



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 2GBL / pdb_00002gbl
Title : Crystal Structure of Full Length Circadian Clock Protein KaiC with Phosphorylation Sites
Authors : Pattanayek, R.; Williams, D.R.; Pattanayek, S.; Xu, Y.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.
Deposited on : 2006-03-10
Resolution : 2.80 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:

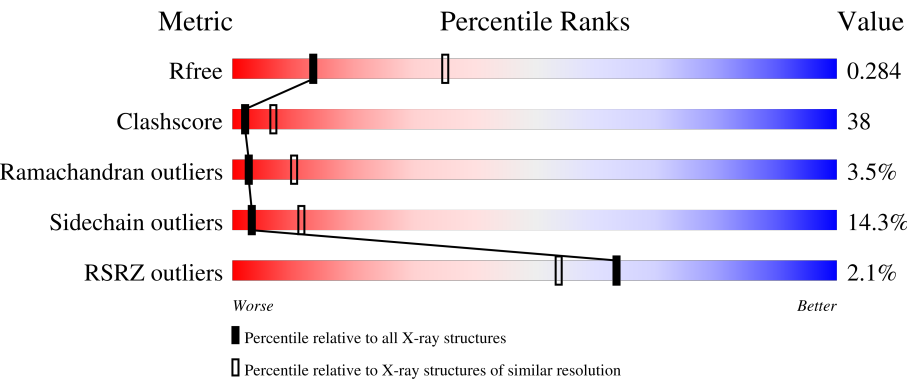
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	519	3% 38%45%11% . .
1	B	519	3% 39%42%12% . 5%
1	E	519	% 41%37%14% . 5%
1	F	519	2% 40%41%13% . .

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Mol	Chain	Length	Quality of chain
2	C	519	
2	D	519	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	431	-	X	X	-
1	SEP	B	431	-	X	X	-
1	SEP	F	431	-	X	-	-
1	TPO	F	432	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23872 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 Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3994	2509	701	767	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3886	2445	679	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2509	701	767	2	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	SEP	SER	modified residue	UNP Q79PF4
A	432	TPO	THR	modified residue	UNP Q79PF4
B	431	SEP	SER	modified residue	UNP Q79PF4
B	432	TPO	THR	modified residue	UNP Q79PF4
E	431	SEP	SER	modified residue	UNP Q79PF4
E	432	TPO	THR	modified residue	UNP Q79PF4
F	431	SEP	SER	modified residue	UNP Q79PF4
F	432	TPO	THR	modified residue	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	15			

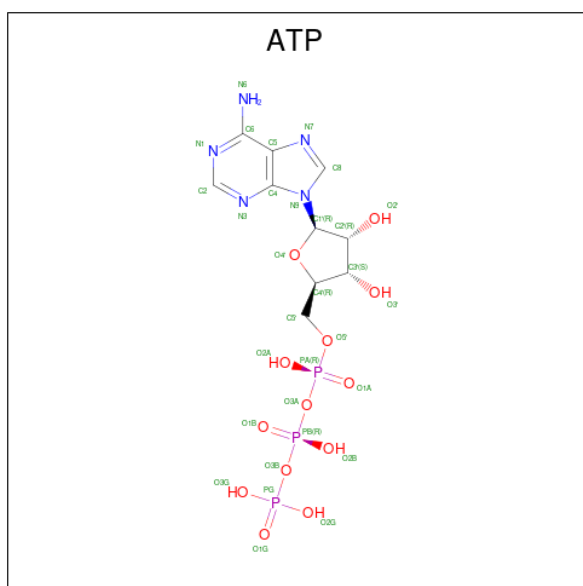
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	432	TPO	THR	modified residue	UNP Q79PF4
D	432	TPO	THR	modified residue	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0	0

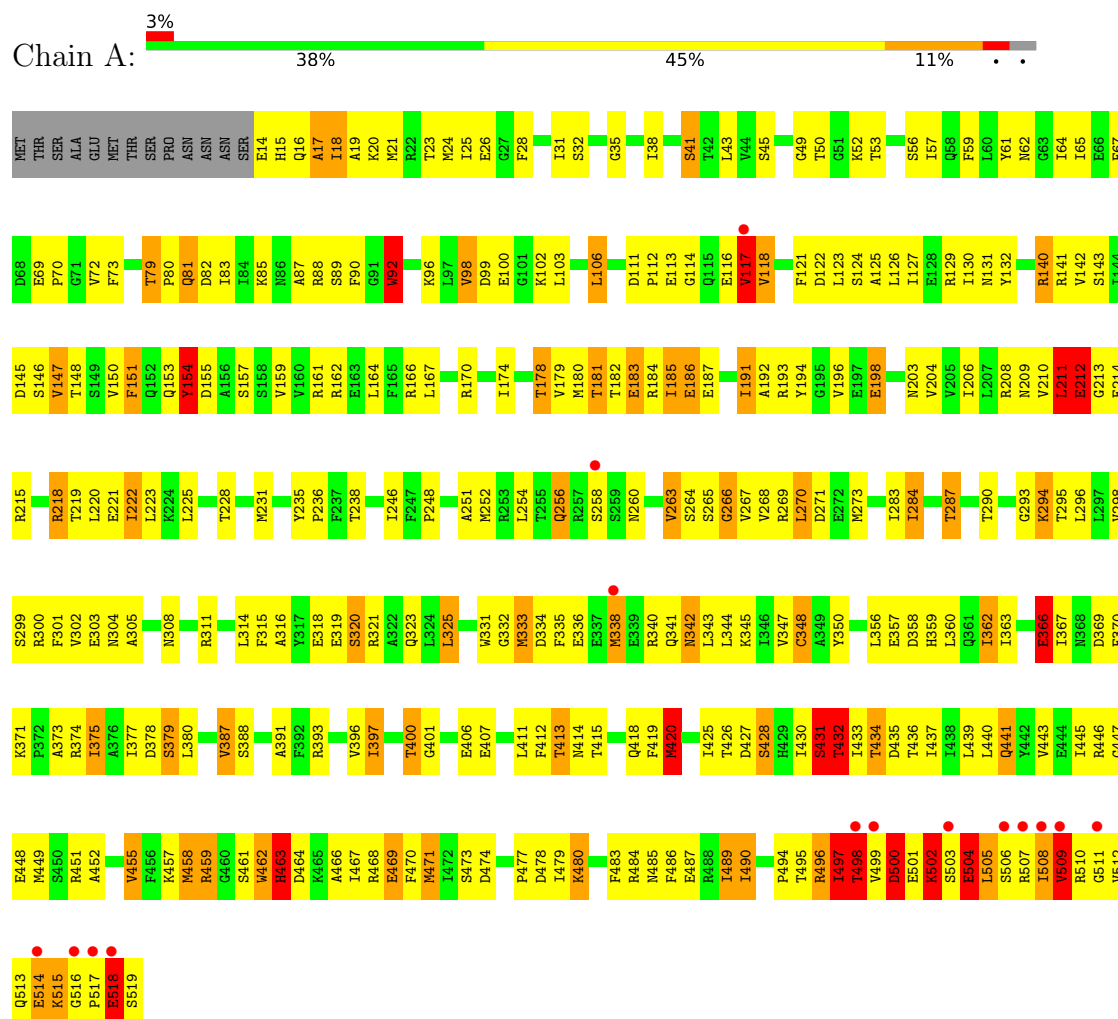
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total 8	O 8	0	0
5	B	5	Total 5	O 5	0	0
5	C	7	Total 7	O 7	0	0
5	D	13	Total 13	O 13	0	0
5	E	10	Total 10	O 10	0	0
5	F	23	Total 23	O 23	0	0

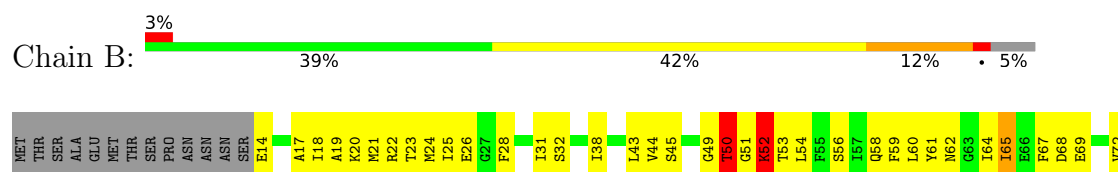
3 Residue-property plots

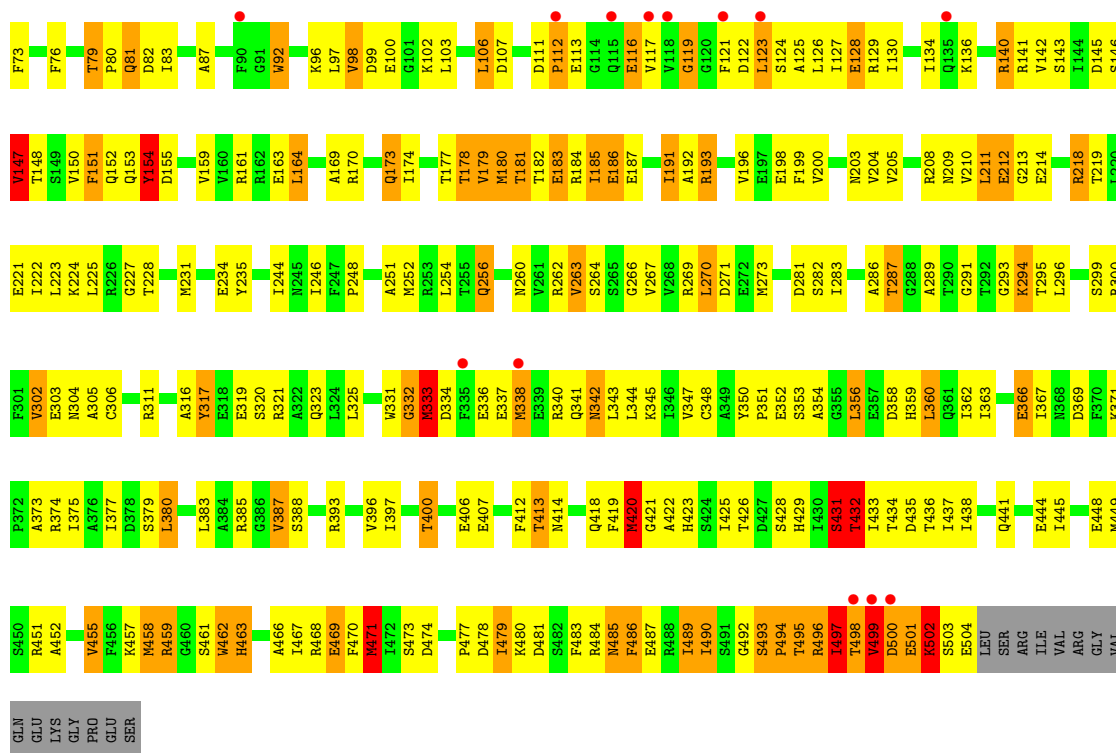
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Circadian clock protein kinase kaiC

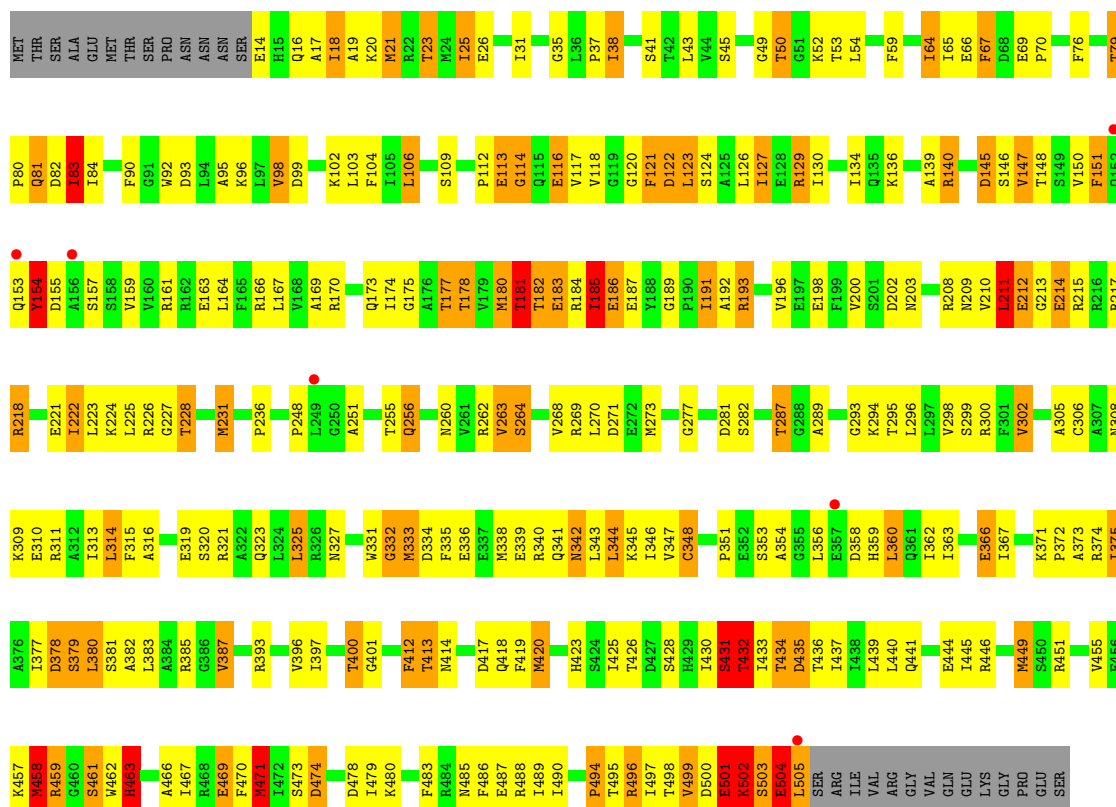
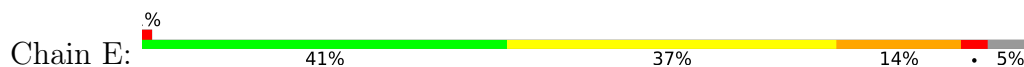


