



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:11 AM UTC

PDB ID : 5X2B / pdb_00005x2b
Title : Crystal structure of mouse sulfotransferase SULT7A1 complexed with PAP
Authors : Kanekiyo, M.; Teramoto, T.; Kakuta, Y.
Deposited on : 2017-01-31
Resolution : 2.08 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)
Xtriage (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

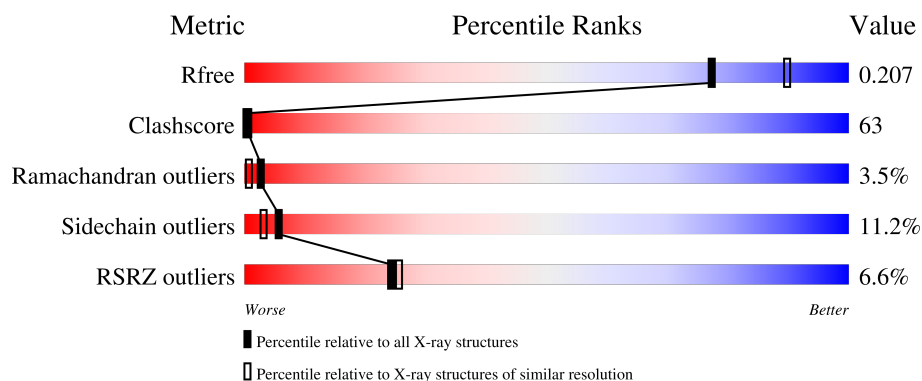
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	283	8% 25% 59% 14% ..
1	B	283	5% 30% 56% 11% .
1	C	283	8% 25% 57% 17% .
1	E	283	5% 29% 53% 15% ..
1	I	283	6% 30% 52% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	283	
1	L	283	
2	D	281	
3	F	282	
3	G	282	
3	H	282	
3	J	282	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A3P	A	301	-	-	X	-
4	A3P	D	301	-	-	X	-
4	A3P	G	301	-	-	X	-
4	A3P	J	301	-	-	X	-
4	A3P	L	301	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29402 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 Sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	282	Total	C	N	O	S	0	4	0
			2313	1485	384	431	13			
1	A	281	Total	C	N	O	S	0	1	0
			2293	1472	383	426	12			
1	B	275	Total	C	N	O	S	0	3	0
			2272	1463	376	422	11			
1	E	277	Total	C	N	O	S	0	1	0
			2264	1456	378	418	12			
1	I	277	Total	C	N	O	S	0	1	0
			2261	1453	377	419	12			
1	K	281	Total	C	N	O	S	0	4	0
			2316	1487	388	429	12			
1	L	283	Total	C	N	O	S	0	5	0
			2327	1494	387	433	13			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ALA	-	expression tag	UNP B7ZWN4
C	263	GLY	VAL	conflict	UNP B7ZWN4
C	288	ALA	-	expression tag	UNP B7ZWN4
A	6	ALA	-	expression tag	UNP B7ZWN4
A	263	GLY	VAL	conflict	UNP B7ZWN4
A	288	ALA	-	expression tag	UNP B7ZWN4
B	6	ALA	-	expression tag	UNP B7ZWN4
B	263	GLY	VAL	conflict	UNP B7ZWN4
B	288	ALA	-	expression tag	UNP B7ZWN4
E	6	ALA	-	expression tag	UNP B7ZWN4
E	263	GLY	VAL	conflict	UNP B7ZWN4
E	288	ALA	-	expression tag	UNP B7ZWN4
I	6	ALA	-	expression tag	UNP B7ZWN4
I	263	GLY	VAL	conflict	UNP B7ZWN4
I	288	ALA	-	expression tag	UNP B7ZWN4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	6	ALA	-	expression tag	UNP B7ZWN4
K	263	GLY	VAL	conflict	UNP B7ZWN4
K	288	ALA	-	expression tag	UNP B7ZWN4
L	6	ALA	-	expression tag	UNP B7ZWN4
L	263	GLY	VAL	conflict	UNP B7ZWN4
L	288	ALA	-	expression tag	UNP B7ZWN4

- Molecule 2 is a protein called Sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	276	Total	C	N	O	S	0	2	0
			2266	1455	378	421	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	8	ALA	-	expression tag	UNP B7ZWN4
D	9	ILE	-	expression tag	UNP B7ZWN4
D	263	GLY	VAL	conflict	UNP B7ZWN4
D	288	ALA	-	expression tag	UNP B7ZWN4

- Molecule 3 is a protein called Sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	279	Total	C	N	O	S	0	2	0
			2277	1465	378	423	11			
3	G	276	Total	C	N	O	S	0	2	0
			2264	1454	377	421	12			
3	H	278	Total	C	N	O	S	0	1	0
			2265	1457	377	420	11			
3	J	274	Total	C	N	O	S	0	2	0
			2249	1448	373	417	11			

There are 8 discrepancies between the modelled and reference sequences:

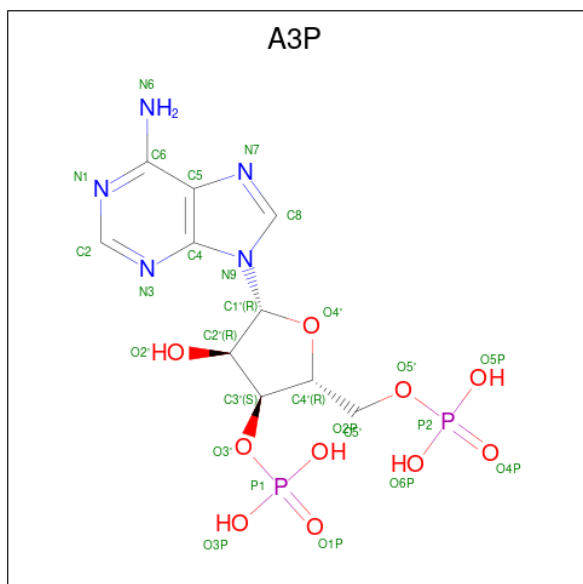
Chain	Residue	Modelled	Actual	Comment	Reference
F	263	GLY	VAL	conflict	UNP B7ZWN4
F	288	ALA	-	expression tag	UNP B7ZWN4
G	263	GLY	VAL	conflict	UNP B7ZWN4
G	288	ALA	-	expression tag	UNP B7ZWN4
H	263	GLY	VAL	conflict	UNP B7ZWN4
H	288	ALA	-	expression tag	UNP B7ZWN4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	263	GLY	VAL	conflict	UNP B7ZWN4
J	288	ALA	-	expression tag	UNP B7ZWN4

- Molecule 4 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

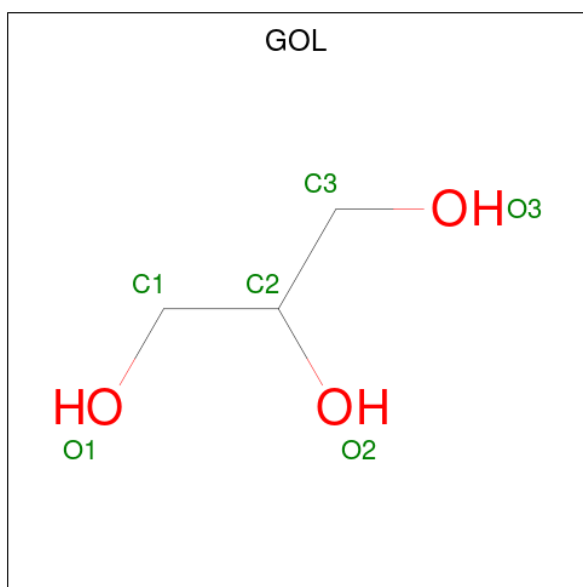
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	A	2	Total	Ca	0	0
			2	2		
5	B	3	Total	Ca	0	0
			3	3		
5	D	3	Total	Ca	0	0
			3	3		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	G	2	Total	Ca	0	0
			2	2		
5	H	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	J	2	Total	Ca	0	0
			2	2		
5	K	2	Total	Ca	0	0
			2	2		
5	L	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	126	Total	O	0	0
			126	126		
7	A	149	Total	O	0	0
			149	149		
7	B	151	Total	O	0	0
			151	151		
7	D	169	Total	O	0	0
			169	169		
7	E	136	Total	O	0	0
			136	136		
7	F	108	Total	O	0	0
			108	108		
7	G	172	Total	O	0	0
			172	172		
7	H	131	Total	O	0	0
			131	131		
7	I	131	Total	O	0	0
			131	131		
7	J	157	Total	O	0	0
			157	157		

Continued on next page...

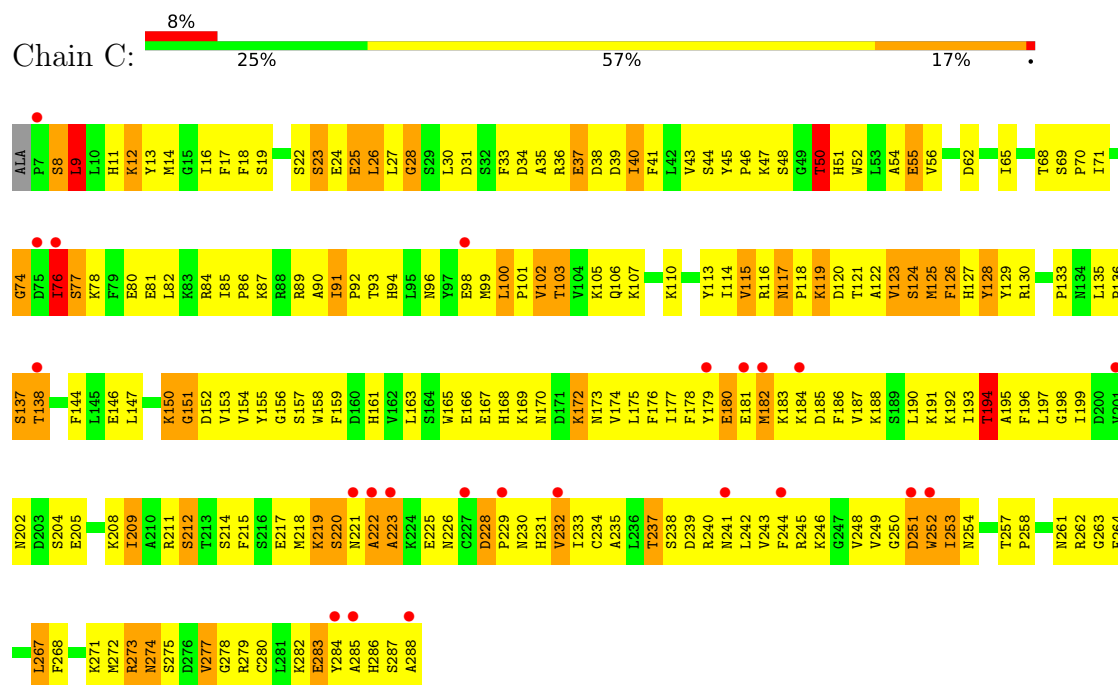
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	151	Total 151	O 151	0	0
7	L	98	Total 98	O 98	0	0

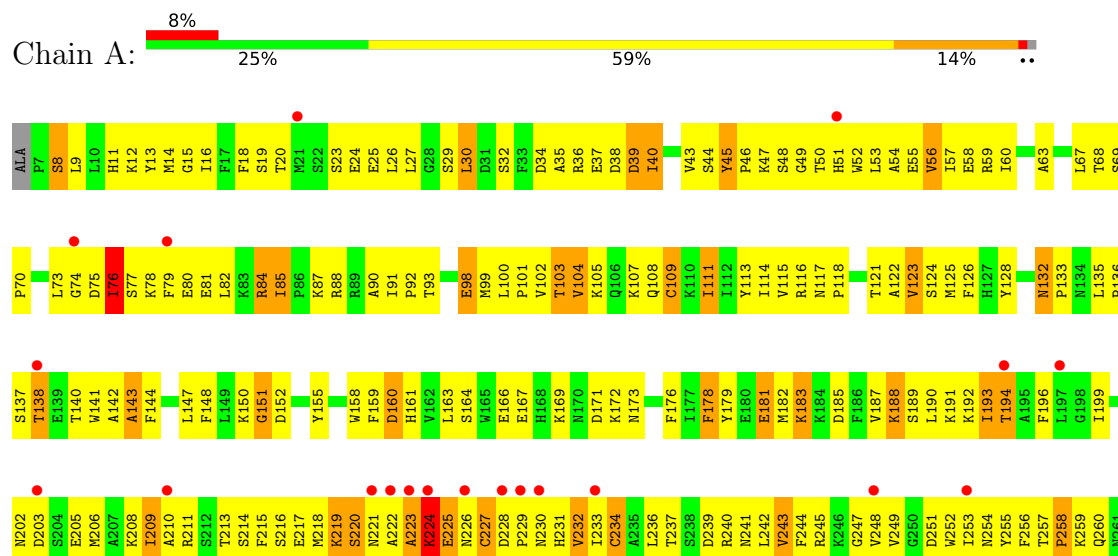
3 Residue-property plots

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: Sulfotransferase

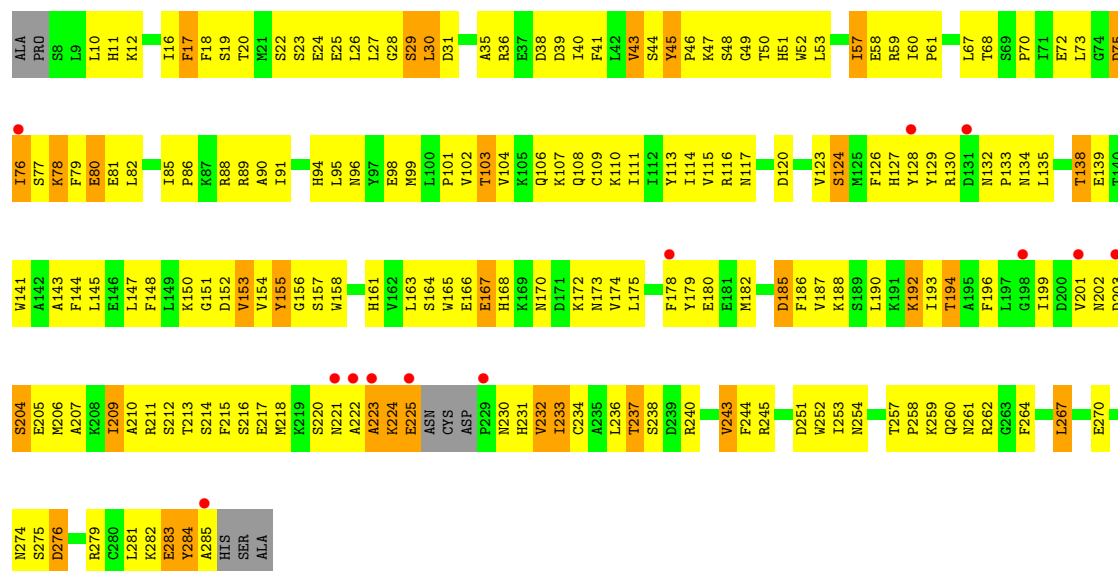


• Molecule 1: Sulfotransferase

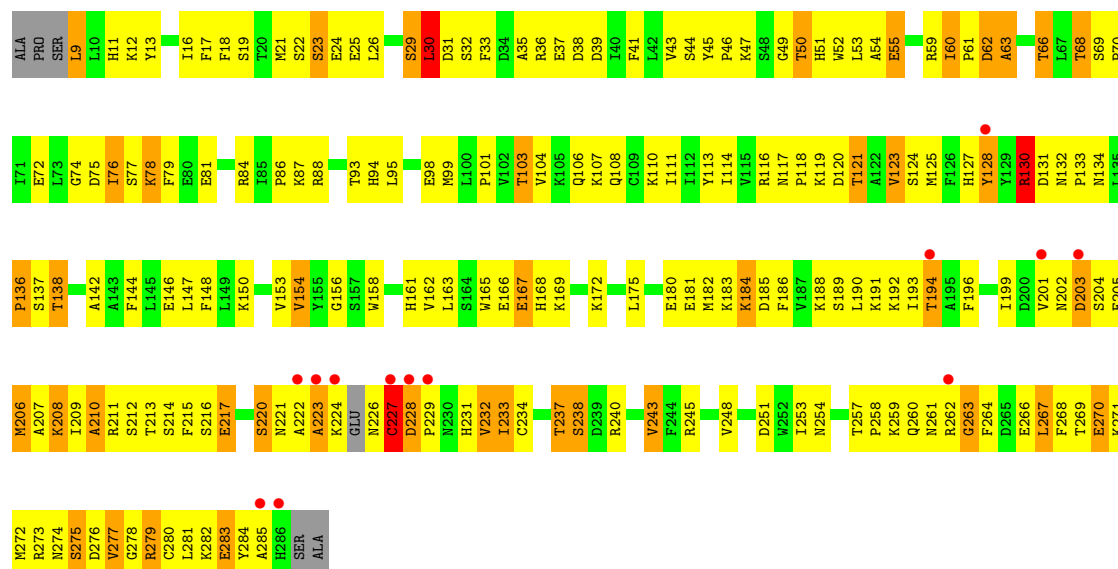




• Molecule 1: Sulfotransferase

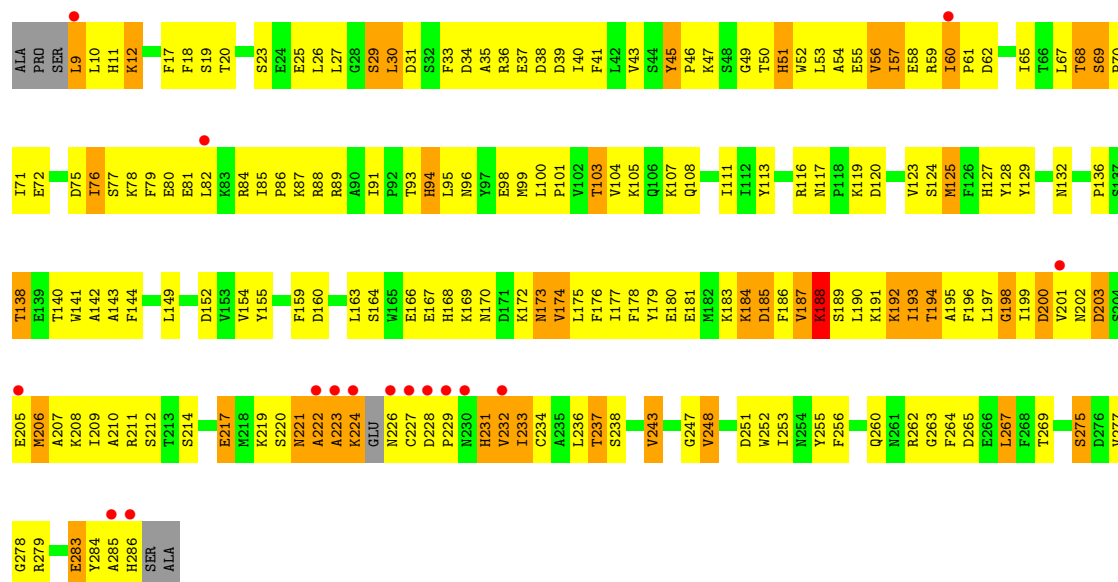


• Molecule 1: Sulfotransferase

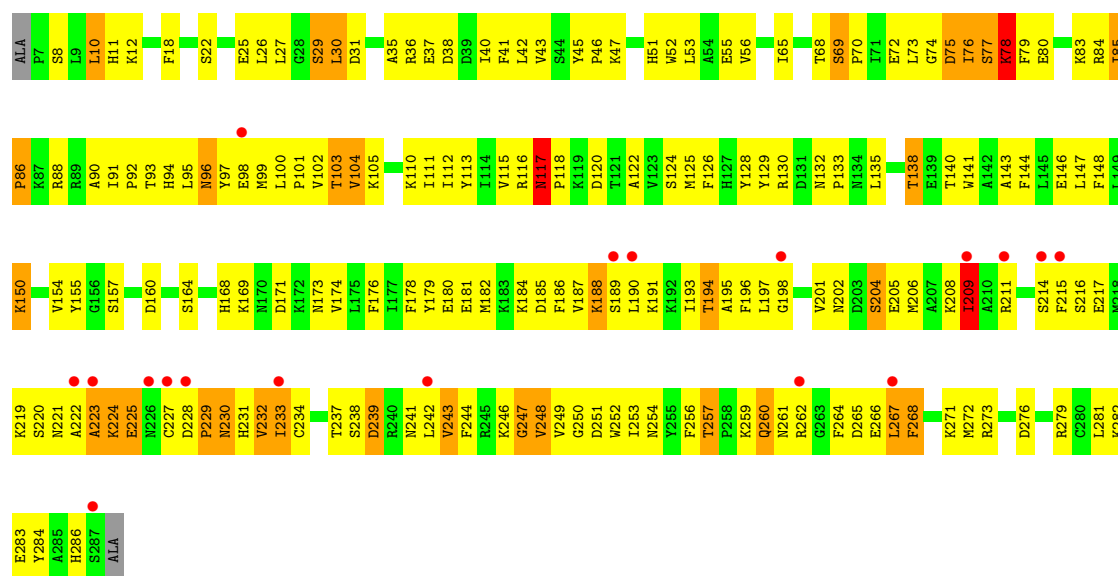


• Molecule 1: Sulfotransferase

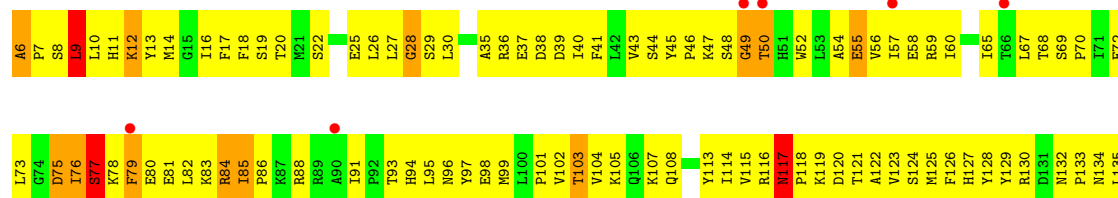


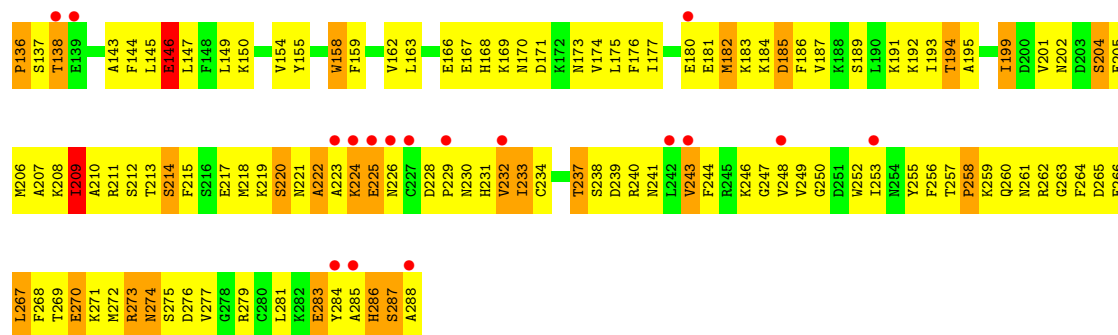


• Molecule 1: Sulfotransferase

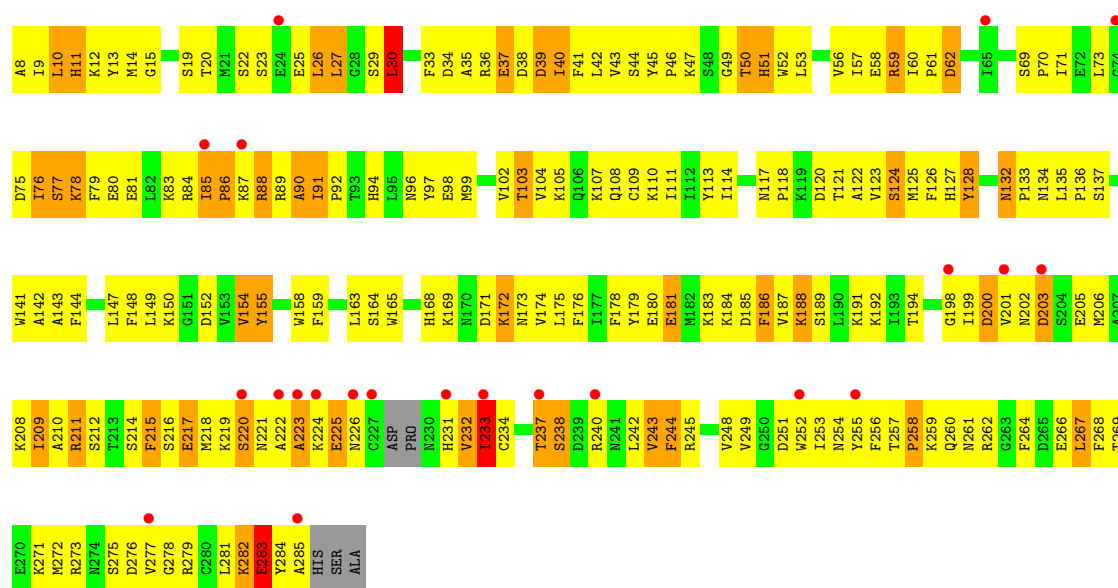


• Molecule 1: Sulfotransferase

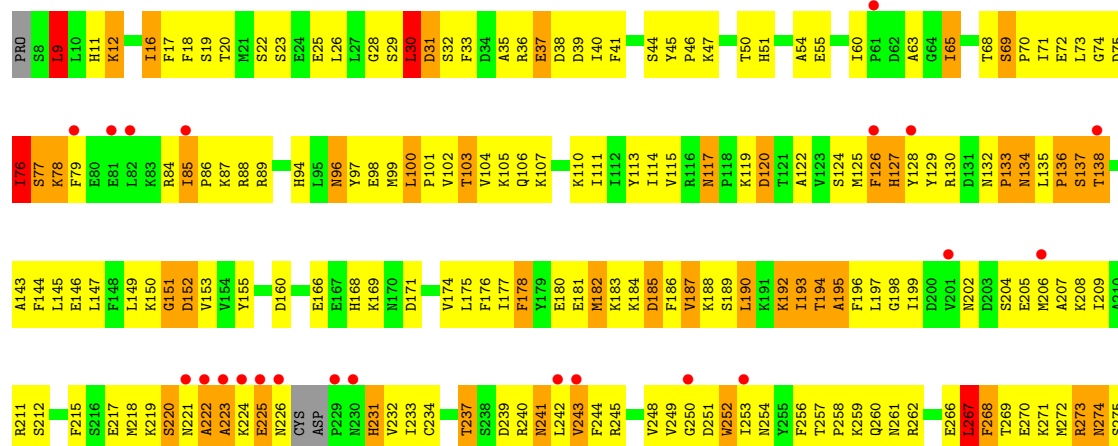


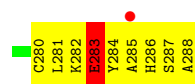


• Molecule 2: Sulfotransferase

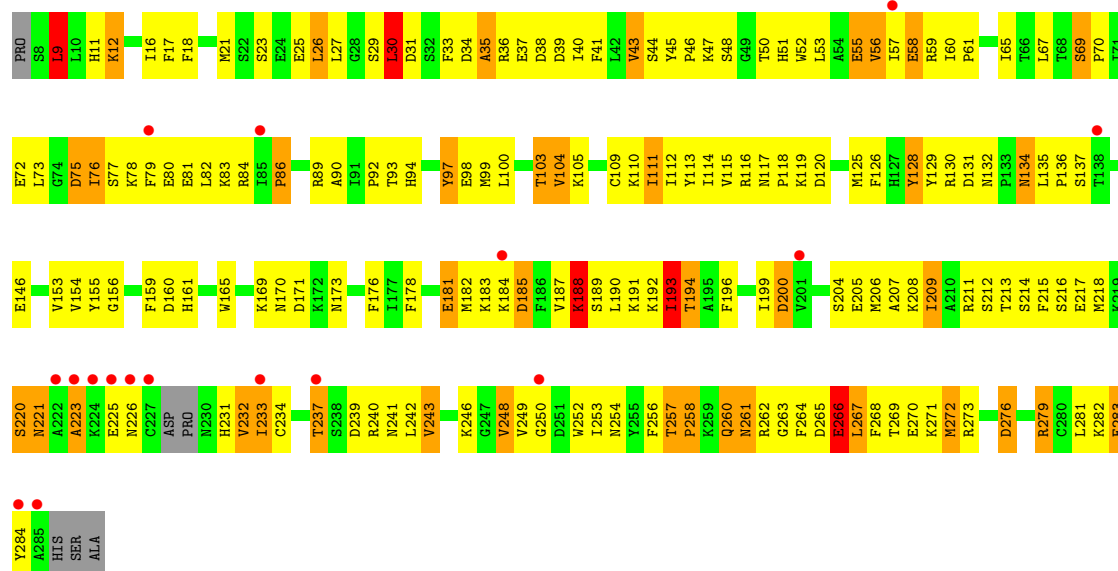


• Molecule 3: Sulfotransferase

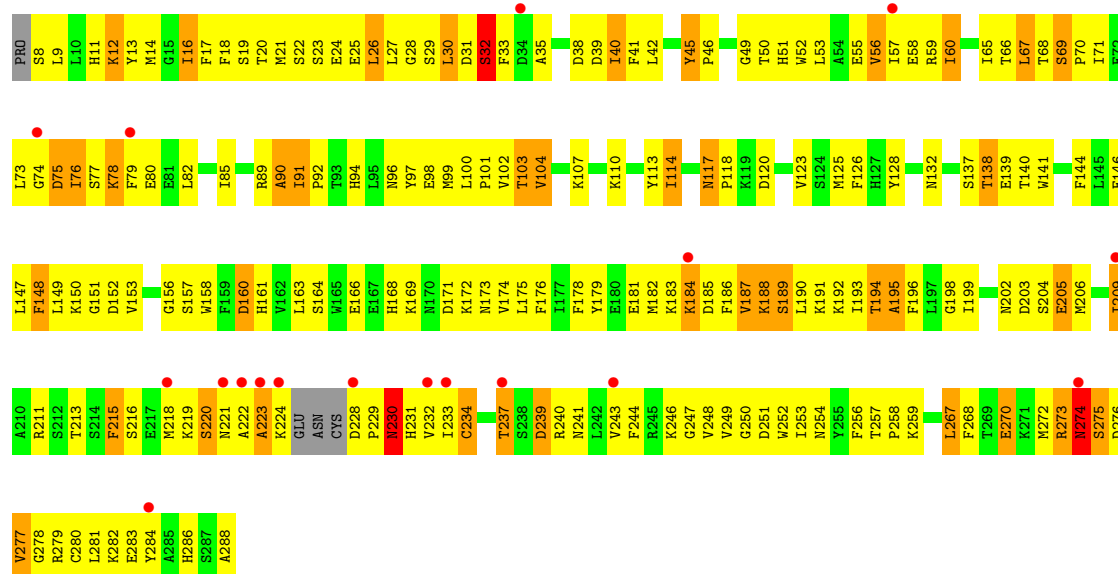




• Molecule 3: Sulfotransferase



• Molecule 3: Sulfotransferase



• Molecule 3: Sulfotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	166.17Å 81.13Å 166.18Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.08 50.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.08) 99.5 (50.00-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.236 (Not available) , 0.207	Depositor DCC
R_{free} test set	11949 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.000 for h,-k,-h-l 0.248 for -h-l,-k,l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.907 for H, K, L 0.093 for H+L, -K, -L	Depositor
Outliers	11 of 229863 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29402	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5363e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, GOL, 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	1.18	4/2350 (0.2%)	1.32	24/3173 (0.8%)
1	B	1.20	4/2327 (0.2%)	1.26	11/3138 (0.4%)
1	C	1.24	4/2379 (0.2%)	1.32	26/3211 (0.8%)
1	E	1.25	5/2318 (0.2%)	1.32	19/3127 (0.6%)
1	I	1.28	8/2315 (0.3%)	1.31	17/3124 (0.5%)
1	K	1.17	4/2379 (0.2%)	1.29	18/3210 (0.6%)
1	L	1.17	5/2393 (0.2%)	1.27	17/3230 (0.5%)
2	D	1.20	7/2319 (0.3%)	1.31	21/3128 (0.7%)
3	F	1.19	5/2337 (0.2%)	1.33	24/3153 (0.8%)
3	G	1.22	7/2320 (0.3%)	1.34	23/3129 (0.7%)
3	H	1.18	6/2319 (0.3%)	1.25	10/3130 (0.3%)
3	J	1.32	8/2306 (0.3%)	1.35	20/3110 (0.6%)
All	All	1.22	67/28062 (0.2%)	1.31	230/37863 (0.6%)

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	91	ILE	CA-CB	-9.39	1.46	1.54
3	J	65	ILE	CA-CB	-8.52	1.43	1.54
1	C	91	ILE	CA-CB	-7.90	1.47	1.54
1	B	90	ALA	CA-CB	-7.29	1.43	1.53
3	H	90	ALA	CA-CB	-7.17	1.43	1.53
3	J	123	VAL	CA-CB	7.16	1.62	1.54
1	L	185	ASP	CA-C	-6.99	1.47	1.53
3	F	185	ASP	CA-C	-6.96	1.43	1.53
3	H	40	ILE	CA-CB	-6.50	1.46	1.54
3	H	91	ILE	CA-C	-6.26	1.47	1.52
3	J	277	VAL	CA-CB	-6.25	1.46	1.54
3	G	65	ILE	CA-CB	-6.24	1.46	1.54
1	I	185	ASP	CA-C	-6.22	1.46	1.53
1	B	185	ASP	CA-C	-6.18	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	ILE	CA-CB	-6.14	1.46	1.54
1	L	127	HIS	CA-C	-6.14	1.44	1.52
3	F	269	THR	CA-CB	-6.12	1.43	1.53
3	G	266	GLU	CA-C	-6.00	1.45	1.52
1	K	209	ILE	CA-CB	-5.98	1.47	1.54
3	J	276	ASP	CA-C	-5.94	1.45	1.52
1	E	130	ARG	N-CA	-5.94	1.38	1.46
3	G	232	VAL	CA-CB	-5.88	1.47	1.54
1	B	17	PHE	CA-C	-5.84	1.45	1.52
1	C	102	VAL	CA-CB	-5.76	1.47	1.54
3	J	79	PHE	CA-C	-5.74	1.45	1.52
1	I	255	TYR	CA-C	-5.70	1.45	1.52
3	H	104	VAL	CA-CB	-5.63	1.46	1.54
1	I	127	HIS	CA-C	-5.62	1.44	1.52
3	G	261	ASN	N-CA	-5.61	1.39	1.46
2	D	244	PHE	CA-C	-5.60	1.47	1.53
1	K	260	GLN	CA-C	-5.60	1.45	1.52
1	E	88	ARG	CA-C	-5.56	1.45	1.52
2	D	39	ASP	CA-C	-5.56	1.46	1.52
1	L	255	TYR	CA-C	-5.53	1.46	1.52
1	E	270	GLU	N-CA	-5.51	1.39	1.46
2	D	174	VAL	CA-CB	-5.49	1.47	1.54
1	I	51	HIS	CA-C	-5.48	1.45	1.52
3	G	193	ILE	CA-C	-5.45	1.45	1.52
3	F	16	ILE	CA-C	-5.44	1.46	1.52
3	J	185	ASP	CA-C	-5.40	1.47	1.53
1	C	40	ILE	CA-CB	-5.38	1.46	1.55
1	K	157	SER	CA-C	-5.36	1.45	1.52
1	A	40	ILE	CA-CB	-5.34	1.47	1.54
1	E	136	PRO	CA-C	-5.33	1.47	1.52
3	H	91	ILE	N-CA	-5.26	1.41	1.46
2	D	39	ASP	CB-CG	-5.26	1.38	1.52
1	L	40	ILE	CA-CB	-5.25	1.48	1.54
1	I	260	GLN	CA-C	-5.22	1.46	1.52
1	A	123	VAL	CA-C	-5.22	1.46	1.52
2	D	90	ALA	CA-CB	-5.19	1.46	1.53
1	A	39	ASP	CA-C	-5.17	1.46	1.52
3	G	185	ASP	CA-C	-5.15	1.45	1.52
1	I	40	ILE	CA-CB	-5.15	1.48	1.54
3	G	276	ASP	CA-C	-5.14	1.46	1.52
1	C	91	ILE	N-CA	-5.13	1.41	1.46
1	K	10	LEU	CA-C	5.12	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	260	GLN	CA-C	-5.12	1.46	1.52
2	D	90	ALA	CA-C	-5.10	1.46	1.52
1	B	91	ILE	CA-CB	-5.09	1.48	1.53
1	E	121	THR	N-CA	-5.08	1.40	1.46
1	L	91	ILE	CA-C	-5.05	1.49	1.53
1	I	91	ILE	CA-CB	-5.05	1.50	1.54
3	J	31	ASP	CA-C	-5.04	1.45	1.52
1	I	187	VAL	CA-CB	-5.03	1.48	1.54
3	F	122	ALA	CA-CB	-5.03	1.45	1.53
3	F	127	HIS	CA-C	-5.03	1.45	1.52
1	A	76	ILE	CA-C	5.00	1.59	1.52

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	74	GLY	N-CA-C	13.92	125.62	111.56
1	A	74	GLY	N-CA-C	11.90	123.58	111.56
1	L	85	ILE	CA-C-N	9.83	132.12	119.84
1	L	85	ILE	C-N-CA	9.83	132.12	119.84
3	J	210	ALA	N-CA-C	-9.64	99.54	111.11
2	D	91	ILE	CA-C-N	9.26	131.42	119.84
2	D	91	ILE	C-N-CA	9.26	131.42	119.84
3	H	60	ILE	CA-C-N	9.00	129.35	119.90
3	H	60	ILE	C-N-CA	9.00	129.35	119.90
1	K	117	ASN	CA-C-N	8.95	128.60	119.56
1	K	117	ASN	C-N-CA	8.95	128.60	119.56
1	K	209	ILE	CB-CA-C	-8.79	100.71	111.97
3	H	209	ILE	CB-CA-C	-8.78	100.28	112.14
1	C	277	VAL	N-CA-C	-8.76	102.29	110.53
1	K	268	PHE	N-CA-C	-8.73	101.77	111.28
3	J	209	ILE	CB-CA-C	-8.62	101.03	111.81
3	F	104	VAL	N-CA-C	-8.36	101.88	111.00
3	J	82	LEU	N-CA-C	-8.28	102.21	111.07
1	I	206	MET	N-CA-C	-8.09	102.41	111.07
3	F	96	ASN	N-CA-C	-8.08	100.10	110.53
3	J	206	MET	N-CA-C	-8.07	101.17	111.02
1	A	45	TYR	N-CA-C	-8.00	99.67	109.83
3	F	268	PHE	N-CA-C	-7.94	102.56	111.14
1	E	60	ILE	N-CA-C	7.85	115.38	108.63
3	J	161	HIS	N-CA-C	-7.70	102.97	111.36
3	G	257	THR	CA-C-N	7.65	129.40	119.84
3	G	257	THR	C-N-CA	7.65	129.40	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	LEU	CA-C-N	7.56	128.02	119.93
1	C	100	LEU	C-N-CA	7.56	128.02	119.93
1	E	206	MET	N-CA-C	-7.47	103.08	111.07
3	J	281	LEU	N-CA-C	-7.37	103.24	111.28
1	A	181	GLU	N-CA-C	-7.25	103.41	111.82
1	A	183	LYS	N-CA-C	-7.17	103.39	111.07
3	J	257	THR	N-CA-C	-7.17	100.39	110.29
3	F	151	GLY	N-CA-C	-7.15	106.10	115.47
3	G	207	ALA	N-CA-C	-7.08	103.56	111.28
1	A	100	LEU	CA-C-N	7.04	127.46	119.93
1	A	100	LEU	C-N-CA	7.04	127.46	119.93
1	L	82	LEU	N-CA-C	-7.03	103.55	111.07
1	B	58	GLU	N-CA-C	-6.98	104.64	113.01
1	I	60	ILE	CA-C-N	6.94	128.52	119.84
1	I	60	ILE	C-N-CA	6.94	128.52	119.84
1	C	180	GLU	N-CA-C	-6.94	102.56	111.02
3	F	100	LEU	CA-C-N	6.89	128.46	119.84
3	F	100	LEU	C-N-CA	6.89	128.46	119.84
3	F	211	ARG	N-CA-C	-6.86	103.73	111.14
1	E	277	VAL	N-CA-C	6.80	117.50	110.36
3	J	55	GLU	N-CA-C	-6.79	103.95	111.36
3	G	40	ILE	CB-CA-C	-6.79	101.13	110.77
3	J	75	ASP	CB-CA-C	-6.79	102.44	113.37
1	L	79	PHE	N-CA-C	6.72	118.69	111.36
1	C	85	ILE	CA-C-N	6.71	126.66	119.28
1	C	85	ILE	C-N-CA	6.71	126.66	119.28
1	K	160	ASP	N-CA-C	-6.71	103.44	111.69
1	I	188	LYS	N-CA-C	-6.68	103.10	111.11
2	D	51	HIS	N-CA-C	-6.63	103.97	111.07
3	F	60	ILE	CA-C-N	6.62	126.85	119.90
3	F	60	ILE	C-N-CA	6.62	126.85	119.90
3	G	45	TYR	N-CA-C	-6.57	100.65	110.24
1	L	209	ILE	CB-CA-C	-6.56	100.53	111.29
1	L	193	ILE	CB-CA-C	-6.56	103.28	111.94
3	F	63	ALA	N-CA-C	-6.55	105.29	113.28
1	B	204	SER	N-CA-C	-6.51	103.30	111.11
1	C	102	VAL	CB-CA-C	-6.51	103.52	112.04
3	G	111	ILE	CB-CA-C	-6.46	100.89	110.33
1	L	158	TRP	N-CA-C	-6.46	104.24	111.28
1	C	209	ILE	CB-CA-C	-6.45	103.32	112.22
1	K	122	ALA	N-CA-C	-6.45	104.17	111.07
1	C	25	GLU	N-CA-C	-6.43	104.19	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	141	TRP	N-CA-C	-6.42	104.21	111.14
3	H	193	ILE	CB-CA-C	-6.42	103.61	112.02
3	F	190	LEU	N-CA-C	6.38	118.32	111.36
3	G	260	GLN	N-CA-C	-6.37	104.38	111.71
3	G	199	ILE	N-CA-C	6.34	117.92	108.54
1	E	193	ILE	CB-CA-C	-6.32	103.61	112.14
3	G	46	PRO	CA-C-O	-6.32	114.35	121.43
1	K	43	VAL	N-CA-C	6.29	116.98	108.17
1	K	78	LYS	N-CA-C	-6.29	104.35	111.14
3	F	45	TYR	N-CA-C	-6.29	100.96	110.39
1	E	62	ASP	N-CA-C	-6.28	102.80	111.28
2	D	111	ILE	CB-CA-C	-6.28	101.34	110.63
1	I	194	THR	N-CA-C	-6.28	103.58	111.11
3	F	267	LEU	N-CA-C	-6.24	104.58	111.82
1	B	209	ILE	CB-CA-C	-6.20	103.77	112.14
1	B	91	ILE	N-CA-C	6.18	114.21	107.60
1	E	68	THR	N-CA-C	6.17	118.84	109.95
3	G	55	GLU	N-CA-C	-6.16	104.48	111.07
3	G	257	THR	N-CA-C	-6.14	102.36	110.40
3	J	241	ASN	N-CA-C	-6.14	104.65	111.71
3	H	195	ALA	N-CA-C	6.13	118.76	111.71
1	C	172	LYS	N-CA-C	6.10	117.93	111.28
1	E	69	SER	CA-C-N	-6.09	113.70	119.85
1	E	69	SER	C-N-CA	-6.09	113.70	119.85
1	B	124	SER	N-CA-C	-6.07	104.67	111.28
1	C	65	ILE	N-CA-C	6.05	116.64	108.17
3	F	134	ASN	N-CA-C	-6.05	104.75	111.71
2	D	132	ASN	CA-C-N	6.05	125.67	119.56
2	D	132	ASN	C-N-CA	6.05	125.67	119.56
1	A	178	PHE	N-CA-C	6.03	118.55	108.96
1	A	193	ILE	CB-CA-C	-5.99	104.06	112.14
1	L	146	GLU	N-CA-C	-5.98	104.84	111.36
2	D	233	ILE	CA-C-N	-5.97	114.58	123.00
2	D	233	ILE	C-N-CA	-5.97	114.58	123.00
1	A	143	ALA	N-CA-C	-5.96	104.69	111.07
3	G	188	LYS	N-CA-C	-5.95	105.52	112.89
2	D	211	ARG	N-CA-C	-5.94	104.49	110.97
1	B	126	PHE	N-CA-C	-5.93	104.89	111.71
1	L	143	ALA	N-CA-C	-5.93	103.79	111.02
1	I	198	GLY	N-CA-C	-5.92	104.84	113.48
2	D	85	ILE	CA-C-N	5.91	125.61	119.64
2	D	85	ILE	C-N-CA	5.91	125.61	119.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	GLY	N-CA-C	5.90	117.52	111.56
1	E	131	ASP	N-CA-C	5.88	120.29	113.18
1	I	94	HIS	N-CA-C	-5.87	106.03	112.72
1	K	104	VAL	CB-CA-C	-5.86	104.23	112.14
1	I	40	ILE	CB-CA-C	-5.84	102.12	110.83
3	J	32	SER	N-CA-C	-5.84	106.14	113.20
2	D	186	PHE	N-CA-C	5.81	117.31	110.97
1	B	80	GLU	N-CA-C	-5.81	104.86	111.07
3	G	279	ARG	N-CA-C	-5.81	104.87	111.14
1	L	199	ILE	N-CA-C	5.81	116.51	107.28
1	E	277	VAL	CB-CA-C	-5.80	104.45	111.88
1	E	210	ALA	N-CA-C	-5.79	104.33	111.33
3	G	97	TYR	N-CA-C	5.79	117.39	111.14
1	L	9	LEU	N-CA-C	-5.77	106.37	113.41
2	D	104	VAL	CB-CA-C	-5.77	104.35	112.14
1	B	153	VAL	N-CA-C	-5.74	99.48	108.95
1	A	104	VAL	CB-CA-C	-5.72	104.65	111.97
3	J	79	PHE	N-CA-C	-5.71	104.74	110.97
3	F	192	LYS	N-CA-C	-5.69	104.98	111.07
3	J	239	ASP	N-CA-C	5.69	119.59	107.70
1	B	45	TYR	N-CA-C	-5.65	102.06	110.20
1	A	224	LYS	N-CA-C	5.65	115.56	108.45
1	I	196	PHE	N-CA-C	-5.65	105.12	111.28
3	G	75	ASP	CB-CA-C	-5.64	99.85	110.51
1	B	27	LEU	N-CA-C	-5.63	105.14	111.28
3	H	193	ILE	N-CA-C	5.63	115.82	110.53
3	J	267	LEU	N-CA-C	-5.63	105.14	111.28
3	F	166	GLU	N-CA-C	-5.62	105.92	112.89
1	A	111	ILE	CB-CA-C	-5.61	102.32	110.63
3	G	56	VAL	N-CA-C	-5.60	104.40	110.23
2	D	269	THR	N-CA-C	-5.59	105.10	111.14
1	L	193	ILE	N-CA-C	5.59	115.83	110.74
3	G	272	MET	N-CA-C	-5.58	106.31	113.23
1	E	55	GLU	N-CA-C	-5.57	104.84	111.69
1	A	132	ASN	CA-C-N	5.56	125.23	119.56
1	A	132	ASN	C-N-CA	5.56	125.23	119.56
1	C	9	LEU	N-CA-C	-5.55	105.62	112.90
1	C	168	HIS	N-CA-C	-5.54	105.21	112.41
1	A	219	LYS	N-CA-C	-5.53	104.48	111.11
3	F	178	PHE	CB-CA-C	-5.52	100.64	109.75
1	E	280	CYS	N-CA-C	5.52	116.97	111.07
1	A	276	ASP	N-CA-C	-5.52	105.35	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	VAL	N-CA-C	-5.51	104.49	110.23
3	H	160	ASP	N-CA-C	-5.50	105.36	111.36
3	F	193	ILE	CB-CA-C	-5.50	104.94	111.81
1	L	55	GLU	N-CA-C	-5.49	105.19	111.07
1	I	193	ILE	N-CA-C	5.48	115.73	110.74
1	I	260	GLN	N-CA-C	-5.48	104.95	111.69
1	I	174	VAL	N-CA-C	5.47	116.35	108.48
2	D	88	ARG	N-CA-C	-5.46	101.96	110.10
1	L	6	ALA	CA-C-N	-5.46	114.08	119.92
1	L	6	ALA	C-N-CA	-5.46	114.08	119.92
3	J	52	TRP	N-CA-C	-5.43	105.05	110.97
1	A	234	CYS	N-CA-C	-5.43	100.39	109.24
3	H	90	ALA	N-CA-C	-5.42	99.68	108.52
3	J	221	ASN	N-CA-C	5.42	122.35	110.80
1	C	55	GLU	N-CA-C	-5.42	105.54	111.82
3	J	45	TYR	N-CA-C	-5.41	102.95	109.83
1	K	193	ILE	CB-CA-C	-5.41	104.95	112.04
1	C	65	ILE	CB-CA-C	-5.41	102.77	110.83
3	F	250	GLY	N-CA-C	5.39	122.77	115.32
1	C	119	LYS	N-CA-C	-5.39	105.06	111.69
1	I	173	ASN	N-CA-C	-5.38	106.75	113.15
1	K	197	LEU	N-CA-C	-5.38	106.56	113.23
1	A	160	ASP	N-CA-C	-5.37	105.09	111.69
3	F	9	LEU	N-CA-C	5.36	122.22	110.80
1	A	227	CYS	N-CA-C	-5.35	100.18	108.42
3	F	120	ASP	N-CA-C	-5.34	105.46	111.28
1	K	143	ALA	N-CA-C	-5.34	105.36	111.07
1	I	192	LYS	N-CA-C	-5.33	105.47	111.28
3	J	174	VAL	N-CA-C	5.33	115.79	108.12
3	F	65	ILE	N-CA-C	5.32	115.51	107.80
3	G	104	VAL	CB-CA-C	-5.32	105.07	112.04
1	E	275	SER	N-CA-C	-5.32	102.04	109.96
2	D	238	SER	N-CA-C	-5.30	105.17	111.69
1	C	115	VAL	N-CA-C	5.29	115.99	108.42
1	C	151	GLY	N-CA-C	-5.29	107.49	115.32
3	H	45	TYR	N-CA-C	-5.28	102.80	110.08
1	E	63	ALA	N-CA-C	-5.26	106.92	113.55
2	D	11	HIS	N-CA-C	5.26	117.24	108.99
3	J	130	ARG	N-CA-C	-5.24	106.40	112.89
1	E	78	LYS	N-CA-C	-5.23	105.66	111.36
3	F	133	PRO	N-CA-C	-5.23	106.22	113.81
1	L	224	LYS	N-CA-C	5.23	116.75	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CA-C-N	-5.22	117.59	123.02
1	A	84	ARG	C-N-CA	-5.22	117.59	123.02
1	I	34	ASP	N-CA-C	5.22	117.13	108.20
3	G	212	SER	N-CA-C	5.22	119.65	113.28
1	C	40	ILE	N-CA-C	5.22	116.88	108.85
1	I	221	ASN	CB-CA-C	-5.21	100.66	110.51
1	C	115	VAL	CB-CA-C	-5.21	101.80	111.18
1	E	133	PRO	N-CA-C	-5.21	107.26	113.98
1	C	166	GLU	N-CA-C	-5.20	106.20	112.54
1	C	263	GLY	N-CA-C	-5.19	106.51	112.73
2	D	134	ASN	N-CA-C	-5.18	106.79	113.01
1	E	66	THR	N-CA-C	-5.18	99.32	108.23
1	K	96	ASN	N-CA-C	-5.17	103.86	110.53
1	C	117	ASN	CA-C-N	5.16	125.61	120.04
1	C	117	ASN	C-N-CA	5.16	125.61	120.04
1	L	117	ASN	N-CA-C	-5.15	102.68	109.84
3	G	35	ALA	N-CA-C	-5.15	103.74	110.53
3	J	31	ASP	N-CA-C	-5.12	106.98	113.18
1	E	270	GLU	N-CA-C	-5.12	104.96	111.11
2	D	27	LEU	N-CA-C	5.12	116.86	111.28
1	B	57	ILE	CB-CA-C	-5.11	105.24	112.14
1	K	257	THR	N-CA-C	-5.11	103.03	110.08
1	K	184	LYS	N-CA-C	5.10	116.53	111.07
1	K	74	GLY	N-CA-C	5.09	120.88	112.84
2	D	86	PRO	N-CA-C	-5.09	107.11	114.18
3	G	134	ASN	N-CA-C	-5.09	106.58	112.89
3	G	170	ASN	CB-CA-C	-5.08	100.86	110.01
3	H	148	PHE	N-CA-C	-5.08	104.83	111.02
1	K	239	ASP	N-CA-C	5.08	116.90	108.02
2	D	124	SER	N-CA-C	-5.07	105.20	111.33
1	C	28	GLY	N-CA-C	-5.06	108.69	115.32
3	G	65	ILE	N-CA-C	5.04	115.57	108.36
1	A	199	ILE	N-CA-C	5.04	115.02	107.51
1	I	45	TYR	N-CA-C	-5.04	103.13	110.08
1	A	87	LYS	N-CA-C	5.01	117.60	109.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2293	0	2259	299	0
1	B	2272	0	2242	281	1
1	C	2313	0	2288	292	1
1	E	2264	0	2241	289	1
1	I	2261	0	2233	287	0
1	K	2316	0	2291	234	2
1	L	2327	0	2304	322	2
2	D	2266	0	2235	309	2
3	F	2277	0	2248	280	1
3	G	2264	0	2237	304	1
3	H	2265	0	2232	310	0
3	J	2249	0	2229	291	1
4	A	27	0	10	14	0
4	B	27	0	11	5	0
4	C	27	0	11	5	0
4	D	27	0	11	9	0
4	E	27	0	11	8	0
4	F	27	0	11	7	0
4	G	27	0	11	26	0
4	H	27	0	11	7	0
4	I	27	0	11	3	0
4	J	27	0	11	10	0
4	K	27	0	11	8	0
4	L	27	0	11	16	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
6	F	6	0	8	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	6	0	8	0	0
7	A	149	0	0	70	1
7	B	151	0	0	60	0
7	C	126	0	0	50	0
7	D	169	0	0	65	1
7	E	136	0	0	53	0
7	F	108	0	0	57	1
7	G	172	0	0	78	2
7	H	131	0	0	57	2
7	I	131	0	0	61	1
7	J	157	0	0	66	0
7	K	151	0	0	38	0
7	L	98	0	0	45	0
All	All	29402	0	27186	3448	10

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 63.

