



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 PM UTC

PDB ID : 4J7C / pdb_00004j7c
Title : KtrAB potassium transporter from *Bacillus subtilis*
Authors : Vieira-Pires, R.S.; Morais-Cabral, J.H.
Deposited on : 2013-02-13
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

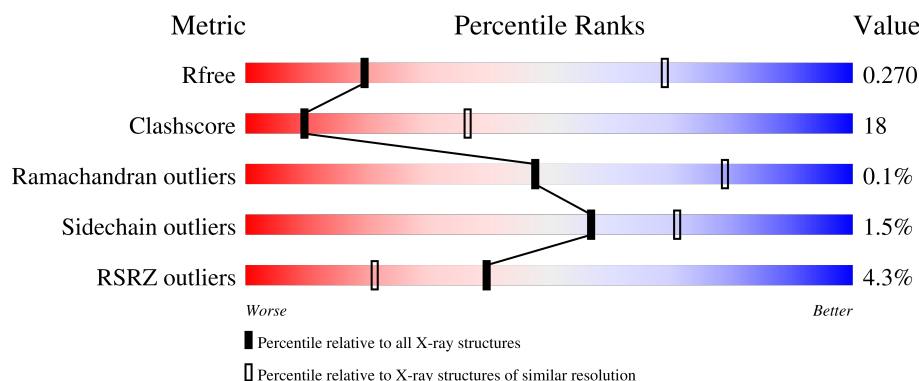
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	222	10% 77% 20% .
1	B	222	5% 81% 16% ..
1	C	222	5% 75% 21% ..
1	D	222	5% 81% 16% ..
1	E	222	5% 74% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	222	5% 80% 17% ••
1	G	222	8% 75% 21% •
1	H	222	2% 77% 19% ••
2	I	465	2% 60% 31% •8%
2	J	465	3% 62% 29% •8%
2	K	465	4% 58% 33% •8%
2	L	465	2% 60% 30% •8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26996 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 Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1699	1079	292	321	7			
1	B	217	Total	C	N	O	S	0	0	0
			1707	1083	294	323	7			
1	C	216	Total	C	N	O	S	0	0	0
			1699	1079	292	321	7			
1	D	217	Total	C	N	O	S	0	0	0
			1707	1083	294	323	7			
1	E	216	Total	C	N	O	S	0	0	0
			1699	1079	292	321	7			
1	F	217	Total	C	N	O	S	0	0	0
			1707	1083	294	323	7			
1	G	216	Total	C	N	O	S	0	0	0
			1699	1079	292	321	7			
1	H	217	Total	C	N	O	S	0	0	0
			1707	1083	294	323	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	VAL	CYS	engineered mutation	UNP O32080
B	22	VAL	CYS	engineered mutation	UNP O32080
C	22	VAL	CYS	engineered mutation	UNP O32080
D	22	VAL	CYS	engineered mutation	UNP O32080
E	22	VAL	CYS	engineered mutation	UNP O32080
F	22	VAL	CYS	engineered mutation	UNP O32080
G	22	VAL	CYS	engineered mutation	UNP O32080
H	22	VAL	CYS	engineered mutation	UNP O32080

- Molecule 2 is a protein called Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	429	Total	C	N	O	S	0	0	0
			3280	2188	510	567	15			
2	J	429	Total	C	N	O	S	0	0	0
			3280	2188	510	567	15			
2	K	429	Total	C	N	O	S	0	0	0
			3280	2188	510	567	15			
2	L	429	Total	C	N	O	S	0	0	0
			3280	2188	510	567	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-19	MET	-	expression tag	UNP O32081
I	-18	GLY	-	expression tag	UNP O32081
I	-17	SER	-	expression tag	UNP O32081
I	-16	SER	-	expression tag	UNP O32081
I	-15	HIS	-	expression tag	UNP O32081
I	-14	HIS	-	expression tag	UNP O32081
I	-13	HIS	-	expression tag	UNP O32081
I	-12	HIS	-	expression tag	UNP O32081
I	-11	HIS	-	expression tag	UNP O32081
I	-10	HIS	-	expression tag	UNP O32081
I	-9	SER	-	expression tag	UNP O32081
I	-8	SER	-	expression tag	UNP O32081
I	-7	GLY	-	expression tag	UNP O32081
I	-6	LEU	-	expression tag	UNP O32081
I	-5	VAL	-	expression tag	UNP O32081
I	-4	PRO	-	expression tag	UNP O32081
I	-3	ARG	-	expression tag	UNP O32081
I	-2	GLY	-	expression tag	UNP O32081
I	-1	SER	-	expression tag	UNP O32081
I	0	HIS	-	expression tag	UNP O32081
J	-19	MET	-	expression tag	UNP O32081
J	-18	GLY	-	expression tag	UNP O32081
J	-17	SER	-	expression tag	UNP O32081
J	-16	SER	-	expression tag	UNP O32081
J	-15	HIS	-	expression tag	UNP O32081
J	-14	HIS	-	expression tag	UNP O32081
J	-13	HIS	-	expression tag	UNP O32081
J	-12	HIS	-	expression tag	UNP O32081
J	-11	HIS	-	expression tag	UNP O32081
J	-10	HIS	-	expression tag	UNP O32081
J	-9	SER	-	expression tag	UNP O32081

Continued on next page...

Continued from previous page...

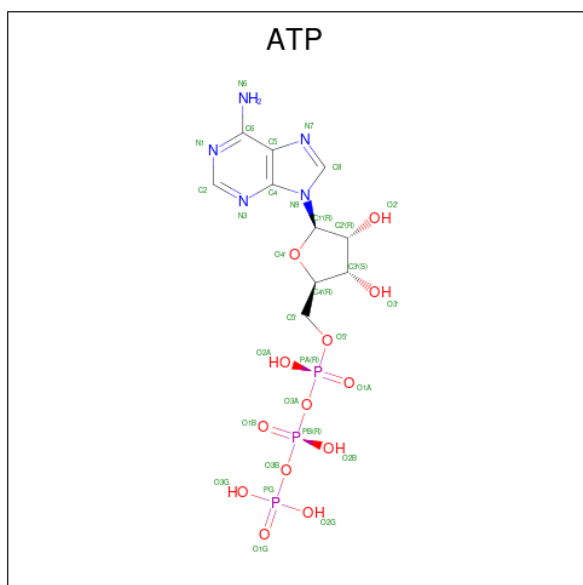
Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	SER	-	expression tag	UNP O32081
J	-7	GLY	-	expression tag	UNP O32081
J	-6	LEU	-	expression tag	UNP O32081
J	-5	VAL	-	expression tag	UNP O32081
J	-4	PRO	-	expression tag	UNP O32081
J	-3	ARG	-	expression tag	UNP O32081
J	-2	GLY	-	expression tag	UNP O32081
J	-1	SER	-	expression tag	UNP O32081
J	0	HIS	-	expression tag	UNP O32081
K	-19	MET	-	expression tag	UNP O32081
K	-18	GLY	-	expression tag	UNP O32081
K	-17	SER	-	expression tag	UNP O32081
K	-16	SER	-	expression tag	UNP O32081
K	-15	HIS	-	expression tag	UNP O32081
K	-14	HIS	-	expression tag	UNP O32081
K	-13	HIS	-	expression tag	UNP O32081
K	-12	HIS	-	expression tag	UNP O32081
K	-11	HIS	-	expression tag	UNP O32081
K	-10	HIS	-	expression tag	UNP O32081
K	-9	SER	-	expression tag	UNP O32081
K	-8	SER	-	expression tag	UNP O32081
K	-7	GLY	-	expression tag	UNP O32081
K	-6	LEU	-	expression tag	UNP O32081
K	-5	VAL	-	expression tag	UNP O32081
K	-4	PRO	-	expression tag	UNP O32081
K	-3	ARG	-	expression tag	UNP O32081
K	-2	GLY	-	expression tag	UNP O32081
K	-1	SER	-	expression tag	UNP O32081
K	0	HIS	-	expression tag	UNP O32081
L	-19	MET	-	expression tag	UNP O32081
L	-18	GLY	-	expression tag	UNP O32081
L	-17	SER	-	expression tag	UNP O32081
L	-16	SER	-	expression tag	UNP O32081
L	-15	HIS	-	expression tag	UNP O32081
L	-14	HIS	-	expression tag	UNP O32081
L	-13	HIS	-	expression tag	UNP O32081
L	-12	HIS	-	expression tag	UNP O32081
L	-11	HIS	-	expression tag	UNP O32081
L	-10	HIS	-	expression tag	UNP O32081
L	-9	SER	-	expression tag	UNP O32081
L	-8	SER	-	expression tag	UNP O32081
L	-7	GLY	-	expression tag	UNP O32081

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	LEU	-	expression tag	UNP O32081
L	-5	VAL	-	expression tag	UNP O32081
L	-4	PRO	-	expression tag	UNP O32081
L	-3	ARG	-	expression tag	UNP O32081
L	-2	GLY	-	expression tag	UNP O32081
L	-1	SER	-	expression tag	UNP O32081
L	0	HIS	-	expression tag	UNP O32081

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



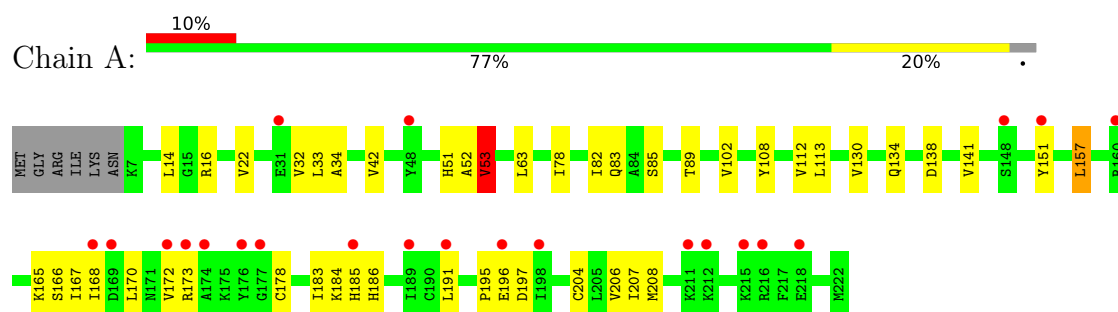
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total 1	K 1	0	0
4	J	1	Total 1	K 1	0	0
4	K	1	Total 1	K 1	0	0
4	L	1	Total 1	K 1	0	0

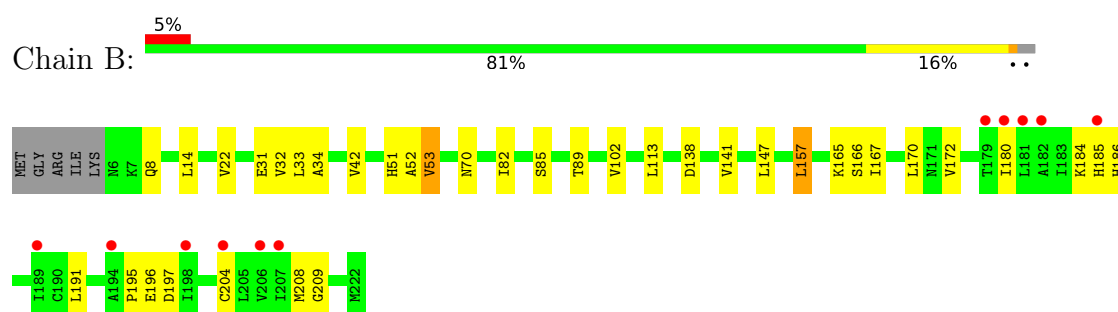
3 Residue-property plots

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.

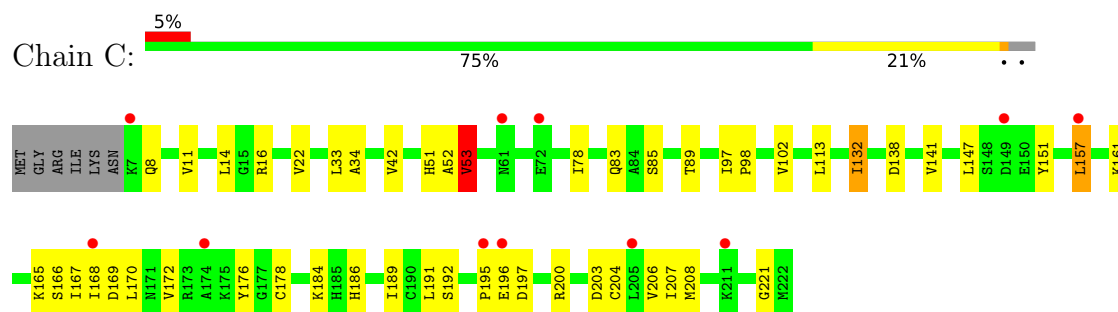
- Molecule 1: Ktr system potassium uptake protein A



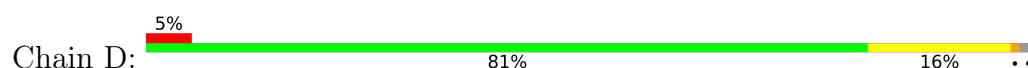
- Molecule 1: Ktr system potassium uptake protein A

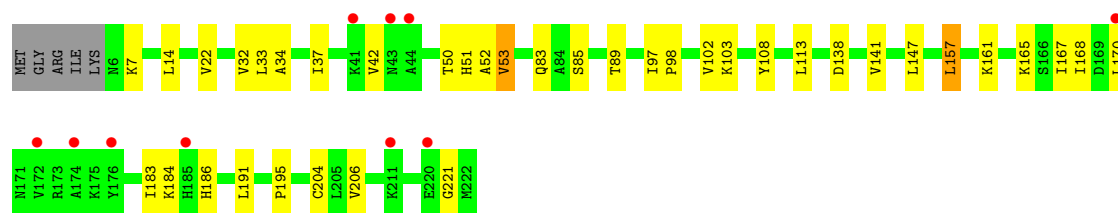


- Molecule 1: Ktr system potassium uptake protein A

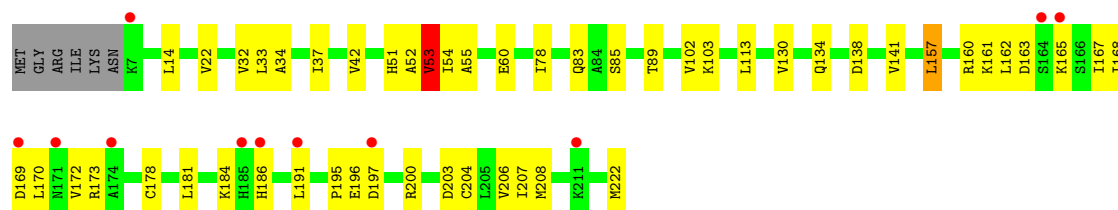
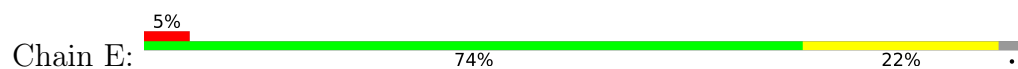


- Molecule 1: Ktr system potassium uptake protein A

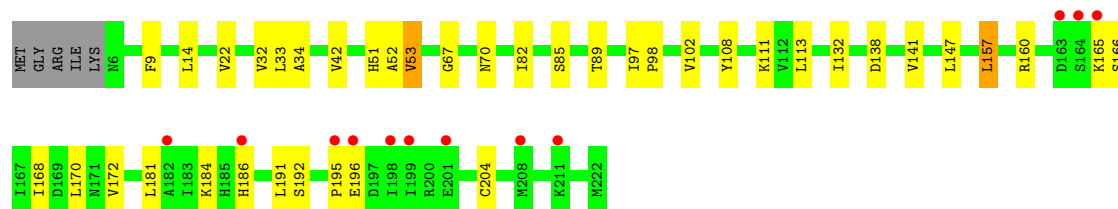
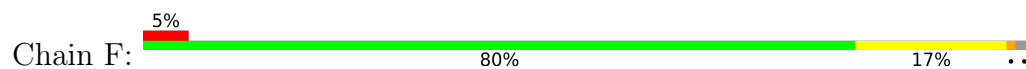




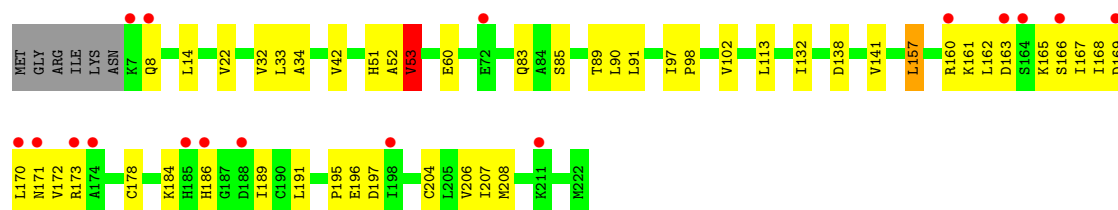
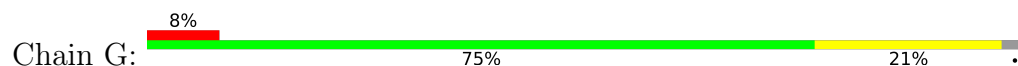
• Molecule 1: Ktr system potassium uptake protein A



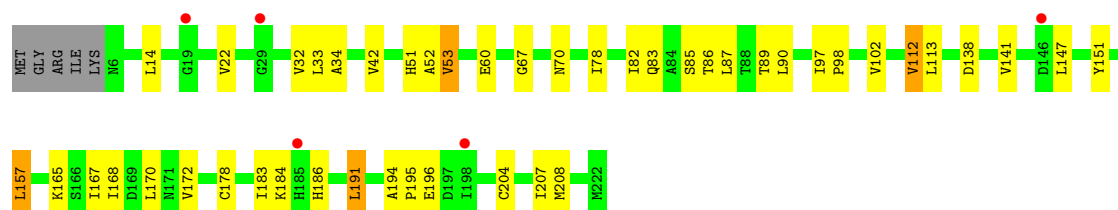
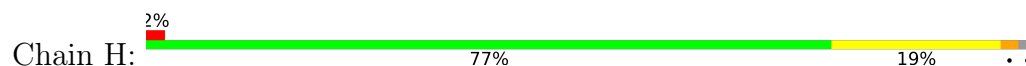
• Molecule 1: Ktr system potassium uptake protein A



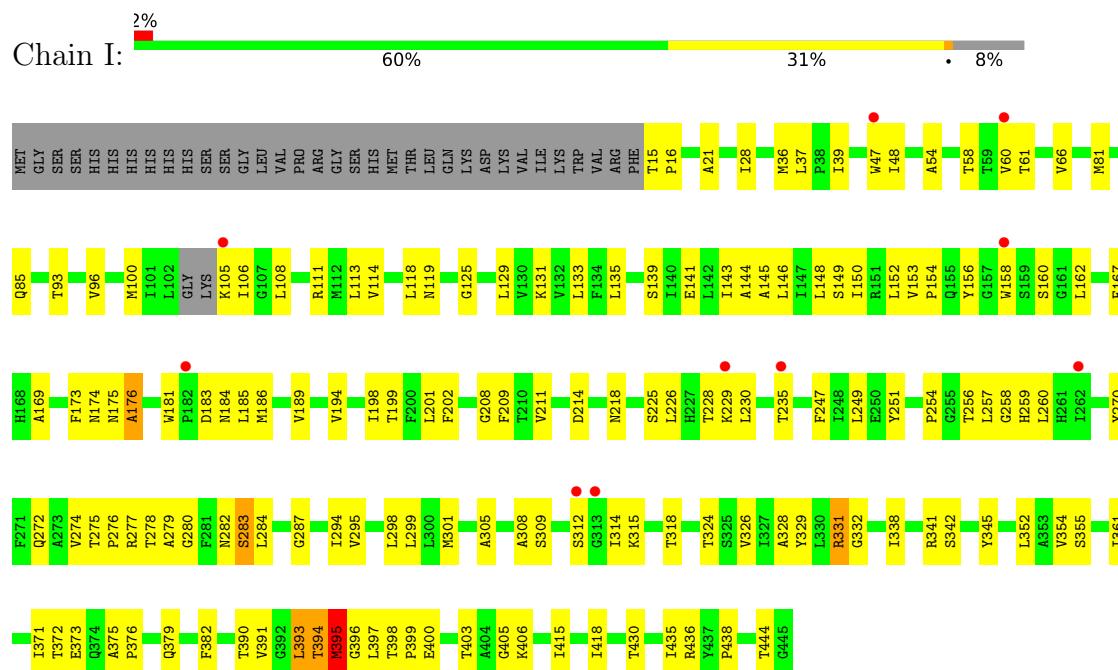
• Molecule 1: Ktr system potassium uptake protein A



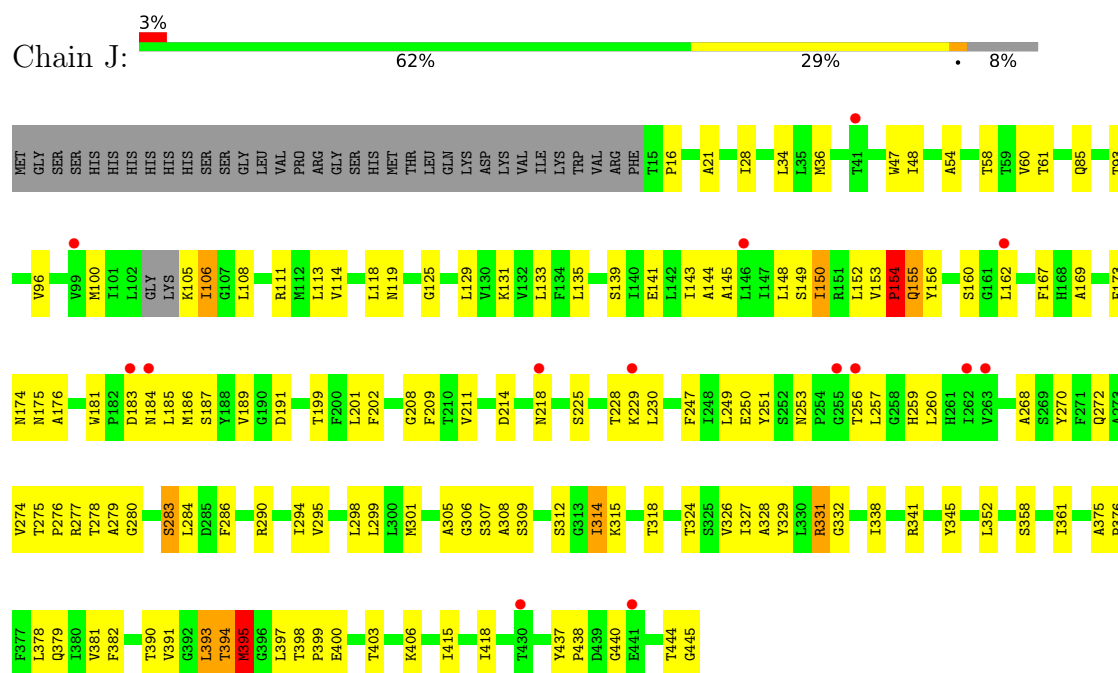
• Molecule 1: Ktr system potassium uptake protein A



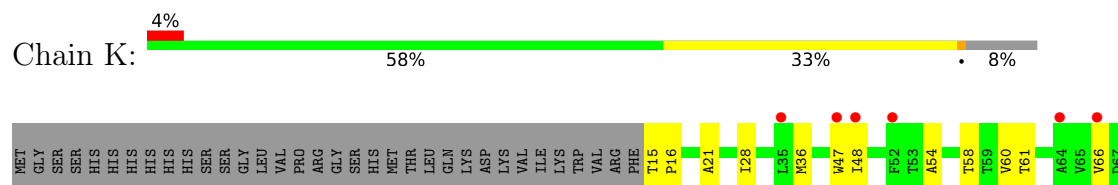
• Molecule 2: Ktr system potassium uptake protein B