• Molecule 1: Circadian clock protein kinase kaiC





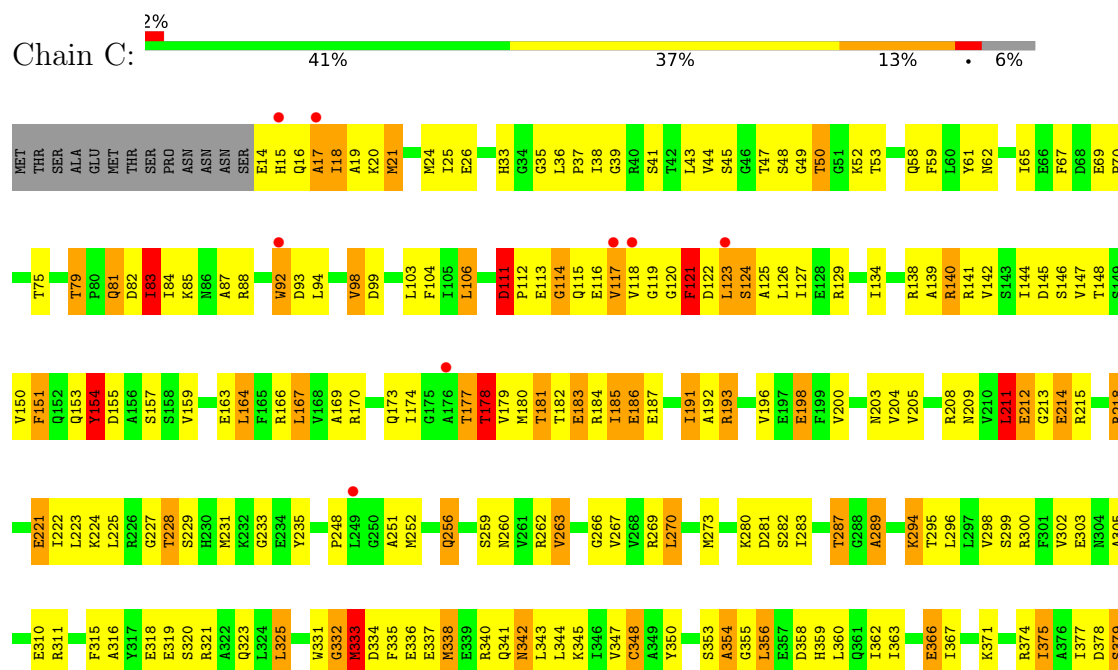
• Molecule 1: Circadian clock protein kinase kaiC

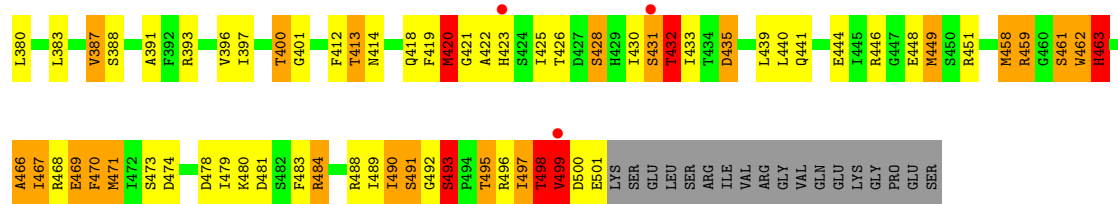


• Molecule 1: Circadian clock protein kinase kaiC

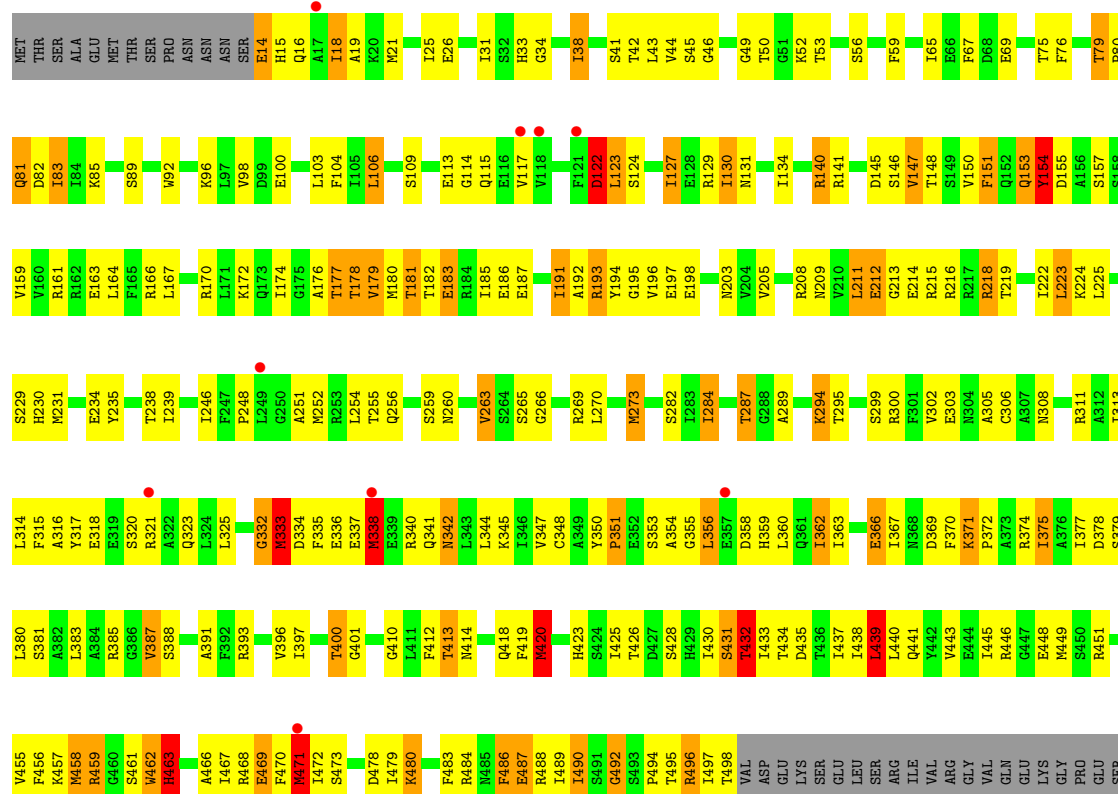
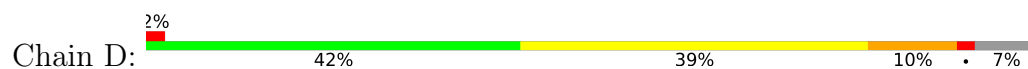


• Molecule 2: Circadian clock protein kinase kaiC





• Molecule 2: Circadian clock protein kinase kaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.87Å 135.58Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.83	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.80) 89.6 (30.00-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.290 0.232 , 0.284	Depositor DCC
R_{free} test set	4041 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23872	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.20	18/4038 (0.4%)	1.38	38/5437 (0.7%)
1	B	1.06	10/3921 (0.3%)	1.36	39/5282 (0.7%)
1	E	1.33	25/3929 (0.6%)	1.47	43/5293 (0.8%)
1	F	1.28	15/4038 (0.4%)	1.45	51/5437 (0.9%)
2	C	1.09	11/3903 (0.3%)	1.36	37/5259 (0.7%)
2	D	1.30	16/3879 (0.4%)	1.41	30/5226 (0.6%)
All	All	1.21	95/23708 (0.4%)	1.40	238/31934 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	E	0	2
1	F	0	3
2	C	0	2
2	D	0	2
All	All	0	14

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	21	MET	SD-CE	-10.64	1.52	1.79
1	A	508	ILE	CA-CB	10.46	1.68	1.54
1	B	499	VAL	CA-CB	9.57	1.65	1.54
1	B	498	THR	CA-CB	9.34	1.69	1.53
1	F	509	VAL	C-N	9.28	1.46	1.33
1	B	52	LYS	N-CA	8.06	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	21	MET	SD-CE	-7.86	1.59	1.79
1	B	92	TRP	CE3-CZ3	7.58	1.61	1.38
1	B	471	MET	SD-CE	7.42	1.98	1.79
1	E	21	MET	SD-CE	-7.26	1.61	1.79
2	D	53	THR	CA-C	7.22	1.62	1.52
2	D	458	MET	CG-SD	-7.17	1.62	1.80
1	E	503	SER	CA-C	7.05	1.60	1.52
1	F	514	GLU	CA-C	6.94	1.60	1.52
1	A	92	TRP	CE3-CZ3	6.87	1.59	1.38
2	C	499	VAL	CA-CB	6.86	1.63	1.54
1	E	458	MET	SD-CE	-6.67	1.62	1.79
1	A	53	THR	CA-C	6.65	1.61	1.52
1	A	517	PRO	CA-C	6.55	1.61	1.52
2	C	213	GLY	C-O	-6.51	1.15	1.23
1	F	15	HIS	CA-C	6.46	1.60	1.53
1	E	499	VAL	CA-CB	6.46	1.63	1.54
1	E	500	ASP	CA-CB	6.44	1.60	1.53
1	A	509	VAL	CA-CB	6.43	1.63	1.54
2	C	449	MET	SD-CE	-6.37	1.63	1.79
2	C	204	VAL	CA-CB	-6.30	1.46	1.54
2	D	130	ILE	CA-CB	6.29	1.62	1.54
1	A	204	VAL	CA-CB	6.29	1.62	1.54
1	F	516	GLY	CA-C	6.27	1.56	1.51
1	B	333	MET	SD-CE	-6.26	1.63	1.79
1	A	507	ARG	CA-C	6.24	1.61	1.52
1	E	92	TRP	CG-CD1	-6.15	1.21	1.36
1	A	498	THR	CA-CB	6.14	1.63	1.53
1	F	191	ILE	CA-CB	6.12	1.61	1.54
1	A	455	VAL	CA-CB	6.06	1.61	1.53
2	D	462	TRP	N-CA	-6.06	1.38	1.46
1	F	510	ARG	N-CA	6.00	1.53	1.46
1	A	212	GLU	CA-C	5.98	1.60	1.52
2	C	498	THR	CA-CB	5.95	1.63	1.53
1	F	41	SER	C-O	-5.94	1.16	1.23
1	E	17	ALA	CA-CB	-5.92	1.43	1.53
1	E	23	THR	CA-C	-5.92	1.44	1.52
1	F	92	TRP	CG-CD1	-5.91	1.22	1.36
1	E	504	GLU	CA-C	5.91	1.58	1.53
2	D	246	ILE	CA-C	-5.89	1.45	1.52
1	F	471	MET	SD-CE	5.88	1.94	1.79
1	A	500	ASP	N-CA	5.86	1.53	1.46
1	A	518	GLU	CA-C	5.84	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	502	LYS	CA-C	5.78	1.60	1.52
2	D	238	THR	CA-C	-5.78	1.45	1.52
2	D	56	SER	N-CA	-5.74	1.39	1.46
1	A	508	ILE	CA-C	5.70	1.59	1.52
2	D	338	MET	SD-CE	5.69	1.93	1.79
2	C	420	MET	SD-CE	5.64	1.93	1.79
2	D	443	VAL	CA-CB	-5.62	1.47	1.54
2	D	471	MET	CG-SD	5.60	1.94	1.80
2	C	87	ALA	CA-CB	-5.58	1.43	1.53
1	A	515	LYS	CA-C	5.53	1.59	1.52
1	E	412	PHE	CA-C	-5.52	1.46	1.52
1	E	471	MET	SD-CE	5.51	1.93	1.79
1	E	92	TRP	CB-CG	-5.49	1.33	1.50
1	E	499	VAL	CA-C	5.48	1.59	1.52
1	F	420	MET	SD-CE	5.46	1.93	1.79
1	A	498	THR	CA-C	5.42	1.60	1.52
2	D	434	THR	CA-C	5.42	1.59	1.52
1	F	338	MET	SD-CE	5.38	1.93	1.79
1	B	180	MET	SD-CE	5.37	1.93	1.79
2	D	273	MET	SD-CE	-5.37	1.66	1.79
2	D	333	MET	SD-CE	-5.37	1.66	1.79
2	C	92	TRP	CG-CD1	-5.35	1.23	1.36
2	C	467	ILE	CA-CB	-5.35	1.47	1.53
1	E	53	THR	CB-OG1	5.33	1.52	1.43
1	F	134	ILE	CA-CB	5.32	1.60	1.54
2	C	466	ALA	CA-CB	-5.28	1.45	1.53
1	E	83	ILE	CA-CB	5.27	1.60	1.54
1	E	65	ILE	CA-CB	5.27	1.60	1.54
1	E	180	MET	SD-CE	-5.26	1.66	1.79
2	D	239	ILE	C-O	-5.24	1.18	1.24
1	A	206	ILE	CA-CB	5.21	1.60	1.54
2	D	420	MET	SD-CE	5.21	1.92	1.79
1	B	92	TRP	CG-CD1	-5.21	1.24	1.36
1	E	66	GLU	CA-C	-5.20	1.45	1.52
1	F	135	GLN	CD-NE2	5.19	1.44	1.33
2	D	238	THR	C-O	-5.15	1.17	1.23
1	B	498	THR	CA-C	5.13	1.59	1.52
1	B	52	LYS	C-N	5.11	1.40	1.33
1	A	338	MET	SD-CE	5.11	1.92	1.79
1	E	503	SER	N-CA	5.08	1.52	1.46
1	E	501	GLU	CA-C	5.07	1.59	1.52
1	E	18	ILE	CA-CB	-5.04	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	346	ILE	CA-CB	-5.01	1.48	1.54
1	A	500	ASP	CA-C	5.01	1.59	1.52
1	F	41	SER	CA-C	-5.01	1.46	1.52
1	E	449	MET	SD-CE	-5.00	1.67	1.79
1	E	231	MET	SD-CE	-5.00	1.67	1.79

