:279:THR:HG22	1:B:283:VAL:HG23	1.75	0.68
2:C:473:GLU:HG3	2:C:474:LYS:H	1.58	0.68
2:D:231:LEU:HG	2:D:243:ILE:HG12	1.75	0.68
2:D:408:ASP:HB3	2:D:411:LYS:HG3	1.74	0.68
2:D:51:ILE:HG23	5:I:701:DC:H5'	1.73	0.68
2:C:24:ARG:NH1	2:C:86:THR:HA	2.08	0.68
2:D:240:TYR:CE1	2:D:253:ASP:HB2	2.28	0.68
2:C:418:ARG:NH2	2:C:446:MET:HA	2.08	0.68
2:D:193:LEU:HD23	2:D:273:ILE:HD11	1.73	0.68
2:D:301:ASP:HB3	2:D:304:LYS:CB	2.23	0.68
2:D:309:MET:HG3	2:D:310:ALA:N	2.06	0.68
1:A:122:ARG:O	1:A:126:LYS:HG3	1.94	0.68
1:A:202:PRO:HB2	1:A:205:SER:HB2	1.75	0.68
1:B:219:MET:CE	1:B:221:LEU:HD11	2.23	0.68
2:C:78:ILE:HG12	2:C:223:PHE:CD1	2.28	0.68
2:C:193:LEU:HD23	2:C:273:ILE:HD11	1.73	0.68
2:D:78:ILE:HG12	2:D:223:PHE:CD1	2.27	0.68
2:D:414:GLU:OE1	2:D:452:ILE:HD12	1.93	0.68
2:C:301:ASP:HB3	2:C:304:LYS:CB	2.23	0.68
1:B:124:ILE:O	1:B:128:LEU:HD13	1.94	0.68
2:C:195:ASN:C	2:C:197:ASN:H	2.02	0.68
2:D:269:PHE:CE1	2:D:272:ASN:HA	2.28	0.67
2:D:317:ARG:O	2:D:321:GLY:HA2	1.93	0.67
2:C:78:ILE:HG12	2:C:223:PHE:CE1	2.29	0.67
2:C:470:ILE:HG23	2:C:477:ILE:HG12	1.76	0.67
2:D:195:ASN:C	2:D:197:ASN:H	2.03	0.67
2:D:331:MET:HA	2:D:331:MET:HE3	1.76	0.67
1:B:287:GLN:HG3	1:B:291:PHE:CE1	2.29	0.67
2:D:325:ASP:OD2	2:D:327:LYS:HB3	1.95	0.67
1:B:164:ILE:HD11	1:B:174:LEU:HD11	1.77	0.67
1:B:239:LEU:HA	1:B:243:VAL:CG2	2.24	0.67
2:D:24:ARG:NH1	2:D:86:THR:HA	2.09	0.67
2:C:349:LYS:HG3	2:C:350:ASP:H	1.57	0.67
2:D:418:ARG:NH2	2:D:446:MET:HA	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ALA:O	1:B:208:MET:HE2	1.94	0.67
2:D:355:LYS:HG3	2:D:356:LYS:H	1.60	0.67
2:C:355:LYS:HG3	2:C:356:LYS:N	2.09	0.67
2:C:355:LYS:HG3	2:C:356:LYS:H	1.60	0.67
2:D:282:LEU:HD12	2:D:285:MET:HB3	1.75	0.67
2:D:349:LYS:HE3	2:D:350:ASP:OD1	1.94	0.67
2:D:355:LYS:HG3	2:D:356:LYS:N	2.09	0.67
1:B:52:LYS:HE2	2:C:376:ASP:CB	2.19	0.67
2:D:78:ILE:HG12	2:D:223:PHE:CE1	2.29	0.67
2:D:235:PRO:HD2	2:D:467:HIS:ND1	2.10	0.67
2:D:331:MET:HG3	2:D:442:LEU:HA	1.76	0.66
2:D:443:LEU:HA	2:D:446:MET:CE	2.24	0.66
1:B:53:LEU:HB3	1:B:58:ILE:HG13	1.77	0.66
2:C:93:LYS:HG2	6:C:600:U5P:O2	1.95	0.66
2:C:258:ARG:N	2:C:382:GLU:OE2	2.29	0.66
1:A:43:LEU:HD23	1:A:74:HIS:HB2	1.77	0.66
1:A:88:ILE:HD11	2:D:211:ARG:HD2	1.77	0.66
2:C:309:MET:HG3	2:C:310:ALA:N	2.08	0.66
2:C:328:ARG:HA	2:C:328:ARG:NH1	2.06	0.66
1:B:191:PRO:O	1:B:210:LEU:HD21	1.96	0.66
2:C:409:LYS:HG2	2:C:455:TYR:CZ	2.30	0.66
2:D:162:SER:HB3	2:D:249:ASN:HD22	1.60	0.66
2:D:176:LEU:C	2:D:273:ILE:HG22	2.21	0.66
2:D:409:LYS:HG2	2:D:455:TYR:CZ	2.30	0.66
1:A:215:THR:OG1	1:A:218:ASN:HB2	1.96	0.66
2:D:404:ILE:HB	2:D:458:THR:HG23	1.77	0.66
2:C:143:ASN:HA	2:C:146:ASN:ND2	2.04	0.66
2:C:279:THR:O	2:C:283:LEU:HD23	1.96	0.66
2:C:317:ARG:O	2:C:321:GLY:HA2	1.95	0.66
1:A:276:PHE:HZ	1:A:285:PHE:CD2	2.14	0.66
2:D:176:LEU:HB3	2:D:273:ILE:HB	1.78	0.66
1:A:150:THR:HG23	1:A:179:PRO:HB3	1.78	0.65
1:A:164:ILE:HD11	1:A:174:LEU:HD11	1.78	0.65
2:C:176:LEU:HB3	2:C:273:ILE:HB	1.78	0.65
2:D:235:PRO:HD2	2:D:467:HIS:CE1	2.31	0.65
2:C:60:LYS:CE	2:C:67:VAL:HB	2.25	0.65
2:C:280:PHE:HA	2:C:429:MET:HE1	1.78	0.65
2:C:414:GLU:OE1	2:C:452:ILE:HD12	1.96	0.65
2:D:134:MET:HA	2:D:134:MET:HE3	1.78	0.65
2:C:199:ARG:NH1	2:C:304:LYS:HA	2.12	0.65
2:C:443:LEU:HA	2:C:446:MET:CE	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:SER:HB2	2:D:200:TYR:HB2	1.79	0.65
3:F:606:DC:C2'	3:F:607:U:H5''	2.27	0.65
2:D:228:ASN:HB3	2:D:473:GLU:OE2	1.96	0.65
3:F:607:U:H5'	3:F:608:U:C5	2.32	0.65
1:A:191:PRO:O	1:A:210:LEU:HD21	1.97	0.65
1:A:219:MET:CE	1:A:221:LEU:HD11	2.26	0.65
1:B:131:SER:HA	2:C:466:ARG:N	2.09	0.65
2:D:279:THR:O	2:D:283:LEU:HD23	1.97	0.65
2:D:109:THR:HG21	5:I:703:U:OP2	1.97	0.65
2:D:174:GLU:O	2:D:178:ARG:HG2	1.96	0.65
2:D:308:ARG:HG2	2:D:308:ARG:NH1	2.11	0.65
1:A:88:ILE:C	1:A:89:ILE:HG13	2.22	0.65
2:C:230:ILE:HG22	2:C:471:ASN:ND2	2.11	0.65
1:B:278:THR:O	1:B:281:ALA:HB3	1.97	0.64
2:D:331:MET:HA	2:D:331:MET:CE	2.24	0.64
2:C:404:ILE:HB	2:C:458:THR:HG23	1.79	0.64
2:C:310:ALA:HA	2:C:313:LEU:HD12	1.79	0.64
2:D:51:ILE:HG23	5:I:701:DC:C5'	2.27	0.64
2:C:276:VAL:O	2:C:281:GLN:HG3	1.98	0.64
2:C:331:MET:HB3	2:C:332:PRO:CD	2.23	0.64
2:C:331:MET:HG3	2:C:442:LEU:HA	1.78	0.64
2:D:245:ASP:HB3	2:D:249:ASN:N	2.13	0.64
2:D:258:ARG:N	2:D:382:GLU:OE2	2.31	0.64
3:E:601:DC:O2	3:E:602:U:H5'	1.97	0.64
1:A:287:GLN:HG3	1:A:291:PHE:CE1	2.32	0.64
1:B:276:PHE:HZ	1:B:285:PHE:CD2	2.16	0.64
2:C:282:LEU:HD22	2:C:312:MET:CB	2.28	0.64
2:C:300:LYS:O	2:C:302:PRO:HD3	1.96	0.64
2:C:408:ASP:HB3	2:C:411:LYS:HG3	1.79	0.64
1:B:257:GLU:OE1	1:B:257:GLU:N	2.31	0.64
1:A:208:MET:HE2	1:A:236:MET:HE2	1.79	0.64
2:C:176:LEU:C	2:C:273:ILE:HG22	2.23	0.64
1:A:61:GLY:HA2	1:A:88:ILE:HG22	1.80	0.64
2:C:235:PRO:HD2	2:C:467:HIS:CE1	2.33	0.64
2:C:235:PRO:HD2	2:C:467:HIS:ND1	2.12	0.64
1:A:278:THR:O	1:A:281:ALA:HB3	1.98	0.63
2:D:143:ASN:HA	2:D:146:ASN:ND2	2.08	0.63
2:D:266:PRO:HD3	2:D:430:LEU:CD2	2.28	0.63
1:A:206:ALA:O	1:A:208:MET:HE2	1.97	0.63
2:C:162:SER:HB3	2:C:249:ASN:HD22	1.63	0.63
2:D:199:ARG:NH1	2:D:304:LYS:HA	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LEU:HD23	2:D:243:ILE:HD12	1.80	0.63
2:D:234:ILE:HD12	2:D:234:ILE:N	2.12	0.63
2:D:60:LYS:CE	2:D:67:VAL:HB	2.28	0.63
2:D:349:LYS:HG3	2:D:350:ASP:H	1.61	0.63
1:B:88:ILE:C	1:B:89:ILE:HG13	2.24	0.63
1:B:267:LEU:HA	1:B:270:VAL:HG23	1.80	0.63
2:C:84:LYS:HA	2:C:87:GLN:OE1	1.98	0.63
1:B:150:THR:HG23	1:B:179:PRO:HB3	1.80	0.63
1:B:184:TRP:HH2	1:B:224:VAL:HG12	1.63	0.63
2:C:225:THR:HG21	2:C:227:ASN:HB2	1.81	0.63
2:D:222:LYS:HB2	2:D:229:ILE:HD11	1.79	0.63
1:B:208:MET:HE2	1:B:236:MET:HE2	1.80	0.63
2:D:297:ASP:HA	2:D:300:LYS:HD3	1.81	0.63
2:C:222:LYS:HD2	2:C:227:ASN:O	1.98	0.63
2:C:228:ASN:HB3	2:C:473:GLU:OE2	1.98	0.63
2:C:325:ASP:OD2	2:C:327:LYS:HB3	1.99	0.63
2:D:310:ALA:HA	2:D:313:LEU:HD12	1.81	0.63
2:C:335:CYS:C	2:C:336:ILE:HD13	2.24	0.63
2:C:349:LYS:CG	2:C:350:ASP:N	2.61	0.63
2:D:328:ARG:HG3	2:D:441:ASP:HA	1.81	0.63
1:B:56:HIS:HA	2:C:388:VAL:HG21	1.79	0.63
2:C:184:ILE:HD12	2:C:262:MET:SD	2.39	0.63
2:C:308:ARG:HG2	2:C:308:ARG:NH1	2.12	0.63
2:D:177:ARG:N	2:D:273:ILE:HG22	2.14	0.63
1:A:267:LEU:HA	1:A:270:VAL:HG23	1.81	0.62
2:C:59:ASN:O	2:C:60:LYS:C	2.41	0.62
2:C:297:ASP:HA	2:C:300:LYS:HD3	1.81	0.62
2:D:87:GLN:N	2:D:87:GLN:CD	2.57	0.62
2:D:276:VAL:O	2:D:281:GLN:HG3	1.99	0.62
1:A:52:LYS:CE	2:D:376:ASP:HB3	2.23	0.62
1:A:88:ILE:O	1:A:89:ILE:HG13	1.98	0.62
2:C:76:ASP:O	2:C:77:ARG:C	2.41	0.62
2:D:300:LYS:O	2:D:302:PRO:HD3	1.98	0.62
2:D:470:ILE:HG23	2:D:477:ILE:HG12	1.81	0.62
2:C:24:ARG:HH12	2:C:86:THR:HA	1.62	0.62
2:C:185:CYS:O	2:C:276:VAL:HG23	1.98	0.62
2:C:337:ILE:CD1	2:C:412:VAL:HG22	2.30	0.62
2:C:418:ARG:HH22	2:C:446:MET:HA	1.64	0.62
2:D:280:PHE:HA	2:D:429:MET:HE1	1.81	0.62
1:B:43:LEU:HD23	1:B:74:HIS:HB2	1.80	0.62
2:D:185:CYS:O	2:D:276:VAL:HG23	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:ASN:ND2	2:D:246:GLU:HB2	2.12	0.62
2:D:449:ARG:HH11	2:D:449:ARG:HA	1.63	0.62
1:A:46:GLU:O	1:A:50:LEU:HD23	1.99	0.62
2:C:188:SER:HB2	2:C:200:TYR:HB2	1.82	0.62
2:C:227:ASN:ND2	2:C:246:GLU:HB2	2.13	0.62
2:C:433:GLY:O	2:C:435:TYR:HD2	1.83	0.62
2:D:24:ARG:HH12	2:D:86:THR:HA	1.62	0.62
1:A:60:ASP:CB	2:D:238:ARG:HH11	2.13	0.62
2:C:328:ARG:HG3	2:C:441:ASP:HA	1.82	0.62
2:D:69:THR:HG21	2:D:224:ILE:O	2.00	0.62
2:D:317:ARG:HA	2:D:322:ILE:H	1.63	0.62
2:C:142:LEU:HD21	2:C:298:LEU:HD11	1.81	0.62
2:C:266:PRO:HD3	2:C:430:LEU:CD2	2.29	0.62
2:C:309:MET:HA	2:C:309:MET:HE3	1.82	0.62
2:D:331:MET:O	2:D:332:PRO:C	2.42	0.62
1:A:167:LEU:O	1:A:168:ASN:C	2.41	0.62
1:B:167:LEU:O	1:B:168:ASN:C	2.42	0.62
2:C:449:ARG:HA	2:C:449:ARG:HH11	1.64	0.62
2:D:142:LEU:HD21	2:D:298:LEU:HD11	1.81	0.62
1:A:265:PHE:HA	1:A:268:ARG:HD2	1.81	0.62
2:C:245:ASP:HB3	2:C:249:ASN:N	2.15	0.62
2:C:331:MET:O	2:C:332:PRO:C	2.43	0.62
2:C:408:ASP:HB3	2:C:411:LYS:HD2	1.82	0.62
2:D:178:ARG:HA	2:D:178:ARG:HH11	1.65	0.62
2:D:184:ILE:HD12	2:D:262:MET:SD	2.39	0.62
2:D:186:TYR:HB3	2:D:276:VAL:CG2	2.30	0.62
2:D:225:THR:HG21	2:D:227:ASN:HB2	1.82	0.62
2:D:433:GLY:O	2:D:435:TYR:HD2	1.83	0.62
1:A:184:TRP:HH2	1:A:224:VAL:HG12	1.65	0.61
2:C:225:THR:CG2	2:C:227:ASN:HB2	2.30	0.61
2:C:234:ILE:N	2:C:234:ILE:HD12	2.14	0.61
2:D:331:MET:HB3	2:D:332:PRO:CD	2.24	0.61
2:D:337:ILE:CD1	2:D:412:VAL:HG22	2.30	0.61
1:A:58:ILE:HG13	1:A:59:LEU:N	2.15	0.61
2:C:177:ARG:N	2:C:273:ILE:HG22	2.15	0.61
2:D:84:LYS:HA	2:D:87:GLN:OE1	2.00	0.61
1:B:215:THR:OG1	1:B:218:ASN:HB2	2.00	0.61
1:A:58:ILE:HD11	1:A:134:ILE:HG12	1.82	0.61
1:B:231:ASN:ND2	1:B:235:LYS:HD2	2.14	0.61
2:C:191:LEU:HD12	2:C:308:ARG:HB3	1.82	0.61
2:D:59:ASN:C	2:D:59:ASN:ND2	2.57	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:ILE:HG22	2:D:471:ASN:ND2	2.15	0.61
2:D:443:LEU:CA	2:D:446:MET:HE3	2.24	0.61
1:B:88:ILE:O	1:B:89:ILE:HG13	1.99	0.61
1:B:129:HIS:ND1	1:B:130:PRO:HA	2.16	0.61
2:D:76:ASP:O	2:D:77:ARG:C	2.43	0.61
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.65	0.61
2:C:45:THR:C	2:C:47:PHE:H	2.09	0.61
2:C:69:THR:HG21	2:C:224:ILE:O	2.00	0.61
2:C:87:GLN:CD	2:C:87:GLN:N	2.59	0.61
2:C:205:ILE:C	2:C:206:LEU:HD23	2.25	0.61
2:C:292:ILE:HG23	2:C:293:ASP:H	1.65	0.61
2:D:270:ILE:O	2:D:271:ASP:HB2	1.99	0.61
1:A:94:ILE:HG23	1:A:112:VAL:HB	1.83	0.61
1:B:61:GLY:HA2	1:B:88:ILE:HG22	1.83	0.61
2:C:186:TYR:HB3	2:C:276:VAL:CG2	2.30	0.61
2:C:261:THR:O	2:C:265:VAL:HG23	2.00	0.61
2:D:222:LYS:HE2	2:D:473:GLU:HB3	1.83	0.61
2:D:309:MET:HA	2:D:309:MET:HE3	1.83	0.61
1:A:221:LEU:N	1:A:221:LEU:HD12	2.15	0.61
2:D:349:LYS:C	2:D:351:TYR:H	2.08	0.61
2:C:116:THR:O	2:C:117:ILE:HG13	2.00	0.61
2:C:413:HIS:NE2	2:C:415:ILE:HG13	2.16	0.61
2:D:222:LYS:HD2	2:D:227:ASN:O	2.00	0.61
2:D:335:CYS:C	2:D:336:ILE:HD13	2.26	0.61
1:A:43:LEU:O	1:A:47:LEU:HB2	2.01	0.61
2:C:222:LYS:HB2	2:C:229:ILE:HD11	1.80	0.61
2:C:270:ILE:O	2:C:271:ASP:HB2	2.00	0.61
2:D:261:THR:O	2:D:265:VAL:HG23	2.01	0.61
2:C:331:MET:HA	2:C:331:MET:CE	2.27	0.60