All (3448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:103:THR:HB	7:J:470:HOH:O	1.21	1.30
1:K:25:GLU:O	1:K:29:SER:OG	1.58	1.18
2:D:245:ARG:N	7:D:402:HOH:O	1.81	1.14
1:C:19:SER:N	7:C:401:HOH:O	1.83	1.09
1:L:218:MET:SD	7:L:406:HOH:O	2.10	1.07
1:E:183:LYS:N	7:E:403:HOH:O	1.88	1.06
1:I:194:THR:OG1	1:I:199:ILE:O	1.72	1.06
1:K:202:ASN:N	1:K:205:GLU:OE2	1.89	1.05
1:K:103:THR:HB	7:K:468:HOH:O	1.54	1.05
1:E:103:THR:HB	7:E:472:HOH:O	1.56	1.04
3:F:240:ARG:NH2	7:F:406:HOH:O	1.90	1.04
3:H:40:ILE:C	7:H:401:HOH:O	2.00	1.04
1:A:215:PHE:N	7:A:403:HOH:O	1.89	1.04
1:B:133:PRO:HA	2:D:211:ARG:HH12	1.22	1.04
1:B:133:PRO:HA	2:D:211:ARG:NH1	1.73	1.04
3:F:262:ARG:NH2	7:F:405:HOH:O	1.89	1.02
1:K:98[B]:GLU:OE1	1:K:98[B]:GLU:N	1.91	1.02
3:H:276:ASP:OD1	3:H:279:ARG:NH1	1.93	1.02
1:L:124:SER:OG	4:L:301:A3P:O2P	1.77	1.01
1:B:199:ILE:C	7:B:405:HOH:O	2.04	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:50:THR:OG1	4:G:301:A3P:O4P	1.78	1.00
1:B:276:ASP:OD2	1:B:276:ASP:N	1.91	1.00
3:H:25:GLU:HB3	3:H:76:ILE:HG23	1.40	1.00
3:H:189:SER:O	3:H:192:LYS:N	1.94	0.99
1:I:168:HIS:NE2	7:I:403:HOH:O	1.88	0.99
1:C:39:ASP:OD2	1:C:89:ARG:NH2	1.95	0.99
3:H:202:ASN:OD1	3:H:205:GLU:N	1.96	0.99
1:I:269:THR:OG1	7:I:401:HOH:O	1.80	0.99
1:E:190:LEU:O	1:E:194:THR:HB	1.63	0.98
1:K:221:ASN:O	7:K:401:HOH:O	1.80	0.98
3:H:40:ILE:O	7:H:401:HOH:O	1.81	0.98
1:L:260:GLN:N	7:L:405:HOH:O	1.96	0.98
1:B:194:THR:N	7:B:407:HOH:O	1.96	0.98
1:A:231:HIS:ND1	7:A:409:HOH:O	1.96	0.97
1:A:39:ASP:OD1	7:A:401:HOH:O	1.82	0.97
1:K:191:LYS:O	7:K:402:HOH:O	1.82	0.97
1:E:146:GLU:OE1	7:E:401:HOH:O	1.82	0.97
3:H:166:GLU:O	7:H:403:HOH:O	1.82	0.97
3:F:262:ARG:HG3	7:F:412:HOH:O	1.63	0.96
2:D:173:ASN:O	7:D:404:HOH:O	1.82	0.96
1:K:117:ASN:ND2	1:K:120:ASP:OD2	1.97	0.96
1:B:28:GLY:O	7:B:401:HOH:O	1.83	0.96
1:A:51:HIS:N	7:A:412:HOH:O	1.97	0.96
2:D:50:THR:HG23	4:D:301:A3P:O5P	1.65	0.96
1:C:125:MET:O	1:C:126:PHE:C	2.06	0.96
3:J:182:MET:SD	7:J:550:HOH:O	2.23	0.96
3:H:192:LYS:O	7:H:402:HOH:O	1.82	0.96
2:D:58:GLU:O	7:D:401:HOH:O	1.81	0.95
3:F:38:ASP:OD1	7:F:401:HOH:O	1.84	0.95
3:H:219:LYS:HA	3:H:244:PHE:CD2	2.01	0.95
2:D:37:GLU:OE1	7:D:403:HOH:O	1.82	0.95
1:E:266:GLU:OE1	7:E:402:HOH:O	1.82	0.95
1:L:138:THR:O	7:L:401:HOH:O	1.81	0.95
1:E:52:TRP:CD2	1:E:182:MET:HE3	2.02	0.94
3:G:86:PRO:HD2	7:G:530:HOH:O	1.65	0.94
3:G:190:LEU:O	3:G:194:THR:HB	1.66	0.94
3:J:69:SER:OG	7:J:401:HOH:O	1.86	0.94
3:J:282:LYS:O	3:J:284:TYR:N	2.00	0.94
1:C:194:THR:HG23	1:C:199:ILE:O	1.67	0.94
1:A:214:SER:OG	7:A:402:HOH:O	1.85	0.94
2:D:273:ARG:HB2	1:E:106:GLN:HE22	1.33	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:160:ASP:OD1	7:F:402:HOH:O	1.84	0.93
1:L:218:MET:O	1:L:221:ASN:ND2	2.01	0.93
3:H:219:LYS:HG3	3:H:244:PHE:HB2	1.47	0.93
1:E:266:GLU:HB2	7:E:402:HOH:O	1.69	0.93
3:F:182:MET:O	7:F:403:HOH:O	1.87	0.93
3:G:98[A]:GLU:HG2	1:I:98:GLU:HG2	1.50	0.93
1:K:171:ASP:OD1	7:K:403:HOH:O	1.84	0.93
1:B:39:ASP:OD1	7:B:402:HOH:O	1.84	0.92
3:H:163:LEU:O	7:H:404:HOH:O	1.87	0.92
2:D:60:ILE:O	7:D:405:HOH:O	1.86	0.92
3:G:98[A]:GLU:OE1	7:G:402:HOH:O	1.87	0.92
1:C:98[B]:GLU:OE2	7:C:403:HOH:O	1.86	0.92
1:C:273:ARG:N	7:C:411:HOH:O	2.03	0.92
3:H:204:SER:OG	3:H:205:GLU:OE1	1.86	0.92
1:I:107:LYS:O	7:I:402:HOH:O	1.87	0.92
3:H:240:ARG:NE	7:H:410:HOH:O	2.02	0.92
2:D:50:THR:OG1	7:D:406:HOH:O	1.89	0.91
3:H:240:ARG:CZ	7:H:410:HOH:O	2.19	0.91
1:I:77:SER:C	7:I:410:HOH:O	2.12	0.91
1:A:284:TYR:O	1:A:286:HIS:N	2.04	0.91
1:L:67:LEU:HD21	1:L:233:ILE:HG21	1.53	0.91
2:D:40:ILE:O	2:D:91:ILE:N	2.02	0.91
1:B:98:GLU:OE2	7:B:403:HOH:O	1.88	0.91
3:G:137:SER:N	7:G:401:HOH:O	1.86	0.91
1:L:288:ALA:O	7:L:402:HOH:O	1.88	0.90
3:J:75:ASP:HB2	7:J:402:HOH:O	1.70	0.90
3:F:288:ALA:O	7:F:404:HOH:O	1.88	0.90
1:C:221:ASN:OD1	7:C:404:HOH:O	1.88	0.90
3:H:25:GLU:O	3:H:29:SER:OG	1.88	0.90
1:I:181:GLU:HA	1:I:184:LYS:HD3	1.53	0.90
1:B:194:THR:HG23	1:B:199:ILE:O	1.72	0.90
3:H:35:ALA:H	3:H:103:THR:CG2	1.84	0.90
1:L:75:ASP:HB3	1:L:77:SER:H	1.37	0.89
1:A:217:GLU:O	1:A:220:SER:OG	1.89	0.89
3:J:96:ASN:HA	3:J:165:TRP:HE1	1.36	0.89
1:B:173:ASN:HA	7:B:414:HOH:O	1.73	0.89
2:D:279:ARG:HD2	3:F:274:ASN:OD1	1.73	0.89
1:L:220:SER:O	1:L:221:ASN:OD1	1.91	0.89
1:B:194:THR:CA	7:B:407:HOH:O	2.21	0.89
3:F:79:PHE:N	7:F:410:HOH:O	2.05	0.89
2:D:39:ASP:OD2	2:D:89:ARG:NH2	2.06	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:GLU:HB2	2:D:184:LYS:NZ	1.88	0.89
1:I:224:LYS:NZ	7:I:413:HOH:O	2.05	0.88
1:A:63:ALA:O	7:A:404:HOH:O	1.90	0.88
1:B:23:SER:OG	1:B:25[B]:GLU:HG3	1.72	0.88
3:H:219:LYS:HG3	3:H:244:PHE:CB	2.02	0.88
1:I:85:ILE:O	7:I:404:HOH:O	1.90	0.88
3:J:59:ARG:NH2	7:J:417:HOH:O	2.06	0.88
1:C:218:MET:O	1:C:221:ASN:ND2	2.06	0.88
1:A:107:LYS:NZ	7:A:414:HOH:O	2.05	0.88
1:B:49:GLY:O	7:B:404:HOH:O	1.91	0.88
3:G:103:THR:HB	7:G:478:HOH:O	1.74	0.88
3:H:181[B]:GLU:HG2	3:H:184:LYS:NZ	1.89	0.88
1:K:265:ASP:O	7:K:404:HOH:O	1.90	0.88
3:G:173:ASN:O	7:G:403:HOH:O	1.89	0.88
3:J:23:SER:OG	3:J:25[B]:GLU:HG3	1.72	0.88
3:G:47:LYS:HA	4:G:301:A3P:P2	2.15	0.87
3:G:70:PRO:HA	3:G:92:PRO:O	1.74	0.87
3:G:239:ASP:OD2	3:G:242:LEU:HG	1.73	0.87
2:D:62:ASP:O	7:D:409:HOH:O	1.92	0.87
3:H:50:THR:HG23	7:H:482:HOH:O	1.74	0.87
1:K:256:PHE:HB3	1:K:261:ASN:OD1	1.73	0.87
1:E:12:LYS:HD3	1:E:17:PHE:CE2	2.10	0.87
3:G:265:ASP:OD2	7:G:404:HOH:O	1.91	0.87
2:D:84:ARG:O	2:D:86:PRO:HD3	1.73	0.87
1:I:160:ASP:O	7:I:405:HOH:O	1.91	0.87
1:C:167:GLU:OE2	7:C:405:HOH:O	1.92	0.87
3:G:181:GLU:HB2	3:G:184:LYS:NZ	1.89	0.87
4:H:301:A3P:O4P	7:H:405:HOH:O	1.93	0.87
1:A:103:THR:O	7:A:406:HOH:O	1.91	0.86
3:G:191:LYS:O	7:G:405:HOH:O	1.92	0.86
3:H:195:ALA:C	7:H:407:HOH:O	2.17	0.86
1:L:287:SER:OG	1:L:288:ALA:N	1.99	0.86
2:D:276:ASP:OD1	7:D:408:HOH:O	1.92	0.86
1:E:216:SER:O	1:E:220:SER:OG	1.93	0.86
1:E:114:ILE:N	7:E:408:HOH:O	2.08	0.86
1:I:31:ASP:OD2	7:I:406:HOH:O	1.93	0.86
1:K:237:THR:C	7:K:418:HOH:O	2.19	0.86
1:L:9:LEU:O	7:L:403:HOH:O	1.92	0.86
1:A:213:THR:OG1	7:A:405:HOH:O	1.91	0.86
1:E:124:SER:OG	4:E:301:A3P:O1P	1.94	0.86
3:G:223:ALA:CA	7:G:407:HOH:O	2.24	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:OD2	7:C:406:HOH:O	1.94	0.86
3:F:124:SER:OG	4:F:301:A3P:O1P	1.92	0.86
3:J:119:LYS:NZ	7:J:415:HOH:O	2.03	0.86
3:G:221:ASN:OD1	7:G:406:HOH:O	1.93	0.86
3:J:50:THR:OG1	4:J:301:A3P:O5P	1.94	0.86
1:C:125:MET:O	1:C:128:TYR:N	2.08	0.85
1:B:151:GLY:O	1:B:156:GLY:HA2	1.76	0.85
3:F:262:ARG:NE	7:F:412:HOH:O	2.09	0.85
3:G:223:ALA:O	7:G:407:HOH:O	1.94	0.85
1:I:81:GLU:HG3	7:I:410:HOH:O	1.74	0.85
1:L:270:GLU:O	1:L:273:ARG:HD3	1.76	0.85
1:C:23:SER:HB2	1:C:25:GLU:OE1	1.75	0.85
3:J:77:SER:N	7:J:402:HOH:O	1.92	0.85
1:B:199:ILE:O	7:B:405:HOH:O	1.92	0.85
1:B:202:ASN:O	1:B:205:GLU:HB2	1.77	0.85
3:J:52:TRP:O	7:J:403:HOH:O	1.94	0.85
1:A:211:ARG:O	7:A:407:HOH:O	1.93	0.85
2:D:226:ASN:HB3	7:D:511:HOH:O	1.77	0.85
1:K:224:LYS:HD3	1:K:228:ASP:HA	1.57	0.85
1:E:137:SER:O	7:E:404:HOH:O	1.94	0.85
3:H:38:ASP:OD2	7:H:406:HOH:O	1.94	0.85
1:L:123:VAL:HG21	1:L:252:TRP:HA	1.58	0.85
3:G:84:ARG:HG3	7:G:414:HOH:O	1.76	0.85
1:K:116:ARG:NH2	7:K:411:HOH:O	2.09	0.85
1:K:222:ALA:N	7:K:409:HOH:O	2.04	0.85
3:J:52:TRP:C	7:J:403:HOH:O	2.18	0.84
1:E:108:GLN:O	7:E:405:HOH:O	1.95	0.84
3:H:51:HIS:N	7:H:405:HOH:O	2.09	0.84
1:I:265:ASP:HA	7:I:414:HOH:O	1.78	0.84
4:K:301:A3P:O4'	7:K:405:HOH:O	1.95	0.84
3:G:223:ALA:N	7:G:407:HOH:O	2.11	0.84
1:A:107:LYS:HB2	7:A:406:HOH:O	1.78	0.84
1:A:171:ASP:OD1	7:A:408:HOH:O	1.95	0.84
1:B:26:LEU:CD1	1:B:79:PHE:CZ	2.60	0.84
1:C:195:ALA:O	1:C:198:GLY:N	2.10	0.84
1:C:212:SER:OG	7:C:407:HOH:O	1.95	0.84
3:F:30:LEU:O	3:F:32:SER:N	2.11	0.84
3:G:183:LYS:O	7:G:408:HOH:O	1.95	0.84
1:C:125:MET:O	1:C:127:HIS:N	2.10	0.84
2:D:98[A]:GLU:HG2	1:E:98:GLU:CG	2.08	0.84
3:F:181[B]:GLU:HG2	3:F:184:LYS:NZ	1.93	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:59:ARG:NE	7:G:420:HOH:O	2.10	0.83
3:H:220:SER:O	3:H:221:ASN:OD1	1.94	0.83
3:F:181[B]:GLU:HG2	3:F:184:LYS:CE	2.08	0.83
3:F:272:MET:O	7:F:407:HOH:O	1.95	0.83
3:G:171:ASP:OD1	7:G:409:HOH:O	1.95	0.83
3:J:125:MET:HE1	3:J:153:VAL:HB	1.58	0.83
3:J:246:LYS:NZ	7:J:412:HOH:O	2.02	0.83
3:H:195:ALA:O	7:H:407:HOH:O	1.95	0.83
3:H:219:LYS:HA	3:H:244:PHE:CG	2.12	0.83
3:J:250:GLY:O	7:J:404:HOH:O	1.95	0.83
1:E:95:LEU:HD23	1:E:99:MET:HE3	1.58	0.83
1:L:98[A]:GLU:OE2	7:L:404:HOH:O	1.95	0.83
1:I:186:PHE:O	1:I:189:SER:HB2	1.79	0.83
1:L:44:SER:HB3	1:L:114:ILE:HG22	1.61	0.83
3:G:128:TYR:OH	3:G:237:THR:HB	1.79	0.83
1:I:184:LYS:HG2	1:I:185:ASP:N	1.94	0.83
1:K:83:LYS:HG2	7:K:406:HOH:O	1.76	0.83
1:K:96:ASN:N	7:K:412:HOH:O	2.10	0.83
3:H:138:THR:O	7:H:408:HOH:O	1.96	0.83
1:B:254:ASN:O	7:B:406:HOH:O	1.96	0.83
3:G:131:ASP:OD2	7:G:410:HOH:O	1.96	0.83
1:K:194:THR:HG22	7:K:402:HOH:O	1.79	0.83
1:E:220:SER:C	1:E:221:ASN:OD1	2.22	0.83
1:L:77:SER:O	1:L:77:SER:OG	1.93	0.83
3:H:26:LEU:HB2	3:H:75:ASP:O	1.78	0.82
3:F:206:MET:O	3:F:209:ILE:N	2.11	0.82
3:J:220:SER:O	3:J:221:ASN:OD1	1.96	0.82
1:A:234:CYS:HB3	1:A:237:THR:CG2	2.09	0.82
2:D:77:SER:O	2:D:80:GLU:N	2.12	0.82
2:D:78:LYS:O	2:D:81:GLU:N	2.12	0.82
1:K:98[B]:GLU:H	1:K:98[B]:GLU:CD	1.78	0.82
3:G:82:LEU:O	3:G:89:ARG:NH1	2.12	0.82
3:H:178:PHE:O	3:H:181[B]:GLU:N	2.11	0.82
1:A:117:ASN:OD1	7:A:411:HOH:O	1.96	0.82
3:H:280:CYS:HA	3:H:283:GLU:OE2	1.80	0.82
1:I:79:PHE:O	1:I:82:LEU:N	2.13	0.82
3:J:216:SER:OG	7:J:405:HOH:O	1.96	0.82
1:K:231:HIS:CG	1:K:231:HIS:O	2.31	0.82
1:A:234:CYS:SG	7:A:483:HOH:O	2.35	0.82
3:G:261:ASN:O	7:G:404:HOH:O	1.96	0.82
1:I:185:ASP:OD1	7:I:407:HOH:O	1.96	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:181:GLU:OE2	7:G:411:HOH:O	1.98	0.82
3:G:249:VAL:O	7:G:412:HOH:O	1.98	0.82
1:I:231:HIS:HA	7:I:423:HOH:O	1.79	0.82
2:D:181:GLU:HB2	2:D:184:LYS:CE	2.10	0.82
3:G:173:ASN:CA	7:G:403:HOH:O	2.27	0.81
3:J:146:GLU:O	7:J:407:HOH:O	1.98	0.81
1:A:51:HIS:ND1	4:A:301:A3P:O4P	2.11	0.81
3:G:263:GLY:O	3:G:266:GLU:HB2	1.79	0.81
4:A:301:A3P:O4P	7:A:412:HOH:O	1.98	0.81
1:E:184:LYS:N	7:E:403:HOH:O	2.01	0.81
3:F:160:ASP:HA	7:F:402:HOH:O	1.78	0.81
3:G:35:ALA:H	3:G:103:THR:HG21	1.43	0.81
3:G:98[A]:GLU:HG2	1:I:98:GLU:CG	2.10	0.81
1:C:172:LYS:NZ	1:B:174:VAL:O	2.13	0.81
1:B:170:ASN:OD1	7:B:408:HOH:O	1.98	0.81
3:G:70:PRO:HD3	3:G:233:ILE:HA	1.61	0.81
1:L:219:LYS:NZ	1:L:244:PHE:O	2.14	0.81
1:C:102:VAL:HG13	1:C:103:THR:N	1.94	0.81
2:D:217:GLU:OE1	2:D:217:GLU:HA	1.79	0.81
3:F:195:ALA:O	3:F:198:GLY:N	2.13	0.81
1:A:205:GLU:O	1:A:209:ILE:HG12	1.81	0.81
3:F:181[B]:GLU:HG2	3:F:184:LYS:HE2	1.63	0.81
3:H:9:LEU:O	7:H:409:HOH:O	1.96	0.81
3:J:253:ILE:CG2	7:J:404:HOH:O	2.28	0.81
2:D:110:LYS:HA	7:D:404:HOH:O	1.79	0.81
1:A:268:PHE:O	1:A:272:MET:N	2.14	0.81
1:K:262[B]:ARG:NE	7:K:414:HOH:O	2.13	0.81
1:C:51:HIS:O	1:C:52:TRP:C	2.22	0.80
1:B:214:SER:HB3	1:B:217:GLU:CB	2.10	0.80
3:J:53:LEU:HA	7:J:403:HOH:O	1.79	0.80
1:C:248:VAL:N	7:C:409:HOH:O	2.01	0.80
3:G:185:ASP:OD1	7:G:413:HOH:O	1.98	0.80
3:G:211:ARG:HH21	3:J:131:ASP:HA	1.46	0.80
3:J:52:TRP:CE2	3:J:182:MET:HE3	2.17	0.80
1:B:17:PHE:CB	1:B:154:VAL:HA	2.11	0.80
7:D:409:HOH:O	3:H:258:PRO:HD3	1.80	0.80
1:L:6:ALA:N	1:L:7:PRO:HD2	1.97	0.80
2:D:36:ARG:NH1	2:D:85:ILE:O	2.14	0.80
2:D:51:HIS:N	7:D:406:HOH:O	2.13	0.80
3:F:150:LYS:HB3	3:F:152:ASP:OD2	1.82	0.80
3:F:257:THR:H	3:F:260:GLN:NE2	1.79	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:301:A3P:O4P	7:J:408:HOH:O	1.99	0.80
1:L:274:ASN:ND2	7:L:411:HOH:O	2.13	0.80
1:C:239:ASP:OD1	1:C:241:ASN:N	2.14	0.80
3:H:13:TYR:CE1	3:H:14:MET:HG2	2.15	0.80
1:I:152:ASP:OD1	7:I:408:HOH:O	1.99	0.80
3:J:146:GLU:OE1	7:J:409:HOH:O	2.00	0.80
2:D:136:PRO:HA	7:D:425:HOH:O	1.80	0.80
4:C:301:A3P:O2'	4:C:301:A3P:O1P	2.00	0.80
1:B:114:ILE:O	7:B:409:HOH:O	1.99	0.80
1:E:282:LYS:O	1:E:284:TYR:O	2.00	0.80
3:F:184:LYS:HG2	3:F:185:ASP:N	1.95	0.80
1:B:194:THR:CG2	1:B:199:ILE:O	2.30	0.80
2:D:98[A]:GLU:HG2	1:E:98:GLU:CD	2.07	0.80
3:F:194:THR:HG23	3:F:199:ILE:O	1.81	0.80
1:L:49:GLY:O	1:L:114:ILE:HG21	1.81	0.80
1:A:44:SER:HB3	1:A:114:ILE:CG2	2.12	0.79
3:F:220:SER:O	3:F:221:ASN:CG	2.25	0.79
3:G:173:ASN:C	7:G:403:HOH:O	2.23	0.79
3:J:98[A]:GLU:CD	3:J:98[A]:GLU:H	1.90	0.79
3:F:29:SER:O	3:F:32:SER:OG	1.99	0.79
3:F:54:ALA:C	7:F:419:HOH:O	2.24	0.79
1:L:132:ASN:OD1	1:L:134:ASN:HB2	1.82	0.79
3:G:267:LEU:O	3:G:268:PHE:C	2.26	0.79
3:H:35:ALA:H	3:H:103:THR:HG21	1.45	0.79
1:I:221:ASN:C	1:I:221:ASN:OD1	2.26	0.79
2:D:49:GLY:O	2:D:53:LEU:N	2.16	0.79
1:K:36:ARG:NH2	7:K:406:HOH:O	2.14	0.79
2:D:169:LYS:HD2	2:D:176:PHE:CD1	2.18	0.79
2:D:198:GLY:O	7:D:410:HOH:O	1.99	0.79
3:G:173:ASN:HA	7:G:403:HOH:O	1.83	0.79
1:K:83:LYS:O	7:K:406:HOH:O	1.99	0.79
1:B:43:VAL:O	1:B:113:TYR:HA	1.81	0.79
3:F:181[B]:GLU:OE2	3:F:184:LYS:HE2	1.83	0.79
3:G:146:GLU:HB3	7:G:448:HOH:O	1.82	0.79
1:K:276:ASP:HA	1:K:279:ARG:NH2	1.97	0.79
1:C:205:GLU:O	7:C:408:HOH:O	1.99	0.79
1:B:225:GLU:C	7:B:410:HOH:O	2.24	0.79
1:I:143:ALA:O	7:I:409:HOH:O	2.01	0.79
1:K:164[A]:SER:O	7:K:407:HOH:O	2.00	0.79
1:B:224:LYS:O	7:B:410:HOH:O	2.01	0.78
1:I:39:ASP:OD1	7:I:411:HOH:O	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215:PHE:HA	4:L:301:A3P:N6	1.98	0.78
1:C:184:LYS:HG2	1:C:185:ASP:N	1.99	0.78
3:J:25[B]:GLU:CD	3:J:76:ILE:HD13	2.08	0.78
1:L:45:TYR:HB3	1:L:48:SER:OG	1.83	0.78
1:C:282:LYS:O	1:C:286:HIS:HB2	1.84	0.78
2:D:89:ARG:O	7:D:411:HOH:O	2.00	0.78
2:D:243:VAL:C	7:D:402:HOH:O	2.26	0.78
2:D:164:SER:O	7:D:412:HOH:O	2.01	0.78
3:J:117:ASN:OD1	7:J:411:HOH:O	2.02	0.78
1:C:80:GLU:OE1	1:C:80:GLU:HA	1.82	0.78
2:D:98[A]:GLU:HG2	1:E:98:GLU:HG2	1.65	0.78
1:I:25:GLU:O	1:I:29:SER:OG	2.01	0.78
7:D:478:HOH:O	1:E:98:GLU:HG2	1.83	0.78
1:E:37:GLU:HG2	7:E:467:HOH:O	1.84	0.78
3:H:277:VAL:O	3:H:280:CYS:N	2.17	0.78
1:I:181:GLU:HB2	1:I:184:LYS:NZ	1.99	0.78
3:J:214:SER:HB2	7:J:418:HOH:O	1.83	0.78
2:D:77:SER:O	2:D:78:LYS:C	2.26	0.78
1:A:234:CYS:HB3	1:A:237:THR:HG22	1.66	0.78
1:L:50:THR:HG21	1:L:94:HIS:CE1	2.19	0.78
1:E:183:LYS:CA	7:E:403:HOH:O	2.29	0.78
3:G:261:ASN:C	7:G:404:HOH:O	2.27	0.78
1:B:216:SER:OG	7:B:412:HOH:O	2.02	0.77
1:I:71:ILE:HG22	1:I:93:THR:HB	1.66	0.77
1:K:253:ILE:HG13	1:K:254:ASN:OD1	1.84	0.77
1:L:181:GLU:HB2	1:L:184:LYS:NZ	1.99	0.77
3:G:52:TRP:O	3:G:56:VAL:HG23	1.84	0.77
3:G:200:ASP:OD2	7:G:415:HOH:O	2.02	0.77
3:H:276:ASP:CG	3:H:279:ARG:NH1	2.43	0.77
3:J:12:LYS:HD3	3:J:17:PHE:CE2	2.19	0.77
3:J:176:PHE:O	7:J:410:HOH:O	2.00	0.77
3:J:220:SER:O	3:J:221:ASN:CG	2.27	0.77
1:B:12:LYS:HD3	1:B:17:PHE:CE2	2.20	0.77
3:H:25:GLU:HB3	3:H:76:ILE:CG2	2.15	0.77
3:F:160:ASP:OD2	7:F:408:HOH:O	2.03	0.77
3:J:96:ASN:C	3:J:96:ASN:OD1	2.27	0.77
1:E:35:ALA:CB	1:E:103:THR:HG23	2.15	0.77
1:E:50:THR:HG23	4:E:301:A3P:O4P	1.84	0.77
1:E:142:ALA:O	7:E:409:HOH:O	2.03	0.77
3:J:60:ILE:HG23	3:J:61:PRO:HD2	1.65	0.77
1:K:26:LEU:HD12	1:K:79:PHE:CZ	2.20	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:THR:O	7:L:406:HOH:O	2.02	0.77
1:B:107:LYS:O	7:B:411:HOH:O	2.02	0.77
1:E:114:ILE:O	7:E:408:HOH:O	2.03	0.77
3:G:70:PRO:HG3	3:G:233:ILE:O	1.84	0.77
3:G:80:GLU:OE2	7:G:414:HOH:O	2.01	0.77
3:J:125:MET:CE	3:J:153:VAL:HB	2.14	0.77
1:K:31:ASP:OD1	7:K:408:HOH:O	2.01	0.77
1:C:11:HIS:O	1:C:18:PHE:N	2.13	0.76
1:A:255:TYR:O	7:A:413:HOH:O	2.03	0.76
1:E:202:ASN:O	1:E:205:GLU:N	2.18	0.76
1:I:181:GLU:HA	1:I:184:LYS:CD	2.14	0.76
1:A:181:GLU:HG3	7:A:447:HOH:O	1.86	0.76
2:D:38:ASP:OD1	2:D:39:ASP:N	2.19	0.76
3:G:76:ILE:HD13	3:G:76:ILE:H	1.51	0.76
3:H:174:VAL:O	1:I:172:LYS:NZ	2.18	0.76
3:J:96:ASN:CA	3:J:165:TRP:HE1	1.96	0.76
3:J:253:ILE:HG23	7:J:404:HOH:O	1.83	0.76
1:B:17:PHE:O	1:B:155:TYR:N	2.17	0.76
2:D:173:ASN:CA	7:D:404:HOH:O	2.34	0.76
3:F:204:SER:O	3:F:207:ALA:HB3	1.86	0.76
3:F:239:ASP:O	3:F:242:LEU:HB2	1.85	0.76
1:A:267:LEU:HD22	1:A:271:LYS:HG2	1.66	0.76
1:E:184:LYS:O	7:E:411:HOH:O	2.04	0.76
3:F:240:ARG:O	3:F:242:LEU:N	2.18	0.76
3:F:251:ASP:O	3:F:253:ILE:N	2.18	0.76
1:I:31:ASP:CG	7:I:406:HOH:O	2.29	0.76
3:J:25[B]:GLU:OE1	3:J:75:ASP:HB3	1.86	0.76
3:G:47:LYS:HA	4:G:301:A3P:O5'	1.86	0.76
1:L:169:LYS:O	7:L:407:HOH:O	2.03	0.76
1:B:44:SER:HB3	1:B:114:ILE:CG2	2.15	0.76
1:E:128:TYR:OH	1:E:237:THR:HB	1.85	0.76
3:F:150:LYS:HE3	3:F:152:ASP:OD2	1.86	0.76
3:H:70:PRO:HD3	3:H:232:VAL:O	1.86	0.76
1:I:284:TYR:O	1:I:286:HIS:N	2.19	0.76
1:A:8:SER:O	1:A:20:THR:HG21	1.85	0.76
1:B:214:SER:HB3	1:B:217:GLU:HB2	1.66	0.76
3:H:276:ASP:O	3:H:279:ARG:HB3	1.85	0.76
3:J:114:ILE:O	7:J:413:HOH:O	2.02	0.76
1:C:25:GLU:O	7:C:412:HOH:O	2.04	0.76
2:D:75:ASP:OD2	7:D:414:HOH:O	2.04	0.76
3:F:55:GLU:N	7:F:419:HOH:O	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:ILE:CG1	1:L:88:ARG:HD3	2.16	0.76
1:C:274:ASN:ND2	7:C:410:HOH:O	2.03	0.75
1:I:176:PHE:O	7:I:412:HOH:O	2.03	0.75
1:I:183:LYS:NZ	1:I:247:GLY:O	2.18	0.75
3:J:200:ASP:OD2	7:J:414:HOH:O	2.03	0.75
1:C:22:SER:O	1:C:23:SER:C	2.29	0.75
3:F:94:HIS:HB2	3:F:155:TYR:CE1	2.21	0.75
1:K:238:SER:N	7:K:418:HOH:O	2.19	0.75
1:L:276:ASP:OD1	1:L:279:ARG:NH1	2.19	0.75
1:B:75:ASP:OD1	7:B:413:HOH:O	2.04	0.75
1:I:252:TRP:HB2	1:I:256:PHE:CE1	2.22	0.75
1:L:48:SER:O	1:L:116:ARG:HB2	1.85	0.75
1:A:248:VAL:HG22	1:A:249:VAL:H	1.51	0.75
1:I:123:VAL:HG11	1:I:251:ASP:OD2	1.86	0.75
3:H:146:GLU:OE1	7:H:413:HOH:O	2.04	0.75
3:H:230:ASN:CG	7:H:427:HOH:O	2.29	0.75
1:A:23:SER:HB2	1:A:25:GLU:OE1	1.86	0.75
2:D:41:PHE:HA	2:D:91:ILE:O	1.87	0.75
2:D:283:GLU:O	7:D:413:HOH:O	2.04	0.75
3:G:237:THR:HB	7:G:464:HOH:O	1.86	0.75
3:J:56:VAL:CG2	7:J:403:HOH:O	2.35	0.75
3:H:65:ILE:O	7:H:412:HOH:O	2.04	0.75
1:K:190:LEU:O	1:K:194:THR:HB	1.87	0.75
1:A:190:LEU:O	1:A:194:THR:HB	1.86	0.74
3:G:188:LYS:O	7:G:416:HOH:O	2.04	0.74
3:J:52:TRP:CH2	3:J:182:MET:HB3	2.22	0.74
3:F:231:HIS:CD2	3:F:231:HIS:O	2.40	0.74
1:K:97:TYR:N	1:K:98[B]:GLU:OE1	2.21	0.74
1:L:286:HIS:CG	1:L:286:HIS:O	2.39	0.74
1:C:251:ASP:O	1:C:253:ILE:N	2.20	0.74
1:A:188:LYS:HG2	7:A:424:HOH:O	1.87	0.74
1:L:44:SER:HB3	1:L:114:ILE:CG2	2.17	0.74
1:I:224:LYS:CE	7:I:413:HOH:O	2.34	0.74
1:L:43:VAL:HG22	1:L:93:THR:CG2	2.17	0.74
1:L:224:LYS:HB2	1:L:228:ASP:O	1.87	0.74
2:D:237:THR:O	7:D:415:HOH:O	2.06	0.74
3:H:98:GLU:OE1	7:H:414:HOH:O	2.06	0.74
3:J:266:GLU:OE2	3:J:267:LEU:N	2.20	0.74
3:H:211:ARG:NH1	7:H:426:HOH:O	2.20	0.74
1:I:173:ASN:CG	7:I:419:HOH:O	2.31	0.74
1:A:44:SER:HB3	1:A:114:ILE:HG23	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LYS:NZ	7:E:413:HOH:O	2.11	0.74
1:E:167:GLU:HG3	7:E:424:HOH:O	1.87	0.74
1:L:65:ILE:HG12	1:L:88:ARG:HD3	1.70	0.74
1:L:270:GLU:HA	1:L:270:GLU:OE2	1.88	0.74
3:F:256:PHE:O	7:F:409:HOH:O	2.05	0.74
3:F:12:LYS:HD2	3:F:17:PHE:CD2	2.23	0.73
1:K:256:PHE:CB	1:K:261:ASN:OD1	2.36	0.73
1:L:44:SER:HB2	1:L:114:ILE:HG23	1.68	0.73
1:B:153:VAL:O	7:B:415:HOH:O	2.05	0.73
2:D:169:LYS:HD2	2:D:176:PHE:CG	2.23	0.73
3:F:36:ARG:CD	7:F:413:HOH:O	2.35	0.73
3:F:220:SER:O	3:F:221:ASN:OD1	2.05	0.73
3:G:239:ASP:OD1	3:G:241:ASN:HB2	1.88	0.73
3:H:25:GLU:OE1	7:H:415:HOH:O	2.06	0.73
1:I:77:SER:O	7:I:410:HOH:O	2.01	0.73
1:L:194:THR:HG23	1:L:199:ILE:O	1.88	0.73
1:C:12:LYS:HD2	1:C:17:PHE:CD2	2.22	0.73
1:E:184:LYS:HG2	1:E:185:ASP:N	2.02	0.73
3:G:78:LYS:O	3:G:78:LYS:HD3	1.87	0.73
1:K:26:LEU:CD1	1:K:79:PHE:CZ	2.71	0.73
1:B:72:GLU:OE2	7:B:417:HOH:O	2.06	0.73
1:B:98:GLU:CD	7:B:403:HOH:O	2.29	0.73
2:D:172:LYS:HG2	2:D:173:ASN:N	2.04	0.73
3:G:35:ALA:H	3:G:103:THR:CG2	2.01	0.73
3:G:110:LYS:HD3	7:G:403:HOH:O	1.88	0.73
1:I:194:THR:HG23	1:I:195:ALA:N	2.02	0.73
1:L:48:SER:HA	1:L:116:ARG:HB3	1.70	0.73
3:G:50:THR:CB	4:G:301:A3P:O4P	2.36	0.73
1:L:239:ASP:OD1	1:L:241:ASN:ND2	2.20	0.73
1:B:82:LEU:O	7:B:416:HOH:O	2.06	0.73
3:H:181[B]:GLU:HG2	3:H:184:LYS:HZ3	1.50	0.73
3:J:139:GLU:O	7:J:416:HOH:O	2.04	0.73
1:L:75:ASP:HB3	1:L:77:SER:N	2.02	0.73
1:B:172:LYS:O	7:B:414:HOH:O	2.05	0.73
3:G:223:ALA:C	7:G:407:HOH:O	2.31	0.73
3:F:225:GLU:HG2	3:F:231:HIS:CD2	2.23	0.73
1:B:35:ALA:H	1:B:103:THR:CG2	2.01	0.73
2:D:221:ASN:ND2	7:D:426:HOH:O	2.22	0.73
1:E:50:THR:CG2	4:E:301:A3P:O4P	2.36	0.73
3:F:12:LYS:HE3	3:F:17:PHE:CD1	2.23	0.73
3:F:132:ASN:O	3:F:135:LEU:N	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:GLU:OE1	7:I:415:HOH:O	2.06	0.73
1:C:11:HIS:ND1	1:C:18:PHE:O	2.17	0.73
1:B:29:SER:OG	7:B:418:HOH:O	2.06	0.73
3:H:40:ILE:O	3:H:90:ALA:HA	1.89	0.73
1:B:44:SER:HB3	1:B:114:ILE:HG22	1.69	0.72
3:H:103:THR:HB	7:H:429:HOH:O	1.89	0.72
3:H:123:VAL:HG21	3:H:252:TRP:HA	1.71	0.72
1:K:228:ASP:HB2	1:K:229:PRO:HD3	1.70	0.72
1:B:50:THR:HA	7:B:404:HOH:O	1.89	0.72
2:D:152:ASP:OD1	7:D:416:HOH:O	2.06	0.72
1:K:239:ASP:OD2	1:K:241:ASN:HB2	1.89	0.72
1:L:144:PHE:O	1:L:147:LEU:N	2.22	0.72
1:A:25:GLU:H	1:A:25:GLU:CD	1.96	0.72
3:F:187:VAL:HG12	3:F:188:LYS:N	2.02	0.72
1:C:178:PHE:O	1:C:181:GLU:N	2.22	0.72
2:D:173:ASN:C	7:D:404:HOH:O	2.29	0.72
2:D:200:ASP:OD1	7:D:410:HOH:O	2.05	0.72
3:G:209:ILE:HA	7:G:433:HOH:O	1.90	0.72
1:K:188:LYS:O	7:K:410:HOH:O	2.05	0.72
1:C:279:ARG:HG2	1:C:283:GLU:OE2	1.90	0.72
2:D:279:ARG:HG2	2:D:283:GLU:OE2	1.89	0.72
3:F:287:SER:HA	3:F:288:ALA:HB2	1.70	0.72
3:G:211:ARG:O	7:G:417:HOH:O	2.05	0.72
3:J:172:LYS:HE2	1:L:169:LYS:O	1.90	0.72
1:L:26:LEU:HD11	1:L:79:PHE:CE1	2.24	0.72
3:F:143:ALA:O	3:F:146:GLU:HB3	1.88	0.72
1:I:265:ASP:OD1	7:I:414:HOH:O	2.06	0.72
3:H:23:SER:OG	3:H:74:GLY:O	2.07	0.72
3:H:28:GLY:O	7:H:416:HOH:O	2.07	0.72
3:G:25:GLU:O	3:G:29:SER:OG	2.06	0.72
3:G:59:ARG:CZ	7:G:420:HOH:O	2.35	0.72
3:H:98:GLU:CD	7:H:414:HOH:O	2.33	0.72
1:L:128:TYR:OH	1:L:237:THR:HB	1.90	0.72
1:L:276:ASP:OD1	7:L:408:HOH:O	2.07	0.72
1:A:203:ASP:O	7:A:416:HOH:O	2.08	0.71
1:B:35:ALA:HB3	1:B:103:THR:HG23	1.69	0.71
1:E:59:ARG:NH1	1:E:212:SER:HB2	2.05	0.71
3:H:45:TYR:CE1	3:H:158:TRP:HA	2.25	0.71
3:J:211:ARG:O	7:J:418:HOH:O	2.08	0.71
1:L:49:GLY:HA3	1:L:114:ILE:HD13	1.72	0.71
1:A:270:GLU:OE2	7:A:415:HOH:O	2.08	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TYR:O	1:C:48:SER:OG	2.02	0.71
1:B:134:ASN:OD1	7:B:419:HOH:O	2.07	0.71
1:B:267:LEU:O	1:B:267:LEU:HD22	1.90	0.71
1:C:37:GLU:OE1	7:C:414:HOH:O	2.08	0.71
2:D:98[A]:GLU:HG3	1:E:98:GLU:OE2	1.90	0.71
3:G:100:LEU:HB3	3:G:105:LYS:HE3	1.72	0.71
3:H:230:ASN:ND2	7:H:427:HOH:O	2.24	0.71
1:I:33:PHE:CE1	1:I:82:LEU:HD13	2.26	0.71
1:C:129:TYR:OH	7:C:415:HOH:O	2.09	0.71
2:D:221:ASN:N	7:D:423:HOH:O	2.16	0.71
3:H:96:ASN:CG	3:H:98:GLU:OE1	2.34	0.71
3:J:169:LYS:NZ	7:J:429:HOH:O	2.23	0.71
3:J:208:LYS:O	3:J:211:ARG:HB3	1.90	0.71
1:C:238:SER:OG	7:C:413:HOH:O	2.08	0.71
1:E:276:ASP:O	1:E:279:ARG:HB3	1.90	0.71
3:F:125:MET:O	3:F:126:PHE:C	2.33	0.71
3:G:160:ASP:OD1	7:G:419:HOH:O	2.08	0.71
1:I:184:LYS:HE2	7:I:421:HOH:O	1.90	0.71
1:E:268:PHE:O	1:E:272:MET:N	2.21	0.71
3:G:70:PRO:HG3	3:G:233:ILE:C	2.16	0.71
3:H:79:PHE:O	7:H:417:HOH:O	2.07	0.71
3:H:194:THR:HG23	3:H:199:ILE:O	1.90	0.71
3:H:240:ARG:NH2	7:H:410:HOH:O	2.22	0.71
3:H:256:PHE:O	7:H:418:HOH:O	2.08	0.71
2:D:50:THR:CG2	4:D:301:A3P:O5P	2.37	0.71
1:E:52:TRP:CE3	1:E:182:MET:HE3	2.25	0.71
1:E:181:GLU:OE2	7:E:412:HOH:O	2.09	0.71
3:F:223:ALA:O	7:F:411:HOH:O	2.08	0.71
1:I:54:ALA:CB	1:I:233:ILE:HD12	2.21	0.71
1:A:216:SER:N	7:A:402:HOH:O	2.24	0.71
2:D:51:HIS:CG	7:D:406:HOH:O	2.43	0.71
2:D:103:THR:HB	7:D:461:HOH:O	1.90	0.71
1:L:8:SER:O	7:L:409:HOH:O	2.09	0.71
3:J:77:SER:CB	7:J:402:HOH:O	2.39	0.70
1:C:157:SER:O	1:C:158:TRP:C	2.34	0.70
1:A:178:PHE:HB2	1:A:181:GLU:HB2	1.72	0.70
2:D:194:THR:OG1	2:D:199:ILE:O	2.09	0.70
1:E:120:ASP:O	1:E:121:THR:C	2.32	0.70
3:F:262:ARG:O	3:F:266:GLU:HG3	1.91	0.70
3:J:204:SER:O	3:J:207:ALA:HB3	1.90	0.70
4:K:301:A3P:C5'	7:K:405:HOH:O	2.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:SER:HB3	7:C:438:HOH:O	1.91	0.70
2:D:152:ASP:OD2	7:D:418:HOH:O	2.09	0.70
2:D:205:GLU:O	2:D:209:ILE:HG13	1.91	0.70
3:H:38:ASP:OD2	7:H:419:HOH:O	2.08	0.70
3:H:172:LYS:NZ	1:I:174:VAL:O	2.24	0.70
3:F:190:LEU:HA	3:F:193:ILE:HD12	1.72	0.70
1:L:234:CYS:HB3	1:L:237:THR:HG23	1.74	0.70
1:C:84:ARG:NH1	7:C:423:HOH:O	2.24	0.70
1:A:79:PHE:O	1:A:82:LEU:N	2.24	0.70
3:H:178:PHE:HB2	3:H:181[B]:GLU:HB2	1.72	0.70
1:L:77:SER:C	7:L:434:HOH:O	2.34	0.70
1:C:25:GLU:HB3	1:C:76:ILE:HG23	1.73	0.70
1:B:170:ASN:HA	7:B:408:HOH:O	1.92	0.70
1:E:59:ARG:NH1	1:E:212:SER:CB	2.54	0.70
3:J:192:LYS:O	7:J:419:HOH:O	2.09	0.70
2:D:96:ASN:C	2:D:96:ASN:OD1	2.34	0.70
1:E:231:HIS:ND1	1:E:231:HIS:O	2.25	0.70
3:H:153:VAL:HA	7:H:422:HOH:O	1.92	0.70
1:I:79:PHE:O	1:I:80:GLU:C	2.33	0.70
2:D:192:LYS:NZ	7:D:407:HOH:O	1.91	0.70
3:G:47:LYS:NZ	4:G:301:A3P:O5P	2.25	0.70
3:H:220:SER:O	3:H:221:ASN:CG	2.34	0.70
3:J:138:THR:CG2	3:J:139:GLU:N	2.54	0.70
1:C:119:LYS:HE3	1:C:264:PHE:CD1	2.26	0.70
1:A:98:GLU:OE2	7:A:417:HOH:O	2.08	0.70
1:B:128:TYR:OH	1:B:237:THR:HB	1.91	0.70
1:B:261:ASN:ND2	7:B:429:HOH:O	2.25	0.70
1:I:85:ILE:HB	7:I:404:HOH:O	1.92	0.70
4:K:301:A3P:O3P	4:K:301:A3P:O2'	2.09	0.70
3:F:225:GLU:OE1	3:F:226:ASN:N	2.25	0.70
1:I:11:HIS:CE1	1:I:19:SER:O	2.45	0.70
2:D:203:ASP:O	7:D:417:HOH:O	2.08	0.69
1:K:265:ASP:C	7:K:404:HOH:O	2.35	0.69
2:D:276:ASP:O	2:D:279:ARG:N	2.24	0.69
3:J:239:ASP:OD2	3:J:242:LEU:HG	1.93	0.69
1:B:26:LEU:HD11	1:B:79:PHE:CZ	2.27	0.69
1:E:203:ASP:O	1:E:204:SER:C	2.34	0.69
3:F:98:GLU:H	3:F:98:GLU:CD	2.00	0.69
1:L:202:ASN:N	1:L:205:GLU:OE2	2.25	0.69
1:A:224:LYS:HD3	1:A:228:ASP:HA	1.74	0.69
2:D:211:ARG:NH1	7:D:429:HOH:O	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:LEU:CD2	3:F:136:PRO:HD3	2.23	0.69
3:H:168:HIS:HB3	3:H:171:ASP:OD2	1.93	0.69
1:I:181:GLU:HB2	1:I:184:LYS:HZ1	1.57	0.69
1:C:12:LYS:HD3	1:C:17:PHE:CE2	2.28	0.69
1:C:52:TRP:O	1:C:56:VAL:HG23	1.93	0.69
1:A:35:ALA:HB3	1:A:103:THR:HG23	1.74	0.69
1:A:237:THR:HB	7:A:483:HOH:O	1.92	0.69
4:B:301:A3P:O4P	7:B:420:HOH:O	2.09	0.69
1:E:76:ILE:H	1:E:76:ILE:HD13	1.58	0.69
1:E:98:GLU:HG2	7:E:418:HOH:O	1.92	0.69
3:G:11:HIS:HD2	7:G:446:HOH:O	1.74	0.69
3:G:240:ARG:O	3:G:243:VAL:HG13	1.92	0.69
3:H:57:ILE:O	3:H:60:ILE:HG13	1.92	0.69
1:I:59:ARG:O	1:I:60:ILE:C	2.35	0.69
1:L:25:GLU:HB3	1:L:76:ILE:HG23	1.72	0.69
1:B:35:ALA:H	1:B:103:THR:HG21	1.57	0.69
2:D:175:LEU:HD11	2:D:192:LYS:HE2	1.74	0.69
1:I:10:LEU:HD22	1:I:154:VAL:HG12	1.73	0.69
3:J:185:ASP:OD1	7:J:420:HOH:O	2.11	0.69
1:B:50:THR:N	4:B:301:A3P:O5P	2.23	0.69
1:B:50:THR:OG1	1:B:94:HIS:HE1	1.74	0.69
1:E:181:GLU:HB2	1:E:184:LYS:CE	2.22	0.69
3:H:50:THR:N	7:H:405:HOH:O	2.25	0.69
1:L:44:SER:CB	1:L:114:ILE:CG2	2.71	0.69
1:A:25:GLU:O	1:A:29:SER:OG	2.04	0.69
1:B:221:ASN:C	7:B:422:HOH:O	2.36	0.69
2:D:39:ASP:CG	2:D:89:ARG:HH21	2.00	0.69
3:F:69:SER:O	3:F:70:PRO:C	2.35	0.69
1:A:84:ARG:O	7:A:418:HOH:O	2.10	0.69
3:H:160:ASP:OD2	7:H:421:HOH:O	2.11	0.69
1:E:188:LYS:CE	7:E:406:HOH:O	2.39	0.69
3:F:50:THR:OG1	4:F:301:A3P:O5P	2.05	0.69
1:I:120:ASP:OD1	1:I:252:TRP:HD1	1.76	0.69
1:A:76:ILE:HD13	1:A:76:ILE:H	1.58	0.68
1:A:191:LYS:O	7:A:421:HOH:O	2.11	0.68
1:A:231:HIS:CE1	7:A:409:HOH:O	2.42	0.68
3:H:100:LEU:O	7:H:420:HOH:O	2.09	0.68
1:L:117:ASN:OD1	1:L:120:ASP:HB2	1.93	0.68
3:F:100:LEU:O	3:F:105:LYS:HE3	1.93	0.68
3:H:181[B]:GLU:OE2	3:H:189:SER:OG	2.11	0.68
3:H:184:LYS:HG2	3:H:185:ASP:N	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:GLU:HA	1:L:184:LYS:HD3	1.75	0.68
1:A:225:GLU:HB3	1:A:231:HIS:CE1	2.27	0.68
3:J:56:VAL:HG23	7:J:403:HOH:O	1.93	0.68
1:E:208:LYS:O	1:E:211:ARG:HB3	1.92	0.68
3:H:49:GLY:HA3	3:H:114:ILE:HD13	1.74	0.68
1:I:52:TRP:O	1:I:56:VAL:HG23	1.93	0.68
4:J:301:A3P:P2	7:J:408:HOH:O	2.51	0.68
2:D:276:ASP:OD2	3:F:274:ASN:HB3	1.92	0.68
1:I:11:HIS:HE1	1:I:19:SER:O	1.75	0.68
1:I:194:THR:CG2	1:I:195:ALA:N	2.56	0.68
1:C:220:SER:O	1:C:221:ASN:CG	2.37	0.68
3:J:203:ASP:O	3:J:204:SER:C	2.36	0.68
1:E:181:GLU:HB2	1:E:184:LYS:HE2	1.75	0.68
1:E:251:ASP:OD1	1:E:254:ASN:ND2	2.26	0.68
3:G:117:ASN:HA	3:G:281:LEU:HD22	1.75	0.68
1:K:234:CYS:HB3	1:K:237:THR:HG22	1.75	0.68
1:B:128:TYR:OH	1:B:237:THR:CG2	2.42	0.68
1:B:133:PRO:CA	2:D:211:ARG:NH1	2.53	0.68
2:D:70:PRO:HD3	2:D:232:VAL:O	1.94	0.68
3:H:12:LYS:HD2	3:H:17:PHE:CE2	2.29	0.68
3:H:35:ALA:HB3	3:H:103:THR:HG23	1.75	0.68
3:H:69:SER:OG	3:H:78:LYS:NZ	2.19	0.68
1:K:38:ASP:OD1	7:K:413:HOH:O	2.11	0.68
1:L:184:LYS:HG2	1:L:185:ASP:N	2.08	0.68
1:A:251:ASP:OD2	7:A:422:HOH:O	2.11	0.68
2:D:35:ALA:CB	2:D:103:THR:HG23	2.24	0.68
3:J:247:GLY:N	4:J:301:A3P:O3P	2.24	0.68
1:L:215:PHE:CZ	1:L:246:LYS:O	2.47	0.68
1:C:9:LEU:HD21	1:C:133:PRO:O	1.93	0.68
1:C:50:THR:OG1	4:C:301:A3P:O5P	2.08	0.68
1:C:234:CYS:HB3	1:C:237:THR:HG23	1.76	0.68
2:D:257:THR:O	2:D:260:GLN:N	2.27	0.68
3:F:286:HIS:C	3:F:288:ALA:HA	2.19	0.68
3:J:221:ASN:ND2	7:J:432:HOH:O	2.27	0.68
1:L:219:LYS:HG3	1:L:244:PHE:HB2	1.75	0.68
1:B:16:ILE:HG22	1:B:17:PHE:N	2.10	0.67
3:H:12:LYS:HD2	3:H:17:PHE:CD2	2.28	0.67
1:L:181:GLU:HB2	1:L:184:LYS:CE	2.22	0.67
1:L:213:THR:OG1	7:L:410:HOH:O	2.13	0.67
1:C:102:VAL:CG1	1:C:103:THR:N	2.56	0.67
1:A:231:HIS:CE1	1:A:240:ARG:NH1	2.62	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:OD2	1:A:242:LEU:HG	1.93	0.67
3:G:225:GLU:HG2	3:G:231:HIS:CE1	2.29	0.67
1:C:26:LEU:HD12	1:C:26:LEU:O	1.94	0.67
1:E:35:ALA:HB3	1:E:103:THR:HG23	1.76	0.67
3:H:82:LEU:HB2	7:H:417:HOH:O	1.93	0.67
3:H:202:ASN:ND2	3:H:205:GLU:HG2	2.10	0.67
3:H:230:ASN:N	3:H:230:ASN:OD1	2.23	0.67
1:I:177:ILE:HD13	1:I:192:LYS:HE2	1.76	0.67
1:A:37:GLU:OE1	7:A:420:HOH:O	2.11	0.67
2:D:148:PHE:O	7:D:419:HOH:O	2.11	0.67
1:E:81:GLU:O	7:E:414:HOH:O	2.12	0.67
1:L:225:GLU:CD	1:L:231:HIS:HB2	2.18	0.67
1:C:202:ASN:N	1:C:205:GLU:OE2	2.23	0.67
1:A:79:PHE:O	1:A:80:GLU:C	2.37	0.67
1:B:18:PHE:HZ	1:B:99:MET:HE1	1.60	0.67
1:E:234:CYS:HB3	1:E:237:THR:CG2	2.25	0.67
1:A:116:ARG:NH2	4:A:301:A3P:O3P	2.26	0.67
3:F:262:ARG:CD	7:F:412:HOH:O	2.42	0.67
3:G:234:CYS:HB3	3:G:237:THR:HG23	1.77	0.67
3:J:160:ASP:OD2	7:J:424:HOH:O	2.12	0.67
3:J:243:VAL:O	7:J:421:HOH:O	2.11	0.67
1:K:276:ASP:OD2	1:K:279:ARG:NH2	2.25	0.67
3:G:67:LEU:HA	3:G:90:ALA:HB3	1.77	0.67
3:J:130:ARG:HG3	7:J:423:HOH:O	1.94	0.67
3:J:130:ARG:O	7:J:423:HOH:O	2.12	0.67
1:L:215:PHE:HA	4:L:301:A3P:C6	2.24	0.67
1:C:251:ASP:O	1:C:254:ASN:N	2.28	0.67
1:A:185:ASP:OD2	7:A:423:HOH:O	2.13	0.67
1:A:234:CYS:CB	1:A:237:THR:HG22	2.25	0.67
2:D:39:ASP:HA	7:D:411:HOH:O	1.94	0.67
1:I:77:SER:OG	7:I:410:HOH:O	2.12	0.67
3:J:206:MET:O	3:J:209:ILE:N	2.27	0.67
1:A:98:GLU:HG2	7:A:491:HOH:O	1.93	0.67
2:D:243:VAL:O	7:D:402:HOH:O	2.13	0.67
3:J:110:LYS:O	3:J:111:ILE:HD13	1.95	0.67
1:E:95:LEU:CD2	1:E:99:MET:HE3	2.25	0.67
3:F:187:VAL:O	3:F:188:LYS:C	2.34	0.67
3:G:206:MET:HA	3:G:209:ILE:HG13	1.76	0.67
3:H:213:THR:O	4:H:301:A3P:N6	2.28	0.67
1:I:78:LYS:O	1:I:82:LEU:HG	1.95	0.67
3:J:188:LYS:O	7:J:422:HOH:O	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:HIS:NE2	7:L:416:HOH:O	2.26	0.67
1:E:188:LYS:NZ	7:E:406:HOH:O	1.95	0.66
3:G:181:GLU:HG3	7:G:475:HOH:O	1.94	0.66
3:H:221:ASN:O	3:H:241:ASN:ND2	2.26	0.66
3:J:22:SER:OG	3:J:72:GLU:O	2.11	0.66
3:J:205:GLU:O	3:J:209:ILE:HG12	1.95	0.66
1:K:276:ASP:CG	1:K:279:ARG:HH22	2.03	0.66
1:A:231:HIS:CE1	1:A:240:ARG:HH11	2.13	0.66
1:B:175:LEU:HD11	1:B:192:LYS:HE3	1.77	0.66
2:D:76:ILE:HD13	2:D:76:ILE:H	1.59	0.66
3:G:51:HIS:O	7:G:422:HOH:O	2.12	0.66
3:G:240:ARG:O	3:G:241:ASN:C	2.38	0.66
3:H:45:TYR:OH	3:H:156:GLY:O	2.07	0.66
3:J:234:CYS:HB3	3:J:237:THR:CG2	2.25	0.66
1:L:38:ASP:OD2	7:L:413:HOH:O	2.13	0.66
1:L:130:ARG:HD2	7:L:401:HOH:O	1.94	0.66
1:E:35:ALA:H	1:E:103:THR:CG2	2.08	0.66
1:E:266:GLU:CB	7:E:402:HOH:O	2.33	0.66
3:H:202:ASN:HD21	3:H:205:GLU:HG2	1.60	0.66
3:J:114:ILE:HD12	7:J:550:HOH:O	1.94	0.66
3:J:207:ALA:O	3:J:208:LYS:C	2.39	0.66
1:K:276:ASP:OD1	7:K:415:HOH:O	2.14	0.66
1:L:181:GLU:HB2	1:L:184:LYS:HE2	1.77	0.66
1:C:40:ILE:HG22	1:C:41:PHE:N	2.10	0.66
3:F:286:HIS:O	3:F:288:ALA:HA	1.96	0.66
1:I:18:PHE:HZ	1:I:99:MET:HE1	1.60	0.66
1:I:98:GLU:CD	1:I:98:GLU:H	2.03	0.66
1:C:229:PRO:O	7:C:416:HOH:O	2.12	0.66
3:G:256:PHE:HA	3:G:260:GLN:OE1	1.94	0.66
1:K:30:LEU:HB2	7:K:446:HOH:O	1.95	0.66
1:E:39:ASP:OD1	7:E:415:HOH:O	2.13	0.66
3:F:99:MET:HA	7:F:435:HOH:O	1.95	0.66
3:F:138:THR:HG21	3:F:144:PHE:HB2	1.77	0.66
3:F:195:ALA:O	3:F:196:PHE:C	2.39	0.66
3:J:194:THR:HG23	3:J:199:ILE:O	1.96	0.66
3:G:181:GLU:HG3	3:G:189:SER:OG	1.96	0.66
3:G:239:ASP:CG	3:G:242:LEU:HG	2.20	0.66
3:J:53:LEU:CA	7:J:403:HOH:O	2.37	0.66
1:L:47:LYS:N	4:L:301:A3P:O5P	2.24	0.66
1:C:25:GLU:CD	1:C:25:GLU:H	2.04	0.66
1:I:181:GLU:HB2	1:I:184:LYS:CE	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ALA:O	1:C:196:PHE:C	2.38	0.66
1:B:116:ARG:HB2	1:B:179:TYR:HB2	1.77	0.66
3:G:98[A]:GLU:CG	1:I:98:GLU:CG	2.74	0.66
3:J:60:ILE:CG2	3:J:61:PRO:HD2	2.25	0.66
1:L:213:THR:HB	7:L:406:HOH:O	1.94	0.66
1:L:239:ASP:OD2	7:L:412:HOH:O	2.13	0.66
1:L:281:LEU:HA	1:L:284:TYR:HD2	1.60	0.66
1:C:40:ILE:HB	1:C:90:ALA:HA	1.78	0.66
1:B:17:PHE:HB2	1:B:154:VAL:HA	1.76	0.66
2:D:168:HIS:HE1	1:E:167:GLU:HG3	1.61	0.66
3:H:185:ASP:OD1	7:H:423:HOH:O	2.13	0.66
3:H:211:ARG:NH2	7:H:426:HOH:O	2.29	0.66
3:J:25[B]:GLU:OE1	3:J:76:ILE:HD13	1.95	0.66
1:K:76:ILE:H	1:K:76:ILE:HD13	1.61	0.66
1:K:217:GLU:O	1:K:220:SER:OG	2.11	0.66
2:D:40:ILE:HB	2:D:90:ALA:HA	1.78	0.65
3:F:75:ASP:OD2	7:F:416:HOH:O	2.14	0.65
3:G:89:ARG:NH1	7:G:435:HOH:O	2.28	0.65
1:I:184:LYS:HG2	1:I:185:ASP:H	1.60	0.65
3:J:258:PRO:O	3:J:262:ARG:HG2	1.96	0.65
1:A:105:LYS:NZ	7:A:417:HOH:O	2.29	0.65
2:D:43:VAL:HG11	2:D:165:TRP:CZ2	2.30	0.65
3:F:9:LEU:HD23	3:F:136:PRO:HD3	1.78	0.65
1:I:94:HIS:HB2	1:I:155:TYR:CZ	2.31	0.65
1:I:199:ILE:HG22	1:I:201:VAL:HG23	1.77	0.65
1:C:211:ARG:HB3	7:C:429:HOH:O	1.94	0.65
1:B:10:LEU:HD22	1:B:154:VAL:CG1	2.27	0.65
2:D:60:ILE:O	7:D:421:HOH:O	2.14	0.65
3:J:222:ALA:O	3:J:223:ALA:HB2	1.94	0.65
1:A:68:THR:O	1:A:92:PRO:CD	2.45	0.65
1:A:188:LYS:O	7:A:424:HOH:O	2.14	0.65
1:B:151:GLY:O	7:B:415:HOH:O	2.12	0.65
3:G:261:ASN:O	3:G:262:ARG:C	2.40	0.65
1:I:10:LEU:HD22	1:I:154:VAL:CG1	2.26	0.65
1:K:221:ASN:O	1:K:221:ASN:OD1	2.15	0.65
1:B:117:ASN:ND2	1:B:180:GLU:OE2	2.29	0.65
2:D:11:HIS:CE1	2:D:20:THR:HA	2.32	0.65
2:D:137:SER:O	7:D:420:HOH:O	2.13	0.65
1:E:98:GLU:CG	7:E:418:HOH:O	2.44	0.65
3:G:99:MET:O	3:G:100:LEU:C	2.37	0.65
3:J:205:GLU:O	3:J:206:MET:C	2.39	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLU:OE1	1:C:283:GLU:N	2.29	0.65
1:B:216:SER:CB	7:B:412:HOH:O	2.44	0.65
2:D:51:HIS:HA	2:D:233:ILE:HD11	1.77	0.65
3:H:12:LYS:HE3	3:H:17:PHE:CG	2.31	0.65
3:H:31:ASP:C	3:H:33:PHE:H	2.05	0.65
1:I:78:LYS:HA	7:I:410:HOH:O	1.96	0.65
1:A:160:ASP:OD1	7:A:425:HOH:O	2.15	0.65
1:A:257:THR:O	1:A:259:LYS:N	2.30	0.65
1:B:258:PRO:O	1:B:262:ARG:HG2	1.97	0.65
2:D:257:THR:O	2:D:258:PRO:C	2.39	0.65
3:F:181[B]:GLU:CG	3:F:184:LYS:HE2	2.26	0.65
3:J:263:GLY:O	3:J:266:GLU:HB3	1.96	0.65
1:C:12:LYS:CD	1:C:17:PHE:CD2	2.79	0.65
2:D:25:GLU:HB3	2:D:76:ILE:HD12	1.78	0.65
2:D:191:LYS:O	2:D:194:THR:HG22	1.97	0.65
2:D:245:ARG:HB2	7:D:402:HOH:O	1.97	0.65
3:F:115:VAL:O	3:F:115:VAL:HG13	1.94	0.65
3:G:47:LYS:HZ1	4:G:301:A3P:H5'1	1.61	0.65
3:G:196:PHE:CZ	7:G:403:HOH:O	2.50	0.65
3:H:186:PHE:CD1	3:H:186:PHE:C	2.75	0.65
1:I:37:GLU:CD	1:I:107:LYS:HD3	2.22	0.65
3:J:182:MET:HG3	7:J:550:HOH:O	1.95	0.65
1:K:26:LEU:O	1:K:29:SER:N	2.29	0.65
1:A:67:LEU:HA	1:A:90:ALA:HB3	1.79	0.65
2:D:98[A]:GLU:CG	1:E:98:GLU:CD	2.69	0.65
2:D:181:GLU:HB2	2:D:184:LYS:HE2	1.78	0.65
1:K:205:GLU:HA	1:K:208:LYS:HD2	1.78	0.65
1:K:234:CYS:HB3	1:K:237:THR:CG2	2.26	0.65
1:L:206:MET:HA	1:L:209:ILE:HG13	1.78	0.65
1:C:184:LYS:CG	1:C:185:ASP:N	2.60	0.65
1:A:234:CYS:HB3	1:A:237:THR:HG21	1.78	0.65
3:F:79:PHE:CD1	7:F:410:HOH:O	2.49	0.65
3:H:218:MET:O	3:H:221:ASN:ND2	2.30	0.65
1:L:55:GLU:HB2	1:L:218:MET:HE3	1.78	0.65
1:A:205:GLU:O	1:A:209:ILE:CG1	2.45	0.64
1:B:45:TYR:CD2	1:B:158:TRP:HD1	2.15	0.64
3:G:205:GLU:O	3:G:208:LYS:CB	2.45	0.64
3:G:239:ASP:OD1	3:G:241:ASN:N	2.30	0.64
1:K:70:PRO:O	1:K:78:LYS:NZ	2.25	0.64
2:D:234:CYS:SG	2:D:237:THR:HG23	2.38	0.64
1:E:181:GLU:HA	1:E:184:LYS:HD3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:PHE:O	7:F:414:HOH:O	2.14	0.64
3:G:98[A]:GLU:OE2	1:I:98:GLU:HG3	1.96	0.64
3:G:188:LYS:HD2	7:G:475:HOH:O	1.98	0.64
3:H:30:LEU:HA	3:H:79:PHE:HZ	1.62	0.64
1:A:44:SER:OG	1:A:50:THR:OG1	2.08	0.64
4:E:301:A3P:H3'	7:E:433:HOH:O	1.97	0.64
1:K:272:MET:O	1:K:273:ARG:C	2.40	0.64
3:F:36:ARG:O	3:F:37:GLU:C	2.37	0.64
3:G:239:ASP:OD1	3:G:239:ASP:C	2.38	0.64
1:I:284:TYR:C	1:I:286:HIS:H	2.05	0.64
1:C:39:ASP:CG	1:C:89:ARG:HE	2.06	0.64
2:D:96:ASN:OD1	2:D:98[A]:GLU:N	2.31	0.64
3:F:114:ILE:O	7:F:415:HOH:O	2.14	0.64
1:I:79:PHE:HB3	7:I:441:HOH:O	1.96	0.64
3:J:96:ASN:HA	3:J:165:TRP:NE1	2.09	0.64
3:J:177:ILE:HD13	3:J:192:LYS:HE2	1.78	0.64
1:K:42:LEU:N	1:K:91:ILE:O	2.25	0.64
1:C:285:ALA:HA	1:C:288:ALA:HB3	1.80	0.64
1:E:98:GLU:CD	7:E:418:HOH:O	2.40	0.64
1:I:181:GLU:HB2	1:I:184:LYS:HE2	1.80	0.64
3:J:266:GLU:OE2	3:J:267:LEU:CA	2.45	0.64
1:C:205:GLU:HG2	7:C:479:HOH:O	1.96	0.64
1:B:243:VAL:O	4:B:301:A3P:H2'	1.98	0.64
3:G:36:ARG:N	3:G:39:ASP:OD2	2.22	0.64
1:I:116:ARG:HB2	1:I:179:TYR:HB2	1.80	0.64
1:A:245:ARG:NH1	1:A:251:ASP:OD2	2.28	0.64
1:B:139:GLU:OE2	7:B:423:HOH:O	2.15	0.64
3:F:36:ARG:HD2	7:F:413:HOH:O	1.94	0.64
3:H:101:PRO:HB2	3:H:104:VAL:HG23	1.79	0.64
1:K:95:LEU:HA	7:K:412:HOH:O	1.96	0.64
1:K:100:LEU:O	1:K:105:LYS:HE3	1.98	0.64
1:K:222:ALA:O	1:K:223:ALA:CB	2.46	0.64
1:C:36:ARG:HB3	1:C:38:ASP:OD1	1.98	0.64
1:B:35:ALA:CB	1:B:103:THR:HG23	2.28	0.64
1:E:22:SER:OG	1:E:72:GLU:O	2.15	0.64
3:F:225:GLU:HB3	7:F:496:HOH:O	1.98	0.64
1:I:168:HIS:CE1	7:I:403:HOH:O	2.42	0.64
3:J:113:TYR:OH	3:J:161:HIS:HD2	1.81	0.64
1:L:70:PRO:O	1:L:78:LYS:NZ	2.30	0.64
3:F:124:SER:CB	4:F:301:A3P:O1P	2.46	0.64
3:H:157:SER:O	3:H:158:TRP:C	2.41	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:GLU:OE2	7:L:415:HOH:O	2.14	0.64
1:C:70:PRO:HG3	1:C:233:ILE:O	1.98	0.63
1:C:120:ASP:OD1	1:C:252:TRP:HD1	1.81	0.63
1:A:228:ASP:O	1:A:229:PRO:C	2.39	0.63
3:F:76:ILE:HD13	3:F:76:ILE:H	1.63	0.63
3:F:117:ASN:OD1	3:F:120:ASP:CG	2.41	0.63
1:I:269:THR:HA	7:I:417:HOH:O	1.98	0.63
3:J:250:GLY:O	3:J:253:ILE:HG12	1.98	0.63
1:C:9:LEU:O	7:C:417:HOH:O	2.15	0.63
1:B:214:SER:HB3	1:B:217:GLU:HB3	1.80	0.63
1:B:222:ALA:O	1:B:223:ALA:HB2	1.97	0.63
3:F:125:MET:O	3:F:127:HIS:N	2.31	0.63
3:H:23:SER:OG	3:H:26:LEU:HB2	1.98	0.63
3:H:150:LYS:HE3	3:H:152:ASP:OD2	1.98	0.63
1:C:115:VAL:O	1:C:115:VAL:HG13	1.98	0.63
1:A:23:SER:O	1:A:27:LEU:HG	1.98	0.63
2:D:98[A]:GLU:CG	1:E:98:GLU:CG	2.77	0.63
2:D:234:CYS:HB3	2:D:237:THR:HG23	1.79	0.63
1:E:206:MET:O	1:E:209:ILE:HB	1.99	0.63
3:H:166:GLU:HA	3:H:176:PHE:CZ	2.33	0.63
3:J:52:TRP:CD2	3:J:182:MET:HE3	2.34	0.63
1:C:193:ILE:O	1:C:194:THR:C	2.42	0.63
1:C:280:CYS:HA	1:C:283:GLU:HG2	1.80	0.63
3:F:36:ARG:O	3:F:39:ASP:N	2.29	0.63
3:F:234:CYS:HB3	3:F:237:THR:CG2	2.29	0.63
1:B:44:SER:CB	1:B:114:ILE:HG23	2.29	0.63
1:I:128:TYR:OH	1:I:237:THR:HB	1.97	0.63
3:J:100:LEU:HB3	3:J:105:LYS:HE3	1.81	0.63
3:J:161:HIS:HB2	7:J:463:HOH:O	1.97	0.63
1:A:272:MET:O	1:A:273:ARG:C	2.38	0.63
2:D:220:SER:O	7:D:422:HOH:O	2.16	0.63
1:K:29:SER:O	1:K:79:PHE:CZ	2.51	0.63
1:C:12:LYS:HE3	1:C:17:PHE:CD1	2.34	0.63
1:B:132:ASN:OD1	1:B:134:ASN:HB2	1.99	0.63
3:J:282:LYS:O	3:J:283:GLU:C	2.42	0.63
1:K:180:GLU:HG2	1:K:284:TYR:HB3	1.80	0.63
1:A:70:PRO:HA	1:A:92:PRO:O	1.99	0.63
1:E:220:SER:C	1:E:221:ASN:CG	2.66	0.63
3:F:36:ARG:O	3:F:38:ASP:N	2.32	0.63
3:H:239:ASP:C	3:H:239:ASP:OD1	2.42	0.63
3:J:25[B]:GLU:CD	3:J:76:ILE:CD1	2.72	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:39:ASP:O	3:J:109:CYS:HB3	1.98	0.63
1:K:79:PHE:O	1:K:80:GLU:C	2.39	0.63
2:D:258:PRO:O	2:D:262:ARG:HG2	1.98	0.63
1:E:12:LYS:CD	1:E:17:PHE:CD2	2.82	0.62
3:G:39:ASP:HB2	3:G:109:CYS:SG	2.38	0.62
3:G:218:MET:HA	7:G:442:HOH:O	1.98	0.62
3:H:16:ILE:O	3:H:18:PHE:CD1	2.52	0.62
1:I:173:ASN:HB3	7:I:419:HOH:O	1.99	0.62
3:J:173:ASN:HB3	7:J:533:HOH:O	1.98	0.62
1:L:73:LEU:O	1:L:78:LYS:NZ	2.31	0.62
1:L:186:PHE:CD1	1:L:186:PHE:C	2.77	0.62
1:A:188:LYS:HG2	7:A:529:HOH:O	1.99	0.62
1:B:70:PRO:HG3	1:B:233:ILE:O	2.00	0.62
1:E:191:LYS:O	1:E:194:THR:HG22	1.98	0.62
3:H:211:ARG:CZ	7:H:426:HOH:O	2.47	0.62
2:D:50:THR:HG23	4:D:301:A3P:P2	2.39	0.62
1:I:54:ALA:HB3	1:I:233:ILE:HD12	1.81	0.62
1:I:88:ARG:NH2	7:I:416:HOH:O	2.14	0.62
1:I:269:THR:O	7:I:417:HOH:O	2.16	0.62
1:C:123:VAL:O	1:C:124:SER:C	2.41	0.62
1:C:202:ASN:OD1	1:C:205:GLU:HG3	1.99	0.62
1:B:43:VAL:O	1:B:114:ILE:N	2.32	0.62
1:E:35:ALA:H	1:E:103:THR:HG21	1.65	0.62
1:E:59:ARG:NH1	1:E:212:SER:OG	2.33	0.62
1:E:137:SER:N	7:E:404:HOH:O	2.32	0.62
1:E:271:LYS:HE3	7:E:470:HOH:O	2.00	0.62
3:F:128:TYR:OH	3:F:237:THR:HB	2.00	0.62
3:G:132:ASN:O	3:G:135:LEU:N	2.29	0.62
3:H:172:LYS:HE2	1:I:169:LYS:O	1.99	0.62
3:H:277:VAL:O	3:H:278:GLY:C	2.40	0.62
3:J:98[A]:GLU:CD	3:J:98[A]:GLU:N	2.56	0.62
1:K:102:VAL:HG13	1:K:103:THR:N	2.12	0.62
1:L:48:SER:HA	1:L:116:ARG:CB	2.28	0.62
1:C:77:SER:O	1:C:80:GLU:N	2.33	0.62
1:A:49:GLY:C	7:A:412:HOH:O	2.41	0.62
1:E:222:ALA:O	1:E:223:ALA:CB	2.47	0.62
3:F:186:PHE:N	7:F:428:HOH:O	2.31	0.62
1:K:264:PHE:C	1:K:264:PHE:CD1	2.78	0.62
1:C:70:PRO:O	1:C:78:LYS:NZ	2.33	0.62
1:C:117:ASN:HD21	1:C:120:ASP:CG	2.07	0.62
3:F:78:LYS:HB3	7:F:410:HOH:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:218:MET:O	3:F:221:ASN:ND2	2.33	0.62
1:I:79:PHE:C	7:I:441:HOH:O	2.43	0.62
3:J:182:MET:CG	7:J:550:HOH:O	2.43	0.62
1:L:260:GLN:CA	7:L:405:HOH:O	2.40	0.62
2:D:248:VAL:HG22	2:D:249:VAL:H	1.65	0.62
1:C:11:HIS:HE1	1:C:19:SER:O	1.83	0.62
1:C:103:THR:HA	1:C:106:GLN:HG3	1.80	0.62
1:E:25:GLU:HB3	1:E:76:ILE:HD12	1.82	0.62
1:E:217:GLU:O	1:E:221:ASN:OD1	2.18	0.62
1:I:37:GLU:HG2	7:I:508:HOH:O	1.99	0.62
1:L:52:TRP:O	1:L:56:VAL:HG23	2.00	0.62
1:C:184:LYS:HG2	1:C:185:ASP:H	1.63	0.62
1:C:215:PHE:O	1:C:219:LYS:N	2.32	0.62
1:A:98:GLU:HG3	7:B:537:HOH:O	1.99	0.62
2:D:11:HIS:HE1	2:D:19:SER:O	1.83	0.62
3:G:261:ASN:O	3:G:264:PHE:N	2.33	0.62
1:I:185:ASP:HA	7:I:407:HOH:O	2.00	0.62
1:K:279:ARG:NH2	1:L:274:ASN:HB3	2.14	0.62
1:L:6:ALA:N	1:L:7:PRO:CD	2.61	0.62
1:L:116:ARG:CG	1:L:121:THR:OG1	2.48	0.62
1:C:11:HIS:CE1	1:C:19:SER:O	2.53	0.62
1:C:127:HIS:CD2	1:C:245:ARG:NH2	2.68	0.62
1:A:101:PRO:HB2	1:A:104:VAL:HG23	1.81	0.62
3:G:41:PHE:HB2	3:G:111:ILE:HD13	1.82	0.62
3:G:231:HIS:CG	3:G:231:HIS:O	2.53	0.62
3:H:56:VAL:O	3:H:57:ILE:C	2.43	0.62
1:L:286:HIS:CE1	7:L:416:HOH:O	2.52	0.62
2:D:30:LEU:HA	2:D:79:PHE:HZ	1.65	0.61
3:F:33:PHE:CE2	3:F:35:ALA:HA	2.34	0.61
3:G:44:SER:HB3	3:G:114:ILE:CG2	2.29	0.61
3:J:234:CYS:HB3	3:J:237:THR:HG23	1.82	0.61
1:B:16:ILE:CG2	1:B:17:PHE:N	2.63	0.61
1:E:125:MET:CE	1:E:153:VAL:HB	2.30	0.61
1:C:187:VAL:HG12	1:C:191:LYS:HE3	1.81	0.61
3:H:196:PHE:C	7:H:407:HOH:O	2.44	0.61
3:H:250:GLY:O	3:H:253:ILE:HG12	2.00	0.61
3:H:270:GLU:O	3:H:273:ARG:NE	2.30	0.61
1:A:222:ALA:N	7:A:437:HOH:O	2.32	0.61
1:A:251:ASP:CG	7:A:422:HOH:O	2.44	0.61
3:G:128:TYR:OH	3:G:237:THR:CB	2.48	0.61
1:K:252:TRP:C	1:K:254:ASN:H	2.07	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LYS:HA	1:C:173:ASN:O	2.00	0.61
1:C:220:SER:O	1:C:221:ASN:OD1	2.19	0.61
1:C:268:PHE:CE1	1:C:272:MET:HG3	2.36	0.61
3:G:184:LYS:HG2	3:G:185:ASP:N	2.14	0.61
1:C:77:SER:O	1:C:80:GLU:HB3	2.00	0.61
1:B:151:GLY:HA2	1:B:157:SER:HA	1.81	0.61
4:D:301:A3P:H3'	7:D:466:HOH:O	2.00	0.61
3:F:12:LYS:HE3	3:F:17:PHE:CG	2.36	0.61
1:I:228:ASP:N	1:I:229:PRO:HD2	2.16	0.61
3:G:136:PRO:HA	7:G:401:HOH:O	2.01	0.61
3:J:257:THR:OG1	7:J:426:HOH:O	2.16	0.61
1:C:170:ASN:HA	1:B:172:LYS:HE2	1.83	0.61
1:A:68:THR:OG1	1:A:91:ILE:HA	2.01	0.61
1:A:136:PRO:HA	7:A:419:HOH:O	2.00	0.61
1:B:102:VAL:O	1:B:106:GLN:HG3	2.01	0.61
1:E:267:LEU:O	1:E:270:GLU:N	2.33	0.61
3:G:47:LYS:CA	4:G:301:A3P:P2	2.88	0.61
3:J:129:TYR:O	3:J:137:SER:HA	2.01	0.61
1:K:40:ILE:O	1:K:91:ILE:N	2.27	0.61
2:D:208:LYS:O	2:D:211:ARG:HB3	2.01	0.61
3:G:47:LYS:NZ	4:G:301:A3P:H5'1	2.16	0.61
3:H:26:LEU:CB	3:H:75:ASP:O	2.49	0.61
3:H:67:LEU:HA	3:H:90:ALA:O	2.00	0.61
3:J:164:SER:HB3	7:J:438:HOH:O	2.00	0.61
3:J:209:ILE:O	3:J:210:ALA:C	2.42	0.61
1:K:228:ASP:CB	1:K:229:PRO:HD3	2.31	0.61
1:K:257:THR:OG1	1:K:260:GLN:HG3	2.01	0.61
1:A:188:LYS:CG	7:A:529:HOH:O	2.49	0.61
1:B:113:TYR:O	1:B:113:TYR:CD1	2.54	0.61
2:D:211:ARG:O	7:D:424:HOH:O	2.16	0.61
3:F:102:VAL:O	3:F:106:GLN:HG3	2.00	0.61
3:F:151:GLY:C	3:F:153:VAL:H	2.08	0.61
3:G:35:ALA:HB3	3:G:103:THR:HG23	1.81	0.61
3:H:33:PHE:O	3:H:103:THR:HG21	2.01	0.61
1:L:26:LEU:HD11	1:L:79:PHE:CZ	2.36	0.61
2:D:51:HIS:ND1	7:D:406:HOH:O	2.30	0.60
2:D:96:ASN:OD1	2:D:98[B]:GLU:N	2.34	0.60
3:F:271:LYS:NZ	7:F:408:HOH:O	2.29	0.60
1:I:76:ILE:HD13	1:I:76:ILE:H	1.65	0.60
1:K:40:ILE:HD11	1:K:88:ARG:CZ	2.31	0.60
1:L:76:ILE:HD13	1:L:76:ILE:H	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:HD11	1:C:192:LYS:HE2	1.83	0.60
1:A:150:LYS:C	1:A:152:ASP:N	2.58	0.60
1:B:282:LYS:O	1:B:284:TYR:N	2.34	0.60
1:E:55:GLU:O	1:E:59:ARG:HG2	2.00	0.60
3:G:26:LEU:C	3:G:26:LEU:HD12	2.26	0.60
3:H:181[B]:GLU:OE1	3:H:184:LYS:HE2	2.01	0.60
3:H:239:ASP:OD1	3:H:240:ARG:N	2.35	0.60
3:J:172:LYS:HE2	1:L:170:ASN:HA	1.82	0.60
1:K:128:TYR:O	1:K:132:ASN:CB	2.48	0.60
1:L:52:TRP:CD1	7:L:406:HOH:O	2.54	0.60
2:D:273:ARG:CB	1:E:106:GLN:HE22	2.07	0.60
3:F:70:PRO:O	3:F:78:LYS:NZ	2.34	0.60
3:H:77:SER:O	3:H:80:GLU:N	2.33	0.60
1:I:79:PHE:HA	1:I:82:LEU:HD12	1.83	0.60
1:K:97:TYR:O	1:K:100:LEU:HB3	2.00	0.60
1:L:286:HIS:O	7:L:416:HOH:O	2.16	0.60
1:C:76:ILE:H	1:C:76:ILE:HD13	1.67	0.60
1:C:214[B]:SER:OG	1:C:217:GLU:HB2	2.00	0.60
1:B:230:ASN:ND2	7:B:436:HOH:O	2.34	0.60
3:F:120:ASP:OD1	3:F:252:TRP:HD1	1.84	0.60
3:G:181:GLU:HB2	3:G:184:LYS:HZ1	1.66	0.60
1:I:89:ARG:HD3	7:I:404:HOH:O	2.01	0.60
1:I:108:GLN:O	7:I:418:HOH:O	2.16	0.60
3:J:266:GLU:OE2	3:J:267:LEU:HA	2.01	0.60
1:L:169:LYS:HD2	1:L:176:PHE:CG	2.37	0.60
1:C:25:GLU:CD	1:C:25:GLU:N	2.60	0.60
1:A:140:THR:OG1	1:A:143:ALA:HB2	2.00	0.60
1:E:272:MET:O	1:E:273:ARG:C	2.44	0.60
3:F:30:LEU:C	3:F:32:SER:H	2.08	0.60
3:G:128:TYR:OH	3:G:237:THR:CG2	2.49	0.60
3:J:206:MET:O	3:J:207:ALA:C	2.43	0.60
3:J:280:CYS:HB3	7:J:453:HOH:O	2.00	0.60
1:B:261:ASN:O	1:B:264:PHE:HB3	2.01	0.60
1:E:186:PHE:CD1	1:E:186:PHE:C	2.78	0.60
1:E:188:LYS:O	1:E:191:LYS:HB2	2.02	0.60
3:F:270:GLU:O	3:F:273:ARG:HG2	2.01	0.60
3:H:181[B]:GLU:HG2	3:H:184:LYS:HZ1	1.66	0.60
1:A:27:LEU:O	1:A:30:LEU:HD22	2.01	0.60
1:A:70:PRO:HG3	1:A:233:ILE:C	2.27	0.60
1:B:199:ILE:N	7:B:405:HOH:O	2.35	0.60
2:D:87:LYS:NZ	7:H:433:HOH:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:ASN:OD1	2:D:133:PRO:HD2	2.02	0.60
1:E:51:HIS:HE1	1:E:237:THR:HG21	1.67	0.60
3:F:55:GLU:CA	7:F:419:HOH:O	2.49	0.60
3:H:32:SER:O	3:H:32:SER:OG	2.19	0.60
1:I:79:PHE:CA	7:I:441:HOH:O	2.49	0.60
3:J:98[B]:GLU:CD	1:K:98[B]:GLU:HG2	2.26	0.60
1:B:144:PHE:O	1:B:147:LEU:N	2.34	0.60
2:D:141:TRP:HB3	7:D:482:HOH:O	2.01	0.60
2:D:245:ARG:CB	7:D:402:HOH:O	2.50	0.60
3:G:181:GLU:HA	3:G:184:LYS:CD	2.31	0.60
3:G:211:ARG:HH21	3:J:131:ASP:CA	2.13	0.60
3:J:10:LEU:HD22	3:J:154:VAL:HG12	1.83	0.60
3:J:282:LYS:C	3:J:284:TYR:N	2.60	0.60
1:L:27:LEU:O	1:L:29:SER:N	2.34	0.60
1:C:40:ILE:O	1:C:91:ILE:N	2.34	0.60
3:H:69:SER:N	3:H:231:HIS:HE1	2.00	0.60
1:I:284:TYR:C	1:I:286:HIS:N	2.60	0.60
3:J:205:GLU:HA	3:J:208:LYS:HB2	1.83	0.60
1:L:67:LEU:HD21	1:L:233:ILE:CG2	2.30	0.60
1:L:168:HIS:HB3	1:L:171:ASP:OD2	2.01	0.60
2:D:217:GLU:HG2	7:D:424:HOH:O	2.02	0.60
2:D:222:ALA:O	2:D:223:ALA:HB2	2.01	0.60
1:C:231:HIS:CG	1:C:231:HIS:O	2.54	0.59
1:C:248:VAL:HG22	1:C:249:VAL:H	1.66	0.59
1:A:173:ASN:O	1:A:196:PHE:HZ	1.85	0.59
3:F:240:ARG:O	3:F:241:ASN:C	2.45	0.59
3:G:264:PHE:HB3	7:G:404:HOH:O	2.01	0.59
1:C:146:GLU:O	1:C:150:LYS:HD3	2.02	0.59
1:C:253:ILE:HG13	1:C:254:ASN:OD1	2.01	0.59
3:G:183:LYS:HD3	4:G:301:A3P:H2	1.84	0.59
1:I:60:ILE:HG23	1:I:61:PRO:HD2	1.83	0.59
1:A:276:ASP:HA	1:A:279:ARG:NH2	2.17	0.59
2:D:98[A]:GLU:CG	1:E:98:GLU:OE2	2.50	0.59
1:E:29:SER:OG	7:E:416:HOH:O	2.16	0.59
3:G:211:ARG:NH2	3:J:131:ASP:C	2.60	0.59
3:H:98:GLU:CD	3:H:98:GLU:H	2.10	0.59
1:I:59:ARG:NH1	1:I:212:SER:HB2	2.17	0.59
1:K:252:TRP:C	1:K:254:ASN:N	2.55	0.59
3:F:175:LEU:HD22	3:F:196:PHE:HB2	1.85	0.59
3:F:240:ARG:C	3:F:242:LEU:N	2.58	0.59
3:G:47:LYS:HD2	4:G:301:A3P:O5P	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:216:SER:O	7:G:423:HOH:O	2.16	0.59
3:H:11:HIS:CE1	3:H:20:THR:HA	2.37	0.59
1:I:181:GLU:HA	1:I:184:LYS:CE	2.32	0.59
1:B:44:SER:HB2	1:B:114:ILE:HG23	1.84	0.59
1:B:154:VAL:C	1:B:156:GLY:H	2.11	0.59
1:B:167:GLU:OE2	7:B:424:HOH:O	2.16	0.59
1:B:193:ILE:HG22	7:B:407:HOH:O	2.03	0.59
3:F:175:LEU:HD11	3:F:192:LYS:HE2	1.83	0.59
3:H:25:GLU:HG2	3:H:76:ILE:HD12	1.85	0.59
1:I:101:PRO:HB2	1:I:104:VAL:HG23	1.84	0.59
1:L:202:ASN:ND2	1:L:205:GLU:OE1	2.36	0.59
1:E:228:ASP:N	1:E:229:PRO:HD2	2.18	0.59
3:F:132:ASN:HB3	3:F:135:LEU:HD12	1.84	0.59
3:H:276:ASP:O	3:H:280:CYS:N	2.26	0.59
1:C:273:ARG:CB	7:C:411:HOH:O	2.51	0.59
1:A:202:ASN:ND2	7:A:441:HOH:O	2.35	0.59
1:B:85:ILE:HB	7:B:416:HOH:O	2.02	0.59
1:B:194:THR:HA	7:B:407:HOH:O	1.97	0.59
2:D:36:ARG:HB2	2:D:38:ASP:OD1	2.02	0.59
3:F:78:LYS:CB	7:F:410:HOH:O	2.50	0.59