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	LYS	N-CA-C	-12.87	96.23	114.12
2	C	214	GLU	N-CA-C	-11.90	95.65	110.88
1	A	459	ARG	N-CA-C	11.80	123.69	111.07
1	E	129	ARG	N-CA-C	-11.66	98.60	111.07
1	E	380	LEU	N-CA-C	-11.45	97.61	111.69
1	E	459	ARG	N-CA-C	11.18	123.47	111.28
1	F	380	LEU	N-CA-C	-11.15	99.10	111.14
2	D	380	LEU	N-CA-C	-11.13	99.23	111.36
1	E	214	GLU	N-CA-C	-11.13	97.17	112.30
1	A	116	GLU	N-CA-C	10.98	126.78	110.52
1	B	380	LEU	N-CA-C	-10.82	99.56	111.36
2	D	459	ARG	N-CA-C	10.72	123.05	111.36
2	C	380	LEU	N-CA-C	-10.71	99.68	111.36
1	A	512	VAL	N-CA-C	-10.29	98.23	111.09
1	F	459	ARG	N-CA-C	10.04	121.98	111.14
2	C	332	GLY	N-CA-C	-9.79	99.41	111.45
1	A	380	LEU	N-CA-C	-9.47	100.84	111.82
1	F	121	PHE	N-CA-C	-9.43	101.20	112.89
2	D	16	GLN	N-CA-C	9.27	122.34	109.18
1	B	459	ARG	N-CA-C	9.27	121.15	111.14
1	F	122	ASP	N-CA-C	-9.08	100.79	112.23
2	C	459	ARG	N-CA-C	8.97	120.83	111.14
1	A	114	GLY	N-CA-C	8.93	122.19	111.93
1	E	213	GLY	N-CA-C	-8.64	96.26	110.95
1	A	266	GLY	N-CA-C	-8.47	103.33	115.27
1	F	114	GLY	N-CA-C	8.32	132.90	113.18
1	F	147	VAL	N-CA-C	-8.23	102.41	110.72
1	F	332	GLY	N-CA-C	-8.14	99.11	111.24
1	E	501	GLU	N-CA-C	8.07	119.71	111.07
1	E	435	ASP	N-CA-C	8.01	119.79	111.14
1	B	497	ILE	N-CA-C	7.93	118.73	110.72
1	F	498	THR	N-CA-C	7.90	124.21	107.70
2	C	213	GLY	N-CA-C	-7.85	94.57	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	ASP	CA-C-N	7.82	127.48	119.82
1	F	111	ASP	C-N-CA	7.82	127.48	119.82
1	F	373	ALA	N-CA-C	-7.82	103.96	113.97
2	D	155	ASP	N-CA-C	7.75	121.66	109.81
1	E	332	GLY	N-CA-C	-7.59	99.93	111.24
1	E	503	SER	N-CA-C	7.55	120.86	107.80
1	E	147	VAL	N-CA-C	-7.45	101.78	111.09
1	F	513	GLN	N-CA-C	7.44	121.08	110.14
1	F	210	VAL	N-CA-C	7.43	119.17	109.58
1	B	489	ILE	CB-CA-C	-7.42	102.54	111.81
1	B	92	TRP	CB-CA-C	7.39	121.03	110.24
1	E	155	ASP	N-CA-C	7.39	121.00	110.14
1	A	497	ILE	N-CA-C	7.36	124.64	109.34
2	C	493	SER	CA-C-N	7.36	127.27	120.21
2	C	493	SER	C-N-CA	7.36	127.27	120.21
1	B	266	GLY	N-CA-C	-7.21	105.11	115.27
1	E	178	THR	N-CA-C	7.12	121.28	109.95
1	F	474	ASP	N-CA-C	-7.12	103.26	112.23
1	A	194	TYR	N-CA-C	7.11	121.79	113.18
2	D	147	VAL	N-CA-C	-7.08	103.57	110.72
2	C	193	ARG	N-CA-C	7.04	122.92	111.37
1	F	155	ASP	N-CA-C	7.01	120.93	109.85
1	F	235	TYR	CA-C-N	7.00	126.76	119.76
1	F	235	TYR	C-N-CA	7.00	126.76	119.76
1	F	514	GLU	N-CA-C	6.90	121.86	112.68
1	A	516	GLY	N-CA-C	-6.89	98.29	112.34
1	B	455	VAL	N-CA-C	-6.89	96.41	106.88
1	B	152	GLN	N-CA-C	-6.85	103.88	113.20
2	D	480	LYS	N-CA-C	6.84	114.39	108.78
1	E	504	GLU	N-CA-C	6.82	119.61	108.08
1	B	155	ASP	N-CA-C	6.81	120.23	109.81
2	D	178	THR	N-CA-C	6.79	120.75	109.95
1	A	507	ARG	N-CA-C	-6.77	104.03	112.90
2	C	178	THR	N-CA-C	6.76	120.48	109.59
1	B	500	ASP	N-CA-C	-6.65	100.39	110.70
1	F	512	VAL	O-C-N	-6.62	114.37	122.18
2	D	480	LYS	CA-C-O	6.61	121.77	117.94
1	A	222	ILE	N-CA-C	-6.60	97.67	107.51
1	A	193	ARG	N-CA-C	6.59	122.17	111.37
2	C	155	ASP	N-CA-C	6.57	120.23	109.85
1	A	210	VAL	N-CA-C	6.55	117.53	108.89
2	C	481	ASP	N-CA-C	6.54	120.14	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	VAL	N-CA-C	-6.49	102.94	111.05
1	E	210	VAL	N-CA-C	6.49	117.41	109.30
2	C	266	GLY	N-CA-C	-6.48	106.49	114.92
1	B	178	THR	N-CA-C	6.46	120.16	110.14
1	E	64	ILE	N-CA-C	6.45	116.59	110.53
2	D	216	ARG	NE-CZ-NH1	-6.40	115.10	121.50
2	D	266	GLY	N-CA-C	-6.36	106.30	115.27
2	D	492	GLY	N-CA-C	-6.36	105.98	114.25
1	B	497	ILE	CB-CA-C	-6.35	103.46	112.22
1	F	439	LEU	N-CA-C	6.32	118.81	108.52
1	A	373	ALA	N-CA-C	-6.31	105.71	113.41
1	A	178	THR	N-CA-C	6.30	119.97	109.95
2	C	111	ASP	CA-C-N	6.29	127.70	119.84
2	C	111	ASP	C-N-CA	6.29	127.70	119.84
1	A	155	ASP	N-CA-C	6.28	119.37	110.14
1	E	373	ALA	N-CA-C	-6.24	105.83	113.50
1	E	114	GLY	N-CA-C	6.23	127.95	113.18
1	F	499	VAL	N-CA-C	-6.23	103.31	112.04
1	F	193	ARG	N-CA-C	6.22	121.57	111.37
1	F	124	SER	N-CA-C	-6.21	105.36	113.12
1	F	266	GLY	N-CA-C	-6.20	106.76	115.32
1	B	244	ILE	N-CA-C	6.19	117.01	108.84
1	B	493	SER	CA-C-N	6.12	127.49	119.84
1	B	493	SER	C-N-CA	6.12	127.49	119.84
1	A	391	ALA	N-CA-C	-6.11	104.70	111.36
1	F	509	VAL	O-C-N	-6.09	114.96	122.57
1	B	193	ARG	N-CA-C	6.06	121.37	111.37
2	D	463	HIS	N-CA-C	6.05	123.68	110.80
1	F	508	ILE	O-C-N	6.04	130.12	122.57
1	E	136	LYS	N-CA-C	6.02	118.34	111.11
1	F	516	GLY	N-CA-C	6.01	122.42	115.09
1	E	213	GLY	O-C-N	-5.96	115.93	122.90
2	D	193	ARG	N-CA-C	5.95	123.47	110.80
1	A	502	LYS	N-CA-C	5.94	123.45	110.80
1	A	511	GLY	N-CA-C	-5.94	106.27	116.01
1	A	508	ILE	CA-C-N	5.90	132.59	121.97
1	A	508	ILE	C-N-CA	5.90	132.59	121.97
1	B	98	VAL	N-CA-C	-5.90	104.98	110.53
1	B	50	THR	CA-C-N	-5.89	117.06	123.30
1	B	50	THR	C-N-CA	-5.89	117.06	123.30
1	F	280	LYS	N-CA-C	-5.88	104.78	111.07
1	A	98	VAL	N-CA-C	-5.87	104.80	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	204	VAL	N-CA-C	5.86	116.45	107.77
1	B	332	GLY	N-CA-C	-5.85	99.32	113.18
2	D	410	GLY	N-CA-C	5.83	119.62	110.71
2	D	434	THR	N-CA-C	5.82	119.03	109.72
1	B	210	VAL	N-CA-C	5.79	116.54	109.30
1	F	127	ILE	N-CA-C	-5.76	104.24	110.23
1	B	495	THR	N-CA-C	-5.75	98.25	108.13
2	C	470	PHE	N-CA-C	5.73	117.98	108.99
1	E	222	ILE	N-CA-C	-5.70	98.85	107.73
1	E	193	ARG	N-CA-C	5.69	122.92	110.80
2	D	332	GLY	N-CA-C	-5.67	99.75	113.18
1	E	167	LEU	N-CA-C	5.67	117.91	111.11
1	F	215	ARG	CA-C-N	-5.67	114.44	122.94
1	F	215	ARG	C-N-CA	-5.67	114.44	122.94
1	E	474	ASP	N-CA-C	-5.66	105.87	112.89
2	C	355	GLY	N-CA-C	-5.66	101.75	112.51
1	E	185	ILE	CB-CA-C	-5.63	104.54	110.62
2	C	98	VAL	N-CA-C	-5.62	105.05	110.72
1	A	258	SER	N-CA-C	5.59	117.97	108.02
2	C	490	ILE	N-CA-C	-5.59	103.45	111.17
1	F	111	ASP	N-CA-C	5.58	117.71	109.62
1	F	469	GLU	N-CA-C	-5.58	101.44	110.32
1	B	65	ILE	N-CA-C	5.58	119.84	112.76
1	B	173	GLN	N-CA-C	-5.55	104.92	110.97
1	E	463	HIS	N-CA-C	5.55	122.62	110.80
1	B	28	PHE	N-CA-C	5.55	117.33	111.28
2	C	435	ASP	N-CA-C	5.55	118.17	111.40
1	F	294	LYS	N-CA-C	-5.54	105.25	111.28
1	E	310	GLU	N-CA-C	-5.53	101.12	109.85
1	A	474	ASP	N-CA-C	-5.52	105.41	111.82
1	F	198	GLU	CB-CA-C	-5.51	101.30	110.68
2	D	439	LEU	N-CA-C	5.49	117.36	108.41
1	A	362	ILE	CB-CA-C	-5.47	103.67	112.16
2	D	284	ILE	CB-CA-C	-5.47	103.39	110.84
1	F	402	TYR	N-CA-C	-5.47	105.00	110.97
1	A	441	GLN	N-CA-C	5.47	118.10	108.75
2	C	222	ILE	N-CA-C	-5.43	99.93	108.23
1	A	366	GLU	CA-CB-CG	-5.42	103.25	114.10
1	E	213	GLY	CA-C-N	-5.40	113.13	122.14
1	E	213	GLY	C-N-CA	-5.40	113.13	122.14
1	E	38	ILE	N-CA-C	5.39	116.65	109.37
1	B	481	ASP	N-CA-C	5.39	118.44	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	ALA	N-CA-C	-5.39	107.07	113.97
1	B	486	PHE	N-CA-C	5.38	118.00	109.50
2	C	167	LEU	N-CA-C	5.38	116.83	111.07
2	D	265	SER	N-CA-C	-5.37	106.72	113.28
1	B	116	GLU	N-CA-C	5.37	115.33	108.24
1	A	23	THR	N-CA-C	-5.35	106.92	113.50
1	B	479	ILE	N-CA-C	5.35	116.08	107.73
2	C	484	ARG	N-CA-C	5.34	117.10	111.28
2	D	282	SER	N-CA-C	5.33	116.64	108.42
2	C	198	GLU	CB-CA-C	-5.33	101.61	110.68
2	D	362	ILE	CB-CA-C	-5.33	105.06	112.04
2	D	176	ALA	N-CA-C	5.33	118.61	110.20
1	F	448	GLU	N-CA-C	5.32	117.91	109.50
1	F	178	THR	N-CA-C	5.32	118.40	109.95
1	E	504	GLU	CB-CA-C	-5.31	110.47	116.63
2	D	153	GLN	N-CA-C	-5.30	107.37	113.88
1	A	159	VAL	N-CA-C	-5.29	105.37	110.72
2	C	118	VAL	N-CA-C	-5.28	106.72	113.22
1	F	176	ALA	N-CA-C	5.28	118.54	110.20
2	C	93	ASP	N-CA-C	5.28	117.30	108.23
1	E	434	THR	N-CA-C	5.28	118.00	109.40
1	A	147	VAL	N-CA-C	-5.25	104.53	111.09
1	A	290	THR	N-CA-C	-5.25	103.21	110.35
1	B	437	ILE	N-CA-C	5.25	115.14	107.37
1	F	241	ASP	N-CA-C	-5.24	106.84	113.18
1	A	117	VAL	N-CA-C	5.22	120.20	109.34
1	A	397	ILE	N-CA-C	-5.22	105.30	110.62
1	B	502	LYS	CA-C-N	5.22	129.59	122.34
1	B	502	LYS	C-N-CA	5.22	129.59	122.34
1	B	496	ARG	N-CA-C	-5.21	101.97	110.20
1	F	287	THR	CB-CA-C	-5.20	98.51	109.38
1	E	298	VAL	CB-CA-C	-5.20	105.32	111.97
2	C	221	GLU	CA-C-N	-5.19	115.88	122.37
2	C	221	GLU	C-N-CA	-5.19	115.88	122.37
1	F	18	ILE	N-CA-C	5.19	115.38	108.11
1	A	92	TRP	CB-CA-C	5.19	118.73	109.65
1	E	264	SER	N-CA-C	5.19	118.57	110.32
1	A	308	ASN	N-CA-C	-5.18	105.68	112.41
2	C	474	ASP	N-CA-C	-5.17	105.71	112.23
1	E	25	ILE	CB-CA-C	-5.17	102.80	111.29
1	E	145	ASP	N-CA-C	5.17	116.73	108.41
1	B	92	TRP	CB-CG-CD1	-5.16	119.16	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	280	LYS	N-CA-C	-5.16	105.55	111.07
2	C	123	LEU	CB-CA-C	-5.16	110.22	117.23
2	D	34	GLY	N-CA-C	5.16	119.09	113.58
2	D	459	ARG	CA-C-N	-5.16	111.31	121.41
2	D	459	ARG	C-N-CA	-5.16	111.31	121.41
2	C	84	ILE	N-CA-C	5.15	115.88	110.62
2	D	456	PHE	N-CA-C	5.15	116.58	111.07
1	B	306	CYS	N-CA-C	-5.15	107.13	113.41
2	C	463	HIS	N-CA-C	5.13	121.72	110.80
1	E	486	PHE	N-CA-C	5.12	117.92	109.72
1	E	181	THR	N-CA-CB	-5.12	102.44	110.69
1	A	198	GLU	CB-CA-C	-5.12	102.62	110.81
2	C	83	ILE	N-CA-C	-5.11	105.00	110.36
1	A	25	ILE	N-CA-C	-5.11	100.98	108.54
1	E	67	PHE	N-CA-C	-5.10	106.61	114.16
2	C	92	TRP	CB-CA-C	5.10	118.57	109.65
1	F	221	GLU	CA-C-N	-5.09	116.26	122.93
1	F	221	GLU	C-N-CA	-5.09	116.26	122.93
1	E	378	ASP	CA-C-N	5.09	131.26	121.54
1	E	378	ASP	C-N-CA	5.09	131.26	121.54
2	D	355	GLY	N-CA-C	-5.09	102.84	112.51
2	D	486	PHE	N-CA-C	5.09	117.54	109.50
1	E	38	ILE	CB-CA-C	-5.08	103.30	111.59
2	C	227	GLY	N-CA-C	5.07	120.84	114.25
2	C	310	GLU	N-CA-C	-5.07	102.69	110.14
1	E	175	GLY	CA-C-O	5.06	124.87	119.06
1	B	136	LYS	N-CA-C	5.05	116.79	111.28
1	F	16	GLN	N-CA-C	-5.05	99.40	108.48
1	A	463	HIS	N-CA-C	5.04	121.54	110.80
1	F	481	ASP	N-CA-C	5.04	117.92	110.46
1	F	251	ALA	N-CA-C	-5.04	106.82	113.17
1	F	157	SER	N-CA-C	5.04	121.53	110.80
1	E	98	VAL	O-C-N	5.03	126.84	121.91
1	F	509	VAL	CA-C-N	5.03	131.15	121.54
1	F	509	VAL	C-N-CA	5.03	131.15	121.54
1	F	516	GLY	CA-C-O	-5.03	116.52	119.69
2	D	25	ILE	N-CA-C	-5.01	102.23	108.84