2:C:400:PHE:CE2	2:C:402:ASN:HB2	2.36	0.60
2:D:292:ILE:HG23	2:D:293:ASP:H	1.65	0.60
1:B:94:ILE:HG23	1:B:112:VAL:HB	1.84	0.60
2:D:418:ARG:HH22	2:D:446:MET:HA	1.66	0.60
2:C:242:VAL:HA	2:C:253:ASP:HA	1.81	0.60
2:C:328:ARG:HH11	2:C:328:ARG:CA	2.07	0.60
1:A:79:ARG:HD2	1:A:106:LEU:HD13	1.82	0.60
1:A:257:GLU:OE1	1:A:257:GLU:N	2.35	0.60
2:C:217:LEU:HD23	2:C:243:ILE:HD12	1.84	0.60
2:D:205:ILE:C	2:D:206:LEU:HD23	2.26	0.60
2:C:39:ARG:O	2:C:43:LYS:N	2.32	0.60
2:C:88:THR:O	2:C:94:LEU:HD21	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:ARG:HA	2:C:322:ILE:H	1.65	0.60
1:B:265:PHE:HA	1:B:268:ARG:HD2	1.82	0.60
2:C:331:MET:HA	2:C:331:MET:HE3	1.82	0.60
1:A:231:ASN:ND2	1:A:235:LYS:HD2	2.16	0.60
1:B:79:ARG:HD2	1:B:106:LEU:HD13	1.83	0.60
1:B:107:ARG:CZ	2:C:477:ILE:HG21	2.31	0.60
2:D:189:TYR:CE2	2:D:193:LEU:HD11	2.37	0.60
2:C:222:LYS:HE2	2:C:473:GLU:HB3	1.84	0.60
2:D:63:PHE:CD2	2:D:171:LEU:HA	2.36	0.60
2:D:225:THR:CG2	2:D:227:ASN:HB2	2.32	0.60
1:B:72:GLY:HA3	1:B:75:ILE:HD12	1.83	0.60
2:D:53:VAL:O	2:D:57:LYS:HG3	2.02	0.60
2:C:328:ARG:NH1	2:C:329:ASN:H	1.98	0.60
2:D:88:THR:O	2:D:94:LEU:HD21	2.02	0.60
2:D:349:LYS:CG	2:D:350:ASP:N	2.65	0.60
2:D:413:HIS:NE2	2:D:415:ILE:HG13	2.17	0.60
1:B:201:ALA:O	1:B:202:PRO:C	2.45	0.59
2:C:134:MET:HA	2:C:134:MET:HE3	1.84	0.59
1:B:122:ARG:HH11	1:B:122:ARG:HG3	1.67	0.59
2:C:63:PHE:CD2	2:C:171:LEU:HA	2.36	0.59
2:D:81:TYR:C	2:D:83:SER:H	2.09	0.59
2:D:282:LEU:HD22	2:D:312:MET:CB	2.28	0.59
1:A:107:ARG:CZ	2:D:477:ILE:HG21	2.32	0.59
2:C:54:SER:HA	2:C:57:LYS:HD2	1.85	0.59
2:C:60:LYS:O	2:C:64:PHE:C	2.46	0.59
2:D:45:THR:C	2:D:47:PHE:H	2.11	0.59
1:B:58:ILE:HD11	1:B:134:ILE:HG12	1.85	0.59
2:D:242:VAL:HA	2:D:253:ASP:HA	1.82	0.59
2:D:328:ARG:HD2	2:D:441:ASP:HB3	1.84	0.59
2:D:391:ILE:HA	2:D:395:ILE:O	2.01	0.59
2:C:138:ALA:HB2	2:C:310:ALA:HB2	1.85	0.59
2:C:443:LEU:CA	2:C:446:MET:HE3	2.27	0.59
2:D:191:LEU:HD12	2:D:308:ARG:HB3	1.85	0.59
1:B:45:GLY:HA2	1:B:196:MET:HE1	1.84	0.59
2:C:136:GLU:HA	2:C:139:ARG:NH2	2.18	0.59
1:B:43:LEU:O	1:B:47:LEU:HB2	2.03	0.59
1:B:46:GLU:O	1:B:50:LEU:HD23	2.02	0.59
1:B:286:LEU:O	1:B:287:GLN:C	2.45	0.59
2:C:349:LYS:C	2:C:351:TYR:H	2.09	0.59
1:B:60:ASP:HB3	2:C:238:ARG:HH11	1.67	0.59
1:B:101:PRO:C	1:B:103:LEU:H	2.09	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:VAL:O	2:C:57:LYS:HG3	2.03	0.59
2:C:408:ASP:HB3	2:C:411:LYS:CD	2.33	0.59
2:D:59:ASN:O	2:D:60:LYS:C	2.44	0.59
2:C:285:MET:HG2	2:C:312:MET:HE1	1.85	0.59
1:A:129:HIS:ND1	1:A:130:PRO:HA	2.18	0.58
1:A:221:LEU:CD1	1:B:221:LEU:CD1	2.81	0.58
2:C:199:ARG:O	2:C:199:ARG:HG3	2.02	0.58
2:D:39:ARG:O	2:D:43:LYS:N	2.33	0.58
2:D:282:LEU:HD12	2:D:285:MET:CB	2.33	0.58
1:A:201:ALA:O	1:A:202:PRO:C	2.46	0.58
1:B:58:ILE:HG13	1:B:59:LEU:N	2.17	0.58
1:A:286:LEU:O	1:A:287:GLN:C	2.45	0.58
2:C:60:LYS:HZ3	2:C:67:VAL:H	1.51	0.58
2:C:427:TYR:CE1	2:C:431:THR:HG21	2.38	0.58
1:A:60:ASP:HB3	2:D:238:ARG:HH11	1.68	0.58
1:A:258:TYR:O	1:A:261:PHE:HB3	2.02	0.58
1:B:221:LEU:HD12	1:B:221:LEU:N	2.18	0.58
2:C:282:LEU:HD12	2:C:285:MET:CB	2.34	0.58
2:D:53:VAL:HA	2:D:78:ILE:CD1	2.32	0.58
1:A:165:SER:HG	1:B:189:TYR:HE1	1.51	0.58
1:A:190:ILE:HD12	1:A:210:LEU:HD22	1.83	0.58
1:A:221:LEU:HD11	1:B:221:LEU:HD13	1.85	0.58
2:C:53:VAL:HA	2:C:78:ILE:CD1	2.32	0.58
2:C:351:TYR:CD2	2:C:438:CYS:HB2	2.39	0.58
2:D:54:SER:HA	2:D:57:LYS:HD2	1.86	0.58
2:D:328:ARG:HH11	2:D:328:ARG:CA	2.10	0.58
1:A:101:PRO:C	1:A:103:LEU:H	2.10	0.58
2:C:178:ARG:HH11	2:C:178:ARG:HA	1.69	0.58
2:C:360:TYR:N	2:C:398:THR:O	2.26	0.58
2:D:104:LEU:HD21	2:D:219:PHE:CG	2.38	0.58
2:D:138:ALA:HB2	2:D:310:ALA:HB2	1.86	0.58
2:C:19:GLU:HG2	2:C:26:PRO:HD3	1.85	0.58
1:A:279:THR:O	1:A:280:LYS:C	2.45	0.58
2:C:391:ILE:HA	2:C:395:ILE:O	2.03	0.58
2:C:413:HIS:CD2	2:C:415:ILE:H	2.21	0.58
2:C:416:SER:C	2:C:418:ARG:N	2.60	0.58
2:D:62:ARG:HB3	2:D:63:PHE:CD1	2.39	0.58
2:D:413:HIS:CD2	2:D:415:ILE:H	2.21	0.58
1:B:20:LEU:HD22	1:B:237:TYR:HE2	1.68	0.57
2:D:276:VAL:O	2:D:277:ASP:C	2.46	0.57
1:A:45:GLY:HA2	1:A:196:MET:HE1	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:ILE:H	2:D:91:ILE:CD1	1.96	0.57
2:D:404:ILE:HB	2:D:458:THR:CG2	2.34	0.57
1:A:70:ALA:HB1	1:A:98:HIS:O	2.04	0.57
1:A:239:LEU:HD12	1:A:243:VAL:HB	1.87	0.57
2:C:202:ASP:HB2	9:C:1001:HOH:O	2.03	0.57
2:C:292:ILE:HG23	2:C:293:ASP:N	2.19	0.57
2:C:476:ILE:HD12	6:C:600:U5P:O2'	2.04	0.57
2:D:136:GLU:HA	2:D:139:ARG:NH2	2.20	0.57
1:B:190:ILE:HD12	1:B:210:LEU:HD22	1.84	0.57
2:C:211:ARG:O	2:C:215:ILE:HG13	2.04	0.57
2:C:258:ARG:NH2	2:C:380:ASP:O	2.37	0.57
2:D:199:ARG:HG3	2:D:199:ARG:O	2.03	0.57
2:D:435:TYR:O	2:D:436:LYS:C	2.47	0.57
2:D:109:THR:HG21	5:I:703:U:P	2.44	0.57
2:D:268:ILE:HG13	2:D:277:ASP:HA	1.86	0.57
2:D:358:LEU:N	2:D:396:MET:O	2.37	0.57
2:C:333:MET:HG3	2:C:346:VAL:HG13	1.85	0.57
2:C:358:LEU:N	2:C:396:MET:O	2.37	0.57
2:D:19:GLU:HG2	2:D:26:PRO:HD3	1.85	0.57
2:D:60:LYS:O	2:D:64:PHE:C	2.48	0.57
2:D:64:PHE:HE1	2:D:171:LEU:HD21	1.69	0.57
2:D:292:ILE:HG23	2:D:293:ASP:N	2.20	0.57
2:D:323:VAL:O	2:D:323:VAL:HG13	2.04	0.57
2:D:391:ILE:O	2:D:391:ILE:HG22	2.05	0.57
2:C:139:ARG:HG3	2:C:306:ASN:ND2	2.19	0.57
2:C:215:ILE:O	2:C:218:ALA:HB3	2.04	0.57
2:D:258:ARG:NH2	2:D:380:ASP:O	2.37	0.57
2:D:416:SER:C	2:D:418:ARG:N	2.62	0.57
2:C:104:LEU:HD21	2:C:219:PHE:CG	2.40	0.57
1:A:20:LEU:HD22	1:A:237:TYR:HE2	1.70	0.57
1:A:248:VAL:HG21	1:A:261:PHE:CD2	2.40	0.57
1:B:79:ARG:HH11	1:B:79:ARG:HG2	1.70	0.57
2:C:333:MET:HG3	2:C:346:VAL:CG1	2.35	0.57
2:C:349:LYS:C	2:C:349:LYS:HD2	2.30	0.57
2:D:174:GLU:CD	2:D:178:ARG:HD3	2.30	0.57
2:D:408:ASP:HB3	2:D:411:LYS:CD	2.35	0.57
2:C:291:GLN:HE21	2:C:293:ASP:HB3	1.70	0.56
2:D:75:LYS:O	2:D:79:LEU:HG	2.05	0.56
2:D:408:ASP:HB3	2:D:411:LYS:HD2	1.87	0.56
2:D:416:SER:C	2:D:418:ARG:H	2.13	0.56
1:B:2:ASP:C	1:B:246:LYS:HZ3	2.12	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TYR:O	1:B:261:PHE:HB3	2.05	0.56
1:B:248:VAL:HG21	1:B:261:PHE:CD2	2.40	0.56
2:C:59:ASN:C	2:C:59:ASN:ND2	2.62	0.56
2:C:91:ILE:H	2:C:91:ILE:CD1	1.95	0.56
2:C:189:TYR:CE2	2:C:193:LEU:HD11	2.40	0.56
2:C:413:HIS:O	2:C:416:SER:HB2	2.04	0.56
2:D:13:ILE:O	2:D:17:ILE:HG12	2.05	0.56
2:D:60:LYS:HZ3	2:D:67:VAL:H	1.52	0.56
2:D:211:ARG:O	2:D:215:ILE:HG13	2.05	0.56
1:B:239:LEU:HD12	1:B:243:VAL:HB	1.88	0.56
2:C:81:TYR:C	2:C:83:SER:H	2.13	0.56
2:D:268:ILE:CG1	2:D:277:ASP:HA	2.36	0.56
2:D:328:ARG:NH1	2:D:329:ASN:H	2.02	0.56
1:A:72:GLY:HA3	1:A:75:ILE:HD12	1.87	0.56
1:A:160:GLN:HB3	1:A:174:LEU:HD22	1.86	0.56
2:C:148:ALA:HB3	2:C:299:SER:OG	2.06	0.56
2:D:21:TYR:CG	2:D:41:ILE:HG23	2.40	0.56
2:D:115:LEU:HD22	2:D:174:GLU:HB3	1.87	0.56
2:D:285:MET:HG2	2:D:312:MET:HE1	1.88	0.56
2:C:69:THR:HA	2:C:73:GLU:OE1	2.06	0.56
2:C:209:ASN:O	2:C:211:ARG:N	2.39	0.56
2:C:328:ARG:HD2	2:C:441:ASP:HB3	1.88	0.56
2:D:427:TYR:CE1	2:D:431:THR:HG21	2.40	0.56
1:A:53:LEU:HB3	1:A:58:ILE:CG1	2.35	0.56
2:C:21:TYR:CZ	2:C:85:GLN:HG2	2.40	0.56
2:C:62:ARG:HB3	2:C:63:PHE:CD1	2.41	0.56
2:C:64:PHE:HE1	2:C:171:LEU:HD21	1.71	0.56
2:D:104:LEU:HD21	2:D:219:PHE:CD1	2.40	0.56
2:D:215:ILE:O	2:D:218:ALA:HB3	2.05	0.56
2:D:328:ARG:HA	2:D:328:ARG:NH1	2.08	0.56
2:D:351:TYR:CD2	2:D:438:CYS:HB2	2.41	0.56
1:B:235:LYS:O	1:B:238:TYR:HB3	2.06	0.56
1:B:225:THR:O	1:B:228:ASP:HB2	2.06	0.56
2:C:174:GLU:CD	2:C:178:ARG:HD3	2.31	0.56
2:C:276:VAL:O	2:C:277:ASP:C	2.48	0.56
2:C:416:SER:C	2:C:418:ARG:H	2.14	0.56
2:D:162:SER:HB3	2:D:249:ASN:ND2	2.20	0.56
2:D:400:PHE:CE2	2:D:402:ASN:HB2	2.41	0.56
5:I:700:DC:H2 ⁷	5:I:701:DC:OP1	2.06	0.56
2:C:97:ILE:O	2:C:101:GLN:HG3	2.05	0.56
1:B:60:ASP:CB	2:C:238:ARG:HH11	2.18	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:ASN:OD1	2:D:197:ASN:HB2	2.06	0.55
2:D:280:PHE:HZ	2:D:430:LEU:HD11	1.70	0.55
2:D:348:THR:HB	2:D:352:PHE:HD1	1.70	0.55
1:A:251:PHE:CZ	1:A:253:TYR:HB2	2.41	0.55
2:C:413:HIS:HD2	2:C:414:GLU:N	2.05	0.55
2:D:214:LEU:HD22	2:D:243:ILE:HG13	1.87	0.55
2:D:423:HIS:HA	2:D:426:LEU:HD12	1.87	0.55
6:C:600:U5P:O1P	6:C:600:U5P:O4'	2.24	0.55
2:D:139:ARG:HG3	2:D:306:ASN:ND2	2.20	0.55
1:A:98:HIS:CE1	1:A:113:THR:HG21	2.41	0.55
2:C:13:ILE:O	2:C:17:ILE:HG12	2.06	0.55
2:C:74:ILE:HD13	2:C:77:ARG:CZ	2.36	0.55
2:D:268:ILE:HB	2:D:275:ILE:CG1	2.37	0.55
2:D:349:LYS:O	2:D:351:TYR:N	2.39	0.55
1:B:219:MET:HE3	1:B:221:LEU:HD21	1.89	0.55
2:C:60:LYS:NZ	2:C:67:VAL:H	2.03	0.55
2:D:413:HIS:O	2:D:416:SER:HB2	2.05	0.55
3:F:606:DC:H1'	3:F:607:U:C5'	2.37	0.55
1:A:79:ARG:HG2	1:A:79:ARG:HH11	1.72	0.55
2:C:21:TYR:CG	2:C:41:ILE:HG23	2.41	0.55
2:C:323:VAL:HG13	2:C:323:VAL:O	2.06	0.55
2:D:74:ILE:HD13	2:D:77:ARG:CZ	2.36	0.55
2:D:116:THR:O	2:D:117:ILE:HG13	2.06	0.55
2:D:360:TYR:N	2:D:398:THR:O	2.26	0.55
1:B:194:ASN:HB2	2:C:371:LEU:HG	1.88	0.55
2:C:22:LEU:HD22	2:C:24:ARG:CZ	2.36	0.55
2:D:245:ASP:CB	2:D:249:ASN:HB2	2.37	0.55
2:D:270:ILE:O	2:D:270:ILE:HG23	2.05	0.55
1:B:160:GLN:HB3	1:B:174:LEU:HD22	1.88	0.55
1:B:279:THR:O	1:B:280:LYS:C	2.48	0.55
2:D:257:ILE:HA	2:D:382:GLU:OE1	2.06	0.55
1:A:244:ARG:HA	1:A:258:TYR:CD2	2.41	0.55
2:C:115:LEU:HD22	2:C:174:GLU:HB3	1.89	0.55
2:C:176:LEU:HD21	2:C:185:CYS:HB2	1.88	0.55
2:C:280:PHE:CE1	2:C:426:LEU:HA	2.41	0.55
2:D:291:GLN:HE21	2:D:293:ASP:HB3	1.72	0.55
2:D:333:MET:HG3	2:D:346:VAL:HG13	1.87	0.55
1:A:235:LYS:O	1:A:238:TYR:HB3	2.07	0.55
1:B:244:ARG:HA	1:B:258:TYR:CD2	2.41	0.55
2:D:333:MET:HG3	2:D:346:VAL:CG1	2.37	0.55
2:C:335:CYS:O	2:C:336:ILE:HD13	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:GLN:H	2:D:85:GLN:CD	2.14	0.54
2:C:404:ILE:HB	2:C:458:THR:CG2	2.38	0.54
2:D:29:ASN:O	2:D:31:TYR:N	2.40	0.54
2:D:285:MET:HE3	2:D:312:MET:HE1	1.89	0.54
3:F:606:DC:H1'	3:F:607:U:H5''	1.89	0.54
1:B:125:LYS:HD3	1:B:167:LEU:HA	1.89	0.54
2:C:75:LYS:O	2:C:79:LEU:HG	2.07	0.54
2:C:162:SER:HB3	2:C:249:ASN:ND2	2.22	0.54
2:C:245:ASP:CG	2:C:246:GLU:N	2.65	0.54
2:D:209:ASN:O	2:D:211:ARG:N	2.41	0.54
1:B:20:LEU:HD22	1:B:237:TYR:CE2	2.42	0.54
2:C:257:ILE:HA	2:C:382:GLU:OE1	2.06	0.54