3:J:175:LEU:HD11	3:J:192:LYS:HE3	1.82	0.59
1:L:115:VAL:HA	7:L:427:HOH:O	2.01	0.59
1:B:17:PHE:HB3	1:B:154:VAL:HA	1.83	0.59
1:B:22:SER:OG	1:B:72:GLU:O	2.18	0.59
2:D:231:HIS:O	2:D:232:VAL:C	2.45	0.59
3:F:168:HIS:HB3	3:F:171:ASP:OD2	2.02	0.59
3:H:191:LYS:O	3:H:192:LYS:C	2.46	0.59
1:I:173:ASN:CB	7:I:419:HOH:O	2.51	0.59
1:I:217:GLU:O	1:I:220:SER:N	2.29	0.59
3:J:204:SER:OG	7:J:427:HOH:O	2.16	0.59
1:L:16:ILE:HA	7:L:458:HOH:O	2.03	0.59
1:C:55:GLU:OE2	7:C:418:HOH:O	2.16	0.59
1:C:113:TYR:CD1	1:C:176:PHE:CE2	2.91	0.59
1:C:239:ASP:OD1	1:C:239:ASP:C	2.46	0.59
2:D:47:LYS:HG3	2:D:125:MET:HA	1.83	0.59
2:D:181:GLU:HA	2:D:184:LYS:HD3	1.84	0.59
2:D:214:SER:HB2	2:D:217:GLU:HB2	1.85	0.59
1:K:117:ASN:HD21	1:K:120:ASP:CG	2.09	0.59
1:C:22:SER:O	1:C:23:SER:O	2.20	0.58
1:C:35:ALA:H	1:C:103:THR:HG21	1.68	0.58
1:C:126:PHE:HB2	1:C:144:PHE:CD1	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HG23	1:A:93:THR:O	2.02	0.58
1:E:269:THR:O	1:E:270:GLU:C	2.45	0.58
3:H:219:LYS:HG3	3:H:244:PHE:HB3	1.85	0.58
1:K:132:ASN:HB3	1:K:135:LEU:HD12	1.85	0.58
1:A:150:LYS:O	1:A:151:GLY:C	2.43	0.58
3:F:194:THR:CG2	3:F:199:ILE:O	2.50	0.58
1:I:78:LYS:O	1:I:81:GLU:HB2	2.03	0.58
1:I:94:HIS:HB2	1:I:155:TYR:CE1	2.38	0.58
1:K:262[B]:ARG:CZ	7:K:414:HOH:O	2.51	0.58
2:D:11:HIS:CE1	2:D:22:SER:O	2.55	0.58
1:E:36:ARG:HB3	1:E:38:ASP:OD1	2.04	0.58
1:A:115:VAL:HG13	1:A:115:VAL:O	2.04	0.58
1:A:251:ASP:OD1	7:A:422:HOH:O	2.17	0.58
2:D:201:VAL:O	2:D:206:MET:HG3	2.02	0.58
1:E:44:SER:HA	7:E:408:HOH:O	2.04	0.58
3:G:92:PRO:HB2	3:G:233:ILE:O	2.03	0.58
1:I:264:PHE:CD1	1:I:264:PHE:C	2.81	0.58
3:J:12:LYS:HD3	3:J:17:PHE:CD2	2.38	0.58
3:J:95:LEU:HD23	3:J:99:MET:HE3	1.84	0.58
3:J:172:LYS:HG3	1:L:170:ASN:O	2.03	0.58
1:A:104:VAL:HA	7:A:406:HOH:O	2.01	0.58
1:E:87:LYS:HG3	7:E:407:HOH:O	2.03	0.58
3:H:276:ASP:CG	3:H:279:ARG:HH11	2.10	0.58
1:I:45:TYR:CD2	1:I:46:PRO:HD2	2.37	0.58
1:B:166:GLU:C	1:B:168:HIS:N	2.60	0.58
1:B:166:GLU:O	1:B:168:HIS:N	2.36	0.58
3:F:39:ASP:CG	3:F:89:ARG:HH21	2.11	0.58
3:F:192:LYS:O	7:F:417:HOH:O	2.16	0.58
3:G:265:ASP:CG	7:G:404:HOH:O	2.43	0.58
3:H:23:SER:HG	3:H:26:LEU:HB2	1.69	0.58
1:C:110:LYS:HA	1:C:173:ASN:HB2	1.85	0.58
1:C:212:SER:CB	7:C:407:HOH:O	2.49	0.58
1:B:253:ILE:HG13	1:B:254:ASN:N	2.17	0.58
2:D:240:ARG:O	2:D:243:VAL:HG13	2.04	0.58
1:E:101:PRO:HB2	1:E:104:VAL:HG23	1.85	0.58
3:H:125:MET:HB3	3:H:144:PHE:CZ	2.38	0.58
1:C:150:LYS:HE3	1:C:152:ASP:OD2	2.03	0.58
3:F:225:GLU:CB	7:F:496:HOH:O	2.50	0.58
3:G:267:LEU:C	3:G:269:THR:N	2.59	0.58
1:I:35:ALA:H	1:I:103:THR:CG2	2.16	0.58
1:I:59:ARG:HH12	1:I:212:SER:HB2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:264:PHE:O	1:L:267:LEU:N	2.36	0.58
1:B:50:THR:CA	7:B:404:HOH:O	2.49	0.58
1:E:189:SER:O	1:E:192:LYS:N	2.36	0.58
3:F:143:ALA:O	3:F:146:GLU:CB	2.52	0.58
3:H:77:SER:O	3:H:78:LYS:C	2.45	0.58
3:J:61:PRO:O	3:J:62:ASP:C	2.47	0.58
1:L:181:GLU:HB2	1:L:184:LYS:HZ1	1.66	0.58
1:A:178:PHE:O	1:A:181:GLU:N	2.36	0.58
1:B:44:SER:CB	1:B:114:ILE:CG2	2.82	0.58
2:D:25:GLU:O	2:D:29:SER:OG	2.08	0.58
2:D:27:LEU:HA	2:D:30:LEU:HD22	1.86	0.58
2:D:52:TRP:CZ3	4:D:301:A3P:C2	2.86	0.58
2:D:76:ILE:H	2:D:76:ILE:CD1	2.12	0.58
3:F:184:LYS:CG	3:F:185:ASP:N	2.66	0.58
3:G:34:ASP:O	7:G:424:HOH:O	2.17	0.58
3:J:110:LYS:C	3:J:111:ILE:HD13	2.28	0.58
1:C:35:ALA:H	1:C:103:THR:CG2	2.16	0.57
1:C:47:LYS:HA	1:C:47:LYS:HE3	1.86	0.57
1:C:273:ARG:CA	7:C:411:HOH:O	2.48	0.57
1:A:25:GLU:HB3	1:A:76:ILE:HD12	1.84	0.57
1:B:36:ARG:NH1	1:B:89:ARG:HD3	2.19	0.57
1:B:221:ASN:N	7:B:422:HOH:O	2.14	0.57
3:G:47:LYS:N	4:G:301:A3P:O4P	2.36	0.57
3:G:181:GLU:HB2	3:G:184:LYS:CE	2.33	0.57
3:G:181:GLU:HA	3:G:184:LYS:CE	2.34	0.57
4:K:301:A3P:H5'2	7:K:405:HOH:O	2.02	0.57
1:C:87:LYS:HG3	7:C:443:HOH:O	2.03	0.57
1:E:35:ALA:HB2	1:E:103:THR:CG2	2.34	0.57
3:F:36:ARG:NH1	3:F:85:ILE:O	2.36	0.57
3:F:94:HIS:HB2	3:F:155:TYR:CZ	2.39	0.57
3:G:117:ASN:CA	3:G:281:LEU:HD22	2.34	0.57
3:G:213:THR:O	3:G:218:MET:SD	2.62	0.57
3:H:150:LYS:HB3	3:H:152:ASP:OD2	2.04	0.57
1:L:232:VAL:CG2	1:L:233:ILE:N	2.66	0.57
1:A:37:GLU:OE2	1:A:107:LYS:HD3	2.03	0.57
2:D:89:ARG:N	7:D:411:HOH:O	2.36	0.57
1:E:172:LYS:NZ	3:F:174:VAL:O	2.33	0.57
1:E:181:GLU:HB2	1:E:184:LYS:NZ	2.19	0.57
3:F:11:HIS:CE1	3:F:20:THR:HA	2.39	0.57
3:G:37:GLU:HG2	7:G:512:HOH:O	2.03	0.57
3:G:258:PRO:O	3:G:262:ARG:HG2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:71:ILE:HG22	3:J:93:THR:HB	1.84	0.57
1:L:272:MET:O	1:L:273:ARG:C	2.47	0.57
1:C:80:GLU:O	1:C:81:GLU:C	2.45	0.57
3:G:128:TYR:O	3:G:132:ASN:N	2.36	0.57
3:H:107:LYS:NZ	7:H:435:HOH:O	2.37	0.57
3:H:172:LYS:HG3	1:I:170:ASN:O	2.03	0.57
3:H:188:LYS:O	3:H:191:LYS:HB2	2.05	0.57
1:I:243:VAL:O	4:I:301:A3P:H2'	2.04	0.57
1:K:138:THR:HG21	1:K:144:PHE:HB2	1.85	0.57
1:K:276:ASP:HA	1:K:279:ARG:HH22	1.69	0.57
1:L:159:PHE:HB2	1:L:271:LYS:HE3	1.86	0.57
1:C:31:ASP:OD1	1:C:101:PRO:HA	2.04	0.57
3:F:12:LYS:HD2	3:F:17:PHE:CE2	2.39	0.57
3:F:181[B]:GLU:CD	3:F:184:LYS:HE2	2.29	0.57
1:I:78:LYS:O	1:I:78:LYS:HD3	2.05	0.57
1:K:205:GLU:O	1:K:208:LYS:HB2	2.04	0.57
1:L:37:GLU:OE2	1:L:107:LYS:HD2	2.04	0.57
1:L:52:TRP:NE1	7:L:410:HOH:O	2.27	0.57
1:C:115:VAL:O	1:C:115:VAL:CG1	2.51	0.57
2:D:39:ASP:OD1	2:D:89:ARG:NE	2.34	0.57
2:D:70:PRO:HD3	2:D:233:ILE:HA	1.87	0.57
2:D:232:VAL:HG21	7:D:449:HOH:O	2.04	0.57
1:E:12:LYS:HD3	1:E:17:PHE:CD2	2.39	0.57
3:F:225:GLU:HG2	3:F:231:HIS:CG	2.39	0.57
3:G:220:SER:O	3:G:221:ASN:CG	2.48	0.57
3:H:169:LYS:O	1:I:172:LYS:HE2	2.05	0.57
1:C:125:MET:C	1:C:127:HIS:N	2.61	0.57
1:C:127:HIS:CD2	1:C:245:ARG:HD2	2.39	0.57
1:B:128:TYR:OH	1:B:237:THR:CB	2.52	0.57
3:F:107:LYS:NZ	7:F:433:HOH:O	2.38	0.57
3:J:266:GLU:OE2	3:J:266:GLU:C	2.48	0.57
1:A:78:LYS:O	1:A:81:GLU:HB2	2.04	0.57
3:G:47:LYS:HA	4:G:301:A3P:O5P	2.03	0.57
3:H:126:PHE:HB2	3:H:144:PHE:CD1	2.39	0.57
3:H:178:PHE:O	3:H:181[A]:GLU:N	2.12	0.57
3:J:208:LYS:NZ	7:J:427:HOH:O	2.27	0.57
1:K:276:ASP:CG	1:L:274:ASN:HB2	2.28	0.57
1:L:44:SER:CB	1:L:114:ILE:HG23	2.32	0.57
1:L:45:TYR:CG	1:L:46:PRO:HD2	2.40	0.57
1:L:115:VAL:HG22	1:L:116:ARG:N	2.19	0.57
1:B:77:SER:O	1:B:80:GLU:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:288:ALA:C	7:F:404:HOH:O	2.43	0.57
3:J:84:ARG:O	3:J:86:PRO:HD3	2.05	0.57
7:C:410:HOH:O	1:A:279:ARG:HB3	2.05	0.57
1:A:56:VAL:O	1:A:59:ARG:HB2	2.04	0.57
3:F:9:LEU:N	7:F:423:HOH:O	2.22	0.57
3:G:200:ASP:N	7:G:426:HOH:O	2.20	0.57
3:G:211:ARG:NH2	3:J:131:ASP:CA	2.68	0.57
1:I:59:ARG:HH12	1:I:212:SER:CB	2.18	0.57
3:J:253:ILE:HG21	7:J:404:HOH:O	1.97	0.57
1:K:243:VAL:O	4:K:301:A3P:H2'	2.05	0.57
1:K:259:LYS:HD2	7:K:544:HOH:O	2.05	0.57
1:L:124:SER:CB	4:L:301:A3P:O2P	2.53	0.57
1:L:144:PHE:O	1:L:145:LEU:C	2.46	0.57
1:A:226:ASN:C	1:A:227:CYS:SG	2.88	0.56
3:F:102:VAL:HG13	3:F:103:THR:N	2.20	0.56
3:F:149:LEU:HD22	3:F:267:LEU:HD12	1.86	0.56
3:G:181:GLU:HA	3:G:184:LYS:HD3	1.87	0.56
1:I:78:LYS:CA	7:I:410:HOH:O	2.51	0.56
3:J:205:GLU:O	3:J:208:LYS:CB	2.53	0.56
1:L:116:ARG:HG2	1:L:121:THR:OG1	2.05	0.56
1:L:260:GLN:HG3	7:L:405:HOH:O	2.04	0.56
1:A:50:THR:N	7:A:412:HOH:O	2.38	0.56
1:B:150:LYS:C	1:B:152:ASP:H	2.11	0.56
1:E:45:TYR:CD2	1:E:46:PRO:HD2	2.40	0.56
3:G:254:ASN:ND2	7:G:425:HOH:O	2.19	0.56
1:C:24:GLU:HA	1:C:27:LEU:HD12	1.87	0.56
1:C:242:LEU:HD12	7:C:425:HOH:O	2.04	0.56
1:C:279:ARG:CG	1:C:283:GLU:OE2	2.52	0.56
1:C:282:LYS:O	1:C:286:HIS:CB	2.52	0.56
1:A:59:ARG:O	1:A:60:ILE:C	2.49	0.56
2:D:35:ALA:H	2:D:103:THR:HG21	1.69	0.56
1:E:125:MET:HE1	1:E:153:VAL:HB	1.87	0.56
1:E:154:VAL:C	1:E:156:GLY:H	2.13	0.56
3:F:11:HIS:CE1	3:F:19:SER:O	2.58	0.56
3:F:185:ASP:O	3:F:186:PHE:C	2.48	0.56
3:G:51:HIS:CD2	3:G:233:ILE:HD11	2.40	0.56
3:G:80:GLU:HG3	7:G:414:HOH:O	2.04	0.56
3:G:81:GLU:O	3:G:84:ARG:N	2.35	0.56
3:G:100:LEU:O	3:G:105:LYS:HE3	2.06	0.56
3:G:205:GLU:O	3:G:208:LYS:HB2	2.04	0.56
3:G:266:GLU:O	3:G:269:THR:HB	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:THR:CG2	7:H:482:HOH:O	2.39	0.56
3:H:69:SER:CA	3:H:231:HIS:HE1	2.18	0.56
3:H:70:PRO:HG3	3:H:233:ILE:O	2.05	0.56
3:H:125:MET:HB3	3:H:144:PHE:HZ	1.70	0.56
3:H:150:LYS:CB	3:H:152:ASP:OD2	2.53	0.56
3:H:273:ARG:O	3:H:275:SER:N	2.39	0.56
1:I:18:PHE:CZ	1:I:99:MET:HE1	2.41	0.56
1:I:191:LYS:HA	1:I:206:MET:HE1	1.87	0.56
1:L:45:TYR:O	1:L:46:PRO:C	2.47	0.56
1:C:186:PHE:C	1:C:186:PHE:CD1	2.82	0.56
1:B:141:TRP:CZ2	1:B:145:LEU:HD22	2.40	0.56
1:B:168:HIS:NE2	7:B:425:HOH:O	2.18	0.56
1:E:35:ALA:CB	1:E:103:THR:CG2	2.83	0.56
3:F:31:ASP:OD1	3:F:101:PRO:HA	2.04	0.56
3:F:47:LYS:HA	3:F:47:LYS:HE3	1.88	0.56
3:G:76:ILE:H	3:G:76:ILE:CD1	2.11	0.56
3:G:181:GLU:CG	3:G:189:SER:OG	2.53	0.56
1:K:128:TYR:O	1:K:132:ASN:N	2.38	0.56
1:L:171:ASP:HB3	1:L:173:ASN:OD1	2.05	0.56
1:A:55:GLU:O	1:A:56:VAL:C	2.49	0.56
1:B:107:LYS:O	1:B:108:GLN:HB2	2.06	0.56
1:E:202:ASN:O	1:E:203:ASP:C	2.49	0.56
3:H:35:ALA:N	3:H:103:THR:CG2	2.64	0.56
3:H:189:SER:O	3:H:190:LEU:C	2.47	0.56
1:K:132:ASN:O	1:K:135:LEU:N	2.30	0.56
2:D:38:ASP:O	2:D:39:ASP:C	2.44	0.56
2:D:169:LYS:CD	2:D:176:PHE:CD1	2.88	0.56
3:F:65:ILE:HG12	3:F:88:ARG:HD3	1.86	0.56
3:G:50:THR:HB	4:G:301:A3P:P2	2.45	0.56
1:I:26:LEU:O	1:I:30:LEU:HD13	2.05	0.56
1:I:138:THR:CG2	1:I:140:THR:O	2.54	0.56
1:K:231:HIS:O	1:K:232:VAL:C	2.44	0.56
1:L:264:PHE:O	1:L:265:ASP:C	2.49	0.56
1:C:167:GLU:HG3	7:C:405:HOH:O	2.06	0.56
1:C:251:ASP:C	1:C:253:ILE:N	2.63	0.56
1:A:68:THR:O	1:A:92:PRO:CG	2.54	0.56
1:B:77:SER:O	1:B:81:GLU:HG3	2.06	0.56
1:B:202:ASN:N	1:B:205:GLU:OE2	2.37	0.56
2:D:35:ALA:HB3	2:D:103:THR:HG23	1.87	0.56
3:H:14:MET:N	3:H:14:MET:SD	2.78	0.56
3:J:214:SER:HB2	3:J:217:GLU:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:125:MET:O	1:L:126:PHE:C	2.43	0.56
1:C:277:VAL:O	1:C:278:GLY:C	2.49	0.56
1:A:55:GLU:N	7:A:446:HOH:O	2.37	0.56
1:B:202:ASN:ND2	1:B:205:GLU:OE2	2.39	0.56
3:F:240:ARG:O	3:F:243:VAL:N	2.34	0.56
1:I:33:PHE:CE1	1:I:82:LEU:CD1	2.88	0.56
3:J:114:ILE:CD1	7:J:550:HOH:O	2.50	0.56
3:J:138:THR:HG22	3:J:139:GLU:N	2.20	0.56
3:J:268:PHE:CZ	3:J:272:MET:HG3	2.40	0.56
1:L:205:GLU:O	1:L:206:MET:C	2.48	0.56
1:C:45:TYR:CG	1:C:46:PRO:HD2	2.41	0.56
1:A:169:LYS:HD2	1:A:176:PHE:CG	2.41	0.56
1:B:234:CYS:SG	1:B:237:THR:CG2	2.94	0.56
2:D:88:ARG:HG3	7:D:411:HOH:O	2.05	0.56
2:D:175:LEU:HD11	2:D:192:LYS:CE	2.35	0.56
1:E:13:TYR:HB3	1:E:18:PHE:CE1	2.41	0.56
3:F:97:TYR:O	3:F:100:LEU:N	2.39	0.56
3:F:100:LEU:HD12	3:F:101:PRO:HD2	1.88	0.56
3:G:100:LEU:HD23	3:G:105:LYS:HG2	1.87	0.56
3:H:49:GLY:HA3	3:H:114:ILE:CD1	2.36	0.56
3:H:52:TRP:O	3:H:56:VAL:HG23	2.06	0.56
1:I:141:TRP:O	1:I:144:PHE:N	2.39	0.56
3:J:117:ASN:HA	3:J:281:LEU:HD22	1.88	0.56
1:L:80:GLU:O	1:L:83:LYS:N	2.39	0.56
1:L:116:ARG:HD3	1:L:121:THR:OG1	2.06	0.56
1:C:36:ARG:C	1:C:38:ASP:N	2.63	0.56
2:D:173:ASN:HB2	7:D:404:HOH:O	2.04	0.56
2:D:257:THR:O	2:D:259:LYS:N	2.38	0.56
1:E:29:SER:O	1:E:31:ASP:N	2.39	0.56
3:F:202:ASN:N	3:F:205[A]:GLU:OE2	2.37	0.56
3:F:231:HIS:O	3:F:231:HIS:CG	2.58	0.56
3:G:116:ARG:NH2	4:G:301:A3P:O1P	2.33	0.56
3:G:239:ASP:OD2	3:G:242:LEU:CG	2.50	0.56
3:H:286:HIS:C	3:H:288:ALA:HA	2.31	0.56
1:I:173:ASN:HA	7:I:471:HOH:O	2.06	0.56
1:I:208:LYS:O	1:I:211:ARG:HB3	2.05	0.56
2:D:183:LYS:HD3	4:D:301:A3P:H2	1.86	0.55
4:F:301:A3P:H4'	7:F:425:HOH:O	2.04	0.55
1:I:224:LYS:HB2	1:I:228:ASP:O	2.06	0.55
1:L:221:ASN:O	1:L:222:ALA:HB2	2.06	0.55
1:C:44:SER:O	1:C:94:HIS:HA	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:CZ	1:B:99:MET:HE1	2.41	0.55
3:F:9:LEU:HA	7:F:423:HOH:O	2.05	0.55
3:F:245:ARG:NH2	7:F:432:HOH:O	2.38	0.55
3:G:159:PHE:HD1	3:G:272:MET:SD	2.29	0.55
1:K:228:ASP:O	1:K:229:PRO:O	2.23	0.55
1:L:55:GLU:CB	1:L:218:MET:HE3	2.35	0.55
1:L:205:GLU:O	1:L:208:LYS:N	2.39	0.55
1:L:212:SER:OG	1:L:213:THR:HG23	2.05	0.55
1:C:179:TYR:O	1:C:182:MET:HB2	2.05	0.55
2:D:205:GLU:O	2:D:209:ILE:CG1	2.54	0.55
1:E:262:ARG:O	1:E:264:PHE:N	2.39	0.55
3:F:258:PRO:O	3:F:261:ASN:N	2.39	0.55
3:F:282:LYS:O	3:F:285:ALA:N	2.40	0.55
3:H:26:LEU:HD22	3:H:75:ASP:O	2.06	0.55
3:H:185:ASP:O	3:H:188:LYS:HB3	2.07	0.55
1:C:102:VAL:O	1:C:106:GLN:HG3	2.07	0.55
1:A:183:LYS:O	7:A:426:HOH:O	2.18	0.55
1:B:10:LEU:HD22	1:B:154:VAL:HG12	1.87	0.55
1:B:220:SER:O	1:B:221:ASN:CG	2.49	0.55
2:D:77:SER:OG	2:D:78:LYS:N	2.39	0.55
2:D:137:SER:N	7:D:425:HOH:O	2.20	0.55
1:E:11:HIS:CE1	1:E:22:SER:O	2.60	0.55
1:E:12:LYS:HD2	1:E:17:PHE:CD2	2.41	0.55
1:E:166:GLU:O	1:E:168:HIS:N	2.39	0.55
1:I:202:ASN:C	1:I:202:ASN:OD1	2.49	0.55
3:J:31:ASP:OD1	3:J:102:VAL:N	2.37	0.55
1:K:84:ARG:HB2	7:K:448:HOH:O	2.06	0.55
1:K:132:ASN:OD1	1:K:133:PRO:HD2	2.07	0.55
1:L:10:LEU:HD22	1:L:154:VAL:HG12	1.87	0.55
1:L:68:THR:C	1:L:231:HIS:CE1	2.83	0.55
1:L:181:GLU:HA	1:L:184:LYS:CD	2.37	0.55
1:C:179:TYR:O	1:C:180:GLU:C	2.50	0.55
1:C:180:GLU:O	1:C:182:MET:N	2.39	0.55
1:C:226:ASN:HA	7:C:437:HOH:O	2.06	0.55
1:A:26:LEU:HD12	1:A:26:LEU:C	2.31	0.55
1:B:221:ASN:ND2	7:B:441:HOH:O	2.39	0.55
3:F:115:VAL:O	3:F:115:VAL:CG1	2.54	0.55
3:H:41:PHE:CA	7:H:401:HOH:O	2.54	0.55
3:H:146:GLU:O	3:H:150:LYS:HD3	2.07	0.55
1:I:35:ALA:H	1:I:103:THR:HG23	1.72	0.55
1:I:45:TYR:CG	1:I:46:PRO:HD2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:279:ARG:HD2	3:J:283:GLU:OE2	2.06	0.55
1:L:88:ARG:NH1	7:L:422:HOH:O	2.25	0.55
1:L:240:ARG:O	1:L:243:VAL:HG13	2.05	0.55
1:C:283:GLU:C	1:C:286:HIS:HB3	2.31	0.55
1:A:23:SER:OG	1:A:26:LEU:CB	2.55	0.55
1:A:45:TYR:HD1	1:A:161:HIS:CG	2.24	0.55
1:A:226:ASN:O	1:A:227:CYS:SG	2.63	0.55
3:F:51:HIS:CD2	3:F:233:ILE:HD11	2.41	0.55
3:G:154:VAL:C	3:G:156:GLY:H	2.15	0.55
3:G:256:PHE:CD2	3:G:261:ASN:OD1	2.60	0.55
3:H:178:PHE:HB2	3:H:181[A]:GLU:HB3	1.88	0.55
3:J:55:GLU:O	3:J:59:ARG:HG2	2.06	0.55
3:J:120:ASP:OD1	3:J:252:TRP:HD1	1.89	0.55
3:J:221:ASN:CG	7:J:432:HOH:O	2.50	0.55
1:K:256:PHE:HA	1:K:260:GLN:OE1	2.06	0.55
1:L:13:TYR:CE1	1:L:14[B]:MET:SD	2.99	0.55
1:C:248:VAL:HG22	1:C:249:VAL:N	2.21	0.55
1:B:51:HIS:CD2	1:B:233:ILE:HD11	2.42	0.55
2:D:122:ALA:O	2:D:126:PHE:N	2.39	0.55
3:J:214:SER:CB	3:J:217:GLU:HB2	2.37	0.55
1:K:126:PHE:CZ	1:K:130:ARG:HD2	2.41	0.55
1:C:147:LEU:O	1:C:152:ASP:N	2.34	0.55
1:B:41:PHE:HB2	1:B:111:ILE:HD13	1.88	0.55
1:E:184:LYS:C	7:E:411:HOH:O	2.49	0.55
3:F:55:GLU:HA	7:F:419:HOH:O	2.05	0.55
3:G:196:PHE:HZ	7:G:403:HOH:O	1.88	0.55
1:I:231:HIS:ND1	1:I:231:HIS:O	2.40	0.55
1:I:252:TRP:CH2	1:I:253:ILE:HG22	2.42	0.55
3:J:206:MET:O	3:J:209:ILE:HB	2.05	0.55
1:L:47:LYS:N	1:L:47:LYS:HD2	2.21	0.55
1:L:67:LEU:O	1:L:231:HIS:NE2	2.39	0.55
1:C:279:ARG:O	1:C:283:GLU:CD	2.50	0.55
1:E:227:CYS:HB3	1:E:229:PRO:HG2	1.87	0.55
1:E:270:GLU:O	1:E:273:ARG:NE	2.36	0.55
3:F:18:PHE:HZ	3:F:99:MET:HE1	1.71	0.55
3:F:257:THR:H	3:F:260:GLN:HE21	1.53	0.55
3:J:240:ARG:O	3:J:243:VAL:HG13	2.06	0.55
1:L:281:LEU:O	1:L:284:TYR:HB2	2.06	0.55
2:D:78:LYS:O	2:D:79:PHE:C	2.47	0.55
3:F:28:GLY:O	6:F:303:GOL:O1	2.24	0.55
3:H:31:ASP:O	3:H:33:PHE:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:191:LYS:O	3:J:194:THR:HB	2.07	0.55
1:L:57:ILE:O	1:L:60:ILE:N	2.29	0.55
2:D:181:GLU:HA	2:D:184:LYS:CD	2.37	0.54
2:D:234:CYS:CB	2:D:237:THR:HG23	2.37	0.54
3:F:110:LYS:HD3	3:F:196:PHE:CZ	2.41	0.54
1:I:252:TRP:HB2	1:I:256:PHE:CD1	2.42	0.54
1:L:260:GLN:CG	7:L:405:HOH:O	2.54	0.54
1:C:222:ALA:O	1:C:223:ALA:HB2	2.07	0.54
1:A:205:GLU:HA	1:A:208:LYS:HD2	1.88	0.54
1:B:251:ASP:OD1	1:B:251:ASP:O	2.25	0.54
2:D:45:TYR:CD2	2:D:46:PRO:HD2	2.42	0.54
3:G:47:LYS:HA	3:G:47:LYS:HE3	1.89	0.54
3:G:70:PRO:HD3	3:G:233:ILE:CA	2.36	0.54
1:I:59:ARG:NH1	1:I:212:SER:CB	2.70	0.54
1:L:208:LYS:O	1:L:211:ARG:HB3	2.06	0.54
1:C:214[B]:SER:OG	7:C:420:HOH:O	2.18	0.54
1:B:166:GLU:O	1:B:167:GLU:C	2.50	0.54
1:B:254:ASN:HA	7:B:406:HOH:O	2.07	0.54
2:D:159:PHE:O	2:D:163:LEU:HG	2.06	0.54
2:D:168:HIS:HE1	1:E:167:GLU:CG	2.20	0.54
3:G:84:ARG:HB2	7:G:450:HOH:O	2.07	0.54
3:G:115:VAL:O	3:G:115:VAL:CG1	2.55	0.54
3:G:261:ASN:CA	7:G:404:HOH:O	2.53	0.54
1:I:37:GLU:OE1	1:I:107:LYS:HD3	2.07	0.54
1:L:219:LYS:HG3	1:L:244:PHE:CB	2.38	0.54
1:A:282:LYS:O	1:A:284:TYR:N	2.40	0.54
1:B:127:HIS:CG	1:B:245:ARG:HD2	2.41	0.54
1:B:150:LYS:HB3	1:B:152:ASP:OD2	2.07	0.54
3:J:201:VAL:O	3:J:206:MET:HE3	2.08	0.54
3:J:282:LYS:C	3:J:284:TYR:H	2.15	0.54
1:L:205:GLU:O	1:L:208:LYS:HB2	2.07	0.54
1:A:253:ILE:HG13	1:A:254:ASN:OD1	2.07	0.54
1:B:52:TRP:O	1:B:53:LEU:C	2.51	0.54
2:D:36:ARG:HD3	3:H:140:THR:HG21	1.89	0.54
2:D:86:PRO:HA	3:H:140:THR:HA	1.90	0.54
3:F:194:THR:O	3:F:198:GLY:N	2.34	0.54
3:H:125:MET:O	3:H:126:PHE:C	2.50	0.54
3:J:129:TYR:OH	7:J:406:HOH:O	1.97	0.54
1:K:35:ALA:H	1:K:103:THR:HG21	1.72	0.54
1:L:35:ALA:H	1:L:103:THR:HG21	1.73	0.54
1:L:149:LEU:HD22	1:L:267:LEU:HD12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:MET:O	1:L:273:ARG:O	2.26	0.54
1:C:181:GLU:HA	1:C:184:LYS:HD3	1.90	0.54
1:C:205:GLU:C	7:C:408:HOH:O	2.47	0.54
1:A:221:ASN:O	1:A:221:ASN:OD1	2.26	0.54
1:E:59:ARG:HH12	1:E:212:SER:HB2	1.71	0.54
3:F:253:ILE:HG13	3:F:254:ASN:N	2.22	0.54
3:G:50:THR:N	4:G:301:A3P:O4P	2.35	0.54
3:G:80:GLU:CD	7:G:414:HOH:O	2.48	0.54
3:H:234:CYS:SG	3:H:237:THR:CG2	2.95	0.54
1:I:166:GLU:OE2	1:I:277:VAL:HG23	2.08	0.54
1:L:175:LEU:HD11	1:L:192:LYS:HE2	1.89	0.54
1:C:234:CYS:CB	1:C:237:THR:HG23	2.38	0.54
2:D:25:GLU:H	2:D:25:GLU:CD	2.15	0.54
2:D:59:ARG:HA	7:D:401:HOH:O	2.07	0.54
1:E:113:TYR:C	7:E:408:HOH:O	2.47	0.54
3:F:119:LYS:HB3	3:F:252:TRP:CB	2.38	0.54
1:K:138:THR:CG2	1:K:140:THR:O	2.56	0.54
1:C:205:GLU:CA	7:C:408:HOH:O	2.56	0.54
1:A:150:LYS:O	1:A:152:ASP:N	2.41	0.54
3:G:35:ALA:CB	3:G:103:THR:HG23	2.37	0.54
3:J:50:THR:HB	4:J:301:A3P:O6P	2.07	0.54
1:L:184:LYS:HG3	1:L:185:ASP:HB2	1.89	0.54
2:D:73:LEU:HD22	2:D:232:VAL:HG21	1.89	0.54
3:G:153:VAL:HA	7:G:434:HOH:O	2.07	0.54
3:H:70:PRO:HG3	3:H:233:ILE:C	2.33	0.54
1:K:94:HIS:HB2	1:K:155:TYR:CE1	2.43	0.54
1:C:127:HIS:CD2	1:C:245:ARG:CZ	2.90	0.54
1:A:11:HIS:HE1	1:A:19:SER:O	1.89	0.54
1:A:68:THR:O	1:A:92:PRO:HD3	2.08	0.54
1:A:222:ALA:O	1:A:223:ALA:CB	2.56	0.54
1:B:120:ASP:OD1	1:B:252:TRP:HD1	1.91	0.54
1:E:43:VAL:HG22	1:E:93:THR:CG2	2.38	0.54
3:F:219:LYS:HG3	3:F:244:PHE:HB2	1.90	0.54
3:F:284:TYR:O	3:F:287:SER:N	2.40	0.54
3:J:23:SER:OG	3:J:25[B]:GLU:CG	2.51	0.54
3:J:102:VAL:HG13	3:J:103:THR:N	2.22	0.54
1:C:268:PHE:C	1:C:268:PHE:CD2	2.86	0.53
1:A:276:ASP:HA	1:A:279:ARG:HH22	1.73	0.53
1:E:214:SER:O	1:E:215:PHE:C	2.52	0.53
3:F:206:MET:O	3:F:207:ALA:C	2.51	0.53
3:F:251:ASP:O	3:F:252:TRP:C	2.50	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:49:GLY:C	7:H:405:HOH:O	2.49	0.53
1:K:40:ILE:O	1:K:90:ALA:HA	2.08	0.53
1:K:237:THR:HG23	1:K:237:THR:O	2.06	0.53
1:B:75:ASP:OD1	1:B:75:ASP:N	2.40	0.53
1:E:11:HIS:HE1	1:E:22:SER:O	1.90	0.53
3:G:267:LEU:O	3:G:269:THR:N	2.41	0.53
3:H:23:SER:O	3:H:27:LEU:HG	2.08	0.53
1:K:252:TRP:O	1:K:254:ASN:N	2.40	0.53
1:K:279:ARG:NH2	1:L:274:ASN:CB	2.70	0.53
1:L:37:GLU:CD	1:L:107:LYS:HD2	2.33	0.53
1:B:25[A]:GLU:O	1:B:29:SER:OG	2.20	0.53
2:D:33:PHE:HB2	2:D:79:PHE:CE1	2.43	0.53
3:F:68:THR:O	7:F:418:HOH:O	2.18	0.53
3:H:183:LYS:CD	4:H:301:A3P:H2	2.39	0.53
3:H:188:LYS:HA	3:H:191:LYS:HD2	1.90	0.53
3:J:180:GLU:OE1	3:J:180:GLU:N	2.39	0.53
1:A:169:LYS:HD2	1:A:176:PHE:HB2	1.90	0.53
2:D:276:ASP:O	2:D:277:VAL:C	2.49	0.53
1:E:181:GLU:C	7:E:403:HOH:O	2.51	0.53
3:F:181[B]:GLU:HG2	3:F:184:LYS:HZ3	1.72	0.53
3:G:56:VAL:HA	3:G:213:THR:HG21	1.90	0.53
1:I:166:GLU:C	1:I:168:HIS:N	2.64	0.53
1:A:43:VAL:O	1:A:114:ILE:N	2.39	0.53
1:A:122:ALA:O	1:A:126:PHE:N	2.27	0.53
1:A:210:ALA:O	1:A:211:ARG:C	2.50	0.53
1:B:178:PHE:O	1:B:179:TYR:C	2.50	0.53
2:D:231:HIS:O	2:D:231:HIS:CG	2.59	0.53
3:F:117:ASN:HA	3:F:281:LEU:HD22	1.90	0.53
3:F:129:TYR:HA	3:F:135:LEU:HB2	1.91	0.53
3:G:26:LEU:HD12	3:G:26:LEU:O	2.08	0.53
3:G:194:THR:HG22	7:G:405:HOH:O	2.07	0.53
3:H:19:SER:C	3:H:21:MET:N	2.66	0.53
1:K:68:THR:O	7:K:419:HOH:O	2.19	0.53
1:K:252:TRP:C	1:K:252:TRP:CE3	2.86	0.53
1:L:230:ASN:OD1	1:L:230:ASN:N	2.41	0.53
1:L:248:VAL:HG22	1:L:249:VAL:N	2.23	0.53
1:C:151:GLY:C	1:C:153:VAL:H	2.15	0.53
1:C:234:CYS:HB3	1:C:237:THR:CG2	2.39	0.53
1:A:47:LYS:HA	4:A:301:A3P:P2	2.49	0.53
2:D:219:LYS:HG3	2:D:244:PHE:CB	2.38	0.53
3:G:80:GLU:CG	7:G:414:HOH:O	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:98[A]:GLU:HG2	1:I:98:GLU:CD	2.34	0.53
3:G:181:GLU:HB2	3:G:184:LYS:HZ3	1.73	0.53
3:H:251:ASP:O	3:H:252:TRP:C	2.50	0.53
1:L:55:GLU:HA	1:L:55:GLU:OE2	2.07	0.53
1:C:13:TYR:OH	1:C:28:GLY:HA2	2.09	0.53
1:E:269:THR:HA	7:E:444:HOH:O	2.08	0.53
3:F:194:THR:HG22	3:F:195:ALA:N	2.24	0.53
3:J:129:TYR:O	3:J:137:SER:CA	2.56	0.53
4:J:301:A3P:O3P	4:J:301:A3P:O2'	2.23	0.53
1:A:179:TYR:O	1:A:182:MET:HB2	2.09	0.53
1:B:49:GLY:C	7:B:404:HOH:O	2.44	0.53
2:D:184:LYS:NZ	2:D:284:TYR:OH	2.39	0.53
2:D:256:PHE:HB3	2:D:261:ASN:OD1	2.09	0.53
1:E:44:SER:HB3	1:E:114:ILE:CG2	2.38	0.53
1:E:269:THR:O	1:E:273:ARG:HD3	2.09	0.53
3:H:19:SER:C	3:H:21:MET:H	2.15	0.53
1:A:38:ASP:CG	7:A:433:HOH:O	2.51	0.53
1:A:69:SER:HA	1:A:232:VAL:O	2.09	0.53
1:B:240:ARG:O	1:B:243:VAL:HG13	2.09	0.53
1:B:284:TYR:O	7:B:426:HOH:O	2.19	0.53
2:D:71:ILE:O	2:D:71:ILE:HG12	2.09	0.53
1:E:52:TRP:CH2	1:E:182:MET:HB3	2.44	0.53
1:I:10:LEU:CD2	1:I:154:VAL:CG1	2.86	0.53
3:J:96:ASN:C	3:J:165:TRP:NE1	2.66	0.53
1:K:80:GLU:OE1	1:K:80:GLU:HA	2.08	0.53
1:K:224:LYS:HB2	1:K:227:CYS:O	2.08	0.53
1:L:12:LYS:HE3	1:L:17:PHE:CD1	2.44	0.53
1:L:287:SER:HG	1:L:288:ALA:H	1.51	0.53
1:C:40:ILE:CG2	1:C:41:PHE:N	2.72	0.53
1:C:167:GLU:CG	7:C:405:HOH:O	2.57	0.53
1:A:132:ASN:HB3	1:A:135:LEU:HD12	1.91	0.53
1:A:159:PHE:O	1:A:163:LEU:HG	2.09	0.53
1:A:164[A]:SER:O	1:A:167:GLU:HB2	2.08	0.53
2:D:47:LYS:HG3	2:D:125:MET:CA	2.39	0.53
1:E:257:THR:O	1:E:260:GLN:N	2.42	0.53
3:F:125:MET:O	3:F:128:TYR:N	2.28	0.53
3:G:98[A]:GLU:CG	1:I:98:GLU:HG2	2.30	0.53
3:H:279:ARG:O	3:H:282:LYS:HB2	2.09	0.53
1:I:84:ARG:O	1:I:86:PRO:HD3	2.09	0.53
1:I:200:ASP:O	1:I:201:VAL:HG23	2.09	0.53
3:J:208:LYS:O	3:J:211:ARG:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:GLU:O	1:K:72:GLU:HG2	2.09	0.53
1:L:29:SER:O	1:L:79:PHE:HE2	1.92	0.53
1:C:115:VAL:O	1:C:178:PHE:HA	2.08	0.52
1:A:239:ASP:C	1:A:239:ASP:OD1	2.50	0.52
1:B:96:ASN:ND2	7:B:444:HOH:O	2.42	0.52
2:D:117:ASN:HA	2:D:281:LEU:HD22	1.90	0.52
1:E:50:THR:HG23	4:E:301:A3P:P2	2.49	0.52
3:F:47:LYS:CA	7:F:425:HOH:O	2.56	0.52
3:F:100:LEU:O	3:F:105:LYS:CE	2.56	0.52
3:H:35:ALA:CB	3:H:103:THR:HG23	2.37	0.52
1:I:78:LYS:N	7:I:410:HOH:O	2.38	0.52
1:I:207:ALA:O	1:I:208:LYS:C	2.52	0.52
1:I:209:ILE:O	1:I:210:ALA:C	2.50	0.52
3:J:153:VAL:O	3:J:154:VAL:C	2.51	0.52
1:L:9:LEU:HD21	1:L:133:PRO:O	2.09	0.52
1:C:36:ARG:O	1:C:38:ASP:N	2.42	0.52
1:C:121:THR:O	1:C:122:ALA:C	2.53	0.52
1:C:174:VAL:O	1:B:172:LYS:NZ	2.43	0.52
1:C:183:LYS:HE2	1:C:248:VAL:HA	1.92	0.52
1:A:44:SER:HB3	1:A:114:ILE:HG22	1.90	0.52
1:B:25[B]:GLU:O	1:B:29:SER:OG	2.21	0.52
1:E:66:THR:OG1	7:E:407:HOH:O	1.96	0.52
1:A:239:ASP:CG	1:A:242:LEU:HG	2.34	0.52
1:B:206:MET:O	1:B:207:ALA:C	2.51	0.52
2:D:35:ALA:N	2:D:103:THR:HG21	2.25	0.52
1:E:259:LYS:O	1:E:262:ARG:N	2.43	0.52
3:G:279:ARG:HB2	3:G:279:ARG:CZ	2.39	0.52
3:J:222:ALA:O	3:J:223:ALA:CB	2.58	0.52
3:J:282:LYS:NZ	7:J:445:HOH:O	2.41	0.52
1:K:102:VAL:CG1	1:K:103:THR:N	2.72	0.52
1:K:252:TRP:CE3	1:K:253:ILE:HA	2.44	0.52
1:L:117:ASN:HB3	1:L:180:GLU:OE2	2.09	0.52
1:B:30:LEU:HD12	1:B:79:PHE:HZ	1.74	0.52
1:B:39:ASP:O	1:B:109:CYS:HB3	2.08	0.52
2:D:149:LEU:HD22	2:D:267:LEU:HD12	1.91	0.52
2:D:234:CYS:HB3	2:D:237:THR:CG2	2.39	0.52
3:J:96:ASN:CA	3:J:165:TRP:NE1	2.70	0.52
1:K:45:TYR:CD2	1:K:46:PRO:HD2	2.45	0.52
1:K:171:ASP:HB2	1:K:174:VAL:CG2	2.39	0.52
1:C:11:HIS:CE1	1:C:18:PHE:HB2	2.45	0.52
1:C:250:GLY:O	1:C:251:ASP:C	2.50	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:C	1:A:220:SER:OG	2.52	0.52
1:A:225:GLU:HG2	1:A:231:HIS:H	1.74	0.52
2:D:36:ARG:HD3	7:D:430:HOH:O	2.08	0.52
2:D:73:LEU:HD22	2:D:232:VAL:CG2	2.40	0.52
2:D:110:LYS:HD3	7:D:404:HOH:O	2.08	0.52
3:G:253:ILE:HG13	3:G:254:ASN:OD1	2.09	0.52
3:H:55:GLU:O	3:H:56:VAL:C	2.53	0.52
3:H:279:ARG:HD2	3:H:283:GLU:OE2	2.09	0.52
1:I:33:PHE:HE1	1:I:82:LEU:HD13	1.74	0.52
1:K:29:SER:HB2	1:K:79:PHE:HE2	1.75	0.52
1:K:72:GLU:OE1	1:K:93:THR:OG1	2.19	0.52
1:K:216:SER:O	1:K:219:LYS:HB3	2.10	0.52
1:L:159:PHE:CB	1:L:271:LYS:HE3	2.39	0.52
1:L:257:THR:O	1:L:258:PRO:C	2.53	0.52
1:A:171:ASP:CG	7:A:408:HOH:O	2.50	0.52
1:B:267:LEU:HD22	1:B:267:LEU:C	2.34	0.52
1:E:213:THR:O	4:E:301:A3P:N6	2.43	0.52
1:E:232:VAL:HG13	7:E:483:HOH:O	2.08	0.52
3:F:151:GLY:O	3:F:153:VAL:N	2.42	0.52
3:J:182:MET:CE	7:J:550:HOH:O	2.55	0.52
3:J:182:MET:HE2	7:J:550:HOH:O	2.09	0.52
3:J:229:PRO:C	7:J:447:HOH:O	2.52	0.52
1:L:57:ILE:O	1:L:58:GLU:C	2.52	0.52
1:L:258:PRO:O	1:L:261:ASN:N	2.42	0.52
1:A:43:VAL:O	1:A:113:TYR:HA	2.09	0.52
1:A:70:PRO:HG3	1:A:233:ILE:O	2.09	0.52
1:A:169:LYS:HB2	1:A:176:PHE:CE1	2.45	0.52
1:B:138:THR:CG2	1:B:143:ALA:HB3	2.39	0.52
2:D:39:ASP:CG	2:D:89:ARG:NH2	2.65	0.52
2:D:107:LYS:O	2:D:108:GLN:C	2.52	0.52
2:D:219:LYS:HG3	2:D:244:PHE:HB2	1.91	0.52
1:E:16:ILE:HG22	1:E:17:PHE:N	2.22	0.52
3:G:47:LYS:CE	4:G:301:A3P:O5P	2.58	0.52
3:J:253:ILE:HG13	3:J:254:ASN:N	2.25	0.52
1:L:13:TYR:O	1:L:14[A]:MET:C	2.52	0.52
1:L:48:SER:N	4:L:301:A3P:O4P	2.42	0.52
1:C:157:SER:CB	7:C:438:HOH:O	2.54	0.52
1:A:45:TYR:CG	1:A:46:PRO:HD2	2.45	0.52
1:A:267:LEU:O	1:A:271:LYS:N	2.34	0.52
3:G:48:SER:O	3:G:114:ILE:HG12	2.10	0.52
3:H:96:ASN:ND2	3:H:98:GLU:OE1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:173:ASN:OD1	3:H:173:ASN:N	2.38	0.52
1:I:195:ALA:HB2	7:I:426:HOH:O	2.09	0.52
1:A:267:LEU:HD22	1:A:271:LYS:CG	2.38	0.52
1:E:266:GLU:O	1:E:267:LEU:C	2.51	0.52
3:G:220:SER:O	3:G:221:ASN:OD1	2.28	0.52
1:I:11:HIS:N	1:I:18:PHE:O	2.42	0.52
1:I:186:PHE:N	7:I:407:HOH:O	2.43	0.52
1:K:80:GLU:O	1:K:83:LYS:HB3	2.10	0.52
1:K:125:MET:O	1:K:126:PHE:C	2.52	0.52
1:K:234:CYS:O	1:K:237:THR:HG22	2.10	0.52
1:L:80:GLU:O	1:L:81:GLU:C	2.53	0.52
1:L:102:VAL:HG13	1:L:103:THR:N	2.24	0.52
1:L:128:TYR:O	1:L:132:ASN:HB2	2.10	0.52
1:C:279:ARG:HD3	1:C:283:GLU:OE2	2.09	0.52
1:A:267:LEU:O	1:A:268:PHE:C	2.53	0.52
2:D:84:ARG:O	2:D:86:PRO:CD	2.52	0.52
2:D:191:LYS:HA	2:D:206:MET:HE1	1.92	0.52
2:D:256:PHE:CD2	2:D:261:ASN:OD1	2.63	0.52
2:D:279:ARG:HB2	2:D:279:ARG:CZ	2.39	0.52
1:E:227:CYS:O	1:E:228:ASP:C	2.52	0.52
3:G:113:TYR:OH	3:G:161:HIS:HD2	1.92	0.52
3:G:115:VAL:O	3:G:115:VAL:HG13	2.08	0.52
3:H:24:GLU:HA	3:H:27:LEU:HD12	1.92	0.52
3:H:39:ASP:OD1	7:H:424:HOH:O	2.19	0.52
3:J:185:ASP:OD2	3:J:188:LYS:HB2	2.10	0.52
1:L:36:ARG:NH1	1:L:85:ILE:O	2.30	0.52
1:L:220:SER:O	1:L:221:ASN:CG	2.53	0.52
1:C:127:HIS:HD2	1:C:245:ARG:CZ	2.23	0.51
1:A:45:TYR:CD2	1:A:46:PRO:HD2	2.45	0.51
1:B:67:LEU:HD21	1:B:233:ILE:CG2	2.40	0.51
3:G:215:PHE:C	3:G:215:PHE:CD2	2.88	0.51
3:H:41:PHE:HA	7:H:401:HOH:O	2.10	0.51
1:I:177:ILE:CD1	1:I:192:LYS:HE2	2.40	0.51
1:K:140:THR:HB	7:K:454:HOH:O	2.11	0.51
1:L:183:LYS:HD3	4:L:301:A3P:H2	1.91	0.51
1:C:23:SER:HG	1:C:26:LEU:HB2	1.74	0.51
2:D:35:ALA:H	2:D:103:THR:CG2	2.23	0.51
3:F:44:SER:HB3	3:F:114:ILE:CG2	2.40	0.51
3:F:128:TYR:O	3:F:132:ASN:CB	2.57	0.51
3:G:225:GLU:HG2	3:G:231:HIS:ND1	2.25	0.51
1:I:36:ARG:O	1:I:37:GLU:C	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:TYR:O	3:J:129:TYR:C	2.48	0.51
3:J:130:ARG:HA	3:J:137:SER:CB	2.39	0.51
1:K:80:GLU:O	1:K:83:LYS:CB	2.59	0.51
1:K:171:ASP:HB2	1:K:174:VAL:HG23	1.91	0.51
1:L:68:THR:O	1:L:231:HIS:NE2	2.42	0.51
1:L:181:GLU:O	1:L:184:LYS:HG2	2.10	0.51
1:E:132:ASN:OD1	1:E:134:ASN:HB2	2.10	0.51
3:F:215:PHE:C	3:F:215:PHE:CD2	2.86	0.51
3:J:138:THR:HG22	3:J:140:THR:N	2.25	0.51
1:K:68:THR:HA	7:K:526:HOH:O	2.10	0.51
1:L:119:LYS:HB3	1:L:252:TRP:CB	2.40	0.51
1:L:167:GLU:OE1	7:L:418:HOH:O	2.19	0.51
1:C:230:ASN:N	1:C:230:ASN:OD1	2.42	0.51
2:D:51:HIS:CA	7:D:406:HOH:O	2.55	0.51
1:E:266:GLU:O	1:E:269:THR:HB	2.11	0.51
3:F:47:LYS:HD2	3:F:47:LYS:N	2.25	0.51
3:F:96:ASN:OD1	3:F:99:MET:HB2	2.10	0.51
3:F:114:ILE:HA	3:F:177:ILE:O	2.10	0.51
3:H:77:SER:O	3:H:79:PHE:N	2.43	0.51
1:I:200:ASP:O	1:I:201:VAL:CG2	2.58	0.51
3:J:94:HIS:O	3:J:161:HIS:HE1	1.93	0.51
1:L:75:ASP:N	7:L:434:HOH:O	2.43	0.51
1:C:36:ARG:C	1:C:38:ASP:H	2.17	0.51
1:C:36:ARG:CB	1:C:38:ASP:OD1	2.59	0.51
1:C:172:LYS:HG3	1:B:170:ASN:O	2.11	0.51
1:A:56:VAL:O	1:A:57:ILE:C	2.52	0.51
1:A:194:THR:HG22	7:A:421:HOH:O	2.10	0.51
1:B:45:TYR:CG	1:B:46:PRO:HD2	2.45	0.51
1:B:216:SER:HB2	7:B:412:HOH:O	2.09	0.51
1:E:259:LYS:O	1:E:260:GLN:C	2.52	0.51
3:F:36:ARG:C	3:F:38:ASP:N	2.64	0.51
3:F:136:PRO:O	3:F:137:SER:C	2.54	0.51
3:H:55:GLU:O	3:H:58:GLU:N	2.43	0.51
3:J:47:LYS:N	3:J:47:LYS:HD2	2.25	0.51
3:J:130:ARG:CG	7:J:423:HOH:O	2.57	0.51
1:A:116:ARG:HH22	4:A:301:A3P:P1	2.33	0.51
1:A:125:MET:O	1:A:126:PHE:C	2.49	0.51
1:B:51:HIS:HE1	1:B:237:THR:HG21	1.76	0.51
2:D:186:PHE:CE1	2:D:210:ALA:HA	2.46	0.51
3:F:251:ASP:C	3:F:253:ILE:N	2.69	0.51
3:G:187:VAL:O	3:G:191:LYS:HG3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:187:VAL:O	3:H:188:LYS:C	2.51	0.51
1:K:18:PHE:HZ	1:K:99:MET:HE1	1.74	0.51
1:K:52:TRP:O	1:K:56:VAL:HG23	2.10	0.51
1:A:26:LEU:HD12	1:A:26:LEU:O	2.11	0.51
1:A:115:VAL:HA	7:A:485:HOH:O	2.10	0.51
1:B:116:ARG:HG3	1:B:179:TYR:HB3	1.90	0.51
1:B:151:GLY:HA2	1:B:157:SER:CA	2.41	0.51
2:D:181:GLU:HB2	2:D:184:LYS:HZ3	1.74	0.51
1:E:50:THR:O	1:E:51:HIS:C	2.53	0.51
1:E:110:LYS:HE3	7:E:419:HOH:O	2.11	0.51
1:E:232:VAL:HG23	1:E:233:ILE:N	2.25	0.51
3:G:171:ASP:C	7:H:434:HOH:O	2.53	0.51
3:H:13:TYR:CD1	3:H:14:MET:HG2	2.46	0.51
3:J:95:LEU:CD2	3:J:99:MET:HE3	2.41	0.51
1:K:168:HIS:HB3	1:K:171:ASP:OD2	2.11	0.51
1:A:267:LEU:CD2	1:A:271:LYS:HG2	2.36	0.51
1:B:47:LYS:N	1:B:47:LYS:HD2	2.25	0.51
3:H:222:ALA:O	3:H:223:ALA:HB2	2.10	0.51
3:H:247:GLY:N	4:H:301:A3P:O1P	2.43	0.51
3:H:276:ASP:O	3:H:277:VAL:C	2.54	0.51
1:I:54:ALA:O	1:I:55:GLU:C	2.51	0.51
1:I:123:VAL:HG21	1:I:252:TRP:HA	1.92	0.51
1:I:275:SER:OG	1:I:278:GLY:N	2.28	0.51
1:K:41:PHE:HA	1:K:91:ILE:O	2.10	0.51
1:K:51:HIS:HA	1:K:233:ILE:HD11	1.92	0.51
1:K:229:PRO:C	1:K:230:ASN:OD1	2.53	0.51
1:L:27:LEU:C	1:L:29:SER:N	2.65	0.51
1:L:234:CYS:HB3	1:L:237:THR:CG2	2.41	0.51
1:C:234:CYS:SG	1:C:237:THR:HG23	2.50	0.51
7:C:410:HOH:O	1:A:279:ARG:HD2	2.10	0.51
1:A:108:GLN:NE2	7:A:454:HOH:O	2.44	0.51
2:D:40:ILE:N	2:D:89:ARG:O	2.30	0.51
1:E:23:SER:HB3	1:E:74:GLY:O	2.11	0.51
1:E:275:SER:O	1:E:276:ASP:C	2.53	0.51
3:F:73:LEU:O	3:F:78:LYS:HE3	2.11	0.51
3:H:234:CYS:SG	3:H:237:THR:HG22	2.51	0.51
1:I:23:SER:O	1:I:27:LEU:HG	2.10	0.51
1:I:65:ILE:HA	1:I:88:ARG:O	2.11	0.51
1:I:166:GLU:C	1:I:168:HIS:H	2.19	0.51
1:C:12:LYS:CD	1:C:17:PHE:CE2	2.94	0.51
1:A:225:GLU:HG2	1:A:231:HIS:ND1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:VAL:O	1:B:243:VAL:HG23	2.11	0.51
3:G:50:THR:HB	4:G:301:A3P:O6P	2.11	0.51
3:G:98[A]:GLU:CD	1:I:98:GLU:HG3	2.36	0.51
3:H:53:LEU:O	3:H:56:VAL:HB	2.11	0.51
1:I:189:SER:O	1:I:192:LYS:HB3	2.11	0.51
1:K:36:ARG:NH1	1:K:85:ILE:O	2.44	0.51
1:L:43:VAL:O	1:L:113:TYR:HA	2.11	0.51
1:A:219:LYS:O	1:A:221:ASN:ND2	2.43	0.50
2:D:77:SER:O	2:D:79:PHE:N	2.44	0.50
2:D:248:VAL:HG22	2:D:249:VAL:N	2.25	0.50
1:E:37:GLU:OE1	7:E:417:HOH:O	2.19	0.50
3:H:12:LYS:CD	3:H:17:PHE:CE2	2.94	0.50
3:H:25:GLU:CB	3:H:76:ILE:HG23	2.27	0.50
3:H:31:ASP:C	3:H:33:PHE:N	2.69	0.50
3:J:163:LEU:O	3:J:164:SER:C	2.53	0.50
1:L:132:ASN:HB3	1:L:135:LEU:HD12	1.92	0.50
1:A:228:ASP:O	1:A:229:PRO:O	2.29	0.50
2:D:36:ARG:CZ	3:H:140:THR:HG22	2.40	0.50
1:E:16:ILE:CG2	1:E:17:PHE:N	2.74	0.50
3:F:102:VAL:O	3:F:102:VAL:HG22	2.11	0.50
3:F:132:ASN:OD1	3:F:133:PRO:HD2	2.10	0.50
3:G:72:GLU:OE1	3:G:93:THR:OG1	2.22	0.50
3:G:116:ARG:O	3:G:117:ASN:C	2.51	0.50
1:I:56:VAL:O	1:I:57:ILE:C	2.52	0.50
3:J:52:TRP:CD2	3:J:182:MET:CE	2.94	0.50
1:C:208:LYS:O	1:C:212:SER:OG	2.29	0.50
1:A:30:LEU:HB2	7:A:474:HOH:O	2.11	0.50
2:D:200:ASP:CG	7:D:410:HOH:O	2.54	0.50
2:D:253:ILE:C	2:D:255:TYR:H	2.19	0.50
1:E:207:ALA:O	1:E:208:LYS:C	2.55	0.50
3:H:16:ILE:O	3:H:18:PHE:CE1	2.64	0.50
3:H:147:LEU:HD22	3:H:152:ASP:HB2	1.93	0.50
3:J:95:LEU:HD22	3:J:99:MET:CB	2.41	0.50
1:L:47:LYS:H	4:L:301:A3P:P2	2.34	0.50
1:L:47:LYS:HB2	1:L:121:THR:HG23	1.93	0.50
1:A:218:MET:O	1:A:219:LYS:C	2.54	0.50
1:E:220:SER:O	1:E:221:ASN:CG	2.54	0.50
3:F:223:ALA:CA	7:F:411:HOH:O	2.60	0.50
3:H:12:LYS:HE3	3:H:17:PHE:CD2	2.47	0.50
1:I:71:ILE:HG22	1:I:93:THR:CB	2.39	0.50
3:J:129:TYR:O	3:J:137:SER:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:SER:O	1:K:221:ASN:HB3	2.10	0.50
1:L:26:LEU:CD1	1:L:79:PHE:CZ	2.93	0.50
1:L:27:LEU:O	1:L:28:GLY:C	2.52	0.50
2:D:181:GLU:CB	2:D:184:LYS:HE2	2.42	0.50
3:G:271:LYS:NZ	1:I:31:ASP:OD2	2.36	0.50
3:H:202:ASN:CG	3:H:205:GLU:HG2	2.36	0.50
1:K:224:LYS:HB3	1:K:228:ASP:O	2.11	0.50
1:K:248:VAL:HG22	1:K:249:VAL:H	1.75	0.50
1:L:116:ARG:CD	1:L:121:THR:OG1	2.60	0.50
1:C:188:LYS:HG2	7:C:428:HOH:O	2.11	0.50
1:A:116:ARG:HH12	4:A:301:A3P:P1	2.34	0.50
1:B:254:ASN:CA	7:B:406:HOH:O	2.60	0.50
2:D:13:TYR:O	2:D:14:MET:C	2.53	0.50
1:E:199:ILE:HG22	1:E:201:VAL:HG23	1.93	0.50
3:F:222:ALA:O	3:F:223:ALA:HB2	2.11	0.50
3:G:50:THR:H	4:G:301:A3P:P2	2.35	0.50
3:G:52:TRP:CD2	3:G:182:MET:HE3	2.47	0.50
1:I:59:ARG:HB3	1:I:209:ILE:CD1	2.42	0.50
1:L:132:ASN:O	1:L:135:LEU:N	2.37	0.50
1:L:146:GLU:O	7:L:420:HOH:O	2.20	0.50
1:L:186:PHE:CD1	1:L:187:VAL:N	2.80	0.50
1:L:213:THR:C	7:L:406:HOH:O	2.51	0.50
1:B:202:ASN:O	1:B:205:GLU:CB	2.57	0.50
1:B:222:ALA:O	1:B:223:ALA:CB	2.60	0.50
2:D:88:ARG:CG	7:D:411:HOH:O	2.59	0.50
1:E:172:LYS:HE2	3:F:169:LYS:O	2.12	0.50
3:F:226:ASN:CG	3:F:226:ASN:O	2.55	0.50
3:F:239:ASP:OD2	3:F:242:LEU:HG	2.12	0.50
3:H:33:PHE:O	3:H:103:THR:CG2	2.60	0.50
3:H:215:PHE:O	3:H:216:SER:C	2.52	0.50
1:B:231:HIS:ND1	1:B:231:HIS:O	2.44	0.50
2:D:264:PHE:CD1	2:D:264:PHE:C	2.90	0.50
1:E:183:LYS:HB2	7:E:403:HOH:O	2.10	0.50
1:E:186:PHE:CD1	1:E:186:PHE:O	2.65	0.50
1:I:89:ARG:HG2	7:I:404:HOH:O	2.11	0.50
1:I:234:CYS:HB3	1:I:237:THR:CG2	2.41	0.50
1:L:183:LYS:HA	7:L:467:HOH:O	2.12	0.50
2:D:97:TYR:OH	1:E:167:GLU:OE1	2.21	0.50
2:D:189:SER:O	2:D:192:LYS:N	2.45	0.50
1:E:19:SER:C	1:E:21:MET:N	2.66	0.50
1:E:35:ALA:N	1:E:103:THR:HG21	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:259:LYS:O	7:H:425:HOH:O	2.20	0.50
1:L:80:GLU:O	1:L:84:ARG:N	2.44	0.50
1:L:194:THR:HG22	1:L:195:ALA:N	2.26	0.50
1:A:68:THR:N	1:A:90:ALA:O	2.30	0.49
1:A:123:VAL:HG21	1:A:252:TRP:HA	1.94	0.49
1:A:203:ASP:HA	7:A:416:HOH:O	2.11	0.49
2:D:216:SER:O	2:D:220:SER:OG	2.22	0.49
1:E:41:PHE:HB2	1:E:111:ILE:HD13	1.93	0.49
1:E:114:ILE:C	7:E:408:HOH:O	2.53	0.49
1:E:182:MET:O	1:E:186:PHE:HB2	2.12	0.49
1:E:231:HIS:O	1:E:231:HIS:CG	2.65	0.49
3:F:258:PRO:O	3:F:259:LYS:C	2.55	0.49
3:H:26:LEU:HD22	3:H:74:GLY:C	2.37	0.49
1:L:257:THR:HB	1:L:258:PRO:HD2	1.92	0.49
1:A:51:HIS:O	1:A:52:TRP:C	2.52	0.49
1:A:138:THR:HG21	1:A:144:PHE:HB2	1.94	0.49
1:B:259:LYS:O	1:B:260:GLN:C	2.53	0.49
1:E:110:LYS:NZ	7:E:437:HOH:O	2.45	0.49
3:F:84:ARG:CZ	3:J:130:ARG:NH2	2.75	0.49
3:G:192:LYS:O	3:G:193:ILE:C	2.53	0.49
3:G:225:GLU:CD	3:G:226:ASN:H	2.18	0.49
1:I:85:ILE:CB	7:I:404:HOH:O	2.55	0.49
1:L:44:SER:CB	1:L:114:ILE:HG22	2.33	0.49
1:C:138:THR:O	1:C:138:THR:HG22	2.12	0.49
1:B:213:THR:HA	1:B:218:MET:HG3	1.94	0.49
1:E:98:GLU:HB3	7:E:458:HOH:O	2.11	0.49
1:E:279:ARG:HG3	7:E:454:HOH:O	2.10	0.49
3:G:126:PHE:CZ	3:G:130:ARG:HD2	2.48	0.49
3:G:239:ASP:O	3:G:240:ARG:C	2.54	0.49
3:H:160:ASP:CG	7:H:437:HOH:O	2.54	0.49
3:J:80:GLU:O	3:J:80:GLU:CD	2.56	0.49
1:A:93:THR:O	1:A:93:THR:CG2	2.60	0.49
1:B:113:TYR:CD1	1:B:113:TYR:C	2.88	0.49
1:B:201:VAL:CG1	1:B:205:GLU:HB3	2.42	0.49
2:D:168:HIS:CE1	1:E:167:GLU:CG	2.96	0.49
1:E:158:TRP:O	1:E:162:VAL:HG23	2.12	0.49
3:F:128:TYR:O	3:F:132:ASN:HB2	2.12	0.49
3:F:233:ILE:HD11	7:F:406:HOH:O	2.11	0.49
3:H:41:PHE:N	7:H:401:HOH:O	2.35	0.49
3:H:181[B]:GLU:CD	3:H:189:SER:HG	2.16	0.49
3:H:188:LYS:O	3:H:189:SER:C	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:ASP:OD1	1:K:101:PRO:HA	2.12	0.49
1:L:67:LEU:O	1:L:231:HIS:CE1	2.65	0.49
1:C:190:LEU:O	1:C:193:ILE:HB	2.13	0.49
1:C:284:TYR:O	1:C:287:SER:C	2.55	0.49
2:D:36:ARG:CB	2:D:38:ASP:OD1	2.60	0.49
2:D:98[A]:GLU:HG2	7:E:418:HOH:O	2.11	0.49
3:F:175:LEU:HD22	3:F:196:PHE:CB	2.43	0.49
3:H:51:HIS:N	4:H:301:A3P:O4P	2.35	0.49
3:H:268:PHE:C	3:H:268:PHE:CD2	2.89	0.49
1:I:79:PHE:HD1	1:I:82:LEU:HD12	1.78	0.49
1:I:98:GLU:CD	1:I:98:GLU:N	2.70	0.49
3:J:98[B]:GLU:OE2	1:K:98[B]:GLU:HG2	2.12	0.49
3:J:127:HIS:O	3:J:131:ASP:N	2.45	0.49
1:L:115:VAL:O	1:L:115:VAL:HG13	2.13	0.49
1:L:191:LYS:O	1:L:192:LYS:C	2.53	0.49
1:C:251:ASP:C	1:C:253:ILE:H	2.20	0.49
1:A:35:ALA:H	1:A:103:THR:HG21	1.77	0.49
1:A:189:SER:O	1:A:193:ILE:N	2.32	0.49
1:A:206:MET:HA	1:A:209:ILE:HG13	1.95	0.49
1:B:284:TYR:O	1:B:285:ALA:C	2.55	0.49
1:E:29:SER:O	1:E:30:LEU:C	2.55	0.49
1:E:202:ASN:O	1:E:205:GLU:HB2	2.13	0.49
3:G:41:PHE:HB2	3:G:111:ILE:CD1	2.42	0.49
3:G:56:VAL:O	3:G:57:ILE:C	2.54	0.49
3:H:160:ASP:CG	7:H:421:HOH:O	2.53	0.49
3:H:248:VAL:HG22	3:H:249:VAL:N	2.27	0.49
1:C:205:GLU:HA	7:C:408:HOH:O	2.13	0.49
1:A:79:PHE:O	1:A:81:GLU:N	2.46	0.49
1:A:228:ASP:C	1:A:229:PRO:O	2.55	0.49
1:A:255:TYR:HA	1:I:87:LYS:HD2	1.93	0.49
1:B:16:ILE:HG21	1:B:155:TYR:HA	1.94	0.49
2:D:98[A]:GLU:CD	1:E:98:GLU:HG3	2.38	0.49
2:D:113:TYR:CE2	2:D:165:TRP:CD1	3.00	0.49
2:D:168:HIS:HA	2:D:171:ASP:OD1	2.13	0.49
3:F:97:TYR:O	3:F:100:LEU:HB3	2.13	0.49
3:F:99:MET:O	3:F:100:LEU:C	2.55	0.49
3:G:56:VAL:O	3:G:59:ARG:HB2	2.12	0.49
1:I:55:GLU:O	1:I:56:VAL:C	2.56	0.49
1:I:221:ASN:O	1:I:222:ALA:HB2	2.13	0.49
3:J:138:THR:HG23	3:J:139:GLU:N	2.27	0.49
1:L:50:THR:OG1	4:L:301:A3P:O4P	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:GLU:OE2	1:L:277:VAL:HG23	2.12	0.49
1:C:33:PHE:O	1:C:103:THR:HG21	2.13	0.49
1:B:11:HIS:CE1	1:B:20:THR:HA	2.48	0.49
1:B:12:LYS:CD	1:B:17:PHE:CD2	2.95	0.49
1:B:130:ARG:HD2	7:B:474:HOH:O	2.12	0.49
2:D:35:ALA:HB2	2:D:103:THR:HG23	1.95	0.49
1:E:166:GLU:O	1:E:169:LYS:N	2.38	0.49
3:F:184:LYS:HG2	3:F:185:ASP:H	1.76	0.49
3:G:264:PHE:O	3:G:265:ASP:C	2.52	0.49
1:I:25:GLU:H	1:I:25:GLU:CD	2.17	0.49
1:I:177:ILE:HD13	1:I:192:LYS:CE	2.40	0.49
3:J:23:SER:CB	3:J:74:GLY:O	2.61	0.49
1:L:144:PHE:O	1:L:146:GLU:N	2.45	0.49
1:C:115:VAL:N	1:C:177:ILE:O	2.45	0.49
1:A:47:LYS:HE3	4:A:301:A3P:H5'1	1.95	0.49
2:D:127:HIS:CD2	2:D:245:ARG:HD2	2.47	0.49
3:G:193:ILE:HG22	3:G:194:THR:N	2.25	0.49
1:I:11:HIS:CE1	1:I:20:THR:HA	2.48	0.49
1:I:51:HIS:CE1	1:I:243:VAL:HG11	2.48	0.49
3:J:23:SER:HB3	3:J:74:GLY:O	2.13	0.49
3:J:47:LYS:NZ	4:J:301:A3P:O4P	2.39	0.49
3:J:77:SER:O	3:J:80:GLU:N	2.46	0.49
3:J:161:HIS:CE1	7:J:440:HOH:O	2.65	0.49
3:J:219:LYS:O	3:J:220:SER:C	2.55	0.49
1:K:117:ASN:HA	1:K:281:LEU:HD22	1.94	0.49
1:K:253:ILE:HD11	7:K:436:HOH:O	2.13	0.49
1:L:189:SER:O	1:L:192:LYS:HB3	2.12	0.49
1:L:286:HIS:O	1:L:286:HIS:CD2	2.66	0.49
1:C:119:LYS:NZ	1:C:261:ASN:OD1	2.43	0.49
1:C:239:ASP:OD1	1:C:241:ASN:HB2	2.13	0.49
1:C:283:GLU:OE1	1:C:283:GLU:CA	2.59	0.49
4:C:301:A3P:H3'	7:C:434:HOH:O	2.12	0.49
1:B:182:MET:O	1:B:186[A]:PHE:HB2	2.13	0.49
2:D:45:TYR:CG	2:D:46:PRO:HD2	2.48	0.49
2:D:181:GLU:HB2	2:D:184:LYS:HZ1	1.76	0.49
1:E:138:THR:HB	7:E:432:HOH:O	2.13	0.49
1:E:269:THR:O	1:E:273:ARG:N	2.30	0.49
3:G:94:HIS:CE1	7:G:460:HOH:O	2.65	0.49
3:H:185:ASP:HB3	3:H:188:LYS:HD2	1.95	0.49
3:H:203:ASP:O	3:H:204:SER:C	2.56	0.49
1:K:35:ALA:H	1:K:103:THR:CG2	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:ALA:O	1:K:223:ALA:HB2	2.12	0.49
1:K:250:GLY:C	1:K:252:TRP:N	2.70	0.49
1:L:118:PRO:O	1:L:122:ALA:N	2.42	0.49
1:L:169:LYS:O	1:L:169:LYS:HG3	2.13	0.49
1:C:39:ASP:OD1	1:C:89:ARG:NE	2.36	0.48
1:C:100:LEU:O	1:C:105:LYS:HE3	2.13	0.48
1:C:261:ASN:O	1:C:262:ARG:C	2.56	0.48
1:C:272:MET:O	1:C:273:ARG:C	2.56	0.48
1:A:121:THR:O	1:A:125:MET:N	2.41	0.48
1:A:203:ASP:CA	7:A:416:HOH:O	2.60	0.48
1:E:222:ALA:O	1:E:223:ALA:HB3	2.13	0.48
3:F:38:ASP:OD1	3:F:38:ASP:C	2.56	0.48
1:I:200:ASP:OD2	1:I:200:ASP:N	2.31	0.48
1:K:45:TYR:CG	1:K:46:PRO:HD2	2.48	0.48
1:L:52:TRP:NE1	7:L:406:HOH:O	2.45	0.48
1:L:207:ALA:O	1:L:208:LYS:C	2.56	0.48
1:C:12:LYS:HD2	1:C:17:PHE:CG	2.48	0.48
1:C:100:LEU:HD22	1:C:165:TRP:HH2	1.77	0.48
1:A:48:SER:O	1:A:114:ILE:HG12	2.13	0.48
1:A:240:ARG:O	1:A:241:ASN:C	2.56	0.48
1:B:16:ILE:CG2	1:B:155:TYR:C	2.86	0.48
1:B:17:PHE:O	1:B:154:VAL:HA	2.13	0.48
1:B:234:CYS:SG	1:B:237:THR:HG23	2.52	0.48
2:D:25:GLU:CD	2:D:25:GLU:N	2.71	0.48
2:D:36:ARG:C	2:D:38:ASP:N	2.71	0.48
2:D:187:VAL:O	2:D:191:LYS:HG3	2.13	0.48
3:F:47:LYS:HA	4:F:301:A3P:O5'	2.13	0.48
3:G:47:LYS:H	4:G:301:A3P:P2	2.35	0.48
3:G:67:LEU:HD12	3:G:90:ALA:HB3	1.95	0.48
3:H:149:LEU:HD22	3:H:267:LEU:HD12	1.95	0.48
1:I:100:LEU:HD23	1:I:105:LYS:HG2	1.95	0.48
1:L:47:LYS:HA	4:L:301:A3P:P2	2.53	0.48
1:L:50:THR:CG2	1:L:94:HIS:CE1	2.95	0.48
1:A:203:ASP:C	7:A:416:HOH:O	2.54	0.48
1:B:116:ARG:O	1:B:117:ASN:C	2.49	0.48
2:D:45:TYR:CD2	2:D:158:TRP:HD1	2.30	0.48
1:I:197:LEU:O	1:I:198:GLY:C	2.56	0.48
1:I:222:ALA:O	1:I:223:ALA:HB2	2.12	0.48
1:I:252:TRP:O	1:I:256:PHE:HD1	1.96	0.48
3:J:117:ASN:CA	3:J:281:LEU:HD22	2.43	0.48
3:J:123:VAL:O	3:J:124:SER:C	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:VAL:HG22	1:L:93:THR:HG22	1.94	0.48
1:L:102:VAL:O	1:L:105:LYS:HB2	2.13	0.48
1:A:56:VAL:O	1:A:59:ARG:N	2.32	0.48
1:B:202:ASN:C	1:B:202:ASN:OD1	2.57	0.48
3:F:33:PHE:CE2	3:F:35:ALA:CA	2.96	0.48
3:F:86:PRO:HG2	3:F:87:LYS:H	1.78	0.48
3:G:264:PHE:C	3:G:266:GLU:N	2.67	0.48
3:H:183:LYS:HD3	4:H:301:A3P:H2	1.95	0.48
1:I:194:THR:CG2	1:I:195:ALA:H	2.26	0.48
3:J:264:PHE:O	3:J:268:PHE:N	2.34	0.48
1:C:84:ARG:O	1:C:86:PRO:HD3	2.13	0.48
1:A:54:ALA:C	7:A:446:HOH:O	2.55	0.48
1:A:76:ILE:H	1:A:76:ILE:CD1	2.22	0.48
1:A:188:LYS:O	1:A:191:LYS:HB2	2.13	0.48
1:B:16:ILE:HD13	7:B:444:HOH:O	2.12	0.48
2:D:98[B]:GLU:HG3	7:D:442:HOH:O	2.12	0.48
2:D:173:ASN:HA	7:D:404:HOH:O	2.06	0.48
1:E:43:VAL:HG22	1:E:93:THR:HG22	1.96	0.48
3:F:36:ARG:HD3	7:F:413:HOH:O	2.07	0.48
3:F:206:MET:O	3:F:209:ILE:HB	2.12	0.48
3:H:73:LEU:CD2	3:H:232:VAL:HG21	2.44	0.48
3:H:181[B]:GLU:CD	3:H:189:SER:OG	2.55	0.48
1:I:9:LEU:HD12	1:I:10:LEU:H	1.77	0.48
1:I:78:LYS:HD3	1:I:78:LYS:C	2.38	0.48
1:I:82:LEU:HB2	7:I:441:HOH:O	2.13	0.48
3:J:187:VAL:HG12	3:J:188:LYS:N	2.29	0.48
1:K:252:TRP:O	1:K:253:ILE:C	2.55	0.48
1:C:161:HIS:O	1:C:165:TRP:HD1	1.96	0.48
1:A:12:LYS:HA	1:A:16:ILE:O	2.12	0.48
1:A:24:GLU:O	1:A:25:GLU:C	2.54	0.48
1:A:52:TRP:CE2	4:A:301:A3P:C6	2.97	0.48
1:B:128:TYR:OH	1:B:237:THR:HG22	2.13	0.48
2:D:147:LEU:O	2:D:148:PHE:C	2.54	0.48
3:F:36:ARG:NH1	7:F:413:HOH:O	2.11	0.48
3:F:144:PHE:O	3:F:145:LEU:C	2.56	0.48
3:G:264:PHE:C	3:G:264:PHE:CD1	2.91	0.48
1:I:53:LEU:O	1:I:56:VAL:HB	2.13	0.48
1:I:116:ARG:O	1:I:117:ASN:C	2.55	0.48
3:J:19:SER:C	3:J:21:MET:H	2.20	0.48
3:J:138:THR:HG22	3:J:140:THR:H	1.79	0.48
1:L:225:GLU:OE2	1:L:231:HIS:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:ASP:O	1:L:229:PRO:C	2.57	0.48
4:L:301:A3P:O1P	7:L:419:HOH:O	2.20	0.48
1:C:26:LEU:HD12	1:C:26:LEU:C	2.37	0.48
1:C:68:THR:O	1:C:92:PRO:CD	2.62	0.48
1:A:137:SER:N	7:A:419:HOH:O	2.10	0.48
1:B:101:PRO:HB2	1:B:104:VAL:HG23	1.96	0.48
1:B:114:ILE:HG21	7:B:404:HOH:O	2.13	0.48
1:E:52:TRP:CH2	1:E:182:MET:CB	2.96	0.48
1:E:243:VAL:O	4:E:301:A3P:H2'	2.14	0.48
3:F:97:TYR:O	3:F:98:GLU:C	2.57	0.48
3:G:23:SER:OG	3:G:26:LEU:HB3	2.14	0.48
3:G:77:SER:O	3:G:81:GLU:HG3	2.14	0.48
1:I:9:LEU:HD12	1:I:10:LEU:N	2.27	0.48
3:J:80:GLU:OE1	3:J:80:GLU:HA	2.14	0.48
3:J:187:VAL:O	3:J:188:LYS:C	2.56	0.48
1:K:146:GLU:HB3	7:K:532:HOH:O	2.13	0.48
1:K:252:TRP:CD2	1:K:253:ILE:N	2.81	0.48
1:L:116:ARG:HG2	1:L:117:ASN:O	2.13	0.48
1:L:208:LYS:O	1:L:211:ARG:N	2.46	0.48
1:L:287:SER:O	1:L:288:ALA:C	2.57	0.48
1:C:43:VAL:HG22	1:C:93:THR:CG2	2.43	0.48
1:E:12:LYS:CD	1:E:17:PHE:CE2	2.91	0.48
1:E:116:ARG:O	1:E:117:ASN:C	2.55	0.48
1:E:277:VAL:O	1:E:278:GLY:C	2.52	0.48
3:G:50:THR:CB	4:G:301:A3P:P2	3.01	0.48
3:G:181:GLU:HB2	3:G:184:LYS:HE2	1.96	0.48
3:G:267:LEU:O	3:G:270:GLU:N	2.46	0.48
3:H:23:SER:CB	3:H:74:GLY:O	2.61	0.48
3:H:228:ASP:N	3:H:229:PRO:CD	2.77	0.48
1:I:203:ASP:OD1	1:I:203:ASP:N	2.45	0.48
3:J:33:PHE:O	3:J:103:THR:HG21	2.13	0.48
3:J:201:VAL:HG13	3:J:205:GLU:OE2	2.13	0.48
3:J:206:MET:O	3:J:209:ILE:CB	2.61	0.48
1:K:282:LYS:O	1:K:286:HIS:CD2	2.67	0.48
1:L:101:PRO:HB2	1:L:104:VAL:HG23	1.96	0.48
1:L:269:THR:O	1:L:273:ARG:HD2	2.13	0.48
1:C:69:SER:OG	1:C:232:VAL:HG13	2.14	0.48
1:B:234:CYS:HB3	1:B:237:THR:HG23	1.96	0.48
2:D:27:LEU:O	2:D:30:LEU:HD22	2.14	0.48
3:F:71:ILE:HG23	3:F:72:GLU:N	2.29	0.48
3:F:96:ASN:ND2	3:F:99:MET:HE2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:43:VAL:O	3:G:113:TYR:HA	2.13	0.48
3:G:98[A]:GLU:CG	1:I:98:GLU:CD	2.86	0.48
3:H:101:PRO:HB3	7:H:429:HOH:O	2.12	0.48
1:I:89:ARG:CG	7:I:404:HOH:O	2.62	0.48
1:I:119:LYS:HB3	1:I:252:TRP:CB	2.44	0.48
1:I:149:LEU:HB2	7:I:434:HOH:O	2.14	0.48
3:J:138:THR:CG2	3:J:140:THR:H	2.27	0.48
1:K:46:PRO:HG2	1:K:125:MET:HE3	1.96	0.48
1:K:228:ASP:CB	1:K:229:PRO:CD	2.91	0.48
1:L:285:ALA:C	1:L:287:SER:H	2.21	0.48
1:C:251:ASP:O	1:C:252:TRP:C	2.57	0.48
1:A:234:CYS:O	1:A:237:THR:HG22	2.13	0.48
1:B:11:HIS:HE1	1:B:19:SER:O	1.97	0.48
1:B:26:LEU:HD12	1:B:26:LEU:O	2.13	0.48
1:B:110:LYS:HB3	1:B:196:PHE:CE2	2.49	0.48
2:D:94:HIS:HB2	2:D:155:TYR:CE1	2.49	0.48
2:D:262:ARG:O	2:D:266:GLU:HG3	2.14	0.48
1:E:212:SER:HA	1:E:217:GLU:HG3	1.95	0.48
1:E:228:ASP:O	1:E:229:PRO:C	2.57	0.48
3:F:132:ASN:C	3:F:134:ASN:N	2.70	0.48
3:F:144:PHE:O	3:F:147:LEU:N	2.45	0.48
3:G:187:VAL:O	3:G:187:VAL:CG1	2.61	0.48
3:G:211:ARG:NH2	3:J:131:ASP:HA	2.21	0.48
3:G:239:ASP:OD1	3:G:241:ASN:CB	2.60	0.48
3:H:8:SER:O	3:H:20:THR:HG21	2.12	0.48
3:J:125:MET:HE2	3:J:129:TYR:HE1	1.78	0.48
3:J:172:LYS:HB3	7:J:436:HOH:O	2.14	0.48
1:L:13:TYR:CE1	1:L:14[B]:MET:HG3	2.48	0.48
1:L:258:PRO:O	1:L:261:ASN:CB	2.62	0.48
1:C:273:ARG:HB2	7:C:411:HOH:O	2.11	0.47
1:A:183:LYS:CD	4:A:301:A3P:H2	2.44	0.47
1:B:167:GLU:OE1	7:B:427:HOH:O	2.20	0.47
2:D:282:LYS:O	2:D:284:TYR:N	2.46	0.47
3:F:41:PHE:HB2	3:F:111:ILE:HD13	1.96	0.47
1:I:193:ILE:O	1:I:194:THR:C	2.56	0.47
3:J:72:GLU:OE1	3:J:72:GLU:N	2.43	0.47
3:J:172:LYS:CE	7:L:407:HOH:O	2.62	0.47
3:J:202:ASN:C	3:J:202:ASN:OD1	2.55	0.47
1:K:115:VAL:HG22	1:K:116:ARG:N	2.29	0.47
1:L:202:ASN:OD1	1:L:202:ASN:C	2.56	0.47
1:B:12:LYS:HD3	1:B:17:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:GLU:O	2:D:184:LYS:N	2.47	0.47
3:F:36:ARG:N	3:F:39:ASP:OD2	2.47	0.47
3:F:245:ARG:HH21	4:F:301:A3P:P1	2.37	0.47
3:H:45:TYR:CG	3:H:46:PRO:HD2	2.49	0.47
1:I:75:ASP:C	1:I:77:SER:H	2.21	0.47
1:I:98:GLU:HG2	7:I:499:HOH:O	2.13	0.47
3:J:177:ILE:CD1	3:J:192:LYS:HE2	2.42	0.47
1:L:41:PHE:CE1	1:L:104:VAL:HG13	2.48	0.47
1:C:13:TYR:O	1:C:14[B]:MET:HB2	2.15	0.47
1:C:41:PHE:HA	1:C:91:ILE:O	2.14	0.47
1:C:62:ASP:N	7:C:444:HOH:O	2.46	0.47
1:C:173:ASN:ND2	7:C:426:HOH:O	2.29	0.47
1:C:215:PHE:CZ	1:C:244:PHE:HB3	2.49	0.47
1:A:52:TRP:CD2	1:A:182:MET:HE3	2.49	0.47
1:A:239:ASP:HB3	7:A:469:HOH:O	2.14	0.47
4:D:301:A3P:O1P	4:D:301:A3P:O2'	2.30	0.47
1:E:224:LYS:C	7:E:425:HOH:O	2.57	0.47
3:F:40:ILE:HD11	3:F:88:ARG:CZ	2.45	0.47
3:F:46:PRO:HG2	3:F:125:MET:HE3	1.96	0.47
3:F:245:ARG:NH2	4:F:301:A3P:O2P	2.47	0.47
3:G:79:PHE:O	3:G:80:GLU:C	2.56	0.47
3:H:22:SER:O	3:H:23:SER:C	2.57	0.47
3:H:96:ASN:C	3:H:96:ASN:OD1	2.56	0.47
3:H:102:VAL:HG13	3:H:103:THR:N	2.29	0.47
1:K:128:TYR:O	1:K:132:ASN:HB2	2.14	0.47
1:L:98[A]:GLU:H	1:L:98[A]:GLU:CD	2.23	0.47
1:L:128:TYR:OH	1:L:237:THR:CB	2.61	0.47
1:B:166:GLU:C	1:B:168:HIS:H	2.20	0.47
1:B:214:SER:OG	1:B:216:SER:OG	2.28	0.47
1:B:225:GLU:HG2	1:B:231:HIS:ND1	2.30	0.47
2:D:179:TYR:CE2	2:D:183:LYS:HG3	2.50	0.47
1:E:18:PHE:CZ	1:E:99:MET:HE1	2.49	0.47
1:E:166:GLU:O	1:E:167:GLU:C	2.58	0.47
1:E:228:ASP:CB	1:E:229:PRO:CD	2.92	0.47
3:G:18:PHE:HZ	3:G:99:MET:HE1	1.80	0.47
1:I:232:VAL:HG13	7:I:439:HOH:O	2.14	0.47
1:L:16:ILE:O	1:L:18:PHE:CD1	2.68	0.47
1:L:114:ILE:HA	1:L:177:ILE:O	2.14	0.47
1:C:173:ASN:HA	7:C:490:HOH:O	2.15	0.47
1:A:173:ASN:OD1	1:A:173:ASN:N	2.38	0.47
1:A:221:ASN:OD1	1:A:241:ASN:OD1	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HD3	7:B:416:HOH:O	2.14	0.47
2:D:76:ILE:HD13	2:D:76:ILE:N	2.29	0.47
3:F:119:LYS:HB3	3:F:252:TRP:CG	2.49	0.47
3:G:257:THR:OG1	3:G:260:GLN:HG3	2.15	0.47
3:H:12:LYS:HE3	3:H:17:PHE:CD1	2.49	0.47
3:H:279:ARG:HG2	3:H:283:GLU:OE1	2.14	0.47
1:I:49:GLY:O	1:I:50:THR:C	2.57	0.47
3:J:70:PRO:O	3:J:71:ILE:C	2.58	0.47
1:K:55:GLU:OE2	7:K:420:HOH:O	2.20	0.47
1:L:46:PRO:C	1:L:47:LYS:HG2	2.40	0.47
1:C:71:ILE:HG13	1:C:71:ILE:O	2.14	0.47
1:C:78:LYS:O	1:C:82:LEU:HG	2.14	0.47
1:A:51:HIS:HD1	4:A:301:A3P:P2	2.31	0.47
1:B:75:ASP:O	1:B:78:LYS:HB3	2.14	0.47
1:B:115:VAL:O	1:B:179:TYR:N	2.40	0.47
1:B:134:ASN:HA	7:B:419:HOH:O	2.15	0.47
1:B:154:VAL:C	1:B:156:GLY:N	2.72	0.47
1:B:205:GLU:O	1:B:206:MET:C	2.57	0.47
1:B:230:ASN:OD1	1:B:230:ASN:N	2.46	0.47
3:F:280:CYS:O	3:F:284:TYR:CD2	2.68	0.47
3:H:68:THR:C	3:H:69:SER:O	2.52	0.47
1:I:11:HIS:ND1	1:I:20:THR:HA	2.29	0.47
3:J:99:MET:O	3:J:100:LEU:C	2.57	0.47
3:J:172:LYS:CE	1:L:169:LYS:O	2.61	0.47