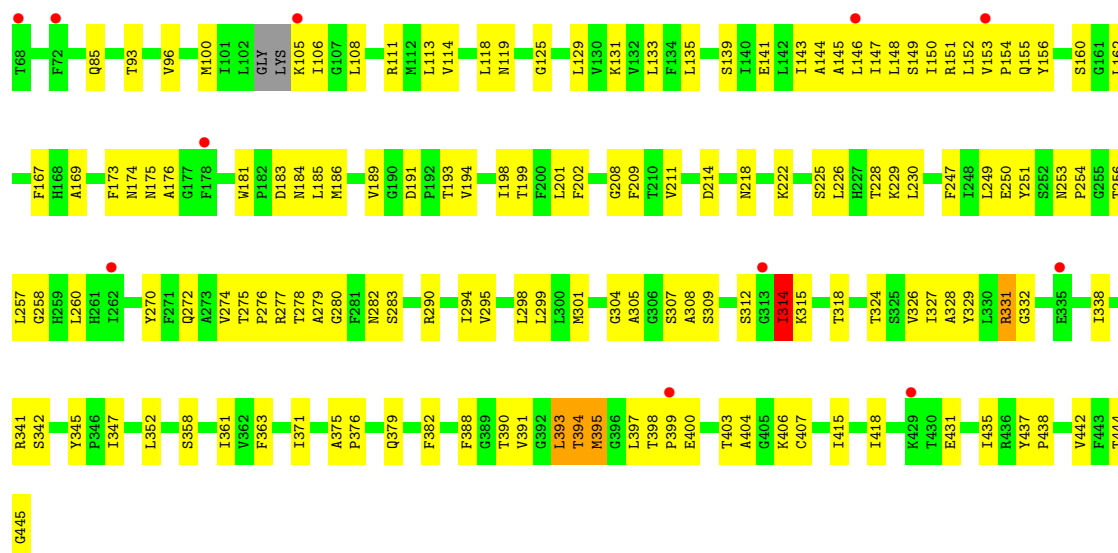


• Molecule 2: Ktr system potassium uptake protein B

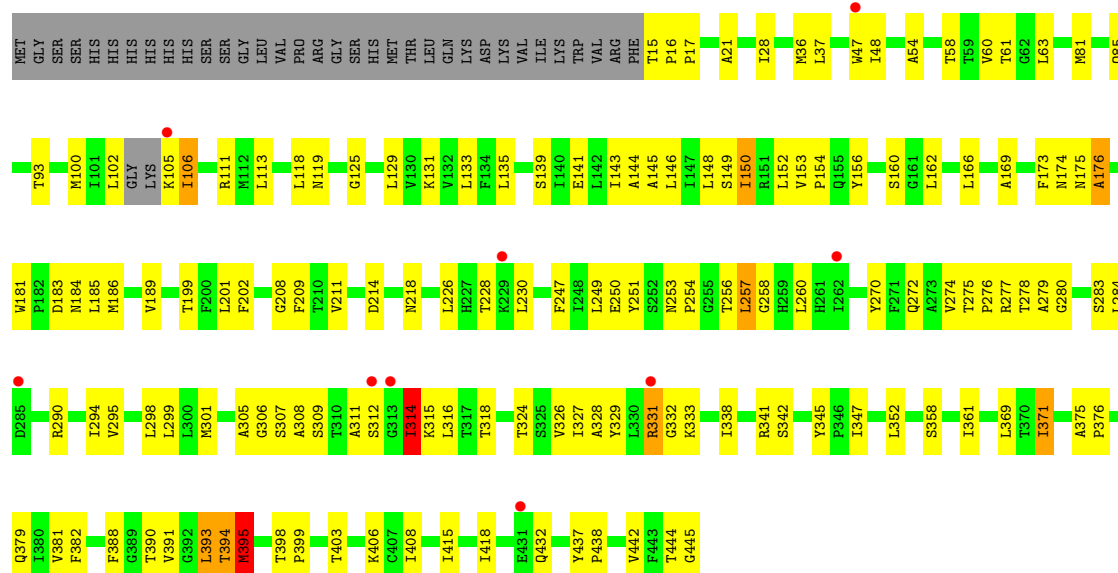


• Molecule 2: Ktr system potassium uptake protein B





• Molecule 2: Ktr system potassium uptake protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.52Å 140.19Å 153.93Å 90.00° 105.69° 90.00°	Depositor
Resolution (Å)	147.44 – 3.50 147.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	79.6 (147.44-3.50) 79.7 (147.44-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.273 0.256 , 0.270	Depositor DCC
R_{free} test set	3121 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	26996	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	4/1725 (0.2%)	0.85	4/2330 (0.2%)
1	B	0.64	4/1733 (0.2%)	0.84	3/2341 (0.1%)
1	C	0.61	2/1725 (0.1%)	0.83	4/2330 (0.2%)
1	D	0.68	4/1733 (0.2%)	0.83	3/2341 (0.1%)
1	E	0.75	4/1725 (0.2%)	0.85	4/2330 (0.2%)
1	F	0.67	3/1733 (0.2%)	0.88	5/2341 (0.2%)
1	G	0.66	2/1725 (0.1%)	0.86	4/2330 (0.2%)
1	H	0.73	5/1733 (0.3%)	0.92	6/2341 (0.3%)
2	I	0.59	2/3351 (0.1%)	1.00	10/4556 (0.2%)
2	J	0.65	3/3351 (0.1%)	1.02	12/4556 (0.3%)
2	K	0.60	0/3351	0.99	6/4556 (0.1%)
2	L	0.61	0/3351	1.01	9/4556 (0.2%)
All	All	0.65	33/27236 (0.1%)	0.93	70/36908 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
2	J	0	2
2	K	0	1
2	L	0	3
All	All	0	7

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	HIS	CG-ND1	-13.29	1.23	1.38
1	H	51	HIS	CG-CD2	-13.02	1.21	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CG-ND1	-12.22	1.24	1.38
1	G	51	HIS	ND1-CE1	10.85	1.43	1.32
1	E	51	HIS	CE1-NE2	-10.28	1.22	1.32
1	A	51	HIS	CE1-NE2	-10.27	1.22	1.32
1	D	51	HIS	CE1-NE2	-9.24	1.23	1.32
1	F	51	HIS	ND1-CE1	9.01	1.41	1.32
2	J	155	GLN	CD-NE2	8.73	1.51	1.33
2	J	155	GLN	CB-CG	8.59	1.78	1.52
1	D	51	HIS	CG-ND1	-8.21	1.29	1.38
1	D	51	HIS	ND1-CE1	7.30	1.39	1.32
1	B	51	HIS	ND1-CE1	6.64	1.39	1.32
1	H	51	HIS	CB-CG	-6.55	1.41	1.50
1	E	51	HIS	CA-C	-6.35	1.44	1.52
1	H	51	HIS	CA-C	-6.07	1.44	1.52
1	A	51	HIS	ND1-CE1	6.05	1.38	1.32
1	F	51	HIS	CE1-NE2	-6.04	1.26	1.32
1	A	51	HIS	CA-C	-5.92	1.45	1.52
1	D	51	HIS	CA-C	-5.87	1.45	1.52
1	H	51	HIS	CE1-NE2	-5.83	1.26	1.32
1	F	51	HIS	CG-ND1	-5.80	1.31	1.38
1	C	51	HIS	CE1-NE2	-5.74	1.26	1.32
1	B	51	HIS	CE1-NE2	-5.72	1.26	1.32
1	G	51	HIS	CE1-NE2	-5.68	1.26	1.32
1	B	51	HIS	CG-ND1	-5.47	1.32	1.38
2	J	259	HIS	CG-CD2	5.42	1.41	1.35
1	B	51	HIS	N-CA	-5.38	1.40	1.46
1	E	51	HIS	ND1-CE1	5.32	1.37	1.32
2	I	259	HIS	CG-CD2	5.22	1.41	1.35
2	I	259	HIS	CE1-NE2	5.10	1.37	1.32
1	H	51	HIS	ND1-CE1	-5.08	1.27	1.32
1	C	51	HIS	CG-CD2	-5.01	1.30	1.35

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	51	HIS	ND1-CE1-NE2	-12.68	95.72	108.40
2	L	395	MET	N-CA-C	-9.78	94.75	110.20
2	I	395	MET	N-CA-C	-9.72	95.89	110.28
2	K	395	MET	N-CA-C	-9.68	95.95	110.28
2	J	395	MET	N-CA-C	-9.21	94.48	109.96
1	H	51	HIS	CE1-NE2-CD2	8.75	117.75	109.00
2	J	155	GLN	N-CA-C	-8.40	102.59	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	51	HIS	CA-CB-CG	-8.16	105.64	113.80
1	H	51	HIS	CB-CA-C	-7.86	95.78	110.16
1	F	192	SER	CA-C-N	7.81	127.81	119.76
1	F	192	SER	C-N-CA	7.81	127.81	119.76
2	I	15	THR	CA-C-N	-7.78	112.37	120.38
2	I	15	THR	C-N-CA	-7.78	112.37	120.38
2	L	331	ARG	N-CA-C	7.75	119.51	111.14
1	E	51	HIS	CB-CA-C	-7.57	96.31	110.16
1	B	51	HIS	CA-CB-CG	-7.45	106.35	113.80
1	A	51	HIS	CB-CA-C	-7.44	96.54	110.16
2	L	181	TRP	CA-C-N	6.92	128.48	119.84
2	L	181	TRP	C-N-CA	6.92	128.48	119.84
1	E	51	HIS	CG-CD2-NE2	6.80	114.00	107.20
2	J	154	PRO	CA-N-CD	-6.79	102.49	112.00
1	D	51	HIS	CB-CA-C	-6.78	97.75	110.16
1	A	51	HIS	CG-CD2-NE2	6.76	113.96	107.20
2	J	155	GLN	CB-CA-C	-6.69	99.26	110.56
2	J	181	TRP	CA-C-N	6.63	128.12	119.84
2	J	181	TRP	C-N-CA	6.63	128.12	119.84
2	K	181	TRP	CA-C-N	6.62	128.12	119.84
2	K	181	TRP	C-N-CA	6.62	128.12	119.84
2	I	331	ARG	N-CA-C	6.54	119.38	111.40
2	J	331	ARG	N-CA-C	6.52	119.71	111.69
2	J	314	ILE	N-CA-C	-6.45	98.84	108.46
2	I	181	TRP	CA-C-N	6.45	127.90	119.84
2	I	181	TRP	C-N-CA	6.45	127.90	119.84
2	L	314	ILE	N-CA-C	-6.41	98.96	108.45
1	G	51	HIS	ND1-CG-CD2	-6.27	99.83	106.10
1	G	51	HIS	CA-CB-CG	-6.24	107.56	113.80
1	G	51	HIS	CG-CD2-NE2	6.15	113.35	107.20
1	D	51	HIS	CG-CD2-NE2	5.97	113.17	107.20
1	H	51	HIS	N-CA-C	5.97	118.20	108.76
2	K	151	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	C	51	HIS	N-CA-C	5.93	117.41	108.46
1	D	51	HIS	ND1-CG-CD2	-5.87	100.23	106.10
1	F	51	HIS	ND1-CG-CD2	-5.85	100.25	106.10
2	K	331	ARG	N-CA-C	5.81	118.49	111.40
1	H	112	VAL	N-CA-CB	5.77	118.39	110.54
1	F	51	HIS	CG-CD2-NE2	5.77	112.97	107.20
1	G	53	VAL	CB-CA-C	-5.75	101.20	110.28
1	C	192	SER	CA-C-N	5.74	125.67	119.76
1	C	192	SER	C-N-CA	5.74	125.67	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
2	K	314	ILE	N-CA-C	-5.71	99.89	108.12
1	H	51	HIS	CG-ND1-CE1	5.65	118.91	109.30
2	I	283	SER	N-CA-C	-5.51	106.23	113.12
1	B	51	HIS	N-CA-C	5.50	116.77	108.46
1	C	53	VAL	CB-CA-C	-5.48	101.62	110.28
1	B	51	HIS	ND1-CG-CD2	-5.34	100.76	106.10
1	E	53	VAL	CB-CA-C	-5.31	101.88	110.28
2	L	257	LEU	N-CA-CB	-5.31	108.11	114.17
2	L	37	LEU	CA-C-N	5.28	126.44	119.84
2	L	37	LEU	C-N-CA	5.28	126.44	119.84
1	A	53	VAL	CB-CA-C	-5.24	102.01	110.28
2	L	371	ILE	N-CA-C	-5.17	107.71	111.90
2	J	154	PRO	CA-CB-CG	5.16	114.30	104.50
2	J	283	SER	N-CA-C	-5.11	106.73	113.12
2	I	396	GLY	N-CA-C	5.08	125.21	113.18
1	A	51	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
2	J	154	PRO	CA-C-N	-5.04	114.59	122.65
2	J	154	PRO	C-N-CA	-5.04	114.59	122.65
2	I	37	LEU	CA-C-N	5.01	126.11	119.84
2	I	37	LEU	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	394	THR	Peptide
2	J	394	THR	Peptide
2	J	395	MET	Peptide
2	K	394	THR	Peptide
2	L	314	ILE	Peptide
2	L	394	THR	Peptide
2	L	395	MET	Peptide

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	1699	0	1728	46	1
1	B	1707	0	1734	32	0
1	C	1699	0	1728	63	0
1	D	1707	0	1734	34	0
1	E	1699	0	1728	58	18
1	F	1707	0	1734	36	1
1	G	1699	0	1728	60	19
1	H	1707	0	1734	43	0
2	I	3280	0	3461	160	1
2	J	3280	0	3461	160	0
2	K	3280	0	3461	196	0
2	L	3280	0	3461	165	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	3	0
3	E	31	0	12	3	0
3	F	31	0	12	0	0
3	G	31	0	12	0	0
3	H	31	0	12	2	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26996	0	27788	967	20

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 18.