2:C:349:LYS:O	2:C:351:TYR:N	2.40	0.54
2:D:342:ARG:O	2:D:343:ILE:HG13	2.08	0.54
1:A:50:LEU:H	1:A:50:LEU:HD22	1.73	0.54
2:C:270:ILE:O	2:C:270:ILE:HG23	2.07	0.54
1:A:225:THR:O	1:A:228:ASP:HB2	2.08	0.54
2:C:60:LYS:NZ	2:C:67:VAL:HB	2.23	0.54
2:C:193:LEU:O	2:C:194:ILE:HD13	2.06	0.54
2:C:268:ILE:HB	2:C:275:ILE:CG1	2.37	0.54
2:C:391:ILE:O	2:C:391:ILE:HG22	2.08	0.54
2:D:69:THR:HG22	2:D:77:ARG:NH2	2.23	0.54
2:D:225:THR:HB	2:D:227:ASN:H	1.72	0.54
2:D:247:ASN:O	2:D:248:ASP:HB2	2.06	0.54
2:D:413:HIS:HD2	2:D:415:ILE:H	1.55	0.54
1:B:130:PRO:HG2	2:C:466:ARG:HA	1.89	0.54
2:C:214:LEU:HD22	2:C:243:ILE:HG13	1.89	0.54
2:D:247:ASN:HB2	2:D:249:ASN:OD1	2.07	0.54
1:A:162:VAL:O	1:A:163:MET:C	2.50	0.54
1:B:79:ARG:CD	1:B:106:LEU:HD13	2.38	0.54
2:C:69:THR:HG22	2:C:77:ARG:NH2	2.23	0.54
2:C:247:ASN:HB2	2:C:249:ASN:OD1	2.07	0.54
2:C:268:ILE:CG1	2:C:277:ASP:HA	2.38	0.54
2:D:280:PHE:CE1	2:D:426:LEU:HA	2.42	0.54
2:D:316:VAL:HG23	2:D:317:ARG:N	2.23	0.54
1:A:289:SER:O	1:A:292:ARG:HB3	2.08	0.54
1:B:289:SER:O	1:B:292:ARG:HB3	2.07	0.54
2:C:393:ASP:C	2:C:394:ASN:CG	2.74	0.54
2:C:450:ASP:O	2:C:452:ILE:N	2.39	0.54
2:D:64:PHE:CE1	2:D:171:LEU:HD21	2.43	0.54
2:D:69:THR:HA	2:D:73:GLU:OE1	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LYS:C	2:D:349:LYS:HD2	2.32	0.54
1:A:79:ARG:CD	1:A:106:LEU:HD13	2.38	0.54
1:A:125:LYS:HD3	1:A:167:LEU:HA	1.89	0.54
1:A:192:HIS:O	1:A:212:SER:HB3	2.08	0.54
2:C:207:GLN:NE2	2:C:213:PHE:CD2	2.76	0.54
2:D:52:PHE:HE1	2:D:56:VAL:CG2	2.21	0.54
2:D:413:HIS:HD2	2:D:414:GLU:N	2.06	0.54
1:B:162:VAL:O	1:B:163:MET:C	2.50	0.53
2:C:285:MET:HE3	2:C:312:MET:HE1	1.90	0.53
2:D:73:GLU:HG2	2:D:77:ARG:NH1	2.20	0.53
2:D:148:ALA:HB3	2:D:299:SER:OG	2.08	0.53
2:C:252:ILE:HD12	9:C:1001:HOH:O	2.08	0.53
1:A:131:SER:HA	2:D:466:ARG:N	2.21	0.53
1:A:294:LEU:HD12	1:A:296:ILE:HD11	1.89	0.53
1:B:192:HIS:O	1:B:212:SER:HB3	2.08	0.53
2:C:225:THR:HB	2:C:227:ASN:H	1.73	0.53
2:C:227:ASN:HD22	2:C:228:ASN:H	1.57	0.53
2:C:295:LEU:C	2:C:297:ASP:H	2.17	0.53
2:C:348:THR:HB	2:C:352:PHE:HD1	1.73	0.53
2:D:29:ASN:O	2:D:30:GLU:C	2.52	0.53
1:A:149:SER:OG	1:A:151:ALA:HB3	2.08	0.53
1:B:20:LEU:HB3	1:B:237:TYR:HD2	1.73	0.53
2:D:50:ASP:OD2	5:I:700:DC:C5	2.61	0.53
2:D:282:LEU:O	2:D:282:LEU:HD12	2.09	0.53
2:D:332:PRO:HD3	2:D:442:LEU:HD12	1.89	0.53
2:D:335:CYS:SG	2:D:346:VAL:HG22	2.49	0.53
2:D:476:ILE:HD12	6:D:602:U5P:H1'	1.90	0.53
1:A:20:LEU:HD22	1:A:237:TYR:CE2	2.43	0.53
1:A:250:ASN:ND2	1:A:251:PHE:N	2.56	0.53
1:B:208:MET:CE	1:B:236:MET:HE2	2.38	0.53
2:C:333:MET:CG	2:C:346:VAL:HG13	2.38	0.53
2:C:435:TYR:O	2:C:436:LYS:C	2.51	0.53
2:C:467:HIS:CD2	3:F:608:U:C4	2.97	0.53
2:D:195:ASN:C	2:D:197:ASN:N	2.67	0.53
2:D:394:ASN:O	2:D:395:ILE:HD13	2.09	0.53
1:A:219:MET:HE3	1:A:221:LEU:HD21	1.90	0.53
1:B:98:HIS:CE1	1:B:113:THR:HG21	2.43	0.53
2:C:64:PHE:CE1	2:C:171:LEU:HD21	2.44	0.53
2:C:195:ASN:OD1	2:C:197:ASN:HB2	2.09	0.53
2:C:268:ILE:HG13	2:C:277:ASP:HA	1.90	0.53
2:D:22:LEU:HD22	2:D:24:ARG:CZ	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ASP:CG	2:D:246:GLU:N	2.67	0.53
1:B:70:ALA:HB1	1:B:98:HIS:O	2.09	0.53
1:B:188:PHE:CD1	1:B:188:PHE:N	2.77	0.53
2:C:52:PHE:HE1	2:C:56:VAL:CG2	2.22	0.53
2:C:258:ARG:H	2:C:382:GLU:CD	2.17	0.53
2:C:327:LYS:C	2:C:327:LYS:HD3	2.34	0.53
2:C:337:ILE:HG13	2:C:412:VAL:HG22	1.91	0.53
2:C:406:LEU:HD23	2:C:457:HIS:HA	1.91	0.53
2:C:413:HIS:HD2	2:C:415:ILE:H	1.57	0.53
1:A:188:PHE:N	1:A:188:PHE:CD1	2.77	0.53
1:B:3:VAL:HB	1:B:249:VAL:CG1	2.38	0.53
1:B:55:ARG:NH1	2:C:378:SER:O	2.40	0.53
1:B:132:LYS:NZ	2:C:238:ARG:HH12	2.07	0.53
2:C:335:CYS:SG	2:C:346:VAL:HG22	2.49	0.53
2:D:316:VAL:HG23	2:D:317:ARG:H	1.74	0.53
1:B:149:SER:OG	1:B:151:ALA:HB3	2.08	0.53
2:C:316:VAL:HG23	2:C:317:ARG:N	2.24	0.53
2:C:415:ILE:O	2:C:418:ARG:HB2	2.09	0.53
3:E:601:DC:H1'	3:E:602:U:C5'	2.38	0.53
2:C:177:ARG:HH11	2:C:177:ARG:HG3	1.74	0.52
2:C:344:VAL:CG1	2:C:345:THR:H	2.04	0.52
2:D:207:GLN:NE2	2:D:213:PHE:CD2	2.77	0.52
1:B:16:ILE:O	1:B:235:LYS:HE3	2.09	0.52
2:C:85:GLN:H	2:C:85:GLN:CD	2.16	0.52
2:D:47:PHE:CE1	5:I:703:U:C2	2.96	0.52
2:D:60:LYS:NZ	2:D:67:VAL:H	2.06	0.52
2:D:192:TYR:CD1	2:D:196:PRO:HA	2.44	0.52
2:D:328:ARG:CG	2:D:441:ASP:HA	2.39	0.52
1:A:231:ASN:HD21	1:A:235:LYS:CD	2.21	0.52
1:B:231:ASN:HD21	1:B:235:LYS:CD	2.20	0.52
2:C:142:LEU:CA	2:C:145:MET:HE3	2.32	0.52
2:C:283:LEU:HD12	2:C:422:ALA:HA	1.91	0.52
2:D:172:MET:HB2	2:D:203:ILE:CD1	2.39	0.52
2:D:393:ASP:C	2:D:394:ASN:CG	2.76	0.52
1:A:279:THR:C	1:A:281:ALA:N	2.62	0.52
1:B:21:ASP:O	1:B:23:GLU:HG3	2.09	0.52
2:C:69:THR:HG22	2:C:77:ARG:HH22	1.75	0.52
2:C:195:ASN:C	2:C:197:ASN:N	2.68	0.52
2:C:247:ASN:O	2:C:248:ASP:HB2	2.09	0.52
2:D:60:LYS:NZ	2:D:67:VAL:HB	2.25	0.52
2:D:471:ASN:OD1	2:D:474:LYS:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:MET:CE	1:A:236:MET:HE2	2.39	0.52
1:B:50:LEU:H	1:B:50:LEU:HD22	1.75	0.52
2:C:342:ARG:O	2:C:343:ILE:HG13	2.10	0.52
2:D:97:ILE:O	2:D:101:GLN:HG3	2.09	0.52
1:A:2:ASP:C	1:A:246:LYS:HZ3	2.17	0.52
1:A:240:ASN:HA	1:A:244:ARG:HD3	1.92	0.52
2:C:282:LEU:O	2:C:282:LEU:HD12	2.10	0.52
2:C:396:MET:HE1	2:C:427:TYR:CD2	2.45	0.52
1:A:34:LEU:HB2	1:A:37:GLN:OE1	2.09	0.52
1:B:189:TYR:HB3	1:B:221:LEU:HB3	1.91	0.52
2:C:44:ILE:O	2:C:47:PHE:HB3	2.09	0.52
2:C:85:GLN:NE2	2:C:85:GLN:N	2.49	0.52
2:C:407:SER:HB3	2:C:413:HIS:HA	1.92	0.52
2:D:185:CYS:SG	2:D:186:TYR:N	2.83	0.52
2:C:41:ILE:HD11	2:C:98:ILE:HD13	1.91	0.52
2:C:245:ASP:CB	2:C:249:ASN:HB2	2.40	0.52
2:C:355:LYS:HG3	2:C:356:LYS:HG3	1.92	0.52
2:D:69:THR:HG22	2:D:77:ARG:HH22	1.75	0.52
1:B:52:LYS:NZ	2:C:376:ASP:HA	2.25	0.52
1:B:53:LEU:HB3	1:B:58:ILE:CG1	2.39	0.52
2:D:172:MET:HE2	2:D:205:ILE:HD13	1.92	0.52
2:D:283:LEU:HD12	2:D:422:ALA:HA	1.91	0.52
1:A:273:ASN:O	1:A:274:LYS:C	2.53	0.52
2:D:21:TYR:CZ	2:D:85:GLN:HG2	2.44	0.52
2:D:50:ASP:O	2:D:53:VAL:N	2.43	0.52
2:D:337:ILE:HG13	2:D:412:VAL:HG22	1.92	0.52
2:D:355:LYS:HG3	2:D:356:LYS:HG3	1.92	0.52
2:D:368:SER:O	2:D:371:LEU:HB3	2.10	0.52
1:A:3:VAL:HB	1:A:249:VAL:CG1	2.40	0.51
1:B:273:ASN:O	1:B:274:LYS:C	2.53	0.51
2:C:328:ARG:CG	2:C:441:ASP:HA	2.40	0.51
2:D:283:LEU:HG	2:D:429:MET:CE	2.40	0.51
2:D:295:LEU:C	2:D:297:ASP:H	2.18	0.51
1:B:128:LEU:O	2:C:466:ARG:NH2	2.44	0.51
2:C:199:ARG:HH22	2:C:304:LYS:HB2	1.76	0.51
2:C:332:PRO:HD3	2:C:442:LEU:HD12	1.91	0.51
2:D:44:ILE:O	2:D:47:PHE:HB3	2.09	0.51
2:D:147:VAL:HG13	2:D:451:LYS:HB3	1.92	0.51
2:D:245:ASP:HB3	2:D:249:ASN:CB	2.40	0.51
2:D:335:CYS:O	2:D:336:ILE:HD13	2.10	0.51
2:D:342:ARG:C	2:D:343:ILE:HG13	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLN:NE2	1:A:174:LEU:HD22	2.26	0.51
1:B:251:PHE:CZ	1:B:253:TYR:HB2	2.45	0.51
2:C:172:MET:HB2	2:C:203:ILE:CD1	2.40	0.51
2:C:283:LEU:HG	2:C:429:MET:CE	2.40	0.51
2:D:227:ASN:HD22	2:D:228:ASN:H	1.59	0.51
2:C:73:GLU:HG2	2:C:77:ARG:NH1	2.21	0.51
2:C:101:GLN:O	2:C:105:VAL:HG23	2.11	0.51
2:D:74:ILE:CD1	2:D:224:ILE:HA	2.40	0.51
2:D:459:GLU:OE1	2:D:459:GLU:HA	2.10	0.51
2:C:50:ASP:O	2:C:53:VAL:N	2.44	0.51
2:C:104:LEU:HD21	2:C:219:PHE:CD1	2.45	0.51
2:C:219:PHE:O	2:C:220:LEU:C	2.54	0.51
2:D:41:ILE:HD11	2:D:98:ILE:HD13	1.91	0.51
2:D:466:ARG:HG2	2:D:467:HIS:N	2.25	0.51
1:A:114:ARG:HD3	1:A:120:TYR:CE1	2.46	0.51
1:A:239:LEU:HD12	1:A:243:VAL:CB	2.40	0.51
2:C:21:TYR:OH	2:C:98:ILE:HG12	2.11	0.51
2:C:406:LEU:HD22	2:C:406:LEU:N	2.25	0.51
2:C:466:ARG:HG2	2:C:467:HIS:N	2.25	0.51
2:D:219:PHE:O	2:D:220:LEU:C	2.54	0.51
1:A:20:LEU:HB3	1:A:237:TYR:HD2	1.74	0.51
2:C:23:GLY:O	2:C:24:ARG:HB3	2.10	0.51
2:C:45:THR:O	2:C:47:PHE:N	2.34	0.51
2:C:412:VAL:O	2:C:413:HIS:C	2.53	0.51
2:D:21:TYR:CD1	2:D:41:ILE:HG23	2.44	0.51
2:D:85:GLN:NE2	2:D:85:GLN:N	2.50	0.51
1:A:16:ILE:O	1:A:235:LYS:HE3	2.10	0.51
1:A:157:TYR:O	1:A:161:ASN:ND2	2.44	0.51
1:A:187:ASP:HB3	1:A:224:VAL:O	2.10	0.51
1:B:250:ASN:ND2	1:B:251:PHE:N	2.58	0.51
2:C:280:PHE:HZ	2:C:430:LEU:HD11	1.75	0.51
2:C:467:HIS:CD2	3:F:608:U:C5	2.98	0.51
2:D:74:ILE:HD11	2:D:224:ILE:HA	1.92	0.51
2:D:75:LYS:HG2	2:D:79:LEU:HD11	1.92	0.51
2:D:298:LEU:HD12	2:D:305:PHE:CD1	2.46	0.51
2:D:333:MET:CG	2:D:346:VAL:HG13	2.40	0.51
2:D:390:LEU:O	2:D:396:MET:HA	2.10	0.51
3:F:607:U:O2'	3:F:608:U:H5'	2.11	0.51
1:A:43:LEU:O	1:A:43:LEU:HD13	2.11	0.51
1:A:221:LEU:HD13	1:B:221:LEU:CD1	2.40	0.51
1:B:215:THR:C	2:C:364:ASN:HD21	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ARG:H	2:D:382:GLU:CD	2.19	0.51
2:D:328:ARG:HG3	2:D:441:ASP:O	2.10	0.51
2:D:344:VAL:CG1	2:D:345:THR:H	2.06	0.51
1:A:49:PHE:CZ	1:A:53:LEU:HD11	2.46	0.51
1:A:100:ASP:OD1	1:A:102:ILE:HG12	2.12	0.51
2:C:86:THR:CB	2:C:87:GLN:NE2	2.70	0.51
2:D:143:ASN:O	2:D:144:SER:C	2.54	0.51
2:D:227:ASN:ND2	2:D:246:GLU:CD	2.69	0.51
1:A:50:LEU:HD22	1:A:50:LEU:N	2.26	0.50
1:B:77:TYR:CE2	1:B:290:ILE:HA	2.46	0.50
1:B:114:ARG:HD3	1:B:120:TYR:CE1	2.46	0.50
2:C:227:ASN:ND2	2:C:246:GLU:CD	2.69	0.50
7:C:801:3AT:H5'2	7:C:801:3AT:PB	2.50	0.50
2:D:227:ASN:HD21	2:D:246:GLU:CD	2.19	0.50
1:A:221:LEU:HD13	1:B:221:LEU:HD11	1.93	0.50
1:B:239:LEU:HD12	1:B:243:VAL:CB	2.41	0.50
2:C:192:TYR:CB	2:C:198:ILE:HG22	2.40	0.50
2:D:422:ALA:O	2:D:423:HIS:C	2.54	0.50
1:A:189:TYR:HB3	1:A:221:LEU:HB3	1.92	0.50
1:B:157:TYR:O	1:B:161:ASN:ND2	2.45	0.50
2:C:471:ASN:OD1	2:C:474:LYS:HB2	2.11	0.50
2:D:142:LEU:CA	2:D:145:MET:HE3	2.35	0.50
1:B:49:PHE:CZ	1:B:53:LEU:HD11	2.46	0.50
1:B:96:GLY:HA3	1:B:115:PHE:CE2	2.46	0.50
1:B:251:PHE:CE2	1:B:261:PHE:HA	2.47	0.50
1:B:294:LEU:HD12	1:B:296:ILE:HD11	1.92	0.50
2:C:76:ASP:O	2:C:79:LEU:N	2.44	0.50
2:C:227:ASN:HD21	2:C:246:GLU:CD	2.19	0.50
2:C:423:HIS:HA	2:C:426:LEU:HD12	1.92	0.50
1:A:61:GLY:HA2	1:A:88:ILE:O	2.12	0.50
2:C:192:TYR:CD1	2:C:196:PRO:HA	2.46	0.50
2:C:249:ASN:N	2:C:249:ASN:OD1	2.44	0.50
2:C:413:HIS:CD2	2:C:414:GLU:N	2.79	0.50
2:C:414:GLU:C	2:C:416:SER:H	2.18	0.50
2:D:51:ILE:O	2:D:55:LEU:HG	2.12	0.50
2:D:138:ALA:O	2:D:142:LEU:HB2	2.11	0.50
1:A:96:GLY:HA3	1:A:115:PHE:CE2	2.47	0.50
2:C:21:TYR:CD1	2:C:41:ILE:HG23	2.45	0.50