1:K:147:LEU:O	1:K:150:LYS:N	2.48	0.47
1:L:11:HIS:CE1	1:L:20:THR:HA	2.50	0.47
1:L:35:ALA:H	1:L:103:THR:CG2	2.28	0.47
1:L:181:GLU:CB	1:L:184:LYS:NZ	2.73	0.47
1:L:215:PHE:CE1	1:L:246:LYS:O	2.67	0.47
1:C:62:ASP:HA	7:C:444:HOH:O	2.15	0.47
1:A:79:PHE:C	1:A:81:GLU:N	2.70	0.47
1:B:127:HIS:CD2	1:B:245:ARG:NH1	2.83	0.47
1:B:147:LEU:O	1:B:148:PHE:C	2.55	0.47
1:B:231:HIS:O	1:B:231:HIS:CG	2.67	0.47
1:B:234:CYS:O	1:B:236:LEU:N	2.47	0.47
2:D:36:ARG:C	2:D:38:ASP:H	2.23	0.47
2:D:42:LEU:N	2:D:91:ILE:O	2.44	0.47
2:D:168:HIS:O	2:D:171:ASP:CB	2.62	0.47
2:D:284:TYR:O	2:D:285:ALA:C	2.56	0.47
1:E:59:ARG:CZ	1:E:212:SER:HB2	2.44	0.47
1:E:166:GLU:C	1:E:168:HIS:N	2.71	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ASN:O	1:E:275:SER:C	2.49	0.47
3:F:136:PRO:O	3:F:136:PRO:HG2	2.15	0.47
3:G:181:GLU:HA	3:G:184:LYS:HE2	1.96	0.47
3:G:217:GLU:C	7:G:442:HOH:O	2.58	0.47
3:G:231:HIS:NE2	7:G:428:HOH:O	2.34	0.47
3:H:202:ASN:O	3:H:206:MET:N	2.41	0.47
3:H:280:CYS:CA	3:H:283:GLU:OE2	2.59	0.47
1:I:58:GLU:CD	1:I:67:LEU:HD23	2.40	0.47
1:I:178:PHE:O	1:I:179:TYR:C	2.57	0.47
3:J:68:THR:HG23	3:J:90:ALA:O	2.15	0.47
3:J:277:VAL:O	3:J:278:GLY:C	2.57	0.47
1:K:96:ASN:C	1:K:98[B]:GLU:OE1	2.57	0.47
1:K:201:VAL:O	1:K:206:MET:HE3	2.14	0.47
1:K:261:ASN:O	1:K:264:PHE:HB3	2.14	0.47
1:L:126:PHE:O	1:L:129:TYR:HB2	2.15	0.47
1:L:247:GLY:HA2	4:L:301:A3P:H1'	1.96	0.47
1:L:252:TRP:CZ2	1:L:253:ILE:HG22	2.50	0.47
1:C:12:LYS:HA	1:C:16:ILE:O	2.15	0.47
1:C:193:ILE:C	1:C:195:ALA:N	2.70	0.47
1:C:231:HIS:O	1:C:231:HIS:ND1	2.48	0.47
1:A:45:TYR:O	1:A:48:SER:HB2	2.14	0.47
1:A:234:CYS:O	1:A:237:THR:CG2	2.62	0.47
1:B:116:ARG:HB2	1:B:179:TYR:CB	2.43	0.47
1:B:178:PHE:HE1	1:B:281:LEU:HG	1.80	0.47
1:E:70:PRO:HG3	1:E:233:ILE:O	2.14	0.47
1:E:262:ARG:C	1:E:264:PHE:N	2.70	0.47
3:F:150:LYS:CB	3:F:152:ASP:OD2	2.59	0.47
3:G:184:LYS:CG	3:G:185:ASP:N	2.77	0.47
3:H:38:ASP:CB	7:H:406:HOH:O	2.62	0.47
3:H:45:TYR:HD1	3:H:161:HIS:CG	2.33	0.47
1:I:206:MET:O	1:I:209:ILE:HB	2.15	0.47
1:I:267:LEU:HD23	1:I:267:LEU:HA	1.65	0.47
3:J:55:GLU:HA	3:J:55:GLU:OE2	2.14	0.47
3:J:246:LYS:HE3	3:J:251:ASP:OD1	2.14	0.47
1:K:231:HIS:C	1:K:232:VAL:O	2.56	0.47
1:A:178:PHE:O	1:A:179:TYR:C	2.58	0.47
1:B:116:ARG:HG3	1:B:179:TYR:CD2	2.50	0.47
2:D:11:HIS:CE1	2:D:19:SER:O	2.65	0.47
1:E:35:ALA:N	1:E:103:THR:CG2	2.75	0.47
3:G:181:GLU:CB	3:G:184:LYS:HE2	2.44	0.47
1:I:61:PRO:O	1:I:62:ASP:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:26:LEU:O	3:J:30:LEU:HD13	2.15	0.47
3:J:59:ARG:O	3:J:60:ILE:C	2.57	0.47
1:L:37:GLU:OE2	1:L:107:LYS:CD	2.63	0.47
1:L:158:TRP:O	1:L:162:VAL:HG23	2.14	0.47
1:C:274:ASN:N	7:C:411:HOH:O	2.44	0.47
1:A:279:ARG:CZ	1:A:279:ARG:HB2	2.44	0.47
1:B:45:TYR:O	1:B:48:SER:HB2	2.15	0.47
1:B:128:TYR:O	1:B:132:ASN:N	2.48	0.47
2:D:168:HIS:O	2:D:171:ASP:CG	2.58	0.47
1:E:194:THR:HG21	1:E:206:MET:CE	2.45	0.47
3:G:12:LYS:HA	3:G:16:ILE:O	2.14	0.47
3:G:26:LEU:CD1	3:G:79:PHE:CZ	2.98	0.47
3:G:128:TYR:HH	3:G:237:THR:HB	1.77	0.47
3:G:187:VAL:N	7:G:413:HOH:O	2.12	0.47
3:H:68:THR:O	3:H:92:PRO:CD	2.63	0.47
3:H:69:SER:HA	3:H:231:HIS:HE1	1.80	0.47
3:H:166:GLU:O	3:H:166:GLU:HG2	2.15	0.47
3:H:173:ASN:O	3:H:196:PHE:HZ	1.97	0.47
3:J:76:ILE:HD13	3:J:76:ILE:H	1.79	0.47
1:L:116:ARG:HB3	1:L:121:THR:OG1	2.14	0.47
1:C:267:LEU:CD2	1:C:271:LYS:HG3	2.45	0.46
1:A:18:PHE:HZ	1:A:99:MET:HE1	1.80	0.46
2:D:276:ASP:C	2:D:278:GLY:N	2.70	0.46
1:E:189:SER:O	1:E:192:LYS:HB3	2.15	0.46
1:E:267:LEU:HD22	1:E:271:LYS:HG2	1.96	0.46
3:F:35:ALA:HA	3:F:39:ASP:OD2	2.16	0.46
3:F:38:ASP:O	3:F:39:ASP:C	2.56	0.46
3:F:113:TYR:CD1	3:F:176:PHE:CE2	3.03	0.46
3:G:33:PHE:CE2	3:G:35:ALA:HA	2.50	0.46
1:I:142:ALA:O	1:I:143:ALA:C	2.57	0.46
3:J:47:LYS:HA	4:J:301:A3P:P2	2.54	0.46
3:J:95:LEU:HD22	3:J:99:MET:HB3	1.97	0.46
3:J:129:TYR:C	3:J:137:SER:HA	2.40	0.46
3:J:257:THR:O	3:J:260:GLN:HB2	2.15	0.46
1:K:47:LYS:HG3	1:K:125:MET:HA	1.97	0.46
1:L:256:PHE:HA	1:L:260:GLN:OE1	2.15	0.46
1:A:9:LEU:O	1:A:20:THR:HG23	2.14	0.46
1:A:53:LEU:HD22	1:A:114:ILE:HB	1.97	0.46
1:A:57:ILE:C	1:A:59:ARG:N	2.73	0.46
1:A:188:LYS:HE2	7:A:423:HOH:O	2.14	0.46
1:A:282:LYS:NZ	7:A:457:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:HA	1:B:16:ILE:O	2.16	0.46
2:D:251:ASP:OD1	2:D:254:ASN:ND2	2.42	0.46
2:D:267:LEU:HD23	2:D:267:LEU:HA	1.80	0.46
1:E:107:LYS:O	1:E:108:GLN:HB2	2.15	0.46
1:E:234:CYS:SG	1:E:237:THR:HG22	2.55	0.46
1:E:268:PHE:O	1:E:269:THR:C	2.58	0.46
3:F:84:ARG:NH2	3:J:130:ARG:NH2	2.62	0.46
3:G:47:LYS:CE	4:G:301:A3P:H5'1	2.45	0.46
3:H:246:LYS:N	4:H:301:A3P:O1P	2.46	0.46
3:H:251:ASP:O	3:H:253:ILE:N	2.48	0.46
3:H:277:VAL:O	3:H:279:ARG:N	2.48	0.46
1:I:71:ILE:CG2	1:I:93:THR:HB	2.43	0.46
3:J:194:THR:OG1	3:J:206:MET:HE2	2.14	0.46
3:J:267:LEU:HA	3:J:267:LEU:HD23	1.62	0.46
1:K:113:TYR:CD1	1:K:176:PHE:CE2	3.04	0.46
1:C:279:ARG:CD	1:C:283:GLU:OE2	2.63	0.46
1:A:104:VAL:CA	7:A:406:HOH:O	2.59	0.46
1:A:150:LYS:C	1:A:152:ASP:H	2.22	0.46
1:A:217:GLU:O	1:A:220:SER:CB	2.63	0.46
2:D:8:ALA:N	7:D:451:HOH:O	2.48	0.46
1:E:101:PRO:C	1:E:103:THR:N	2.70	0.46
1:E:274:ASN:O	1:E:276:ASP:N	2.48	0.46
3:F:115:VAL:O	3:F:178:PHE:HA	2.15	0.46
3:F:150:LYS:C	3:F:152:ASP:H	2.23	0.46
1:I:214[B]:SER:OG	1:I:217:GLU:HB2	2.16	0.46
3:J:8:SER:O	3:J:20:THR:HG21	2.15	0.46
3:J:10:LEU:CD2	3:J:154:VAL:HG12	2.45	0.46
3:J:52:TRP:CZ2	3:J:182:MET:HE3	2.51	0.46
1:C:45:TYR:OH	1:C:156:GLY:O	2.28	0.46
1:A:70:PRO:HD3	1:A:232:VAL:O	2.15	0.46
1:A:140:THR:O	1:A:143:ALA:HB3	2.15	0.46
1:A:155:TYR:HE2	1:A:236:LEU:HD21	1.80	0.46
1:B:185:ASP:CG	1:B:188:LYS:HB2	2.40	0.46
1:B:210:ALA:O	1:B:211:ARG:C	2.59	0.46
1:B:282:LYS:C	1:B:284:TYR:N	2.73	0.46
1:E:12:LYS:HA	1:E:16:ILE:O	2.16	0.46
1:E:125:MET:HB3	1:E:144:PHE:CZ	2.51	0.46
1:E:191:LYS:HA	1:E:194:THR:CG2	2.46	0.46
3:F:100:LEU:O	3:F:105:LYS:NZ	2.48	0.46
3:G:82:LEU:C	7:G:435:HOH:O	2.58	0.46
3:H:35:ALA:N	3:H:103:THR:HG21	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:PHE:CD2	3:J:101:PRO:HG2	2.51	0.46
3:J:125:MET:HE2	3:J:129:TYR:CE1	2.50	0.46
1:C:115:VAL:CG1	1:C:178:PHE:CD1	2.99	0.46
1:C:180:GLU:C	1:C:182:MET:N	2.72	0.46
1:C:217:GLU:OE2	1:C:217:GLU:HA	2.12	0.46
1:A:126:PHE:HB2	1:A:144:PHE:CD1	2.51	0.46
2:D:52:TRP:O	2:D:56:VAL:HG23	2.16	0.46
1:E:94:HIS:O	1:E:161:HIS:HE1	1.99	0.46
1:E:119:LYS:HE3	1:E:264:PHE:CE1	2.51	0.46
3:G:178:PHE:HE1	3:G:281:LEU:HG	1.81	0.46
3:G:218:MET:O	3:G:221:ASN:ND2	2.49	0.46
3:G:279:ARG:HD2	3:H:274:ASN:ND2	2.30	0.46
3:H:46:PRO:HA	3:H:94:HIS:CE1	2.51	0.46
1:C:126:PHE:O	1:C:127:HIS:C	2.55	0.46
1:C:202:ASN:OD1	1:C:205:GLU:CG	2.63	0.46
1:A:117:ASN:HA	1:A:281:LEU:HD22	1.95	0.46
1:A:225:GLU:CD	1:A:227:CYS:O	2.58	0.46
2:D:10:LEU:HD21	2:D:154:VAL:HG13	1.98	0.46
2:D:125:MET:HG2	2:D:144:PHE:HZ	1.81	0.46
2:D:188:LYS:HD2	7:D:484:HOH:O	2.14	0.46
1:E:78:LYS:O	1:E:78:LYS:HD3	2.16	0.46
3:F:47:LYS:C	7:F:425:HOH:O	2.58	0.46
3:F:186:PHE:CB	7:F:426:HOH:O	2.64	0.46
3:J:130:ARG:HA	3:J:137:SER:HB2	1.97	0.46
1:K:75:ASP:O	1:K:76:ILE:C	2.58	0.46
1:K:126:PHE:HE1	1:K:138:THR:HG22	1.80	0.46
1:L:78:LYS:N	7:L:434:HOH:O	2.48	0.46
1:A:52:TRP:CZ2	4:A:301:A3P:N1	2.83	0.46
1:A:147:LEU:O	1:A:150:LYS:N	2.49	0.46
1:B:221:ASN:ND2	7:B:450:HOH:O	2.49	0.46
2:D:142:ALA:O	2:D:143:ALA:C	2.58	0.46
2:D:267:LEU:HD22	2:D:271:LYS:HG2	1.97	0.46
1:E:234:CYS:HB3	1:E:237:THR:HG23	1.97	0.46
3:F:151:GLY:C	3:F:153:VAL:N	2.67	0.46
3:G:181:GLU:CA	3:G:184:LYS:HE2	2.46	0.46
3:H:98:GLU:CD	3:H:98:GLU:N	2.74	0.46
3:H:188:LYS:HB3	3:H:189:SER:H	1.63	0.46
1:I:37:GLU:OE1	1:I:37:GLU:HA	2.15	0.46
1:I:59:ARG:O	1:I:60:ILE:O	2.32	0.46
1:I:262:ARG:O	1:I:263:GLY:C	2.58	0.46
3:J:148:PHE:C	3:J:148:PHE:CD2	2.94	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:LYS:HA	4:K:301:A3P:O5'	2.16	0.46
1:K:115:VAL:CG1	1:K:178:PHE:CD1	2.99	0.46
1:C:34:ASP:HA	1:C:103:THR:HG21	1.98	0.46
1:C:228:ASP:HB2	1:C:229:PRO:HD3	1.98	0.46
1:A:188:LYS:HA	1:A:191:LYS:HD2	1.97	0.46
1:E:147:LEU:O	1:E:148:PHE:C	2.57	0.46
3:G:47:LYS:CA	3:G:47:LYS:HE3	2.46	0.46
1:K:225:GLU:OE1	1:K:231:HIS:HB3	2.16	0.46
1:L:54:ALA:O	1:L:58:GLU:HG3	2.16	0.46
1:L:186:PHE:HD1	1:L:187:VAL:N	2.13	0.46
1:L:214[A]:SER:OG	7:L:414:HOH:O	2.14	0.46
1:A:138:THR:CG2	1:A:140:THR:O	2.64	0.46
1:A:143:ALA:HB2	7:A:466:HOH:O	2.15	0.46
1:B:203:ASP:O	1:B:207:ALA:N	2.37	0.46
2:D:36:ARG:NH2	2:D:83:LYS:O	2.49	0.46
2:D:61:PRO:O	2:D:62:ASP:C	2.59	0.46
2:D:209:ILE:O	2:D:210:ALA:C	2.59	0.46
1:E:95:LEU:HD22	1:E:99:MET:CB	2.46	0.46
3:G:97:TYR:CE2	3:G:105:LYS:HE2	2.51	0.46
3:H:97:TYR:CE2	3:H:168:HIS:NE2	2.84	0.46
3:J:188:LYS:O	3:J:191:LYS:HB2	2.16	0.46
3:J:210:ALA:O	3:J:211:ARG:C	2.58	0.46
1:K:202:ASN:C	1:K:202:ASN:OD1	2.57	0.46
1:L:268:PHE:O	1:L:269:THR:C	2.58	0.46
1:C:228:ASP:CB	1:C:229:PRO:CD	2.94	0.46
1:A:141:TRP:O	1:A:142:ALA:C	2.59	0.46
1:A:181:GLU:OE2	1:A:284:TYR:OH	2.28	0.46
1:A:183:LYS:HD3	4:A:301:A3P:H2	1.98	0.46
1:B:41:PHE:HB2	1:B:111:ILE:CD1	2.46	0.46
1:E:29:SER:O	1:E:32:SER:OG	2.31	0.46
3:F:18:PHE:CZ	3:F:99:MET:HE1	2.50	0.46
3:F:26:LEU:HD12	3:F:79:PHE:CZ	2.51	0.46
3:G:27:LEU:O	3:G:30:LEU:HD22	2.15	0.46
3:G:272:MET:O	3:G:273:ARG:C	2.59	0.46
3:H:35:ALA:CB	3:H:103:THR:CG2	2.94	0.46
3:H:205:GLU:O	3:H:209:ILE:HG12	2.16	0.46
1:K:69:SER:HB3	1:K:78:LYS:NZ	2.31	0.46
1:K:276:ASP:OD2	1:K:279:ARG:NH1	2.49	0.46
1:L:47:LYS:HD2	4:L:301:A3P:O5P	2.15	0.46
1:L:202:ASN:CG	1:L:205:GLU:CD	2.83	0.46
1:L:209:ILE:O	1:L:210:ALA:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:O	1:C:81:GLU:N	2.44	0.45
1:C:193:ILE:HG22	1:C:194:THR:N	2.31	0.45
1:A:258:PRO:O	1:A:262:ARG:NH1	2.48	0.45
1:B:153:VAL:O	1:B:156:GLY:N	2.46	0.45
1:B:190:LEU:HA	1:B:193:ILE:HD12	1.97	0.45
2:D:73:LEU:CD2	2:D:232:VAL:CG2	2.94	0.45
2:D:98[A]:GLU:OE2	1:E:98:GLU:HG3	2.15	0.45
1:E:18:PHE:CE2	1:E:99:MET:HE1	2.51	0.45
1:E:50:THR:HG21	1:E:94:HIS:HE1	1.81	0.45
3:F:47:LYS:HG3	3:F:125:MET:HA	1.97	0.45
3:H:248:VAL:HG22	3:H:249:VAL:H	1.81	0.45
3:H:281:LEU:HA	3:H:284:TYR:HD2	1.80	0.45
1:I:41:PHE:HB2	1:I:111:ILE:HD13	1.97	0.45
1:I:119:LYS:HB3	1:I:252:TRP:CG	2.51	0.45
3:J:118:PRO:HG2	3:J:264:PHE:HZ	1.80	0.45
3:J:172:LYS:HG3	1:L:170:ASN:C	2.40	0.45
1:L:79:PHE:N	1:L:79:PHE:CD1	2.84	0.45
1:C:119:LYS:HG3	1:C:264:PHE:CE1	2.50	0.45
1:A:23:SER:OG	1:A:26:LEU:HB3	2.16	0.45
2:D:180:GLU:HG3	2:D:249:VAL:HG22	1.98	0.45
2:D:284:TYR:HB3	2:D:285:ALA:H	1.35	0.45
1:E:136:PRO:C	7:E:404:HOH:O	2.59	0.45
3:F:9:LEU:CD2	3:F:136:PRO:CD	2.94	0.45
3:F:96:ASN:OD1	3:F:96:ASN:C	2.57	0.45
3:F:206:MET:O	3:F:209:ILE:CB	2.64	0.45
1:K:181:GLU:OE2	1:K:284:TYR:OH	2.19	0.45
1:K:253:ILE:CG1	1:K:254:ASN:OD1	2.60	0.45
1:L:181:GLU:HG3	1:L:189:SER:OG	2.17	0.45
1:L:232:VAL:HG23	1:L:233:ILE:N	2.30	0.45
1:C:51:HIS:O	1:C:52:TRP:O	2.35	0.45
1:C:191:LYS:C	1:C:193:ILE:N	2.71	0.45
1:C:250:GLY:O	1:C:252:TRP:N	2.49	0.45
1:A:36:ARG:NH1	1:A:85:ILE:O	2.48	0.45
1:A:109:CYS:O	1:A:173:ASN:HB2	2.17	0.45
1:A:132:ASN:O	1:A:135:LEU:N	2.43	0.45
1:A:219:LYS:HA	1:A:244:PHE:CG	2.51	0.45
1:B:10:LEU:CD2	1:B:154:VAL:CG1	2.94	0.45
1:E:45:TYR:CG	1:E:46:PRO:HD2	2.51	0.45
1:E:208:LYS:O	1:E:211:ARG:CB	2.63	0.45
3:F:259:LYS:O	3:F:262:ARG:N	2.49	0.45
3:G:267:LEU:HD23	3:G:267:LEU:HA	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:25:GLU:CB	3:H:76:ILE:HD12	2.45	0.45
3:H:232:VAL:O	3:H:232:VAL:HG23	2.15	0.45
3:J:269:THR:O	3:J:273:ARG:N	2.40	0.45
1:K:96:ASN:C	1:K:96:ASN:OD1	2.59	0.45
1:L:136:PRO:O	1:L:137:SER:C	2.59	0.45
1:C:69:SER:O	1:C:70:PRO:C	2.56	0.45
1:A:35:ALA:CB	1:A:103:THR:HG23	2.46	0.45
1:A:49:GLY:O	1:A:114:ILE:HD13	2.15	0.45
1:A:169:LYS:HD2	1:A:176:PHE:CB	2.46	0.45
1:B:36:ARG:HB3	1:B:38:ASP:OD1	2.17	0.45
2:D:257:THR:OG1	2:D:260:GLN:HG3	2.16	0.45
3:G:98[A]:GLU:CD	1:I:98:GLU:CG	2.90	0.45
1:I:79:PHE:O	1:I:82:LEU:HB2	2.15	0.45
1:I:163:LEU:O	1:I:164:SER:C	2.59	0.45
1:I:175:LEU:HD11	1:I:192:LYS:CE	2.46	0.45
3:J:77:SER:HB3	7:J:402:HOH:O	2.09	0.45
3:J:82:LEU:HD23	3:J:82:LEU:HA	1.78	0.45
1:K:47:LYS:HB3	1:K:124:SER:OG	2.17	0.45
1:K:96:ASN:CG	1:K:98[B]:GLU:OE1	2.59	0.45
1:L:205:GLU:O	1:L:208:LYS:CB	2.64	0.45
1:L:208:LYS:O	1:L:211:ARG:CB	2.64	0.45
1:C:147:LEU:O	1:C:151:GLY:N	2.50	0.45
1:C:228:ASP:HB2	1:C:229:PRO:CD	2.46	0.45
1:A:98:GLU:OE2	1:A:98:GLU:HA	2.17	0.45
1:B:150:LYS:C	1:B:152:ASP:N	2.74	0.45
2:D:40:ILE:HG22	2:D:41:PHE:N	2.31	0.45
1:E:128:TYR:O	1:E:132:ASN:N	2.48	0.45
1:E:185:ASP:CG	1:E:188:LYS:HB2	2.41	0.45
3:F:46:PRO:C	3:F:47:LYS:HG2	2.42	0.45
3:G:9:LEU:HD13	3:G:134:ASN:O	2.16	0.45
3:G:35:ALA:CB	3:G:103:THR:CG2	2.95	0.45
3:G:205:GLU:O	3:G:208:LYS:N	2.49	0.45
1:I:55:GLU:HA	1:I:55:GLU:OE2	2.16	0.45
1:I:183:LYS:NZ	1:I:248:VAL:HA	2.31	0.45
3:J:47:LYS:HA	3:J:47:LYS:HE3	1.98	0.45
1:K:252:TRP:CZ3	1:K:253:ILE:HA	2.51	0.45
1:K:257:THR:OG1	1:K:260:GLN:CG	2.65	0.45
1:L:49:GLY:O	1:L:114:ILE:HD13	2.16	0.45
1:B:116:ARG:HG3	1:B:179:TYR:CB	2.47	0.45
2:D:118:PRO:HG2	2:D:264:PHE:HZ	1.82	0.45
2:D:186:PHE:O	2:D:189:SER:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:ASN:HB3	3:F:180:GLU:OE2	2.17	0.45
3:G:29:SER:O	3:G:31:ASP:N	2.49	0.45
3:G:154:VAL:C	3:G:156:GLY:N	2.74	0.45
3:H:126:PHE:HE1	3:H:138:THR:HG22	1.81	0.45
3:H:251:ASP:C	3:H:253:ILE:N	2.72	0.45
1:I:12:LYS:HD2	1:I:17:PHE:CD2	2.52	0.45
1:I:243:VAL:O	1:I:243:VAL:HG23	2.17	0.45
3:J:231:HIS:CG	3:J:231:HIS:O	2.70	0.45
1:K:250:GLY:C	1:K:252:TRP:H	2.24	0.45
1:L:234:CYS:CB	1:L:237:THR:HG23	2.46	0.45
1:C:282:LYS:CG	7:C:516:HOH:O	2.65	0.45
1:A:70:PRO:O	1:A:78:LYS:NZ	2.49	0.45
1:B:138:THR:HG23	1:B:143:ALA:HB3	1.98	0.45
1:B:213:THR:O	4:B:301:A3P:N6	2.45	0.45
2:D:282:LYS:C	2:D:284:TYR:N	2.74	0.45
1:E:84:ARG:O	1:E:86:PRO:HD3	2.17	0.45
3:F:221:ASN:O	3:F:222:ALA:HB2	2.16	0.45
3:G:113:TYR:CD1	3:G:176:PHE:CE2	3.04	0.45
3:G:191:LYS:O	3:G:194:THR:HG22	2.16	0.45
1:I:93:THR:OG1	1:I:95:LEU:HG	2.16	0.45
3:J:96:ASN:C	3:J:165:TRP:HE1	2.25	0.45
1:K:120:ASP:OD1	1:K:252:TRP:HD1	2.00	0.45
1:K:148:PHE:C	1:K:148:PHE:CD2	2.94	0.45
1:L:115:VAL:CG2	1:L:116:ARG:N	2.79	0.45
1:C:101:PRO:HB3	7:C:430:HOH:O	2.17	0.45
4:C:301:A3P:HO2'	4:C:301:A3P:P1	2.37	0.45
2:D:45:TYR:CG	2:D:46:PRO:CD	3.00	0.45
2:D:117:ASN:CA	2:D:281:LEU:HD22	2.47	0.45
2:D:237:THR:O	2:D:237:THR:OG1	2.35	0.45
1:E:267:LEU:O	1:E:270:GLU:HB3	2.16	0.45
3:F:150:LYS:C	3:F:152:ASP:N	2.70	0.45
3:G:67:LEU:HD12	3:G:90:ALA:CB	2.47	0.45
3:G:129:TYR:HA	3:G:135:LEU:CB	2.46	0.45
3:G:248:VAL:HG13	7:G:412:HOH:O	2.16	0.45
1:I:47:LYS:HA	1:I:47:LYS:HE3	1.99	0.45
1:I:125:MET:HG2	1:I:144:PHE:HZ	1.82	0.45
1:I:187:VAL:O	1:I:191:LYS:HG3	2.17	0.45
3:J:172:LYS:NZ	7:L:407:HOH:O	2.32	0.45
1:L:215:PHE:CA	4:L:301:A3P:N6	2.76	0.45
1:C:80:GLU:C	1:C:82:LEU:N	2.73	0.45
1:A:243:VAL:O	1:A:243:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:HA	1:A:260:GLN:OE1	2.17	0.45
1:B:201:VAL:CG1	1:B:205:GLU:CB	2.95	0.45
1:E:44:SER:HB3	1:E:114:ILE:HG23	1.99	0.45
1:E:262:ARG:O	1:E:263:GLY:C	2.59	0.45
3:F:25:GLU:N	3:F:25:GLU:CD	2.75	0.45
3:G:103:THR:HG22	3:G:104:VAL:N	2.31	0.45
3:G:239:ASP:CG	3:G:239:ASP:O	2.57	0.45
3:H:45:TYR:CD1	3:H:158:TRP:HA	2.51	0.45
3:J:13:TYR:HB3	3:J:18:PHE:CE1	2.52	0.45
3:J:206:MET:HA	3:J:209:ILE:HG12	1.99	0.45
1:K:115:VAL:O	1:K:115:VAL:HG13	2.16	0.45
1:K:267:LEU:HD22	1:K:271:LYS:HG2	1.99	0.45
1:L:67:LEU:CD2	1:L:233:ILE:HG21	2.36	0.45
1:C:70:PRO:HD3	1:C:232:VAL:O	2.17	0.45
1:A:116:ARG:HB3	1:A:121:THR:OG1	2.17	0.45
1:B:16:ILE:HG23	1:B:156:GLY:N	2.32	0.45
1:B:60:ILE:HG23	1:B:61:PRO:HD2	1.99	0.45
1:B:94:HIS:O	1:B:161:HIS:HE1	2.00	0.45
1:B:182:MET:O	1:B:186[B]:PHE:HB2	2.17	0.45
2:D:184:LYS:HG2	2:D:185:ASP:N	2.32	0.45
1:E:32:SER:O	1:E:33:PHE:C	2.57	0.45
1:E:35:ALA:H	1:E:103:THR:HG23	1.79	0.45
3:F:102:VAL:CG1	3:F:103:THR:N	2.79	0.45
3:F:252:TRP:O	3:F:256:PHE:HD1	2.00	0.45
3:H:148:PHE:O	3:H:151:GLY:N	2.48	0.45
3:H:178:PHE:O	3:H:179:TYR:C	2.60	0.45
1:I:180:GLU:H	1:I:180:GLU:CD	2.24	0.45
1:I:184:LYS:CG	1:I:185:ASP:N	2.72	0.45
1:I:209:ILE:O	1:I:212:SER:N	2.50	0.45
3:J:280:CYS:O	3:J:284:TYR:CD2	2.70	0.45
4:J:301:A3P:H3'	7:J:421:HOH:O	2.17	0.45
1:K:173:ASN:C	1:K:196:PHE:HZ	2.24	0.45
1:K:221:ASN:OD1	1:K:221:ASN:C	2.60	0.45
1:K:276:ASP:CB	1:K:279:ARG:HH22	2.30	0.45
1:L:97:TYR:CE2	1:L:168:HIS:NE2	2.85	0.45
1:L:263:GLY:HA3	7:L:423:HOH:O	2.17	0.45
1:C:51:HIS:HD2	1:C:233:ILE:HD11	1.82	0.44
1:C:193:ILE:O	1:C:196:PHE:N	2.50	0.44
2:D:76:ILE:O	2:D:77:SER:C	2.59	0.44
3:F:251:ASP:C	3:F:253:ILE:H	2.25	0.44
3:F:262:ARG:CG	7:F:412:HOH:O	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:71:ILE:O	3:H:71:ILE:CG1	2.64	0.44
3:H:172:LYS:CE	1:I:169:LYS:O	2.63	0.44
1:I:181:GLU:CB	1:I:184:LYS:NZ	2.77	0.44
2:D:36:ARG:NH1	2:D:89:ARG:HD3	2.33	0.44
2:D:168:HIS:O	2:D:171:ASP:N	2.43	0.44
1:E:19:SER:C	1:E:21:MET:H	2.24	0.44
1:E:45:TYR:OH	1:E:156:GLY:O	2.19	0.44
1:E:180:GLU:C	7:E:403:HOH:O	2.60	0.44
1:E:206:MET:O	1:E:209:ILE:N	2.50	0.44
1:E:267:LEU:HA	1:E:267:LEU:HD23	1.71	0.44
3:G:50:THR:HG23	7:G:460:HOH:O	2.17	0.44
3:G:267:LEU:HD22	3:G:271:LYS:HG2	1.98	0.44
1:I:129:TYR:HD2	1:I:136:PRO:O	1.99	0.44
1:L:262:ARG:O	1:L:266:GLU:HG3	2.18	0.44
1:C:126:PHE:N	1:C:144:PHE:CZ	2.85	0.44
1:A:13:TYR:HB3	1:A:18:PHE:CE1	2.52	0.44
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.69	0.44
1:B:206:MET:O	1:B:209:ILE:N	2.49	0.44
2:D:209:ILE:O	2:D:212:SER:N	2.50	0.44
1:E:16:ILE:HG22	1:E:17:PHE:O	2.17	0.44
1:E:154:VAL:C	1:E:156:GLY:N	2.75	0.44
1:E:209:ILE:O	1:E:210:ALA:C	2.60	0.44
3:G:117:ASN:N	3:G:281:LEU:HD22	2.32	0.44
3:G:191:LYS:HB2	7:G:416:HOH:O	2.17	0.44
3:H:272:MET:O	3:H:273:ARG:C	2.61	0.44
1:I:50:THR:OG1	4:I:301:A3P:O5P	2.31	0.44
1:I:55:GLU:HG2	7:I:429:HOH:O	2.16	0.44
1:I:71:ILE:HG23	1:I:72:GLU:N	2.33	0.44
1:I:269:THR:CA	7:I:417:HOH:O	2.61	0.44
3:J:19:SER:C	3:J:21:MET:N	2.75	0.44
3:J:132:ASN:OD1	3:J:133:PRO:HD2	2.17	0.44
3:J:159:PHE:O	3:J:162:VAL:N	2.50	0.44
1:L:12:LYS:HE3	1:L:17:PHE:CG	2.52	0.44
1:C:12:LYS:HD2	1:C:17:PHE:HA	1.99	0.44
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.64	0.44
1:B:39:ASP:CG	1:B:89:ARG:HE	2.25	0.44
1:B:168:HIS:CE1	7:B:425:HOH:O	2.67	0.44
2:D:98[A]:GLU:CD	1:E:98:GLU:CG	2.90	0.44
2:D:172:LYS:HG2	2:D:173:ASN:H	1.82	0.44
1:E:47:LYS:HA	1:E:47:LYS:HE3	1.98	0.44
1:E:52:TRP:CD2	1:E:182:MET:CE	2.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:VAL:O	1:E:127:HIS:CD2	2.70	0.44
3:F:96:ASN:CG	3:F:99:MET:HE2	2.42	0.44
1:I:55:GLU:O	1:I:58:GLU:N	2.48	0.44
1:I:75:ASP:C	1:I:77:SER:N	2.75	0.44
1:I:231:HIS:O	1:I:231:HIS:CG	2.71	0.44
3:J:179:TYR:OH	4:J:301:A3P:N3	2.43	0.44
3:J:243:VAL:HG22	3:J:244:PHE:CD2	2.53	0.44
1:K:282:LYS:O	1:K:286:HIS:HD2	2.00	0.44
1:L:154:VAL:O	1:L:155:TYR:HB2	2.16	0.44
1:C:37:GLU:HG2	1:C:107:LYS:HD2	1.98	0.44
1:C:102:VAL:HG22	1:C:106:GLN:CG	2.48	0.44
1:A:237:THR:HG23	1:A:237:THR:O	2.18	0.44
1:B:31:ASP:HB2	7:B:498:HOH:O	2.17	0.44
1:E:50:THR:OG1	1:E:51:HIS:N	2.48	0.44
3:F:174:VAL:O	7:F:421:HOH:O	2.21	0.44
3:F:183:LYS:HE3	3:F:183:LYS:HB3	1.78	0.44
3:F:268:PHE:CE2	3:F:282:LYS:HD2	2.53	0.44
3:H:189:SER:O	3:H:192:LYS:CA	2.64	0.44
1:K:115:VAL:O	1:K:178:PHE:HA	2.17	0.44
1:K:202:ASN:OD1	1:K:205:GLU:HG3	2.18	0.44
1:L:47:LYS:N	4:L:301:A3P:P2	2.91	0.44
1:L:47:LYS:O	1:L:116:ARG:HD3	2.18	0.44
1:L:187:VAL:O	1:L:191:LYS:HG3	2.17	0.44
1:C:180:GLU:C	1:C:182:MET:H	2.25	0.44
1:B:16:ILE:CG2	1:B:155:TYR:CA	2.96	0.44
2:D:128:TYR:O	2:D:132:ASN:N	2.50	0.44
1:E:146:GLU:O	1:E:150:LYS:HG3	2.18	0.44
3:G:165:TRP:HB3	3:G:176:PHE:HZ	1.82	0.44
3:J:9:LEU:O	7:J:428:HOH:O	2.21	0.44
1:K:35:ALA:HB3	1:K:103:THR:HG23	2.00	0.44
1:K:110:LYS:NZ	1:K:196:PHE:O	2.32	0.44
1:L:55:GLU:O	1:L:58:GLU:HB2	2.18	0.44
1:L:102:VAL:CG1	1:L:103:THR:N	2.81	0.44
1:C:40:ILE:C	1:C:41:PHE:CD1	2.95	0.44
1:C:190:LEU:O	1:C:191:LYS:C	2.59	0.44
1:A:8:SER:O	1:A:20:THR:CG2	2.62	0.44
1:A:70:PRO:CD	1:A:232:VAL:HG23	2.48	0.44
1:A:245:ARG:NH2	1:A:251:ASP:OD2	2.49	0.44
1:A:254:ASN:O	1:I:87:LYS:NZ	2.32	0.44
1:B:116:ARG:HG3	1:B:179:TYR:CG	2.53	0.44
2:D:44:SER:HB3	2:D:114:ILE:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ALA:O	2:D:144:PHE:C	2.60	0.44
2:D:171:ASP:OD1	2:D:171:ASP:N	2.50	0.44
1:E:113:TYR:C	1:E:113:TYR:CD1	2.95	0.44
3:G:110:LYS:HA	7:G:403:HOH:O	2.18	0.44
3:G:169:LYS:HD2	3:G:176:PHE:HB2	1.99	0.44
3:H:110:LYS:HG3	7:H:480:HOH:O	2.17	0.44
3:H:257:THR:O	3:H:258:PRO:C	2.58	0.44
1:I:185:ASP:CA	7:I:407:HOH:O	2.63	0.44
3:J:13:TYR:CE1	3:J:14:MET:HG2	2.52	0.44
3:J:34:ASP:OD1	1:K:273:ARG:NH1	2.41	0.44
3:J:172:LYS:NZ	1:L:174:VAL:O	2.50	0.44
1:K:93:THR:OG1	1:K:94:HIS:N	2.51	0.44
1:L:128:TYR:O	1:L:132:ASN:CB	2.65	0.44
1:L:220:SER:C	1:L:221:ASN:CG	2.85	0.44
1:C:47:LYS:HA	1:C:47:LYS:CE	2.48	0.44
1:C:118:PRO:HB3	1:C:158:TRP:CE2	2.53	0.44
1:C:122:ALA:O	1:C:125:MET:HB3	2.18	0.44
1:A:11:HIS:CE1	1:A:19:SER:O	2.69	0.44
1:A:282:LYS:C	1:A:284:TYR:N	2.75	0.44
1:B:202:ASN:CG	1:B:205:GLU:OE2	2.60	0.44
2:D:97:TYR:CE2	2:D:105:LYS:HE2	2.53	0.44
2:D:98[A]:GLU:HG2	7:D:478:HOH:O	2.18	0.44
1:E:43:VAL:HG11	1:E:165:TRP:CZ2	2.53	0.44
3:G:39:ASP:O	3:G:109:CYS:HB3	2.18	0.44
3:G:125:MET:O	3:G:126:PHE:C	2.60	0.44
3:G:173:ASN:O	3:G:196:PHE:HZ	2.01	0.44
3:H:16:ILE:HB	3:H:18:PHE:CE1	2.53	0.44
3:H:147:LEU:HD22	3:H:152:ASP:CB	2.48	0.44
1:K:96:ASN:OD1	1:K:98[B]:GLU:OE1	2.35	0.44
1:C:70:PRO:HG3	1:C:233:ILE:C	2.42	0.44
1:B:203:ASP:O	1:B:204:SER:C	2.61	0.44
2:D:26:LEU:C	2:D:26:LEU:HD12	2.42	0.44
2:D:243:VAL:O	4:D:301:A3P:H2'	2.18	0.44
2:D:245:ARG:NE	4:D:301:A3P:O2P	2.42	0.44
1:E:19:SER:O	1:E:22:SER:N	2.46	0.44
1:E:262:ARG:C	1:E:264:PHE:H	2.26	0.44
3:F:130:ARG:HG3	7:F:434:HOH:O	2.17	0.44
3:G:79:PHE:O	3:G:82:LEU:N	2.51	0.44
3:H:175:LEU:HD11	3:H:192:LYS:HE2	2.00	0.44
1:I:17:PHE:CB	1:I:154:VAL:HA	2.48	0.44
1:I:190:LEU:O	1:I:193:ILE:HB	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:LYS:CA	4:L:301:A3P:P2	3.06	0.44
1:A:118:PRO:HD3	1:A:158:TRP:CZ2	2.53	0.43
1:B:201:VAL:HG13	1:B:205:GLU:HB3	1.99	0.43
2:D:272:MET:O	2:D:273:ARG:C	2.59	0.43
1:E:75:ASP:HB3	1:E:77:SER:H	1.82	0.43
1:E:224:LYS:HD3	1:E:228:ASP:HA	1.99	0.43
3:F:222:ALA:N	7:F:442:HOH:O	2.51	0.43
3:G:239:ASP:HB3	3:G:242:LEU:HD12	2.00	0.43
3:H:26:LEU:CD2	3:H:74:GLY:C	2.91	0.43
3:H:254:ASN:HA	7:H:433:HOH:O	2.18	0.43
3:J:220:SER:O	3:J:221:ASN:CB	2.64	0.43
1:K:29:SER:O	1:K:79:PHE:CE2	2.70	0.43
1:K:91:ILE:HA	1:K:92:PRO:HD3	1.86	0.43
1:K:205:GLU:O	1:K:209:ILE:HG12	2.18	0.43
1:L:11:HIS:HE1	1:L:19:SER:O	2.00	0.43
1:L:27:LEU:C	1:L:29:SER:H	2.26	0.43
1:L:35:ALA:HB3	1:L:103:THR:HG23	2.00	0.43
1:A:247:GLY:N	4:A:301:A3P:O1P	2.42	0.43
1:B:144:PHE:O	1:B:145:LEU:C	2.59	0.43
1:B:186[A]:PHE:CD1	1:B:186[A]:PHE:C	2.94	0.43
2:D:121:THR:O	2:D:125:MET:HB2	2.17	0.43
2:D:284:TYR:O	2:D:285:ALA:O	2.36	0.43
1:E:125:MET:HE2	1:E:153:VAL:HB	2.01	0.43
1:E:203:ASP:O	1:E:206:MET:N	2.51	0.43
3:G:12:LYS:HD3	3:G:17:PHE:CE2	2.54	0.43
3:G:41:PHE:O	3:G:112:ILE:N	2.34	0.43
3:G:47:LYS:N	4:G:301:A3P:P2	2.92	0.43
3:H:98:GLU:OE2	3:H:164:SER:HB2	2.18	0.43
1:I:36:ARG:NH1	7:I:404:HOH:O	2.49	0.43
1:I:174:VAL:CG1	1:I:175:LEU:N	2.81	0.43
1:K:229:PRO:C	1:K:230:ASN:CG	2.86	0.43
1:K:252:TRP:CE3	1:K:253:ILE:N	2.86	0.43
1:L:55:GLU:HB2	1:L:218:MET:CE	2.46	0.43
1:L:214[B]:SER:OG	1:L:217:GLU:HB2	2.18	0.43
1:L:215:PHE:CD1	1:L:247:GLY:HA3	2.52	0.43
1:C:22:SER:C	1:C:23:SER:O	2.59	0.43
1:C:23:SER:OG	1:C:26:LEU:HB2	2.18	0.43
1:A:25:GLU:CB	1:A:76:ILE:HD12	2.47	0.43
1:A:147:LEU:O	1:A:148:PHE:C	2.61	0.43
2:D:169:LYS:HB2	2:D:176:PHE:CE1	2.54	0.43
2:D:221:ASN:C	7:D:423:HOH:O	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:MET:HB3	1:E:144:PHE:HZ	1.83	0.43
1:E:203:ASP:C	1:E:205:GLU:N	2.71	0.43
1:E:257:THR:O	1:E:258:PRO:C	2.61	0.43
1:E:260:GLN:O	1:E:261:ASN:C	2.61	0.43
1:E:284:TYR:O	1:E:285:ALA:HB3	2.18	0.43
3:F:160:ASP:CG	7:F:408:HOH:O	2.54	0.43
3:F:217:GLU:OE2	3:F:217:GLU:HA	2.19	0.43
3:G:156:GLY:HA2	7:G:468:HOH:O	2.18	0.43
3:G:231:HIS:O	3:G:231:HIS:ND1	2.50	0.43
3:H:128:TYR:O	3:H:132:ASN:HB3	2.18	0.43
3:H:186:PHE:CD1	3:H:186:PHE:O	2.72	0.43
3:H:202:ASN:OD1	3:H:205:GLU:HG2	2.18	0.43
1:I:60:ILE:HA	1:I:61:PRO:HD3	1.84	0.43
1:I:124:SER:HB2	4:I:301:A3P:O2P	2.18	0.43
1:I:219:LYS:O	1:I:219:LYS:CG	2.66	0.43
1:L:41:PHE:CE1	1:L:104:VAL:CG1	3.01	0.43
1:C:195:ALA:C	1:C:197:LEU:N	2.71	0.43
1:A:219:LYS:HA	1:A:244:PHE:CD2	2.53	0.43
1:A:225:GLU:OE2	1:A:229:PRO:O	2.36	0.43
1:A:257:THR:C	1:A:259:LYS:H	2.27	0.43
1:B:70:PRO:O	1:B:73:LEU:HB3	2.18	0.43
1:B:202:ASN:H	1:B:205:GLU:CD	2.27	0.43
2:D:35:ALA:HB2	2:D:103:THR:CG2	2.48	0.43
3:F:182:MET:HA	3:F:186:PHE:HA	2.00	0.43
3:F:240:ARG:C	3:F:242:LEU:H	2.24	0.43
3:H:219:LYS:CG	3:H:244:PHE:CB	2.86	0.43
1:I:234:CYS:O	1:I:236:LEU:N	2.51	0.43
1:K:173:ASN:O	1:K:196:PHE:HZ	2.01	0.43
1:L:47:LYS:N	1:L:47:LYS:CD	2.80	0.43
1:L:50:THR:HG21	1:L:94:HIS:HE1	1.75	0.43
1:L:95:LEU:HD22	1:L:99:MET:HE3	2.01	0.43
1:C:268:PHE:CZ	1:C:272:MET:HG3	2.54	0.43
2:D:225:GLU:HB2	2:D:226:ASN:H	1.65	0.43
1:E:119:LYS:HE2	1:E:264:PHE:CD1	2.53	0.43
3:G:60:ILE:HA	3:G:61:PRO:HD3	1.88	0.43
3:H:166:GLU:HA	3:H:176:PHE:HZ	1.82	0.43
3:H:272:MET:C	3:H:273:ARG:O	2.61	0.43
1:I:187:VAL:O	1:I:188:LYS:C	2.61	0.43
3:J:30:LEU:HD12	3:J:30:LEU:HA	1.83	0.43
1:K:51:HIS:CG	1:K:233:ILE:HD11	2.53	0.43
1:K:100:LEU:HB3	1:K:105:LYS:HE3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:THR:C	1:L:231:HIS:NE2	2.75	0.43
1:C:23:SER:CB	1:C:74:GLY:O	2.67	0.43
1:C:169:LYS:NZ	7:C:440:HOH:O	2.41	0.43
1:A:248:VAL:HG22	1:A:249:VAL:N	2.27	0.43
1:B:234:CYS:O	1:B:237:THR:HG23	2.17	0.43
2:D:29:SER:O	2:D:30:LEU:C	2.61	0.43
2:D:50:THR:HG21	2:D:94:HIS:HE1	1.83	0.43
2:D:169:LYS:HD2	2:D:176:PHE:HB2	2.01	0.43
1:E:50:THR:HG22	4:E:301:A3P:O4P	2.17	0.43
1:E:118:PRO:HD3	1:E:281:LEU:HD13	2.01	0.43
1:E:266:GLU:CD	7:E:402:HOH:O	2.45	0.43
3:F:47:LYS:HB3	7:F:425:HOH:O	2.17	0.43
3:F:186:PHE:O	3:F:189:SER:HB2	2.18	0.43
3:G:44:SER:CB	3:G:114:ILE:HG23	2.49	0.43
3:G:84:ARG:CD	7:G:414:HOH:O	2.67	0.43
3:H:30:LEU:HA	3:H:79:PHE:CZ	2.49	0.43
3:H:191:LYS:HA	3:H:206:MET:HE1	1.99	0.43
1:I:164:SER:HB3	7:I:405:HOH:O	2.19	0.43
1:I:172:LYS:C	1:I:174:VAL:H	2.25	0.43
3:J:33:PHE:HE2	3:J:104:VAL:HG22	1.84	0.43
3:J:125:MET:HG2	3:J:144:PHE:CZ	2.53	0.43
1:K:86:PRO:HD2	7:K:514:HOH:O	2.17	0.43
1:K:129:TYR:HA	1:K:135:LEU:CB	2.48	0.43
1:L:9:LEU:CD2	1:L:133:PRO:O	2.67	0.43
1:C:154:VAL:O	1:C:155:TYR:HB2	2.18	0.43
1:A:23:SER:OG	1:A:26:LEU:HB2	2.19	0.43
1:A:37:GLU:CD	7:A:420:HOH:O	2.58	0.43
1:A:166:GLU:OE2	1:A:277:VAL:HG23	2.18	0.43
1:A:216:SER:O	1:A:220:SER:OG	2.34	0.43
2:D:70:PRO:CD	2:D:232:VAL:O	2.65	0.43
2:D:91:ILE:HA	2:D:92:PRO:HD3	1.52	0.43
2:D:123:VAL:O	2:D:124:SER:C	2.62	0.43
2:D:242:LEU:HD23	2:D:242:LEU:HA	1.89	0.43
1:E:25:GLU:O	1:E:29:SER:OG	2.25	0.43
3:F:25:GLU:O	3:F:26:LEU:C	2.62	0.43
3:F:132:ASN:CG	3:F:134:ASN:HB2	2.44	0.43
3:G:120:ASP:OD1	3:G:252:TRP:HD1	2.01	0.43
3:G:276:ASP:HB2	7:G:462:HOH:O	2.18	0.43
3:H:157:SER:CB	7:H:421:HOH:O	2.66	0.43
1:I:219:LYS:O	1:I:219:LYS:HG2	2.18	0.43
1:I:221:ASN:OD1	1:I:221:ASN:O	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:205:GLU:O	3:J:208:LYS:N	2.52	0.43
3:J:267:LEU:O	3:J:267:LEU:HD22	2.19	0.43
1:L:182:MET:O	1:L:183:LYS:C	2.60	0.43
1:E:101:PRO:C	1:E:103:THR:H	2.26	0.43
1:E:282:LYS:O	1:E:283:GLU:C	2.61	0.43
3:H:76:ILE:H	3:H:76:ILE:HD13	1.84	0.43
3:H:139:GLU:HA	7:H:408:HOH:O	2.18	0.43
1:I:39:ASP:OD2	1:I:89:ARG:NH2	2.45	0.43
1:I:166:GLU:O	1:I:168:HIS:N	2.51	0.43
1:I:181:GLU:CB	1:I:184:LYS:HE2	2.46	0.43
1:I:181:GLU:CA	1:I:184:LYS:HE2	2.48	0.43
1:K:65:ILE:HG12	1:K:88:ARG:HD3	2.00	0.43
1:K:116:ARG:HG3	1:K:179:TYR:HB3	1.99	0.43
1:K:221:ASN:C	7:K:401:HOH:O	2.47	0.43
1:L:177:ILE:CD1	1:L:192:LYS:HD3	2.49	0.43
1:E:61:PRO:O	1:E:62:ASP:C	2.59	0.43
3:G:58:GLU:OE1	7:G:428:HOH:O	2.21	0.43
3:G:217:GLU:HG3	7:G:442:HOH:O	2.19	0.43
3:H:45:TYR:CD2	3:H:158:TRP:HD1	2.36	0.43
1:I:30:LEU:HD12	1:I:30:LEU:HA	1.66	0.43
1:I:43:VAL:HB	1:I:113:TYR:HD2	1.84	0.43
1:I:206:MET:O	1:I:207:ALA:C	2.61	0.43
3:J:81:GLU:O	3:J:82:LEU:C	2.61	0.43
1:K:243:VAL:HG22	1:K:244:PHE:CE2	2.54	0.43
1:K:252:TRP:C	1:K:252:TRP:CD2	2.97	0.43
1:C:9:LEU:HB3	1:C:136:PRO:HD3	2.00	0.43
1:C:257:THR:O	1:C:258:PRO:C	2.60	0.43
1:A:47:LYS:HB3	1:A:124:SER:OG	2.18	0.43
1:A:80:GLU:OE2	1:A:84:ARG:HD2	2.19	0.43
1:B:173:ASN:C	1:B:196:PHE:HZ	2.27	0.43
1:B:215:PHE:CE1	1:B:244:PHE:HB3	2.54	0.43
1:B:234:CYS:C	1:B:236:LEU:N	2.77	0.43
2:D:86:PRO:O	3:H:141:TRP:N	2.44	0.43
1:E:66:THR:OG1	1:E:87:LYS:HB2	2.19	0.43
1:E:70:PRO:CD	1:E:232:VAL:HG22	2.49	0.43
1:E:271:LYS:CE	7:E:470:HOH:O	2.62	0.43
3:G:21:MET:O	3:G:73:LEU:HD12	2.19	0.43
3:G:80:GLU:O	3:G:83:LYS:HB3	2.19	0.43
3:H:11:HIS:ND1	3:H:20:THR:HA	2.33	0.43
1:I:205:GLU:O	1:I:206:MET:C	2.60	0.43
1:I:252:TRP:HE3	1:I:256:PHE:CD1	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:10:LEU:CD2	3:J:154:VAL:CG1	2.97	0.43
3:J:36:ARG:HB3	3:J:38:ASP:OD1	2.18	0.43
1:K:215:PHE:CE2	1:K:219:LYS:HE2	2.53	0.43
1:L:44:SER:HB2	1:L:114:ILE:O	2.18	0.43
1:L:128:TYR:OH	1:L:237:THR:CG2	2.67	0.43
1:C:62:ASP:CA	7:C:444:HOH:O	2.67	0.42
1:C:123:VAL:C	1:C:125:MET:N	2.76	0.42
1:B:202:ASN:O	1:B:205:GLU:N	2.52	0.42
1:E:13:TYR:N	1:E:16:ILE:O	2.39	0.42
3:F:207:ALA:O	3:F:208:LYS:C	2.61	0.42
3:G:47:LYS:HE3	4:G:301:A3P:H5'1	2.01	0.42
3:G:47:LYS:CD	4:G:301:A3P:O5P	2.66	0.42
3:G:281:LEU:HA	3:G:284:TYR:HD2	1.84	0.42
3:H:42:LEU:HD12	3:H:67:LEU:HD11	2.01	0.42
3:H:55:GLU:HA	3:H:55:GLU:OE2	2.19	0.42
1:I:35:ALA:CB	1:I:103:THR:HG23	2.49	0.42
1:I:70:PRO:O	1:I:71:ILE:C	2.58	0.42
3:J:25[B]:GLU:OE2	3:J:76:ILE:CD1	2.67	0.42
3:J:205:GLU:O	3:J:208:LYS:HB3	2.19	0.42
1:K:256:PHE:CG	1:K:261:ASN:OD1	2.72	0.42
1:L:133:PRO:C	1:L:135:LEU:N	2.75	0.42
1:A:47:LYS:HA	1:A:47:LYS:HE3	2.00	0.42
1:B:88:ARG:NH1	7:B:452:HOH:O	2.51	0.42
1:B:138:THR:HG21	1:B:143:ALA:HB3	2.01	0.42
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.88	0.42
1:B:275:SER:C	1:B:276:ASP:OD2	2.56	0.42
2:D:10:LEU:HD12	2:D:10:LEU:HA	1.78	0.42
2:D:225:GLU:H	2:D:225:GLU:HG3	1.74	0.42
1:E:43:VAL:HA	1:E:93:THR:O	2.19	0.42
1:E:75:ASP:C	1:E:77:SER:N	2.73	0.42
1:E:273:ARG:C	1:E:275:SER:H	2.27	0.42
3:F:100:LEU:HB3	3:F:105:LYS:HE3	2.01	0.42
3:G:29:SER:O	3:G:30:LEU:C	2.62	0.42
3:G:38:ASP:OD1	3:G:38:ASP:N	2.40	0.42
3:G:268:PHE:O	3:G:269:THR:C	2.60	0.42
3:H:45:TYR:CE1	3:H:158:TRP:CA	3.00	0.42
3:H:138:THR:HG21	3:H:144:PHE:HB2	2.01	0.42
1:I:154:VAL:O	1:I:155:TYR:HB2	2.19	0.42
3:J:186:PHE:CE1	3:J:210:ALA:HA	2.53	0.42
1:K:27:LEU:HA	1:K:30:LEU:HD22	2.01	0.42
1:K:97:TYR:O	1:K:100:LEU:CB	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:PRO:O	1:L:259:LYS:C	2.61	0.42
1:C:120:ASP:OD1	1:C:252:TRP:CD1	2.67	0.42
1:C:123:VAL:O	1:C:125:MET:N	2.53	0.42
1:C:194:THR:HG22	1:C:195:ALA:N	2.33	0.42
7:A:527:HOH:O	1:B:98:GLU:HG3	2.19	0.42
1:B:89:ARG:HG3	7:B:402:HOH:O	2.18	0.42
1:B:215:PHE:O	1:B:216:SER:C	2.62	0.42
3:H:25:GLU:CG	3:H:76:ILE:HD12	2.49	0.42
3:H:53:LEU:O	3:H:53:LEU:HD12	2.19	0.42
3:H:126:PHE:CE1	3:H:138:THR:HG22	2.54	0.42
1:I:36:ARG:C	1:I:38:ASP:N	2.74	0.42
3:J:137:SER:OG	3:J:138:THR:N	2.52	0.42
1:K:10:LEU:HD22	1:K:154:VAL:CG1	2.49	0.42
1:L:45:TYR:CD1	1:L:46:PRO:HD2	2.54	0.42
1:L:101:PRO:O	1:L:102:VAL:C	2.59	0.42
1:L:149:LEU:HA	1:L:149:LEU:HD23	1.75	0.42
1:L:159:PHE:O	1:L:163:LEU:HG	2.19	0.42
1:L:232:VAL:O	1:L:233:ILE:HG23	2.19	0.42
1:C:71:ILE:O	1:C:71:ILE:CG1	2.65	0.42
1:C:113:TYR:HE2	1:C:161:HIS:CE1	2.37	0.42
1:A:132:ASN:C	1:A:132:ASN:OD1	2.62	0.42
1:A:188:LYS:HD2	7:A:488:HOH:O	2.20	0.42
1:B:43:VAL:O	1:B:113:TYR:CA	2.60	0.42
1:E:9:LEU:HD21	7:E:536:HOH:O	2.20	0.42
1:E:60:ILE:HG22	1:E:63:ALA:HB2	2.01	0.42
3:F:206:MET:HA	3:F:209:ILE:CG1	2.49	0.42
3:F:259:LYS:O	3:F:260:GLN:C	2.61	0.42
3:G:93:THR:OG1	3:G:94:HIS:N	2.53	0.42
1:I:55:GLU:CG	7:I:429:HOH:O	2.67	0.42
3:J:119:LYS:HG2	3:J:256:PHE:CZ	2.54	0.42
1:L:80:GLU:OE2	1:L:84:ARG:HG3	2.19	0.42
1:L:119:LYS:HD3	1:L:252:TRP:CE3	2.54	0.42
1:C:96:ASN:CG	1:C:99:MET:HE2	2.45	0.42
1:A:35:ALA:H	1:A:103:THR:CG2	2.32	0.42
1:A:209:ILE:HG12	1:A:209:ILE:H	1.55	0.42
1:B:276:ASP:HB3	1:B:279:ARG:NH1	2.35	0.42
2:D:276:ASP:C	2:D:279:ARG:H	2.26	0.42
1:E:70:PRO:HG3	1:E:233:ILE:C	2.44	0.42
3:H:113:TYR:OH	3:H:161:HIS:ND1	2.44	0.42
1:I:68:THR:OG1	1:I:69:SER:N	2.48	0.42
3:J:12:LYS:CD	3:J:17:PHE:CD2	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:TYR:CD1	1:K:176:PHE:CZ	3.08	0.42
1:K:135:LEU:HA	1:K:135:LEU:HD23	1.73	0.42
1:K:169:LYS:HD2	1:K:176:PHE:HB2	2.01	0.42
1:K:179:TYR:CD2	1:K:179:TYR:C	2.97	0.42
4:K:301:A3P:HO2'	4:K:301:A3P:P1	2.40	0.42
1:C:47:LYS:HE3	1:C:47:LYS:CA	2.47	0.42
1:C:172:LYS:HG2	1:B:172:LYS:HA	2.01	0.42
1:C:261:ASN:O	1:C:264:PHE:N	2.53	0.42
1:B:260:GLN:O	1:B:261:ASN:C	2.61	0.42
1:B:262:ARG:C	1:B:264:PHE:N	2.76	0.42
2:D:59:ARG:HA	2:D:59:ARG:HD3	1.76	0.42
1:E:119:LYS:CE	1:E:264:PHE:CD1	3.03	0.42
3:F:129:TYR:HA	3:F:135:LEU:CB	2.49	0.42
3:F:239:ASP:O	3:F:240:ARG:C	2.61	0.42
3:H:56:VAL:O	3:H:59:ARG:HB2	2.20	0.42
3:H:219:LYS:HB2	3:H:244:PHE:HB3	2.02	0.42
3:H:253:ILE:HG13	3:H:254:ASN:N	2.34	0.42
1:I:29:SER:O	1:I:30:LEU:C	2.63	0.42
3:J:200:ASP:CB	7:J:414:HOH:O	2.67	0.42
1:K:47:LYS:HA	4:K:301:A3P:P2	2.59	0.42
1:K:204:SER:O	1:K:205:GLU:C	2.60	0.42
1:K:225:GLU:CD	1:K:231:HIS:HB3	2.45	0.42
1:C:273:ARG:HB2	1:C:274:ASN:H	1.76	0.42
1:A:265:ASP:OD1	1:A:265:ASP:N	2.53	0.42
1:A:276:ASP:OD1	7:A:427:HOH:O	2.22	0.42
1:B:16:ILE:HG21	1:B:155:TYR:CA	2.50	0.42
1:B:201:VAL:HG12	1:B:205:GLU:HB2	2.01	0.42
1:B:274:ASN:O	1:B:275:SER:C	2.61	0.42
1:E:175:LEU:HD22	1:E:196:PHE:HB2	2.02	0.42
3:F:195:ALA:O	3:F:197:LEU:N	2.53	0.42
3:H:117:ASN:ND2	3:H:120:ASP:HB2	2.34	0.42
1:I:117:ASN:HD21	1:I:120:ASP:CG	2.28	0.42
1:I:191:LYS:O	1:I:195:ALA:CB	2.67	0.42
3:J:35:ALA:H	3:J:103:THR:CG2	2.32	0.42
3:J:95:LEU:HD22	3:J:99:MET:HB2	2.01	0.42
1:K:115:VAL:HG13	1:K:178:PHE:CD1	2.55	0.42
1:K:202:ASN:O	1:K:206:MET:HG3	2.19	0.42
1:L:119:LYS:HB3	1:L:252:TRP:CG	2.55	0.42
1:L:132:ASN:CB	1:L:135:LEU:HD12	2.50	0.42
1:A:45:TYR:O	1:A:48:SER:CB	2.67	0.42
1:A:77:SER:O	1:A:78:LYS:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HA	7:A:510:HOH:O	2.20	0.42
1:B:128:TYR:O	1:B:132:ASN:CB	2.68	0.42
2:D:23:SER:HB2	2:D:25:GLU:OE1	2.20	0.42
3:F:195:ALA:C	3:F:197:LEU:N	2.75	0.42
3:F:252:TRP:HB2	3:F:256:PHE:CE1	2.55	0.42
3:G:250:GLY:C	3:G:252:TRP:N	2.73	0.42
3:H:46:PRO:HG2	3:H:125:MET:CE	2.50	0.42
1:I:262:ARG:O	1:I:264:PHE:N	2.52	0.42
3:J:77:SER:O	3:J:78:LYS:C	2.63	0.42
3:J:110:LYS:NZ	7:J:430:HOH:O	2.23	0.42
3:J:159:PHE:O	3:J:160:ASP:C	2.62	0.42
3:J:206:MET:CA	3:J:209:ILE:HG12	2.49	0.42
1:K:97:TYR:CE2	1:K:105:LYS:HE2	2.55	0.42
1:L:13:TYR:CZ	1:L:14[B]:MET:HG3	2.55	0.42
1:L:107:LYS:O	1:L:108:GLN:C	2.63	0.42
1:L:181:GLU:HG3	1:L:182:MET:N	2.32	0.42
1:C:240:ARG:C	1:C:242:LEU:N	2.77	0.42
2:D:73:LEU:CD2	2:D:232:VAL:HG21	2.49	0.42
2:D:102:VAL:HG13	2:D:103:THR:N	2.35	0.42
2:D:208:LYS:O	2:D:211:ARG:CB	2.68	0.42
2:D:219:LYS:HA	2:D:244:PHE:CD2	2.55	0.42
1:E:43:VAL:O	1:E:113:TYR:HA	2.20	0.42
1:E:268:PHE:C	1:E:268:PHE:CD2	2.97	0.42
3:F:22:SER:O	3:F:23:SER:C	2.63	0.42
3:F:30:LEU:O	3:F:31:ASP:C	2.62	0.42
3:F:97:TYR:O	3:F:100:LEU:CB	2.68	0.42
3:G:55:GLU:O	3:G:56:VAL:C	2.63	0.42
3:H:49:GLY:CA	3:H:114:ILE:HD13	2.46	0.42
3:H:66:THR:O	3:H:89:ARG:HA	2.20	0.42
1:I:25:GLU:OE1	1:I:25:GLU:N	2.31	0.42
1:I:58:GLU:OE2	1:I:67:LEU:HD23	2.20	0.42
1:I:79:PHE:O	1:I:81:GLU:N	2.52	0.42
1:I:100:LEU:O	1:I:105:LYS:HE3	2.19	0.42
1:I:181:GLU:HA	1:I:184:LYS:HE2	2.02	0.42
1:I:194:THR:O	1:I:197:LEU:N	2.53	0.42
1:C:190:LEU:C	1:C:190:LEU:HD12	2.43	0.42
1:A:9:LEU:O	1:A:20:THR:N	2.35	0.42
1:A:102:VAL:O	1:A:102:VAL:HG22	2.20	0.42
1:A:116:ARG:NH1	4:A:301:A3P:O3'	2.52	0.42
1:A:140:THR:HG1	1:A:143:ALA:HB2	1.85	0.42
1:B:244:PHE:HE1	4:B:301:A3P:N7	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:O	1:B:262:ARG:N	2.53	0.42
2:D:52:TRP:O	2:D:52:TRP:CD1	2.73	0.42
2:D:276:ASP:O	2:D:279:ARG:HB3	2.19	0.42
1:E:205:GLU:O	1:E:206:MET:C	2.60	0.42
1:E:240:ARG:O	1:E:243:VAL:HG13	2.19	0.42
3:F:248:VAL:HG22	3:F:249:VAL:N	2.35	0.42
3:G:213:THR:C	3:G:218:MET:SD	3.03	0.42
3:H:273:ARG:H	3:H:273:ARG:HG2	1.62	0.42
1:I:33:PHE:O	1:I:103:THR:HG21	2.20	0.42
1:I:129:TYR:CD2	1:I:136:PRO:O	2.73	0.42
3:J:45:TYR:O	3:J:46:PRO:C	2.62	0.42
3:J:101:PRO:HB2	3:J:104:VAL:HG23	2.02	0.42
3:J:113:TYR:OH	3:J:161:HIS:CD2	2.67	0.42
3:J:172:LYS:HE3	7:L:472:HOH:O	2.19	0.42
3:J:195:ALA:HB3	7:J:419:HOH:O	2.18	0.42
1:K:279:ARG:HD2	7:L:411:HOH:O	2.19	0.42
1:L:201:VAL:CG1	1:L:205:GLU:HB2	2.50	0.42
1:L:218:MET:HE2	1:L:218:MET:HB3	1.94	0.42
1:C:18:PHE:N	1:C:18:PHE:CD1	2.88	0.41
1:C:70:PRO:HG2	1:C:235:ALA:N	2.35	0.41
1:B:163:LEU:C	1:B:165:TRP:N	2.77	0.41
1:B:234:CYS:C	1:B:236:LEU:H	2.28	0.41
2:D:37:GLU:CD	2:D:107:LYS:HD3	2.45	0.41
3:F:132:ASN:HA	3:F:133:PRO:HD3	1.78	0.41
3:G:47:LYS:HD2	7:G:430:HOH:O	2.19	0.41
3:G:234:CYS:HB3	3:G:237:THR:CG2	2.47	0.41
3:G:242:LEU:HD23	3:G:242:LEU:HA	1.80	0.41
1:I:128:TYR:OH	1:I:237:THR:CB	2.66	0.41
1:I:149:LEU:HD22	1:I:267:LEU:HD12	2.01	0.41
1:K:103:THR:HG22	1:K:104:VAL:N	2.35	0.41
1:K:242:LEU:HD23	1:K:242:LEU:HA	1.79	0.41
1:L:26:LEU:HD22	1:L:75:ASP:O	2.19	0.41
1:L:202:ASN:OD1	1:L:205:GLU:HG3	2.20	0.41
1:L:225:GLU:HB2	1:L:226:ASN:H	1.67	0.41
1:L:250:GLY:O	1:L:253:ILE:HG23	2.19	0.41
1:A:185:ASP:CB	7:A:423:HOH:O	2.68	0.41
2:D:62:ASP:OD1	2:D:62:ASP:N	2.53	0.41
2:D:253:ILE:HG13	2:D:254:ASN:N	2.35	0.41
1:E:125:MET:CG	1:E:144:PHE:HZ	2.33	0.41
1:E:253:ILE:HG13	1:E:254:ASN:N	2.35	0.41
3:F:196:PHE:CD2	3:F:197:LEU:HD23	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:9:LEU:HD22	3:G:9:LEU:HA	1.80	0.41
3:G:129:TYR:HA	3:G:135:LEU:HB3	2.02	0.41
3:H:46:PRO:HG2	3:H:125:MET:HE3	2.02	0.41
3:H:69:SER:N	3:H:231:HIS:CE1	2.84	0.41
1:I:93:THR:OG1	1:I:95:LEU:HD12	2.21	0.41
3:J:10:LEU:HD21	3:J:154:VAL:CG1	2.50	0.41
3:J:154:VAL:O	3:J:155:TYR:HB2	2.19	0.41
1:K:11:HIS:HE1	1:K:22:SER:O	2.02	0.41
1:K:117:ASN:HA	1:K:118:PRO:HD3	1.90	0.41
1:K:132:ASN:O	1:K:135:LEU:HB2	2.20	0.41
1:L:120:ASP:OD1	1:L:252:TRP:HD1	2.03	0.41
1:L:204:SER:O	1:L:207:ALA:HB3	2.21	0.41
1:C:119:LYS:HE3	1:C:264:PHE:CE1	2.56	0.41
1:A:40:ILE:HD11	1:A:88:ARG:CZ	2.50	0.41
1:A:214:SER:O	1:A:215:PHE:C	2.64	0.41
1:A:269:THR:O	1:A:270:GLU:C	2.60	0.41
1:A:282:LYS:HE2	7:A:457:HOH:O	2.20	0.41
1:B:67:LEU:HG	1:B:68:THR:N	2.33	0.41
1:B:163:LEU:O	1:B:164:SER:C	2.62	0.41
2:D:132:ASN:HA	2:D:133:PRO:HD2	1.77	0.41
2:D:168:HIS:O	2:D:171:ASP:HB2	2.21	0.41
2:D:178:PHE:HB2	2:D:181:GLU:HB3	2.01	0.41
1:E:205:GLU:O	1:E:209:ILE:HG12	2.20	0.41
3:F:73:LEU:CD2	3:F:232:VAL:HG21	2.50	0.41
3:F:225:GLU:OE2	3:F:231:HIS:HB3	2.20	0.41
3:G:135:LEU:HD23	3:G:135:LEU:HA	1.85	0.41
3:G:183:LYS:HE3	3:G:183:LYS:HB3	1.92	0.41
3:H:40:ILE:O	3:H:91:ILE:N	2.49	0.41
3:H:219:LYS:HA	3:H:244:PHE:CE2	2.53	0.41
3:J:36:ARG:C	3:J:38:ASP:N	2.77	0.41
3:J:101:PRO:O	3:J:102:VAL:C	2.62	0.41
3:J:212:SER:HA	3:J:217:GLU:HG2	2.02	0.41
1:K:73:LEU:O	1:K:78:LYS:HE3	2.20	0.41
1:K:80:GLU:C	1:K:80:GLU:CD	2.88	0.41
1:K:246:LYS:O	1:K:247:GLY:C	2.63	0.41
1:C:13:TYR:O	1:C:14[A]:MET:HB2	2.17	0.41
1:C:77:SER:O	1:C:80:GLU:CB	2.66	0.41
1:C:179:TYR:CD2	1:C:179:TYR:C	2.98	0.41
1:C:183:LYS:O	7:C:421:HOH:O	2.22	0.41
1:C:258:PRO:O	1:C:262:ARG:HG2	2.21	0.41
1:B:132:ASN:OD1	1:B:134:ASN:CB	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:CG2	1:B:233:ILE:N	2.83	0.41
2:D:98[A]:GLU:CG	7:D:478:HOH:O	2.68	0.41
2:D:215:PHE:O	2:D:218:MET:N	2.53	0.41
1:E:203:ASP:O	1:E:205:GLU:N	2.53	0.41
3:F:221:ASN:C	7:F:442:HOH:O	2.63	0.41
3:G:69:SER:O	3:G:70:PRO:C	2.61	0.41
3:G:132:ASN:OD1	3:G:134:ASN:HB2	2.20	0.41
3:H:38:ASP:OD1	3:H:38:ASP:N	2.46	0.41
3:H:273:ARG:C	3:H:275:SER:H	2.28	0.41
1:I:47:LYS:HG3	1:I:125:MET:HA	2.02	0.41
1:L:22:SER:OG	1:L:72:GLU:O	2.31	0.41
1:C:232:VAL:CG2	1:C:233:ILE:N	2.80	0.41
1:B:59:ARG:CZ	1:B:212:SER:HB2	2.50	0.41
2:D:147:LEU:O	2:D:150:LYS:N	2.52	0.41
2:D:282:LYS:O	2:D:284:TYR:O	2.38	0.41
3:F:73:LEU:HB3	3:F:78:LYS:HZ1	1.84	0.41
3:F:267:LEU:HD23	3:F:267:LEU:HA	1.85	0.41
3:G:25:GLU:H	3:G:25:GLU:CD	2.28	0.41
3:G:132:ASN:C	3:G:134:ASN:N	2.76	0.41
1:L:59:ARG:O	1:L:60:ILE:C	2.59	0.41
1:L:144:PHE:C	1:L:146:GLU:N	2.71	0.41
1:L:169:LYS:HD2	1:L:176:PHE:CD1	2.54	0.41
1:C:19:SER:HB3	7:C:401:HOH:O	2.21	0.41
1:A:208:LYS:O	1:A:211:ARG:HB3	2.21	0.41
1:B:26:LEU:HD12	1:B:26:LEU:C	2.44	0.41
1:B:132:ASN:C	1:B:134:ASN:N	2.77	0.41
1:E:132:ASN:C	1:E:134:ASN:N	2.76	0.41
3:F:204:SER:O	3:F:207:ALA:CB	2.64	0.41
3:G:75:ASP:HB2	3:G:77:SER:H	1.85	0.41
3:G:208:LYS:O	3:G:211:ARG:HB3	2.21	0.41
1:I:262:ARG:C	1:I:264:PHE:N	2.77	0.41
3:J:205:GLU:O	3:J:209:ILE:N	2.46	0.41
1:K:53:LEU:HD21	1:K:112:ILE:CG2	2.51	0.41
1:C:114:ILE:HD12	1:C:182:MET:HE2	2.02	0.41
1:C:183:LYS:HE3	1:C:183:LYS:HB3	1.67	0.41
1:C:240:ARG:O	1:C:242:LEU:N	2.54	0.41
1:A:171:ASP:HA	7:A:408:HOH:O	2.21	0.41
1:A:254:ASN:O	1:I:87:LYS:CD	2.69	0.41
1:A:282:LYS:C	1:A:284:TYR:H	2.29	0.41
1:B:16:ILE:HG23	1:B:155:TYR:C	2.45	0.41
1:B:76:ILE:O	1:B:77:SER:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:CYS:HB3	1:B:237:THR:CG2	2.51	0.41
1:E:54:ALA:HB3	1:E:233:ILE:HD12	2.02	0.41
1:E:78:LYS:CE	7:E:413:HOH:O	2.64	0.41
1:E:123:VAL:O	1:E:127:HIS:HD2	2.04	0.41
3:F:28:GLY:O	6:F:303:GOL:C1	2.68	0.41
3:F:143:ALA:O	3:F:146:GLU:N	2.54	0.41
3:G:78:LYS:HD3	3:G:78:LYS:C	2.45	0.41
3:G:282:LYS:C	3:G:284:TYR:N	2.76	0.41
3:H:51:HIS:O	3:H:52:TRP:C	2.62	0.41
1:I:33:PHE:HE1	1:I:82:LEU:CD1	2.31	0.41
1:I:159:PHE:O	1:I:163:LEU:HG	2.20	0.41
3:J:11:HIS:HE1	3:J:19:SER:O	2.03	0.41
3:J:55:GLU:O	3:J:59:ARG:N	2.53	0.41
3:J:130:ARG:HA	3:J:137:SER:OG	2.21	0.41
1:K:265:ASP:HA	7:K:425:HOH:O	2.21	0.41
1:L:50:THR:CG2	1:L:94:HIS:HE1	2.32	0.41
1:L:213:THR:CA	7:L:406:HOH:O	2.69	0.41
1:L:276:ASP:O	1:L:279:ARG:HB3	2.20	0.41
1:C:31:ASP:C	1:C:33:PHE:H	2.28	0.41
1:C:115:VAL:HG22	1:C:116:ARG:N	2.35	0.41
1:A:215:PHE:C	1:A:215:PHE:CD2	2.99	0.41
1:B:147:LEU:HA	1:B:147:LEU:HD23	1.81	0.41
3:G:261:ASN:HA	7:G:404:HOH:O	2.17	0.41
1:I:96:ASN:C	1:I:96:ASN:OD1	2.63	0.41
3:J:35:ALA:H	3:J:103:THR:HG21	1.86	0.41
3:J:60:ILE:CG2	3:J:61:PRO:CD	2.95	0.41
3:J:159:PHE:HE1	3:J:268:PHE:CD1	2.39	0.41
1:K:253:ILE:HG13	1:K:254:ASN:N	2.35	0.41
1:C:158:TRP:O	1:C:159:PHE:C	2.64	0.41
1:C:191:LYS:O	1:C:193:ILE:N	2.52	0.41
1:C:218:MET:HB3	1:C:244:PHE:CZ	2.55	0.41
1:A:30:LEU:C	1:A:32:SER:H	2.29	0.41
1:A:172:LYS:HG3	1:A:173:ASN:N	2.35	0.41
1:A:257:THR:C	1:A:259:LYS:N	2.77	0.41
1:A:267:LEU:O	1:A:270:GLU:N	2.54	0.41
1:B:44:SER:HA	1:B:114:ILE:O	2.20	0.41
1:B:76:ILE:C	1:B:78:LYS:N	2.76	0.41
1:B:129:TYR:HA	1:B:135:LEU:HB2	2.03	0.41
1:B:132:ASN:HB3	1:B:135:LEU:HD12	2.03	0.41
1:B:257:THR:O	1:B:258:PRO:C	2.63	0.41
1:B:262:ARG:C	1:B:264:PHE:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:MET:HE3	2:D:99:MET:HB2	1.85	0.41
2:D:141:TRP:O	2:D:142:ALA:C	2.64	0.41
2:D:176:PHE:O	2:D:192:LYS:NZ	2.53	0.41
2:D:191:LYS:HG2	2:D:206:MET:HE1	2.02	0.41
2:D:275:SER:O	2:D:279:ARG:N	2.54	0.41
1:E:52:TRP:CG	1:E:182:MET:HE3	2.54	0.41
3:F:47:LYS:HA	7:F:425:HOH:O	2.20	0.41
3:F:226:ASN:O	3:F:226:ASN:OD1	2.39	0.41
3:G:51:HIS:CG	3:G:233:ILE:HD11	2.56	0.41
3:G:82:LEU:HB2	7:G:435:HOH:O	2.20	0.41
3:G:98[A]:GLU:CD	3:G:98[A]:GLU:H	2.28	0.41
3:G:103:THR:CG2	3:G:104:VAL:N	2.83	0.41
3:G:117:ASN:HB2	3:G:118:PRO:HD2	2.03	0.41
3:G:276:ASP:OD2	3:H:274:ASN:HB3	2.20	0.41
3:H:25:GLU:HB3	3:H:76:ILE:HD12	2.03	0.41
3:H:27:LEU:C	3:H:29:SER:H	2.29	0.41
3:H:118:PRO:HB3	3:H:158:TRP:CD2	2.56	0.41
3:H:150:LYS:HB2	3:H:152:ASP:OD2	2.21	0.41
3:H:189:SER:O	3:H:192:LYS:CB	2.69	0.41
3:H:276:ASP:O	3:H:279:ARG:CB	2.64	0.41
3:J:119:LYS:HE3	3:J:264:PHE:CD1	2.56	0.41
3:J:272:MET:O	3:J:273:ARG:C	2.63	0.41
3:J:276:ASP:O	3:J:279:ARG:N	2.54	0.41
3:J:284:TYR:O	3:J:285:ALA:C	2.64	0.41
1:K:267:LEU:O	1:K:268:PHE:C	2.63	0.41
1:L:39:ASP:OD1	7:L:421:HOH:O	2.21	0.41
1:L:65:ILE:HG12	1:L:88:ARG:CD	2.46	0.41
1:L:266:GLU:O	1:L:267:LEU:C	2.63	0.41
1:C:135:LEU:O	1:C:137:SER:N	2.54	0.41
1:A:73:LEU:CD2	1:A:232:VAL:HG21	2.51	0.41
1:A:115:VAL:O	1:A:115:VAL:CG1	2.68	0.41
1:B:57:ILE:C	1:B:59:ARG:N	2.76	0.41
1:E:49:GLY:O	1:E:50:THR:C	2.63	0.41
1:E:50:THR:O	1:E:53:LEU:N	2.54	0.41
1:E:95:LEU:HD22	1:E:99:MET:HB3	2.01	0.41
1:E:163:LEU:C	1:E:165:TRP:N	2.78	0.41
3:F:75:ASP:C	3:F:77:SER:N	2.78	0.41
3:F:132:ASN:C	7:F:424:HOH:O	2.63	0.41
3:F:281:LEU:HD23	3:F:281:LEU:HA	1.89	0.41
3:G:53:LEU:O	3:G:56:VAL:HB	2.20	0.41
1:I:12:LYS:HD3	1:I:17:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:128:TYR:O	1:I:132:ASN:CB	2.69	0.41
1:K:101:PRO:O	1:K:102:VAL:C	2.63	0.41
1:K:117:ASN:H	1:K:180:GLU:CD	2.29	0.41
1:K:185:ASP:O	1:K:186:PHE:C	2.63	0.41
1:K:234:CYS:HB3	1:K:237:THR:HG21	2.01	0.41
1:L:96:ASN:CG	1:L:98[A]:GLU:OE1	2.63	0.41
1:L:276:ASP:CG	1:L:279:ARG:NH1	2.79	0.41
1:A:12:LYS:HE2	1:A:15:GLY:O	2.20	0.40
1:A:234:CYS:C	1:A:237:THR:HG22	2.46	0.40
1:A:258:PRO:CB	1:A:262:ARG:HH12	2.35	0.40
1:B:40:ILE:HD11	1:B:88:ARG:CZ	2.51	0.40
1:B:76:ILE:O	1:B:78:LYS:N	2.55	0.40
2:D:57:ILE:C	2:D:59:ARG:N	2.79	0.40
2:D:222:ALA:O	2:D:223:ALA:CB	2.67	0.40
1:E:26:LEU:CD1	1:E:79:PHE:CZ	3.04	0.40
1:E:191:LYS:HA	1:E:194:THR:HG22	2.03	0.40
3:H:14:MET:CE	3:H:14:MET:HA	2.49	0.40
3:H:239:ASP:OD1	3:H:241:ASN:N	2.38	0.40
1:I:143:ALA:C	7:I:409:HOH:O	2.59	0.40
1:K:215:PHE:O	1:K:219:LYS:N	2.49	0.40
1:L:145:LEU:O	1:L:149:LEU:HG	2.21	0.40
1:L:215:PHE:CE2	1:L:246:LYS:O	2.74	0.40
1:C:187:VAL:CG1	1:C:191:LYS:HE3	2.51	0.40
1:A:188:LYS:HG3	7:A:529:HOH:O	2.17	0.40
1:A:219:LYS:HG3	1:A:244:PHE:CB	2.51	0.40
1:B:12:LYS:CD	1:B:17:PHE:CE2	2.99	0.40
1:B:115:VAL:O	1:B:178:PHE:HA	2.21	0.40
1:B:123:VAL:O	1:B:124:SER:C	2.62	0.40
1:B:151:GLY:HA2	1:B:157:SER:N	2.36	0.40
2:D:13:TYR:C	2:D:15:GLY:N	2.77	0.40
2:D:98[B]:GLU:OE1	2:D:98[B]:GLU:HA	2.20	0.40
2:D:164:SER:CA	7:D:412:HOH:O	2.69	0.40
2:D:217:GLU:OE1	2:D:217:GLU:CA	2.60	0.40
2:D:267:LEU:O	2:D:268:PHE:C	2.61	0.40
1:E:166:GLU:C	1:E:168:HIS:H	2.29	0.40
3:F:223:ALA:C	7:F:411:HOH:O	2.61	0.40
3:F:283:GLU:HA	3:F:283:GLU:OE1	2.21	0.40
3:G:205:GLU:OE2	7:G:427:HOH:O	2.21	0.40
3:H:98:GLU:OE2	3:H:164:SER:CB	2.70	0.40
3:H:183:LYS:NZ	3:H:247:GLY:O	2.36	0.40
3:H:198:GLY:C	3:H:199:ILE:HG13	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:GLU:CD	7:I:429:HOH:O	2.64	0.40
1:I:175:LEU:HD11	1:I:192:LYS:HE3	2.02	0.40
3:J:15:GLY:C	3:J:16:ILE:HG13	2.46	0.40
3:J:240:ARG:O	3:J:241:ASN:C	2.61	0.40
1:K:26:LEU:CD1	1:K:79:PHE:CE1	3.04	0.40
1:C:51:HIS:O	1:C:54:ALA:N	2.54	0.40
1:C:220:SER:C	1:C:221:ASN:CG	2.89	0.40
1:A:44:SER:HB2	1:A:48:SER:HB2	2.03	0.40
1:A:132:ASN:HA	1:A:133:PRO:HD2	1.84	0.40
1:A:279:ARG:HG2	1:A:283:GLU:OE2	2.22	0.40
3:F:73:LEU:O	3:F:78:LYS:NZ	2.53	0.40
3:G:84:ARG:HD2	7:G:414:HOH:O	2.21	0.40
3:G:115:VAL:CG1	3:G:178:PHE:CD1	3.03	0.40
3:G:128:TYR:O	3:G:132:ASN:CB	2.70	0.40
4:G:301:A3P:O5P	7:G:430:HOH:O	2.22	0.40
3:H:189:SER:O	3:H:191:LYS:N	2.54	0.40
3:H:189:SER:HA	3:H:192:LYS:HB2	2.03	0.40
1:I:252:TRP:CE3	1:I:252:TRP:C	3.00	0.40
1:K:47:LYS:HA	1:K:47:LYS:HE3	2.04	0.40
1:K:209:ILE:HG12	1:K:209:ILE:H	1.54	0.40
1:K:215:PHE:O	1:K:216:SER:C	2.64	0.40
1:B:95:LEU:HD22	1:B:99:MET:HE3	2.03	0.40
2:D:13:TYR:CZ	2:D:14:MET:HG2	2.56	0.40
2:D:36:ARG:CD	3:H:140:THR:HG21	2.50	0.40
2:D:120:ASP:OD1	2:D:252:TRP:HD1	2.04	0.40
1:E:277:VAL:C	1:E:279:ARG:N	2.78	0.40
3:G:119:LYS:HG2	3:G:256:PHE:CZ	2.56	0.40
4:G:301:A3P:O3P	4:G:301:A3P:O2'	2.36	0.40
3:H:68:THR:HG21	3:H:91:ILE:HG12	2.02	0.40
3:H:96:ASN:OD1	3:H:99:MET:N	2.45	0.40
1:I:138:THR:HG22	1:I:140:THR:O	2.21	0.40
1:I:173:ASN:OD1	7:I:419:HOH:O	2.21	0.40
3:J:114:ILE:HA	3:J:177:ILE:O	2.21	0.40
3:J:185:ASP:CG	3:J:188:LYS:HB2	2.46	0.40
1:K:195:ALA:O	1:K:198:GLY:N	2.53	0.40
1:L:45:TYR:HD2	1:L:46:PRO:O	2.04	0.40
1:L:259:LYS:O	1:L:260:GLN:C	2.61	0.40
4:C:301:A3P:O2'	4:C:301:A3P:P1	2.79	0.40
1:A:13:TYR:O	1:A:14:MET:C	2.64	0.40
1:A:233:ILE:CG1	1:A:234:CYS:N	2.84	0.40
1:A:239:ASP:CG	1:A:239:ASP:O	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TYR:O	1:A:285:ALA:C	2.61	0.40
1:B:51:HIS:HD2	1:B:233:ILE:HD11	1.85	0.40
1:B:234:CYS:CB	1:B:237:THR:HG23	2.51	0.40
1:E:41:PHE:HB2	1:E:111:ILE:CD1	2.52	0.40
1:E:51:HIS:CD2	1:E:233:ILE:HD11	2.56	0.40
1:E:134:ASN:ND2	1:E:238:SER:OG	2.55	0.40
3:F:219:LYS:HG3	3:F:244:PHE:CB	2.52	0.40
3:H:110:LYS:CE	7:H:466:HOH:O	2.69	0.40
1:I:194:THR:HG23	7:I:437:HOH:O	2.22	0.40
1:K:69:SER:HB3	1:K:78:LYS:HZ1	1.87	0.40
1:K:264:PHE:O	1:K:265:ASP:C	2.61	0.40
1:L:46:PRO:C	1:L:47:LYS:CG	2.95	0.40
1:L:258:PRO:O	1:L:261:ASN:HB3	2.21	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:PHE:O	7:G:519:HOH:O[1_545]	1.43	0.77
2:D:135:LEU:O	7:H:426:HOH:O[2_646]	1.78	0.42
1:L:211:ARG:NH1	7:A:419:HOH:O[2_657]	1.99	0.21
1:E:130:ARG:O	1:K:211:ARG:NH2[2_747]	2.04	0.16
2:D:137:SER:N	7:H:426:HOH:O[2_646]	2.06	0.14
1:L:288:ALA:O	7:I:476:HOH:O[2_657]	2.07	0.13
1:B:86:PRO:O	7:D:482:HOH:O[2_656]	2.10	0.10
3:G:254:ASN:O	3:J:87:LYS:NZ[2_647]	2.13	0.07
7:F:414:HOH:O	7:G:519:HOH:O[1_545]	2.15	0.05
1:C:211:ARG:NH1	1:K:135:LEU:O[2_646]	2.16	0.04