All (967) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:155:GLN:CB	2:J:155:GLN:CG	1.78	1.55
2:K:150:ILE:HD12	2:K:162:LEU:CD2	1.39	1.53
2:K:150:ILE:CD1	2:K:162:LEU:HD21	1.44	1.43
1:C:167:ILE:CG2	1:C:195:PRO:HA	1.59	1.30
2:K:150:ILE:CD1	2:K:162:LEU:CD2	2.06	1.25
2:I:152:LEU:HD23	2:I:152:LEU:O	1.40	1.22
2:L:145:ALA:HB2	2:L:169:ALA:CB	1.71	1.20
2:I:312:SER:CB	2:I:315:LYS:HD3	1.70	1.20
2:I:145:ALA:HB2	2:I:169:ALA:CB	1.72	1.19
2:L:208:GLY:HA2	2:L:308:ALA:HB2	1.24	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:LYS:HD2	1:E:222:MET:O	1.38	1.17
2:J:145:ALA:HB2	2:J:169:ALA:CB	1.73	1.17
2:K:145:ALA:HB2	2:K:169:ALA:CB	1.74	1.17
2:L:145:ALA:CB	2:L:169:ALA:HB2	1.74	1.17
1:A:172:VAL:HG11	1:A:207:ILE:HD11	1.28	1.16
1:C:167:ILE:HG22	1:C:196:GLU:HA	1.19	1.16
2:J:145:ALA:CB	2:J:169:ALA:HB2	1.75	1.15
2:K:145:ALA:CB	2:K:169:ALA:HB2	1.77	1.14
2:L:208:GLY:HA2	2:L:308:ALA:CB	1.77	1.14
2:I:145:ALA:CB	2:I:169:ALA:HB2	1.77	1.13
2:K:208:GLY:HA2	2:K:308:ALA:HB2	1.14	1.13
2:I:312:SER:HB2	2:I:315:LYS:HD3	1.26	1.13
2:I:312:SER:HB2	2:I:315:LYS:CD	1.78	1.12
2:J:208:GLY:HA2	2:J:308:ALA:HB2	1.15	1.11
2:J:208:GLY:HA2	2:J:308:ALA:CB	1.82	1.10
2:K:150:ILE:HD11	2:K:162:LEU:HD21	1.20	1.10
2:L:208:GLY:CA	2:L:308:ALA:HB2	1.80	1.09
2:I:208:GLY:HA2	2:I:308:ALA:HB2	1.15	1.09
2:I:208:GLY:HA2	2:I:308:ALA:CB	1.83	1.08
2:K:208:GLY:HA2	2:K:308:ALA:CB	1.83	1.07
1:C:167:ILE:CG2	1:C:196:GLU:HA	1.84	1.07
2:J:312:SER:HB2	2:J:315:LYS:CD	1.85	1.07
2:K:150:ILE:HD12	2:K:162:LEU:HD23	1.28	1.07
2:L:209:PHE:H	2:L:308:ALA:CB	1.67	1.07
2:L:145:ALA:CB	2:L:169:ALA:CB	2.31	1.06
2:J:312:SER:HB2	2:J:315:LYS:CE	1.84	1.06
2:J:145:ALA:CB	2:J:169:ALA:CB	2.33	1.06
1:C:167:ILE:HG21	1:C:195:PRO:HA	1.09	1.05
2:K:208:GLY:CA	2:K:308:ALA:HB2	1.87	1.05
1:A:167:ILE:HD11	1:A:183:ILE:HD11	1.35	1.05
2:K:145:ALA:CB	2:K:169:ALA:CB	2.33	1.04
1:G:167:ILE:CG2	1:G:195:PRO:HA	1.87	1.04
2:I:208:GLY:CA	2:I:308:ALA:HB2	1.87	1.04
2:L:312:SER:HB2	2:L:315:LYS:CE	1.87	1.04
2:J:145:ALA:HB2	2:J:169:ALA:HB2	1.32	1.03
2:J:208:GLY:CA	2:J:308:ALA:HB2	1.87	1.03
2:L:145:ALA:HB2	2:L:169:ALA:HB2	1.30	1.03
2:I:145:ALA:CB	2:I:169:ALA:CB	2.32	1.03
2:L:272:GLN:HE22	2:L:283:SER:HB3	1.23	1.03
2:K:28:ILE:HG12	2:K:58:THR:HG21	1.40	1.02
2:L:28:ILE:HG12	2:L:58:THR:HG21	1.40	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:312:SER:HB2	2:I:315:LYS:CE	1.89	1.01
2:J:28:ILE:HG12	2:J:58:THR:HG21	1.39	1.01
2:J:272:GLN:HE22	2:J:283:SER:HB3	1.24	1.01
2:J:312:SER:HB2	2:J:315:LYS:HD3	1.40	1.01
2:K:312:SER:HB2	2:K:315:LYS:HD3	1.41	1.01
2:L:15:THR:CG2	2:L:17:PRO:HD2	1.89	1.01
1:G:168:ILE:HB	1:G:195:PRO:HB3	1.43	1.01
2:L:15:THR:HG22	2:L:17:PRO:HD2	1.00	1.00
2:I:314:ILE:HD12	2:I:355:SER:HA	1.38	0.99
2:J:209:PHE:H	2:J:308:ALA:CB	1.74	0.99
2:K:394:THR:HG21	2:K:398:THR:OG1	1.60	0.99
2:I:209:PHE:H	2:I:308:ALA:CB	1.75	0.99
2:K:272:GLN:HE22	2:K:283:SER:HB3	1.27	0.99
2:K:145:ALA:HB2	2:K:169:ALA:HB2	1.33	0.99
2:K:209:PHE:H	2:K:308:ALA:CB	1.75	0.98
2:I:28:ILE:HG12	2:I:58:THR:HG21	1.44	0.98
2:I:145:ALA:HB2	2:I:169:ALA:HB2	1.32	0.98
2:I:312:SER:HB2	2:I:315:LYS:HE2	1.46	0.97
2:L:394:THR:HG21	2:L:398:THR:OG1	1.62	0.97
2:I:394:THR:HG21	2:I:398:THR:OG1	1.65	0.96
2:L:15:THR:HG22	2:L:17:PRO:CD	1.95	0.96
2:I:272:GLN:HE22	2:I:283:SER:HB3	1.27	0.96
1:C:167:ILE:HG21	1:C:195:PRO:CA	1.94	0.96
2:L:312:SER:HB2	2:L:315:LYS:CD	1.97	0.95
1:C:167:ILE:CG2	1:C:195:PRO:CA	2.45	0.95
2:K:152:LEU:HD21	2:K:191:ASP:OD2	1.65	0.94
1:G:172:VAL:HG11	1:G:207:ILE:HD11	1.47	0.94
1:A:168:ILE:HB	1:A:195:PRO:HB3	1.49	0.94
1:E:161:LYS:CD	1:E:222:MET:O	2.16	0.94
2:L:209:PHE:H	2:L:308:ALA:HB1	1.32	0.94
2:K:152:LEU:CD2	2:K:193:THR:HB	1.98	0.94
1:E:167:ILE:CG2	1:E:195:PRO:HA	1.98	0.93
2:J:28:ILE:HG12	2:J:58:THR:CG2	1.98	0.93
1:E:22:VAL:HG23	1:E:32:VAL:HG11	1.47	0.93
1:A:22:VAL:HG23	1:A:32:VAL:HG11	1.51	0.93
1:G:167:ILE:HG21	1:G:195:PRO:HA	1.51	0.93
1:A:167:ILE:HD11	1:A:183:ILE:CD1	1.98	0.92
2:K:152:LEU:HD22	2:K:193:THR:HB	1.49	0.92
2:K:379:GLN:HA	2:K:395:MET:CE	2.00	0.92
2:J:153:VAL:HG12	2:J:153:VAL:O	1.70	0.92
2:J:394:THR:HG21	2:J:398:THR:OG1	1.68	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:312:SER:HB2	2:K:315:LYS:CD	1.98	0.91
2:J:312:SER:CB	2:J:315:LYS:HD3	2.00	0.91
2:K:28:ILE:HG12	2:K:58:THR:CG2	2.00	0.91
1:E:22:VAL:HG23	1:E:32:VAL:CG1	2.02	0.90
2:L:28:ILE:HG12	2:L:58:THR:CG2	2.00	0.90
1:E:167:ILE:HG22	1:E:197:ASP:H	1.35	0.89
1:A:167:ILE:HD12	1:A:197:ASP:HB2	1.54	0.89
2:I:28:ILE:HG12	2:I:58:THR:CG2	2.02	0.89
2:L:312:SER:HB2	2:L:315:LYS:HE3	1.53	0.89
1:D:22:VAL:HG23	1:D:32:VAL:HG11	1.54	0.89
2:K:308:ALA:HB3	2:K:309:SER:HA	1.54	0.89
1:G:167:ILE:HG22	1:G:196:GLU:HA	1.53	0.88
1:C:167:ILE:HG22	1:C:196:GLU:CA	2.03	0.88
2:I:308:ALA:HB3	2:I:309:SER:HA	1.54	0.88
1:H:22:VAL:HG23	1:H:32:VAL:HG11	1.57	0.87
2:J:145:ALA:HB1	2:J:169:ALA:HB2	1.55	0.87
2:J:209:PHE:H	2:J:308:ALA:HB1	1.37	0.86
2:K:209:PHE:H	2:K:308:ALA:HB1	1.38	0.86
2:J:308:ALA:HB3	2:J:309:SER:HA	1.57	0.86
2:I:209:PHE:H	2:I:308:ALA:HB1	1.38	0.86
2:I:152:LEU:O	2:I:152:LEU:CD2	2.23	0.86
2:L:145:ALA:HB1	2:L:169:ALA:HB2	1.54	0.86
2:K:185:LEU:HD11	2:K:194:VAL:HG11	1.58	0.85
2:I:145:ALA:HB1	2:I:169:ALA:HB2	1.57	0.85
1:D:22:VAL:HG23	1:D:32:VAL:CG1	2.07	0.85
2:L:153:VAL:HG12	2:L:153:VAL:O	1.74	0.85
2:L:209:PHE:N	2:L:308:ALA:CB	2.40	0.84
1:H:172:VAL:HG11	1:H:207:ILE:HD11	1.57	0.84
2:K:147:ILE:O	2:K:150:ILE:HG22	1.77	0.84
1:A:22:VAL:HG23	1:A:32:VAL:CG1	2.08	0.84
2:K:155:GLN:O	2:K:155:GLN:HG2	1.77	0.84
1:G:22:VAL:HG23	1:G:32:VAL:HG11	1.57	0.83
2:L:308:ALA:HB3	2:L:309:SER:HA	1.60	0.83
2:L:312:SER:HB2	2:L:315:LYS:HD3	1.58	0.83
1:G:167:ILE:HG22	1:G:197:ASP:H	1.43	0.83
2:K:185:LEU:HG	2:K:185:LEU:O	1.78	0.83
2:K:145:ALA:HB1	2:K:169:ALA:HB2	1.57	0.83
2:J:150:ILE:O	2:J:154:PRO:HD3	1.77	0.82
2:I:145:ALA:HB2	2:I:169:ALA:HB1	1.59	0.82
2:L:312:SER:CB	2:L:315:LYS:HD3	2.09	0.82
2:K:379:GLN:HA	2:K:395:MET:HE2	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:CG1	1:C:178:CYS:HB2	2.09	0.81
2:J:145:ALA:HB2	2:J:169:ALA:HB1	1.60	0.81
2:L:145:ALA:HB2	2:L:169:ALA:HB1	1.59	0.81
2:K:153:VAL:HG12	2:K:153:VAL:O	1.80	0.80
1:F:168:ILE:HB	1:F:195:PRO:HB3	1.63	0.80
1:H:22:VAL:HG23	1:H:32:VAL:CG1	2.12	0.80
2:K:152:LEU:HD22	2:K:193:THR:CB	2.10	0.80
2:K:257:LEU:HD23	2:K:257:LEU:O	1.80	0.80
2:K:145:ALA:HB2	2:K:169:ALA:HB1	1.62	0.80
2:I:379:GLN:HA	2:I:395:MET:CE	2.12	0.80
2:K:111:ARG:NH1	2:K:125:GLY:HA2	1.97	0.79
1:E:89:THR:HG21	1:E:102:VAL:HG11	1.65	0.79
2:I:153:VAL:HG12	2:I:153:VAL:O	1.82	0.79
2:J:379:GLN:HA	2:J:395:MET:CE	2.13	0.79
1:E:172:VAL:HG11	1:E:207:ILE:HD11	1.65	0.79
1:F:70:ASN:HD21	2:L:111:ARG:CD	1.96	0.78
1:E:167:ILE:HG23	1:E:195:PRO:HA	1.65	0.78
1:G:167:ILE:CG2	1:G:196:GLU:HA	2.14	0.78
2:K:211:VAL:HG13	2:K:228:THR:HG23	1.65	0.78
2:L:111:ARG:NH1	2:L:125:GLY:HA2	1.97	0.78
1:B:22:VAL:HG23	1:B:32:VAL:HG11	1.65	0.78
2:K:394:THR:HB	2:K:395:MET:O	1.84	0.77
2:J:111:ARG:NH1	2:J:125:GLY:HA2	2.00	0.77
2:J:211:VAL:HG13	2:J:228:THR:HG23	1.65	0.77
1:C:167:ILE:HG23	1:C:195:PRO:HB3	1.67	0.76
1:G:189:ILE:HG13	1:G:191:LEU:HD12	1.66	0.76
2:L:211:VAL:HG13	2:L:228:THR:HG23	1.67	0.76
1:H:89:THR:HG21	1:H:102:VAL:HG11	1.66	0.76
2:J:209:PHE:N	2:J:308:ALA:CB	2.48	0.76
1:C:172:VAL:HG11	1:C:178:CYS:HB2	1.67	0.76
2:I:111:ARG:NH1	2:I:125:GLY:HA2	2.00	0.76
1:A:172:VAL:CG1	1:A:207:ILE:HD11	2.13	0.75
1:A:191:LEU:HG	1:B:208:MET:HE2	1.68	0.75
1:F:22:VAL:HG23	1:F:32:VAL:HG11	1.68	0.75
2:L:209:PHE:N	2:L:308:ALA:HB2	2.01	0.75
2:I:314:ILE:CD1	2:I:355:SER:HA	2.16	0.75
1:G:89:THR:HG21	1:G:102:VAL:HG11	1.68	0.74
1:G:22:VAL:HG23	1:G:32:VAL:CG1	2.16	0.74
1:G:172:VAL:CG1	1:G:178:CYS:HB2	2.17	0.74
1:B:89:THR:HG21	1:B:102:VAL:HG11	1.66	0.74
1:E:167:ILE:HG22	1:E:197:ASP:N	2.01	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:209:PHE:N	2:K:308:ALA:CB	2.50	0.74
1:H:167:ILE:HD11	1:H:183:ILE:HD11	1.68	0.74
2:J:379:GLN:HA	2:J:395:MET:HE3	1.69	0.74
2:L:208:GLY:HA2	2:L:308:ALA:HB3	1.69	0.74
2:I:209:PHE:N	2:I:308:ALA:CB	2.50	0.74
2:I:211:VAL:HG13	2:I:228:THR:HG23	1.69	0.74
2:K:214:ASP:OD1	2:K:218:ASN:ND2	2.21	0.74
1:A:167:ILE:CD1	1:A:183:ILE:HD11	2.15	0.73
1:C:11:VAL:HG11	1:C:22:VAL:HG23	1.70	0.73
1:C:89:THR:HG21	1:C:102:VAL:HG11	1.69	0.73
2:I:185:LEU:O	2:I:185:LEU:HD23	1.89	0.73
2:K:152:LEU:HG	2:K:152:LEU:O	1.87	0.73
1:G:168:ILE:HB	1:G:195:PRO:CB	2.19	0.73
2:L:106:ILE:CG2	2:L:106:ILE:O	2.36	0.73
1:E:53:VAL:HG11	2:I:435:ILE:HD12	1.70	0.72
1:A:89:THR:HG21	1:A:102:VAL:HG11	1.70	0.72
2:J:375:ALA:HB1	2:J:376:PRO:HD2	1.70	0.72
1:G:189:ILE:CG1	1:G:191:LEU:CD1	2.68	0.72
1:G:189:ILE:HG12	1:G:191:LEU:HD11	1.72	0.72
2:I:280:GLY:HA2	2:I:393:LEU:HD22	1.72	0.71
1:D:167:ILE:HD11	1:D:183:ILE:HD11	1.72	0.71
2:K:312:SER:HB3	2:K:315:LYS:HG2	1.71	0.71
1:F:22:VAL:HG23	1:F:32:VAL:CG1	2.19	0.71
1:G:189:ILE:HG12	1:G:191:LEU:CD1	2.20	0.71
1:D:89:THR:HG21	1:D:102:VAL:HG11	1.72	0.71
2:J:280:GLY:HA2	2:J:393:LEU:HD22	1.71	0.70
2:K:314:ILE:HG13	2:K:314:ILE:O	1.92	0.70
2:K:150:ILE:CD1	2:K:162:LEU:HD23	1.97	0.70
2:J:312:SER:HB2	2:J:315:LYS:HE2	1.71	0.70
2:J:272:GLN:NE2	2:J:283:SER:HB3	2.05	0.70
2:J:312:SER:CB	2:J:315:LYS:CD	2.64	0.70
1:F:89:THR:HG21	1:F:102:VAL:HG11	1.72	0.70
2:K:314:ILE:HG21	2:K:358:SER:OG	1.92	0.69
1:A:167:ILE:CD1	1:A:197:ASP:HB2	2.22	0.69
1:F:70:ASN:HD21	2:L:111:ARG:HD3	1.56	0.69
2:I:214:ASP:OD1	2:I:218:ASN:ND2	2.24	0.69
1:A:168:ILE:HB	1:A:195:PRO:CB	2.23	0.69
2:I:158:TRP:HE3	2:I:162:LEU:HD11	1.58	0.69
1:C:167:ILE:HG23	1:C:195:PRO:HA	1.70	0.69
1:G:167:ILE:HG22	1:G:197:ASP:N	2.06	0.69
2:I:403:THR:HA	2:I:406:LYS:HE3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:375:ALA:HB1	2:L:376:PRO:HD2	1.73	0.69
2:K:141:GLU:O	2:K:145:ALA:HB3	1.92	0.69
2:L:186:MET:O	2:L:189:VAL:HG23	1.93	0.68
2:J:209:PHE:N	2:J:308:ALA:HB2	2.08	0.68
1:B:22:VAL:HG23	1:B:32:VAL:CG1	2.22	0.68
2:I:375:ALA:HB1	2:I:376:PRO:HD2	1.75	0.68
2:J:403:THR:HA	2:J:406:LYS:HE3	1.76	0.68
2:K:312:SER:CB	2:K:315:LYS:HD3	2.21	0.68
2:K:251:TYR:HA	2:K:257:LEU:CD2	2.24	0.68
2:I:186:MET:O	2:I:189:VAL:HG23	1.92	0.67
2:K:314:ILE:CG2	2:K:358:SER:OG	2.41	0.67
2:K:403:THR:HA	2:K:406:LYS:HE3	1.75	0.67
2:K:445:GLY:O	2:L:315:LYS:NZ	2.26	0.67
2:I:141:GLU:O	2:I:145:ALA:HB3	1.93	0.67
2:I:324:THR:HG21	2:I:338:ILE:HD11	1.76	0.67
2:L:403:THR:HA	2:L:406:LYS:HE3	1.74	0.67
2:I:230:LEU:HD21	2:I:338:ILE:HG21	1.76	0.67
2:K:152:LEU:HD21	2:K:191:ASP:CG	2.20	0.67
1:E:55:ALA:HB2	2:I:435:ILE:HG22	1.76	0.67
2:I:209:PHE:N	2:I:308:ALA:HB2	2.09	0.67
2:K:230:LEU:HD21	2:K:338:ILE:HG21	1.75	0.67
1:A:172:VAL:HG11	1:A:207:ILE:CD1	2.17	0.66
1:C:167:ILE:HG23	1:C:195:PRO:CB	2.25	0.66
2:J:209:PHE:H	2:J:308:ALA:HB2	1.60	0.66
2:K:250:GLU:O	2:K:257:LEU:HD22	1.95	0.66
1:E:89:THR:CG2	1:E:102:VAL:HG11	2.25	0.66
1:E:167:ILE:HG22	1:E:196:GLU:HA	1.77	0.66
1:E:54:ILE:HB	2:I:436:ARG:HB2	1.77	0.66
2:J:186:MET:O	2:J:189:VAL:HG23	1.96	0.66
2:K:375:ALA:HB1	2:K:376:PRO:HD2	1.76	0.66
1:C:189:ILE:HG13	1:C:191:LEU:HD12	1.76	0.66
2:I:60:VAL:HG12	2:I:60:VAL:O	1.94	0.66
2:L:60:VAL:HG12	2:L:60:VAL:O	1.96	0.66
2:L:257:LEU:HD12	2:L:284:LEU:HD11	1.78	0.66
2:L:324:THR:HG21	2:L:338:ILE:HD11	1.77	0.66
1:D:168:ILE:HB	1:D:195:PRO:HB3	1.76	0.66
2:L:185:LEU:HD23	2:L:185:LEU:O	1.95	0.66
2:L:230:LEU:HD21	2:L:338:ILE:HG21	1.78	0.65
2:K:209:PHE:H	2:K:308:ALA:HB2	1.61	0.65
2:K:324:THR:HG21	2:K:338:ILE:HD11	1.78	0.65
2:L:280:GLY:HA2	2:L:393:LEU:HD22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:THR:CG2	1:H:102:VAL:HG11	2.26	0.65
2:K:209:PHE:N	2:K:308:ALA:HB2	2.09	0.65
1:E:172:VAL:CG1	1:E:178:CYS:HB2	2.27	0.65
2:K:186:MET:O	2:K:189:VAL:HG23	1.96	0.65
2:L:153:VAL:O	2:L:153:VAL:CG1	2.44	0.65
2:L:214:ASP:OD1	2:L:218:ASN:ND2	2.29	0.65
2:J:257:LEU:HA	2:J:260:LEU:HD13	1.79	0.65
2:K:60:VAL:HG12	2:K:60:VAL:O	1.96	0.65
1:B:89:THR:CG2	1:B:102:VAL:HG11	2.26	0.64
2:I:145:ALA:HB1	2:I:169:ALA:CB	2.21	0.64
2:J:230:LEU:HD21	2:J:338:ILE:HG21	1.77	0.64
2:K:185:LEU:HD11	2:K:194:VAL:CG1	2.26	0.64
2:K:280:GLY:HA2	2:K:393:LEU:HD22	1.78	0.64
2:J:183:ASP:O	2:J:185:LEU:N	2.28	0.64
2:L:312:SER:CB	2:L:315:LYS:CD	2.71	0.64
2:I:272:GLN:NE2	2:I:283:SER:HB3	2.08	0.64
2:J:141:GLU:O	2:J:145:ALA:HB3	1.98	0.64
1:E:161:LYS:HD2	1:E:222:MET:C	2.22	0.64
1:F:82:ILE:HB	1:G:83:GLN:CD	2.23	0.64
2:J:314:ILE:CG2	2:J:358:SER:OG	2.46	0.64
2:L:208:GLY:C	2:L:308:ALA:HB2	2.22	0.63
1:F:184:LYS:HB3	1:F:204:CYS:HB2	1.81	0.63
1:H:78:ILE:HG12	3:H:301:ATP:O4'	1.98	0.63
2:L:272:GLN:NE2	2:L:283:SER:HB3	2.05	0.63
2:J:185:LEU:HD23	2:J:185:LEU:O	1.98	0.63
1:C:167:ILE:HG23	1:C:195:PRO:CA	2.26	0.63
1:G:89:THR:CG2	1:G:102:VAL:HG11	2.27	0.63
2:I:146:LEU:O	2:I:150:ILE:HB	1.98	0.63
2:J:155:GLN:CG	2:J:155:GLN:CA	2.74	0.63
1:A:172:VAL:CG1	1:A:178:CYS:HB2	2.28	0.63
2:K:111:ARG:HH11	2:K:125:GLY:HA2	1.64	0.63
2:K:352:LEU:HD23	2:L:352:LEU:HD23	1.81	0.63
2:L:141:GLU:O	2:L:145:ALA:HB3	1.99	0.63
1:A:89:THR:CG2	1:A:102:VAL:HG11	2.29	0.62
2:J:150:ILE:HD11	2:J:162:LEU:CD2	2.29	0.62
2:K:184:ASN:O	2:K:185:LEU:HB3	1.98	0.62
2:L:105:LYS:HG3	2:L:105:LYS:O	1.98	0.62
2:L:153:VAL:N	2:L:154:PRO:CD	2.62	0.62
1:C:89:THR:CG2	1:C:102:VAL:HG11	2.29	0.62
2:K:272:GLN:NE2	2:K:283:SER:HB3	2.09	0.62
2:L:257:LEU:HA	2:L:260:LEU:HD13	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:HB3	1:F:170:LEU:HD13	1.81	0.62
1:H:165:LYS:HB3	1:H:170:LEU:HD13	1.80	0.62
1:D:89:THR:CG2	1:D:102:VAL:HG11	2.30	0.62
2:K:312:SER:CB	2:K:315:LYS:HG2	2.30	0.62
1:G:165:LYS:HB3	1:G:170:LEU:HD13	1.81	0.62
2:J:152:LEU:HG	2:J:152:LEU:O	1.99	0.62
2:L:149:SER:O	2:L:153:VAL:HB	1.99	0.62
1:G:189:ILE:HG13	1:G:191:LEU:CD1	2.31	0.61
2:J:214:ASP:OD1	2:J:218:ASN:ND2	2.33	0.61
2:J:324:THR:HG21	2:J:338:ILE:HD11	1.81	0.61
2:K:145:ALA:HB1	2:K:169:ALA:CB	2.21	0.61
1:G:167:ILE:HG23	1:G:195:PRO:HA	1.81	0.61
2:I:345:TYR:CE1	2:J:345:TYR:CE1	2.88	0.61
1:E:167:ILE:CG2	1:E:196:GLU:HA	2.31	0.61
2:I:394:THR:HB	2:I:395:MET:O	1.99	0.61
1:F:89:THR:CG2	1:F:102:VAL:HG11	2.30	0.61
2:I:105:LYS:O	2:I:105:LYS:HG3	1.99	0.61
2:K:105:LYS:O	2:K:105:LYS:HG3	1.99	0.61
1:E:165:LYS:HB3	1:E:170:LEU:HD13	1.83	0.60
1:G:172:VAL:HG12	1:G:178:CYS:HB2	1.81	0.60
2:J:100:MET:HE1	2:J:131:LYS:HE2	1.82	0.60
1:A:165:LYS:HB3	1:A:170:LEU:HD13	1.84	0.60
2:L:60:VAL:HG13	2:L:176:ALA:HA	1.83	0.60
1:D:184:LYS:HB3	1:D:204:CYS:HB2	1.82	0.60
1:C:165:LYS:HB3	1:C:170:LEU:HD13	1.83	0.60
2:J:153:VAL:O	2:J:153:VAL:CG1	2.42	0.60
2:J:60:VAL:HG12	2:J:60:VAL:O	2.01	0.60
1:A:208:MET:HE2	1:B:191:LEU:HD22	1.84	0.60
2:L:183:ASP:O	2:L:185:LEU:N	2.33	0.60
1:F:82:ILE:HD13	1:G:83:GLN:NE2	2.17	0.60
1:B:184:LYS:HB3	1:B:204:CYS:HB2	1.82	0.60
1:H:184:LYS:HB3	1:H:204:CYS:HB2	1.84	0.60
2:L:111:ARG:HH11	2:L:125:GLY:HA2	1.63	0.60
1:A:151:TYR:CD1	1:B:191:LEU:HD11	2.37	0.59
1:C:189:ILE:HG12	1:C:191:LEU:HD11	1.84	0.59
1:D:165:LYS:HB3	1:D:170:LEU:HD13	1.84	0.59
2:J:111:ARG:HH11	2:J:125:GLY:HA2	1.67	0.59
2:K:149:SER:O	2:K:153:VAL:HB	2.02	0.59
1:G:167:ILE:HG22	1:G:196:GLU:CA	2.30	0.59
1:E:55:ALA:CB	2:I:435:ILE:HG22	2.33	0.59
1:E:168:ILE:HG22	1:E:196:GLU:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:183:ASP:C	2:I:185:LEU:H	2.10	0.59
2:J:118:LEU:HD13	2:J:129:LEU:HD23	1.84	0.59
1:B:166:SER:OG	1:B:196:GLU:HB2	2.03	0.59
2:L:432:GLN:O	2:L:432:GLN:HG3	2.03	0.59
1:A:184:LYS:HB3	1:A:204:CYS:HB2	1.84	0.59
1:C:189:ILE:CG1	1:C:191:LEU:CD1	2.81	0.59
1:D:83:GLN:HB2	1:E:83:GLN:HB2	1.85	0.59
1:G:167:ILE:HG23	1:G:168:ILE:N	2.17	0.59
2:I:149:SER:O	2:I:153:VAL:HB	2.02	0.59
1:G:208:MET:HE2	1:H:191:LEU:HG	1.84	0.59
2:I:371:ILE:HD11	2:J:249:LEU:HD21	1.83	0.59
2:L:106:ILE:O	2:L:106:ILE:HG22	2.02	0.59
1:F:166:SER:OG	1:F:196:GLU:HB2	2.03	0.58
2:K:345:TYR:CE1	2:L:345:TYR:CE1	2.91	0.58
1:A:33:LEU:HD11	1:A:53:VAL:CG2	2.33	0.58
1:A:108:TYR:OH	1:H:60:GLU:OE1	2.21	0.58
2:I:314:ILE:HD12	2:I:355:SER:CA	2.24	0.58
2:K:312:SER:HB2	2:K:315:LYS:CE	2.32	0.58
1:C:167:ILE:HG23	1:C:168:ILE:N	2.18	0.58
1:F:168:ILE:HB	1:F:195:PRO:CB	2.32	0.58
1:H:168:ILE:HB	1:H:195:PRO:HB3	1.84	0.58
1:B:8:GLN:NE2	2:K:108:LEU:N	2.51	0.58
2:K:100:MET:HE1	2:K:131:LYS:HE2	1.85	0.58
2:I:287:GLY:HA2	2:I:395:MET:HG2	1.84	0.58
1:A:172:VAL:HG12	1:A:178:CYS:HB2	1.83	0.58
1:B:8:GLN:HE21	2:K:108:LEU:N	2.02	0.58
1:E:184:LYS:HB3	1:E:204:CYS:HB2	1.85	0.58
2:K:254:PRO:HA	2:K:258:GLY:HA3	1.86	0.58
1:E:33:LEU:HD11	1:E:53:VAL:CG2	2.33	0.58
1:G:184:LYS:HB3	1:G:204:CYS:HB2	1.86	0.58
2:J:150:ILE:CD1	2:J:162:LEU:CD2	2.81	0.58
1:B:8:GLN:HE21	2:K:108:LEU:H	1.50	0.57
1:E:208:MET:HE2	1:F:191:LEU:HG	1.86	0.57
2:J:105:LYS:HG3	2:J:105:LYS:O	2.02	0.57
2:L:183:ASP:C	2:L:185:LEU:H	2.12	0.57
1:B:165:LYS:HB3	1:B:170:LEU:HD13	1.85	0.57
2:I:54:ALA:O	2:I:58:THR:HG22	2.03	0.57
2:L:307:SER:HA	2:L:315:LYS:HD2	1.87	0.57
1:C:184:LYS:HB3	1:C:204:CYS:HB2	1.86	0.57
2:J:268:ALA:HB1	2:J:284:LEU:HD21	1.85	0.57
1:C:189:ILE:HG12	1:C:191:LEU:CD1	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:152:LEU:HD23	2:K:193:THR:HB	1.82	0.57
2:K:199:THR:HG21	2:K:270:TYR:CE2	2.40	0.57
2:L:379:GLN:HA	2:L:395:MET:HE3	1.85	0.57
2:I:100:MET:HE1	2:I:131:LYS:HE2	1.87	0.57
2:I:60:VAL:HG13	2:I:176:ALA:HA	1.87	0.56
2:K:150:ILE:HD11	2:K:162:LEU:CD2	2.01	0.56
1:G:33:LEU:HD11	1:G:53:VAL:CG2	2.34	0.56
2:I:361:ILE:HD13	2:I:415:ILE:HG21	1.87	0.56
2:K:249:LEU:CD2	2:L:371:ILE:HD11	2.35	0.56
1:E:167:ILE:HG23	1:E:195:PRO:CA	2.35	0.56
1:F:22:VAL:HG21	1:F:34:ALA:HB2	1.87	0.56
2:J:145:ALA:HB1	2:J:169:ALA:CB	2.21	0.56
2:L:145:ALA:HB1	2:L:169:ALA:CB	2.20	0.56
2:L:150:ILE:HG21	2:L:162:LEU:HD23	1.86	0.56
2:L:199:THR:HG21	2:L:270:TYR:HE2	1.71	0.56
1:E:200:ARG:HB2	1:E:203:ASP:OD2	2.05	0.56
2:I:352:LEU:HD23	2:J:352:LEU:HD23	1.87	0.56
2:K:361:ILE:HD13	2:K:415:ILE:HG21	1.87	0.56
2:L:100:MET:HE1	2:L:131:LYS:HE2	1.86	0.56
1:C:11:VAL:HB	1:C:22:VAL:CG2	2.36	0.56
1:C:172:VAL:HG11	1:C:207:ILE:HD11	1.88	0.56
1:E:22:VAL:HG23	1:E:32:VAL:HG12	1.86	0.56
2:I:199:THR:HG21	2:I:270:TYR:CE2	2.41	0.56
2:K:312:SER:CB	2:K:315:LYS:CD	2.80	0.56
2:L:60:VAL:HG11	2:L:174:ASN:O	2.06	0.56
1:C:11:VAL:HB	1:C:22:VAL:HG22	1.88	0.56
1:C:78:ILE:HG23	3:C:601:ATP:H5'2	1.88	0.56
1:G:157:LEU:HD13	1:G:157:LEU:C	2.31	0.56
1:A:173:ARG:HA	1:A:178:CYS:O	2.06	0.56
2:J:361:ILE:HD13	2:J:415:ILE:HG21	1.88	0.56
2:I:225:SER:O	2:I:229:LYS:HG3	2.06	0.56
1:C:33:LEU:HD11	1:C:53:VAL:CG2	2.37	0.55
1:C:167:ILE:HG22	1:C:197:ASP:H	1.70	0.55
1:C:172:VAL:HG13	1:C:176:TYR:HB2	1.89	0.55
2:L:361:ILE:HD13	2:L:415:ILE:HG21	1.88	0.55
1:G:189:ILE:CG1	1:G:191:LEU:HD12	2.30	0.55
2:L:36:MET:CE	2:L:47:TRP:HA	2.36	0.55
1:H:172:VAL:HG12	1:H:178:CYS:HB2	1.87	0.55
2:I:326:VAL:HG22	2:J:352:LEU:HD13	1.89	0.55
2:K:152:LEU:CD2	2:K:191:ASP:OD2	2.48	0.55
2:L:199:THR:HG21	2:L:270:TYR:CE2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:LEU:HD13	1:E:157:LEU:C	2.30	0.55
1:G:168:ILE:HG23	1:G:169:ASP:N	2.21	0.55
2:I:118:LEU:HD13	2:I:129:LEU:HD23	1.89	0.55
2:I:183:ASP:O	2:I:185:LEU:N	2.32	0.55
2:K:60:VAL:HG13	2:K:176:ALA:HA	1.88	0.55
1:H:33:LEU:HD11	1:H:53:VAL:CG1	2.37	0.55
2:K:60:VAL:O	2:K:60:VAL:CG1	2.55	0.55
2:I:153:VAL:O	2:I:153:VAL:CG1	2.54	0.55
2:J:143:ILE:HG13	2:J:144:ALA:N	2.22	0.55
2:K:379:GLN:HG3	2:K:395:MET:HE3	1.88	0.55
1:F:186:HIS:CG	1:F:186:HIS:O	2.60	0.55
2:I:111:ARG:HH11	2:I:125:GLY:HA2	1.67	0.55
2:K:379:GLN:HA	2:K:395:MET:HE1	1.84	0.55
2:K:150:ILE:O	2:K:154:PRO:HD3	2.06	0.55
2:I:60:VAL:O	2:I:60:VAL:CG1	2.54	0.55
1:B:157:LEU:HD13	1:B:157:LEU:C	2.32	0.54
2:J:150:ILE:HD11	2:J:162:LEU:HD23	1.90	0.54
1:G:186:HIS:CG	1:G:186:HIS:O	2.59	0.54
2:I:257:LEU:HA	2:I:260:LEU:HD13	1.89	0.54
2:J:60:VAL:HG13	2:J:176:ALA:HA	1.88	0.54
2:K:249:LEU:HD21	2:L:371:ILE:HD11	1.90	0.54
1:A:186:HIS:CG	1:A:186:HIS:O	2.60	0.54
1:D:186:HIS:CG	1:D:186:HIS:O	2.60	0.54
2:I:36:MET:CE	2:I:47:TRP:HA	2.36	0.54
2:I:183:ASP:C	2:I:185:LEU:N	2.65	0.54
1:C:200:ARG:HB2	1:C:203:ASP:OD2	2.07	0.54
2:J:155:GLN:CG	2:J:155:GLN:H	2.20	0.54
2:J:208:GLY:C	2:J:308:ALA:HB2	2.32	0.54
2:L:143:ILE:HG13	2:L:144:ALA:N	2.22	0.54
2:L:208:GLY:CA	2:L:308:ALA:CB	2.57	0.54
1:C:186:HIS:CG	1:C:186:HIS:O	2.60	0.54
2:I:85:GLN:HA	2:I:174:ASN:ND2	2.23	0.54
2:I:199:THR:HG21	2:I:270:TYR:HE2	1.73	0.54
2:K:202:PHE:CE1	2:K:274:VAL:HG12	2.43	0.54
1:G:167:ILE:CG2	1:G:197:ASP:H	2.19	0.54
2:I:60:VAL:HG11	2:I:174:ASN:O	2.07	0.54
2:J:183:ASP:C	2:J:185:LEU:H	2.15	0.54
2:J:202:PHE:CE1	2:J:274:VAL:HG12	2.43	0.54
2:K:208:GLY:C	2:K:308:ALA:HB2	2.33	0.54
2:L:202:PHE:CE1	2:L:274:VAL:HG12	2.42	0.54
2:J:36:MET:CE	2:J:47:TRP:HA	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:60:VAL:HG11	2:J:174:ASN:O	2.08	0.54
1:B:167:ILE:HD13	1:B:197:ASP:HB2	1.90	0.54
1:B:186:HIS:CG	1:B:186:HIS:O	2.60	0.54
2:K:183:ASP:O	2:K:185:LEU:N	2.38	0.54
2:K:15:THR:HB	2:K:16:PRO:HD2	1.88	0.54
1:H:157:LEU:C	1:H:157:LEU:HD13	2.32	0.54
2:I:208:GLY:C	2:I:308:ALA:HB2	2.33	0.54
1:C:157:LEU:C	1:C:157:LEU:HD13	2.33	0.53
2:K:155:GLN:O	2:K:155:GLN:CG	2.50	0.53
2:L:60:VAL:O	2:L:60:VAL:CG1	2.57	0.53
2:L:118:LEU:HD13	2:L:129:LEU:HD23	1.89	0.53
1:A:157:LEU:C	1:A:157:LEU:HD13	2.33	0.53
1:E:22:VAL:HG21	1:E:34:ALA:HB2	1.89	0.53
2:I:202:PHE:CE1	2:I:274:VAL:HG12	2.43	0.53
2:I:314:ILE:HG13	2:I:354:VAL:HG12	1.91	0.53
2:K:36:MET:CE	2:K:47:TRP:HA	2.37	0.53
2:K:118:LEU:HD13	2:K:129:LEU:HD23	1.89	0.53
2:K:199:THR:HG21	2:K:270:TYR:HE2	1.73	0.53
1:E:191:LEU:HD12	1:E:191:LEU:C	2.33	0.53
1:F:85:SER:O	1:F:89:THR:HG23	2.08	0.53
1:H:67:GLY:O	1:H:70:ASN:HB2	2.09	0.53
2:I:158:TRP:CE3	2:I:162:LEU:HD11	2.43	0.53
2:I:352:LEU:HD13	2:J:326:VAL:HG22	1.90	0.53
2:L:311:ALA:O	2:L:312:SER:OG	2.25	0.53
1:D:157:LEU:HD13	1:D:157:LEU:C	2.33	0.53
2:J:394:THR:HB	2:J:395:MET:O	2.09	0.53
2:J:150:ILE:CD1	2:J:162:LEU:HD23	2.38	0.53
2:K:85:GLN:HA	2:K:174:ASN:ND2	2.24	0.53
2:L:85:GLN:HA	2:L:174:ASN:ND2	2.24	0.53
1:H:22:VAL:HG21	1:H:34:ALA:HB2	1.90	0.53