2:C:190:SER:O	2:C:193:LEU:HB2	2.12	0.50
2:C:227:ASN:ND2	2:C:228:ASN:N	2.59	0.50
2:D:383:SER:HA	2:D:386:ASN:HD22	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:O	1:A:102:ILE:N	2.45	0.50
1:B:61:GLY:HA2	1:B:88:ILE:O	2.12	0.50
1:B:166:ILE:C	1:B:168:ASN:H	2.19	0.50
2:C:316:VAL:HG23	2:C:317:ARG:H	1.77	0.50
2:C:392:HIS:CE1	2:C:393:ASP:OD2	2.65	0.50
2:D:76:ASP:O	2:D:79:LEU:N	2.44	0.50
2:D:408:ASP:HA	2:D:455:TYR:CB	2.41	0.50
1:A:76:ARG:NH1	1:A:102:ILE:O	2.45	0.50
1:A:101:PRO:C	1:A:103:LEU:N	2.68	0.50
1:B:67:ILE:HG21	1:B:163:MET:HE2	1.92	0.50
1:B:160:GLN:NE2	1:B:174:LEU:HD22	2.27	0.50
1:B:184:TRP:O	1:B:185:ILE:HD13	2.11	0.50
2:C:214:LEU:HB2	2:C:231:LEU:HD11	1.94	0.50
2:C:222:LYS:HA	2:C:227:ASN:O	2.12	0.50
2:C:368:SER:O	2:C:371:LEU:HB3	2.12	0.50
2:C:370:ILE:O	2:C:373:LEU:HB2	2.12	0.50
2:C:452:ILE:HG23	2:C:453:PRO:HD2	1.93	0.50
2:D:406:LEU:HD23	2:D:457:HIS:HA	1.94	0.50
1:B:101:PRO:C	1:B:103:LEU:N	2.68	0.50
2:C:74:ILE:CD1	2:C:224:ILE:HA	2.42	0.50
2:C:323:VAL:HG22	2:C:325:ASP:OD1	2.12	0.50
2:C:348:THR:O	2:C:349:LYS:C	2.55	0.50
2:D:309:MET:HE2	2:D:313:LEU:CG	2.40	0.50
2:D:348:THR:O	2:D:349:LYS:C	2.54	0.50
1:B:114:ARG:CG	1:B:115:PHE:N	2.74	0.49
2:C:18:ILE:O	2:C:22:LEU:HB2	2.12	0.49
2:C:114:VAL:O	2:C:115:LEU:C	2.55	0.49
2:C:116:THR:C	2:C:117:ILE:HG13	2.37	0.49
2:C:383:SER:HA	2:C:386:ASN:HD22	1.77	0.49
2:C:394:ASN:O	2:C:395:ILE:HD13	2.12	0.49
2:D:21:TYR:OH	2:D:98:ILE:HG12	2.13	0.49
2:D:78:ILE:O	2:D:82:PHE:HD1	1.95	0.49
2:D:176:LEU:HD21	2:D:185:CYS:HB2	1.94	0.49
2:D:190:SER:O	2:D:193:LEU:HB2	2.12	0.49
2:D:328:ARG:HB2	2:D:444:ASN:CB	2.42	0.49
2:D:452:ILE:HG23	2:D:453:PRO:HD2	1.94	0.49
1:A:4:VAL:HG22	1:A:5:SER:N	2.27	0.49
1:A:77:TYR:CE2	1:A:290:ILE:HA	2.47	0.49
1:B:76:ARG:NH1	1:B:102:ILE:O	2.45	0.49
2:C:234:ILE:O	2:C:236:TYR:N	2.45	0.49
2:C:280:PHE:HE1	2:C:426:LEU:HA	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:298:LEU:HD12	2:C:305:PHE:CD1	2.47	0.49
2:D:44:ILE:HG21	2:D:101:GLN:HE21	1.77	0.49
2:D:234:ILE:O	2:D:236:TYR:N	2.45	0.49
2:D:437:GLN:CD	2:D:437:GLN:N	2.66	0.49
1:A:276:PHE:HZ	1:A:285:PHE:HD2	1.59	0.49
1:B:261:PHE:O	1:B:264:TYR:HB3	2.11	0.49
2:C:51:ILE:O	2:C:55:LEU:HG	2.13	0.49
2:C:116:THR:O	2:C:117:ILE:CG1	2.60	0.49
2:C:331:MET:CB	2:C:332:PRO:CD	2.85	0.49
2:D:249:ASN:N	2:D:249:ASN:OD1	2.45	0.49
2:D:327:LYS:HD3	2:D:327:LYS:C	2.38	0.49
1:A:57:GLY:O	1:A:58:ILE:C	2.55	0.49
1:A:239:LEU:HA	1:A:243:VAL:HG23	1.92	0.49
1:B:4:VAL:HG22	1:B:5:SER:N	2.27	0.49
1:B:240:ASN:HA	1:B:244:ARG:HD3	1.94	0.49
2:C:70:SER:OG	2:C:73:GLU:HB2	2.12	0.49
2:D:415:ILE:O	2:D:418:ARG:HB2	2.12	0.49
2:C:143:ASN:O	2:C:144:SER:C	2.55	0.49
2:C:162:SER:N	2:C:249:ASN:HB3	2.28	0.49
2:C:415:ILE:CA	2:C:418:ARG:HD3	2.33	0.49
2:C:459:GLU:OE1	2:C:459:GLU:HA	2.11	0.49
2:C:475:ASP:O	2:C:476:ILE:HD13	2.11	0.49
2:D:101:GLN:O	2:D:105:VAL:HG23	2.13	0.49
2:D:144:SER:HB3	2:D:449:ARG:HB2	1.95	0.49
2:D:317:ARG:HG2	2:D:317:ARG:HH11	1.78	0.49
2:D:435:TYR:CG	2:D:436:LYS:N	2.81	0.49
2:C:44:ILE:HG21	2:C:101:GLN:HE21	1.77	0.49
2:C:245:ASP:HB3	2:C:249:ASN:CB	2.42	0.49
2:C:435:TYR:CG	2:C:436:LYS:N	2.81	0.49
2:D:234:ILE:N	2:D:234:ILE:CD1	2.74	0.49
2:D:450:ASP:O	2:D:452:ILE:N	2.44	0.49
1:A:53:LEU:O	1:A:58:ILE:HG23	2.13	0.49
2:C:34:LEU:O	2:C:37:GLN:N	2.46	0.49
2:C:78:ILE:O	2:C:82:PHE:HD1	1.95	0.49
2:C:211:ARG:HG2	2:C:211:ARG:HH11	1.77	0.49
2:D:103:VAL:HG11	2:D:215:ILE:HB	1.93	0.49
2:D:233:LYS:C	2:D:234:ILE:HD12	2.38	0.49
1:A:67:ILE:HG21	1:A:163:MET:HE2	1.94	0.49
1:A:114:ARG:CG	1:A:115:PHE:N	2.75	0.49
1:B:79:ARG:HG2	1:B:79:ARG:NH1	2.27	0.49
2:C:74:ILE:HD11	2:C:224:ILE:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:LEU:O	2:C:396:MET:HA	2.12	0.49
2:C:414:GLU:C	2:C:416:SER:N	2.70	0.49
1:A:54:GLN:HB2	1:A:59:LEU:HD23	1.95	0.49
2:C:50:ASP:O	2:C:51:ILE:C	2.55	0.49
2:C:51:ILE:HB	4:G:502:U:C4	2.47	0.49
2:C:103:VAL:HG11	2:C:215:ILE:HB	1.93	0.49
1:A:279:THR:O	1:A:282:LYS:N	2.46	0.49
1:B:67:ILE:HG21	1:B:163:MET:CE	2.43	0.49
1:B:76:ARG:O	1:B:77:TYR:C	2.56	0.49
2:C:232:SER:O	2:C:241:MET:HA	2.13	0.49
2:D:222:LYS:HA	2:D:227:ASN:O	2.13	0.49
2:D:233:LYS:O	2:D:235:PRO:HD3	2.13	0.49
2:C:273:ILE:C	2:C:273:ILE:HD12	2.38	0.48
2:D:18:ILE:O	2:D:22:LEU:HB2	2.13	0.48
2:D:22:LEU:O	2:D:24:ARG:HG2	2.12	0.48
2:D:412:VAL:O	2:D:413:HIS:C	2.55	0.48
1:B:279:THR:C	1:B:281:ALA:N	2.66	0.48
2:C:61:LYS:O	2:C:62:ARG:HB2	2.11	0.48
2:C:214:LEU:HA	2:C:243:ILE:HD11	1.94	0.48
2:C:227:ASN:ND2	2:C:228:ASN:H	2.11	0.48
2:C:328:ARG:HG3	2:C:441:ASP:O	2.12	0.48
2:D:177:ARG:HH11	2:D:177:ARG:HG3	1.78	0.48
2:D:192:TYR:CB	2:D:198:ILE:HG22	2.42	0.48
2:D:427:TYR:O	2:D:431:THR:HG23	2.13	0.48
2:C:237:LEU:HD22	2:C:237:LEU:N	2.28	0.48
2:D:18:ILE:CG2	2:D:26:PRO:HB3	2.43	0.48
2:D:406:LEU:C	2:D:413:HIS:HB2	2.38	0.48
1:A:79:ARG:HG2	1:A:79:ARG:NH1	2.28	0.48
1:A:166:ILE:C	1:A:168:ASN:H	2.20	0.48
1:B:121:LEU:CD1	1:B:163:MET:HA	2.40	0.48
2:C:233:LYS:O	2:C:235:PRO:HD3	2.13	0.48
2:C:328:ARG:HB2	2:C:444:ASN:CB	2.43	0.48
2:D:232:SER:O	2:D:241:MET:HA	2.13	0.48
2:D:396:MET:HE1	2:D:427:TYR:CD2	2.49	0.48
1:A:21:ASP:O	1:A:23:GLU:HG3	2.13	0.48
1:A:121:LEU:CD1	1:A:163:MET:HA	2.39	0.48
1:B:88:ILE:CD1	2:C:211:ARG:HD2	2.38	0.48
2:C:48:ASN:OD1	2:C:50:ASP:HB2	2.14	0.48
2:C:185:CYS:SG	2:C:186:TYR:N	2.87	0.48
2:D:227:ASN:ND2	2:D:228:ASN:N	2.60	0.48
2:D:266:PRO:O	2:D:277:ASP:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:ASN:O	2:D:288:MET:N	2.43	0.48
1:A:3:VAL:HG23	1:A:4:VAL:N	2.28	0.48
2:C:75:LYS:HG2	2:C:79:LEU:HD11	1.95	0.48
2:C:214:LEU:HD13	2:C:231:LEU:HD21	1.95	0.48
2:C:421:CYS:O	2:C:422:ALA:C	2.56	0.48
2:D:192:TYR:HA	2:D:195:ASN:O	2.13	0.48
2:D:195:ASN:O	2:D:197:ASN:N	2.46	0.48
2:D:202:ASP:OD2	7:D:800:3AT:O1G	2.32	0.48
2:D:325:ASP:O	2:D:327:LYS:N	2.46	0.48
2:D:341:ASN:HB3	2:D:343:ILE:HD12	1.96	0.48
2:D:407:SER:HB3	2:D:413:HIS:HA	1.95	0.48
2:D:413:HIS:CD2	2:D:414:GLU:N	2.81	0.48
2:D:423:HIS:HA	2:D:426:LEU:CD1	2.44	0.48
2:C:198:ILE:HG22	2:C:198:ILE:O	2.12	0.48
2:D:331:MET:CB	2:D:332:PRO:CD	2.87	0.48
1:A:52:LYS:HE2	2:D:376:ASP:CB	2.29	0.48
1:B:276:PHE:HZ	1:B:285:PHE:HD2	1.61	0.48
2:C:266:PRO:O	2:C:277:ASP:N	2.46	0.48
2:C:419:GLY:O	2:C:420:LEU:C	2.56	0.48
2:D:273:ILE:C	2:D:273:ILE:HD12	2.39	0.48
2:D:415:ILE:CA	2:D:418:ARG:HD3	2.35	0.48
2:C:12:ASN:ND2	2:C:14:THR:OG1	2.46	0.48
2:C:186:TYR:CE2	2:C:204:ASP:HB3	2.49	0.48
2:C:341:ASN:HB3	2:C:343:ILE:HD12	1.96	0.48
2:D:214:LEU:HA	2:D:243:ILE:HD11	1.95	0.48
2:D:406:LEU:HD22	2:D:406:LEU:N	2.28	0.48
1:A:206:ALA:CA	1:A:236:MET:HE3	2.38	0.48
2:C:211:ARG:HG2	2:C:211:ARG:NH1	2.28	0.48
2:C:317:ARG:HB2	2:C:324:PHE:CE1	2.49	0.48
2:C:342:ARG:C	2:C:343:ILE:HG13	2.37	0.48
2:D:114:VAL:O	2:D:115:LEU:C	2.57	0.48
1:A:184:TRP:O	1:A:185:ILE:HD13	2.14	0.47
1:A:189:TYR:CE2	1:A:223:ARG:HB2	2.49	0.47
2:C:317:ARG:HG2	2:C:317:ARG:HH11	1.79	0.47
2:D:23:GLY:O	2:D:24:ARG:HB3	2.13	0.47
2:D:34:LEU:O	2:D:37:GLN:N	2.47	0.47
2:D:50:ASP:O	2:D:51:ILE:C	2.56	0.47
2:D:186:TYR:CE2	2:D:204:ASP:HB3	2.49	0.47
2:D:227:ASN:ND2	2:D:228:ASN:H	2.12	0.47
1:A:279:THR:HG22	1:A:283:VAL:CG2	2.42	0.47
2:C:29:ASN:O	2:C:30:GLU:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:PRO:HB2	2:C:315:TYR:CD2	2.49	0.47
2:C:422:ALA:O	2:C:423:HIS:C	2.56	0.47
2:D:19:GLU:HG2	2:D:24:ARG:O	2.13	0.47
2:D:45:THR:O	2:D:47:PHE:N	2.37	0.47
2:D:70:SER:OG	2:D:73:GLU:HB2	2.14	0.47
2:D:229:ILE:H	2:D:229:ILE:CD1	2.18	0.47
2:D:280:PHE:HE1	2:D:426:LEU:HA	1.79	0.47
2:D:309:MET:O	2:D:312:MET:HB2	2.14	0.47
2:D:383:SER:HA	2:D:386:ASN:ND2	2.27	0.47
2:C:74:ILE:HD13	2:C:77:ARG:HD2	1.97	0.47
2:C:177:ARG:HA	2:C:272:ASN:O	2.14	0.47
2:D:81:TYR:O	2:D:84:LYS:HG2	2.14	0.47
2:D:241:MET:HE1	2:D:470:ILE:HD11	1.95	0.47
1:A:145:GLY:O	1:A:146:ASN:CB	2.62	0.47
1:B:100:ASP:O	1:B:102:ILE:N	2.48	0.47
2:D:61:LYS:O	2:D:62:ARG:HB2	2.13	0.47
2:D:289:PHE:CE2	2:D:298:LEU:HD13	2.49	0.47
2:D:475:ASP:O	2:D:476:ILE:HD13	2.14	0.47
1:A:60:ASP:HB2	2:D:238:ARG:HH11	1.80	0.47
1:A:251:PHE:CE2	1:A:261:PHE:HA	2.50	0.47
1:B:3:VAL:HG23	1:B:4:VAL:N	2.29	0.47
1:B:50:LEU:HD22	1:B:50:LEU:N	2.29	0.47
2:C:195:ASN:O	2:C:197:ASN:N	2.47	0.47
2:C:233:LYS:C	2:C:234:ILE:HD12	2.40	0.47
2:C:241:MET:HE1	2:C:470:ILE:HD11	1.96	0.47
2:D:188:SER:HB3	7:D:800:3AT:O3B	2.15	0.47
2:D:323:VAL:HG22	2:D:325:ASP:OD1	2.14	0.47
2:D:365:VAL:HG12	2:D:369:ASP:OD2	2.15	0.47
1:A:114:ARG:HG3	1:A:115:PHE:H	1.79	0.47
1:B:57:GLY:O	1:B:58:ILE:C	2.57	0.47
2:C:22:LEU:O	2:C:24:ARG:HG2	2.14	0.47
2:C:53:VAL:HG12	2:C:57:LYS:HE3	1.96	0.47
2:C:147:VAL:HG13	2:C:451:LYS:HB3	1.96	0.47
2:C:234:ILE:N	2:C:234:ILE:CD1	2.76	0.47
2:C:427:TYR:O	2:C:431:THR:HG23	2.15	0.47
2:D:19:GLU:HA	2:D:24:ARG:O	2.15	0.47
2:D:317:ARG:HB2	2:D:324:PHE:CE1	2.50	0.47
1:A:76:ARG:O	1:A:77:TYR:C	2.57	0.47
1:A:121:LEU:CB	1:A:166:ILE:HG21	2.45	0.47
1:B:121:LEU:CB	1:B:166:ILE:HG21	2.44	0.47
2:C:43:LYS:O	2:C:44:ILE:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:SER:C	2:C:165:VAL:N	2.67	0.47
2:C:298:LEU:C	2:C:300:LYS:H	2.23	0.47
2:C:309:MET:O	2:C:312:MET:HB2	2.14	0.47
2:C:355:LYS:CG	2:C:356:LYS:H	2.27	0.47
2:D:18:ILE:HG21	2:D:26:PRO:HB3	1.95	0.47
2:D:39:ARG:O	2:D:40:ASN:C	2.57	0.47
2:D:53:VAL:HG12	2:D:57:LYS:HE3	1.96	0.47
2:D:86:THR:CB	2:D:87:GLN:NE2	2.73	0.47
2:D:162:SER:N	2:D:249:ASN:HB3	2.30	0.47
2:D:188:SER:HB3	7:D:800:3AT:PG	2.55	0.47
2:D:214:LEU:HB2	2:D:231:LEU:HD11	1.96	0.47
2:D:324:PHE:HA	2:D:444:ASN:HD21	1.80	0.47
2:D:349:LYS:C	2:D:351:TYR:N	2.73	0.47
2:D:355:LYS:CG	2:D:356:LYS:H	2.27	0.47
2:D:408:ASP:HA	2:D:455:TYR:HB2	1.96	0.47
2:D:425:LEU:HA	2:D:428:GLN:HB2	1.95	0.47
2:D:435:TYR:O	2:D:438:CYS:N	2.48	0.47
2:C:376:ASP:OD2	2:C:376:ASP:N	2.48	0.47
2:D:409:LYS:HE2	2:D:455:TYR:CZ	2.50	0.47
2:D:414:GLU:C	2:D:416:SER:H	2.21	0.47
1:A:16:ILE:N	1:A:16:ILE:HD12	2.29	0.47
1:B:121:LEU:HB3	1:B:166:ILE:HG21	1.97	0.47
1:B:154:LEU:O	1:B:155:SER:C	2.58	0.47
1:B:198:GLN:OE1	1:B:209:ARG:HD3	2.15	0.47