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	280/283 (99%)	235 (84%)	38 (14%)	7 (2%)	4	1
1	B	274/283 (97%)	242 (88%)	27 (10%)	5 (2%)	6	3
1	C	284/283 (100%)	231 (81%)	36 (13%)	17 (6%)	1	0
1	E	274/283 (97%)	240 (88%)	27 (10%)	7 (3%)	4	1
1	I	274/283 (97%)	230 (84%)	37 (14%)	7 (3%)	4	1
1	K	283/283 (100%)	247 (87%)	30 (11%)	6 (2%)	5	2
1	L	286/283 (101%)	236 (82%)	37 (13%)	13 (4%)	2	0
2	D	274/281 (98%)	234 (85%)	27 (10%)	13 (5%)	2	0
3	F	277/282 (98%)	231 (83%)	31 (11%)	15 (5%)	1	0
3	G	274/282 (97%)	240 (88%)	27 (10%)	7 (3%)	4	1
3	H	275/282 (98%)	237 (86%)	26 (10%)	12 (4%)	2	0
3	J	272/282 (96%)	230 (85%)	36 (13%)	6 (2%)	5	2
All	All	3327/3390 (98%)	2833 (85%)	379 (11%)	115 (4%)	3	1

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	THR
1	C	137	SER
1	C	223	ALA
1	C	228	ASP
1	A	8	SER
1	A	56	VAL
1	A	223	ALA
1	A	285	ALA
1	B	223	ALA
2	D	9	ILE
2	D	30	LEU
2	D	78	LYS
2	D	223	ALA
1	E	30	LEU
1	E	223	ALA
3	F	31	ASP
3	F	222	ALA
3	F	223	ALA
3	F	252	TRP
3	G	30	LEU
3	G	223	ALA
3	H	223	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	277	VAL
1	I	56	VAL
1	I	167	GLU
1	I	223	ALA
1	I	285	ALA
3	J	221	ASN
3	J	223	ALA
3	J	283	GLU
1	K	223	ALA
1	K	229	PRO
1	L	222	ALA
1	L	273	ARG
1	C	8	SER
1	C	37	GLU
1	C	126	PHE
1	C	252	TRP
1	C	273	ARG
1	A	283	GLU
1	B	283	GLU
2	D	37	GLU
2	D	155	TYR
2	D	220	SER
1	E	167	GLU
3	F	76	ILE
3	F	126	PHE
3	F	137	SER
3	F	225	GLU
3	G	86	PRO
3	G	221	ASN
1	I	222	ALA
1	L	49	GLY
1	L	223	ALA
1	L	286	HIS
1	C	124	SER
1	C	125	MET
1	C	194	THR
1	C	222	ALA
2	D	224	LYS
2	D	283	GLU
1	E	203	ASP
1	E	227	CYS
3	F	37	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	241	ASN
3	G	9	LEU
3	H	32	SER
3	H	78	LYS
3	H	188	LYS
3	H	274	ASN
1	I	283	GLU
3	J	142	ALA
3	J	167	GLU
1	K	77	SER
1	L	77	SER
1	L	283	GLU
1	L	287	SER
1	C	23	SER
1	C	76	ILE
1	B	155	TYR
1	B	167	GLU
1	B	284	TYR
1	E	245	ARG
1	E	263	GLY
3	F	30	LEU
3	F	283	GLU
3	G	155	TYR
3	H	75	ASP
3	H	137	SER
3	H	230	ASN
3	J	284	TYR
1	C	123	VAL
1	C	251	ASP
2	D	202	ASN
2	D	215	PHE
3	F	136	PRO
3	F	152	ASP
1	I	57	ILE
1	K	251	ASP
2	D	77	SER
3	F	195	ALA
3	G	283	GLU
3	H	56	VAL
3	H	189	SER
3	H	215	PHE
1	A	151	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	258	PRO
1	L	258	PRO
1	L	28	GLY
1	L	86	PRO
1	A	258	PRO
1	K	86	PRO
1	K	247	GLY
1	L	233	ILE
1	L	136	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/255 (100%)	231 (91%)	24 (9%)	8	5
1	B	252/255 (99%)	229 (91%)	23 (9%)	9	6
1	C	259/255 (102%)	229 (88%)	30 (12%)	5	3
1	E	251/255 (98%)	220 (88%)	31 (12%)	4	2
1	I	251/255 (98%)	222 (88%)	29 (12%)	5	3
1	K	258/255 (101%)	226 (88%)	32 (12%)	4	2
1	L	260/255 (102%)	229 (88%)	31 (12%)	5	2
2	D	251/253 (99%)	221 (88%)	30 (12%)	5	2
3	F	251/255 (98%)	225 (90%)	26 (10%)	7	4
3	G	252/255 (99%)	223 (88%)	29 (12%)	5	3
3	H	249/255 (98%)	219 (88%)	30 (12%)	5	2
3	J	250/255 (98%)	227 (91%)	23 (9%)	8	5
All	All	3039/3058 (99%)	2701 (89%)	338 (11%)	6	3