2:K:308:ALA:CB	2:K:309:SER:HA	2.34	0.53
2:L:54:ALA:O	2:L:58:THR:HG22	2.08	0.53
1:E:167:ILE:HG21	1:E:195:PRO:HA	1.87	0.53
1:E:172:VAL:CG1	1:E:207:ILE:HD11	2.38	0.53
2:K:301:MET:HB2	2:K:391:VAL:HG21	1.91	0.53
1:G:85:SER:O	1:G:89:THR:HG23	2.09	0.52
2:K:36:MET:HE1	2:K:47:TRP:HA	1.91	0.52
2:K:225:SER:O	2:K:229:LYS:HG3	2.09	0.52
2:K:307:SER:HA	2:K:315:LYS:HD2	1.91	0.52
1:E:186:HIS:CG	1:E:186:HIS:O	2.60	0.52
2:J:28:ILE:HG12	2:J:58:THR:HG23	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:149:SER:O	2:J:153:VAL:HB	2.09	0.52
2:J:183:ASP:C	2:J:185:LEU:N	2.67	0.52
2:K:54:ALA:O	2:K:58:THR:HG22	2.09	0.52
2:K:251:TYR:HA	2:K:257:LEU:HD22	1.91	0.52
1:D:85:SER:O	1:D:89:THR:HG23	2.09	0.52
2:L:394:THR:HG21	2:L:398:THR:HG1	1.70	0.52
1:H:53:VAL:HG21	2:K:435:ILE:HD12	1.92	0.52
1:H:186:HIS:CG	1:H:186:HIS:O	2.60	0.52
2:J:199:THR:HG21	2:J:270:TYR:CE2	2.45	0.52
2:K:143:ILE:HG13	2:K:144:ALA:N	2.24	0.52
2:L:106:ILE:O	2:L:106:ILE:HG23	2.09	0.52
2:L:301:MET:HB2	2:L:391:VAL:HG21	1.92	0.52
1:E:55:ALA:HB2	2:I:435:ILE:CG2	2.38	0.52
2:I:28:ILE:HG12	2:I:58:THR:HG23	1.90	0.52
2:I:208:GLY:HA2	2:I:308:ALA:HB3	1.88	0.52
2:J:54:ALA:O	2:J:58:THR:HG22	2.09	0.52
2:L:111:ARG:HH11	2:L:125:GLY:CA	2.23	0.52
1:D:14:LEU:HD21	1:D:34:ALA:HB1	1.92	0.52
2:I:36:MET:HE1	2:I:47:TRP:HA	1.91	0.52
2:K:326:VAL:HG22	2:L:352:LEU:HD13	1.92	0.52
2:L:36:MET:HE1	2:L:47:TRP:HA	1.91	0.52
1:D:168:ILE:HB	1:D:195:PRO:CB	2.40	0.52
1:F:157:LEU:C	1:F:157:LEU:HD13	2.35	0.52
2:I:308:ALA:CB	2:I:309:SER:HA	2.34	0.52
2:K:341:ARG:HG2	2:L:438:PRO:HG2	1.91	0.52
1:C:167:ILE:HG22	1:C:197:ASP:N	2.25	0.52
2:I:156:TYR:O	2:I:160:SER:HB2	2.10	0.52
2:I:257:LEU:HD12	2:I:284:LEU:HD11	1.92	0.52
2:K:153:VAL:N	2:K:154:PRO:HD3	2.25	0.52
1:A:166:SER:HB3	1:A:196:GLU:HB2	1.93	0.51
2:J:36:MET:HE1	2:J:47:TRP:HA	1.92	0.51
2:J:308:ALA:CB	2:J:309:SER:HA	2.36	0.51
2:K:60:VAL:HG11	2:K:174:ASN:O	2.11	0.51
2:K:352:LEU:HD13	2:L:326:VAL:HG22	1.92	0.51
1:D:22:VAL:HG21	1:D:34:ALA:HB2	1.92	0.51
2:J:85:GLN:HA	2:J:174:ASN:ND2	2.25	0.51
1:H:78:ILE:HG23	3:H:301:ATP:H5'2	1.92	0.51
2:J:301:MET:HB2	2:J:391:VAL:HG21	1.93	0.51
1:C:8:GLN:HE21	2:I:108:LEU:H	1.58	0.51
1:G:167:ILE:CG2	1:G:195:PRO:CA	2.76	0.51
2:K:312:SER:HB2	2:K:315:LYS:HE2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:184:ASN:O	2:L:185:LEU:HB3	2.11	0.51
1:D:37:ILE:HB	3:D:301:ATP:C2	2.44	0.51
1:E:78:ILE:HA	3:E:601:ATP:H5'2	1.93	0.51
2:J:307:SER:HA	2:J:315:LYS:HD2	1.93	0.51
2:K:257:LEU:HA	2:K:260:LEU:HD13	1.93	0.51
2:L:183:ASP:C	2:L:185:LEU:N	2.66	0.51
2:J:152:LEU:CD2	2:J:191:ASP:OD2	2.59	0.51
2:L:202:PHE:CD1	2:L:279:ALA:HB2	2.46	0.51
2:L:152:LEU:HD23	2:L:152:LEU:O	2.10	0.50
1:G:14:LEU:HD21	1:G:34:ALA:HB1	1.93	0.50
2:J:155:GLN:CG	2:J:155:GLN:N	2.74	0.50
1:A:83:GLN:HB2	1:H:83:GLN:HB2	1.93	0.50
1:B:14:LEU:HD21	1:B:34:ALA:HB1	1.92	0.50
2:I:438:PRO:HG2	2:J:341:ARG:HG2	1.93	0.50
2:J:312:SER:HB2	2:J:315:LYS:HE3	1.83	0.50
2:L:394:THR:HB	2:L:395:MET:O	2.11	0.50
1:A:14:LEU:HD21	1:A:34:ALA:HB1	1.92	0.50
1:B:33:LEU:HD11	1:B:53:VAL:CG1	2.41	0.50
1:C:208:MET:HE2	1:D:191:LEU:HD22	1.94	0.50
1:F:70:ASN:ND2	2:L:111:ARG:HD3	2.24	0.50
2:J:60:VAL:O	2:J:60:VAL:CG1	2.59	0.50
2:J:314:ILE:HG21	2:J:358:SER:OG	2.11	0.50
1:D:22:VAL:HG23	1:D:32:VAL:HG12	1.91	0.50
2:J:150:ILE:HD11	2:J:162:LEU:HD22	1.92	0.50
2:J:306:GLY:O	2:J:315:LYS:HB3	2.12	0.50
1:G:167:ILE:HG21	1:G:195:PRO:CA	2.35	0.50
2:J:394:THR:HG21	2:J:398:THR:HG1	1.74	0.50
1:G:8:GLN:HE21	2:J:108:LEU:H	1.59	0.50
1:G:102:VAL:HG21	1:G:113:LEU:HD22	1.92	0.50
2:K:16:PRO:HA	2:K:113:LEU:HD23	1.93	0.50
2:K:202:PHE:CD1	2:K:279:ALA:HB2	2.47	0.50
1:C:85:SER:O	1:C:89:THR:HG23	2.11	0.50
2:I:379:GLN:HA	2:I:395:MET:HE3	1.93	0.50
1:E:14:LEU:HD21	1:E:34:ALA:HB1	1.92	0.49
1:F:22:VAL:HG23	1:F:32:VAL:HG12	1.94	0.49
1:G:172:VAL:HG11	1:G:178:CYS:HB2	1.93	0.49
1:H:14:LEU:HD21	1:H:34:ALA:HB1	1.94	0.49
2:I:143:ILE:HG13	2:I:144:ALA:N	2.26	0.49
2:J:150:ILE:O	2:J:154:PRO:CD	2.56	0.49
2:K:379:GLN:CA	2:K:395:MET:CE	2.81	0.49
1:C:189:ILE:HG13	1:C:191:LEU:CD1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:TYR:OH	1:G:60:GLU:HB2	2.11	0.49
1:H:22:VAL:HG23	1:H:32:VAL:HG12	1.94	0.49
1:H:85:SER:O	1:H:89:THR:HG23	2.12	0.49
2:I:294:ILE:HG23	2:I:382:PHE:CD2	2.46	0.49
2:K:144:ALA:O	2:K:148:LEU:HB2	2.12	0.49
2:K:153:VAL:O	2:K:153:VAL:CG1	2.51	0.49
1:D:138:ASP:HB3	1:D:141:VAL:HG12	1.94	0.49
1:G:8:GLN:NE2	2:J:108:LEU:N	2.60	0.49
2:I:16:PRO:HA	2:I:113:LEU:HD23	1.94	0.49
1:A:85:SER:O	1:A:89:THR:HG23	2.12	0.49
1:D:42:VAL:HG13	1:D:52:ALA:HB1	1.94	0.49
2:K:175:ASN:ND2	2:K:278:THR:H	2.10	0.49
1:C:151:TYR:CD1	1:D:191:LEU:HD11	2.48	0.49
2:I:145:ALA:O	2:I:149:SER:HB2	2.13	0.49
2:I:295:VAL:O	2:I:298:LEU:HB2	2.13	0.49
2:K:153:VAL:N	2:K:154:PRO:CD	2.76	0.49
2:K:185:LEU:O	2:K:185:LEU:CG	2.56	0.49
1:D:103:LYS:NZ	3:D:301:ATP:O1G	2.45	0.49
2:J:150:ILE:CD1	2:J:162:LEU:HD22	2.43	0.49
2:J:155:GLN:H	2:J:155:GLN:HG2	1.77	0.49
2:L:175:ASN:ND2	2:L:278:THR:H	2.10	0.49
1:B:70:ASN:OD1	2:K:111:ARG:NH2	2.45	0.49
2:I:202:PHE:CD1	2:I:279:ALA:HB2	2.47	0.49
2:J:202:PHE:CD1	2:J:279:ALA:HB2	2.48	0.49
1:C:138:ASP:HB3	1:C:141:VAL:HG12	1.95	0.49
1:H:138:ASP:HB3	1:H:141:VAL:HG12	1.95	0.49
2:I:144:ALA:O	2:I:148:LEU:HB2	2.13	0.49
2:K:328:ALA:O	2:K:332:GLY:HA2	2.12	0.49
1:C:189:ILE:CG1	1:C:191:LEU:HD12	2.41	0.49
1:H:102:VAL:HG21	1:H:113:LEU:HD22	1.93	0.49
2:K:111:ARG:HH11	2:K:125:GLY:CA	2.24	0.49
2:K:294:ILE:HG23	2:K:382:PHE:CD2	2.48	0.49
1:G:206:VAL:HG21	1:H:147:LEU:HD22	1.94	0.49
2:I:93:THR:HG21	2:I:133:LEU:HD11	1.94	0.49
2:I:398:THR:HB	2:I:399:PRO:HD3	1.94	0.49
2:K:146:LEU:O	2:K:150:ILE:HB	2.13	0.49
2:K:256:THR:O	2:K:257:LEU:HB3	2.12	0.49
1:C:14:LEU:HD21	1:C:34:ALA:HB1	1.95	0.48
1:D:33:LEU:HD11	1:D:53:VAL:CG1	2.43	0.48
1:D:102:VAL:HG21	1:D:113:LEU:HD22	1.94	0.48
2:K:295:VAL:O	2:K:298:LEU:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG23	1:H:90:LEU:HD22	1.95	0.48
2:I:301:MET:HB2	2:I:391:VAL:HG21	1.94	0.48
2:J:199:THR:HG21	2:J:270:TYR:HE2	1.78	0.48
1:B:85:SER:O	1:B:89:THR:HG23	2.13	0.48
1:H:42:VAL:HG13	1:H:52:ALA:HB1	1.93	0.48
2:I:226:LEU:HD22	2:J:440:GLY:HA3	1.96	0.48
2:I:397:LEU:O	2:I:400:GLU:N	2.45	0.48
2:K:28:ILE:HG12	2:K:58:THR:HG23	1.92	0.48
2:I:152:LEU:O	2:I:152:LEU:CG	2.61	0.48
2:J:93:THR:HG21	2:J:133:LEU:HD11	1.94	0.48
2:J:111:ARG:HH11	2:J:125:GLY:CA	2.26	0.48
2:L:16:PRO:HA	2:L:113:LEU:HD23	1.96	0.48
1:C:168:ILE:HB	1:C:195:PRO:HB3	1.96	0.48
1:F:14:LEU:HD21	1:F:34:ALA:HB1	1.94	0.48
2:I:312:SER:OG	2:I:315:LYS:HD3	2.11	0.48
2:J:225:SER:O	2:J:229:LYS:HG3	2.13	0.48
2:L:93:THR:HG21	2:L:133:LEU:HD11	1.95	0.48
1:A:42:VAL:HG13	1:A:52:ALA:HB1	1.95	0.48
1:C:11:VAL:CB	1:C:22:VAL:CG2	2.91	0.48
2:I:111:ARG:HH11	2:I:125:GLY:CA	2.27	0.48
2:J:145:ALA:O	2:J:149:SER:HB2	2.14	0.48
2:K:21:ALA:HA	2:K:418:ILE:HD11	1.94	0.48
2:K:275:THR:N	2:K:276:PRO:CD	2.77	0.48
2:L:256:THR:O	2:L:257:LEU:HB3	2.14	0.48
2:J:175:ASN:ND2	2:J:278:THR:H	2.12	0.48
2:L:295:VAL:O	2:L:298:LEU:HB2	2.14	0.47
1:A:22:VAL:HG21	1:A:34:ALA:HB2	1.96	0.47
1:B:138:ASP:HB3	1:B:141:VAL:HG12	1.97	0.47
1:C:8:GLN:NE2	2:I:108:LEU:N	2.62	0.47
2:J:275:THR:N	2:J:276:PRO:CD	2.77	0.47
2:J:314:ILE:O	2:J:314:ILE:HG13	2.14	0.47
2:L:145:ALA:O	2:L:149:SER:HB2	2.14	0.47
1:D:7:LYS:H	1:D:7:LYS:HD2	1.79	0.47
1:E:42:VAL:HG13	1:E:52:ALA:HB1	1.95	0.47
2:I:21:ALA:HA	2:I:418:ILE:HD11	1.95	0.47
2:I:312:SER:HB3	2:I:315:LYS:HD3	1.80	0.47
2:K:183:ASP:C	2:K:185:LEU:H	2.22	0.47
1:C:102:VAL:HG21	1:C:113:LEU:HD22	1.95	0.47
2:I:48:ILE:HD12	2:I:48:ILE:H	1.80	0.47
2:I:175:ASN:ND2	2:I:278:THR:H	2.12	0.47
2:K:276:PRO:O	2:K:391:VAL:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:ALA:HA	2:L:418:ILE:HD11	1.96	0.47
1:C:206:VAL:HG21	1:D:147:LEU:HD22	1.96	0.47
1:F:33:LEU:HD11	1:F:53:VAL:CG1	2.44	0.47
2:I:341:ARG:HG2	2:J:438:PRO:HG2	1.95	0.47
2:J:295:VAL:O	2:J:298:LEU:HB2	2.14	0.47
2:K:379:GLN:HG3	2:K:395:MET:CE	2.45	0.47
2:L:153:VAL:N	2:L:154:PRO:HD3	2.28	0.47
1:E:168:ILE:HB	1:E:195:PRO:HB3	1.97	0.47
1:G:8:GLN:HE21	2:J:108:LEU:N	2.13	0.47
2:J:28:ILE:CG1	2:J:58:THR:HG21	2.29	0.47
2:J:275:THR:N	2:J:276:PRO:HD3	2.30	0.47
1:E:161:LYS:CD	1:E:222:MET:C	2.83	0.47
1:F:102:VAL:HG21	1:F:113:LEU:HD22	1.97	0.47
2:K:275:THR:N	2:K:276:PRO:HD3	2.30	0.47
1:E:195:PRO:HA	1:E:196:GLU:HA	1.75	0.47
2:I:328:ALA:O	2:I:332:GLY:HA2	2.15	0.47
2:I:372:THR:O	2:I:373:GLU:HG2	2.15	0.47
1:E:172:VAL:HG12	1:E:178:CYS:C	2.41	0.46
1:F:108:TYR:CE1	1:G:91:LEU:HD21	2.50	0.46
1:G:173:ARG:HA	1:G:178:CYS:O	2.14	0.46
2:K:48:ILE:HD12	2:K:48:ILE:H	1.80	0.46
2:L:294:ILE:HG23	2:L:382:PHE:CD2	2.50	0.46
1:A:78:ILE:HA	3:A:601:ATP:H5'2	1.97	0.46
1:A:206:VAL:HG21	1:B:147:LEU:HD22	1.95	0.46
1:B:82:ILE:HB	1:C:83:GLN:CD	2.40	0.46
1:C:147:LEU:HD22	1:D:206:VAL:HG21	1.97	0.46
1:C:168:ILE:HG23	1:C:169:ASP:N	2.30	0.46
1:E:138:ASP:HB3	1:E:141:VAL:HG12	1.96	0.46
1:F:70:ASN:ND2	2:L:111:ARG:CD	2.73	0.46
2:J:331:ARG:N	2:J:332:GLY:HA2	2.30	0.46
2:K:135:LEU:O	2:K:139:SER:HB2	2.15	0.46
2:K:93:THR:HG21	2:K:133:LEU:HD11	1.96	0.46
1:C:42:VAL:HG13	1:C:52:ALA:HB1	1.97	0.46
1:C:167:ILE:HG23	1:C:168:ILE:H	1.80	0.46
2:J:21:ALA:HA	2:J:418:ILE:HD11	1.97	0.46
2:K:183:ASP:C	2:K:185:LEU:N	2.73	0.46
1:A:22:VAL:HG23	1:A:32:VAL:HG12	1.92	0.46
1:F:138:ASP:HB3	1:F:141:VAL:HG12	1.97	0.46
2:J:329:TYR:CD2	2:J:329:TYR:C	2.94	0.46
2:L:156:TYR:O	2:L:160:SER:HB2	2.15	0.46
2:L:256:THR:HB	2:L:284:LEU:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:294:ILE:HG23	2:I:382:PHE:HD2	1.80	0.46
2:J:247:PHE:O	2:J:251:TYR:HB2	2.16	0.46
2:K:308:ALA:HB3	2:K:309:SER:CA	2.36	0.46
2:K:329:TYR:C	2:K:329:TYR:CD2	2.94	0.46
1:B:102:VAL:HG21	1:B:113:LEU:HD22	1.97	0.46
1:H:168:ILE:HB	1:H:195:PRO:CB	2.46	0.46
2:J:327:ILE:O	2:J:331:ARG:HG3	2.15	0.46
2:K:146:LEU:O	2:K:150:ILE:HG22	2.15	0.46
1:F:195:PRO:HA	1:F:196:GLU:HA	1.76	0.46
2:I:275:THR:N	2:I:276:PRO:CD	2.79	0.46
2:I:277:ARG:HH11	2:I:305:ALA:HB2	1.81	0.46
2:I:331:ARG:N	2:I:332:GLY:HA2	2.31	0.46
2:J:135:LEU:O	2:J:139:SER:HB2	2.15	0.46
2:J:184:ASN:O	2:J:185:LEU:HB3	2.16	0.46
2:J:328:ALA:O	2:J:332:GLY:HA2	2.16	0.46
2:K:253:ASN:HD22	2:K:290:ARG:HG2	1.79	0.46
2:L:144:ALA:O	2:L:148:LEU:HB2	2.15	0.46
2:L:257:LEU:HD23	2:L:257:LEU:O	2.16	0.46
2:L:254:PRO:HA	2:L:258:GLY:HA3	1.98	0.46
2:J:16:PRO:HA	2:J:113:LEU:HD23	1.97	0.46
2:J:144:ALA:O	2:J:148:LEU:HB2	2.16	0.46
1:A:16:ARG:NH2	3:B:301:ATP:O2B	2.49	0.45
1:A:138:ASP:HB3	1:A:141:VAL:HG12	1.98	0.45
1:E:168:ILE:CG2	1:E:196:GLU:HB3	2.46	0.45
2:J:105:LYS:HA	2:J:106:ILE:HA	1.78	0.45
2:J:294:ILE:HG23	2:J:382:PHE:CD2	2.50	0.45
1:E:191:LEU:HD12	1:E:191:LEU:O	2.17	0.45
1:H:86:THR:HG21	1:H:112:VAL:HG21	1.97	0.45
2:J:250:GLU:O	2:J:257:LEU:HD22	2.15	0.45
2:J:398:THR:HB	2:J:399:PRO:HD3	1.97	0.45
2:K:145:ALA:O	2:K:149:SER:HB2	2.16	0.45
2:L:184:ASN:O	2:L:185:LEU:CB	2.64	0.45
1:A:102:VAL:HG21	1:A:113:LEU:HD22	1.97	0.45
1:G:166:SER:HB3	1:G:196:GLU:HB2	1.98	0.45
2:I:184:ASN:HB3	2:I:282:ASN:HB2	1.98	0.45
2:J:277:ARG:HA	2:J:278:THR:HA	1.67	0.45
2:K:152:LEU:HD22	2:K:193:THR:OG1	2.17	0.45
2:K:371:ILE:HD11	2:L:249:LEU:HD21	1.98	0.45
2:L:276:PRO:O	2:L:391:VAL:HG13	2.16	0.45
2:L:277:ARG:HA	2:L:278:THR:HA	1.68	0.45
1:H:172:VAL:CG1	1:H:178:CYS:HB2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:MET:SD	2:L:166:LEU:HD23	2.57	0.45
1:E:172:VAL:HG12	1:E:178:CYS:O	2.16	0.45
2:J:397:LEU:O	2:J:400:GLU:N	2.47	0.45
2:L:175:ASN:OD1	2:L:202:PHE:HB2	2.17	0.45
2:K:294:ILE:HG23	2:K:382:PHE:HD2	1.82	0.45
2:L:48:ILE:HD12	2:L:48:ILE:H	1.82	0.45
2:L:135:LEU:O	2:L:139:SER:HB2	2.17	0.45
1:E:85:SER:O	1:E:89:THR:HG23	2.17	0.45
1:G:191:LEU:HG	1:H:208:MET:HE2	1.99	0.45
2:I:135:LEU:O	2:I:139:SER:HB2	2.17	0.45
2:J:253:ASN:HD22	2:J:290:ARG:HG2	1.82	0.45
2:L:275:THR:N	2:L:276:PRO:CD	2.80	0.45
2:L:315:LYS:O	2:L:316:LEU:C	2.56	0.45
1:G:138:ASP:HB3	1:G:141:VAL:HG12	1.99	0.45
2:J:276:PRO:O	2:J:391:VAL:HG13	2.17	0.45
2:K:398:THR:HB	2:K:399:PRO:HD3	1.99	0.45
2:L:294:ILE:HG23	2:L:382:PHE:HD2	1.82	0.45
1:B:42:VAL:HG13	1:B:52:ALA:HB1	1.98	0.44
1:C:161:LYS:HG3	1:C:161:LYS:O	2.17	0.44
1:C:161:LYS:HG3	1:C:221:GLY:O	2.18	0.44
2:K:250:GLU:C	2:K:257:LEU:HD22	2.42	0.44
1:C:166:SER:HB3	1:C:196:GLU:HB2	1.98	0.44
2:I:184:ASN:O	2:I:185:LEU:HB3	2.17	0.44
2:J:152:LEU:O	2:J:152:LEU:CG	2.66	0.44
2:I:175:ASN:OD1	2:I:202:PHE:HB2	2.17	0.44
2:I:376:PRO:HG2	2:I:379:GLN:HB2	1.99	0.44
2:K:156:TYR:O	2:K:160:SER:HB2	2.16	0.44
2:K:318:THR:OG1	2:L:444:THR:O	2.35	0.44
2:K:397:LEU:O	2:K:400:GLU:N	2.51	0.44
2:L:63:LEU:HD22	2:L:394:THR:HG23	1.99	0.44
2:L:250:GLU:O	2:L:257:LEU:HD22	2.17	0.44
2:L:398:THR:HB	2:L:399:PRO:HD3	1.98	0.44
2:I:61:THR:HG23	2:I:390:THR:HA	2.00	0.44
2:I:329:TYR:CD2	2:I:329:TYR:C	2.95	0.44
2:J:208:GLY:HA2	2:J:308:ALA:HB3	1.85	0.44
1:G:189:ILE:HG21	1:H:151:TYR:CD2	2.53	0.44
2:I:256:THR:HB	2:I:284:LEU:HD13	1.99	0.44
2:K:437:TYR:HB2	2:L:342:SER:HB3	2.00	0.44
2:L:329:TYR:C	2:L:329:TYR:CD2	2.96	0.44
2:I:275:THR:N	2:I:276:PRO:HD3	2.33	0.44
2:L:328:ALA:O	2:L:332:GLY:HA2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ILE:HB	3:E:601:ATP:C2	2.52	0.44
2:J:189:VAL:HG22	2:J:283:SER:O	2.17	0.44
2:K:312:SER:CB	2:K:315:LYS:CG	2.95	0.44
2:L:275:THR:N	2:L:276:PRO:HD3	2.33	0.44
1:G:167:ILE:CG2	1:G:168:ILE:N	2.81	0.44
2:I:85:GLN:HA	2:I:174:ASN:HD21	1.82	0.44
2:K:388:PHE:C	2:K:390:THR:H	2.26	0.44
2:L:85:GLN:HA	2:L:174:ASN:HD21	1.82	0.44
1:D:161:LYS:O	1:D:161:LYS:HG3	2.18	0.43
2:K:173:PHE:HB2	2:K:201:LEU:HD22	2.00	0.43
2:K:376:PRO:HG2	2:K:379:GLN:HB2	2.00	0.43
1:F:97:ILE:HA	1:F:98:PRO:HD3	1.91	0.43
2:J:312:SER:OG	2:J:315:LYS:HD3	2.17	0.43
2:K:175:ASN:OD1	2:K:202:PHE:HB2	2.18	0.43
2:K:194:VAL:O	2:K:198:ILE:HB	2.18	0.43
2:K:277:ARG:HA	2:K:278:THR:HA	1.70	0.43
2:K:445:GLY:HA3	2:L:119:ASN:ND2	2.33	0.43
2:L:150:ILE:O	2:L:154:PRO:HD3	2.18	0.43
2:L:247:PHE:O	2:L:251:TYR:HB2	2.18	0.43
2:L:314:ILE:CG2	2:L:358:SER:OG	2.66	0.43
1:G:167:ILE:HG23	1:G:168:ILE:H	1.83	0.43
2:I:194:VAL:O	2:I:198:ILE:HB	2.19	0.43
2:J:294:ILE:HG23	2:J:382:PHE:HD2	1.83	0.43
1:C:16:ARG:NH2	3:D:301:ATP:O2B	2.50	0.43
1:C:196:GLU:OE1	1:C:196:GLU:N	2.50	0.43
1:F:111:LYS:HB2	1:G:90:LEU:HD21	1.99	0.43
1:G:42:VAL:HG13	1:G:52:ALA:HB1	1.99	0.43
2:I:141:GLU:O	2:I:145:ALA:CB	2.64	0.43
2:K:247:PHE:O	2:K:251:TYR:HB2	2.18	0.43
2:K:85:GLN:HA	2:K:174:ASN:HD21	1.83	0.43
2:K:342:SER:HB3	2:L:437:TYR:HB2	2.00	0.43
2:L:105:LYS:HA	2:L:106:ILE:HA	1.75	0.43
1:B:31:GLU:OE1	2:K:108:LEU:N	2.44	0.43
1:B:185:HIS:O	1:B:185:HIS:ND1	2.52	0.43
2:I:276:PRO:O	2:I:391:VAL:HG13	2.19	0.43
1:E:173:ARG:HA	1:E:178:CYS:O	2.18	0.43
2:I:235:THR:HG23	2:I:277:ARG:HH12	1.84	0.43
2:I:331:ARG:HB2	2:I:332:GLY:HA2	2.01	0.43
2:K:146:LEU:O	2:K:150:ILE:CG2	2.66	0.43
2:K:208:GLY:HA2	2:K:308:ALA:HB3	1.88	0.43
2:K:444:THR:O	2:L:318:THR:OG1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:THR:HG23	2:K:222:LYS:NZ	2.34	0.43
1:F:42:VAL:HG13	1:F:52:ALA:HB1	2.01	0.43
2:J:48:ILE:H	2:J:48:ILE:HD12	1.83	0.43
2:L:331:ARG:N	2:L:332:GLY:HA2	2.33	0.43
1:A:185:HIS:O	1:A:185:HIS:ND1	2.52	0.42
2:I:153:VAL:N	2:I:154:PRO:CD	2.82	0.42
2:K:96:VAL:HG21	2:K:114:VAL:CG2	2.49	0.42
2:K:141:GLU:O	2:K:145:ALA:CB	2.64	0.42
1:A:83:GLN:NE2	1:H:82:ILE:HB	2.34	0.42
1:D:161:LYS:HG3	1:D:221:GLY:O	2.19	0.42
1:E:102:VAL:HG21	1:E:113:LEU:HD22	2.00	0.42
2:J:175:ASN:OD1	2:J:202:PHE:HB2	2.19	0.42
2:K:189:VAL:HG11	2:K:260:LEU:HD21	2.01	0.42
1:A:112:VAL:CG2	1:H:90:LEU:HD22	2.49	0.42
1:C:11:VAL:CB	1:C:22:VAL:HG22	2.48	0.42
1:E:181:LEU:HD13	1:F:181:LEU:HD13	2.01	0.42
1:H:195:PRO:HA	1:H:196:GLU:HA	1.75	0.42
1:G:162:LEU:O	1:G:165:LYS:HG2	2.19	0.42
2:I:173:PHE:HB2	2:I:201:LEU:HD22	2.02	0.42
2:I:361:ILE:CD1	2:I:415:ILE:HG21	2.49	0.42
2:K:119:ASN:ND2	2:L:445:GLY:HA3	2.34	0.42
2:K:379:GLN:CA	2:K:395:MET:HE1	2.48	0.42
2:K:431:GLU:OE1	2:L:333:LYS:HE3	2.20	0.42
2:L:28:ILE:HG12	2:L:58:THR:HG23	1.92	0.42
1:E:165:LYS:HD2	1:E:170:LEU:HD11	2.02	0.42
1:H:97:ILE:HA	1:H:98:PRO:HD3	1.89	0.42
2:I:153:VAL:N	2:I:154:PRO:HD3	2.35	0.42
2:J:378:LEU:HG	2:J:395:MET:HE1	2.00	0.42
2:K:442:VAL:HG13	2:L:347:ILE:HG21	2.02	0.42
2:L:301:MET:SD	2:L:391:VAL:HG21	2.59	0.42
1:B:172:VAL:HG21	1:B:180:ILE:HG13	2.02	0.42
1:E:162:LEU:O	1:E:165:LYS:HG2	2.20	0.42
1:H:194:ALA:HA	1:H:195:PRO:HD3	1.89	0.42
2:I:376:PRO:HG2	2:I:379:GLN:CB	2.49	0.42
2:L:256:THR:O	2:L:257:LEU:CB	2.66	0.42
1:A:130:VAL:O	1:A:134:GLN:HG2	2.20	0.42
1:G:168:ILE:CG2	1:G:169:ASP:N	2.82	0.42
2:I:254:PRO:HA	2:I:258:GLY:HA3	2.01	0.42
2:J:96:VAL:HG21	2:J:114:VAL:CG2	2.50	0.42
2:J:118:LEU:O	2:J:119:ASN:C	2.62	0.42
2:J:156:TYR:O	2:J:160:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:312:SER:OG	2:L:315:LYS:HD3	2.19	0.42
2:J:308:ALA:HB3	2:J:309:SER:CA	2.39	0.42
2:K:184:ASN:HB3	2:K:282:ASN:HB2	2.01	0.42
2:L:61:THR:HG23	2:L:390:THR:HA	2.02	0.42
2:L:102:LEU:HD23	2:L:102:LEU:HA	1.80	0.42
1:A:195:PRO:HA	1:A:196:GLU:HA	1.74	0.42
2:I:277:ARG:HA	2:I:278:THR:HA	1.67	0.42
2:K:324:THR:HA	2:K:327:ILE:HD12	2.01	0.42
2:L:277:ARG:HH11	2:L:305:ALA:HB2	1.84	0.42
2:L:369:LEU:HG	2:L:408:ILE:HD11	2.02	0.42
1:B:196:GLU:OE1	1:B:196:GLU:N	2.50	0.42
1:C:165:LYS:HD2	1:C:170:LEU:HD11	2.02	0.42
1:E:206:VAL:HG21	1:F:147:LEU:HD22	2.01	0.42
2:I:318:THR:OG1	2:J:444:THR:O	2.38	0.42
2:J:61:THR:HG23	2:J:390:THR:HA	2.01	0.42
2:J:361:ILE:CD1	2:J:415:ILE:HG21	2.49	0.42
2:K:404:ALA:O	2:K:407:CYS:HB2	2.20	0.42
2:I:247:PHE:O	2:I:251:TYR:HB2	2.19	0.41
2:K:347:ILE:HG21	2:L:442:VAL:HG13	2.01	0.41
2:L:314:ILE:HG22	2:L:358:SER:OG	2.20	0.41
2:I:150:ILE:O	2:I:154:PRO:HD3	2.20	0.41
2:J:186:MET:O	2:J:187:SER:C	2.63	0.41
2:L:253:ASN:HD22	2:L:290:ARG:HG2	1.84	0.41
2:L:376:PRO:HG2	2:L:379:GLN:HB2	2.02	0.41
1:G:167:ILE:CG2	1:G:197:ASP:N	2.80	0.41
2:I:81:MET:HG3	2:I:167:PHE:CD1	2.55	0.41
2:I:96:VAL:HG21	2:I:114:VAL:CG2	2.51	0.41
2:I:301:MET:SD	2:I:391:VAL:HG21	2.60	0.41
2:J:277:ARG:HH11	2:J:305:ALA:HB2	1.85	0.41
2:K:147:ILE:C	2:K:150:ILE:HG22	2.43	0.41
2:L:298:LEU:HD21	2:L:381:VAL:HG12	2.02	0.41
2:J:376:PRO:HG2	2:J:379:GLN:HB2	2.02	0.41
2:L:306:GLY:O	2:L:315:LYS:HB3	2.21	0.41
1:E:130:VAL:O	1:E:134:GLN:HG2	2.20	0.41
2:I:342:SER:HB3	2:J:437:TYR:HB2	2.02	0.41
2:J:272:GLN:HG3	2:J:286:PHE:CZ	2.55	0.41
2:L:146:LEU:O	2:L:150:ILE:HG23	2.20	0.41
1:B:195:PRO:HA	1:B:196:GLU:HA	1.75	0.41
1:C:132:ILE:HD13	1:C:132:ILE:HA	1.94	0.41
1:E:168:ILE:HG23	1:E:169:ASP:N	2.36	0.41
1:F:132:ILE:HD13	1:F:132:ILE:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:ASN:ND2	2:J:445:GLY:HA3	2.35	0.41
2:L:388:PHE:C	2:L:390:THR:H	2.28	0.41
1:B:22:VAL:HG21	1:B:34:ALA:HB2	2.02	0.41
1:C:161:LYS:CG	1:C:221:GLY:O	2.68	0.41
1:E:103:LYS:NZ	3:E:601:ATP:O3G	2.52	0.41
1:H:33:LEU:HD11	1:H:53:VAL:HG12	2.02	0.41
2:I:153:VAL:HG13	2:I:156:TYR:CD2	2.55	0.41
2:J:314:ILE:O	2:J:314:ILE:CG1	2.67	0.41
2:K:438:PRO:HG2	2:L:341:ARG:HG2	2.03	0.41
2:L:152:LEU:C	2:L:154:PRO:HD2	2.46	0.41
1:G:196:GLU:OE1	1:G:196:GLU:N	2.50	0.41
1:D:22:VAL:CG2	1:D:32:VAL:HG11	2.37	0.41
2:I:118:LEU:O	2:I:119:ASN:C	2.64	0.41
2:I:167:PHE:CD2	2:I:167:PHE:C	2.99	0.41
2:I:326:VAL:CG2	2:J:352:LEU:HD13	2.51	0.41
2:J:298:LEU:HD21	2:J:381:VAL:HG12	2.03	0.41
2:K:96:VAL:HG21	2:K:114:VAL:HG22	2.02	0.41
2:K:111:ARG:HH12	2:K:125:GLY:HA2	1.81	0.41
2:K:277:ARG:HH11	2:K:305:ALA:HB2	1.86	0.41
2:K:304:GLY:HA3	2:K:312:SER:OG	2.21	0.41
2:K:363:PHE:CD2	2:K:363:PHE:C	2.99	0.41
1:A:191:LEU:CD1	1:B:209:GLY:HA2	2.51	0.41
1:D:97:ILE:HA	1:D:98:PRO:HD3	1.93	0.41
1:D:161:LYS:CG	1:D:221:GLY:O	2.68	0.41
2:I:372:THR:O	2:I:372:THR:HG22	2.21	0.41
2:I:430:THR:HA	2:J:331:ARG:O	2.21	0.41
2:K:189:VAL:HG22	2:K:283:SER:O	2.21	0.41
2:K:331:ARG:N	2:K:332:GLY:HA2	2.34	0.41
2:K:361:ILE:CD1	2:K:415:ILE:HG21	2.51	0.41
1:A:82:ILE:HG21	1:H:87:LEU:HD11	2.02	0.40
1:C:8:GLN:HE21	2:I:108:LEU:N	2.17	0.40
1:D:108:TYR:OH	1:E:60:GLU:OE1	2.37	0.40
1:F:67:GLY:O	1:F:70:ASN:HB2	2.21	0.40
2:J:167:PHE:CD2	2:J:167:PHE:C	2.99	0.40
2:J:173:PHE:HB2	2:J:201:LEU:HD22	2.03	0.40
2:J:256:THR:O	2:J:257:LEU:HB3	2.20	0.40
2:K:61:THR:HG23	2:K:390:THR:HA	2.02	0.40
2:L:105:LYS:O	2:L:105:LYS:CG	2.67	0.40
2:L:141:GLU:O	2:L:145:ALA:CB	2.68	0.40
2:L:173:PHE:HB2	2:L:201:LEU:HD22	2.03	0.40
2:L:324:THR:HA	2:L:327:ILE:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HA	1:C:98:PRO:HD3	1.93	0.40
1:G:97:ILE:HA	1:G:98:PRO:HD3	1.92	0.40
2:I:111:ARG:HH12	2:I:125:GLY:HA2	1.85	0.40
2:I:184:ASN:O	2:I:185:LEU:CB	2.69	0.40
2:I:308:ALA:HB3	2:I:309:SER:CA	2.36	0.40
2:I:444:THR:O	2:J:318:THR:OG1	2.40	0.40
2:K:167:PHE:CD2	2:K:167:PHE:C	2.98	0.40
2:K:249:LEU:HD23	2:L:371:ILE:HD11	2.03	0.40
1:H:165:LYS:HD2	1:H:170:LEU:HD11	2.03	0.40
2:I:373:GLU:OE2	2:I:405:GLY:HA3	2.21	0.40
1:F:9:PHE:HB2	1:F:32:VAL:HG22	2.03	0.40
1:H:89:THR:CG2	1:H:102:VAL:CG1	2.99	0.40
2:K:16:PRO:HA	2:K:113:LEU:CD2	2.52	0.40
2:L:361:ILE:CD1	2:L:415:ILE:HG21	2.51	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ARG:NH2	1:G:163:ASP:CA[2_646]	1.13	1.07
1:E:160:ARG:NH2	1:G:163:ASP:CB[2_646]	1.34	0.86
1:E:160:ARG:O	1:G:165:LYS:NZ[2_646]	1.40	0.80
1:E:160:ARG:NH1	1:G:163:ASP:N[2_646]	1.52	0.68
1:E:160:ARG:NH2	1:G:163:ASP:C[2_646]	1.61	0.59
1:E:160:ARG:CD	1:G:160:ARG:O[2_646]	1.69	0.51
1:F:160:ARG:CD	2:I:39:ILE:CD1[2_545]	1.75	0.45
1:E:160:ARG:CZ	1:G:163:ASP:N[2_646]	1.81	0.39
1:E:160:ARG:NH2	1:G:163:ASP:N[2_646]	1.81	0.39
1:E:161:LYS:CA	1:G:165:LYS:NZ[2_646]	1.82	0.38
1:E:160:ARG:NH2	1:G:163:ASP:O[2_646]	1.89	0.31
1:E:160:ARG:C	1:G:165:LYS:NZ[2_646]	1.92	0.28
1:A:173:ARG:NH1	1:G:171:ASN:ND2[2_656]	1.94	0.26
1:E:160:ARG:O	1:G:165:LYS:CE[2_646]	1.94	0.26
1:E:163:ASP:OD2	1:G:161:LYS:NZ[2_646]	1.94	0.26
1:E:160:ARG:NE	1:G:160:ARG:O[2_646]	1.96	0.24
1:E:160:ARG:NH1	1:G:162:LEU:C[2_646]	1.96	0.24
1:E:161:LYS:C	1:G:165:LYS:NZ[2_646]	2.06	0.14
1:E:161:LYS:N	1:G:165:LYS:NZ[2_646]	2.07	0.13
1:E:160:ARG:CZ	1:G:163:ASP:CA[2_646]	2.15	0.05