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	SEP	Mainchain
1	A	432	TPO	Mainchain
1	B	317	TYR	Sidechain
1	B	431	SEP	Mainchain
1	B	432	TPO	Mainchain
2	C	235	TYR	Sidechain
2	C	432	TPO	Mainchain
2	D	235	TYR	Sidechain
2	D	432	TPO	Mainchain
1	E	431	SEP	Mainchain
1	E	432	TPO	Mainchain
1	F	431	SEP	Mainchain
1	F	432	TPO	Mainchain
1	F	509	VAL	Mainchain

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	3994	0	3984	325	0
1	B	3878	0	3862	321	0
1	E	3886	0	3872	298	0
1	F	3994	0	3984	339	0
2	C	3850	0	3837	299	0
2	D	3826	0	3818	300	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	62	0	24	12	0
4	B	62	0	24	9	0
4	C	62	0	24	7	0
4	D	62	0	23	7	0
4	E	62	0	24	6	0
4	F	62	0	24	7	0
5	A	8	0	0	0	0
5	B	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	7	0	0	2	0
5	D	13	0	0	2	0
5	E	10	0	0	0	0
5	F	23	0	0	6	0
All	All	23872	0	23500	1778	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:THR:HB	1:B:431:SEP:O3P	1.37	1.22
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.15
1:A:14:GLU:HG3	1:A:15:HIS:H	1.08	1.11
1:A:426:THR:HB	1:A:431:SEP:O2P	1.50	1.10
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.31	1.10
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.16	1.06
2:D:146:SER:H	2:D:181:THR:HG22	1.20	1.05
1:E:146:SER:H	1:E:181:THR:HG22	1.22	1.04
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.40	1.03
1:F:147:VAL:HG11	1:F:180:MET:HE3	1.38	1.02
1:F:486:PHE:CE2	1:F:496:ARG:HD2	1.92	1.02
2:C:123:LEU:HD12	2:C:163:GLU:OE2	1.61	0.99
1:F:146:SER:H	1:F:181:THR:HG22	1.24	0.99
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.45	0.99
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.29	0.98
2:D:446:ARG:N	2:D:496:ARG:HH12	1.60	0.97
1:B:79:THR:HG22	1:B:82:ASP:H	1.29	0.97
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.31	0.96
2:D:79:THR:HG22	2:D:82:ASP:H	1.25	0.96
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.46	0.95
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.29	0.95
1:F:79:THR:HG22	1:F:82:ASP:H	1.31	0.94
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.49	0.94
1:E:431:SEP:O	1:E:434:THR:HG22	1.67	0.94
1:F:509:VAL:O	1:F:512:VAL:HG23	1.66	0.94
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.48	0.94
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.49	0.93
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.33	0.93
2:D:371:LYS:O	2:D:371:LYS:HD3	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.33	0.92
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.00	0.92
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.35	0.91
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.72	0.90
1:B:379:SER:HA	1:B:413:THR:HG22	1.54	0.89
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.36	0.89
1:E:123:LEU:HD22	1:E:166:ARG:HD2	1.54	0.89
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.55	0.87
2:C:287:THR:CG2	2:C:414:ASN:HD22	1.87	0.87
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.85	0.87
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.40	0.87
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.55	0.87
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.57	0.87
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.89	0.87
1:E:293:GLY:HA2	4:E:901:ATP:O1A	1.74	0.87
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.54	0.87
1:A:14:GLU:CG	1:A:15:HIS:H	1.84	0.86
2:D:287:THR:CG2	2:D:414:ASN:HD22	1.87	0.86
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.55	0.86
1:B:431:SEP:O	1:B:434:THR:HG22	1.76	0.86
1:B:471:MET:HE1	1:B:473:SER:OG	1.76	0.86
1:F:45:SER:HB2	1:F:182:THR:HB	1.58	0.86
2:C:146:SER:H	2:C:181:THR:HG22	1.41	0.86
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.58	0.85
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.59	0.85
1:F:426:THR:HG22	1:F:428:SER:H	1.38	0.85
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.40	0.85
1:A:431:SEP:O	1:A:434:THR:HG22	1.76	0.85
1:B:140:ARG:HH11	1:B:140:ARG:CB	1.89	0.85
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.57	0.85
2:D:147:VAL:HG11	2:D:180:MET:CE	2.07	0.84
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.57	0.84
1:B:147:VAL:O	1:B:150:VAL:HG12	1.77	0.84
1:F:191:ILE:HB	1:F:198:GLU:CG	2.08	0.84
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.89	0.84
1:E:147:VAL:HG11	1:E:180:MET:HE3	1.59	0.84
1:F:509:VAL:O	1:F:512:VAL:CG2	2.25	0.84
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.07	0.84
1:F:231:MET:HE1	1:F:251:ALA:HB2	1.59	0.84
1:F:504:GLU:HB3	1:F:507:ARG:NH2	1.90	0.84
1:E:287:THR:CG2	1:E:414:ASN:HD22	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.59	0.84
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.08	0.83
2:C:52:LYS:HE3	4:C:903:ATP:O1B	1.78	0.83
2:D:191:ILE:HB	2:D:198:GLU:CG	2.08	0.83
1:F:145:ASP:OD2	1:F:181:THR:HG21	1.78	0.83
1:E:146:SER:N	1:E:181:THR:HG22	1.92	0.83
2:D:446:ARG:H	2:D:496:ARG:HH12	1.20	0.83
1:B:191:ILE:HB	1:B:198:GLU:CD	2.04	0.83
2:C:347:VAL:O	2:C:348:CYS:HB2	1.78	0.83
1:A:498:THR:HB	1:A:501:GLU:HG3	1.59	0.83
1:A:14:GLU:HG3	1:A:15:HIS:N	1.91	0.82
2:C:147:VAL:O	2:C:150:VAL:HG12	1.79	0.82
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.62	0.82
2:D:146:SER:N	2:D:181:THR:HG22	1.94	0.82
2:D:344:LEU:HD13	2:D:344:LEU:C	2.04	0.82
1:A:147:VAL:O	1:A:150:VAL:HG12	1.80	0.82
2:C:262:ARG:NH2	2:C:461:SER:HB2	1.93	0.82
1:A:379:SER:HA	1:A:413:THR:HG22	1.60	0.82
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.60	0.81
1:F:515:LYS:HG3	1:F:516:GLY:N	1.95	0.81
1:B:191:ILE:HB	1:B:198:GLU:CG	2.10	0.81
2:C:151:PHE:C	2:C:153:GLN:H	1.89	0.81
2:D:79:THR:O	2:D:83:ILE:HD12	1.81	0.81
2:C:495:THR:HA	2:D:487:GLU:OE2	1.81	0.80
1:A:211:LEU:O	1:A:212:GLU:HB3	1.81	0.80
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.45	0.80
1:A:252:MET:HE3	1:F:350:TYR:CE1	2.15	0.80
2:D:315:PHE:CZ	2:D:363:ILE:HG23	2.15	0.80
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.47	0.80
1:E:79:THR:HG22	1:E:82:ASP:H	1.47	0.80
1:F:502:LYS:NZ	1:F:507:ARG:HB3	1.97	0.80
1:A:79:THR:HG22	1:A:82:ASP:H	1.47	0.80
2:D:311:ARG:HD2	2:D:371:LYS:HD2	1.62	0.80
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.64	0.80
1:F:191:ILE:HB	1:F:198:GLU:CD	2.07	0.79
2:C:67:PHE:HB2	2:C:69:GLU:HG3	1.61	0.79
2:D:446:ARG:H	2:D:496:ARG:NH1	1.80	0.79
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.95	0.79
1:B:377:ILE:HD12	1:B:412:PHE:CE2	2.18	0.79
1:B:471:MET:HB3	1:B:480:LYS:NZ	1.97	0.79
2:C:79:THR:HG22	2:C:82:ASP:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:THR:HG22	1:E:428:SER:H	1.47	0.79
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.64	0.79
1:E:449:MET:HE3	1:F:467:ILE:HD11	1.65	0.79
1:E:485:ASN:ND2	1:E:496:ARG:HH11	1.81	0.79
1:F:218:ARG:HD2	5:F:906:HOH:O	1.83	0.79
1:F:486:PHE:HE2	1:F:496:ARG:CD	1.94	0.78
1:B:441:GLN:NE2	1:B:490:ILE:HD13	1.97	0.78
1:F:293:GLY:HA2	4:F:901:ATP:O1A	1.82	0.78
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.18	0.78
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.63	0.78
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.48	0.78
1:E:14:GLU:HG3	1:E:16:GLN:H	1.48	0.78
1:F:146:SER:N	1:F:181:THR:HG22	1.99	0.78
1:A:41:SER:HB3	1:A:178:THR:HB	1.67	0.77
1:E:147:VAL:O	1:E:150:VAL:HG12	1.84	0.77
1:B:147:VAL:HG11	1:B:180:MET:CE	2.14	0.77
1:E:191:ILE:HB	1:E:198:GLU:CG	2.15	0.77
1:E:371:LYS:HD2	1:E:371:LYS:O	1.85	0.77
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.20	0.77
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.77
2:C:300:ARG:HA	2:C:333:MET:HE1	1.66	0.77
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.66	0.76
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.85	0.76
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.67	0.76
1:F:420:MET:HA	5:F:915:HOH:O	1.83	0.76
1:A:426:THR:HG22	1:A:428:SER:H	1.51	0.76
1:F:515:LYS:HG3	1:F:516:GLY:H	1.50	0.76
1:B:363:ILE:O	1:B:367:ILE:HG13	1.86	0.76
1:A:371:LYS:O	1:A:371:LYS:HD3	1.86	0.76
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.85	0.75
1:A:117:VAL:HA	1:A:154:TYR:OH	1.86	0.75
1:E:146:SER:H	1:E:181:THR:CG2	1.99	0.75
2:D:287:THR:HG23	2:D:414:ASN:HB3	1.66	0.75
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.50	0.75
1:E:334:ASP:OD1	1:E:336:GLU:HB2	1.86	0.75
1:E:371:LYS:O	1:E:371:LYS:CD	2.35	0.75
1:F:439:LEU:HD12	1:F:440:LEU:N	2.01	0.75
4:B:901:ATP:H3'	2:C:458:MET:O	1.86	0.75
2:C:81:GLN:NE2	2:C:81:GLN:H	1.84	0.75
2:D:379:SER:HA	2:D:413:THR:HG22	1.66	0.75
1:B:426:THR:CB	1:B:431:SEP:O3P	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.02	0.75
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.52	0.74
1:A:65:ILE:O	1:A:65:ILE:HG22	1.85	0.74
1:B:21:MET:HE1	1:B:141:ARG:HG2	1.69	0.74
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.00	0.74
2:D:140:ARG:HB3	2:D:140:ARG:HH11	1.51	0.74
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.23	0.74
1:A:316:ALA:O	1:A:348:CYS:HA	1.88	0.74
2:D:446:ARG:N	2:D:496:ARG:NH1	2.35	0.74
1:A:426:THR:CB	1:A:431:SEP:O2P	2.32	0.74
2:D:151:PHE:C	2:D:153:GLN:H	1.95	0.74
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.70	0.74
1:E:145:ASP:OD2	1:E:181:THR:HG21	1.86	0.74
1:E:419:PHE:CD2	1:F:425:ILE:HD12	2.23	0.74
1:B:146:SER:H	1:B:181:THR:HG22	1.53	0.74
1:B:21:MET:HE3	1:B:141:ARG:NE	2.03	0.74
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.68	0.74
1:E:323:GLN:HE22	1:F:459:ARG:HD3	1.52	0.74
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.69	0.74
2:D:146:SER:H	2:D:181:THR:CG2	1.99	0.73
1:B:377:ILE:HD12	1:B:412:PHE:HE2	1.53	0.73
1:E:148:THR:HG21	1:E:183:GLU:HG3	1.68	0.73
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.22	0.73
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.69	0.73
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.52	0.73
2:C:79:THR:O	2:C:83:ILE:HD12	1.89	0.73
2:D:147:VAL:O	2:D:150:VAL:HG12	1.88	0.73
2:D:419:PHE:CD2	1:E:425:ILE:HD12	2.24	0.73
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.68	0.73
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.19	0.73
1:E:461:SER:OG	1:E:462:TRP:N	2.16	0.73
1:F:140:ARG:HB3	1:F:140:ARG:NH1	2.04	0.73
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.70	0.73
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.71	0.73
2:C:121:PHE:HD1	2:C:121:PHE:H	1.35	0.73
2:D:148:THR:OG1	2:D:182:THR:HG23	1.89	0.72
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.70	0.72
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.04	0.72
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.24	0.72
2:D:486:PHE:HB2	2:D:489:ILE:HD11	1.71	0.72
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:SER:OG	1:F:462:TRP:N	2.21	0.72
1:A:145:ASP:OD2	1:A:181:THR:HG21	1.89	0.72
1:B:502:LYS:HG3	1:B:504:GLU:O	1.88	0.72
2:D:426:THR:HG22	2:D:428:SER:H	1.52	0.72
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.70	0.72