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	9	LEU
1	C	12	LYS
1	C	26	LEU
1	C	30	LEU
1	C	50	THR
1	C	76	ILE
1	C	77	SER
1	C	103	THR
1	C	128	TYR
1	C	130	ARG
1	C	138	THR
1	C	150	LYS
1	C	182	MET
1	C	194	THR
1	C	204	SER
1	C	209	ILE
1	C	212	SER
1	C	219	LYS
1	C	220	SER
1	C	225	GLU
1	C	232	VAL
1	C	237	THR
1	C	243	VAL
1	C	246	LYS
1	C	253	ILE
1	C	267	LEU
1	C	274	ASN
1	C	275	SER
1	C	283	GLU
1	A	30	LEU
1	A	34	ASP
1	A	58	GLU
1	A	75	ASP
1	A	76	ILE
1	A	85	ILE
1	A	98	GLU
1	A	103	THR
1	A	109	CYS
1	A	111	ILE
1	A	128	TYR
1	A	138	THR
1	A	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	188	LYS
1	A	194	THR
1	A	209	ILE
1	A	220	SER
1	A	224	LYS
1	A	225	GLU
1	A	230	ASN
1	A	232	VAL
1	A	243	VAL
1	A	267	LEU
1	A	275	SER
1	B	24	GLU
1	B	29	SER
1	B	30	LEU
1	B	43	VAL
1	B	75	ASP
1	B	76	ILE
1	B	78	LYS
1	B	103	THR
1	B	138	THR
1	B	187	VAL
1	B	192	LYS
1	B	194	THR
1	B	224	LYS
1	B	225	GLU
1	B	232	VAL
1	B	233	ILE
1	B	237	THR
1	B	238	SER
1	B	243	VAL
1	B	267	LEU
1	B	270	GLU
1	B	276	ASP
1	B	283	GLU
2	D	10	LEU
2	D	12	LYS
2	D	26	LEU
2	D	30	LEU
2	D	34	ASP
2	D	50	THR
2	D	59	ARG
2	D	62	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	69	SER
2	D	76	ILE
2	D	103	THR
2	D	109	CYS
2	D	128	TYR
2	D	154	VAL
2	D	172	LYS
2	D	181	GLU
2	D	188	LYS
2	D	200	ASP
2	D	203	ASP
2	D	209	ILE
2	D	217	GLU
2	D	225	GLU
2	D	232	VAL
2	D	233	ILE
2	D	237	THR
2	D	238	SER
2	D	243	VAL
2	D	267	LEU
2	D	282	LYS
2	D	283	GLU
1	E	9	LEU
1	E	23	SER
1	E	24	GLU
1	E	29	SER
1	E	30	LEU
1	E	50	THR
1	E	68	THR
1	E	76	ILE
1	E	103	THR
1	E	123	VAL
1	E	128	TYR
1	E	130	ARG
1	E	138	THR
1	E	154	VAL
1	E	184	LYS
1	E	194	THR
1	E	208	LYS
1	E	217	GLU
1	E	220	SER
1	E	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	227	CYS
1	E	228	ASP
1	E	232	VAL
1	E	233	ILE
1	E	237	THR
1	E	238	SER
1	E	243	VAL
1	E	248	VAL
1	E	267	LEU
1	E	279	ARG
1	E	283	GLU
3	F	9	LEU
3	F	12	LYS
3	F	16	ILE
3	F	30	LEU
3	F	69	SER
3	F	76	ILE
3	F	77	SER
3	F	78	LYS
3	F	85	ILE
3	F	103	THR
3	F	117	ASN
3	F	138	THR
3	F	182	MET
3	F	187	VAL
3	F	194	THR
3	F	212	SER
3	F	220	SER
3	F	224	LYS
3	F	231	HIS
3	F	237	THR
3	F	243	VAL
3	F	267	LEU
3	F	273	ARG
3	F	274	ASN
3	F	275	SER
3	F	283	GLU
3	G	9	LEU
3	G	12	LYS
3	G	26	LEU
3	G	30	LEU
3	G	43	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	58	GLU
3	G	69	SER
3	G	76	ILE
3	G	103	THR
3	G	128	TYR
3	G	181	GLU
3	G	188	LYS
3	G	193	ILE
3	G	194	THR
3	G	200	ASP
3	G	204	SER
3	G	209	ILE
3	G	214	SER
3	G	220	SER
3	G	232	VAL
3	G	233	ILE
3	G	237	THR
3	G	243	VAL
3	G	246	LYS
3	G	248	VAL
3	G	258	PRO
3	G	266	GLU
3	G	267	LEU
3	G	283	GLU
3	H	12	LYS
3	H	16	ILE
3	H	26	LEU
3	H	30	LEU
3	H	32	SER
3	H	67	LEU
3	H	69	SER
3	H	76	ILE
3	H	85	ILE
3	H	103	THR
3	H	114	ILE
3	H	117	ASN
3	H	138	THR
3	H	182	MET
3	H	184	LYS
3	H	187	VAL
3	H	194	THR
3	H	205	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	220	SER
3	H	224	LYS
3	H	230	ASN
3	H	234	CYS
3	H	237	THR
3	H	239	ASP
3	H	243	VAL
3	H	267	LEU
3	H	270	GLU
3	H	273	ARG
3	H	274	ASN
3	H	275	SER
1	I	9	LEU
1	I	12	LYS
1	I	29	SER
1	I	30	LEU
1	I	68	THR
1	I	69	SER
1	I	76	ILE
1	I	103	THR
1	I	125	MET
1	I	138	THR
1	I	184	LYS
1	I	188	LYS
1	I	200	ASP
1	I	203	ASP
1	I	217	GLU
1	I	224	LYS
1	I	226	ASN
1	I	227	CYS
1	I	231	HIS
1	I	232	VAL
1	I	233	ILE
1	I	237	THR
1	I	238	SER
1	I	243	VAL
1	I	248	VAL
1	I	267	LEU
1	I	275	SER
1	I	279	ARG
1	I	283	GLU
3	J	8	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	12	LYS
3	J	29	SER
3	J	30	LEU
3	J	37	GLU
3	J	75	ASP
3	J	76	ILE
3	J	78	LYS
3	J	102	VAL
3	J	103	THR
3	J	128	TYR
3	J	138	THR
3	J	177	ILE
3	J	214	SER
3	J	220	SER
3	J	224	LYS
3	J	232	VAL
3	J	233	ILE
3	J	237	THR
3	J	243	VAL
3	J	248	VAL
3	J	267	LEU
3	J	275	SER
1	K	8	SER
1	K	12	LYS
1	K	29	SER
1	K	30	LEU
1	K	37	GLU
1	K	69	SER
1	K	75	ASP
1	K	76	ILE
1	K	77	SER
1	K	78	LYS
1	K	85	ILE
1	K	103	THR
1	K	111	ILE
1	K	117	ASN
1	K	138	THR
1	K	150	LYS
1	K	182	MET
1	K	187	VAL
1	K	188	LYS
1	K	194	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	204	SER
1	K	209	ILE
1	K	214	SER
1	K	224	LYS
1	K	225	GLU
1	K	230	ASN
1	K	232	VAL
1	K	233	ILE
1	K	243	VAL
1	K	248	VAL
1	K	267	LEU
1	K	283	GLU
1	L	9	LEU
1	L	12	LYS
1	L	30	LEU
1	L	50	THR
1	L	69	SER
1	L	75	ASP
1	L	76	ILE
1	L	77	SER
1	L	84	ARG
1	L	103	THR
1	L	117	ASN
1	L	138	THR
1	L	146	GLU
1	L	150	LYS
1	L	182	MET
1	L	194	THR
1	L	204	SER
1	L	209	ILE
1	L	214[A]	SER
1	L	214[B]	SER
1	L	220	SER
1	L	225	GLU
1	L	232	VAL
1	L	237	THR
1	L	238	SER
1	L	243	VAL
1	L	267	LEU
1	L	270	GLU
1	L	274	ASN
1	L	275	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	283	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	127	HIS
1	A	11	HIS
1	A	230	ASN
1	B	11	HIS
1	B	94	HIS
1	B	161	HIS
1	B	241	ASN
2	D	11	HIS
1	E	11	HIS
1	E	106	GLN
1	E	127	HIS
1	E	134	ASN
1	E	161	HIS
1	E	241	ASN
3	F	11	HIS
3	F	51	HIS
3	F	170	ASN
3	F	260	GLN
3	F	261	ASN
3	G	11	HIS
3	G	127	HIS
3	G	161	HIS
3	G	168	HIS
3	G	241	ASN
3	H	11	HIS
3	H	108	GLN
3	H	231	HIS
3	H	274	ASN
1	I	11	HIS
1	I	241	ASN
1	I	261	ASN
3	J	11	HIS
3	J	108	GLN
3	J	161	HIS
1	K	11	HIS
1	K	51	HIS
1	K	231	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	286	HIS
1	L	11	HIS
1	L	51	HIS
1	L	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 20 are monoatomic - leaving 14 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
4	A3P	B	301	-	29,29,29	1.64	8 (27%)	44,45,45	2.20	13 (29%)
6	GOL	F	303	-	5,5,5	0.43	0	5,5,5	0.31	0
4	A3P	J	301	-	29,29,29	1.93	7 (24%)	44,45,45	2.04	12 (27%)
4	A3P	A	301	-	29,29,29	1.65	7 (24%)	44,45,45	2.63	16 (36%)
6	GOL	J	304	-	5,5,5	0.39	0	5,5,5	0.88	0
4	A3P	I	301	-	29,29,29	1.90	7 (24%)	44,45,45	1.95	10 (22%)
4	A3P	D	301	-	29,29,29	2.06	9 (31%)	44,45,45	2.03	8 (18%)
4	A3P	L	301	-	29,29,29	1.84	8 (27%)	44,45,45	2.11	13 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A3P	E	301	-	29,29,29	1.83	9 (31%)	44,45,45	2.11	10 (22%)
4	A3P	H	301	-	29,29,29	1.83	8 (27%)	44,45,45	1.91	10 (22%)
4	A3P	K	301	-	29,29,29	2.02	8 (27%)	44,45,45	1.97	8 (18%)
4	A3P	C	301	-	29,29,29	1.68	6 (20%)	44,45,45	1.94	11 (25%)
4	A3P	F	301	-	29,29,29	1.68	5 (17%)	44,45,45	2.07	11 (25%)
4	A3P	G	301	-	29,29,29	1.88	8 (27%)	44,45,45	2.36	15 (34%)