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	214/222 (96%)	209 (98%)	5 (2%)	0	100	100
1	B	215/222 (97%)	211 (98%)	4 (2%)	0	100	100
1	C	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
1	D	215/222 (97%)	212 (99%)	3 (1%)	0	100	100
1	E	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
1	F	215/222 (97%)	210 (98%)	5 (2%)	0	100	100
1	G	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
1	H	215/222 (97%)	211 (98%)	4 (2%)	0	100	100
2	I	425/465 (91%)	372 (88%)	52 (12%)	1 (0%)	43	74
2	J	425/465 (91%)	375 (88%)	49 (12%)	1 (0%)	43	74
2	K	425/465 (91%)	374 (88%)	51 (12%)	0	100	100
2	L	425/465 (91%)	375 (88%)	49 (12%)	1 (0%)	43	74
All	All	3416/3636 (94%)	3179 (93%)	234 (7%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	154	PRO
2	I	176	ALA
2	L	176	ALA

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	185/190 (97%)	182 (98%)	3 (2%)	55	70
1	B	186/190 (98%)	184 (99%)	2 (1%)	65	74
1	C	185/190 (97%)	182 (98%)	3 (2%)	55	70
1	D	186/190 (98%)	184 (99%)	2 (1%)	65	74
1	E	185/190 (97%)	183 (99%)	2 (1%)	65	74
1	F	186/190 (98%)	183 (98%)	3 (2%)	55	70
1	G	185/190 (97%)	182 (98%)	3 (2%)	55	70
1	H	186/190 (98%)	183 (98%)	3 (2%)	55	70
2	I	359/391 (92%)	353 (98%)	6 (2%)	53	70
2	J	359/391 (92%)	354 (99%)	5 (1%)	59	71
2	K	359/391 (92%)	353 (98%)	6 (2%)	53	70
2	L	359/391 (92%)	353 (98%)	6 (2%)	53	70
All	All	2920/3084 (95%)	2876 (98%)	44 (2%)	57	71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	63	LEU
1	A	157	LEU
1	B	53	VAL
1	B	157	LEU
1	C	53	VAL
1	C	132	ILE
1	C	157	LEU
1	D	53	VAL
1	D	157	LEU
1	E	53	VAL
1	E	157	LEU
1	F	53	VAL
1	F	157	LEU
1	F	172	VAL
1	G	53	VAL
1	G	132	ILE
1	G	157	LEU
1	H	53	VAL
1	H	157	LEU
1	H	191	LEU
2	I	66	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	106	ILE
2	I	249	LEU
2	I	299	LEU
2	I	393	LEU
2	I	395	MET
2	J	34	LEU
2	J	106	ILE
2	J	150	ILE
2	J	299	LEU
2	J	393	LEU
2	K	66	VAL
2	K	106	ILE
2	K	226	LEU
2	K	299	LEU
2	K	314	ILE
2	K	393	LEU
2	L	106	ILE
2	L	150	ILE
2	L	226	LEU
2	L	299	LEU
2	L	314	ILE
2	L	393	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	51	HIS
1	A	134	GLN
1	A	210	HIS
1	B	8	GLN
1	B	26	HIS
1	B	51	HIS
1	B	186	HIS
1	B	210	HIS
1	C	8	GLN
1	C	26	HIS
1	C	83	GLN
1	C	186	HIS
1	C	210	HIS
1	D	26	HIS
1	D	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	210	HIS
1	E	26	HIS
1	E	51	HIS
1	E	134	GLN
1	E	210	HIS
1	F	6	ASN
1	F	26	HIS
1	F	51	HIS
1	F	186	HIS
1	F	210	HIS
1	G	26	HIS
1	G	51	HIS
1	G	83	GLN
1	G	134	GLN
1	G	186	HIS
1	G	210	HIS
1	H	6	ASN
1	H	26	HIS
1	H	210	HIS
2	I	175	ASN
2	J	155	GLN
2	J	175	ASN
2	J	272	GLN
2	K	174	ASN
2	K	175	ASN
2	K	272	GLN
2	L	174	ASN
2	L	175	ASN
2	L	272	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
3	ATP	F	301	-	32,33,33	1.57	6 (18%)	48,52,52	2.58	13 (27%)
3	ATP	D	301	-	32,33,33	1.64	7 (21%)	48,52,52	2.77	12 (25%)
3	ATP	H	301	-	32,33,33	1.60	7 (21%)	48,52,52	2.70	11 (22%)
3	ATP	G	601	-	32,33,33	1.68	7 (21%)	48,52,52	2.78	15 (31%)
3	ATP	B	301	-	32,33,33	1.67	8 (25%)	48,52,52	2.77	15 (31%)
3	ATP	C	601	-	32,33,33	1.59	6 (18%)	48,52,52	2.79	11 (22%)
3	ATP	A	601	-	32,33,33	1.50	5 (15%)	48,52,52	2.74	14 (29%)
3	ATP	E	601	-	32,33,33	1.59	6 (18%)	48,52,52	2.69	13 (27%)