2:C:61:LYS:HB2	2:C:61:LYS:HZ3	1.80	0.47
2:C:141:MET:SD	2:C:313:LEU:HD21	2.55	0.47
2:C:309:MET:HE3	2:C:309:MET:CA	2.43	0.47
2:C:383:SER:HA	2:C:386:ASN:ND2	2.28	0.47
2:C:408:ASP:HA	2:C:455:TYR:CB	2.44	0.47
2:C:437:GLN:CD	2:C:437:GLN:N	2.69	0.47
2:D:134:MET:C	2:D:136:GLU:N	2.72	0.47
2:D:298:LEU:C	2:D:300:LYS:H	2.23	0.47
1:A:121:LEU:HB3	1:A:166:ILE:HG21	1.97	0.47
1:A:261:PHE:O	1:A:264:TYR:HB3	2.14	0.47
1:B:145:GLY:O	1:B:146:ASN:CB	2.62	0.47
2:C:45:THR:C	2:C:47:PHE:N	2.72	0.47
2:C:192:TYR:HA	2:C:195:ASN:O	2.15	0.47
2:C:244:LYS:HG2	2:C:250:HIS:HA	1.97	0.47
2:D:43:LYS:O	2:D:44:ILE:C	2.58	0.47
2:D:199:ARG:HH22	2:D:304:LYS:HB2	1.80	0.47
2:D:419:GLY:O	2:D:420:LEU:C	2.57	0.47

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:HG21	1.96	0.46
2:C:22:LEU:O	2:C:86:THR:HA	2.14	0.46
2:C:39:ARG:O	2:C:40:ASN:C	2.58	0.46
2:C:172:MET:HE2	2:C:205:ILE:HD13	1.97	0.46
2:C:209:ASN:O	2:C:210:SER:C	2.56	0.46
2:C:320:HIS:HB2	2:C:322:ILE:HD11	1.97	0.46
2:C:405:LEU:HD12	2:C:415:ILE:HB	1.96	0.46
2:D:13:ILE:O	2:D:16:LYS:HB2	2.15	0.46
2:D:244:LYS:HG2	2:D:250:HIS:HA	1.97	0.46
2:D:309:MET:HE3	2:D:309:MET:CA	2.44	0.46
2:D:421:CYS:O	2:D:422:ALA:C	2.58	0.46
1:B:54:GLN:HB2	1:B:59:LEU:HD23	1.98	0.46
2:C:103:VAL:HG21	2:C:215:ILE:HD13	1.97	0.46
2:D:12:ASN:ND2	2:D:14:THR:OG1	2.47	0.46
2:D:116:THR:C	2:D:117:ILE:HG13	2.40	0.46
2:D:143:ASN:C	2:D:145:MET:N	2.72	0.46
1:B:72:GLY:CA	1:B:75:ILE:HD12	2.45	0.46
1:B:187:ASP:HB3	1:B:224:VAL:O	2.14	0.46
2:C:134:MET:C	2:C:136:GLU:N	2.73	0.46
2:C:166:LYS:HE2	2:C:166:LYS:N	2.29	0.46
2:C:324:PHE:HA	2:C:444:ASN:HD21	1.80	0.46
2:D:19:GLU:CD	2:D:25:VAL:HA	2.40	0.46
2:D:96:THR:HG23	2:D:477:ILE:HG13	1.97	0.46
2:D:168:VAL:C	2:D:170:LYS:N	2.72	0.46
2:D:237:LEU:N	2:D:237:LEU:HD22	2.31	0.46
2:D:392:HIS:CE1	2:D:393:ASP:OD2	2.68	0.46
1:A:225:THR:HG23	1:A:228:ASP:OD2	2.15	0.46
1:B:279:THR:HG22	1:B:283:VAL:CG2	2.44	0.46
2:C:109:THR:HG23	4:G:501:U:O2'	2.15	0.46
2:C:138:ALA:O	2:C:142:LEU:HB2	2.15	0.46
2:C:217:LEU:O	2:C:218:ALA:C	2.59	0.46
2:C:406:LEU:C	2:C:413:HIS:HB2	2.40	0.46
1:B:35:PRO:HG2	1:B:296:ILE:HG23	1.96	0.46
1:B:42:LEU:HD22	1:B:46:GLU:OE2	2.15	0.46
1:B:257:GLU:O	1:B:258:TYR:C	2.58	0.46
2:C:409:LYS:HE2	2:C:455:TYR:CZ	2.50	0.46
2:D:44:ILE:HD13	2:D:101:GLN:HE21	1.80	0.46
2:D:350:ASP:C	2:D:351:TYR:CD1	2.93	0.46
1:A:5:SER:C	1:A:6:LEU:HD23	2.41	0.46
1:A:74:HIS:O	1:A:75:ILE:C	2.58	0.46
1:B:74:HIS:O	1:B:77:TYR:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:O	1:B:75:ILE:C	2.58	0.46
1:B:152:ASP:O	1:B:153:LEU:C	2.58	0.46
2:C:250:HIS:C	2:C:250:HIS:CD2	2.93	0.46
2:D:81:TYR:C	2:D:83:SER:N	2.72	0.46
2:D:291:GLN:O	2:D:292:ILE:C	2.58	0.46
2:D:355:LYS:CG	2:D:356:LYS:N	2.78	0.46
1:A:60:ASP:HB3	2:D:238:ARG:NH1	2.30	0.46
2:C:70:SER:OG	2:C:73:GLU:CB	2.64	0.46
2:C:112:LEU:O	2:C:113:GLY:C	2.58	0.46
2:C:240:TYR:HE1	2:C:253:ASP:HB2	1.79	0.46
2:D:109:THR:HG21	5:I:702:U:O3'	2.15	0.46
2:D:177:ARG:HA	2:D:272:ASN:O	2.16	0.46
2:D:189:TYR:HD1	2:D:200:TYR:CZ	2.34	0.46
2:D:193:LEU:O	2:D:194:ILE:HD13	2.15	0.46
2:D:223:PHE:O	2:D:224:ILE:C	2.58	0.46
2:D:250:HIS:CD2	2:D:250:HIS:C	2.93	0.46
1:A:46:GLU:OE2	1:A:66:TYR:OH	2.25	0.46
1:A:145:GLY:O	1:A:146:ASN:HB3	2.16	0.46
1:B:189:TYR:CE2	1:B:223:ARG:HB2	2.51	0.46
2:C:86:THR:CB	2:C:87:GLN:HE22	2.10	0.46
2:C:189:TYR:HD1	2:C:200:TYR:CZ	2.34	0.46
2:D:61:LYS:HB2	2:D:61:LYS:HZ3	1.81	0.46
2:D:282:LEU:O	2:D:285:MET:CB	2.62	0.46
2:D:405:LEU:HD12	2:D:415:ILE:HB	1.97	0.46
1:A:55:ARG:NH1	2:D:378:SER:O	2.49	0.46
1:B:184:TRP:CH2	1:B:224:VAL:HG12	2.48	0.46
2:C:327:LYS:HD3	2:C:327:LYS:O	2.16	0.46
2:C:349:LYS:C	2:C:351:TYR:N	2.74	0.46
2:D:22:LEU:O	2:D:86:THR:HA	2.15	0.46
2:D:141:MET:SD	2:D:313:LEU:HD21	2.56	0.46
2:D:148:ALA:HB2	2:D:295:LEU:O	2.16	0.46
2:D:148:ALA:O	2:D:149:VAL:C	2.58	0.46
2:D:380:ASP:HB2	2:D:388:VAL:HG13	1.98	0.46
1:A:22:TYR:C	1:A:22:TYR:CD2	2.94	0.46
1:A:74:HIS:O	1:A:77:TYR:N	2.48	0.46
1:B:43:LEU:O	1:B:43:LEU:HD13	2.16	0.46
1:B:166:ILE:C	1:B:168:ASN:N	2.73	0.46
2:C:18:ILE:CG2	2:C:26:PRO:HB3	2.45	0.46
2:C:53:VAL:HG13	2:C:75:LYS:HA	1.98	0.46
2:C:144:SER:HB3	2:C:449:ARG:HB2	1.98	0.46
2:C:214:LEU:CB	2:C:231:LEU:HD11	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:PHE:CE2	2:C:298:LEU:HD13	2.50	0.46
2:C:380:ASP:HB2	2:C:388:VAL:HG13	1.98	0.46
2:C:393:ASP:C	2:C:394:ASN:OD1	2.59	0.46
2:D:287:LYS:HA	2:D:419:GLY:CA	2.46	0.46
1:A:67:ILE:HG21	1:A:163:MET:CE	2.46	0.45
1:A:202:PRO:O	1:A:203:SER:C	2.57	0.45
1:A:232:TYR:O	1:A:233:GLU:C	2.59	0.45
1:B:114:ARG:HG3	1:B:115:PHE:H	1.80	0.45
2:C:17:ILE:HD12	2:C:42:GLN:HG3	1.97	0.45
2:C:143:ASN:C	2:C:145:MET:N	2.73	0.45
2:D:88:THR:HG22	2:D:94:LEU:CG	2.39	0.45
2:D:116:THR:O	2:D:117:ILE:CG1	2.64	0.45
1:B:287:GLN:HG3	1:B:291:PHE:CD1	2.51	0.45
2:C:284:ASN:O	2:C:288:MET:N	2.46	0.45
2:C:425:LEU:O	2:C:428:GLN:HB2	2.17	0.45
2:D:287:LYS:HA	2:D:419:GLY:HA3	1.98	0.45
2:C:19:GLU:CD	2:C:25:VAL:HA	2.42	0.45
2:C:148:ALA:O	2:C:149:VAL:C	2.58	0.45
2:C:168:VAL:C	2:C:170:LYS:N	2.74	0.45
2:C:223:PHE:O	2:C:224:ILE:C	2.59	0.45
2:C:287:LYS:HA	2:C:419:GLY:HA3	1.98	0.45
2:C:425:LEU:HA	2:C:428:GLN:HB2	1.97	0.45
2:D:217:LEU:O	2:D:218:ALA:C	2.60	0.45
2:D:233:LYS:HA	2:D:240:TYR:O	2.16	0.45
3:F:606:DC:C1'	3:F:607:U:H5''	2.47	0.45
1:A:54:GLN:NE2	1:A:87:VAL:HG21	2.32	0.45
1:A:184:TRP:CH2	1:A:224:VAL:HG12	2.49	0.45
2:C:19:GLU:HA	2:C:24:ARG:O	2.17	0.45
2:C:29:ASN:O	2:C:31:TYR:N	2.49	0.45
2:C:96:THR:HG23	2:C:477:ILE:HG13	1.99	0.45
2:C:233:LYS:HA	2:C:240:TYR:O	2.16	0.45
2:C:240:TYR:CZ	2:C:253:ASP:HB2	2.52	0.45
2:C:322:ILE:HG21	2:C:443:LEU:HD12	1.98	0.45
2:C:389:TYR:N	2:C:389:TYR:CD1	2.84	0.45
2:D:414:GLU:C	2:D:416:SER:N	2.74	0.45
1:A:122:ARG:NH2	1:B:186:LYS:HD2	2.31	0.45
1:A:161:ASN:OD1	1:A:191:PRO:HD3	2.17	0.45
1:A:198:GLN:OE1	1:A:209:ARG:HD3	2.17	0.45
1:B:34:LEU:HB2	1:B:37:GLN:OE1	2.16	0.45
1:B:94:ILE:HG23	1:B:112:VAL:CG1	2.47	0.45
2:D:370:ILE:O	2:D:373:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HG23	1:A:112:VAL:CG1	2.46	0.45
1:A:166:ILE:C	1:A:168:ASN:N	2.74	0.45
1:B:279:THR:O	1:B:282:LYS:N	2.49	0.45
2:C:49:LYS:O	2:C:52:PHE:HB3	2.16	0.45
2:C:74:ILE:O	2:C:75:LYS:C	2.59	0.45
2:D:211:ARG:HG2	2:D:211:ARG:HH11	1.82	0.45
2:D:270:ILE:O	2:D:270:ILE:CG2	2.65	0.45
2:D:337:ILE:HD11	2:D:412:VAL:CG1	2.36	0.45
1:A:72:GLY:CA	1:A:75:ILE:HD12	2.47	0.45
1:A:152:ASP:O	1:A:153:LEU:C	2.60	0.45
1:B:22:TYR:C	1:B:22:TYR:CD2	2.94	0.45
1:B:192:HIS:O	1:B:212:SER:CB	2.64	0.45
2:C:229:ILE:H	2:C:229:ILE:CD1	2.21	0.45
2:C:291:GLN:O	2:C:292:ILE:C	2.59	0.45
2:D:45:THR:C	2:D:47:PHE:N	2.74	0.45
2:D:99:GLU:O	2:D:103:VAL:HG23	2.16	0.45
2:D:425:LEU:O	2:D:428:GLN:HB2	2.17	0.45
1:A:285:PHE:O	1:A:286:LEU:C	2.59	0.45
1:B:53:LEU:O	1:B:58:ILE:HG23	2.17	0.45
2:C:81:TYR:O	2:C:84:LYS:HG2	2.16	0.45
2:C:355:LYS:CG	2:C:356:LYS:N	2.77	0.45
2:D:166:LYS:HE2	2:D:166:LYS:N	2.31	0.45
2:D:245:ASP:HB2	2:D:249:ASN:HB2	1.99	0.45
2:D:476:ILE:CD1	6:D:602:U5P:H1'	2.47	0.45
1:A:42:LEU:HD22	1:A:46:GLU:OE2	2.16	0.45
1:B:161:ASN:OD1	1:B:191:PRO:HD3	2.17	0.45
2:C:234:ILE:HB	2:C:240:TYR:HD2	1.82	0.45
2:D:310:ALA:C	2:D:312:MET:N	2.73	0.45
2:D:352:PHE:CE2	2:D:428:GLN:HG3	2.52	0.45
2:D:389:TYR:CE2	2:D:427:TYR:HB2	2.51	0.45
2:C:18:ILE:HG21	2:C:26:PRO:HB3	1.98	0.45
2:C:282:LEU:HD13	2:C:312:MET:CE	2.46	0.45
2:D:74:ILE:O	2:D:75:LYS:C	2.59	0.45
2:D:103:VAL:HG21	2:D:215:ILE:HD13	1.98	0.45
1:B:49:PHE:CD1	1:B:211:LEU:HD22	2.52	0.44
1:B:118:GLU:O	1:B:119:GLU:C	2.58	0.44
1:B:239:LEU:HA	1:B:243:VAL:HG21	1.98	0.44
2:C:19:GLU:CG	2:C:26:PRO:HD3	2.47	0.44
2:D:112:LEU:O	2:D:113:GLY:C	2.60	0.44
2:D:113:GLY:HA3	5:I:702:U:O2	2.17	0.44
2:D:163:SER:C	2:D:165:VAL:N	2.69	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:606:DC:C2	3:F:607:U:C6	3.05	0.44
1:A:49:PHE:CD1	1:A:211:LEU:HD22	2.52	0.44
1:A:150:THR:O	1:A:154:LEU:HG	2.16	0.44
1:B:77:TYR:O	1:B:78:LEU:C	2.60	0.44
1:B:138:ASP:OD1	1:B:209:ARG:NH2	2.51	0.44
2:D:17:ILE:HD12	2:D:42:GLN:HG3	1.98	0.44
2:D:19:GLU:CG	2:D:26:PRO:HD3	2.47	0.44
2:D:49:LYS:O	2:D:52:PHE:HB3	2.17	0.44
2:D:53:VAL:HG13	2:D:75:LYS:HA	1.99	0.44
2:D:216:ASP:O	2:D:217:LEU:C	2.59	0.44
2:D:280:PHE:CZ	2:D:430:LEU:HD11	2.51	0.44
2:D:328:ARG:HB2	2:D:444:ASN:HB2	1.99	0.44
2:D:376:ASP:OD2	2:D:376:ASP:N	2.51	0.44
1:A:128:LEU:O	1:A:129:HIS:C	2.60	0.44
1:B:232:TYR:O	1:B:233:GLU:C	2.61	0.44
1:B:239:LEU:HA	1:B:243:VAL:HG23	1.97	0.44
1:B:282:LYS:O	1:B:283:VAL:C	2.59	0.44
2:C:34:LEU:O	2:C:35:LYS:C	2.60	0.44
2:C:216:ASP:O	2:C:217:LEU:C	2.59	0.44
2:C:303:GLU:HA	2:C:306:ASN:CB	2.46	0.44
2:C:408:ASP:HA	2:C:455:TYR:HB2	1.98	0.44
2:D:301:ASP:C	2:D:303:GLU:N	2.75	0.44
3:F:607:U:H3'	3:F:608:U:C6	2.52	0.44
1:B:5:SER:C	1:B:6:LEU:HD23	2.42	0.44
2:C:63:PHE:CE2	2:C:171:LEU:HA	2.53	0.44
1:A:60:ASP:OD1	2:D:238:ARG:HD3	2.18	0.44
1:A:94:ILE:HG23	1:A:112:VAL:CB	2.48	0.44
1:A:257:GLU:O	1:A:258:TYR:C	2.60	0.44
1:B:202:PRO:HB2	1:B:205:SER:CB	2.45	0.44
1:B:202:PRO:O	1:B:203:SER:C	2.59	0.44
2:C:60:LYS:HZ3	2:C:67:VAL:N	2.14	0.44
2:D:303:GLU:HA	2:D:306:ASN:CB	2.46	0.44
2:D:389:TYR:N	2:D:389:TYR:CD1	2.84	0.44
1:A:35:PRO:HG2	1:A:296:ILE:HG23	1.99	0.44
1:A:77:TYR:O	1:A:78:LEU:C	2.60	0.44
2:C:44:ILE:HD13	2:C:101:GLN:HE21	1.82	0.44
2:C:60:LYS:HG2	2:C:224:ILE:HG23	2.00	0.44
2:C:100:LEU:HD11	2:C:477:ILE:HD11	2.00	0.44
2:C:337:ILE:CG1	2:C:412:VAL:HG22	2.48	0.44
2:C:365:VAL:HG12	2:C:369:ASP:OD2	2.18	0.44
2:C:408:ASP:OD1	2:C:409:LYS:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:SD	2:D:213:PHE:HZ	2.41	0.44
2:D:240:TYR:CZ	2:D:253:ASP:HB2	2.53	0.44
2:D:282:LEU:HD13	2:D:312:MET:CE	2.47	0.44
1:B:40:LEU:O	1:B:41:LYS:C	2.61	0.44
2:C:44:ILE:HG21	2:C:101:GLN:NE2	2.32	0.44
2:C:270:ILE:O	2:C:270:ILE:CG2	2.66	0.44
2:C:337:ILE:HD11	2:C:412:VAL:CG1	2.36	0.44
2:D:44:ILE:HG21	2:D:101:GLN:NE2	2.32	0.44
2:D:473:GLU:HG3	2:D:474:LYS:N	2.31	0.44
1:A:74:HIS:CG	1:A:75:ILE:N	2.86	0.44
1:A:138:ASP:OD1	1:A:209:ARG:NH2	2.51	0.44