1:F:140:ARG:HH11	1:F:140:ARG:CB	2.02	0.72
2:C:79:THR:CG2	2:C:81:GLN:HG2	2.19	0.72
2:C:123:LEU:HD22	2:C:127:ILE:HD11	1.70	0.72
2:C:21:MET:HE3	2:C:141:ARG:NE	2.04	0.72
2:C:45:SER:HB2	2:C:182:THR:HB	1.71	0.72
2:C:218:ARG:HB3	5:C:906:HOH:O	1.89	0.72
2:D:497:ILE:HD12	2:D:497:ILE:O	1.90	0.72
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.71	0.72
1:E:418:GLN:HB2	1:F:423:HIS:O	1.89	0.71
1:E:426:THR:HG22	1:E:428:SER:N	2.04	0.71
1:B:497:ILE:HG13	1:B:498:THR:N	2.04	0.71
2:D:191:ILE:HB	2:D:198:GLU:HG3	1.70	0.71
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.72	0.71
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.20	0.71
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.05	0.71
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.05	0.71
2:D:439:LEU:HD12	2:D:440:LEU:N	2.06	0.71
1:B:106:LEU:C	1:B:106:LEU:HD12	2.16	0.71
1:B:119:GLY:C	1:B:121:PHE:H	1.99	0.71
1:B:462:TRP:O	1:B:463:HIS:O	2.08	0.71
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.26	0.71
1:E:344:LEU:C	1:E:344:LEU:HD13	2.15	0.71
1:F:379:SER:HA	1:F:413:THR:HG22	1.73	0.71
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.04	0.71
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.55	0.71
1:B:273:MET:O	1:B:463:HIS:HA	1.90	0.71
2:D:299:SER:C	2:D:333:MET:HE1	2.16	0.71
1:F:182:THR:HG22	1:F:183:GLU:N	2.06	0.71
2:C:191:ILE:HB	2:C:198:GLU:CG	2.20	0.70
1:B:169:ALA:O	1:B:173:GLN:HG3	1.91	0.70
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.56	0.70
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.06	0.70
2:C:106:LEU:C	2:C:106:LEU:HD12	2.16	0.70
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.54	0.70
2:D:31:ILE:HG22	2:D:222:ILE:HD12	1.73	0.70
1:E:19:ALA:O	1:E:38:ILE:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:CD2	1:E:127:ILE:HD11	2.20	0.70
1:B:498:THR:OG1	2:C:499:VAL:HG21	1.91	0.70
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.74	0.70
1:A:266:GLY:HA3	1:A:300:ARG:O	1.91	0.70
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.72	0.70
2:C:371:LYS:O	2:C:371:LYS:HD3	1.91	0.70
2:C:393:ARG:O	2:C:397:ILE:HG12	1.90	0.70
2:D:145:ASP:OD2	2:D:181:THR:HG21	1.92	0.70
1:A:147:VAL:HG11	1:A:180:MET:CE	2.21	0.70
1:A:451:ARG:HG2	1:A:451:ARG:NH1	1.99	0.70
1:A:499:VAL:O	1:A:499:VAL:HG12	1.92	0.70
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.72	0.70
1:E:273:MET:O	1:E:463:HIS:HA	1.91	0.70
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.73	0.70
1:A:151:PHE:C	1:A:153:GLN:H	2.00	0.70
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.91	0.70
1:B:65:ILE:O	1:B:65:ILE:HG22	1.91	0.69
2:C:14:GLU:HG3	2:C:16:GLN:H	1.57	0.69
2:C:203:ASN:HB3	2:C:225:LEU:HD23	1.74	0.69
1:B:429:HIS:HA	1:B:431:SEP:O1P	1.91	0.69
2:C:379:SER:HA	2:C:413:THR:HG22	1.73	0.69
1:F:151:PHE:C	1:F:153:GLN:H	2.00	0.69
1:F:239:ILE:HB	5:F:916:HOH:O	1.91	0.69
1:F:347:VAL:O	1:F:348:CYS:HB2	1.92	0.69
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.22	0.69
1:B:18:ILE:HB	1:B:228:THR:HG23	1.73	0.69
2:D:345:LYS:HZ2	2:D:366:GLU:HG2	1.57	0.69
1:F:147:VAL:O	1:F:150:VAL:HG12	1.92	0.69
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.22	0.69
1:E:396:VAL:O	1:E:400:THR:HB	1.92	0.69
1:F:502:LYS:HZ1	1:F:507:ARG:HB3	1.55	0.69
1:A:377:ILE:HD12	1:A:412:PHE:HE2	1.58	0.69
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.92	0.69
1:A:89:SER:HB2	1:B:227:GLY:O	1.93	0.69
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.93	0.69
1:E:151:PHE:C	1:E:153:GLN:H	2.01	0.69
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.23	0.69
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.75	0.69
1:F:81:GLN:NE2	1:F:81:GLN:H	1.91	0.69
1:F:509:VAL:HG12	1:F:510:ARG:H	1.57	0.69
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HB2	4:B:903:ATP:O1B	1.93	0.68
2:C:182:THR:HG22	2:C:183:GLU:H	1.57	0.68
1:E:497:ILE:HG22	1:E:498:THR:H	1.58	0.68
1:F:334:ASP:OD1	1:F:336:GLU:HB2	1.93	0.68
1:A:79:THR:O	1:A:83:ILE:HD12	1.93	0.68
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.08	0.68
2:C:287:THR:HG23	2:C:414:ASN:HB3	1.74	0.68
2:C:299:SER:HB3	2:C:333:MET:HE2	1.75	0.68
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.74	0.68
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.06	0.68
2:D:295:THR:HG23	2:D:378:ASP:OD2	1.93	0.68
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.68
1:B:300:ARG:HA	1:B:333:MET:HE1	1.76	0.68
2:C:126:LEU:O	2:C:129:ARG:HB2	1.92	0.68
2:C:146:SER:N	2:C:181:THR:HG22	2.08	0.68
1:A:505:LEU:HD12	1:A:505:LEU:O	1.94	0.68
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.08	0.68
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.58	0.68
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.76	0.68
1:A:18:ILE:N	1:A:18:ILE:HD12	2.08	0.68
2:D:79:THR:HG23	2:D:81:GLN:H	1.59	0.68
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.23	0.68
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.58	0.68
1:A:350:TYR:CE1	1:B:252:MET:HE3	2.29	0.67
1:F:14:GLU:HG2	5:F:923:HOH:O	1.94	0.67
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.76	0.67
2:D:370:PHE:O	2:D:371:LYS:HD2	1.94	0.67
1:A:363:ILE:O	1:A:367:ILE:HG13	1.94	0.67
2:C:17:ALA:C	2:C:18:ILE:HD12	2.19	0.67
2:C:147:VAL:HG11	2:C:180:MET:HE3	1.75	0.67
1:F:273:MET:O	1:F:463:HIS:HA	1.94	0.67
1:F:504:GLU:HA	1:F:507:ARG:NE	2.09	0.67
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.75	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
1:A:471:MET:HE2	1:A:478:ASP:HB2	1.77	0.67
1:B:151:PHE:C	1:B:153:GLN:H	2.02	0.67
2:D:182:THR:HG22	2:D:183:GLU:N	2.09	0.67
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.59	0.67
1:F:504:GLU:HB3	1:F:507:ARG:CZ	2.24	0.67
1:A:503:SER:C	1:A:504:GLU:HG3	2.20	0.67
1:B:295:THR:HG21	1:B:319:GLU:OE2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.08	0.67
1:A:299:SER:C	1:A:333:MET:HE1	2.20	0.67
1:A:471:MET:HE2	1:A:478:ASP:CB	2.25	0.67
2:C:461:SER:OG	2:C:462:TRP:N	2.25	0.67
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.07	0.67
1:A:293:GLY:HA2	4:A:901:ATP:O1A	1.95	0.67
1:B:497:ILE:HD12	1:B:499:VAL:HB	1.74	0.67
2:C:106:LEU:HD13	2:C:129:ARG:NH2	2.10	0.67
1:A:273:MET:O	1:A:463:HIS:HA	1.95	0.67
1:B:497:ILE:HD12	1:B:499:VAL:H	1.60	0.67
2:D:14:GLU:CD	2:D:15:HIS:H	2.03	0.67
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.60	0.67
1:B:461:SER:OG	1:B:462:TRP:N	2.26	0.66
2:D:367:ILE:HG12	2:D:375:ILE:HD11	1.76	0.66
1:A:61:TYR:CE1	1:A:92:TRP:HB2	2.31	0.66
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.77	0.66
1:B:81:GLN:NE2	1:B:81:GLN:H	1.93	0.66
2:D:316:ALA:O	2:D:348:CYS:HA	1.95	0.66
1:E:123:LEU:HD22	1:E:166:ARG:CD	2.25	0.66
1:F:119:GLY:C	1:F:122:ASP:OD2	2.38	0.66
1:A:24:MET:CB	1:A:62:ASN:HD22	2.08	0.66
2:C:273:MET:O	2:C:463:HIS:HA	1.96	0.66
1:F:371:LYS:O	1:F:371:LYS:CD	2.43	0.66
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.95	0.66
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.24	0.66
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.77	0.66
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.76	0.66
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.19	0.66
1:F:471:MET:HB3	1:F:480:LYS:NZ	2.11	0.66
2:C:371:LYS:O	2:C:371:LYS:CD	2.43	0.66
1:F:363:ILE:O	1:F:367:ILE:HG13	1.96	0.66
1:B:426:THR:HG22	1:B:428:SER:H	1.60	0.66
2:C:497:ILE:C	2:C:498:THR:HG22	2.21	0.66
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.09	0.66
2:C:182:THR:HG22	2:C:183:GLU:N	2.10	0.66
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.61	0.65
2:C:334:ASP:OD1	2:C:336:GLU:HB2	1.97	0.65
2:C:419:PHE:O	2:C:420:MET:HB2	1.95	0.65
2:C:470:PHE:HB2	2:C:478:ASP:O	1.96	0.65
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.96	0.65
1:E:359:HIS:O	1:E:363:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.76	0.65
1:A:459:ARG:HD3	1:F:323:GLN:HE22	1.62	0.65
1:B:293:GLY:HA2	4:B:901:ATP:O1A	1.96	0.65
1:B:350:TYR:CE1	2:C:252:MET:HE3	2.32	0.65
1:F:146:SER:H	1:F:181:THR:CG2	2.02	0.65
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.78	0.65
2:D:334:ASP:OD1	2:D:336:GLU:HB2	1.96	0.65
2:D:344:LEU:HD13	2:D:345:LYS:N	2.12	0.65
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.79	0.65
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.27	0.65
1:E:439:LEU:HD12	1:E:440:LEU:N	2.11	0.65
2:D:52:LYS:HE3	4:D:903:ATP:O1B	1.97	0.65
2:D:371:LYS:O	2:D:371:LYS:CD	2.43	0.65
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.30	0.65
1:A:146:SER:H	1:A:181:THR:HG22	1.61	0.65
2:D:299:SER:HB3	2:D:333:MET:HE2	1.79	0.65
2:D:345:LYS:NZ	2:D:366:GLU:HG2	2.10	0.65
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.79	0.65
1:B:371:LYS:O	1:B:371:LYS:HD3	1.97	0.65
2:C:300:ARG:CA	2:C:333:MET:HE1	2.27	0.65
1:F:508:ILE:HG22	1:F:508:ILE:O	1.97	0.65
1:B:444:GLU:OE2	2:C:489:ILE:HG13	1.97	0.64
2:C:41:SER:HB3	2:C:178:THR:HB	1.78	0.64
2:D:49:GLY:O	2:D:218:ARG:NH2	2.30	0.64
2:D:191:ILE:HB	2:D:198:GLU:CD	2.21	0.64
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.79	0.64
2:D:311:ARG:HD2	2:D:371:LYS:CD	2.27	0.64
2:D:471:MET:HE1	2:D:473:SER:OG	1.97	0.64
1:F:432:TPO:O3P	1:F:432:TPO:HG21	1.97	0.64
1:B:79:THR:HG21	1:B:81:GLN:HG2	1.78	0.64
2:C:350:TYR:CE1	2:D:252:MET:HE3	2.32	0.64
2:D:191:ILE:CB	2:D:198:GLU:HG3	2.28	0.64
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.97	0.64
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.78	0.64
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.62	0.64
1:E:79:THR:HG23	1:E:81:GLN:HE21	1.61	0.64
1:E:148:THR:OG1	1:E:182:THR:HG23	1.97	0.64
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.27	0.64
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.27	0.64
1:A:96:LYS:O	1:A:100:GLU:HG3	1.98	0.64
1:A:334:ASP:OD1	1:A:336:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:C	1:A:506:SER:H	2.05	0.64
2:C:18:ILE:HD12	2:C:18:ILE:N	2.11	0.64
2:D:19:ALA:C	2:D:38:ILE:HD12	2.23	0.64
1:F:299:SER:C	1:F:333:MET:HE1	2.23	0.64
1:A:396:VAL:O	1:A:400:THR:HB	1.97	0.64
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.28	0.64
1:E:462:TRP:O	1:E:463:HIS:O	2.16	0.64
1:F:344:LEU:HD22	1:F:345:LYS:N	2.12	0.64
1:F:431:SEP:O	1:F:434:THR:HG22	1.98	0.64
1:F:471:MET:HG2	1:F:480:LYS:HE2	1.79	0.64
1:E:186:GLU:OE2	1:E:187:GLU:N	2.30	0.64
1:B:21:MET:CE	1:B:141:ARG:HG2	2.27	0.64
2:C:305:ALA:HB2	2:C:374:ARG:CD	2.28	0.64
2:D:182:THR:HG22	2:D:183:GLU:H	1.61	0.64
2:D:400:THR:HG22	2:D:401:GLY:N	2.13	0.64
2:D:469:GLU:HG3	2:D:470:PHE:N	2.13	0.64
1:A:315:PHE:CZ	1:A:363:ILE:HG23	2.33	0.64
1:A:371:LYS:O	1:A:371:LYS:CD	2.45	0.64
1:B:45:SER:HB3	1:B:182:THR:HB	1.79	0.64
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.80	0.64
2:D:223:LEU:O	2:D:223:LEU:HD22	1.98	0.64
2:D:393:ARG:O	2:D:397:ILE:HG12	1.98	0.64
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.80	0.63
1:F:106:LEU:C	1:F:106:LEU:HD12	2.23	0.63