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
3	ATP	F	301	-	-	5/22/38/38	0/3/3/3
3	ATP	D	301	-	-	4/22/38/38	0/3/3/3
3	ATP	H	301	-	-	5/22/38/38	0/3/3/3
3	ATP	G	601	-	-	4/22/38/38	0/3/3/3
3	ATP	B	301	-	-	7/22/38/38	0/3/3/3
3	ATP	C	601	-	-	7/22/38/38	0/3/3/3
3	ATP	A	601	-	-	8/22/38/38	0/3/3/3
3	ATP	E	601	-	-	3/22/38/38	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	ATP	C6-N6	3.70	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ATP	C6-N6	3.64	1.43	1.34
3	A	601	ATP	C6-N6	3.62	1.43	1.34
3	F	301	ATP	C6-N6	3.61	1.43	1.34
3	G	601	ATP	C6-N6	3.59	1.43	1.34
3	D	301	ATP	C6-N6	3.55	1.43	1.34
3	B	301	ATP	C6-N6	3.54	1.43	1.34
3	H	301	ATP	C5-N7	-3.49	1.32	1.39
3	H	301	ATP	PB-O3A	-3.48	1.55	1.59
3	H	301	ATP	C6-N6	3.42	1.42	1.34
3	G	601	ATP	PB-O3B	-3.42	1.55	1.59
3	D	301	ATP	C5-N7	-3.38	1.32	1.39
3	C	601	ATP	C5-N7	-3.25	1.33	1.39
3	G	601	ATP	PB-O3A	-3.20	1.56	1.59
3	F	301	ATP	C5-N7	-3.13	1.33	1.39
3	B	301	ATP	C5-N7	-3.07	1.33	1.39
3	B	301	ATP	PB-O3A	-3.02	1.56	1.59
3	D	301	ATP	PB-O3A	-3.00	1.56	1.59
3	B	301	ATP	PB-O3B	-2.98	1.56	1.59
3	G	601	ATP	C5-N7	-2.96	1.33	1.39
3	E	601	ATP	C5-N7	-2.95	1.33	1.39
3	F	301	ATP	PB-O3B	-2.86	1.56	1.59
3	A	601	ATP	C5-N7	-2.83	1.33	1.39
3	E	601	ATP	O4'-C4'	-2.67	1.39	1.45
3	F	301	ATP	PB-O3A	-2.65	1.56	1.59
3	D	301	ATP	PB-O3B	-2.60	1.56	1.59
3	C	601	ATP	O4'-C4'	-2.56	1.39	1.45
3	A	601	ATP	C2'-C3'	-2.52	1.46	1.53
3	B	301	ATP	O4'-C4'	-2.51	1.39	1.45
3	A	601	ATP	PB-O3B	-2.45	1.56	1.59
3	E	601	ATP	C2'-C3'	-2.45	1.46	1.53
3	E	601	ATP	PB-O3B	-2.44	1.56	1.59
3	C	601	ATP	C2'-C3'	-2.42	1.46	1.53
3	G	601	ATP	C2'-C3'	-2.42	1.46	1.53
3	D	301	ATP	C8-N9	-2.40	1.33	1.37
3	A	601	ATP	O4'-C4'	-2.39	1.39	1.45
3	D	301	ATP	C2'-C3'	-2.37	1.46	1.53
3	H	301	ATP	O4'-C4'	-2.33	1.39	1.45
3	F	301	ATP	C2'-C3'	-2.30	1.47	1.53
3	H	301	ATP	C2'-C3'	-2.30	1.47	1.53
3	G	601	ATP	O4'-C4'	-2.29	1.39	1.45
3	B	301	ATP	C2'-C3'	-2.26	1.47	1.53
3	D	301	ATP	O4'-C4'	-2.24	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ATP	C8-N9	-2.22	1.33	1.37
3	C	601	ATP	O2'-C2'	-2.17	1.37	1.43
3	F	301	ATP	O4'-C4'	-2.12	1.40	1.45
3	E	601	ATP	PB-O3A	-2.11	1.57	1.59
3	H	301	ATP	O2'-C2'	-2.10	1.37	1.43
3	G	601	ATP	PA-O3A	-2.07	1.57	1.59
3	H	301	ATP	C8-N9	-2.07	1.34	1.37
3	B	301	ATP	PA-O3A	-2.06	1.57	1.59
3	B	301	ATP	C8-N9	-2.03	1.34	1.37

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	ATP	O3A-PA-O1A	-11.41	76.37	110.70
3	C	601	ATP	O3A-PA-O1A	-10.89	77.93	110.70
3	B	301	ATP	O3A-PA-O1A	-10.22	79.95	110.70
3	A	601	ATP	O3A-PA-O1A	-9.64	81.71	110.70
3	D	301	ATP	O3A-PA-O1A	-9.60	81.81	110.70
3	E	601	ATP	O3A-PA-O1A	-9.59	81.87	110.70
3	G	601	ATP	O3A-PA-O1A	-9.41	82.40	110.70
3	F	301	ATP	O3A-PA-O1A	-7.65	87.68	110.70
3	F	301	ATP	O2A-PA-O1A	-6.85	80.57	112.44
3	C	601	ATP	O2A-PA-O1A	-6.69	81.33	112.44
3	E	601	ATP	O2A-PA-O1A	-6.50	82.22	112.44
3	G	601	ATP	O5'-PA-O1A	-6.49	83.22	108.94
3	A	601	ATP	O2A-PA-O1A	-6.46	82.42	112.44
3	H	301	ATP	O2A-PA-O1A	-6.41	82.63	112.44
3	B	301	ATP	O5'-PA-O1A	-6.28	84.06	108.94
3	D	301	ATP	O5'-PA-O1A	-6.20	84.38	108.94
3	A	601	ATP	O2A-PA-O3A	6.14	123.88	107.27
3	B	301	ATP	N3-C2-N1	-6.08	119.38	128.58
3	D	301	ATP	O2A-PA-O1A	-6.08	84.18	112.44
3	F	301	ATP	O5'-PA-O1A	-5.94	85.40	108.94
3	F	301	ATP	N3-C2-N1	-5.90	119.65	128.58
3	C	601	ATP	N3-C2-N1	-5.87	119.69	128.58
3	G	601	ATP	N3-C2-N1	-5.81	119.78	128.58
3	G	601	ATP	O2A-PA-O1A	-5.80	85.46	112.44
3	D	301	ATP	C5-C4-N3	-5.80	118.73	126.72
3	E	601	ATP	O5'-PA-O1A	-5.63	86.63	108.94
3	F	301	ATP	C5-C4-N3	-5.63	118.97	126.72
3	C	601	ATP	O2A-PA-O3A	5.62	122.47	107.27
3	A	601	ATP	N3-C2-N1	-5.56	120.17	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	ATP	C5-C4-N3	-5.52	119.12	126.72
3	E	601	ATP	O2A-PA-O3A	5.51	122.16	107.27
3	A	601	ATP	O5'-PA-O1A	-5.50	87.14	108.94
3	B	301	ATP	O2A-PA-O1A	-5.49	86.91	112.44
3	E	601	ATP	N3-C2-N1	-5.48	120.28	128.58
3	D	301	ATP	N3-C2-N1	-5.48	120.29	128.58
3	H	301	ATP	N3-C2-N1	-5.39	120.42	128.58
3	H	301	ATP	O2A-PA-O3A	5.28	121.55	107.27
3	C	601	ATP	C5-C4-N3	-5.21	119.54	126.72
3	E	601	ATP	C5-C4-N3	-5.12	119.67	126.72
3	H	301	ATP	C5-C4-N3	-4.95	119.90	126.72
3	B	301	ATP	O2A-PA-O3A	4.81	120.28	107.27
3	B	301	ATP	C5-C4-N3	-4.74	120.19	126.72
3	D	301	ATP	O2A-PA-O3A	4.71	120.01	107.27
3	A	601	ATP	C5-C4-N3	-4.64	120.33	126.72
3	H	301	ATP	O5'-PA-O1A	-4.63	90.57	108.94
3	C	601	ATP	O5'-PA-O1A	-4.57	90.83	108.94
3	D	301	ATP	N3-C4-N9	4.55	134.90	127.17
3	F	301	ATP	N3-C4-N9	4.41	134.66	127.17
3	G	601	ATP	N3-C4-N9	4.39	134.63	127.17
3	D	301	ATP	C5-N7-C8	4.32	110.24	103.45
3	G	601	ATP	O2A-PA-O3A	4.20	118.64	107.27
3	F	301	ATP	O2A-PA-O3A	4.19	118.58	107.27
3	C	601	ATP	C5-N7-C8	4.10	109.90	103.45
3	B	301	ATP	C5-N7-C8	4.08	109.86	103.45
3	E	601	ATP	N3-C4-N9	4.02	134.01	127.17
3	C	601	ATP	N3-C4-N9	4.01	133.99	127.17
3	F	301	ATP	C2-N3-C4	4.00	121.61	111.83
3	G	601	ATP	C5-N7-C8	3.99	109.72	103.45
3	G	601	ATP	C2-N3-C4	3.91	121.38	111.83
3	A	601	ATP	C5-N7-C8	3.87	109.53	103.45
3	D	301	ATP	C2-N3-C4	3.82	121.15	111.83
3	D	301	ATP	C4-C5-N7	-3.77	106.27	110.58
3	H	301	ATP	N3-C4-N9	3.77	133.57	127.17
3	E	601	ATP	C5-N7-C8	3.73	109.31	103.45
3	C	601	ATP	C2-N3-C4	3.73	120.93	111.83
3	C	601	ATP	C4-C5-N7	-3.68	106.37	110.58
3	B	301	ATP	N3-C4-N9	3.68	133.42	127.17
3	B	301	ATP	C2-N3-C4	3.67	120.80	111.83
3	E	601	ATP	C2-N3-C4	3.59	120.61	111.83
3	A	601	ATP	N3-C4-N9	3.59	133.27	127.17
3	F	301	ATP	C5-N7-C8	3.56	109.05	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	ATP	C4-C5-N7	-3.52	106.55	110.58
3	A	601	ATP	C2-N3-C4	3.45	120.26	111.83
3	H	301	ATP	C5-N7-C8	3.41	108.82	103.45
3	G	601	ATP	C4-C5-N7	-3.38	106.72	110.58
3	A	601	ATP	C4-C5-N7	-3.38	106.72	110.58
3	H	301	ATP	C2-N3-C4	3.34	119.98	111.83
3	E	601	ATP	C4-C5-N7	-3.22	106.90	110.58
3	G	601	ATP	C4'-O4'-C1'	-3.22	102.37	109.47
3	B	301	ATP	N9-C8-N7	-3.16	109.45	113.94
3	H	301	ATP	C4-C5-N7	-3.06	107.09	110.58
3	D	301	ATP	N9-C8-N7	-3.05	109.61	113.94
3	A	601	ATP	N9-C8-N7	-3.04	109.62	113.94
3	F	301	ATP	C4-C5-N7	-2.97	107.19	110.58
3	G	601	ATP	N9-C8-N7	-2.83	109.92	113.94
3	C	601	ATP	N9-C8-N7	-2.80	109.96	113.94
3	E	601	ATP	N9-C8-N7	-2.50	110.39	113.94
3	G	601	ATP	O2G-PG-O3B	2.47	112.92	104.64
3	B	301	ATP	O3G-PG-O3B	2.41	112.73	104.64
3	G	601	ATP	O2A-PA-O5'	2.35	118.23	107.57
3	A	601	ATP	O4'-C4'-C3'	2.31	109.73	105.15
3	E	601	ATP	O3G-PG-O3B	2.29	112.33	104.64
3	G	601	ATP	O4'-C4'-C3'	2.29	109.70	105.15
3	B	301	ATP	O2A-PA-O5'	2.27	117.85	107.57
3	F	301	ATP	N9-C8-N7	-2.22	110.79	113.94
3	D	301	ATP	O4'-C4'-C3'	2.22	109.55	105.15
3	H	301	ATP	N9-C8-N7	-2.14	110.90	113.94
3	B	301	ATP	O4'-C4'-C3'	2.11	109.34	105.15
3	A	601	ATP	C4'-O4'-C1'	-2.11	104.82	109.47
3	E	601	ATP	O2A-PA-O5'	2.09	117.03	107.57
3	F	301	ATP	O5'-C5'-C4'	2.05	115.99	108.99
3	F	301	ATP	O2A-PA-O5'	2.05	116.86	107.57
3	A	601	ATP	O2A-PA-O5'	2.01	116.67	107.57
3	B	301	ATP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ATP	C5'-O5'-PA-O3A
3	B	301	ATP	C5'-O5'-PA-O3A
3	C	601	ATP	C5'-O5'-PA-O2A
3	C	601	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

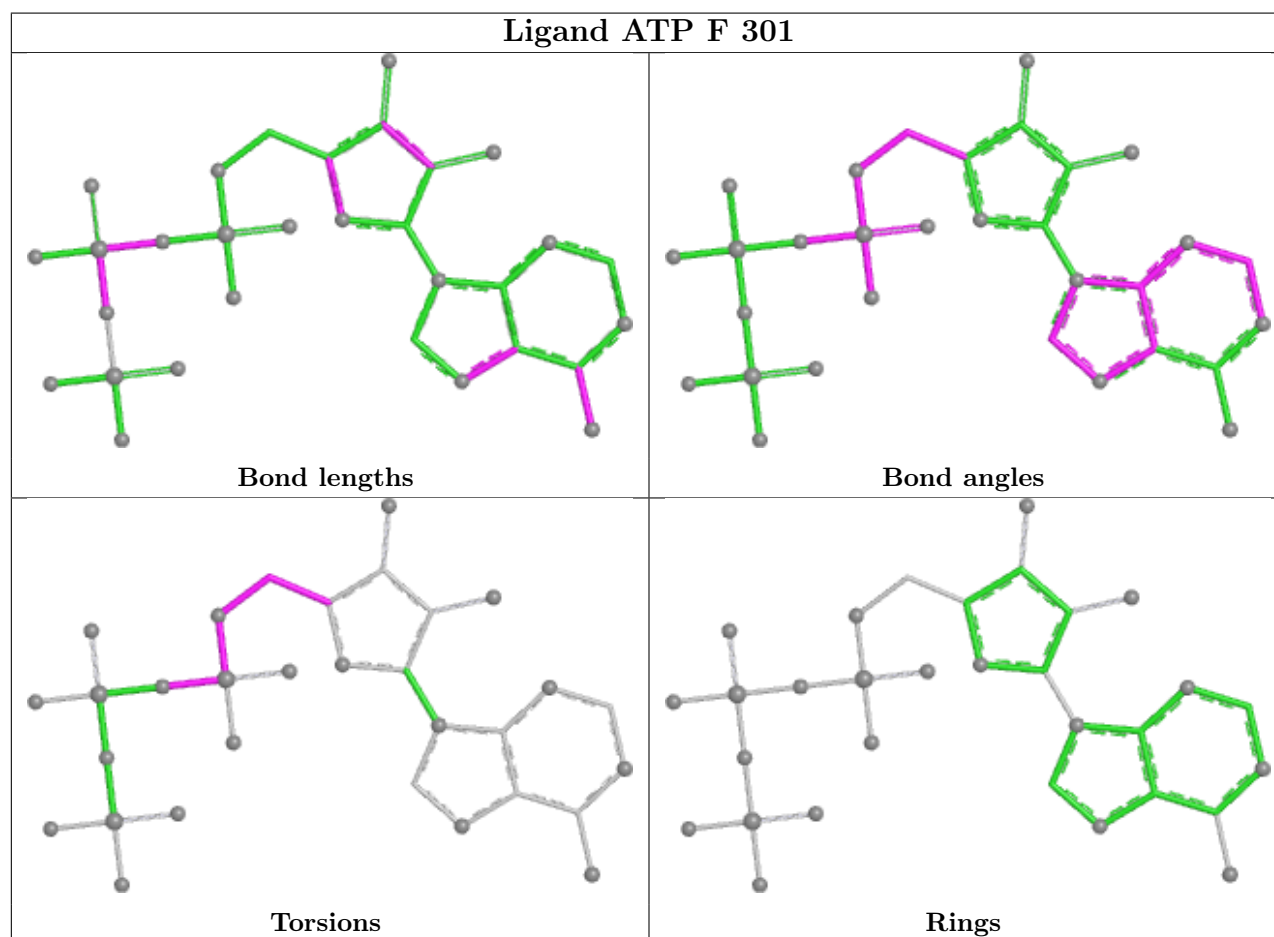
Mol	Chain	Res	Type	Atoms
3	D	301	ATP	C5'-O5'-PA-O3A
3	E	601	ATP	PB-O3A-PA-O5'
3	E	601	ATP	C5'-O5'-PA-O1A
3	E	601	ATP	C5'-O5'-PA-O3A
3	G	601	ATP	C5'-O5'-PA-O3A
3	H	301	ATP	C5'-O5'-PA-O3A
3	H	301	ATP	O4'-C4'-C5'-O5'
3	H	301	ATP	C3'-C4'-C5'-O5'
3	B	301	ATP	O4'-C4'-C5'-O5'
3	C	601	ATP	O4'-C4'-C5'-O5'
3	C	601	ATP	C3'-C4'-C5'-O5'
3	B	301	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
3	G	601	ATP	C3'-C4'-C5'-O5'
3	A	601	ATP	O4'-C4'-C5'-O5'
3	F	301	ATP	O4'-C4'-C5'-O5'
3	D	301	ATP	O4'-C4'-C5'-O5'
3	A	601	ATP	C3'-C4'-C5'-O5'
3	A	601	ATP	PB-O3A-PA-O5'
3	B	301	ATP	PB-O3A-PA-O5'
3	D	301	ATP	PB-O3A-PA-O5'
3	A	601	ATP	C2'-C1'-N9-C8
3	B	301	ATP	C2'-C1'-N9-C8
3	F	301	ATP	PB-O3A-PA-O2A
3	H	301	ATP	C4'-C5'-O5'-PA
3	C	601	ATP	C5'-O5'-PA-O1A
3	D	301	ATP	C5'-O5'-PA-O1A
3	F	301	ATP	C5'-O5'-PA-O1A
3	F	301	ATP	C5'-O5'-PA-O3A
3	A	601	ATP	C2'-C1'-N9-C4
3	C	601	ATP	C4'-C5'-O5'-PA
3	B	301	ATP	O4'-C1'-N9-C8
3	F	301	ATP	C4'-C5'-O5'-PA
3	A	601	ATP	PB-O3A-PA-O1A
3	B	301	ATP	PB-O3A-PA-O1A
3	C	601	ATP	PB-O3A-PA-O2A
3	A	601	ATP	O4'-C1'-N9-C8
3	G	601	ATP	C2'-C1'-N9-C8
3	H	301	ATP	PB-O3A-PA-O2A

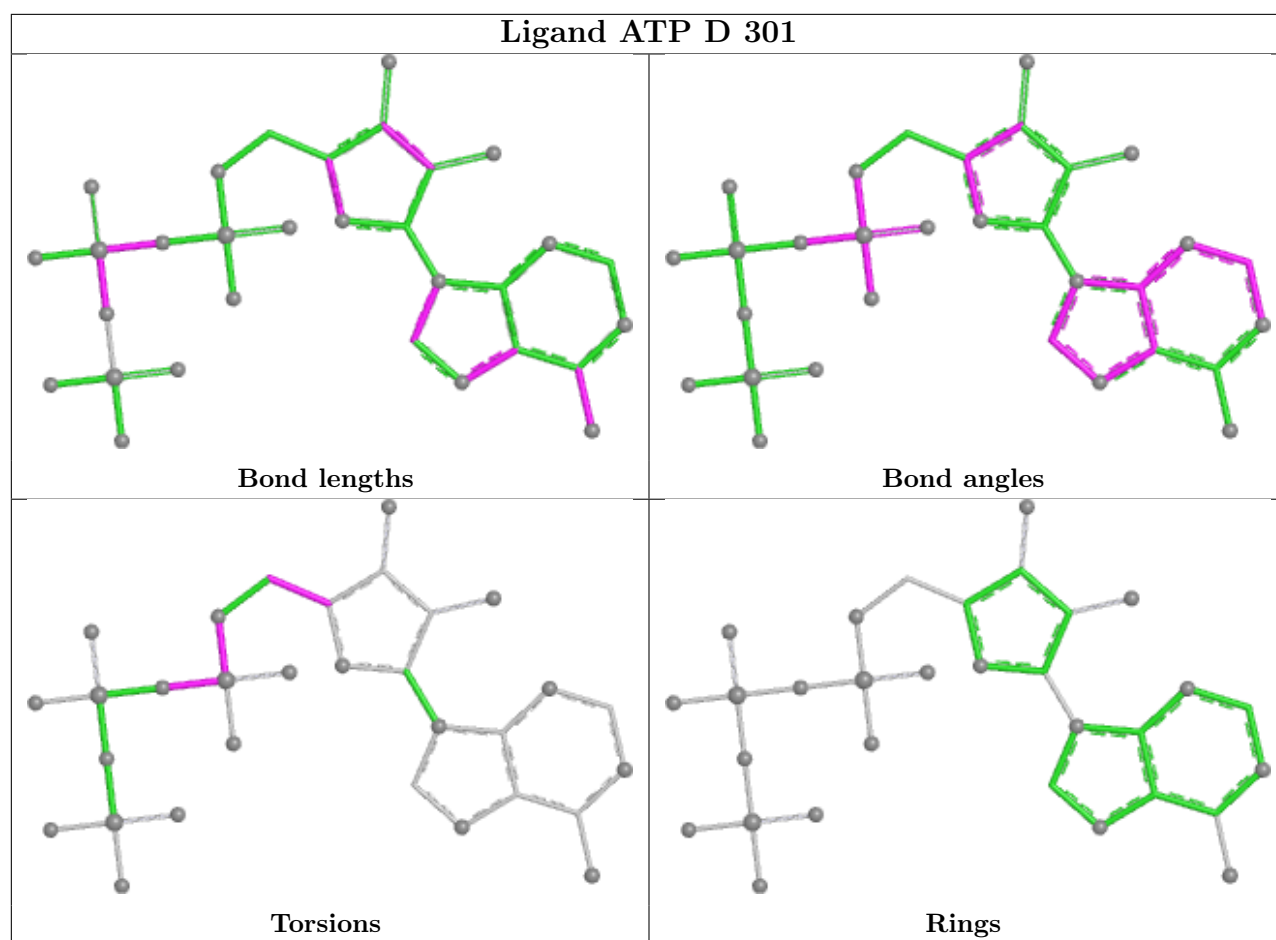
There are no ring outliers.