1:B:50:LEU:HD12	1:B:59:LEU:HD13	2.00	0.44
1:B:74:HIS:CG	1:B:75:ILE:N	2.86	0.44
1:B:132:LYS:N	2:C:465:GLY:HA2	2.33	0.44
1:B:181:PRO:C	1:B:183:GLN:H	2.26	0.44
2:C:88:THR:HG22	2:C:94:LEU:CG	2.39	0.44
2:C:301:ASP:C	2:C:303:GLU:N	2.76	0.44
2:C:389:TYR:CE2	2:C:427:TYR:HB2	2.52	0.44
2:C:408:ASP:CB	2:C:411:LYS:HD2	2.48	0.44
2:C:435:TYR:O	2:C:438:CYS:N	2.51	0.44
2:D:186:TYR:HB3	2:D:276:VAL:HG23	1.99	0.44
2:D:209:ASN:O	2:D:210:SER:C	2.59	0.44
1:A:192:HIS:O	1:A:212:SER:CB	2.66	0.44
2:C:110:ASP:OD2	2:C:110:ASP:N	2.51	0.44
2:C:268:ILE:HB	2:C:275:ILE:HG12	2.00	0.44
2:C:400:PHE:HE2	2:C:402:ASN:HB2	1.82	0.44
2:C:450:ASP:C	2:C:452:ILE:N	2.76	0.44
2:D:107:THR:O	2:D:108:TYR:C	2.59	0.44
2:D:214:LEU:CB	2:D:231:LEU:HD11	2.48	0.44
1:A:187:ASP:OD2	1:A:225:THR:HA	2.17	0.43
1:B:13:PHE:HA	1:B:16:ILE:HD13	2.00	0.43
1:B:16:ILE:HD12	1:B:16:ILE:N	2.33	0.43
1:B:94:ILE:HG23	1:B:112:VAL:CB	2.48	0.43
2:C:328:ARG:HB2	2:C:444:ASN:HB2	1.99	0.43
2:D:393:ASP:C	2:D:394:ASN:OD1	2.60	0.43
1:A:40:LEU:O	1:A:41:LYS:C	2.61	0.43
1:B:206:ALA:CA	1:B:236:MET:HE3	2.42	0.43
2:C:287:LYS:HA	2:C:419:GLY:CA	2.48	0.43
2:D:189:TYR:CD1	2:D:200:TYR:CZ	3.06	0.43
2:D:211:ARG:HG2	2:D:211:ARG:NH1	2.32	0.43
2:D:292:ILE:O	2:D:295:LEU:N	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:TYR:CD2	2:D:427:TYR:HB2	2.54	0.43
1:A:13:PHE:HA	1:A:16:ILE:HD13	2.00	0.43
2:C:418:ARG:HH22	2:C:446:MET:CA	2.30	0.43
2:D:74:ILE:CA	2:D:77:ARG:NH1	2.79	0.43
2:D:214:LEU:HD13	2:D:231:LEU:HD21	1.99	0.43
2:D:278:PRO:HB2	2:D:315:TYR:CD2	2.53	0.43
2:D:365:VAL:O	2:D:366:LEU:C	2.60	0.43
1:A:197:LEU:HD22	1:A:197:LEU:N	2.34	0.43
1:B:87:VAL:HG12	1:B:88:ILE:N	2.33	0.43
1:B:287:GLN:O	1:B:288:GLN:C	2.60	0.43
2:C:13:ILE:O	2:C:16:LYS:HB2	2.19	0.43
2:C:148:ALA:HB2	2:C:295:LEU:O	2.19	0.43
2:C:350:ASP:C	2:C:351:TYR:CD1	2.96	0.43
2:C:423:HIS:HA	2:C:426:LEU:CD1	2.49	0.43
2:C:471:ASN:O	2:C:472:ILE:C	2.60	0.43
2:D:17:ILE:HG22	2:D:41:ILE:HG22	2.00	0.43
2:D:63:PHE:CE2	2:D:171:LEU:HA	2.53	0.43
2:D:147:VAL:HG21	2:D:452:ILE:O	2.18	0.43
2:D:218:ALA:CB	2:D:472:ILE:HD11	2.34	0.43
2:D:240:TYR:HE1	2:D:253:ASP:HB2	1.82	0.43
1:B:4:VAL:N	1:B:247:VAL:O	2.52	0.43
1:B:130:PRO:O	1:B:131:SER:C	2.60	0.43
1:B:145:GLY:O	1:B:146:ASN:HB3	2.19	0.43
1:B:225:THR:HG23	1:B:228:ASP:OD2	2.17	0.43
2:C:74:ILE:CA	2:C:77:ARG:NH1	2.80	0.43
2:C:77:ARG:CD	2:C:223:PHE:O	2.67	0.43
2:C:198:ILE:HD13	2:C:198:ILE:HA	1.80	0.43
2:D:27:SER:OG	2:D:30:GLU:HG3	2.17	0.43
2:D:111:ILE:HG23	2:D:175:TYR:OH	2.19	0.43
2:D:145:MET:O	2:D:147:VAL:N	2.52	0.43
1:A:22:TYR:HB2	1:A:233:GLU:HG2	2.00	0.43
1:A:164:ILE:HD12	1:A:214:TYR:OH	2.19	0.43
1:A:199:PRO:HG3	1:A:262:HIS:CE1	2.54	0.43
2:C:81:TYR:C	2:C:83:SER:N	2.75	0.43
2:C:182:SER:O	2:C:183:CYS:HB2	2.18	0.43
2:C:189:TYR:CD1	2:C:200:TYR:CZ	3.06	0.43
2:C:352:PHE:CE2	2:C:428:GLN:HG3	2.54	0.43
2:C:449:ARG:HB3	2:C:449:ARG:CZ	2.49	0.43
2:D:192:TYR:HD1	2:D:196:PRO:HA	1.82	0.43
2:D:409:LYS:HG2	2:D:455:TYR:CE2	2.53	0.43
1:A:287:GLN:HG3	1:A:291:PHE:CD1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:OD1	2:C:238:ARG:HD3	2.19	0.43
1:B:128:LEU:O	1:B:129:HIS:C	2.61	0.43
2:C:19:GLU:HG2	2:C:24:ARG:O	2.18	0.43
2:C:175:TYR:CE1	2:C:179:HIS:CD2	3.06	0.43
2:C:186:TYR:HB3	2:C:276:VAL:HG23	1.99	0.43
2:C:292:ILE:O	2:C:295:LEU:N	2.39	0.43
2:C:405:LEU:C	2:C:406:LEU:HD22	2.43	0.43
2:D:86:THR:CB	2:D:87:GLN:HE22	2.13	0.43
2:D:182:SER:O	2:D:183:CYS:HB2	2.18	0.43
2:D:442:LEU:HG	2:D:446:MET:HE2	2.00	0.43
1:A:286:LEU:O	1:A:290:ILE:HG13	2.19	0.43
1:B:2:ASP:CA	1:B:246:LYS:HZ3	2.31	0.43
2:C:24:ARG:HH12	2:C:86:THR:CA	2.32	0.43
2:C:389:TYR:CD2	2:C:427:TYR:HB2	2.54	0.43
2:C:409:LYS:HG2	2:C:455:TYR:CE2	2.53	0.43
2:D:34:LEU:O	2:D:35:LYS:C	2.61	0.43
2:D:83:SER:CA	2:D:85:GLN:HE22	2.32	0.43
2:D:198:ILE:HG22	2:D:198:ILE:O	2.17	0.43
2:D:408:ASP:OD1	2:D:409:LYS:N	2.50	0.43
1:B:286:LEU:O	1:B:290:ILE:HG13	2.19	0.43
2:C:17:ILE:HG22	2:C:41:ILE:HG22	2.01	0.43
2:C:298:LEU:C	2:C:300:LYS:N	2.76	0.43
2:C:337:ILE:HG13	2:C:412:VAL:CG2	2.48	0.43
2:D:48:ASN:OD1	2:D:50:ASP:HB2	2.19	0.43
2:D:52:PHE:CD1	2:D:52:PHE:C	2.96	0.43
2:D:61:LYS:HB2	2:D:61:LYS:HZ2	1.80	0.43
2:D:166:LYS:O	2:D:167:ASN:C	2.62	0.43
2:D:175:TYR:CE1	2:D:179:HIS:CD2	3.06	0.43
2:D:328:ARG:HE	2:D:441:ASP:CG	2.27	0.43
2:D:418:ARG:HH22	2:D:446:MET:CA	2.31	0.43
2:D:471:ASN:O	2:D:472:ILE:C	2.62	0.43
1:A:87:VAL:HG12	1:A:88:ILE:N	2.33	0.43
1:A:154:LEU:O	1:A:155:SER:C	2.62	0.43
1:A:168:ASN:OD1	1:B:223:ARG:HD2	2.19	0.43
1:A:270:VAL:HG12	1:A:271:TYR:N	2.32	0.43
1:B:203:SER:O	1:B:240:ASN:HB3	2.19	0.43
2:C:61:LYS:HB2	2:C:61:LYS:HZ2	1.81	0.43
2:C:85:GLN:H	2:C:85:GLN:HE21	1.62	0.43
2:C:99:GLU:O	2:C:103:VAL:HG23	2.18	0.43
2:C:231:LEU:CD2	2:C:241:MET:HE2	2.31	0.43
1:B:181:PRO:O	1:B:183:GLN:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:LEU:O	2:C:286:ILE:HG13	2.19	0.42
2:C:325:ASP:O	2:C:327:LYS:N	2.51	0.42
2:D:52:PHE:CE1	2:D:56:VAL:CG2	3.02	0.42
2:D:60:LYS:HZ3	2:D:67:VAL:N	2.16	0.42
2:D:110:ASP:OD2	2:D:110:ASP:N	2.52	0.42
2:D:372:ASP:C	2:D:374:ASN:H	2.26	0.42
2:D:462:LYS:H	2:D:462:LYS:CD	2.21	0.42
1:A:46:GLU:OE1	1:A:74:HIS:NE2	2.52	0.42
2:D:41:ILE:HD11	2:D:98:ILE:CD1	2.49	0.42
2:D:53:VAL:CG1	2:D:75:LYS:HG3	2.43	0.42
2:D:70:SER:OG	2:D:73:GLU:CB	2.67	0.42
2:D:216:ASP:O	2:D:219:PHE:N	2.52	0.42
2:D:291:GLN:OE1	2:D:403:THR:HG23	2.19	0.42
2:D:320:HIS:HB2	2:D:322:ILE:HD11	2.02	0.42
2:D:322:ILE:HG21	2:D:443:LEU:HD12	2.00	0.42
1:A:118:GLU:O	1:A:119:GLU:C	2.61	0.42
2:C:52:PHE:HE2	2:C:104:LEU:HB3	1.84	0.42
2:C:83:SER:CA	2:C:85:GLN:HE22	2.32	0.42
2:C:331:MET:CG	2:C:332:PRO:HD2	2.47	0.42
2:D:228:ASN:O	2:D:473:GLU:OE2	2.37	0.42
2:D:423:HIS:O	2:D:426:LEU:HB2	2.20	0.42
1:A:114:ARG:HG3	1:A:115:PHE:N	2.34	0.42
1:A:282:LYS:O	1:A:283:VAL:C	2.61	0.42
1:B:22:TYR:HB2	1:B:233:GLU:HG2	2.01	0.42
1:B:181:PRO:C	1:B:183:GLN:N	2.78	0.42
2:C:397:TYR:N	2:C:397:TYR:CD1	2.87	0.42
2:C:471:ASN:HD22	2:C:471:ASN:HA	1.58	0.42
2:D:134:MET:O	2:D:135:GLU:C	2.62	0.42
2:D:268:ILE:O	2:D:274:TYR:HA	2.19	0.42
2:D:337:ILE:HG13	2:D:412:VAL:CG2	2.49	0.42
2:D:337:ILE:HA	2:D:344:VAL:HA	2.01	0.42
2:D:337:ILE:CG1	2:D:412:VAL:HG22	2.49	0.42
1:A:55:ARG:HH11	1:A:55:ARG:HG3	1.84	0.42
1:A:165:SER:OG	1:B:189:TYR:HE1	2.00	0.42
1:A:241:LYS:HG2	1:A:242:ILE:HD13	2.02	0.42
1:A:287:GLN:O	1:A:288:GLN:C	2.61	0.42
1:B:2:ASP:C	1:B:246:LYS:NZ	2.78	0.42
1:B:117:ASP:OD1	1:B:120:TYR:HB2	2.20	0.42
2:C:188:SER:O	2:C:189:TYR:C	2.62	0.42
2:C:291:GLN:HG3	2:C:293:ASP:HB3	2.00	0.42
2:C:473:GLU:HG3	2:C:474:LYS:N	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:SER:HB2	5:I:701:DC:H5	1.84	0.42
2:D:77:ARG:CD	2:D:223:PHE:O	2.68	0.42
7:D:800:3AT:O1G	7:D:800:3AT:O1B	2.38	0.42
3:E:601:DC:C1'	3:E:602:U:O5'	2.60	0.42
1:A:56:HIS:HA	2:D:388:VAL:HG21	2.02	0.42
1:B:241:LYS:HG2	1:B:242:ILE:HD13	2.01	0.42
2:D:60:LYS:HG2	2:D:224:ILE:HG23	2.02	0.42
2:D:198:ILE:HD13	2:D:198:ILE:HA	1.83	0.42
2:D:298:LEU:C	2:D:300:LYS:N	2.77	0.42
2:D:327:LYS:HD3	2:D:327:LYS:O	2.19	0.42
2:D:397:TYR:N	2:D:397:TYR:CD1	2.87	0.42
2:D:415:ILE:O	2:D:415:ILE:HG22	2.19	0.42
1:A:117:ASP:OD1	1:A:120:TYR:HB2	2.20	0.42
1:B:100:ASP:OD1	1:B:102:ILE:HG12	2.20	0.42
1:B:265:PHE:O	1:B:268:ARG:HG2	2.20	0.42
2:C:145:MET:O	2:C:147:VAL:N	2.53	0.42
2:D:19:GLU:HG2	2:D:25:VAL:HA	2.02	0.42
2:D:418:ARG:HH22	2:D:445:SER:C	2.28	0.42
5:I:703:U:OP2	5:I:704:DC:N4	2.51	0.42
1:A:57:GLY:O	1:A:59:LEU:N	2.52	0.42
1:B:124:ILE:O	1:B:125:LYS:C	2.62	0.42
1:B:253:TYR:O	1:B:254:PRO:C	2.62	0.42
2:C:52:PHE:C	2:C:52:PHE:CD1	2.97	0.42
2:C:300:LYS:O	2:C:302:PRO:CD	2.66	0.42
2:D:100:LEU:HD11	2:D:477:ILE:HD11	2.02	0.42
2:D:282:LEU:O	2:D:286:ILE:HG13	2.20	0.42
2:D:325:ASP:C	2:D:327:LYS:N	2.77	0.42
1:A:4:VAL:N	1:A:247:VAL:O	2.53	0.42
1:A:34:LEU:CB	1:A:35:PRO:CD	2.87	0.42
1:A:223:ARG:HB3	1:B:217:GLU:HA	2.01	0.42
1:B:199:PRO:HG3	1:B:262:HIS:CE1	2.55	0.42
1:B:294:LEU:HD12	1:B:296:ILE:CD1	2.49	0.42
2:C:52:PHE:CE1	2:C:56:VAL:CG2	3.03	0.42
2:C:107:THR:O	2:C:108:TYR:C	2.60	0.42
2:C:387:SER:OG	2:C:388:VAL:N	2.53	0.42
2:D:22:LEU:O	2:D:24:ARG:NH1	2.53	0.42
2:D:74:ILE:HD13	2:D:77:ARG:HD2	2.02	0.42
2:D:168:VAL:C	2:D:170:LYS:H	2.27	0.42
2:D:198:ILE:HD12	2:D:308:ARG:NH1	2.34	0.42
2:D:291:GLN:HG3	2:D:293:ASP:HB3	2.00	0.42
2:D:449:ARG:CZ	2:D:449:ARG:HB3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:ASN:HD22	2:D:471:ASN:HA	1.58	0.42
3:E:602:U:O2'	3:E:603:U:O5'	2.38	0.42
1:B:54:GLN:NE2	1:B:87:VAL:HG21	2.35	0.42
1:B:162:VAL:O	1:B:166:ILE:HG12	2.20	0.42
1:B:285:PHE:O	1:B:286:LEU:C	2.62	0.42
2:C:216:ASP:O	2:C:219:PHE:N	2.53	0.42
2:C:372:ASP:C	2:C:374:ASN:H	2.27	0.42
2:C:386:ASN:HB3	2:C:401:SER:HB3	2.02	0.42
2:C:438:CYS:O	2:C:441:ASP:HB2	2.20	0.42
2:D:81:TYR:O	2:D:83:SER:N	2.53	0.42
2:D:205:ILE:O	2:D:206:LEU:HD23	2.20	0.42
2:D:406:LEU:HA	2:D:413:HIS:H	1.85	0.42
1:B:158:ALA:O	1:B:162:VAL:HG23	2.20	0.41
2:C:285:MET:CG	2:C:312:MET:HE1	2.50	0.41
2:D:114:VAL:HG13	2:D:178:ARG:NH2	2.35	0.41
2:D:450:ASP:C	2:D:452:ILE:N	2.78	0.41
1:A:130:PRO:O	1:A:131:SER:C	2.61	0.41
1:A:203:SER:O	1:A:240:ASN:HB3	2.20	0.41
1:A:253:TYR:CG	1:A:254:PRO:HD2	2.54	0.41
1:B:132:LYS:HZ1	2:C:238:ARG:HH12	1.66	0.41
2:D:186:TYR:HB3	2:D:276:VAL:HG21	2.00	0.41
2:D:358:LEU:N	2:D:358:LEU:HD23	2.35	0.41
1:A:50:LEU:H	1:A:50:LEU:CD2	2.33	0.41
1:A:181:PRO:C	1:A:183:GLN:H	2.29	0.41
1:A:221:LEU:CD1	1:B:221:LEU:HD13	2.47	0.41
1:A:283:VAL:O	1:A:284:LEU:C	2.62	0.41
2:C:41:ILE:HD11	2:C:98:ILE:CD1	2.50	0.41
2:C:109:THR:HG21	4:G:501:U:O3'	2.20	0.41
2:C:214:LEU:CA	2:C:243:ILE:HD11	2.49	0.41
2:D:188:SER:HB2	2:D:200:TYR:CB	2.46	0.41
2:D:234:ILE:HB	2:D:240:TYR:HD2	1.85	0.41
1:A:219:MET:CE	1:B:221:LEU:HD13	2.40	0.41
1:B:67:ILE:HD12	1:B:163:MET:SD	2.60	0.41
1:B:108:ASP:OD1	1:B:108:ASP:N	2.45	0.41
1:B:132:LYS:H	2:C:465:GLY:HA2	1.85	0.41
2:C:107:THR:HG21	2:C:212:THR:HG21	2.02	0.41
2:C:142:LEU:HD13	2:C:302:PRO:O	2.20	0.41
2:C:227:ASN:HD22	2:C:228:ASN:N	2.18	0.41
2:C:392:HIS:HE1	2:C:393:ASP:OD2	2.03	0.41