1:A:420:MET:CE	1:B:490:ILE:HG21	2.29	0.63
2:C:170:ARG:O	2:C:174:ILE:HG12	1.99	0.63
2:D:313:ILE:CD1	2:D:372:PRO:HG3	2.28	0.63
1:B:24:MET:CB	1:B:62:ASN:HD22	2.10	0.63
2:C:311:ARG:HD2	2:C:371:LYS:HD2	1.81	0.63
1:F:231:MET:CE	1:F:251:ALA:HB2	2.27	0.63
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.34	0.63
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.63
1:A:106:LEU:C	1:A:106:LEU:HD12	2.24	0.63
2:C:159:VAL:O	2:C:163:GLU:HG2	1.98	0.63
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.79	0.63
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.80	0.63
1:F:120:GLY:HA2	1:F:123:LEU:HB2	1.81	0.63
2:C:61:TYR:CE1	2:C:92:TRP:HB2	2.34	0.63
2:D:345:LYS:HZ3	2:D:366:GLU:CD	2.06	0.62
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.62
1:E:345:LYS:HZ3	1:E:366:GLU:CD	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:ARG:O	1:E:497:ILE:HD13	1.99	0.62
1:A:419:PHE:CD2	1:B:425:ILE:CD1	2.83	0.62
2:C:419:PHE:CD1	2:C:420:MET:HG3	2.34	0.62
1:A:52:LYS:HE3	4:A:903:ATP:O1B	2.00	0.62
2:C:231:MET:HE1	2:C:251:ALA:HB2	1.80	0.62
2:D:340:ARG:O	2:D:342:ASN:N	2.31	0.62
1:B:371:LYS:O	1:B:371:LYS:CD	2.47	0.62
2:D:81:GLN:H	2:D:81:GLN:NE2	1.98	0.62
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.30	0.62
1:A:300:ARG:HA	1:A:333:MET:HE1	1.82	0.62
1:E:170:ARG:O	1:E:174:ILE:HG12	1.99	0.62
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.99	0.62
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.14	0.62
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.64	0.62
2:D:14:GLU:OE1	2:D:14:GLU:HA	1.99	0.62
2:D:377:ILE:HD12	2:D:412:PHE:CE2	2.35	0.62
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.34	0.62
1:E:148:THR:HG21	1:E:183:GLU:CG	2.30	0.62
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.81	0.62
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.82	0.62
1:B:146:SER:H	1:B:181:THR:CG2	2.13	0.62
2:C:145:ASP:OD2	2:C:181:THR:HG21	1.99	0.62
1:E:14:GLU:HG3	1:E:16:GLN:N	2.14	0.62
1:E:347:VAL:HG12	1:E:348:CYS:N	2.14	0.62
1:F:122:ASP:O	1:F:126:LEU:N	2.32	0.62
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.30	0.62
2:C:81:GLN:H	2:C:81:GLN:CD	2.05	0.62
1:A:441:GLN:HG3	1:A:441:GLN:O	2.00	0.61
1:B:287:THR:HG21	1:B:425:ILE:O	1.99	0.61
1:E:294:LYS:HB2	4:E:901:ATP:O1B	1.98	0.61
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.15	0.61
1:A:231:MET:HE1	1:A:251:ALA:HB2	1.82	0.61
1:B:170:ARG:O	1:B:174:ILE:HG12	2.00	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
2:C:203:ASN:HB3	2:C:225:LEU:CD2	2.30	0.61
2:D:79:THR:HG23	2:D:81:GLN:HE21	1.65	0.61
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.78	0.61
1:E:148:THR:OG1	1:E:182:THR:CG2	2.48	0.61
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.81	0.61
1:E:300:ARG:HA	1:E:333:MET:HE1	1.81	0.61
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:ARG:O	1:F:342:ASN:N	2.32	0.61
1:B:51:GLY:O	1:B:52:LYS:C	2.43	0.61
2:C:150:VAL:O	2:C:153:GLN:HG3	2.01	0.61
2:D:446:ARG:H	2:D:496:ARG:HH22	1.47	0.61
2:C:52:LYS:HD3	2:C:182:THR:O	2.01	0.61
1:E:471:MET:HE2	1:E:478:ASP:HB2	1.81	0.61
2:C:19:ALA:O	2:C:38:ILE:HD12	2.00	0.61
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.15	0.61
2:D:418:GLN:HB2	1:E:423:HIS:O	2.00	0.61
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.82	0.61
1:B:146:SER:N	1:B:181:THR:HG22	2.15	0.61
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.83	0.61
2:C:296:LEU:HD13	2:C:331:TRP:CD2	2.36	0.61
1:E:140:ARG:HB3	1:E:140:ARG:NH1	2.15	0.61
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.83	0.61
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.49	0.61
1:F:371:LYS:O	1:F:371:LYS:HD3	1.99	0.61
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.81	0.61
1:A:486:PHE:HB2	1:A:489:ILE:HD11	1.82	0.61
1:B:418:GLN:HG3	1:B:418:GLN:O	2.00	0.61
2:C:148:THR:OG1	2:C:182:THR:HG23	2.01	0.61
2:C:363:ILE:O	2:C:367:ILE:HG13	2.01	0.61
2:D:41:SER:HB3	2:D:178:THR:HB	1.83	0.61
2:D:151:PHE:C	2:D:153:GLN:N	2.58	0.61
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.62	0.61
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.64	0.61
1:B:19:ALA:O	1:B:38:ILE:HD12	2.00	0.61
2:C:431:SER:O	2:C:432:TPO:HG22	2.00	0.61
1:E:159:VAL:O	1:E:163:GLU:HG2	2.01	0.61
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.20	0.61
1:B:283:ILE:HD12	1:B:412:PHE:HE1	1.65	0.61
2:D:347:VAL:O	2:D:348:CYS:HB2	2.00	0.61
1:A:320:SER:HA	1:B:254:LEU:HG	1.82	0.60
1:F:19:ALA:O	1:F:38:ILE:HD12	2.01	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.31	0.60
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.82	0.60
1:A:16:GLN:O	1:A:17:ALA:O	2.20	0.60
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.16	0.60
1:A:347:VAL:O	1:A:348:CYS:HB2	2.01	0.60
1:B:117:VAL:O	1:B:117:VAL:HG12	2.02	0.60
1:B:493:SER:HB3	2:C:488:ARG:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.84	0.60
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.82	0.60
2:D:130:ILE:O	2:D:134:ILE:HG13	2.00	0.60
2:D:449:MET:HE3	1:E:467:ILE:HD11	1.84	0.60
2:C:347:VAL:O	2:C:348:CYS:CB	2.45	0.60
2:C:400:THR:HG22	2:C:401:GLY:N	2.16	0.60
2:D:446:ARG:H	2:D:496:ARG:NH2	1.99	0.60
1:E:268:VAL:O	1:E:271:ASP:HB2	2.02	0.60
1:F:471:MET:HE2	1:F:478:ASP:HB2	1.83	0.60
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.36	0.60
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.32	0.60
1:B:379:SER:CA	1:B:413:THR:HG22	2.30	0.60
2:D:140:ARG:HB3	2:D:140:ARG:NH1	2.16	0.60
1:E:19:ALA:C	1:E:38:ILE:HD12	2.26	0.60
1:F:340:ARG:C	1:F:342:ASN:H	2.09	0.60
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.84	0.60
2:D:79:THR:HG22	2:D:82:ASP:N	2.07	0.60
1:F:316:ALA:O	1:F:348:CYS:HA	2.02	0.60
2:C:340:ARG:O	2:C:342:ASN:N	2.34	0.59
1:E:436:THR:HG23	1:E:458:MET:HG3	1.83	0.59
1:B:299:SER:HB3	1:B:333:MET:HE2	1.83	0.59
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.67	0.59
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.59
2:C:21:MET:CE	2:C:141:ARG:HG2	2.33	0.59
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.84	0.59
2:D:396:VAL:O	2:D:400:THR:HB	2.02	0.59
1:F:378:ASP:HB3	5:F:904:HOH:O	2.02	0.59
2:C:462:TRP:O	2:C:463:HIS:O	2.20	0.59
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.85	0.59
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.36	0.59
2:C:147:VAL:HG11	2:C:180:MET:CE	2.32	0.59
2:D:340:ARG:C	2:D:342:ASN:H	2.10	0.59
1:F:159:VAL:O	1:F:163:GLU:HG2	2.02	0.59
1:F:21:MET:HE1	1:F:141:ARG:HG2	1.85	0.59
2:C:318:GLU:OE2	2:D:432:TPO:O1P	2.21	0.59
1:E:316:ALA:O	1:E:348:CYS:HA	2.03	0.59
1:F:123:LEU:O	1:F:127:ILE:HG12	2.02	0.59
1:F:504:GLU:O	1:F:505:LEU:HB2	2.00	0.59
1:A:379:SER:H	1:A:413:THR:HB	1.67	0.59
2:D:131:ASN:OD1	2:D:174:ILE:HD12	2.03	0.59
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.85	0.59
1:F:218:ARG:HB3	5:F:919:HOH:O	2.03	0.59
1:B:340:ARG:C	1:B:342:ASN:H	2.11	0.59
1:B:471:MET:HB3	1:B:480:LYS:HZ3	1.68	0.59
2:C:113:GLU:O	2:C:114:GLY:C	2.45	0.59
1:A:432:TPO:O1P	1:A:432:TPO:HG22	2.02	0.58
2:C:33:HIS:HD2	2:C:229:SER:OG	1.85	0.58
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.85	0.58
1:E:485:ASN:HD21	1:E:496:ARG:NH1	2.01	0.58
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.33	0.58
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.85	0.58
4:A:901:ATP:H3'	1:B:458:MET:O	2.03	0.58
2:C:79:THR:CG2	2:C:82:ASP:H	2.15	0.58
2:C:419:PHE:CD2	2:D:425:ILE:HD12	2.38	0.58
2:D:439:LEU:HD12	2:D:439:LEU:C	2.28	0.58
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.68	0.58
2:C:294:LYS:HB2	4:C:901:ATP:O1B	2.04	0.58
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.66	0.58
1:B:65:ILE:O	1:B:65:ILE:CG2	2.52	0.58
1:A:420:MET:HE1	1:B:490:ILE:HG21	1.85	0.58
2:D:79:THR:CG2	2:D:82:ASP:H	2.09	0.58
1:E:400:THR:HG22	1:E:401:GLY:N	2.19	0.58
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.86	0.58
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.85	0.58
1:F:503:SER:O	1:F:504:GLU:O	2.21	0.58
1:A:191:ILE:HB	1:A:198:GLU:CG	2.33	0.58
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.37	0.58
1:A:461:SER:OG	1:A:462:TRP:N	2.36	0.58
1:B:98:VAL:HA	1:B:103:LEU:O	2.02	0.58
2:C:344:LEU:HD22	2:C:345:LYS:N	2.18	0.58
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.19	0.58
2:D:446:ARG:HG3	2:D:496:ARG:NH1	2.18	0.58
1:A:19:ALA:C	1:A:38:ILE:HD12	2.29	0.58
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	0.58
1:A:400:THR:HG22	1:A:401:GLY:N	2.18	0.58
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.86	0.58
2:C:88:ARG:HD3	2:D:15:HIS:O	2.04	0.58
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.38	0.58
1:E:123:LEU:CD1	1:E:163:GLU:OE2	2.52	0.57
1:A:462:TRP:O	1:A:463:HIS:O	2.21	0.57
1:E:358:ASP:O	1:E:362:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:THR:HG23	1:F:378:ASP:OD2	2.04	0.57
1:B:119:GLY:C	1:B:121:PHE:N	2.62	0.57
2:D:79:THR:HG21	2:D:81:GLN:HG2	1.84	0.57
2:D:81:GLN:H	2:D:81:GLN:CD	2.13	0.57
1:A:65:ILE:O	1:A:65:ILE:CG2	2.51	0.57
1:E:41:SER:HB3	1:E:178:THR:HB	1.84	0.57
1:A:432:TPO:OG1	1:A:433:ILE:HD12	2.04	0.57
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.86	0.57
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.87	0.57
2:C:419:PHE:O	2:C:420:MET:CB	2.51	0.57
2:D:344:LEU:C	2:D:344:LEU:CD1	2.77	0.57
2:D:345:LYS:NZ	2:D:366:GLU:CG	2.67	0.57
1:E:191:ILE:HB	1:E:198:GLU:CD	2.29	0.57
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.19	0.57
2:C:426:THR:HG22	2:C:428:SER:H	1.70	0.57
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.86	0.57
2:D:164:LEU:CD2	2:D:180:MET:HE1	2.35	0.57
1:F:123:LEU:O	1:F:123:LEU:HD13	2.03	0.57
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.04	0.57
1:E:81:GLN:NE2	1:E:81:GLN:H	2.02	0.57
1:E:231:MET:HE1	1:E:251:ALA:HB2	1.85	0.57
1:A:513:GLN:HG3	1:A:513:GLN:O	2.04	0.57
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.85	0.57
2:C:79:THR:C	2:C:83:ILE:HD12	2.29	0.57
1:E:281:ASP:O	1:E:282:SER:HB3	2.05	0.57
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.86	0.57
2:C:146:SER:H	2:C:181:THR:CG2	2.16	0.57
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.87	0.57
1:E:123:LEU:CD2	1:E:166:ARG:HD2	2.30	0.57
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.87	0.57
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.05	0.57
1:F:182:THR:HG22	1:F:183:GLU:H	1.70	0.57
1:A:15:HIS:C	1:A:16:GLN:OE1	2.47	0.57
1:A:85:LYS:NZ	1:B:14:GLU:HG3	2.20	0.57
2:D:45:SER:HB2	2:D:182:THR:HB	1.87	0.57
2:D:446:ARG:H	2:D:496:ARG:CZ	2.16	0.57
1:E:469:GLU:HB2	1:E:483:PHE:CZ	2.40	0.57
1:F:79:THR:HG23	1:F:81:GLN:H	1.70	0.57
1:F:300:ARG:HA	1:F:333:MET:HE1	1.87	0.57
2:C:45:SER:CB	2:C:182:THR:HB	2.35	0.56
2:D:106:LEU:C	2:D:106:LEU:HD12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.69	0.56
1:A:21:MET:CE	1:A:59:PHE:CZ	2.88	0.56
2:C:444:GLU:OE2	2:D:489:ILE:HG12	2.05	0.56
1:E:471:MET:HE2	1:E:478:ASP:CB	2.34	0.56