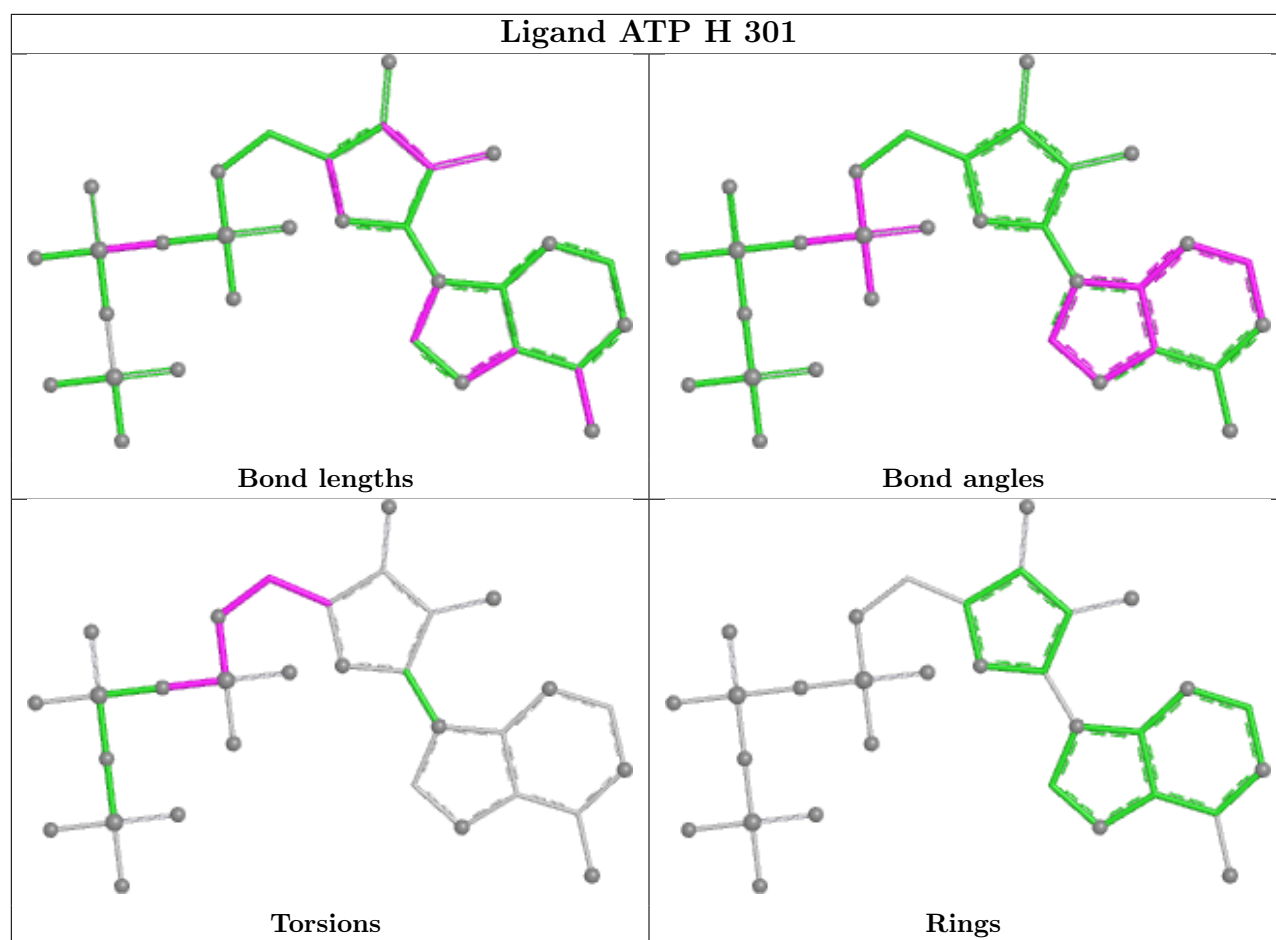
6 monomers are involved in 11 short contacts:

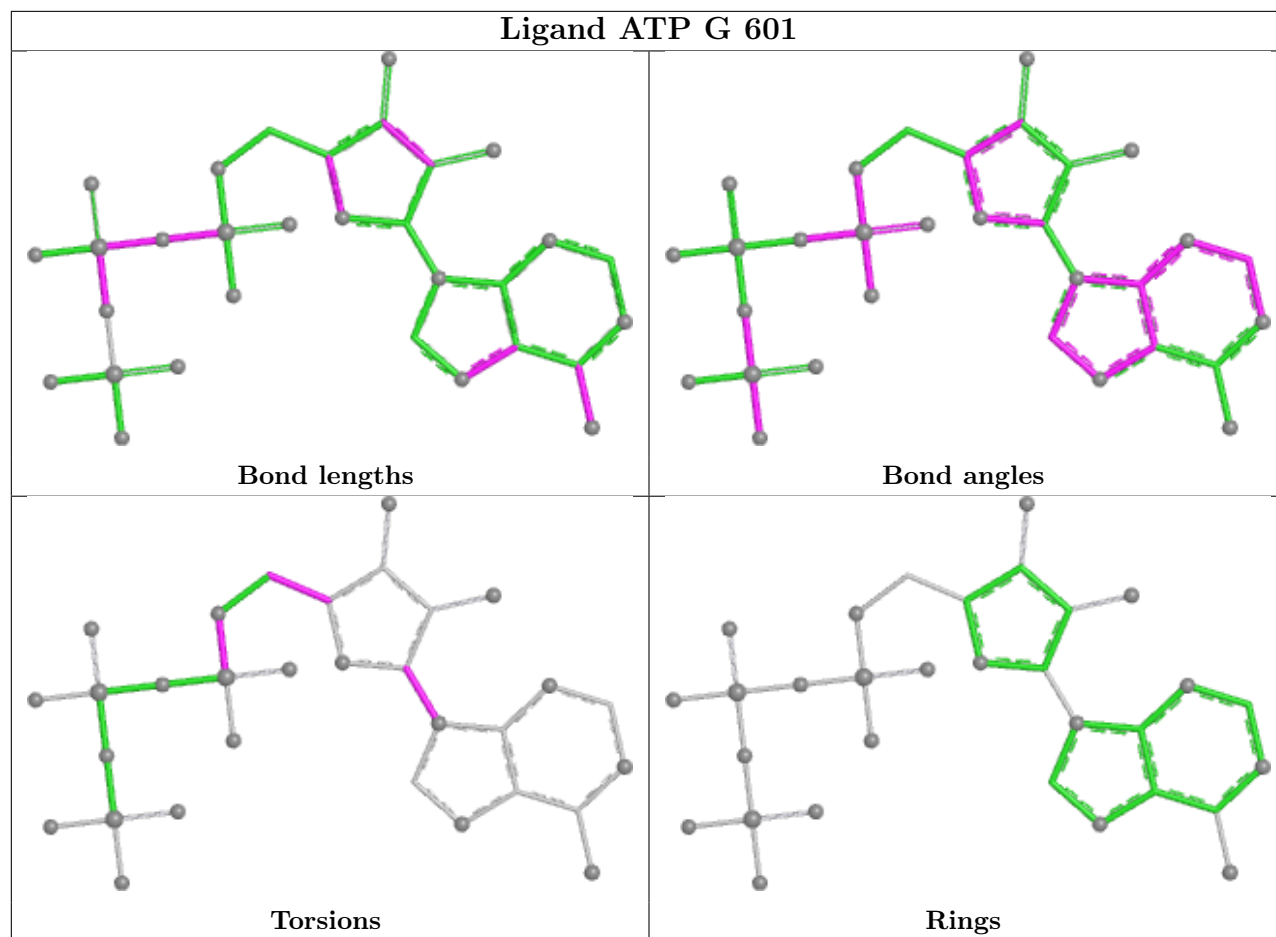
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	ATP	3	0
3	H	301	ATP	2	0
3	B	301	ATP	1	0
3	C	601	ATP	1	0
3	A	601	ATP	1	0
3	E	601	ATP	3	0

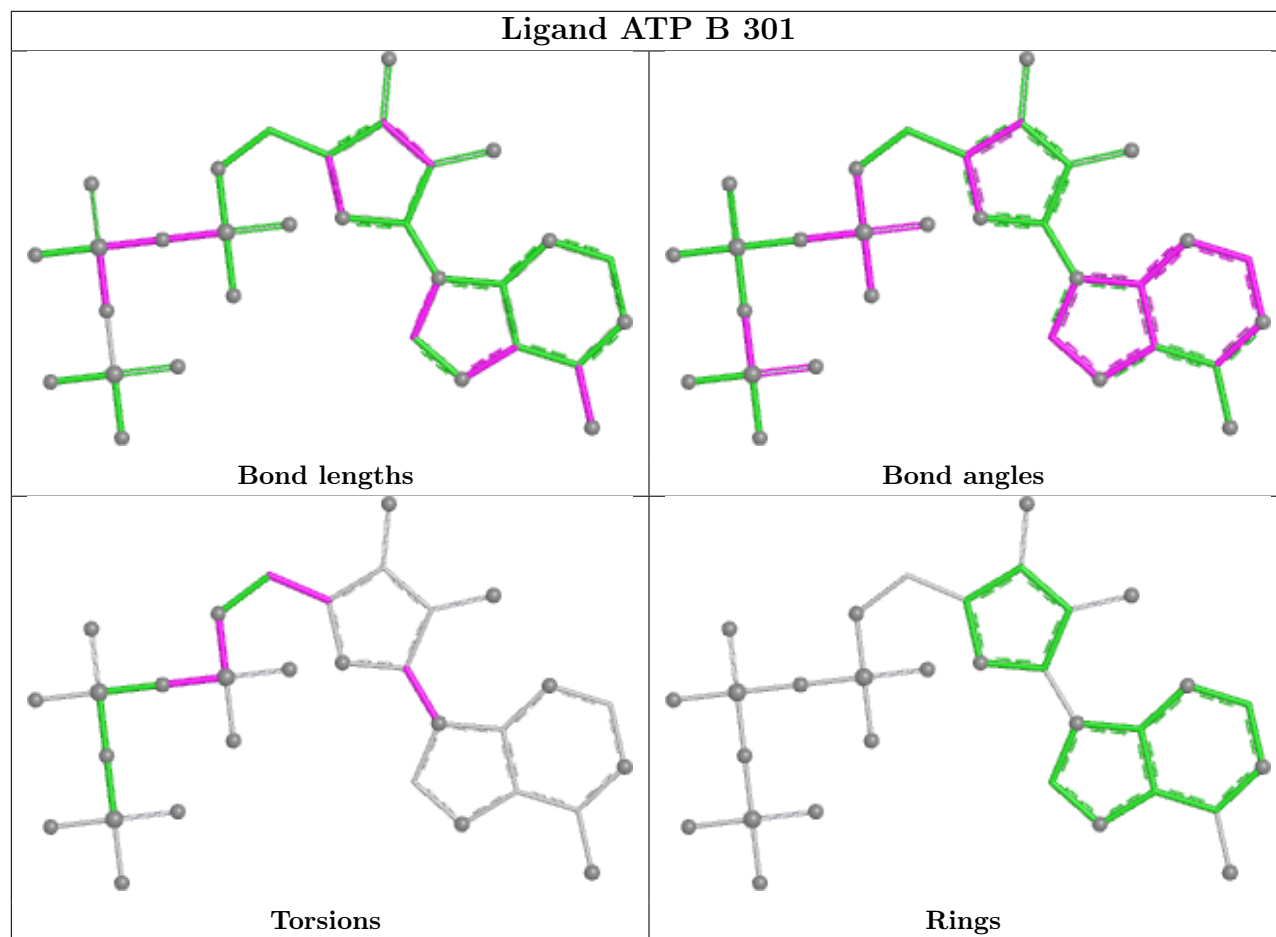
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