2:D:29:ASN:C	2:D:31:TYR:N	2.78	0.41
2:D:103:VAL:HG12	2:D:216:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:ASP:HA	2:D:303:GLU:OE2	2.20	0.41
2:D:329:ASN:OD1	2:D:330:ASN:ND2	2.53	0.41
1:A:279:THR:O	1:A:281:ALA:N	2.54	0.41
1:B:4:VAL:O	1:B:248:VAL:HA	2.20	0.41
1:B:55:ARG:O	1:B:55:ARG:HG2	2.20	0.41
1:B:55:ARG:O	2:C:388:VAL:HG21	2.20	0.41
1:B:88:ILE:HD13	1:B:88:ILE:HA	1.94	0.41
2:C:134:MET:O	2:C:135:GLU:C	2.63	0.41
2:C:192:TYR:HD1	2:C:196:PRO:HA	1.84	0.41
2:C:291:GLN:OE1	2:C:403:THR:HG23	2.21	0.41
2:C:310:ALA:C	2:C:312:MET:N	2.76	0.41
2:C:328:ARG:HE	2:C:441:ASP:CG	2.28	0.41
2:D:268:ILE:HB	2:D:275:ILE:HG13	2.02	0.41
2:D:268:ILE:HG12	2:D:277:ASP:HA	2.03	0.41
2:D:331:MET:CG	2:D:332:PRO:HD2	2.49	0.41
2:D:337:ILE:HD12	2:D:412:VAL:HG22	2.03	0.41
1:A:199:PRO:HG2	1:A:266:MET:SD	2.60	0.41
1:B:60:ASP:HB3	2:C:238:ARG:NH1	2.35	0.41
1:B:69:SER:O	1:B:70:ALA:C	2.63	0.41
2:C:301:ASP:O	2:C:303:GLU:N	2.53	0.41
2:C:405:LEU:CD1	2:C:415:ILE:HB	2.50	0.41
2:D:301:ASP:O	2:D:303:GLU:N	2.54	0.41
2:D:328:ARG:CD	2:D:441:ASP:HB3	2.51	0.41
2:D:352:PHE:CE2	2:D:428:GLN:CD	2.99	0.41
1:B:34:LEU:CB	1:B:35:PRO:CD	2.86	0.41
1:B:164:ILE:HD12	1:B:214:TYR:OH	2.21	0.41
1:B:197:LEU:HD22	1:B:197:LEU:N	2.36	0.41
2:C:27:SER:OG	2:C:30:GLU:HG3	2.20	0.41
2:C:217:LEU:O	2:C:220:LEU:HB3	2.21	0.41
2:C:245:ASP:CG	2:C:246:GLU:H	2.27	0.41
2:C:268:ILE:HG12	2:C:277:ASP:HA	2.03	0.41
2:D:169:ASN:O	2:D:203:ILE:HD11	2.20	0.41
1:A:158:ALA:O	1:A:162:VAL:HG23	2.20	0.41
1:B:46:GLU:OE1	1:B:74:HIS:NE2	2.54	0.41
2:C:109:THR:HG21	4:G:502:U:P	2.61	0.41
2:C:111:ILE:HG23	2:C:175:TYR:OH	2.21	0.41
2:C:188:SER:HB3	7:C:801:3AT:PG	2.60	0.41
2:D:33:MET:HB3	2:D:95:PHE:CE2	2.55	0.41
2:D:188:SER:O	2:D:189:TYR:C	2.64	0.41
1:A:22:TYR:C	1:A:22:TYR:HD2	2.29	0.41
1:A:121:LEU:HD22	1:A:167:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:HA	1:B:246:LYS:NZ	2.36	0.41
2:C:22:LEU:HD23	2:C:22:LEU:HA	1.92	0.41
2:C:61:LYS:O	2:C:62:ARG:CB	2.68	0.41
2:C:245:ASP:HB2	2:C:249:ASN:HB2	2.03	0.41
2:C:280:PHE:HD1	2:C:429:MET:SD	2.44	0.41
2:C:365:VAL:O	2:C:366:LEU:C	2.63	0.41
2:C:416:SER:O	2:C:418:ARG:N	2.53	0.41
7:C:801:3AT:O1B	7:C:801:3AT:O1G	2.39	0.41
2:D:142:LEU:HD13	2:D:302:PRO:O	2.21	0.41
2:D:209:ASN:O	2:D:212:THR:N	2.50	0.41
2:D:242:VAL:HB	2:D:253:ASP:HB3	2.02	0.41
2:D:277:ASP:HA	2:D:278:PRO:HD3	1.96	0.41
2:D:438:CYS:O	2:D:441:ASP:HB2	2.21	0.41
1:B:215:THR:HA	2:C:364:ASN:ND2	2.36	0.41
2:C:15:LEU:HD21	2:C:26:PRO:CG	2.50	0.41
2:C:172:MET:SD	2:C:213:PHE:HZ	2.44	0.41
2:C:186:TYR:HB3	2:C:276:VAL:HG21	2.01	0.41
2:C:415:ILE:C	2:C:418:ARG:HB2	2.46	0.41
2:C:462:LYS:H	2:C:462:LYS:CD	2.22	0.41
2:D:74:ILE:HA	2:D:74:ILE:HD13	1.92	0.41
2:D:115:LEU:HD23	2:D:178:ARG:HG3	2.02	0.41
2:D:189:TYR:O	2:D:192:TYR:HB3	2.21	0.41
2:D:199:ARG:HH12	2:D:304:LYS:CA	2.30	0.41
2:D:245:ASP:CG	2:D:246:GLU:H	2.27	0.41
2:D:390:LEU:HG	2:D:391:ILE:N	2.36	0.41
2:D:413:HIS:CD2	2:D:413:HIS:C	2.99	0.41
2:D:416:SER:O	2:D:418:ARG:N	2.53	0.41
1:A:72:GLY:O	1:A:73:THR:C	2.64	0.40
1:A:77:TYR:C	1:A:77:TYR:CD1	2.98	0.40
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.32	0.40
1:B:250:ASN:ND2	1:B:250:ASN:C	2.79	0.40
2:C:161:VAL:N	2:C:249:ASN:HA	2.36	0.40
2:C:199:ARG:HH12	2:C:304:LYS:CA	2.28	0.40
2:C:242:VAL:HB	2:C:253:ASP:HB3	2.03	0.40
2:D:300:LYS:O	2:D:302:PRO:CD	2.67	0.40
2:D:408:ASP:CB	2:D:411:LYS:HD2	2.51	0.40
1:A:62:ALA:HB2	1:A:132:LYS:HE3	2.03	0.40
1:B:187:ASP:OD2	1:B:225:THR:HA	2.20	0.40
2:C:33:MET:HB3	2:C:95:PHE:CE2	2.56	0.40
2:C:103:VAL:HG12	2:C:216:ASP:OD1	2.22	0.40
2:C:198:ILE:HD12	2:C:308:ARG:NH1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:ALA:O	2:C:308:ARG:C	2.62	0.40
2:D:270:ILE:O	2:D:271:ASP:CB	2.66	0.40
2:D:307:ALA:O	2:D:308:ARG:C	2.62	0.40
2:D:405:LEU:CD1	2:D:415:ILE:HB	2.51	0.40
2:D:422:ALA:O	2:D:426:LEU:HG	2.21	0.40
2:D:425:LEU:O	2:D:426:LEU:C	2.63	0.40
3:F:607:U:H2'	3:F:608:U:C6	2.56	0.40
1:A:88:ILE:HD13	1:A:88:ILE:HA	1.95	0.40
1:A:253:TYR:O	1:A:254:PRO:C	2.63	0.40
2:C:166:LYS:O	2:C:167:ASN:C	2.64	0.40
2:C:228:ASN:O	2:C:473:GLU:OE2	2.39	0.40
2:D:52:PHE:HE2	2:D:104:LEU:HB3	1.86	0.40
2:D:242:VAL:HG13	2:D:242:VAL:O	2.21	0.40
1:A:46:GLU:HB2	1:A:78:LEU:HD11	2.04	0.40
1:A:76:ARG:O	1:A:79:ARG:HB3	2.21	0.40
1:A:146:ASN:O	1:A:147:GLU:HB2	2.21	0.40
1:A:237:TYR:OH	1:A:241:LYS:HD2	2.22	0.40
1:B:253:TYR:CG	1:B:254:PRO:HD2	2.55	0.40
2:C:277:ASP:HA	2:C:278:PRO:HD3	1.96	0.40
2:C:425:LEU:O	2:C:426:LEU:C	2.64	0.40
2:D:195:ASN:ND2	2:D:198:ILE:HG12	2.30	0.40
2:D:286:ILE:CG2	2:D:418:ARG:HB3	2.51	0.40
2:D:331:MET:SD	2:D:441:ASP:HB3	2.61	0.40
6:D:602:U5P:H2'	6:D:602:U5P:H6	1.84	0.40
1:A:124:ILE:O	1:A:125:LYS:C	2.64	0.40
1:A:202:PRO:HB2	1:A:205:SER:CB	2.49	0.40
1:A:240:ASN:HA	1:A:244:ARG:CD	2.51	0.40
1:A:250:ASN:ND2	1:A:250:ASN:C	2.79	0.40
1:A:294:LEU:HD12	1:A:296:ILE:CD1	2.50	0.40
1:B:52:LYS:NZ	2:C:375:ALA:O	2.49	0.40
1:B:107:ARG:NH1	2:C:477:ILE:CG2	2.85	0.40
1:B:114:ARG:HG3	1:B:115:PHE:N	2.36	0.40
1:B:150:THR:O	1:B:154:LEU:HG	2.21	0.40
1:B:163:MET:O	1:B:164:ILE:C	2.65	0.40
2:C:53:VAL:CG1	2:C:75:LYS:HG3	2.45	0.40
2:D:52:PHE:C	2:D:52:PHE:HD1	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/297 (95%)	207 (73%)	57 (20%)	18 (6%)	1	7
1	B	282/297 (95%)	203 (72%)	61 (22%)	18 (6%)	1	7
2	C	439/479 (92%)	293 (67%)	110 (25%)	36 (8%)	0	4
2	D	439/479 (92%)	295 (67%)	109 (25%)	35 (8%)	1	4
All	All	1442/1552 (93%)	998 (69%)	337 (23%)	107 (7%)	1	5

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	146	ASN
1	A	147	GLU
1	A	277	PRO
1	B	2	ASP
1	B	146	ASN
1	B	147	GLU
1	B	277	PRO
2	C	38	ALA
2	C	62	ARG
2	C	146	ASN
2	C	309	MET
2	C	332	PRO
2	C	349	LYS
2	C	350	ASP
2	C	382	GLU
2	C	448	ASN
2	D	38	ALA
2	D	62	ARG
2	D	146	ASN
2	D	210	SER
2	D	309	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	332	PRO
2	D	349	LYS
2	D	350	ASP
2	D	448	ASN
1	A	58	ILE
1	B	58	ILE
1	B	164	ILE
2	C	46	VAL
2	C	210	SER
2	C	270	ILE
2	C	330	ASN
2	C	434	GLU
2	D	30	GLU
2	D	46	VAL
2	D	270	ILE
2	D	326	GLY
2	D	330	ASN
2	D	382	GLU
2	D	434	GLU
1	A	24	PRO
1	A	35	PRO
1	A	101	PRO
1	A	118	GLU
1	A	164	ILE
1	A	182	ASP
1	B	24	PRO
1	B	35	PRO
1	B	101	PRO
1	B	118	GLU
1	B	182	ASP
2	C	24	ARG
2	C	30	GLU
2	C	77	ARG
2	C	116	THR
2	C	163	SER
2	C	183	CYS
2	C	216	ASP
2	C	235	PRO
2	C	250	HIS
2	C	326	GLY
2	C	384	VAL
2	D	77	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	82	PHE
2	D	116	THR
2	D	163	SER
2	D	183	CYS
2	D	216	ASP
2	D	235	PRO
2	D	250	HIS
2	D	384	VAL
1	A	202	PRO
1	B	75	ILE
1	B	202	PRO
2	C	82	PHE
2	C	145	MET
2	C	189	TYR
2	C	213	PHE
2	C	436	LYS
2	D	24	ARG
2	D	145	MET
2	D	189	TYR
2	D	213	PHE
2	D	436	LYS
1	A	70	ALA
1	A	75	ILE
1	B	70	ALA
2	C	196	PRO
2	C	323	VAL
2	D	196	PRO
2	D	323	VAL
2	D	421	CYS
2	C	33	MET
2	C	190	SER
2	C	301	ASP
2	D	301	ASP
1	A	105	GLY
1	B	254	PRO
2	C	344	VAL
2	D	344	VAL
1	A	254	PRO
1	A	181	PRO
1	B	4	VAL
1	B	181	PRO
1	A	4	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	283	VAL

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	266/270 (98%)	247 (93%)	19 (7%)	13	43
1	B	266/270 (98%)	247 (93%)	19 (7%)	13	43
2	C	422/453 (93%)	386 (92%)	36 (8%)	10	35
2	D	422/453 (93%)	385 (91%)	37 (9%)	9	34
All	All	1376/1446 (95%)	1265 (92%)	111 (8%)	11	38

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	18	ASN
1	A	20	LEU
1	A	35	PRO
1	A	47	LEU
1	A	58	ILE
1	A	109	VAL
1	A	118	GLU
1	A	130	PRO
1	A	131	SER
1	A	194	ASN
1	A	202	PRO
1	A	217	GLU
1	A	248	VAL
1	A	257	GLU
1	A	275	THR
1	A	284	LEU
1	A	288	GLN
1	A	295	ASN
1	B	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	ASN
1	B	20	LEU
1	B	35	PRO
1	B	47	LEU
1	B	58	ILE
1	B	109	VAL
1	B	118	GLU
1	B	130	PRO
1	B	131	SER
1	B	194	ASN
1	B	202	PRO
1	B	217	GLU
1	B	248	VAL
1	B	257	GLU
1	B	275	THR
1	B	284	LEU
1	B	288	GLN
1	B	295	ASN
2	C	15	LEU
2	C	39	ARG
2	C	46	VAL
2	C	59	ASN
2	C	61	LYS
2	C	62	ARG
2	C	85	GLN
2	C	91	ILE
2	C	110	ASP
2	C	134	MET
2	C	161	VAL
2	C	166	LYS
2	C	174	GLU
2	C	186	TYR
2	C	198	ILE
2	C	206	LEU
2	C	229	ILE
2	C	231	LEU
2	C	249	ASN
2	C	264	VAL
2	C	292	ILE
2	C	293	ASP
2	C	301	ASP
2	C	308	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	309	MET
2	C	328	ARG
2	C	331	MET
2	C	332	PRO
2	C	333	MET
2	C	349	LYS
2	C	370	ILE
2	C	376	ASP
2	C	394	ASN
2	C	448	ASN
2	C	462	LYS
2	C	471	ASN
2	D	15	LEU
2	D	39	ARG
2	D	46	VAL
2	D	59	ASN
2	D	61	LYS
2	D	62	ARG
2	D	85	GLN
2	D	91	ILE
2	D	110	ASP
2	D	132	THR
2	D	161	VAL
2	D	166	LYS
2	D	174	GLU
2	D	186	TYR
2	D	198	ILE
2	D	206	LEU
2	D	229	ILE
2	D	231	LEU
2	D	249	ASN
2	D	264	VAL
2	D	292	ILE
2	D	293	ASP
2	D	301	ASP
2	D	308	ARG
2	D	309	MET
2	D	328	ARG
2	D	331	MET
2	D	332	PRO
2	D	333	MET
2	D	349	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	358	LEU
2	D	370	ILE
2	D	376	ASP
2	D	394	ASN
2	D	448	ASN
2	D	462	LYS
2	D	471	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	81	HIS
1	A	84	ASN
1	A	98	HIS
1	A	127	GLN
1	A	156	ASN
1	A	183	GLN
1	A	194	ASN
1	A	231	ASN
1	A	250	ASN
1	A	287	GLN
1	A	288	GLN
1	A	295	ASN
1	B	54	GLN
1	B	81	HIS
1	B	84	ASN
1	B	98	HIS
1	B	127	GLN
1	B	156	ASN
1	B	183	GLN
1	B	231	ASN
1	B	250	ASN
1	B	287	GLN
1	B	288	GLN
1	B	295	ASN
2	C	12	ASN
2	C	59	ASN
2	C	87	GLN
2	C	101	GLN
2	C	146	ASN
2	C	227	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	228	ASN
2	C	247	ASN
2	C	259	GLN
2	C	263	ASN
2	C	329	ASN
2	C	330	ASN
2	C	341	ASN
2	C	374	ASN
2	C	386	ASN
2	C	392	HIS
2	C	413	HIS
2	C	428	GLN
2	C	437	GLN
2	C	444	ASN
2	D	12	ASN
2	D	59	ASN
2	D	87	GLN
2	D	101	GLN
2	D	146	ASN
2	D	227	ASN
2	D	228	ASN
2	D	247	ASN
2	D	329	ASN
2	D	330	ASN
2	D	341	ASN
2	D	386	ASN
2	D	392	HIS
2	D	413	HIS
2	D	428	GLN
2	D	437	GLN
2	D	444	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	1/5 (20%)	1 (100%)	0
3	F	1/5 (20%)	0	0
4	G	1/4 (25%)	1 (100%)	0
5	I	1/5 (20%)	1 (100%)	0
All	All	4/19 (21%)	3 (75%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	603	U
4	G	502	U
5	I	703	U

There are no RNA pucker outliers to report.