1:F:96:LYS:O	1:F:100:GLU:HG3	2.05	0.56
1:F:115:GLN:HG3	1:F:116:GLU:N	2.21	0.56
1:B:45:SER:CB	1:B:182:THR:HB	2.35	0.56
1:B:150:VAL:O	1:B:153:GLN:HG3	2.05	0.56
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.86	0.56
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.87	0.56
2:D:96:LYS:O	2:D:100:GLU:HG3	2.05	0.56
2:D:495:THR:HA	1:E:487:GLU:OE2	2.05	0.56
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.40	0.56
1:E:485:ASN:HD21	1:E:496:ARG:HH11	1.50	0.56
1:F:118:VAL:O	1:F:118:VAL:HG13	2.05	0.56
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.87	0.56
1:F:471:MET:HE2	1:F:478:ASP:CB	2.34	0.56
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.20	0.56
1:A:211:LEU:HD12	1:A:215:ARG:O	2.06	0.56
1:A:252:MET:HE3	1:F:350:TYR:CZ	2.39	0.56
2:C:449:MET:HE3	2:D:467:ILE:HD11	1.87	0.56
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.87	0.56
2:D:178:THR:HG22	2:D:179:VAL:N	2.20	0.56
2:D:471:MET:HB3	2:D:480:LYS:NZ	2.20	0.56
1:F:150:VAL:O	1:F:153:GLN:HG3	2.06	0.56
1:B:497:ILE:HG13	1:B:498:THR:H	1.69	0.56
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.86	0.56
2:D:231:MET:CE	2:D:251:ALA:HB2	2.31	0.56
1:B:294:LYS:HB2	4:B:901:ATP:O1B	2.06	0.56
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.21	0.56
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.41	0.56
1:F:497:ILE:C	1:F:497:ILE:HD12	2.30	0.56
1:A:299:SER:HB3	1:A:333:MET:HE2	1.86	0.56
1:A:311:ARG:HD2	1:A:371:LYS:CD	2.35	0.56
1:B:79:THR:CG2	1:B:82:ASP:H	2.11	0.56
1:B:130:ILE:O	1:B:134:ILE:HG13	2.06	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.70	0.56
1:E:499:VAL:O	1:E:499:VAL:HG12	2.06	0.56
1:F:436:THR:OG1	1:F:458:MET:HG2	2.06	0.56
1:A:495:THR:HG22	1:A:497:ILE:CG2	2.36	0.55
1:F:118:VAL:HG22	1:F:122:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD23	1:A:220:LEU:C	2.31	0.55
4:A:901:ATP:O3'	1:B:457:LYS:HB2	2.06	0.55
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.87	0.55
1:F:117:VAL:O	1:F:118:VAL:HB	2.06	0.55
1:F:151:PHE:C	1:F:153:GLN:N	2.63	0.55
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.55
2:D:419:PHE:CD2	1:E:425:ILE:CD1	2.88	0.55
1:A:345:LYS:HZ3	1:A:366:GLU:HG2	1.71	0.55
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.05	0.55
2:C:49:GLY:O	2:C:218:ARG:NH2	2.39	0.55
2:C:104:PHE:CE2	2:C:106:LEU:HB2	2.41	0.55
2:C:377:ILE:HD12	2:C:412:PHE:CE2	2.42	0.55
2:D:21:MET:HE3	2:D:141:ARG:CD	2.36	0.55
2:D:469:GLU:HB2	2:D:483:PHE:CZ	2.42	0.55
1:E:49:GLY:CA	4:E:903:ATP:O2B	2.53	0.55
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.36	0.55
1:E:123:LEU:HD21	1:E:127:ILE:HD11	1.87	0.55
1:E:496:ARG:HG3	1:E:497:ILE:N	2.21	0.55
2:D:42:THR:HG23	2:D:203:ASN:HB2	1.88	0.55
1:F:294:LYS:N	4:F:901:ATP:O1B	2.40	0.55
1:A:433:ILE:HG22	1:A:433:ILE:O	2.06	0.55
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.36	0.55
1:B:448:GLU:HG2	2:C:466:ALA:HA	1.89	0.55
2:C:340:ARG:C	2:C:342:ASN:H	2.14	0.55
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.87	0.55
1:F:439:LEU:HD12	1:F:439:LEU:C	2.31	0.55
1:A:393:ARG:O	1:A:397:ILE:HG12	2.06	0.55
2:C:117:VAL:O	2:C:117:VAL:HG12	2.06	0.55
2:D:140:ARG:HH11	2:D:140:ARG:CB	2.20	0.55
1:A:49:GLY:CA	4:A:903:ATP:O2B	2.54	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.52	0.55
1:B:449:MET:HE3	2:C:467:ILE:HD11	1.87	0.55
1:B:485:ASN:OD1	1:B:485:ASN:N	2.33	0.55
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.89	0.55
2:C:493:SER:HB3	2:D:488:ARG:HG2	1.89	0.55
2:D:377:ILE:HD12	2:D:412:PHE:HE2	1.72	0.55
1:E:151:PHE:C	1:E:153:GLN:N	2.64	0.55
1:A:439:LEU:HD12	1:A:440:LEU:N	2.21	0.55
2:C:169:ALA:O	2:C:173:GLN:HG3	2.07	0.55
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.41	0.55
1:F:501:GLU:HG3	1:F:502:LYS:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HG2	1:B:191:ILE:O	2.06	0.54
1:B:360:LEU:O	1:B:360:LEU:HD22	2.07	0.54
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.21	0.54
1:B:79:THR:O	1:B:83:ILE:HD12	2.07	0.54
1:B:213:GLY:O	1:B:214:GLU:CB	2.55	0.54
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.37	0.54
2:C:148:THR:HG21	2:C:183:GLU:HG3	1.89	0.54
2:C:208:ARG:NH2	2:C:221:GLU:OE2	2.40	0.54
2:D:147:VAL:HG11	2:D:180:MET:HE2	1.86	0.54
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.37	0.54
1:E:485:ASN:ND2	1:E:496:ARG:NH1	2.51	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:B:148:THR:OG1	1:B:182:THR:HG23	2.08	0.54
1:B:159:VAL:O	1:B:163:GLU:HG2	2.08	0.54
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.22	0.54
1:E:121:PHE:CD1	1:E:121:PHE:N	2.74	0.54
1:A:340:ARG:C	1:A:342:ASN:H	2.15	0.54
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.41	0.54
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.88	0.54
1:A:148:THR:OG1	1:A:182:THR:HG23	2.08	0.54
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.89	0.54
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.73	0.54
1:A:451:ARG:HD2	1:A:451:ARG:N	2.23	0.54
1:B:213:GLY:O	1:B:214:GLU:HB2	2.06	0.54
1:B:340:ARG:O	1:B:342:ASN:N	2.40	0.54
2:C:53:THR:HG23	2:C:145:ASP:OD1	2.06	0.54
2:C:356:LEU:CD2	2:C:387:VAL:HG11	2.37	0.54
2:D:387:VAL:CG1	2:D:388:SER:N	2.70	0.54
1:A:57:ILE:HD13	1:A:73:PHE:CE1	2.43	0.54
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.54
1:B:426:THR:HG22	1:B:428:SER:N	2.23	0.54
1:B:503:SER:O	1:B:504:GLU:HB2	2.06	0.54
1:E:471:MET:HB3	1:E:480:LYS:NZ	2.23	0.54
1:F:504:GLU:HA	1:F:507:ARG:HE	1.73	0.54
1:B:299:SER:C	1:B:333:MET:HE1	2.32	0.54
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.43	0.54
2:C:18:ILE:HG21	2:C:37:PRO:HB3	1.89	0.54
2:D:127:ILE:HD11	2:D:167:LEU:HA	1.88	0.54
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.90	0.54
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.73	0.54
1:A:457:LYS:HB2	4:F:901:ATP:O3'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HA	1:B:177:THR:CG2	2.37	0.54
1:B:316:ALA:O	1:B:348:CYS:HA	2.08	0.54
2:D:150:VAL:O	2:D:153:GLN:HG3	2.07	0.54
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.37	0.54
1:E:123:LEU:O	1:E:127:ILE:CG1	2.55	0.54
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.48	0.54
1:F:49:GLY:HA2	4:F:903:ATP:O2B	2.07	0.54
1:F:498:THR:HB	1:F:500:ASP:O	2.08	0.54
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.89	0.54
2:C:81:GLN:CD	2:C:81:GLN:N	2.66	0.54
2:C:150:VAL:HG13	2:C:151:PHE:N	2.22	0.54
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.08	0.54
1:F:122:ASP:OD2	1:F:123:LEU:N	2.41	0.54
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.89	0.54
1:A:311:ARG:HA	1:A:343:LEU:O	2.07	0.54
2:D:211:LEU:HD12	2:D:215:ARG:O	2.08	0.54
2:D:294:LYS:HB2	4:D:901:ATP:O1B	2.07	0.54
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.89	0.54
1:E:118:VAL:O	1:E:118:VAL:HG12	2.08	0.54
1:E:123:LEU:HD23	1:E:127:ILE:CD1	2.37	0.54
1:F:19:ALA:C	1:F:38:ILE:HD12	2.33	0.54
1:A:17:ALA:C	1:A:18:ILE:HD12	2.33	0.53
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.38	0.53
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.73	0.53
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.90	0.53
1:F:20:LYS:C	1:F:38:ILE:HD11	2.32	0.53
1:A:510:ARG:NE	1:A:510:ARG:HA	2.23	0.53
1:E:320:SER:HA	1:F:254:LEU:HG	1.89	0.53
1:F:340:ARG:C	1:F:342:ASN:N	2.65	0.53
1:A:264:SER:HA	1:A:271:ASP:OD1	2.08	0.53
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.89	0.53
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.73	0.53
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.90	0.53
1:E:471:MET:HG2	1:E:480:LYS:HE2	1.90	0.53
1:A:126:LEU:HG	1:A:130:ILE:HD12	1.90	0.53
1:A:503:SER:O	1:A:504:GLU:HG3	2.08	0.53
1:B:358:ASP:O	1:B:362:ILE:HG12	2.09	0.53
2:C:488:ARG:HG3	2:C:488:ARG:HH11	1.71	0.53
2:D:255:THR:O	2:D:255:THR:HG22	2.08	0.53
1:E:255:THR:HG22	1:E:255:THR:O	2.07	0.53
1:A:82:ASP:O	1:A:83:ILE:C	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:HIS:O	2:C:363:ILE:HG13	2.08	0.53
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.90	0.53
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.89	0.53
2:C:433:ILE:O	2:C:433:ILE:HG22	2.08	0.53
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.38	0.53
1:A:150:VAL:HG13	1:A:151:PHE:N	2.23	0.53
1:A:419:PHE:O	1:A:420:MET:HB2	2.08	0.53
1:E:18:ILE:HD11	1:E:227:GLY:C	2.34	0.53
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.73	0.53
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.91	0.53
2:C:211:LEU:O	2:C:212:GLU:HB3	2.08	0.53
2:C:221:GLU:HG3	2:C:233:GLY:O	2.08	0.53
1:F:502:LYS:HZ2	1:F:507:ARG:HB3	1.73	0.53
1:A:426:THR:HG22	1:A:428:SER:N	2.21	0.53
1:B:81:GLN:H	1:B:81:GLN:CD	2.14	0.53
2:C:123:LEU:O	2:C:126:LEU:N	2.41	0.53
2:C:287:THR:HG21	2:C:425:ILE:O	2.08	0.53
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.08	0.53
2:D:345:LYS:HZ3	2:D:366:GLU:CG	2.22	0.53
1:F:500:ASP:O	1:F:501:GLU:HB3	2.08	0.53
1:A:87:ALA:O	1:A:92:TRP:CD1	2.62	0.53
1:B:68:ASP:CG	1:B:102:LYS:HZ1	2.16	0.53
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.32	0.53
1:B:353:SER:O	1:B:354:ALA:HB2	2.08	0.53
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.91	0.53
2:C:52:LYS:HB2	4:C:903:ATP:O1B	2.09	0.53
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.90	0.53
2:D:385:ARG:HG2	1:E:393:ARG:NH1	2.24	0.53
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.73	0.53
1:B:116:GLU:HG2	1:B:117:VAL:H	1.74	0.53
2:C:186:GLU:OE2	2:C:187:GLU:N	2.41	0.53
2:D:353:SER:O	2:D:354:ALA:HB2	2.09	0.53
2:D:359:HIS:O	2:D:363:ILE:HG13	2.09	0.53
1:F:52:LYS:HE3	4:F:903:ATP:O1B	2.09	0.53
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.08	0.52
1:A:146:SER:N	1:A:181:THR:HG22	2.24	0.52
1:A:332:GLY:O	1:A:333:MET:O	2.27	0.52
2:D:212:GLU:HG2	2:D:212:GLU:O	2.08	0.52
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.23	0.52
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.24	0.52
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:MET:O	4:F:901:ATP:H3'	2.10	0.52
2:C:111:ASP:O	2:C:113:GLU:N	2.38	0.52
1:E:191:ILE:CB	1:E:198:GLU:CG	2.87	0.52
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.39	0.52
1:F:379:SER:H	1:F:413:THR:HB	1.74	0.52
1:F:396:VAL:O	1:F:400:THR:HB	2.10	0.52
1:A:451:ARG:NH1	1:A:451:ARG:CG	2.65	0.52
1:B:96:LYS:O	1:B:100:GLU:HG3	2.09	0.52
1:E:123:LEU:O	1:E:127:ILE:HG13	2.09	0.52
1:E:504:GLU:OE1	1:E:505:LEU:HD23	2.10	0.52
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.91	0.52
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.45	0.52
2:C:119:GLY:HA2	2:C:122:ASP:OD1	2.09	0.52
1:E:469:GLU:HG3	1:E:470:PHE:N	2.24	0.52
1:F:49:GLY:CA	4:F:903:ATP:O2B	2.56	0.52
1:A:52:LYS:N	4:A:903:ATP:O1B	2.34	0.52
1:A:213:GLY:O	1:A:214:GLU:HB2	2.09	0.52
1:A:300:ARG:N	1:A:333:MET:HE1	2.24	0.52
2:D:81:GLN:CD	2:D:81:GLN:N	2.68	0.52
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.90	0.52
1:F:191:ILE:HG21	1:F:198:GLU:HG3	1.92	0.52
1:A:56:SER:HB2	1:A:143:SER:HB3	1.91	0.52