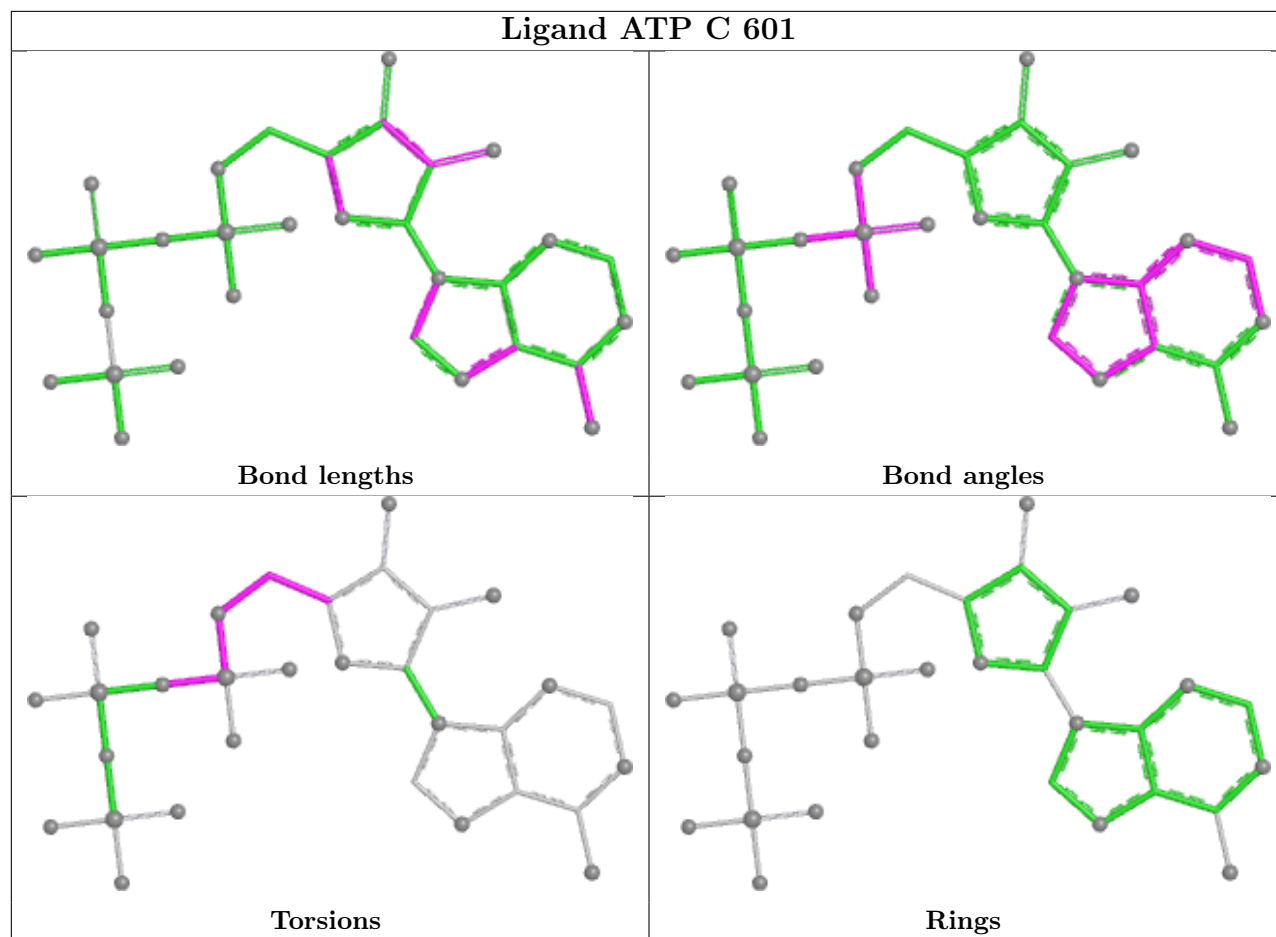


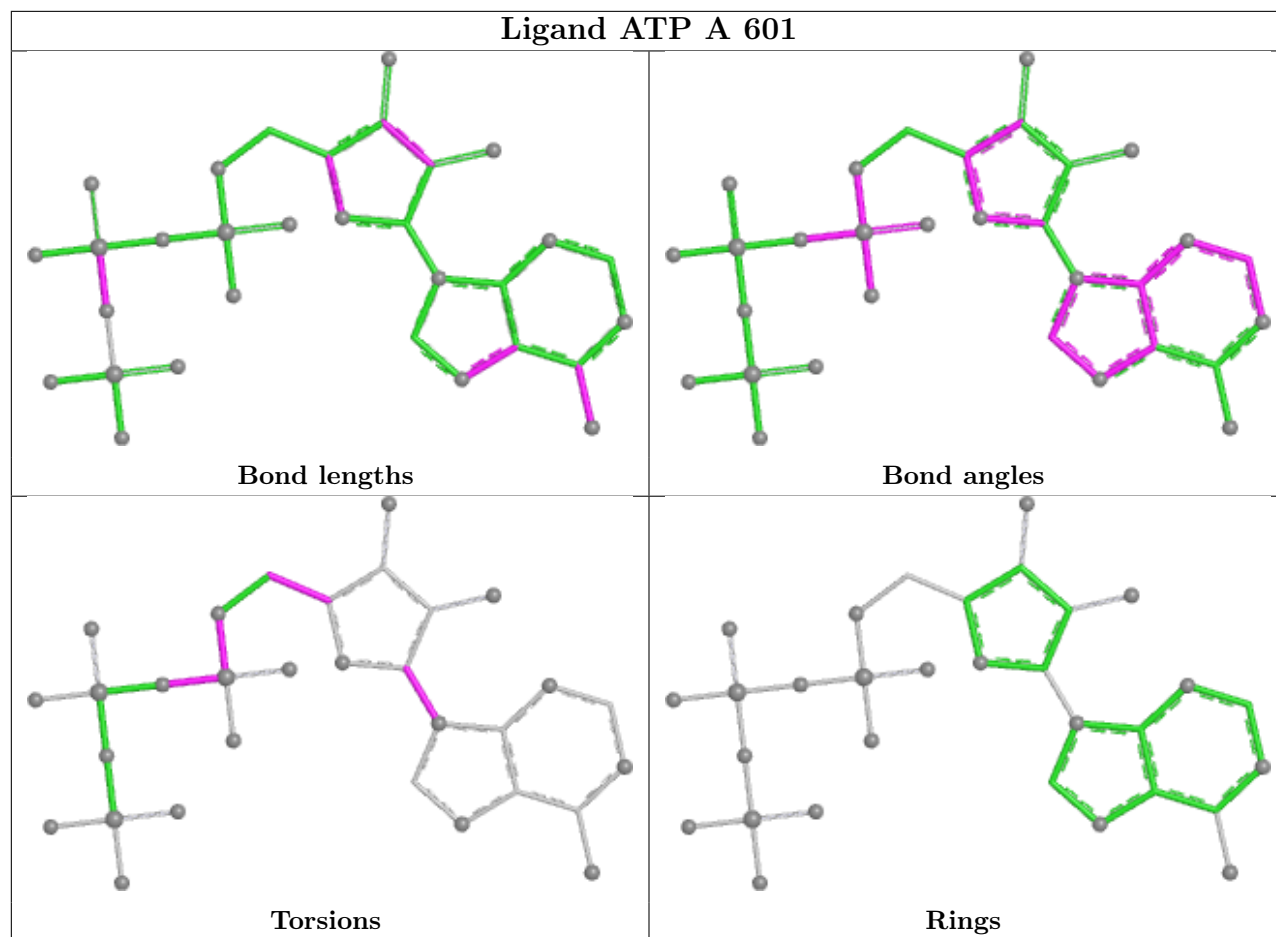


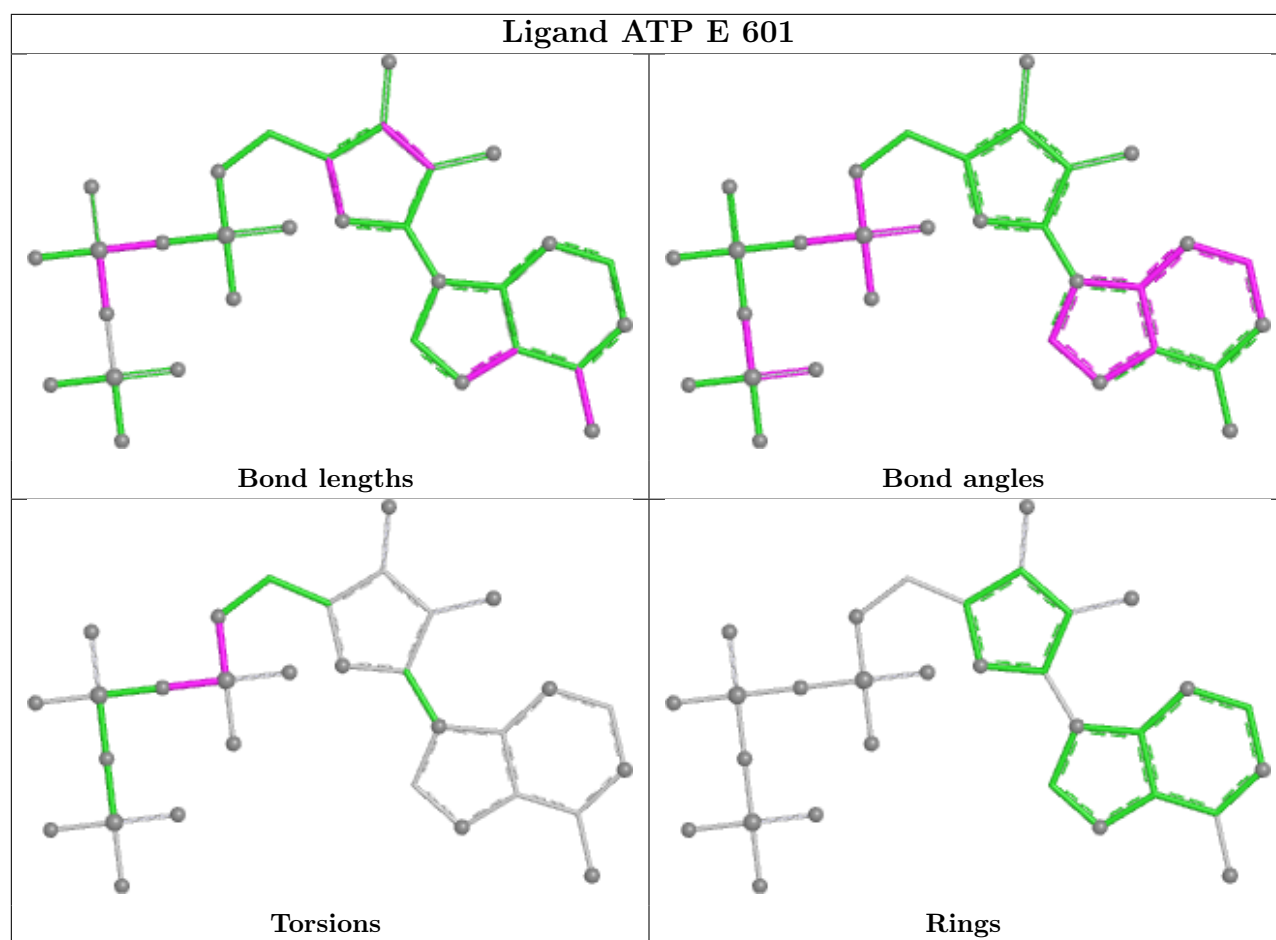












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	216/222 (97%)	0.66	22 (10%) 12 8	27, 62, 143, 176	0
1	B	217/222 (97%)	0.39	11 (5%) 33 19	38, 59, 142, 166	0
1	C	216/222 (97%)	0.41	11 (5%) 33 19	38, 63, 163, 177	0
1	D	217/222 (97%)	0.50	10 (4%) 37 20	35, 69, 153, 178	0
1	E	216/222 (97%)	0.36	11 (5%) 33 19	25, 54, 138, 163	0
1	F	217/222 (97%)	0.45	12 (5%) 30 18	27, 56, 140, 169	0
1	G	216/222 (97%)	0.35	17 (7%) 18 12	28, 49, 127, 155	0
1	H	217/222 (97%)	0.23	5 (2%) 61 37	30, 50, 113, 154	0
2	I	429/465 (92%)	0.30	10 (2%) 61 37	32, 58, 96, 139	0
2	J	429/465 (92%)	0.29	14 (3%) 49 28	28, 48, 88, 136	0
2	K	429/465 (92%)	0.33	17 (3%) 42 23	29, 60, 105, 139	0
2	L	429/465 (92%)	0.22	9 (2%) 63 38	31, 51, 88, 138	0
All	All	3448/3636 (94%)	0.35	149 (4%) 40 21	25, 56, 133, 178	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	6.2
1	G	164	SER	5.8
1	A	173	ARG	5.5
2	I	105	LYS	5.1
1	G	174	ALA	4.6
1	C	72	GLU	4.6
1	E	174	ALA	4.5
1	G	185	HIS	4.5
1	G	169	ASP	4.5
2	J	262	ILE	4.2
2	K	313	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	285	ASP	4.1
1	A	196	GLU	4.0
1	E	211	LYS	3.8
2	L	312	SER	3.8
1	E	169	ASP	3.8
2	L	262	ILE	3.8
1	A	211	LYS	3.8
1	A	168	ILE	3.7
1	A	191	LEU	3.7
1	B	207	ILE	3.7
1	F	186	HIS	3.6
1	G	211	LYS	3.6
1	B	180	ILE	3.6
2	K	68	THR	3.6
1	C	61	ASN	3.5
2	I	312	SER	3.5
1	F	198	ILE	3.4
2	K	399	PRO	3.4
2	K	262	ILE	3.4
1	B	185	HIS	3.3
2	I	235	THR	3.3
1	D	211	LYS	3.3
2	J	256	THR	3.3
2	I	229	LYS	3.3
1	H	146	ASP	3.2
1	C	7	LYS	3.2
2	K	47	TRP	3.2
2	J	255	GLY	3.2
1	E	171	ASN	3.1
1	E	7	LYS	3.1
2	K	64	ALA	3.1
1	F	182	ALA	3.1
2	J	263	VAL	3.1
2	K	52	PHE	3.1
1	G	7	LYS	3.0
1	G	198	ILE	3.0
1	C	196	GLU	2.9
1	E	165	LYS	2.9
1	D	174	ALA	2.9
1	B	194	ALA	2.9
1	A	216	ARG	2.9
2	L	105	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	172	VAL	2.8
1	H	19	GLY	2.8
1	H	29	GLY	2.8
1	G	173	ARG	2.8
1	F	196	GLU	2.8
2	K	146	LEU	2.8
1	A	215	LYS	2.8
1	G	186	HIS	2.8
2	J	41	THR	2.8
1	G	163	ASP	2.8
2	J	441	GLU	2.8
1	B	181	LEU	2.8
1	A	198	ILE	2.7
1	H	185	HIS	2.7
2	I	158	TRP	2.7
1	E	164	SER	2.7
2	L	431	GLU	2.7
1	A	177	GLY	2.7
1	E	197	ASP	2.7
2	I	182	PRO	2.7
2	I	262	ILE	2.7
1	F	211	LYS	2.7
1	G	166	SER	2.6
1	B	189	ILE	2.6
2	J	162	LEU	2.6
1	E	185	HIS	2.6
2	I	47	TRP	2.6
2	J	183	ASP	2.6
1	D	170	LEU	2.6
1	B	198	ILE	2.5
2	K	48	ILE	2.5
2	K	153	VAL	2.5
1	D	43	ASN	2.5
1	G	171	ASN	2.5
1	C	211	LYS	2.5
1	A	185	HIS	2.5
2	J	229	LYS	2.5
2	L	47	TRP	2.5
1	B	179	THR	2.5
1	B	206	VAL	2.5
1	A	48	TYR	2.5
2	K	429	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	99	VAL	2.4
1	A	31	GLU	2.4
2	I	313	GLY	2.4
1	A	176	TYR	2.4
1	E	191	LEU	2.4
1	F	195	PRO	2.4
2	L	229	LYS	2.4
1	A	151	TYR	2.3
2	K	105	LYS	2.3
1	D	220	GLU	2.3
1	F	199	ILE	2.3
1	H	198	ILE	2.3
1	D	185	HIS	2.3
2	K	72	PHE	2.3
1	A	189	ILE	2.3
1	G	72	GLU	2.3
1	G	8	GLN	2.3
2	K	335	GLU	2.3
1	F	163	ASP	2.3
1	E	186	HIS	2.2
1	F	164	SER	2.2
1	B	204	CYS	2.2
2	K	66	VAL	2.2
1	C	157	LEU	2.2
1	F	165	LYS	2.2
1	C	168	ILE	2.2
1	C	174	ALA	2.2
2	I	60	VAL	2.2
1	D	176	TYR	2.2
2	L	313	GLY	2.2
2	J	146	LEU	2.2
1	G	160	ARG	2.1
1	D	172	VAL	2.1
1	A	218	GLU	2.1
2	J	430	THR	2.1
1	A	148	SER	2.1
1	G	170	LEU	2.1
1	B	182	ALA	2.1
1	C	205	LEU	2.1
1	C	149	ASP	2.1
2	J	218	ASN	2.1
1	C	195	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	201	GLU	2.0
2	J	184	ASN	2.0
1	A	160	ARG	2.0
1	A	212	LYS	2.0
1	D	41	LYS	2.0
1	A	169	ASP	2.0
2	K	35	LEU	2.0
1	F	208	MET	2.0
2	L	331	ARG	2.0
1	G	188	ASP	2.0
2	K	178	PHE	2.0
1	D	44	ALA	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(Å ²)	Q<0.9
3	ATP	B	301	31/31	0.97	0.07	37,41,52,53	0
3	ATP	C	601	31/31	0.97	0.07	35,37,43,44	0
3	ATP	D	301	31/31	0.97	0.07	32,34,40,40	0
3	ATP	F	301	31/31	0.97	0.07	33,38,47,47	0
3	ATP	G	601	31/31	0.97	0.06	28,30,35,36	0
3	ATP	H	301	31/31	0.97	0.07	29,30,32,32	0
3	ATP	E	601	31/31	0.98	0.06	23,27,32,33	0
3	ATP	A	601	31/31	0.98	0.06	32,35,38,39	0
4	K	L	501	1/1	0.99	0.20	25,25,25,25	0
4	K	J	501	1/1	1.00	0.20	22,22,22,22	0
4	K	K	501	1/1	1.00	0.14	32,32,32,32	0

Continued on next page...

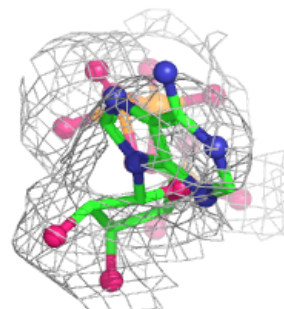
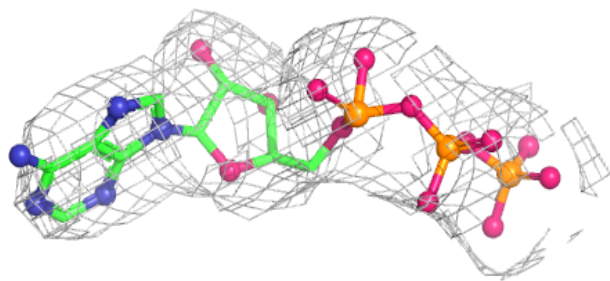
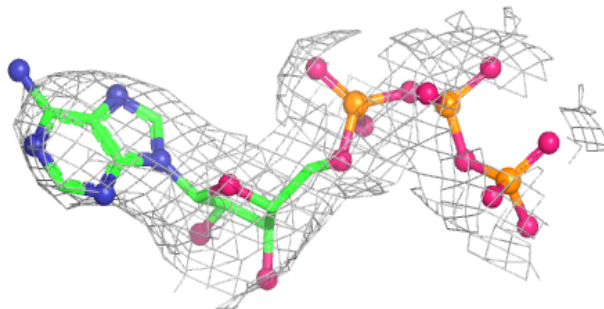
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	I	501	1/1	1.00	0.18	29,29,29,29	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.

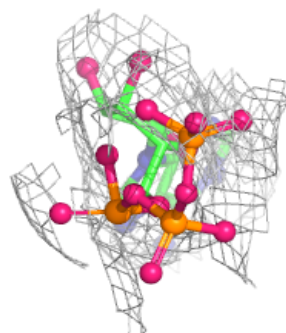
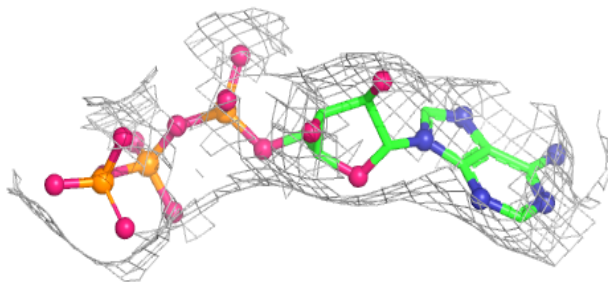
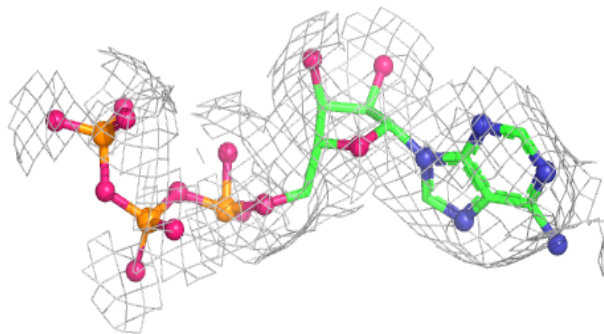
Electron density around ATP B 301:

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

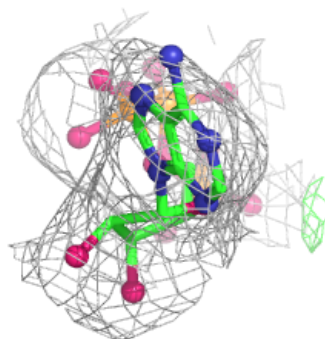
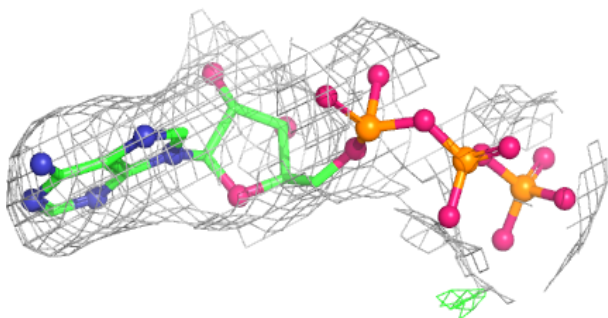
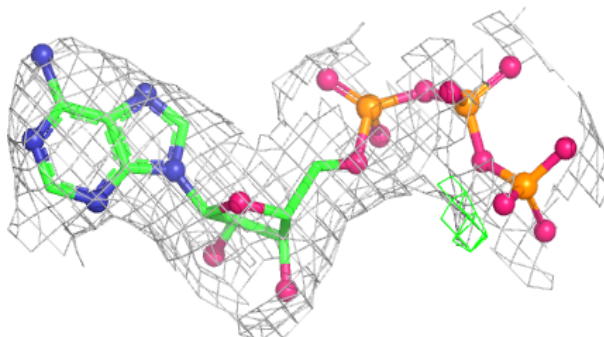


Electron density around ATP C 601:

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

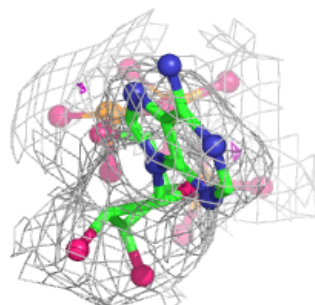
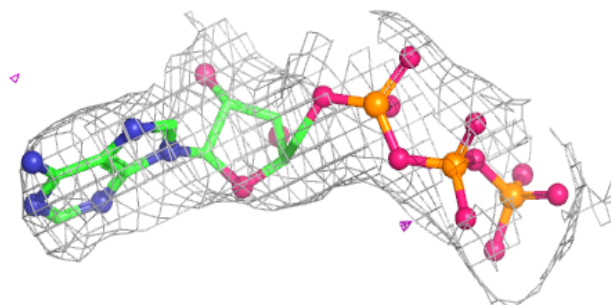
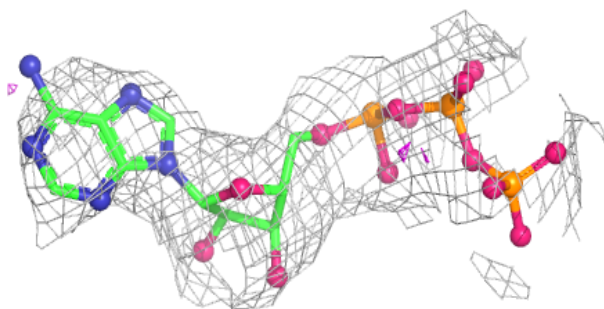
**Electron density around ATP D 301:**

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

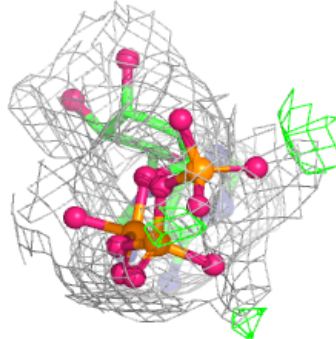
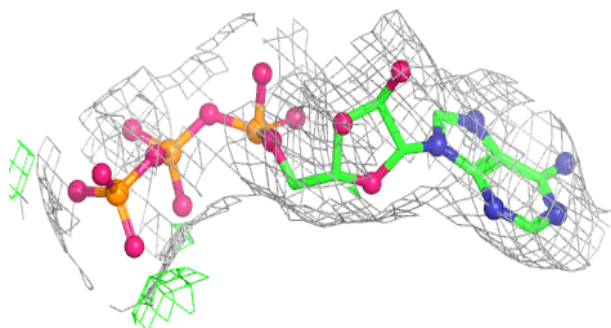
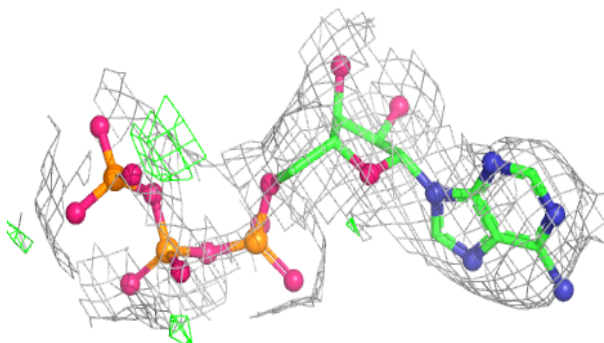


Electron density around ATP F 301:

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

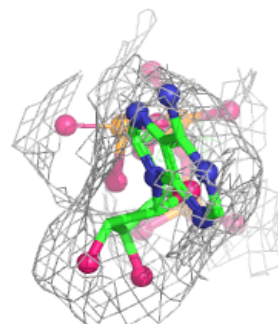
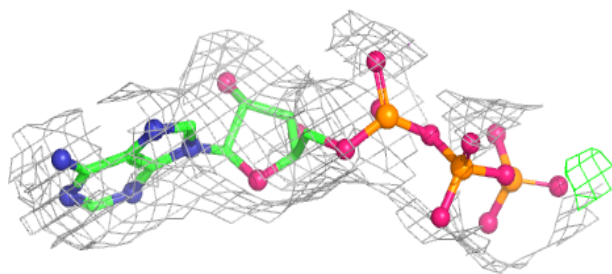
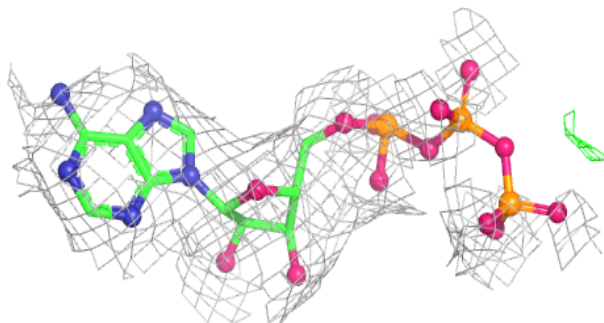
**Electron density around ATP G 601:**

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

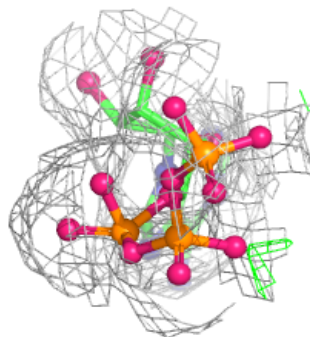
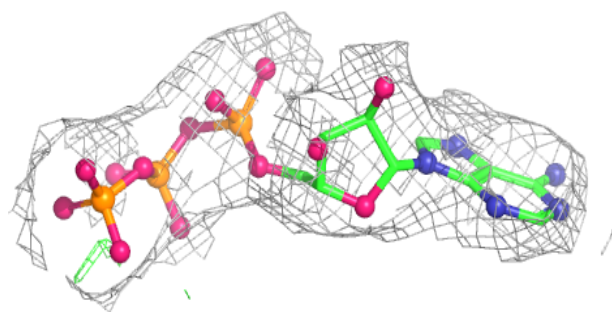
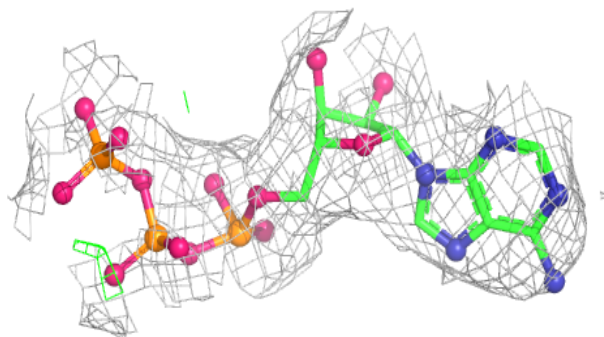


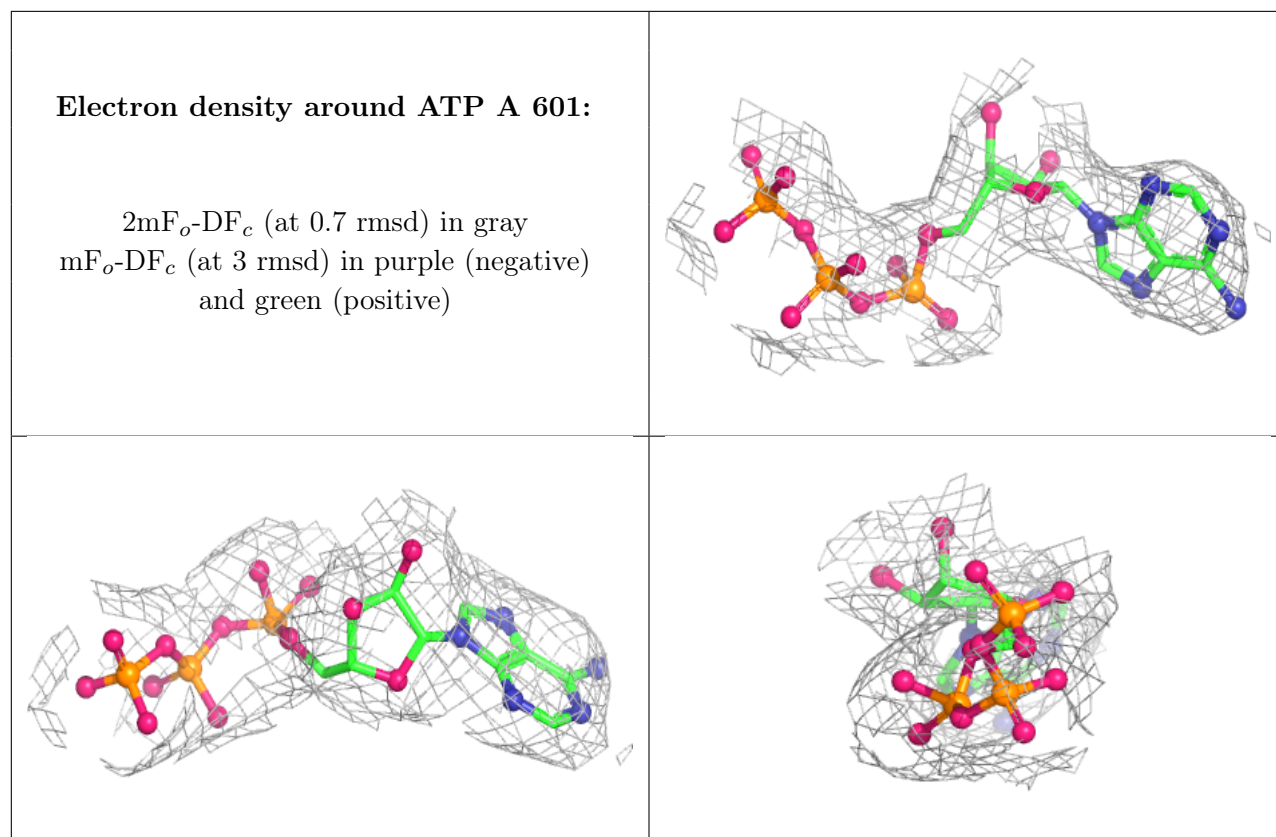
Electron density around ATP H 301:

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

**Electron density around ATP E 601:**

$2mF_o-DF_c$ (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.