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
4	A3P	B	301	-	-	1/15/31/31	0/3/3/3
6	GOL	F	303	-	-	3/4/4/4	-
4	A3P	J	301	-	-	1/15/31/31	0/3/3/3
4	A3P	A	301	-	-	5/15/31/31	0/3/3/3
6	GOL	J	304	-	-	4/4/4/4	-
4	A3P	I	301	-	-	2/15/31/31	0/3/3/3
4	A3P	D	301	-	-	3/15/31/31	0/3/3/3
4	A3P	L	301	-	-	2/15/31/31	0/3/3/3
4	A3P	E	301	-	-	2/15/31/31	0/3/3/3
4	A3P	H	301	-	-	3/15/31/31	0/3/3/3
4	A3P	K	301	-	-	0/15/31/31	0/3/3/3
4	A3P	C	301	-	-	1/15/31/31	0/3/3/3
4	A3P	F	301	-	-	2/15/31/31	0/3/3/3
4	A3P	G	301	-	-	3/15/31/31	0/3/3/3

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	301	A3P	P1-O3'	-5.38	1.50	1.59
4	D	301	A3P	C5-N7	-4.86	1.30	1.39
4	I	301	A3P	C2'-C3'	-4.85	1.42	1.53
4	K	301	A3P	C2'-C3'	-4.72	1.42	1.53
4	H	301	A3P	C2'-C3'	-4.56	1.43	1.53
4	J	301	A3P	P1-O3'	-4.51	1.51	1.59
4	J	301	A3P	C6-N6	4.38	1.45	1.34
4	B	301	A3P	C6-N6	4.27	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	A3P	P1-O3'	-4.26	1.52	1.59
4	C	301	A3P	C2'-C3'	-4.22	1.43	1.53
4	G	301	A3P	C6-N6	4.20	1.44	1.34
4	G	301	A3P	C2'-C3'	-4.16	1.43	1.53
4	J	301	A3P	C2'-C3'	-4.08	1.44	1.53
4	E	301	A3P	C6-N6	4.00	1.44	1.34
4	I	301	A3P	C6-N6	4.00	1.44	1.34
4	K	301	A3P	C6-N6	3.98	1.44	1.34
4	H	301	A3P	C6-N6	3.97	1.44	1.34
4	A	301	A3P	C6-N6	3.96	1.44	1.34
4	D	301	A3P	P1-O3P	-3.92	1.40	1.54
4	F	301	A3P	P1-O3'	-3.91	1.52	1.59
4	I	301	A3P	P1-O3'	-3.78	1.52	1.59
4	E	301	A3P	P1-O3'	-3.75	1.52	1.59
4	D	301	A3P	P1-O2P	-3.74	1.40	1.54
4	F	301	A3P	C6-N6	3.71	1.43	1.34
4	G	301	A3P	P1-O3'	-3.70	1.53	1.59
4	C	301	A3P	P1-O3'	-3.67	1.53	1.59
4	C	301	A3P	C6-N6	3.65	1.43	1.34
4	L	301	A3P	C6-N6	3.64	1.43	1.34
4	F	301	A3P	C2'-C3'	-3.62	1.45	1.53
4	D	301	A3P	P2-O5P	-3.61	1.41	1.54
4	E	301	A3P	C2'-C3'	-3.60	1.45	1.53
4	L	301	A3P	C2'-C3'	-3.56	1.45	1.53
4	D	301	A3P	C5-C4	3.36	1.45	1.39
4	A	301	A3P	C5-N7	-3.32	1.33	1.39
4	A	301	A3P	C2'-C3'	-3.16	1.46	1.53
4	G	301	A3P	C5-N7	-3.14	1.33	1.39
4	H	301	A3P	P2-O6P	-3.08	1.43	1.54
4	J	301	A3P	C2'-C1'	-3.06	1.43	1.53
4	H	301	A3P	C5-N7	-3.05	1.33	1.39
4	H	301	A3P	P1-O3'	-3.03	1.54	1.59
4	I	301	A3P	O4'-C4'	-2.98	1.38	1.45
4	B	301	A3P	C2'-C3'	-2.96	1.46	1.53
4	I	301	A3P	C2'-C1'	-2.90	1.44	1.53
4	L	301	A3P	C5-N7	-2.88	1.33	1.39
4	A	301	A3P	P1-O3'	-2.86	1.54	1.59
4	E	301	A3P	P2-O5P	-2.84	1.44	1.54
4	D	301	A3P	C8-N9	-2.80	1.32	1.37
4	D	301	A3P	O4'-C4'	-2.79	1.38	1.45
4	K	301	A3P	C5-N7	-2.76	1.34	1.39
4	C	301	A3P	C5-N7	-2.71	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	301	A3P	O4'-C4'	-2.67	1.39	1.45
4	J	301	A3P	O4'-C4'	-2.66	1.39	1.45
4	E	301	A3P	O4'-C4'	-2.64	1.39	1.45
4	G	301	A3P	P2-O5P	-2.63	1.45	1.54
4	K	301	A3P	C3'-C4'	-2.60	1.46	1.52
4	H	301	A3P	O4'-C4'	-2.56	1.39	1.45
4	L	301	A3P	C3'-C4'	-2.54	1.46	1.52
4	A	301	A3P	C1'-N9	2.54	1.53	1.46
4	F	301	A3P	C5-N7	-2.53	1.34	1.39
4	I	301	A3P	P2-O6P	-2.46	1.45	1.54
4	G	301	A3P	C3'-C4'	-2.43	1.46	1.52
4	A	301	A3P	P2-O6P	-2.41	1.45	1.54
4	G	301	A3P	C5'-C4'	-2.40	1.44	1.51
4	D	301	A3P	C4-N9	-2.37	1.32	1.37
4	L	301	A3P	C2'-C1'	-2.36	1.46	1.53
4	G	301	A3P	O4'-C4'	-2.35	1.39	1.45
4	L	301	A3P	O4'-C4'	-2.33	1.39	1.45
4	B	301	A3P	P2-O6P	-2.32	1.46	1.54
4	J	301	A3P	C3'-C4'	-2.32	1.46	1.52
4	D	301	A3P	C5-C6	2.31	1.47	1.41
4	K	301	A3P	C2'-C1'	-2.29	1.46	1.53
4	H	301	A3P	C8-N9	-2.29	1.33	1.37
4	H	301	A3P	C2'-C1'	-2.28	1.46	1.53
4	F	301	A3P	C2'-C1'	-2.28	1.46	1.53
4	B	301	A3P	C2'-C1'	-2.25	1.46	1.53
4	B	301	A3P	P1-O3'	-2.22	1.55	1.59
4	K	301	A3P	C5'-C4'	-2.22	1.44	1.51
4	A	301	A3P	O4'-C4'	-2.20	1.40	1.45
4	B	301	A3P	C5-N7	-2.19	1.35	1.39
4	C	301	A3P	O4'-C4'	-2.18	1.40	1.45
4	E	301	A3P	C8-N7	2.17	1.35	1.31
4	L	301	A3P	P2-O5P	-2.17	1.46	1.54
4	C	301	A3P	P2-O4P	-2.16	1.43	1.50
4	E	301	A3P	C5-N7	-2.15	1.35	1.39
4	E	301	A3P	C5'-C4'	-2.15	1.45	1.51
4	B	301	A3P	O4'-C4'	-2.13	1.40	1.45
4	E	301	A3P	C3'-C4'	-2.11	1.47	1.52
4	B	301	A3P	C5'-C4'	-2.03	1.45	1.51
4	I	301	A3P	C3'-C4'	-2.03	1.47	1.52
4	J	301	A3P	P2-O5'	2.02	1.66	1.60

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	A3P	C5-C4-N3	-7.68	116.14	126.72
4	G	301	A3P	C5-C4-N3	-7.54	116.33	126.72
4	D	301	A3P	C5-C4-N3	-7.03	117.03	126.72
4	A	301	A3P	C2'-C1'-N9	7.00	130.69	113.30
4	F	301	A3P	C5-C4-N3	-6.57	117.68	126.72
4	L	301	A3P	C5-C4-N3	-6.55	117.70	126.72
4	B	301	A3P	C5-C4-N3	-6.52	117.75	126.72
4	C	301	A3P	C5-C4-N3	-6.19	118.20	126.72
4	J	301	A3P	C5-C4-N3	-6.03	118.42	126.72
4	K	301	A3P	C5-C4-N3	-5.94	118.54	126.72
4	E	301	A3P	C5-C4-N3	-5.87	118.63	126.72
4	A	301	A3P	O4'-C1'-N9	5.66	118.95	108.09
4	A	301	A3P	N3-C4-N9	5.59	136.67	127.17
4	D	301	A3P	N3-C4-N9	5.56	136.62	127.17
4	H	301	A3P	C5-C4-N3	-5.41	119.26	126.72
4	G	301	A3P	N3-C4-N9	5.40	136.35	127.17
4	I	301	A3P	N3-C2-N1	-5.23	120.67	128.58
4	F	301	A3P	N3-C4-N9	5.12	135.87	127.17
4	E	301	A3P	N3-C2-N1	-5.11	120.84	128.58
4	K	301	A3P	N3-C4-N9	4.95	135.59	127.17
4	I	301	A3P	C5-C4-N3	-4.81	120.09	126.72
4	C	301	A3P	N3-C2-N1	-4.67	121.51	128.58
4	K	301	A3P	N3-C2-N1	-4.61	121.60	128.58
4	G	301	A3P	N3-C2-N1	-4.58	121.64	128.58
4	H	301	A3P	N3-C2-N1	-4.55	121.70	128.58
4	F	301	A3P	N3-C2-N1	-4.50	121.77	128.58
4	L	301	A3P	N3-C2-N1	-4.46	121.83	128.58
4	A	301	A3P	N3-C2-N1	-4.36	121.98	128.58
4	H	301	A3P	N3-C4-N9	4.35	134.56	127.17
4	B	301	A3P	N3-C2-N1	-4.31	122.06	128.58
4	B	301	A3P	N3-C4-N9	4.29	134.46	127.17
4	I	301	A3P	N3-C4-N9	4.25	134.40	127.17
4	D	301	A3P	C2-N3-C4	4.25	122.20	111.83
4	A	301	A3P	C2-N3-C4	4.22	122.13	111.83
4	I	301	A3P	C4-N9-C8	4.12	110.07	105.74
4	J	301	A3P	N3-C4-N9	4.08	134.11	127.17
4	C	301	A3P	C2-N3-C4	4.08	121.79	111.83
4	F	301	A3P	C2-N3-C4	4.05	121.72	111.83
4	G	301	A3P	C2-N3-C4	4.05	121.72	111.83
4	B	301	A3P	C2-N3-C4	4.00	121.60	111.83
4	L	301	A3P	C2-N3-C4	3.96	121.50	111.83
4	I	301	A3P	N9-C8-N7	-3.95	108.33	113.94
4	D	301	A3P	C4-C5-N7	-3.94	106.07	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	301	A3P	N3-C2-N1	-3.93	122.64	128.58
4	E	301	A3P	C2-N3-C4	3.91	121.39	111.83
4	G	301	A3P	O4'-C1'-C2'	-3.84	98.40	106.62
4	G	301	A3P	C5-N7-C8	3.83	109.46	103.45
4	I	301	A3P	C2-N3-C4	3.81	121.14	111.83
4	C	301	A3P	N3-C4-N9	3.81	133.64	127.17
4	L	301	A3P	N3-C4-N9	3.79	133.62	127.17
4	E	301	A3P	C4-C5-N7	-3.69	106.36	110.58
4	E	301	A3P	N3-C4-N9	3.69	133.44	127.17
4	J	301	A3P	C4-C5-N7	-3.68	106.38	110.58
4	J	301	A3P	C2-N3-C4	3.65	120.74	111.83
4	K	301	A3P	C2-N3-C4	3.58	120.58	111.83
4	L	301	A3P	C4-C5-N7	-3.55	106.53	110.58
4	E	301	A3P	C5-N7-C8	3.54	109.02	103.45
4	L	301	A3P	O4'-C1'-C2'	-3.54	99.04	106.62
4	D	301	A3P	N3-C2-N1	-3.52	123.25	128.58
4	D	301	A3P	C5-N7-C8	3.43	108.84	103.45
4	J	301	A3P	O5P-P2-O5'	3.39	115.51	106.67
4	G	301	A3P	C4-C5-N7	-3.38	106.72	110.58
4	B	301	A3P	C4-C5-N7	-3.38	106.72	110.58
4	A	301	A3P	C5-N7-C8	3.37	108.75	103.45
4	B	301	A3P	O4'-C1'-C2'	-3.36	99.42	106.62
4	B	301	A3P	C5-N7-C8	3.30	108.63	103.45
4	E	301	A3P	O4'-C1'-N9	3.27	114.37	108.09
4	E	301	A3P	N9-C8-N7	-3.26	109.31	113.94
4	H	301	A3P	C2-N3-C4	3.24	119.73	111.83
4	H	301	A3P	N9-C8-N7	-3.20	109.40	113.94
4	L	301	A3P	C5-N7-C8	3.19	108.47	103.45
4	B	301	A3P	C2'-C3'-C4'	-3.13	97.77	103.24
4	B	301	A3P	N9-C8-N7	-3.11	109.53	113.94
4	K	301	A3P	C5-N7-C8	3.10	108.33	103.45
4	C	301	A3P	C4-C5-N7	-3.10	107.04	110.58
4	J	301	A3P	C5-N7-C8	3.10	108.32	103.45
4	F	301	A3P	O5'-C5'-C4'	3.05	119.39	108.99
4	K	301	A3P	N9-C8-N7	-3.05	109.61	113.94
4	B	301	A3P	O4'-C1'-N9	3.05	113.94	108.09
4	F	301	A3P	N9-C8-N7	-3.04	109.63	113.94
4	J	301	A3P	N9-C8-N7	-3.04	109.63	113.94
4	H	301	A3P	O5'-C5'-C4'	2.99	119.16	108.99
4	C	301	A3P	C5-N7-C8	2.99	108.14	103.45
4	H	301	A3P	C5-N7-C8	2.98	108.13	103.45
4	J	301	A3P	O4'-C1'-N9	2.96	113.77	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	A3P	C3'-C2'-C1'	2.95	106.38	99.89
4	L	301	A3P	P1-O3'-C3'	-2.90	115.67	123.43
4	A	301	A3P	C4-C5-N7	-2.89	107.28	110.58
4	I	301	A3P	O6P-P2-O5'	2.81	113.99	106.67
4	G	301	A3P	C3'-C2'-C1'	2.80	106.05	99.89
4	G	301	A3P	C6-C5-C4	2.78	120.97	117.18
4	F	301	A3P	C5-N7-C8	2.73	107.74	103.45
4	L	301	A3P	O5P-P2-O5'	2.71	113.73	106.67
4	G	301	A3P	N9-C8-N7	-2.69	110.12	113.94
4	C	301	A3P	N9-C8-N7	-2.69	110.13	113.94
4	B	301	A3P	O2P-P1-O3'	2.68	116.30	105.85
4	J	301	A3P	O5'-C5'-C4'	2.67	118.09	108.99
4	G	301	A3P	O6P-P2-O5P	2.65	117.73	107.80
4	L	301	A3P	C2'-C1'-N9	2.64	119.87	113.30
4	C	301	A3P	O6P-P2-O5'	2.64	113.54	106.67
4	L	301	A3P	C5-C4-N9	2.63	108.67	105.81
4	A	301	A3P	C6-C5-C4	2.62	120.76	117.18
4	H	301	A3P	C4-N9-C8	2.62	108.49	105.74
4	G	301	A3P	C2'-C3'-C4'	-2.59	98.71	103.24
4	I	301	A3P	C5-N7-C8	2.58	107.50	103.45
4	C	301	A3P	C2'-C1'-N9	2.56	119.65	113.30
4	B	301	A3P	P1-O3'-C3'	2.49	130.07	123.43
4	L	301	A3P	N9-C8-N7	-2.48	110.42	113.94
4	J	301	A3P	O2'-C2'-C3'	2.47	118.10	111.19
4	H	301	A3P	C4-C5-N7	-2.46	107.77	110.58
4	A	301	A3P	C4-N9-C1'	2.45	132.37	126.63
4	E	301	A3P	O3P-P1-O2P	2.45	116.98	107.80
4	G	301	A3P	O2P-P1-O3'	2.44	115.36	105.85
4	A	301	A3P	C1'-N9-C8	-2.42	121.72	127.09
4	J	301	A3P	C4-N9-C8	2.34	108.20	105.74
4	K	301	A3P	C4-N9-C8	2.34	108.19	105.74
4	F	301	A3P	O4'-C1'-C2'	-2.30	101.69	106.62
4	D	301	A3P	O4'-C1'-N9	2.29	112.49	108.09
4	C	301	A3P	O4'-C1'-C2'	-2.28	101.74	106.62
4	K	301	A3P	C4-C5-N7	-2.26	108.00	110.58
4	I	301	A3P	C5-C6-N6	-2.23	117.76	123.29
4	F	301	A3P	C5-C6-N6	-2.21	117.82	123.29
4	A	301	A3P	N9-C8-N7	-2.17	110.86	113.94
4	C	301	A3P	C5-C4-N9	2.16	108.16	105.81
4	E	301	A3P	O2P-P1-O1P	-2.15	102.46	110.83
4	A	301	A3P	P1-O3'-C3'	2.14	129.15	123.43
4	L	301	A3P	O3'-C3'-C4'	-2.14	102.50	110.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	A3P	O2P-P1-O1P	-2.13	102.54	110.83
4	G	301	A3P	P1-O3'-C3'	2.12	129.10	123.43
4	D	301	A3P	C2-N1-C6	2.12	122.21	118.73
4	I	301	A3P	O5'-C5'-C4'	2.10	116.14	108.99
4	A	301	A3P	O4'-C4'-C3'	2.10	109.34	104.92
4	G	301	A3P	C1'-N9-C8	-2.07	122.50	127.09
4	F	301	A3P	C4-N9-C8	2.06	107.90	105.74
4	A	301	A3P	O3P-P1-O1P	-2.05	102.84	110.83
4	F	301	A3P	C4-C5-N7	-2.03	108.26	110.58
4	B	301	A3P	O5'-C5'-C4'	2.00	115.82	108.99

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	A3P	C5'-O5'-P2-O4P
4	A	301	A3P	C5'-O5'-P2-O5P
4	H	301	A3P	C5'-O5'-P2-O4P
4	H	301	A3P	C5'-O5'-P2-O5P
4	H	301	A3P	C5'-O5'-P2-O6P
4	I	301	A3P	C5'-O5'-P2-O4P
4	I	301	A3P	C5'-O5'-P2-O5P
6	F	303	GOL	O1-C1-C2-C3
6	J	304	GOL	O1-C1-C2-C3
4	L	301	A3P	C3'-C4'-C5'-O5'
6	F	303	GOL	O1-C1-C2-O2
4	A	301	A3P	C2'-C3'-O3'-P1
4	F	301	A3P	C3'-C4'-C5'-O5'
4	L	301	A3P	O4'-C4'-C5'-O5'
4	A	301	A3P	C4'-C3'-O3'-P1
4	G	301	A3P	C4'-C3'-O3'-P1
6	J	304	GOL	O1-C1-C2-O2
4	G	301	A3P	C3'-C4'-C5'-O5'
4	D	301	A3P	C5'-O5'-P2-O5P
6	J	304	GOL	C1-C2-C3-O3
4	E	301	A3P	C3'-O3'-P1-O3P
4	D	301	A3P	C4'-C3'-O3'-P1
4	B	301	A3P	C3'-O3'-P1-O1P
6	J	304	GOL	O2-C2-C3-O3
4	F	301	A3P	O4'-C4'-C5'-O5'
4	A	301	A3P	C5'-O5'-P2-O6P
4	J	301	A3P	C5'-O5'-P2-O5P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	303	GOL	C1-C2-C3-O3
4	E	301	A3P	C3'-O3'-P1-O2P
4	C	301	A3P	C2'-C3'-O3'-P1
4	D	301	A3P	C2'-C3'-O3'-P1
4	G	301	A3P	C2'-C3'-O3'-P1

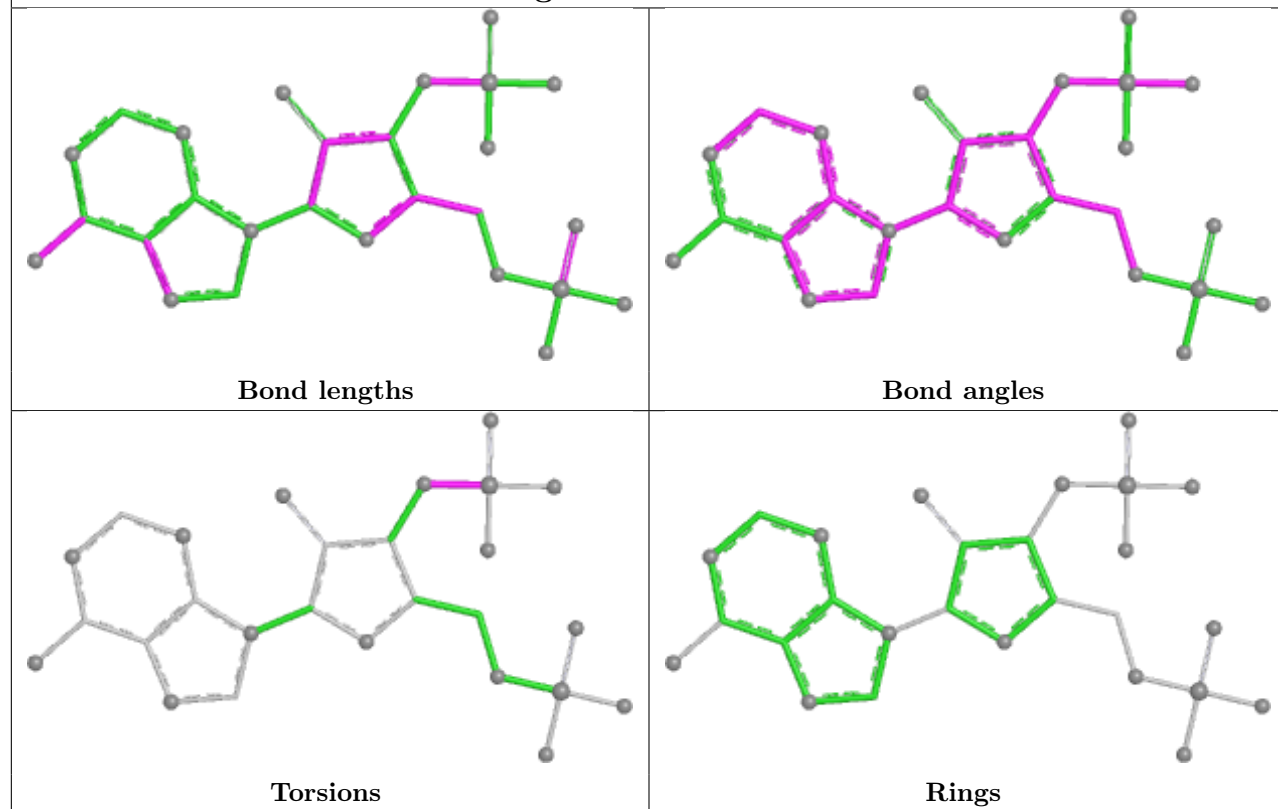
There are no ring outliers.

13 monomers are involved in 120 short contacts:

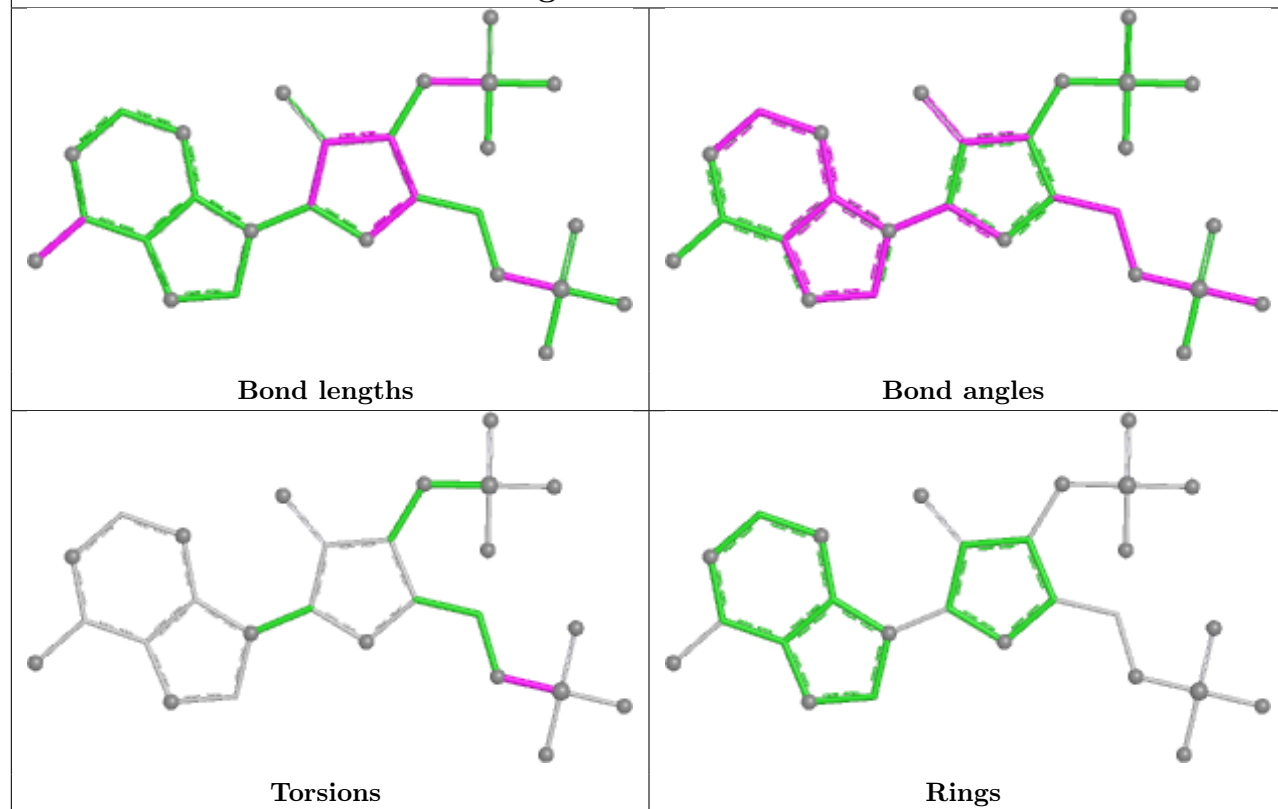
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	A3P	5	0
6	F	303	GOL	2	0
4	J	301	A3P	10	0
4	A	301	A3P	14	0
4	I	301	A3P	3	0
4	D	301	A3P	9	0
4	L	301	A3P	16	0
4	E	301	A3P	8	0
4	H	301	A3P	7	0
4	K	301	A3P	8	0
4	C	301	A3P	5	0
4	F	301	A3P	7	0
4	G	301	A3P	26	0

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.