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U5P	C	600	-	18,21,22	0.48	0	25,30,33	0.64	1 (4%)
6	U5P	D	602	-	18,21,22	0.44	0	25,30,33	0.56	1 (4%)
7	3AT	C	801	8	30,32,32	2.65	7 (23%)	42,50,50	2.07	9 (21%)
7	3AT	D	800	8	30,32,32	2.69	8 (26%)	42,50,50	1.95	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U5P	C	600	-	-	1/7/25/26	0/2/2/2
6	U5P	D	602	-	-	4/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	3AT	C	801	8	-	7/22/34/34	0/3/3/3
7	3AT	D	800	8	-	7/22/34/34	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	800	3AT	PB-O3B	8.63	1.68	1.59
7	C	801	3AT	PA-O3A	7.10	1.67	1.59
7	C	801	3AT	PB-O3A	6.96	1.67	1.59
7	C	801	3AT	PB-O3B	6.79	1.66	1.59
7	D	800	3AT	PB-O3A	5.77	1.65	1.59
7	D	800	3AT	PA-O3A	4.55	1.64	1.59
7	D	800	3AT	C5-C4	3.99	1.46	1.39
7	D	800	3AT	PG-O1G	3.99	1.62	1.50
7	C	801	3AT	PG-O1G	3.52	1.61	1.50
7	D	800	3AT	C4-N3	3.34	1.40	1.34
7	C	801	3AT	C5-C4	3.15	1.44	1.39
7	D	800	3AT	C2-N1	2.62	1.38	1.33
7	C	801	3AT	C4-N3	2.32	1.38	1.34
7	C	801	3AT	PG-O2G	2.04	1.62	1.54
7	D	800	3AT	PG-O2G	2.02	1.62	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	800	3AT	N3-C2-N1	-6.50	118.75	128.58
7	C	801	3AT	N3-C2-N1	-6.45	118.82	128.58
7	C	801	3AT	C5-C4-N3	-4.72	120.22	126.72
7	C	801	3AT	N3-C4-N9	4.66	135.09	127.17
7	D	800	3AT	N3-C4-N9	4.42	134.68	127.17
7	D	800	3AT	C5-C4-N3	-4.29	120.81	126.72
7	C	801	3AT	C2-N3-C4	4.17	122.02	111.83
7	D	800	3AT	C2-N3-C4	3.94	121.45	111.83
7	D	800	3AT	C5-N7-C8	3.10	108.33	103.45
7	C	801	3AT	C5-N7-C8	3.08	108.28	103.45
7	D	800	3AT	C2-N1-C6	2.86	123.43	118.73
7	C	801	3AT	O4'-C1'-C2'	-2.76	103.91	106.51
6	C	600	U5P	O3'-C3'-C2'	-2.74	103.02	111.82
7	C	801	3AT	O4'-C4'-C3'	2.67	108.45	105.07
7	C	801	3AT	O4'-C1'-N9	2.48	112.85	108.09
7	C	801	3AT	C2-N1-C6	2.47	122.80	118.73
7	D	800	3AT	O4'-C1'-N9	2.46	112.82	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	602	U5P	O3'-C3'-C2'	-2.15	104.91	111.82

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	600	U5P	C4'-C5'-O5'-P
6	D	602	U5P	C2'-C1'-N1-C2
6	D	602	U5P	C2'-C1'-N1-C6
7	C	801	3AT	PB-O3B-PG-O3G
7	C	801	3AT	C3'-C4'-C5'-O5'
7	D	800	3AT	PB-O3B-PG-O3G
7	D	800	3AT	O4'-C4'-C5'-O5'
7	D	800	3AT	C3'-C4'-C5'-O5'
7	C	801	3AT	O4'-C4'-C5'-O5'
7	C	801	3AT	C5'-O5'-PA-O1A
7	C	801	3AT	C5'-O5'-PA-O2A
7	C	801	3AT	C5'-O5'-PA-O3A
7	D	800	3AT	C5'-O5'-PA-O1A
7	D	800	3AT	C5'-O5'-PA-O2A
7	D	800	3AT	C5'-O5'-PA-O3A
6	D	602	U5P	O4'-C1'-N1-C6
6	D	602	U5P	O4'-C1'-N1-C2
7	C	801	3AT	PA-O3A-PB-O2B
7	D	800	3AT	PA-O3A-PB-O2B

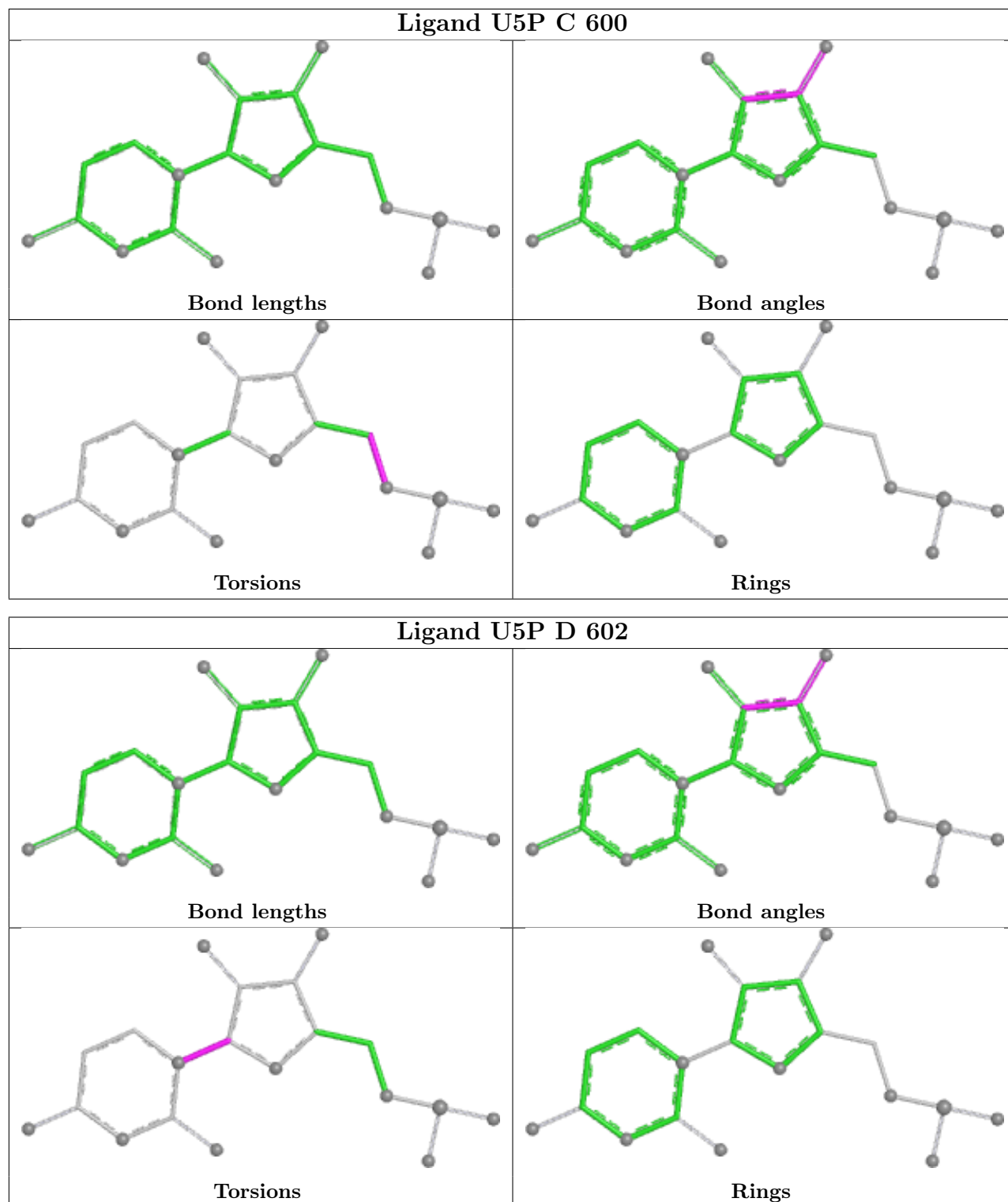
There are no ring outliers.

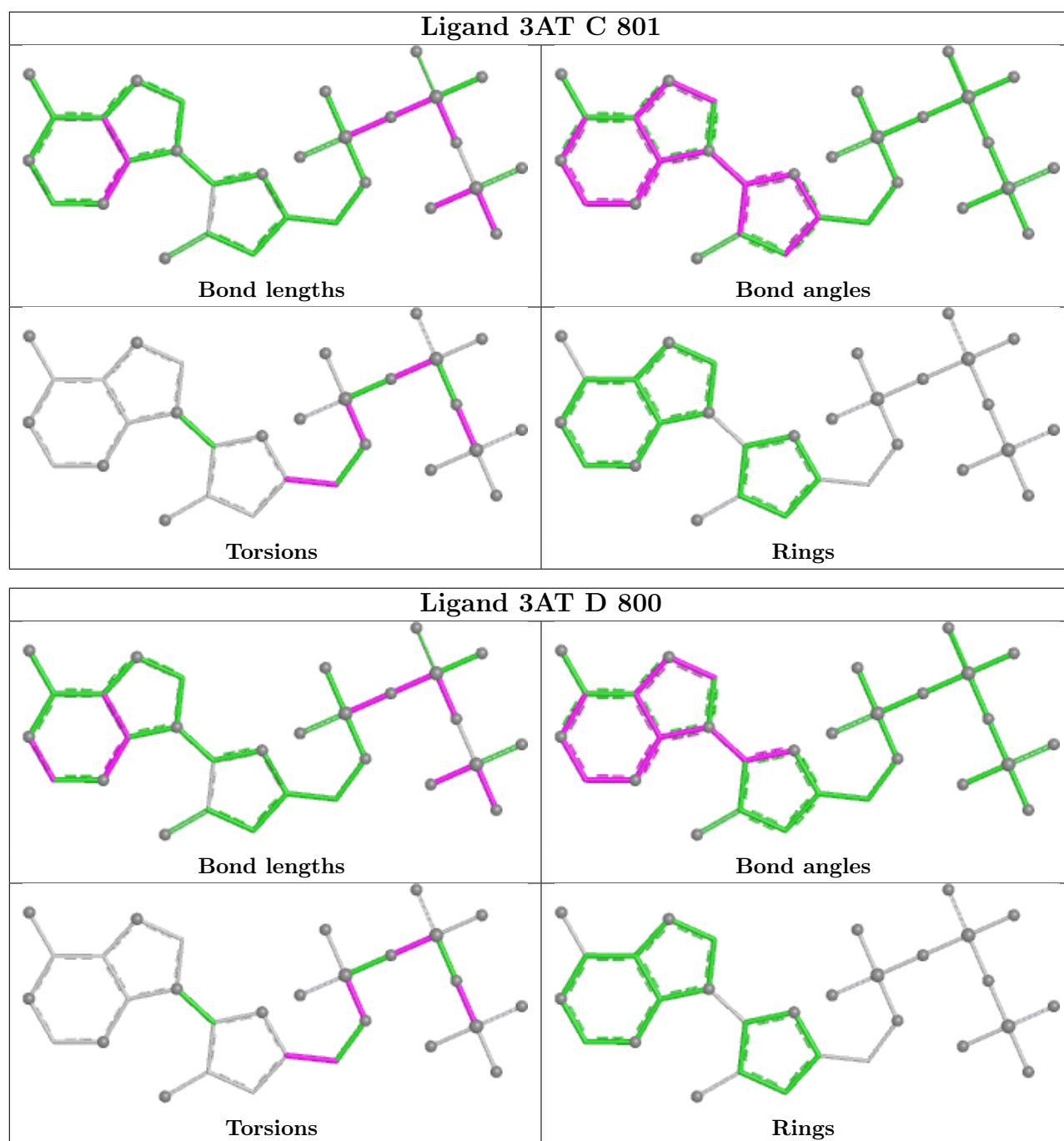
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	600	U5P	3	0
6	D	602	U5P	3	0
7	C	801	3AT	3	0
7	D	800	3AT	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.35	0 100 100	41, 68, 94, 133	0
1	B	288/297 (96%)	-0.31	0 100 100	41, 66, 93, 124	0
2	C	445/479 (92%)	-0.15	1 (0%) 91 85	47, 90, 123, 156	0
2	D	445/479 (92%)	-0.05	0 100 100	41, 94, 130, 162	0
3	E	5/5 (100%)	-0.10	0 100 100	101, 102, 150, 157	0
3	F	5/5 (100%)	-0.21	0 100 100	97, 100, 138, 157	0
4	G	4/4 (100%)	0.13	0 100 100	81, 97, 119, 122	0
5	I	5/5 (100%)	-0.06	0 100 100	95, 101, 116, 116	0
All	All	1485/1571 (94%)	-0.19	1 (0%) 92 89	41, 82, 122, 162	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	91	ILE	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

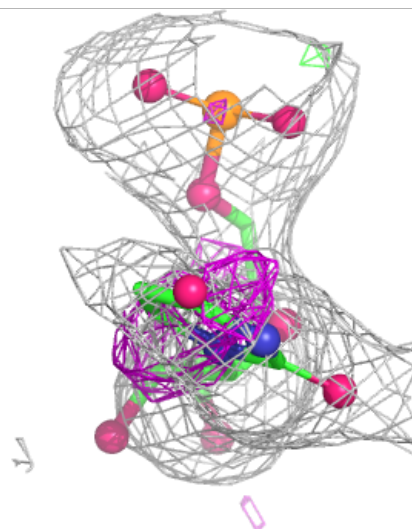
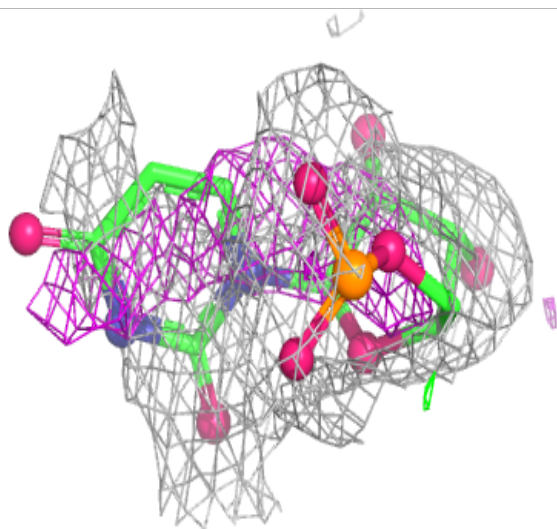
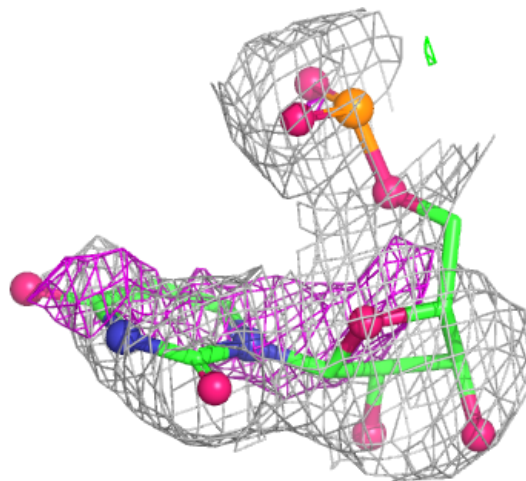
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U5P	D	602	20/21	0.76	0.12	79,79,79,79	0
6	U5P	C	600	20/21	0.77	0.11	79,79,79,79	0
8	CA	C	901	1/1	0.87	0.07	79,79,79,79	0
7	3AT	D	800	30/30	0.93	0.09	79,108,108,108	0
7	3AT	C	801	30/30	0.94	0.08	79,93,97,97	0
8	CA	C	902	1/1	0.94	0.05	79,79,79,79	0
8	CA	D	903	1/1	0.95	0.05	79,79,79,79	0
8	CA	D	904	1/1	0.98	0.04	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

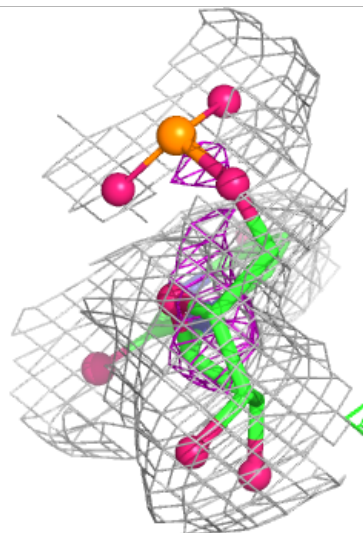
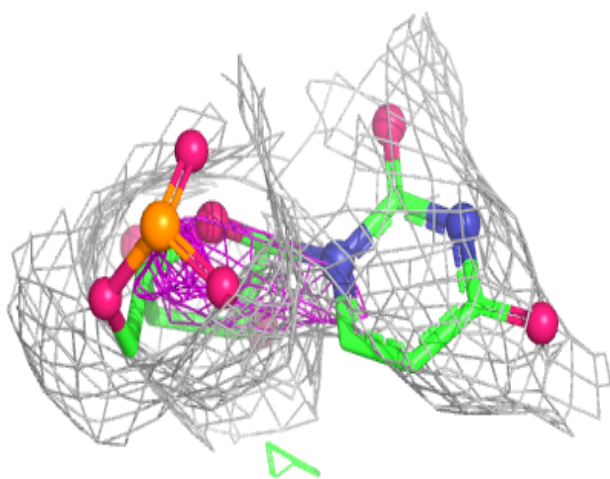
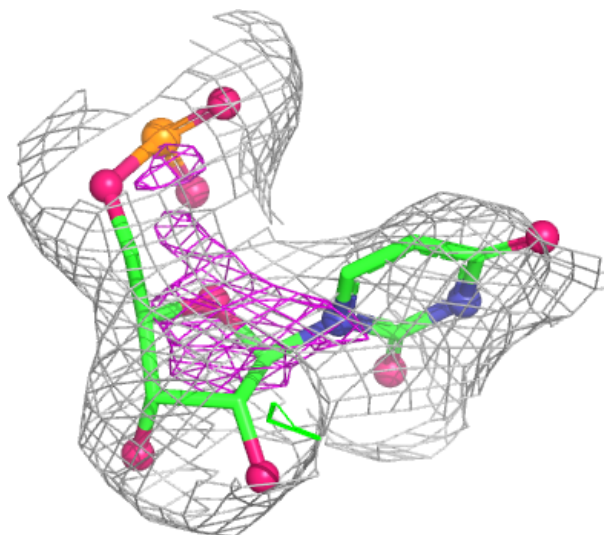
Electron density around U5P D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



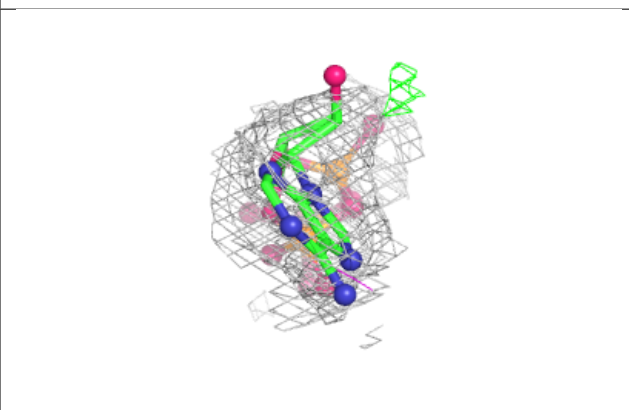
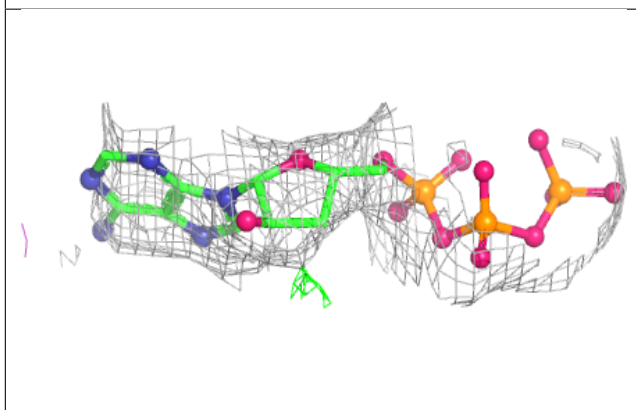
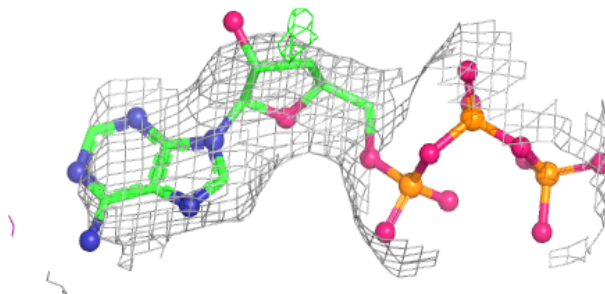
Electron density around U5P C 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

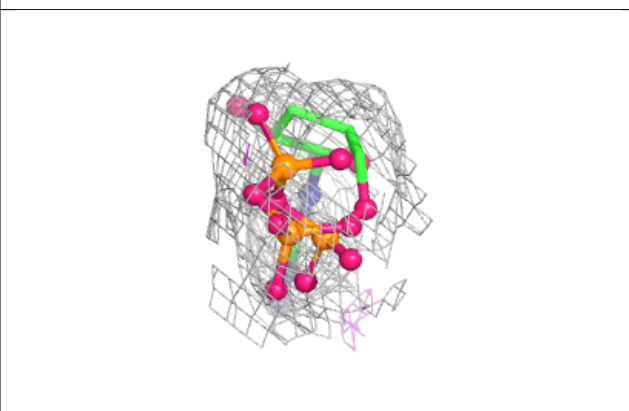
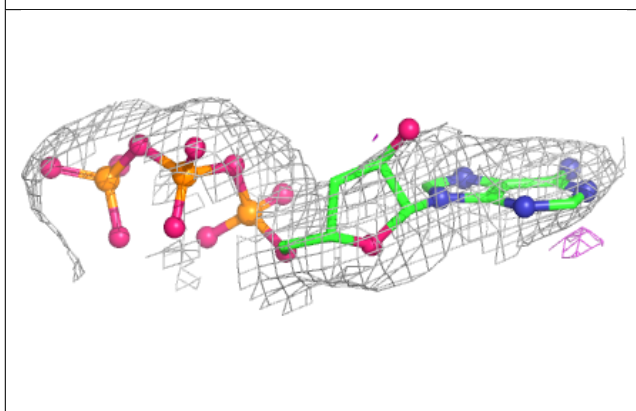
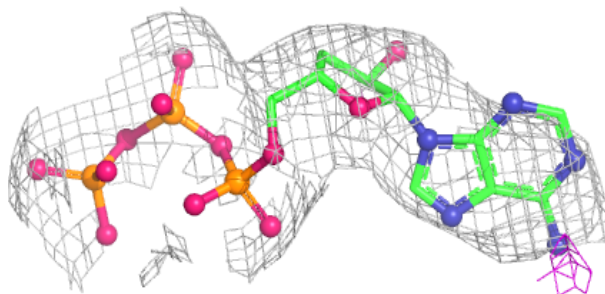


Electron density around 3AT D 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 3AT C 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.