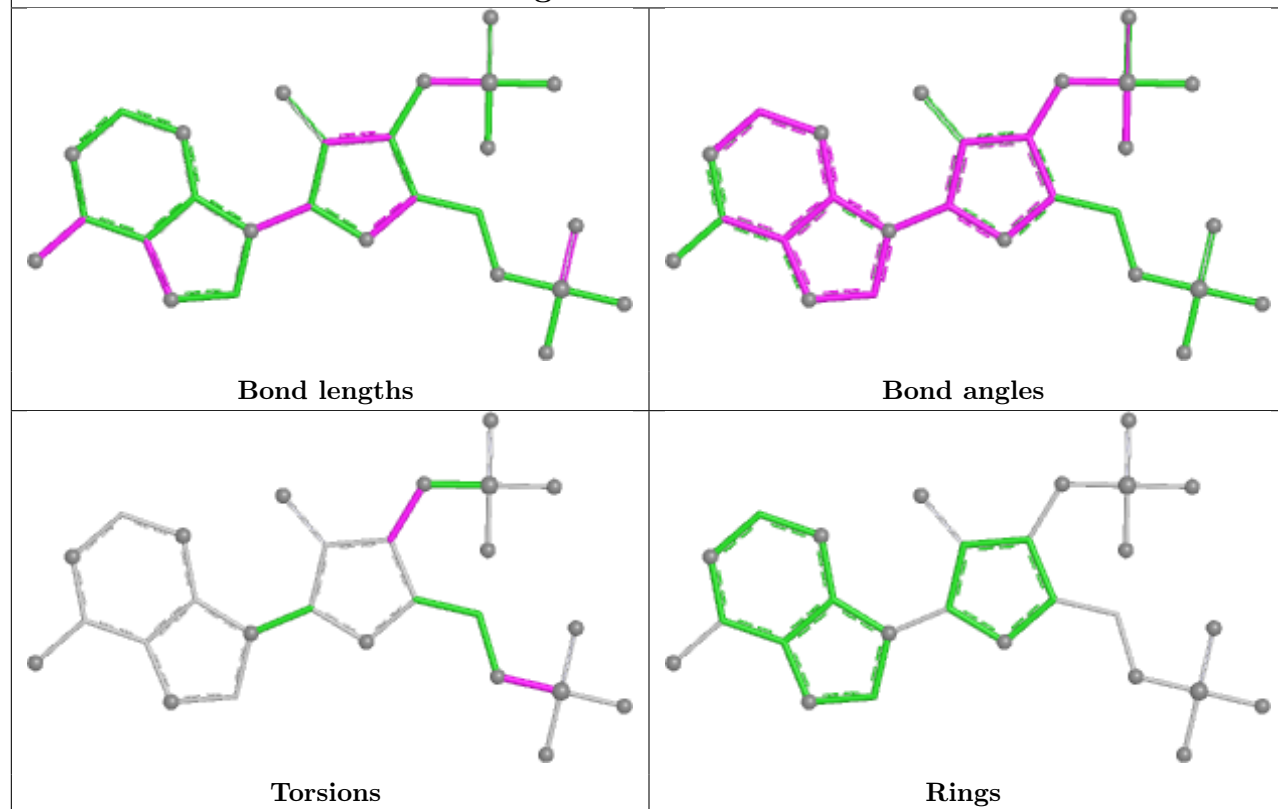
Ligand A3P B 301



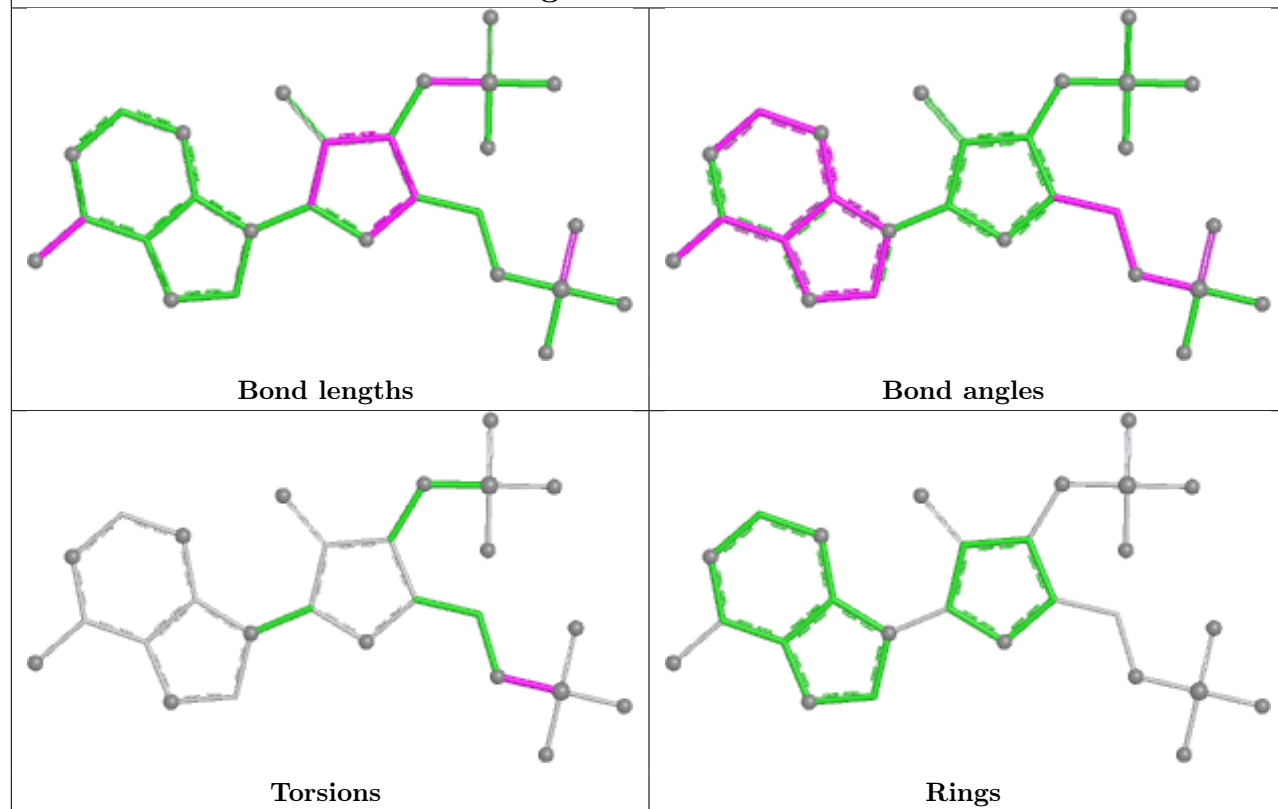
Ligand A3P J 301



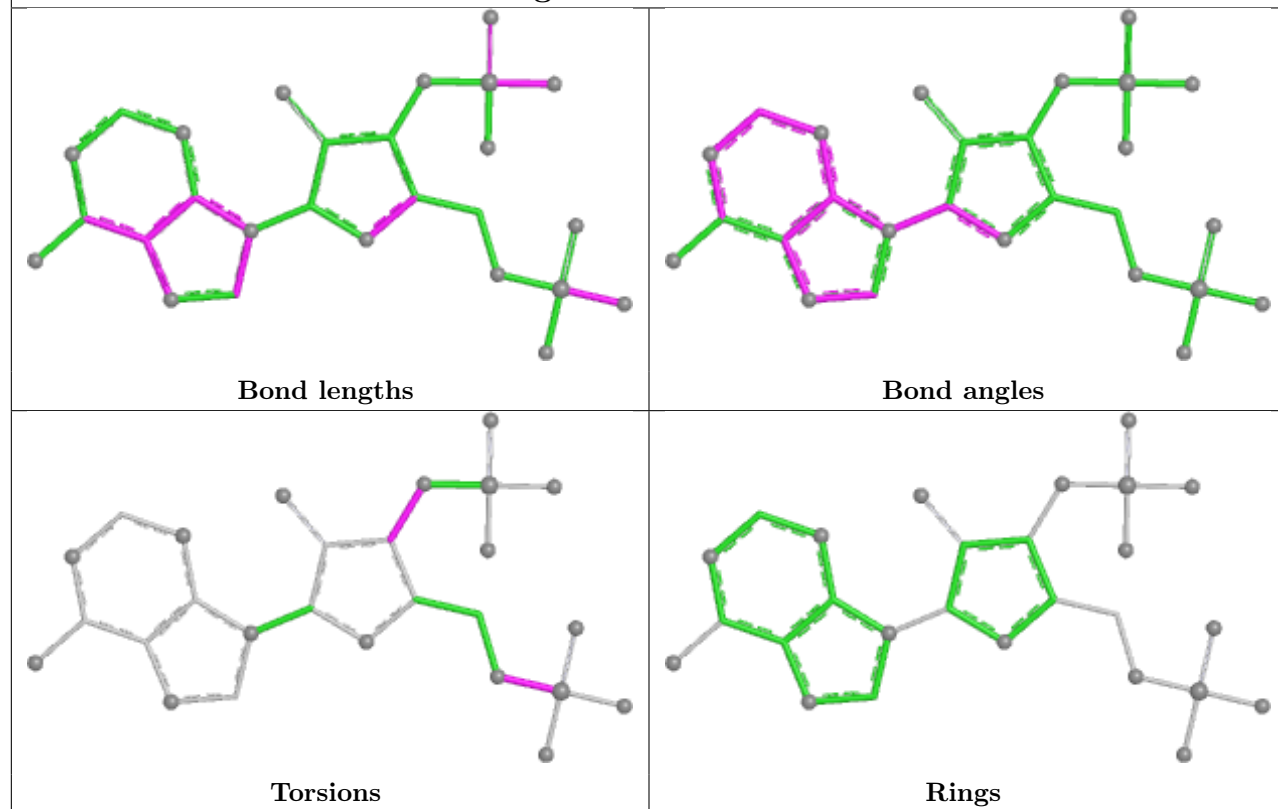
Ligand A3P A 301



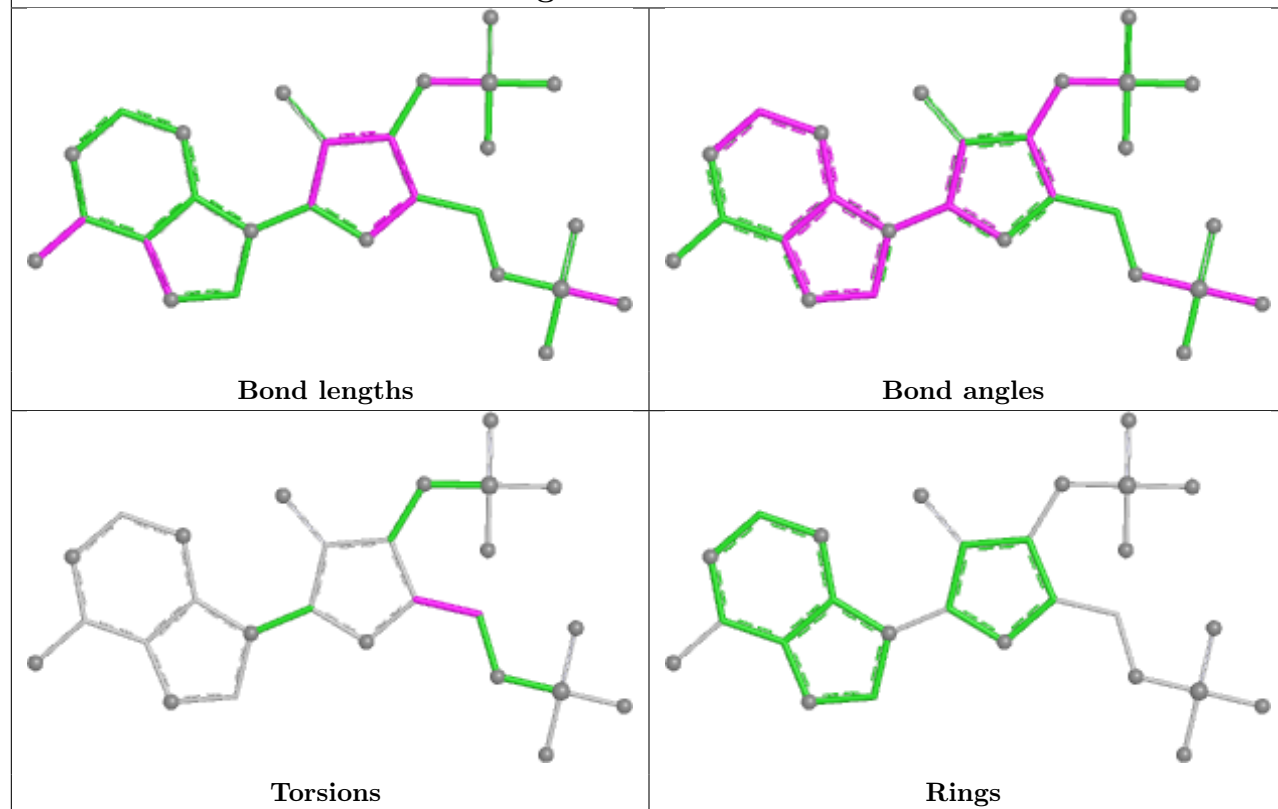
Ligand A3P I 301



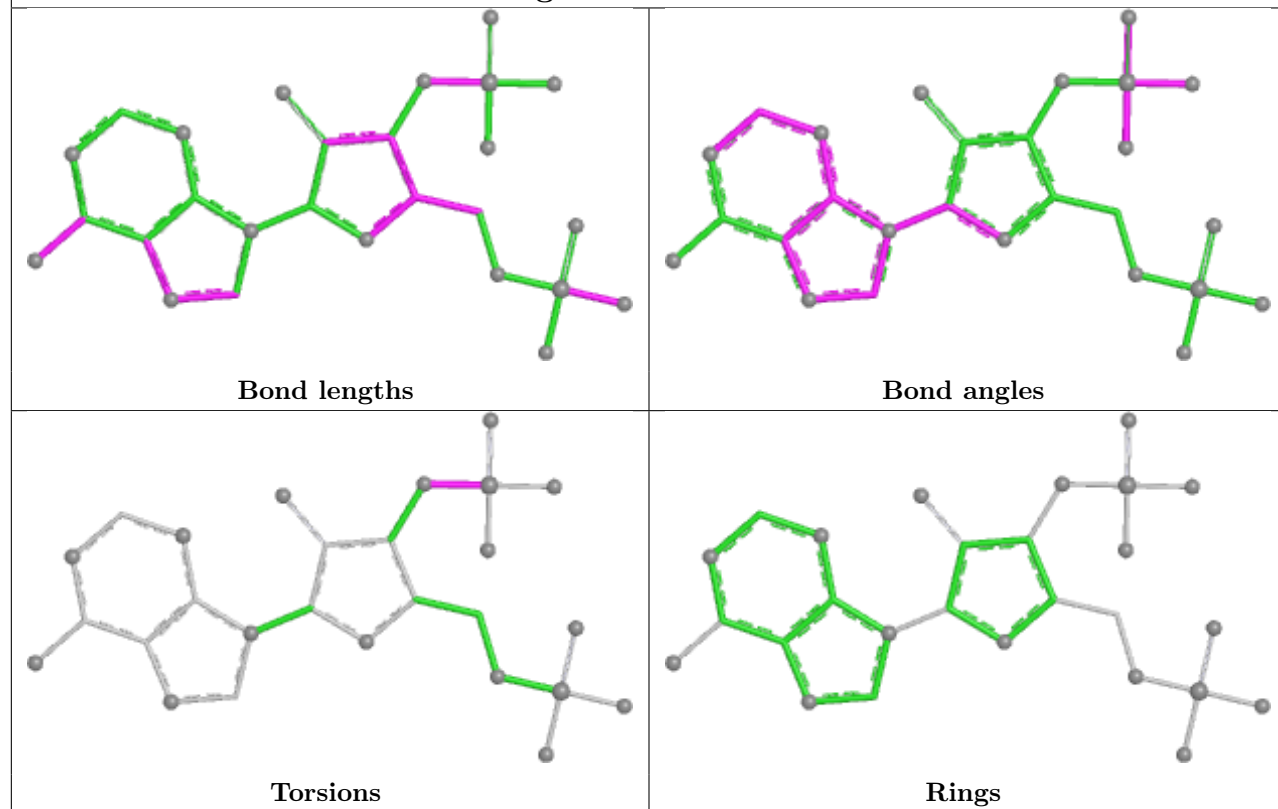
Ligand A3P D 301



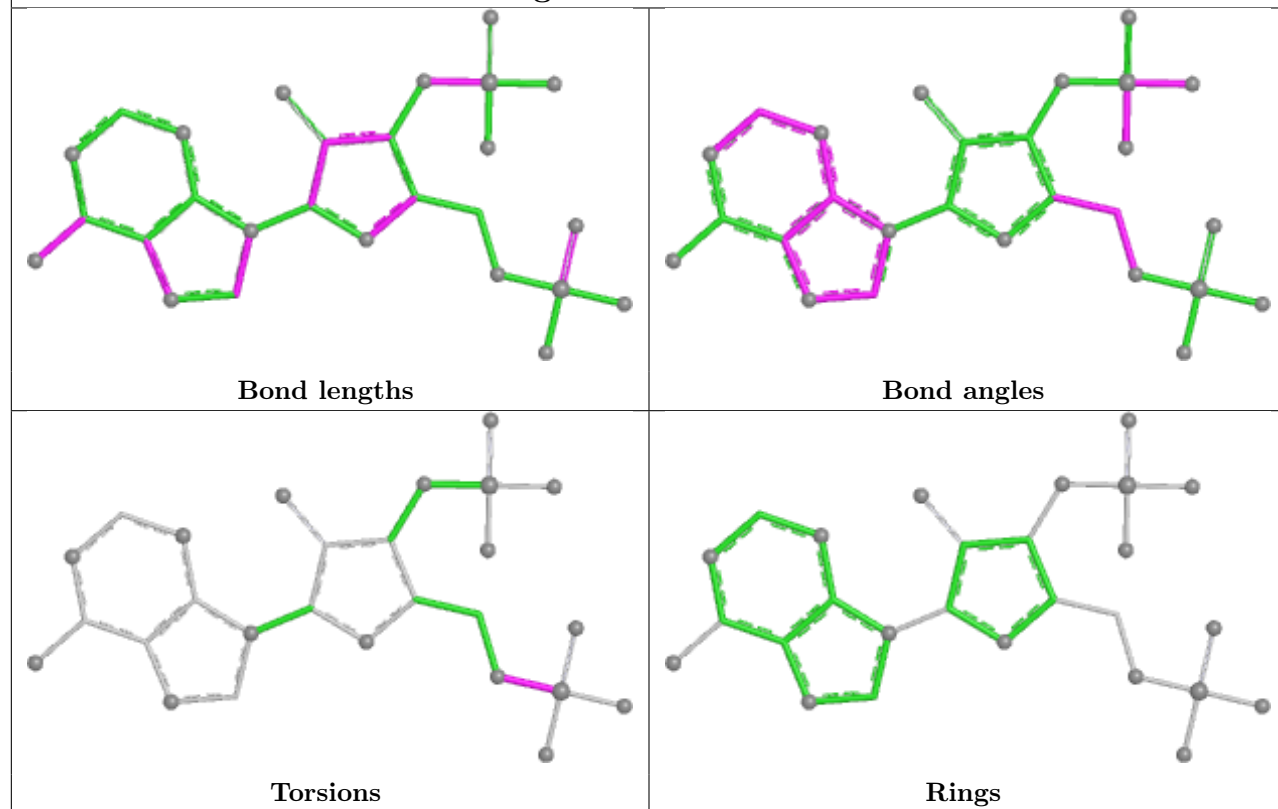
Ligand A3P L 301



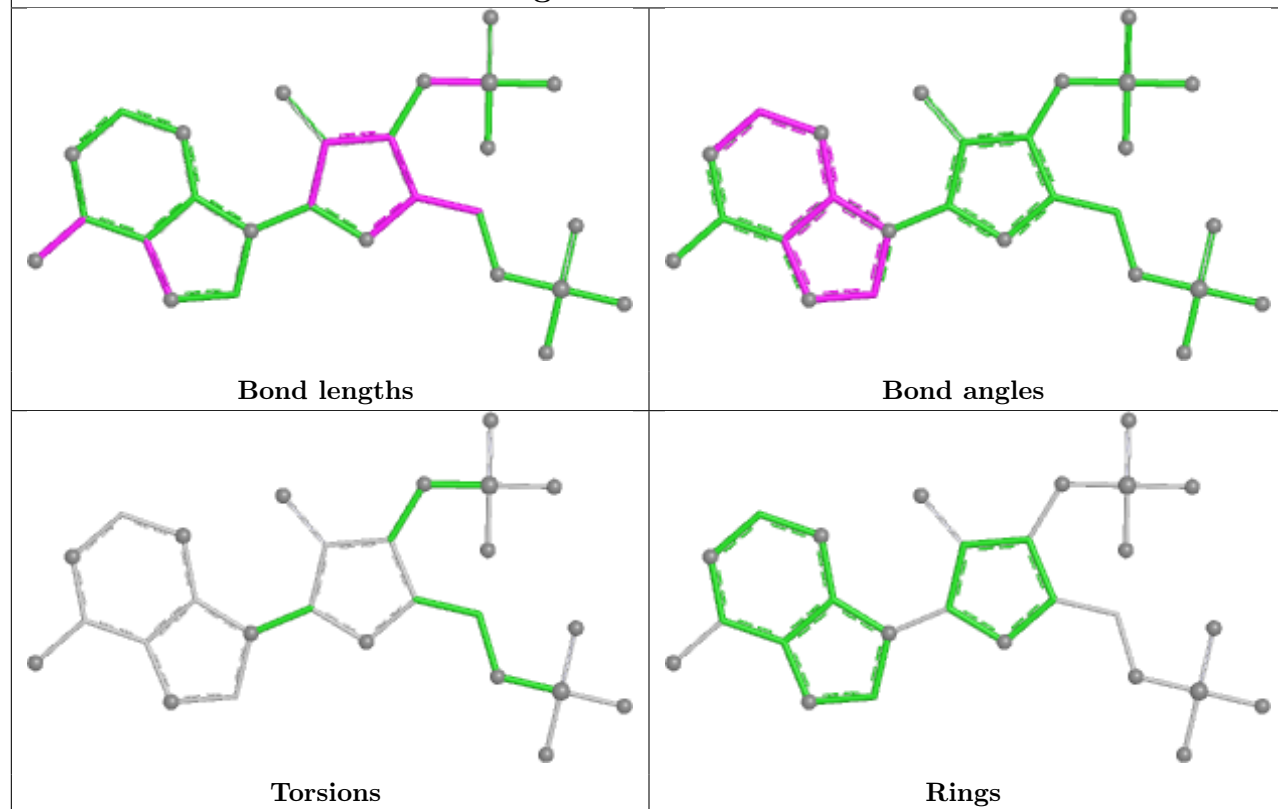
Ligand A3P E 301



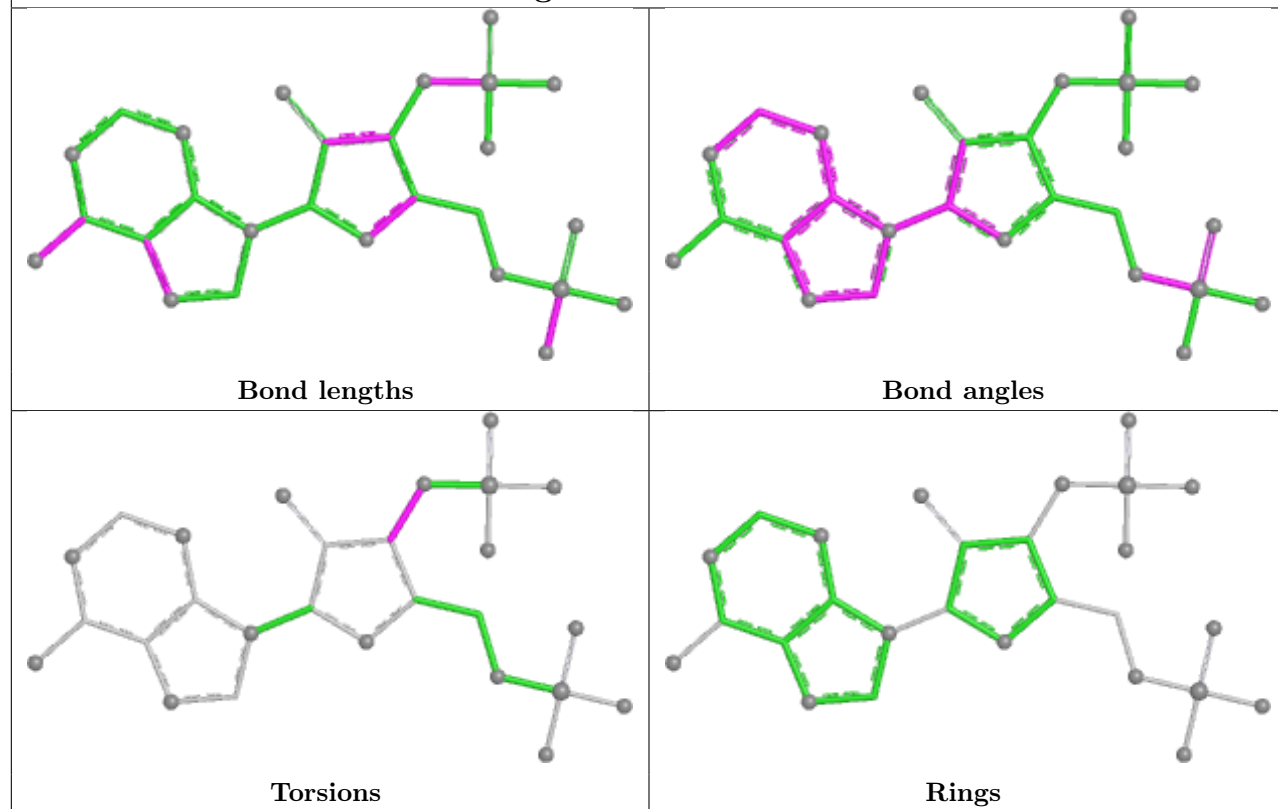
Ligand A3P H 301



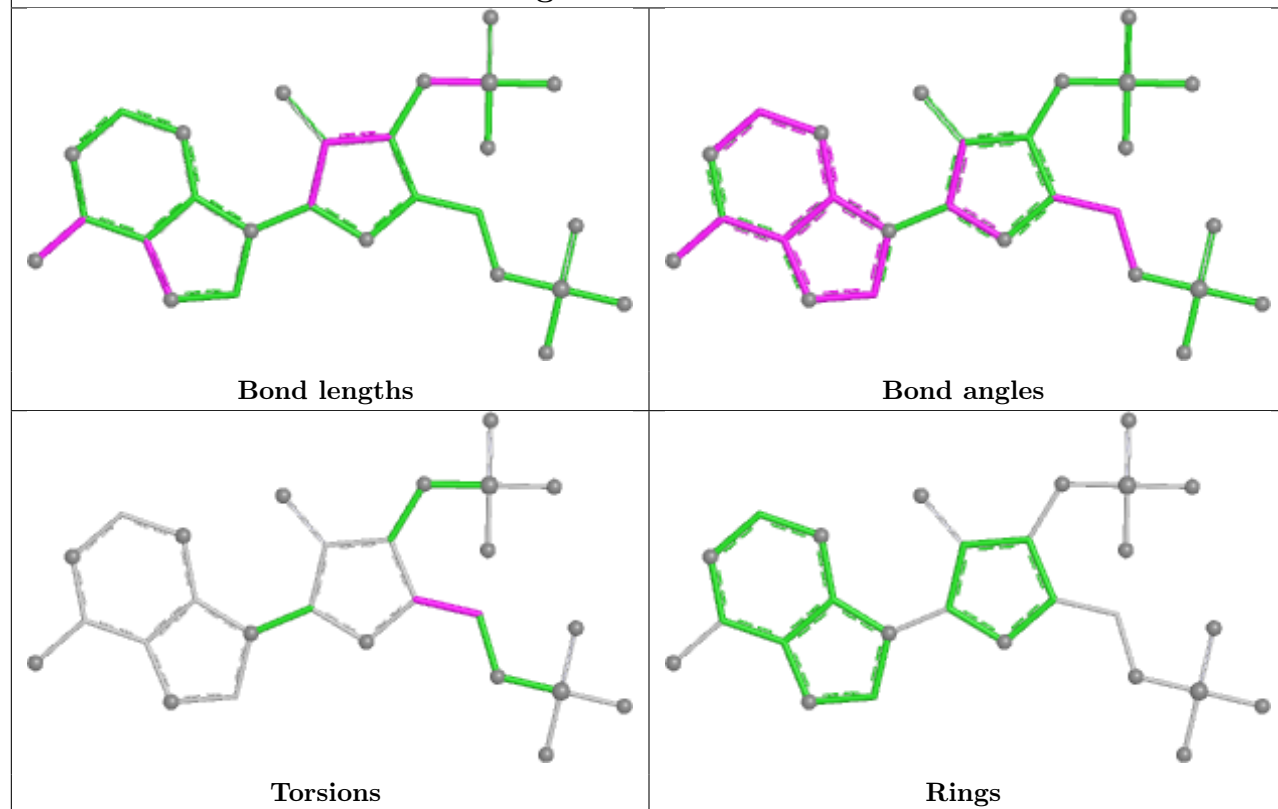
Ligand A3P K 301



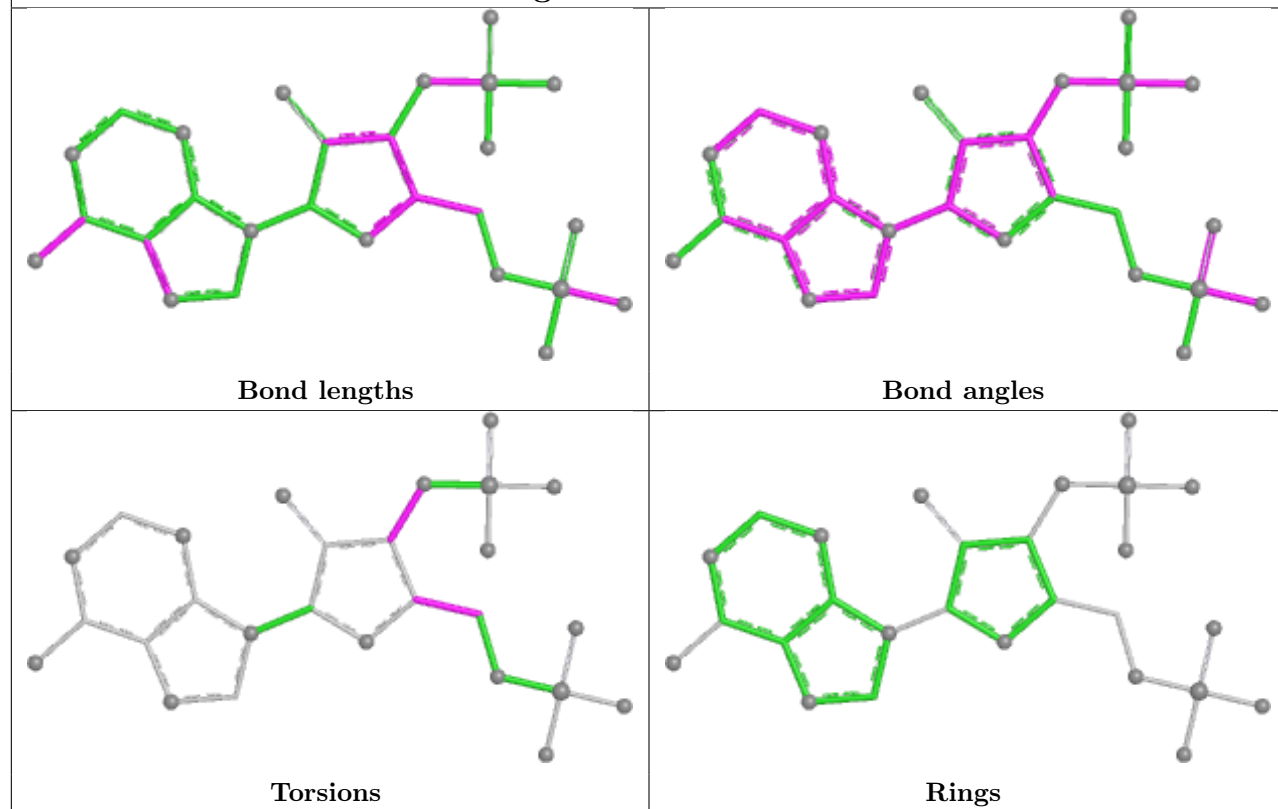
Ligand A3P C 301



Ligand A3P F 301



Ligand A3P G 301



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/283 (99%)	0.63	22 (7%)	19	20	14, 39, 61, 105	1 (0%)
1	B	275/283 (97%)	0.49	13 (4%)	36	38	20, 37, 61, 98	3 (1%)
1	C	282/283 (99%)	0.69	23 (8%)	17	18	18, 41, 66, 107	4 (1%)
1	E	277/283 (97%)	0.52	13 (4%)	36	38	22, 37, 62, 99	1 (0%)
1	I	277/283 (97%)	0.50	16 (5%)	29	30	23, 36, 63, 115	1 (0%)
1	K	281/283 (99%)	0.60	18 (6%)	25	26	15, 38, 62, 107	4 (1%)
1	L	283/283 (100%)	0.74	23 (8%)	18	19	18, 42, 65, 116	5 (1%)
2	D	276/281 (98%)	0.52	22 (7%)	18	19	14, 38, 61, 100	2 (0%)
3	F	279/282 (98%)	0.71	23 (8%)	17	18	25, 41, 65, 99	2 (0%)
3	G	276/282 (97%)	0.64	17 (6%)	26	28	14, 38, 61, 108	2 (0%)
3	H	278/282 (98%)	0.74	18 (6%)	25	26	22, 43, 64, 109	1 (0%)
3	J	274/282 (97%)	0.50	12 (4%)	39	40	18, 37, 61, 104	2 (0%)
All	All	3339/3390 (98%)	0.61	220 (6%)	24	25	14, 39, 64, 116	28 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	227	CYS	7.8
3	H	222	ALA	7.0
3	G	227	CYS	6.8
1	L	223	ALA	6.6
3	G	226	ASN	5.7
1	A	223	ALA	5.3
3	G	222	ALA	5.3
1	C	223	ALA	5.3
1	I	227	CYS	5.2
1	L	66	THR	4.9
2	D	223	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	222	ALA	4.7
3	H	223	ALA	4.7
3	J	229	PRO	4.6
3	F	229	PRO	4.5
1	C	98[A]	GLU	4.5
3	J	223	ALA	4.3
1	I	226	ASN	4.3
1	L	180	GLU	4.3
1	C	222	ALA	4.2
3	J	222	ALA	4.2
1	B	285	ALA	4.2
1	I	223	ALA	4.2
3	F	223	ALA	4.1
1	I	285	ALA	4.1
1	C	285	ALA	3.9
1	L	253	ILE	3.9
3	H	79	PHE	3.7
1	L	49	GLY	3.7
1	K	223	ALA	3.7
3	H	184	LYS	3.6
1	K	215	PHE	3.6
1	K	262[A]	ARG	3.5
1	K	267	LEU	3.5
1	L	225	GLU	3.5
1	K	222	ALA	3.5
1	B	203	ASP	3.5
3	H	237	THR	3.5
3	G	79	PHE	3.4
1	I	229	PRO	3.4
1	B	229	PRO	3.4
1	E	222	ALA	3.3
1	I	201	VAL	3.3
3	H	209	ILE	3.2
1	I	205	GLU	3.2
1	E	223	ALA	3.2
2	D	222	ALA	3.2
1	K	228	ASP	3.2
3	F	226	ASN	3.2
3	F	79	PHE	3.1
1	E	224	LYS	3.1
1	B	223	ALA	3.1
1	L	232	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	285	ALA	3.1
1	K	226	ASN	3.0
1	A	226	ASN	3.0
3	J	285	ALA	3.0
3	J	237	THR	3.0
1	E	229	PRO	3.0
2	D	226	ASN	3.0
3	G	225	GLU	3.0
1	K	98[A]	GLU	2.9
1	C	227	CYS	2.9
3	F	242	LEU	2.9
3	F	138	THR	2.9
1	I	232	VAL	2.9
1	A	138	THR	2.9
3	F	128	TYR	2.9
3	J	224	LYS	2.9
3	F	221	ASN	2.8
1	L	90	ALA	2.8
1	L	50	THR	2.8
1	L	226	ASN	2.8
1	K	190	LEU	2.8
1	A	253	ILE	2.8
1	C	221	ASN	2.8
1	B	225	GLU	2.8
2	D	201	VAL	2.8
1	A	79	PHE	2.7
1	E	194	THR	2.7
3	F	201	VAL	2.7
1	K	233	ILE	2.7
1	I	224	LYS	2.7
3	G	224	LYS	2.7
1	I	228	ASP	2.7
1	B	222	ALA	2.6
1	L	79	PHE	2.6
2	D	231	HIS	2.6
3	F	222	ALA	2.6
1	C	251	ASP	2.6
2	D	87	LYS	2.6
2	D	74	GLY	2.6
1	A	230	ASN	2.6
2	D	224	LYS	2.6
1	K	214	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	284	TYR	2.5
3	H	34	ASP	2.5
3	J	152	ASP	2.5
3	F	206	MET	2.5
1	C	201	VAL	2.5
1	B	128	TYR	2.5
1	K	227	CYS	2.5
1	C	75	ASP	2.5
2	D	203	ASP	2.5
1	C	7	PRO	2.5
1	L	139	GLU	2.5
1	K	242	LEU	2.5
1	C	244	PHE	2.5
1	E	201	VAL	2.5
1	L	243	VAL	2.5
3	G	85	ILE	2.5
2	D	255	TYR	2.5
1	A	51	HIS	2.5
1	L	57	ILE	2.5
2	D	233	ILE	2.5
1	A	228	ASP	2.4
1	C	229	PRO	2.4
3	G	223	ALA	2.4
1	C	182	MET	2.4
1	A	21	MET	2.4
3	G	57	ILE	2.4
1	C	138	THR	2.4
1	C	179	TYR	2.4
1	L	288	ALA	2.4
3	F	230	ASN	2.4
3	H	74	GLY	2.4
3	H	221	ASN	2.4
1	K	209	ILE	2.4
3	F	243	VAL	2.4
3	F	253	ILE	2.4
1	C	184	LYS	2.4
1	L	224	LYS	2.4
3	F	81	GLU	2.3
1	E	228	ASP	2.3
3	H	228	ASP	2.3
1	A	229	PRO	2.3
1	L	229	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	138	THR	2.3
1	L	284	TYR	2.3
1	B	198	GLY	2.3
1	A	203	ASP	2.3
1	E	203	ASP	2.3
1	E	262	ARG	2.3
1	E	286	HIS	2.3
1	I	60	ILE	2.3
1	I	286	HIS	2.3
3	J	138	THR	2.3
3	H	274	ASN	2.3
1	E	285	ALA	2.3
1	A	284	TYR	2.3
2	D	252	TRP	2.3
1	K	211	ARG	2.3
3	H	224	LYS	2.3
3	G	233	ILE	2.3
3	J	60	ILE	2.3
1	C	288	ALA	2.3
3	G	284	TYR	2.3
1	C	232	VAL	2.2
3	F	61	PRO	2.2
3	J	276	ASP	2.2
1	L	242	LEU	2.2
1	B	178	PHE	2.2
3	J	79	PHE	2.2
1	C	241	ASN	2.2
1	A	233	ILE	2.2
1	I	230	ASN	2.2
3	F	85	ILE	2.2
3	G	201	VAL	2.2
1	B	131	ASP	2.2
3	F	250	GLY	2.2
3	G	250	GLY	2.2
1	L	285	ALA	2.2
2	D	285	ALA	2.2
3	G	285	ALA	2.2
1	I	9	LEU	2.2
3	F	82	LEU	2.2
1	L	138	THR	2.2
3	G	237	THR	2.2
3	H	57	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	201	VAL	2.2
3	H	243	VAL	2.2
1	K	287	SER	2.2
2	D	220	SER	2.2
3	F	224	LYS	2.2
3	H	232	VAL	2.1
1	A	221	ASN	2.1
1	E	128	TYR	2.1
1	C	181	GLU	2.1
2	D	24	GLU	2.1
3	H	233	ILE	2.1
1	A	224	LYS	2.1
1	A	194	THR	2.1
1	B	76	ILE	2.1
1	I	82	LEU	2.1
1	K	189	SER	2.1
3	H	284	TYR	2.1
1	K	198	GLY	2.1
2	D	198	GLY	2.1
1	L	248	VAL	2.1
1	C	252	TRP	2.1
1	A	210	ALA	2.1
3	F	225	GLU	2.0
3	F	285	ALA	2.1
3	H	218	MET	2.0
1	A	197	LEU	2.0
3	J	67	LEU	2.0
2	D	227	CYS	2.0
2	D	237	THR	2.0
3	G	184	LYS	2.0
1	C	76	ILE	2.0
2	D	65	ILE	2.0
2	D	85	ILE	2.0
1	A	248	VAL	2.0
2	D	277	VAL	2.0
3	F	126	PHE	2.0
1	A	222	ALA	2.0
1	B	221	ASN	2.0
2	D	240	ARG	2.0
1	E	227	CYS	2.0
1	A	74	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
6	GOL	J	304	6/6	0.63	0.17	42,47,59,67	0
6	GOL	F	303	6/6	0.74	0.12	47,54,66,79	0
5	CA	J	302	1/1	0.81	0.14	58,58,58,58	0
5	CA	L	302	1/1	0.88	0.12	80,80,80,80	0
5	CA	K	303	1/1	0.89	0.10	58,58,58,58	0
4	A3P	L	301	27/27	0.89	0.11	31,44,62,64	0
5	CA	F	302	1/1	0.91	0.10	64,64,64,64	0
4	A3P	D	301	27/27	0.92	0.11	28,40,62,91	0
5	CA	B	303	1/1	0.93	0.12	44,44,44,44	0
5	CA	D	304	1/1	0.95	0.11	58,58,58,58	0
4	A3P	F	301	27/27	0.95	0.08	28,44,53,57	0
5	CA	H	302	1/1	0.95	0.12	49,49,49,49	0
4	A3P	H	301	27/27	0.95	0.09	36,48,63,65	0
4	A3P	I	301	27/27	0.95	0.08	27,37,44,47	0
4	A3P	A	301	27/27	0.95	0.09	28,40,54,60	0
5	CA	A	303	1/1	0.95	0.09	53,53,53,53	0
4	A3P	C	301	27/27	0.95	0.08	33,42,49,54	0
4	A3P	K	301	27/27	0.96	0.08	29,39,52,58	0
5	CA	J	303	1/1	0.96	0.07	63,63,63,63	0
5	CA	K	302	1/1	0.96	0.07	46,46,46,46	0
4	A3P	E	301	27/27	0.96	0.07	28,36,51,67	0
5	CA	A	302	1/1	0.96	0.06	46,46,46,46	0
4	A3P	B	301	27/27	0.96	0.08	20,37,49,53	0
5	CA	I	302	1/1	0.96	0.09	39,39,39,39	0
4	A3P	J	301	27/27	0.97	0.07	24,38,50,55	0
5	CA	E	302	1/1	0.97	0.05	43,43,43,43	0
4	A3P	G	301	27/27	0.97	0.07	20,43,54,63	0

Continued on next page...

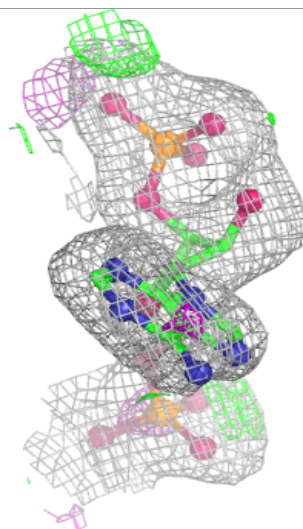
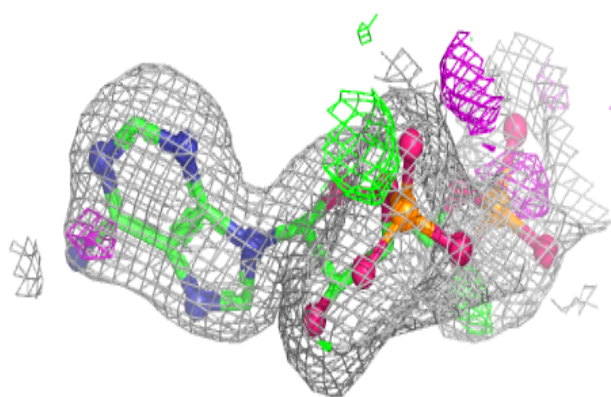
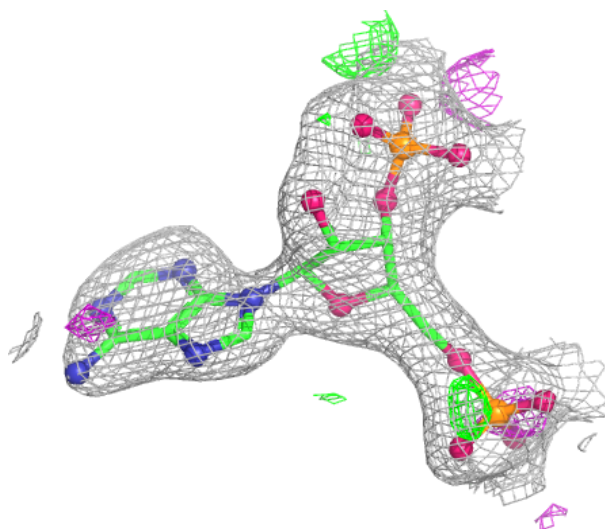
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	G	302	1/1	0.97	0.05	53,53,53,53	0
5	CA	G	303	1/1	0.97	0.05	45,45,45,45	0
5	CA	B	304	1/1	0.97	0.06	69,69,69,69	0
5	CA	D	302	1/1	0.97	0.05	47,47,47,47	0
5	CA	C	302	1/1	0.98	0.06	44,44,44,44	0
5	CA	D	303	1/1	0.98	0.04	43,43,43,43	0
5	CA	B	302	1/1	0.99	0.06	40,40,40,40	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.

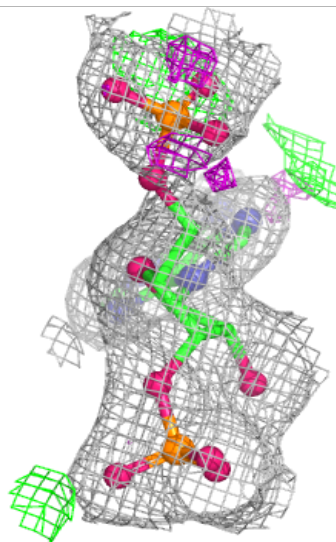
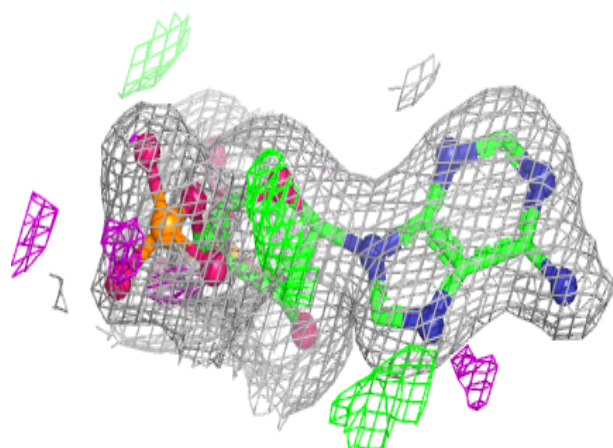
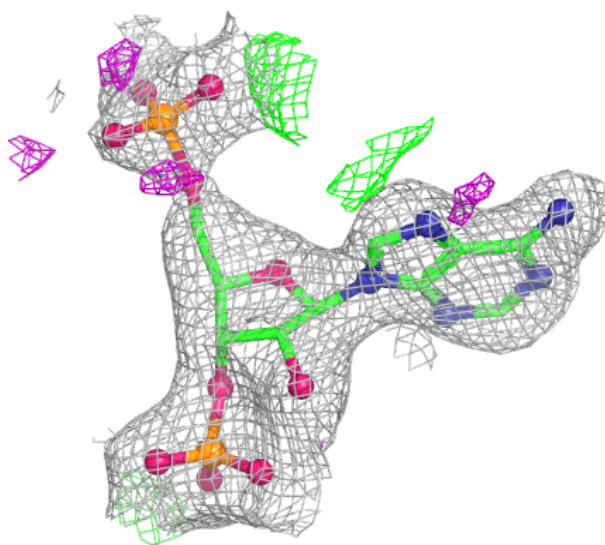
Electron density around A3P L 301:

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



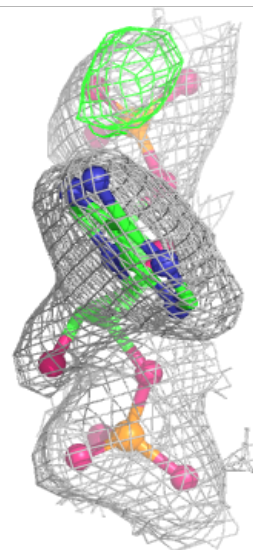
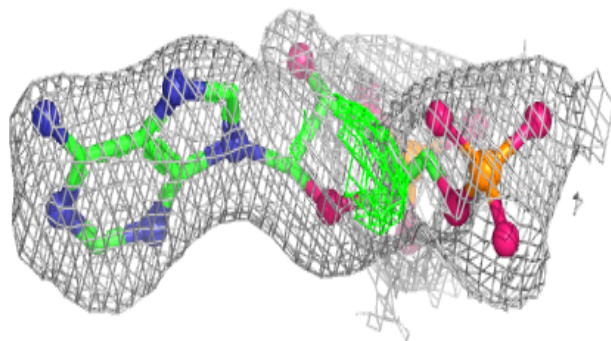
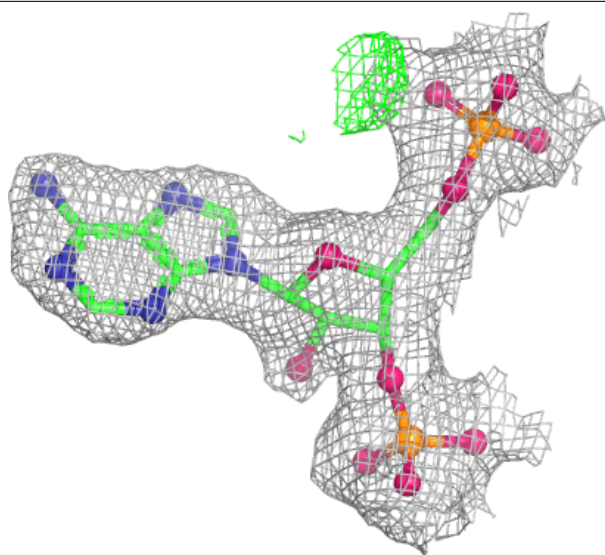
Electron density around A3P D 301:

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



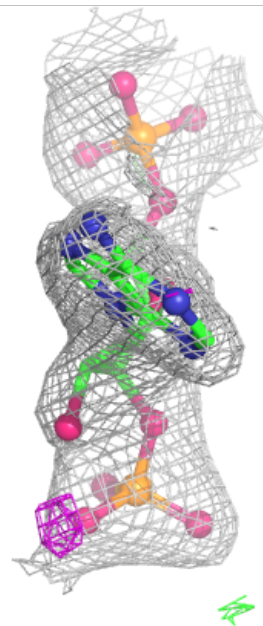
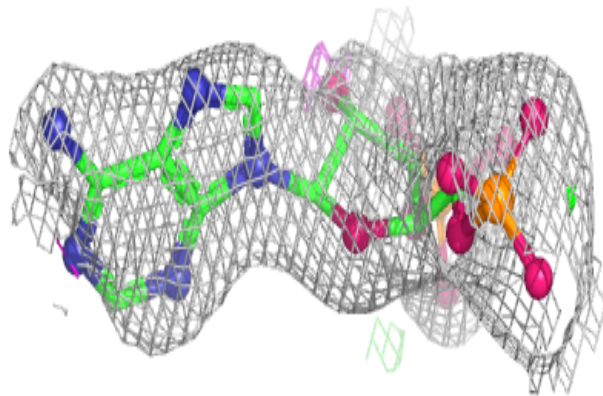
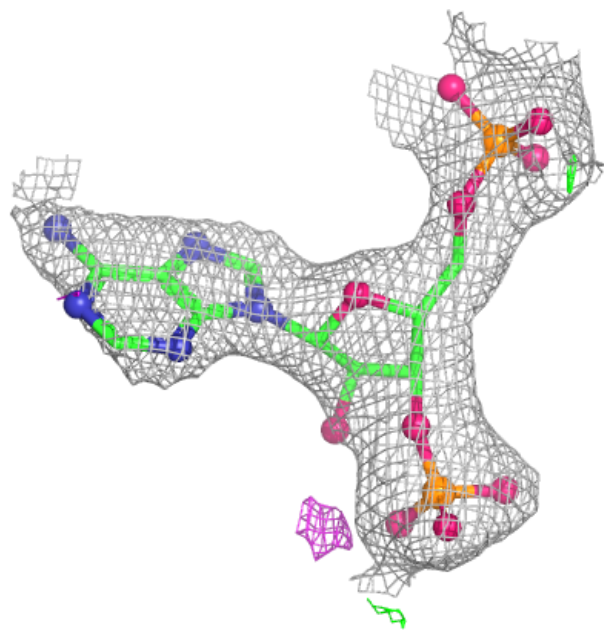
Electron density around A3P F 301:

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



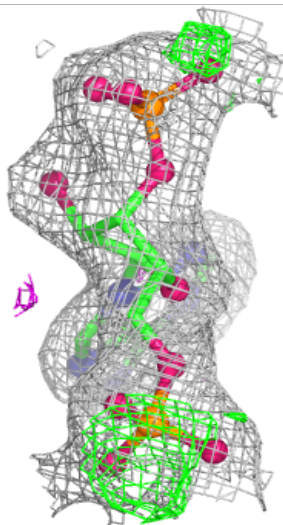
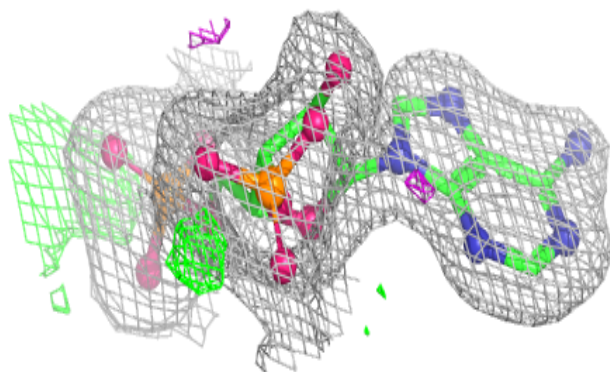
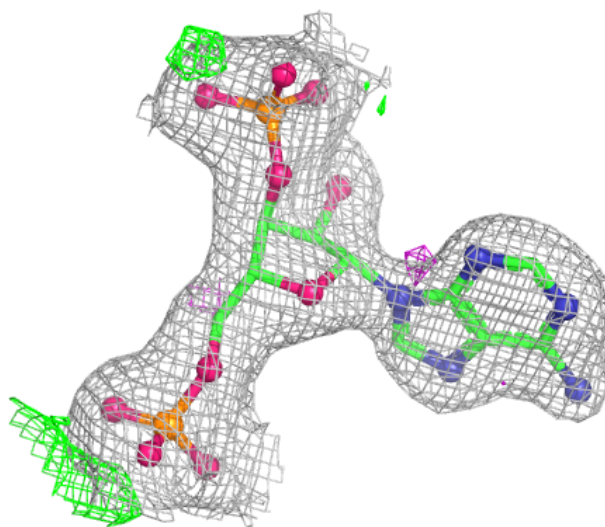
Electron density around A3P H 301:

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



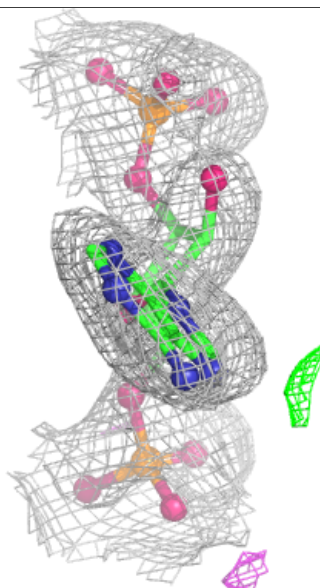
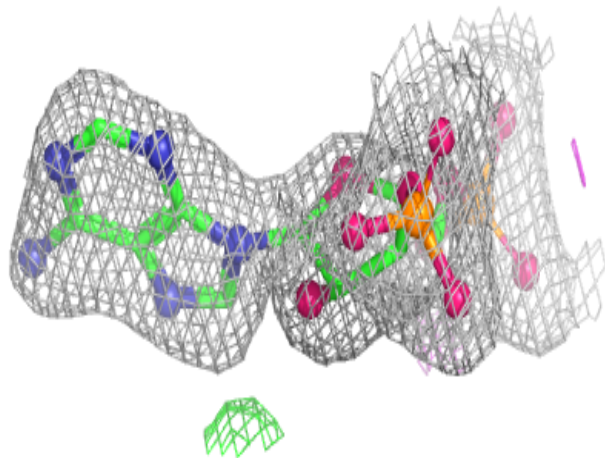
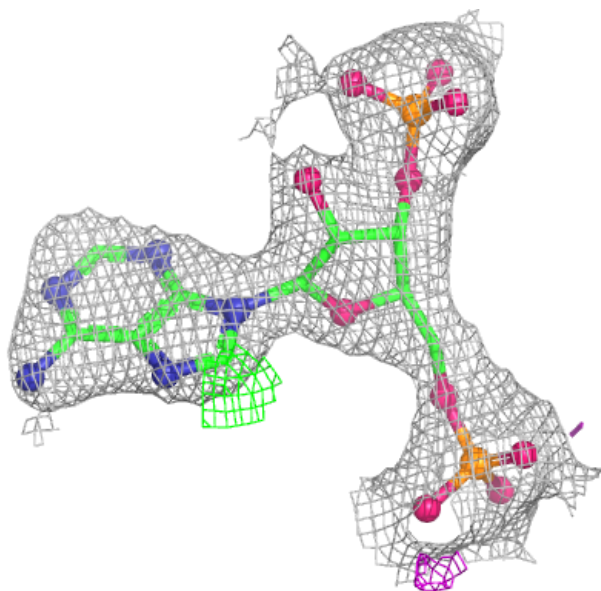
Electron density around A3P I 301:

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



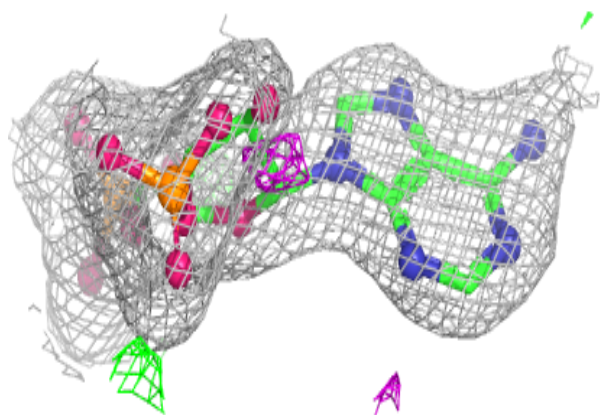
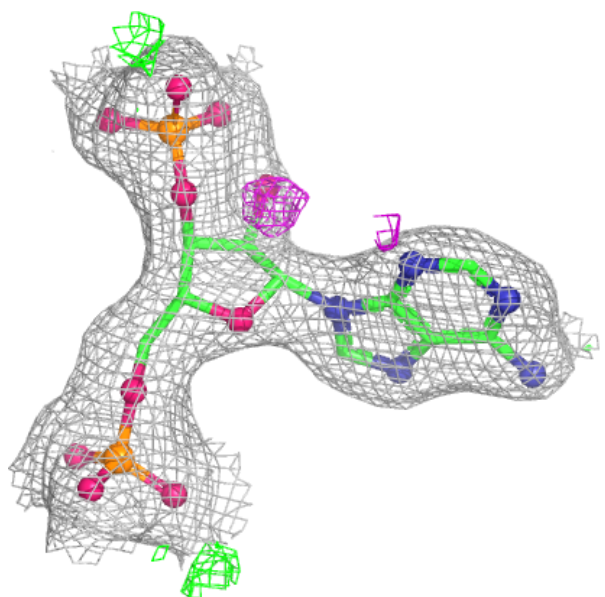
Electron density around A3P A 301:

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



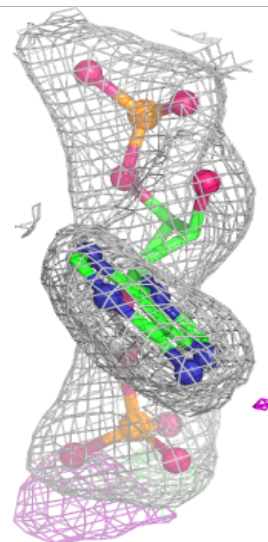
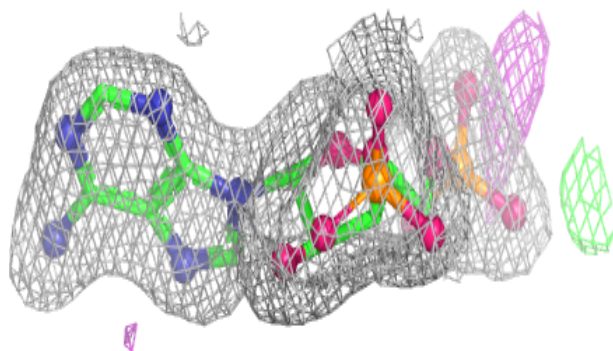
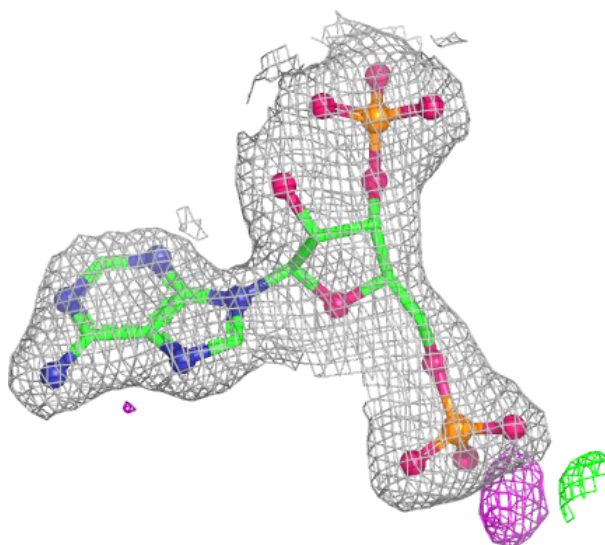
Electron density around A3P C 301:

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



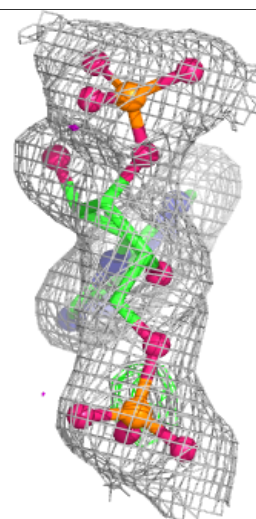
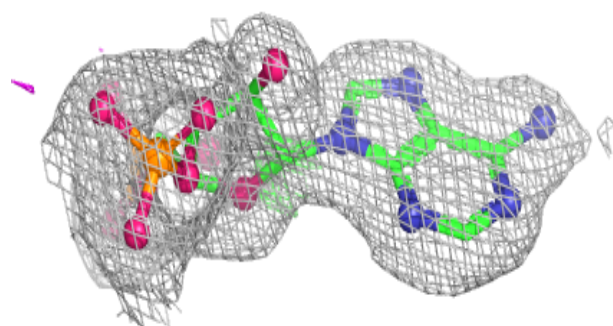
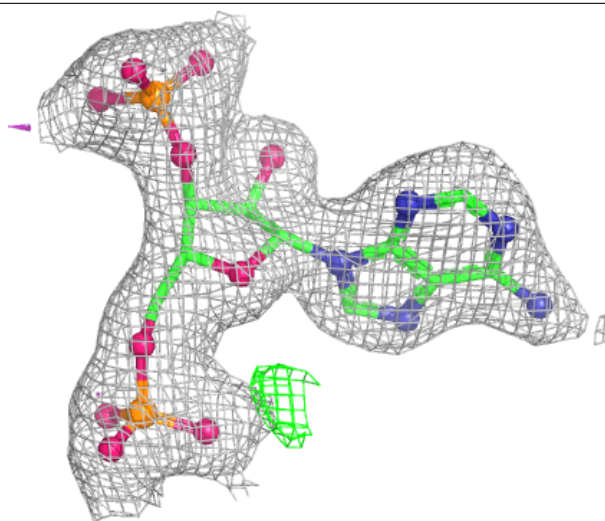
Electron density around A3P K 301:

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



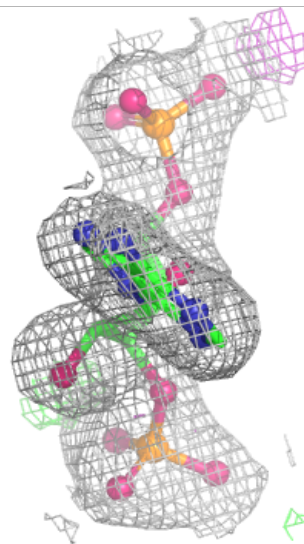
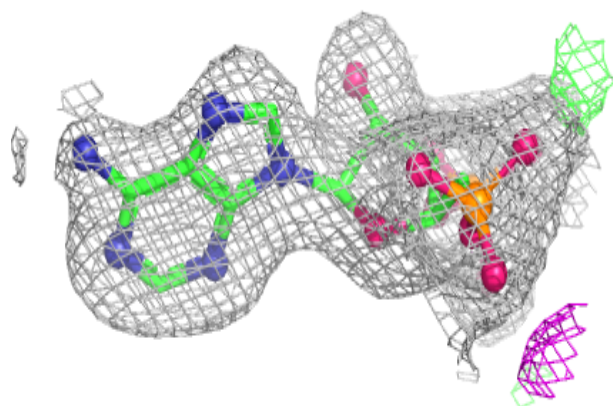
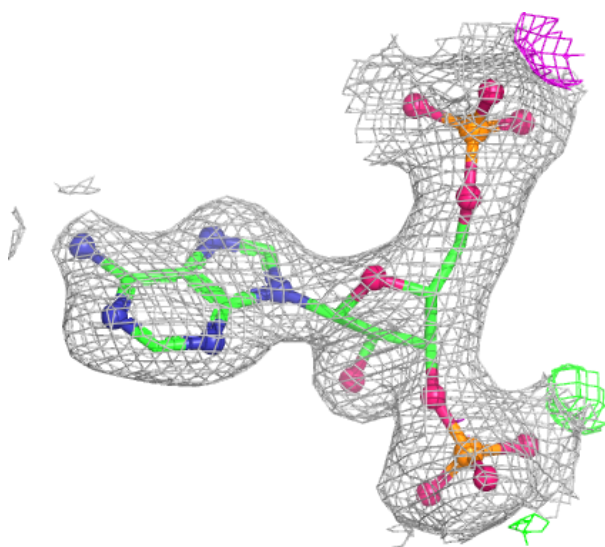
Electron density around A3P E 301:

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



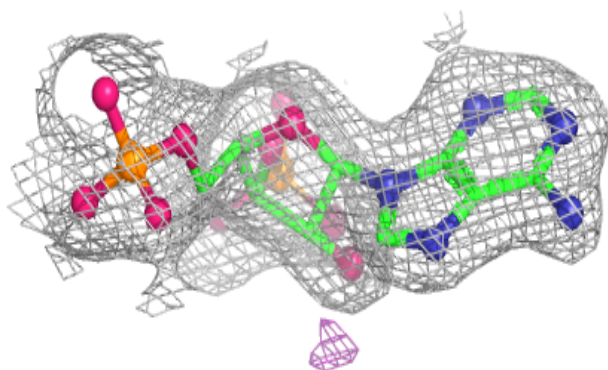
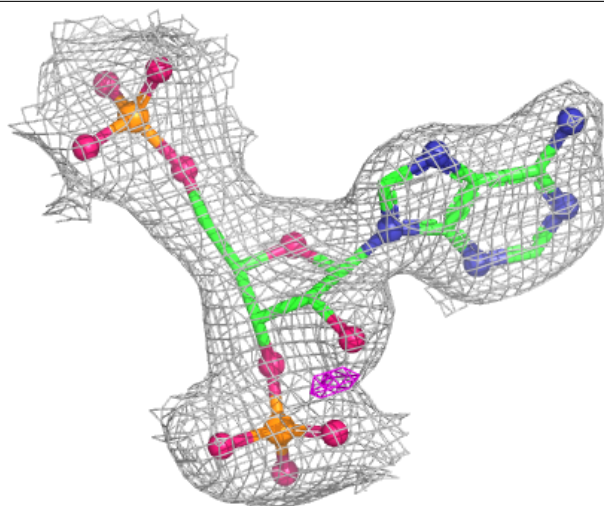
Electron density around A3P B 301:

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



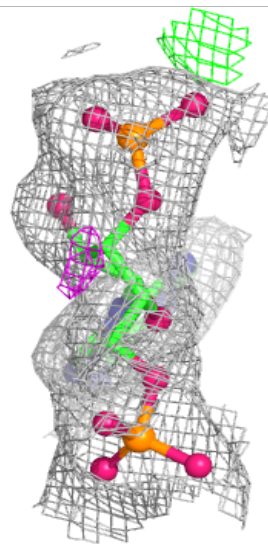
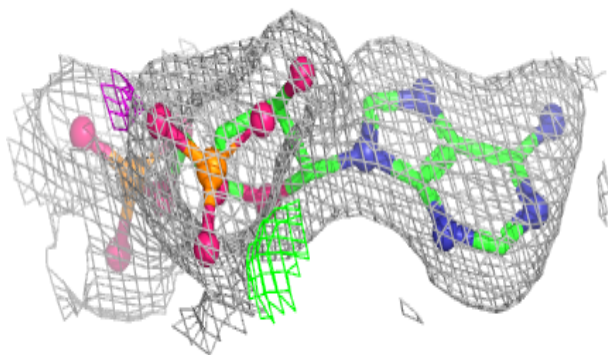
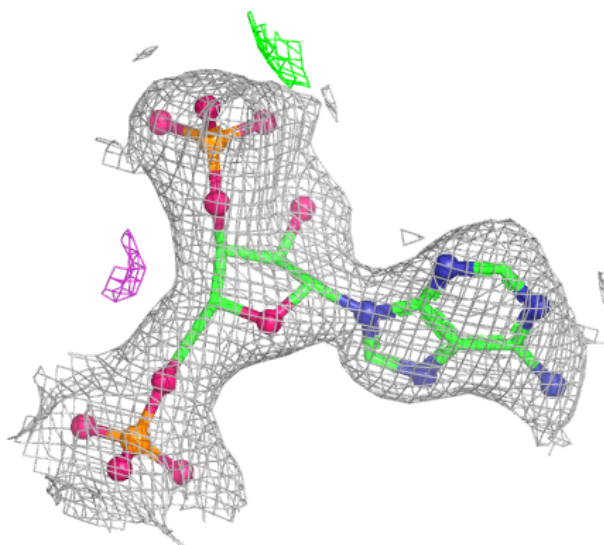
Electron density around A3P J 301:

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



Electron density around A3P G 301:

$2mF_o-DF_c$ (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.