2:C:164:LEU:CD2	2:C:180:MET:HE1	2.39	0.52
1:A:419:PHE:CE2	1:B:425:ILE:HD12	2.45	0.52
1:A:514:GLU:HA	1:A:514:GLU:OE1	2.03	0.52
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.44	0.52
1:A:79:THR:HG23	1:A:81:GLN:H	1.75	0.52
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.24	0.52
1:B:38:ILE:HA	1:B:177:THR:HG23	1.92	0.52
1:B:79:THR:HG23	1:B:81:GLN:HE21	1.74	0.52
2:D:300:ARG:HA	2:D:333:MET:HE1	1.91	0.52
1:F:81:GLN:CD	1:F:81:GLN:N	2.68	0.52
1:A:294:LYS:N	4:A:901:ATP:O1B	2.43	0.52
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.39	0.52
2:C:151:PHE:C	2:C:153:GLN:N	2.55	0.51
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.10	0.51
2:D:65:ILE:O	2:D:65:ILE:HG22	2.08	0.51
2:D:332:GLY:O	2:D:333:MET:O	2.28	0.51
2:D:350:TYR:O	2:D:351:PRO:C	2.50	0.51
1:F:191:ILE:CB	1:F:198:GLU:CG	2.81	0.51
1:A:370:PHE:O	1:A:371:LYS:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.25	0.51
1:B:286:ALA:HA	1:B:438:ILE:O	2.10	0.51
1:E:379:SER:H	1:E:413:THR:HB	1.76	0.51
1:F:197:GLU:H	1:F:197:GLU:CD	2.17	0.51
1:F:353:SER:O	1:F:354:ALA:HB2	2.10	0.51
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.91	0.51
2:D:104:PHE:CE2	2:D:106:LEU:HB2	2.45	0.51
2:D:335:PHE:HA	2:D:338:MET:HG3	1.93	0.51
1:E:49:GLY:HA2	4:E:903:ATP:O2B	2.09	0.51
1:A:294:LYS:HB2	4:A:901:ATP:O1B	2.10	0.51
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.40	0.51
2:C:430:ILE:O	2:C:432:TPO:N	2.44	0.51
2:D:45:SER:CB	2:D:182:THR:HB	2.40	0.51
2:D:471:MET:HB3	2:D:480:LYS:HZ3	1.76	0.51
1:E:437:ILE:HD12	1:E:457:LYS:HE2	1.91	0.51
1:F:170:ARG:O	1:F:174:ILE:HG12	2.10	0.51
1:F:270:LEU:O	1:F:273:MET:HB2	2.10	0.51
1:A:340:ARG:O	1:A:342:ASN:N	2.44	0.51
1:A:359:HIS:O	1:A:363:ILE:HG13	2.10	0.51
1:B:178:THR:HG22	1:B:179:VAL:N	2.26	0.51
2:D:471:MET:HE2	2:D:478:ASP:CB	2.40	0.51
1:A:213:GLY:O	1:A:214:GLU:CB	2.59	0.51
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.92	0.51
2:D:396:VAL:HG11	2:D:430:ILE:HG23	1.91	0.51
1:F:81:GLN:NE2	1:F:81:GLN:N	2.59	0.51
1:F:148:THR:OG1	1:F:182:THR:HG23	2.11	0.51
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.41	0.51
2:C:191:ILE:HB	2:C:198:GLU:CD	2.35	0.51
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.26	0.51
2:C:420:MET:CE	2:D:490:ILE:HG21	2.40	0.51
1:E:471:MET:HG3	1:E:478:ASP:HB3	1.93	0.51
1:E:501:GLU:O	1:E:502:LYS:HE3	2.11	0.51
1:F:501:GLU:HG3	1:F:502:LYS:H	1.75	0.51
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.41	0.51
1:A:166:ARG:HG3	1:F:112:PRO:O	2.11	0.51
1:B:433:ILE:O	1:B:433:ILE:HG22	2.10	0.51
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.91	0.51
1:F:79:THR:HG23	1:F:81:GLN:HE21	1.76	0.51
1:F:509:VAL:HG12	1:F:510:ARG:N	2.25	0.51
1:B:49:GLY:O	1:B:218:ARG:NH2	2.44	0.51
1:B:191:ILE:CG2	1:B:198:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:ILE:HB	2:C:198:GLU:HG3	1.92	0.51
1:E:81:GLN:H	1:E:81:GLN:CD	2.19	0.51
1:E:262:ARG:NH2	1:E:461:SER:HB2	2.26	0.51
1:F:505:LEU:O	1:F:506:SER:HB3	2.11	0.51
1:A:449:MET:HE3	1:B:467:ILE:HD11	1.93	0.51
1:B:246:ILE:O	1:B:248:PRO:HD3	2.10	0.51
1:A:148:THR:HG1	1:A:182:THR:HG23	1.76	0.50
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.93	0.50
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.11	0.50
2:D:80:PRO:HD2	2:D:81:GLN:NE2	2.26	0.50
1:E:191:ILE:CB	1:E:198:GLU:HG3	2.41	0.50
2:C:123:LEU:HD11	2:C:163:GLU:O	2.11	0.50
2:C:295:THR:HG21	2:C:319:GLU:OE2	2.11	0.50
2:C:344:LEU:HD22	2:C:345:LYS:H	1.75	0.50
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.92	0.50
1:E:363:ILE:O	1:E:367:ILE:HG13	2.12	0.50
1:F:115:GLN:CG	1:F:116:GLU:N	2.74	0.50
1:F:344:LEU:HD22	1:F:345:LYS:H	1.76	0.50
1:A:300:ARG:CA	1:A:333:MET:HE1	2.41	0.50
1:B:273:MET:HE3	1:B:468:ARG:HD2	1.93	0.50
2:C:120:GLY:O	2:C:122:ASP:N	2.45	0.50
2:D:273:MET:HE3	2:D:468:ARG:HD2	1.93	0.50
2:D:484:ARG:HB3	2:D:484:ARG:NH1	2.26	0.50
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.92	0.50
1:A:18:ILE:N	1:A:18:ILE:CD1	2.74	0.50
1:A:425:ILE:HD12	1:F:419:PHE:CE2	2.47	0.50
1:A:436:THR:HG23	1:A:458:MET:HG3	1.93	0.50
1:B:79:THR:HG23	1:B:81:GLN:H	1.76	0.50
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.76	0.50
2:C:79:THR:HG21	2:C:81:GLN:HG2	1.92	0.50
2:D:356:LEU:HD21	2:D:387:VAL:HG11	1.94	0.50
2:D:388:SER:OG	2:D:391:ALA:CB	2.59	0.50
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.41	0.50
1:F:120:GLY:O	1:F:123:LEU:HB3	2.11	0.50
2:C:19:ALA:C	2:C:38:ILE:HD12	2.37	0.50
2:D:340:ARG:C	2:D:342:ASN:N	2.68	0.50
2:D:345:LYS:NZ	2:D:366:GLU:OE1	2.43	0.50
1:F:406:GLU:HB3	1:F:408:ILE:HG13	1.93	0.50
1:B:31:ILE:HA	1:B:231:MET:SD	2.52	0.50
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.93	0.50
2:D:419:PHE:CE2	1:E:425:ILE:HD12	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HG	1:F:320:SER:HA	1.94	0.50
1:B:61:TYR:CZ	1:B:92:TRP:HB2	2.46	0.50
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.94	0.50
1:B:436:THR:HG23	1:B:458:MET:HG3	1.94	0.50
2:D:273:MET:CE	2:D:468:ARG:HD2	2.42	0.50
2:D:300:ARG:N	2:D:333:MET:HE1	2.26	0.50
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.11	0.50
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.94	0.50
1:B:433:ILE:O	1:B:433:ILE:CG2	2.60	0.50
2:C:123:LEU:O	2:C:124:SER:C	2.54	0.50
2:D:496:ARG:CG	1:E:487:GLU:OE1	2.60	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.77	0.50
1:F:148:THR:HG21	1:F:183:GLU:CG	2.38	0.50
1:A:52:LYS:HD3	1:A:182:THR:O	2.11	0.50
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.50
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.94	0.50
2:C:38:ILE:HA	2:C:177:THR:HG23	1.94	0.50
2:D:106:LEU:HD13	2:D:129:ARG:NH2	2.27	0.50
1:E:146:SER:CA	1:E:181:THR:HG22	2.41	0.50
1:E:262:ARG:HH22	1:E:461:SER:HB2	1.77	0.50
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.41	0.50
1:B:419:PHE:CD2	2:C:425:ILE:CD1	2.92	0.49
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.22	0.49
2:D:347:VAL:O	2:D:348:CYS:CB	2.59	0.49
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.94	0.49
1:A:425:ILE:HD12	1:F:419:PHE:CD2	2.46	0.49
1:B:287:THR:HG23	1:B:414:ASN:HB3	1.94	0.49
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.93	0.49
2:D:363:ILE:O	2:D:367:ILE:HG13	2.12	0.49
1:F:462:TRP:O	1:F:463:HIS:O	2.29	0.49
1:F:471:MET:CG	1:F:478:ASP:HB3	2.43	0.49
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.77	0.49
1:B:418:GLN:HB2	2:C:423:HIS:O	2.12	0.49
1:B:499:VAL:C	1:B:501:GLU:H	2.21	0.49
2:D:159:VAL:O	2:D:163:GLU:HG2	2.13	0.49
2:D:191:ILE:CB	2:D:198:GLU:CG	2.87	0.49
2:D:313:ILE:HD11	2:D:372:PRO:HG3	1.94	0.49
1:A:218:ARG:O	1:A:236:PRO:HA	2.13	0.49
1:A:504:GLU:C	1:A:506:SER:N	2.68	0.49
2:C:52:LYS:N	4:C:903:ATP:O1B	2.43	0.49
2:C:111:ASP:OD1	2:C:113:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.27	0.49
1:E:347:VAL:O	1:E:348:CYS:HB2	2.12	0.49
1:F:79:THR:CG2	1:F:82:ASP:H	2.13	0.49
1:F:121:PHE:O	1:F:125:ALA:N	2.41	0.49
1:A:433:ILE:O	1:A:433:ILE:CG2	2.61	0.49
1:B:191:ILE:HG21	1:B:198:GLU:HG3	1.94	0.49
1:B:344:LEU:HD13	1:B:344:LEU:C	2.38	0.49
1:B:377:ILE:HD12	1:B:412:PHE:CD2	2.46	0.49
4:B:903:ATP:O3'	2:C:224:LYS:HB2	2.13	0.49
2:C:70:PRO:HG2	2:C:138:ARG:O	2.11	0.49
2:C:396:VAL:O	2:C:400:THR:HB	2.13	0.49
2:D:148:THR:OG1	2:D:182:THR:CG2	2.59	0.49
1:E:294:LYS:N	4:E:901:ATP:O1B	2.43	0.49
1:F:65:ILE:O	1:F:65:ILE:HG22	2.12	0.49
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.13	0.49
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.77	0.49
1:B:347:VAL:O	1:B:348:CYS:HB2	2.12	0.49
2:C:38:ILE:HA	2:C:177:THR:CG2	2.42	0.49
2:D:79:THR:HG23	2:D:81:GLN:N	2.27	0.49
2:D:289:ALA:HB2	2:D:419:PHE:HA	1.93	0.49
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.42	0.49
1:F:471:MET:HB3	1:F:480:LYS:HZ3	1.77	0.49
1:A:267:VAL:O	1:A:271:ASP:OD2	2.31	0.49
1:B:219:THR:HA	1:B:235:TYR:O	2.11	0.49
2:C:350:TYR:CZ	2:D:252:MET:HE3	2.47	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.93	0.49
1:B:107:ASP:C	1:B:107:ASP:OD1	2.56	0.49
1:B:126:LEU:C	1:B:128:GLU:N	2.68	0.49
1:B:396:VAL:O	1:B:400:THR:HB	2.13	0.49
2:C:419:PHE:HD1	2:C:420:MET:HG3	1.76	0.49
2:D:151:PHE:O	2:D:153:GLN:N	2.41	0.49
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.48	0.49
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.95	0.49
1:F:300:ARG:N	1:F:333:MET:HE1	2.27	0.49
1:A:471:MET:HG2	1:A:480:LYS:HE2	1.94	0.49
1:B:281:ASP:O	1:B:282:SER:HB3	2.12	0.49
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.47	0.49
2:C:332:GLY:O	2:C:333:MET:O	2.30	0.49
2:D:461:SER:OG	2:D:462:TRP:N	2.45	0.49
1:E:79:THR:HG23	1:E:81:GLN:H	1.77	0.49
1:A:21:MET:HE1	1:A:141:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:MET:HE2	1:B:478:ASP:HB2	1.94	0.48
2:C:495:THR:HG22	2:D:487:GLU:OE2	2.12	0.48
2:D:21:MET:CE	2:D:141:ARG:HG2	2.44	0.48
1:E:496:ARG:C	1:E:497:ILE:HD13	2.38	0.48
1:F:81:GLN:H	1:F:81:GLN:CD	2.19	0.48
1:F:311:ARG:HD2	1:F:371:LYS:HD2	1.95	0.48
1:A:19:ALA:O	1:A:38:ILE:HD12	2.13	0.48
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.41	0.48
1:A:419:PHE:HD1	1:A:420:MET:HG3	1.77	0.48
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.42	0.48
2:D:98:VAL:HA	2:D:103:LEU:O	2.14	0.48
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.22	0.48
1:E:123:LEU:HD23	1:E:127:ILE:CG1	2.43	0.48
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.95	0.48
1:B:340:ARG:C	1:B:342:ASN:N	2.71	0.48
2:C:98:VAL:HA	2:C:103:LEU:O	2.13	0.48
2:C:305:ALA:CB	2:C:374:ARG:HD2	2.38	0.48
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.43	0.48
1:E:169:ALA:O	1:E:173:GLN:HG3	2.13	0.48
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.29	0.48
1:E:417:ASP:O	1:F:424:SER:HB3	2.13	0.48
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.96	0.48
1:F:426:THR:CG2	1:F:428:SER:OG	2.61	0.48
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.47	0.48
2:C:49:GLY:CA	4:C:903:ATP:O2B	2.61	0.48
2:C:58:GLN:HG3	2:C:92:TRP:CH2	2.49	0.48
2:D:197:GLU:H	2:D:197:GLU:CD	2.19	0.48
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.43	0.48
1:F:79:THR:O	1:F:83:ILE:HD12	2.13	0.48
1:F:169:ALA:O	1:F:173:GLN:HG3	2.12	0.48
1:F:426:THR:HG21	1:F:430:ILE:HG12	1.95	0.48
1:F:471:MET:HB3	1:F:480:LYS:HZ1	1.77	0.48
2:C:44:VAL:HA	2:C:205:VAL:O	2.14	0.48
2:C:469:GLU:HB2	2:C:483:PHE:CZ	2.48	0.48
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.37	0.48
1:B:311:ARG:HA	1:B:343:LEU:O	2.13	0.48
2:C:67:PHE:CB	2:C:69:GLU:HG3	2.40	0.48
2:D:299:SER:HB3	2:D:333:MET:CE	2.43	0.48
1:E:186:GLU:HB3	1:E:189:GLY:HA3	1.96	0.48
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.48
1:F:220:LEU:HD23	1:F:220:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.46	0.48
2:C:41:SER:HA	2:C:178:THR:O	2.13	0.48
2:C:311:ARG:HA	2:C:343:LEU:O	2.14	0.48
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.44	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.42	0.48
1:E:21:MET:CE	1:E:59:PHE:CZ	2.97	0.48
1:A:387:VAL:HG12	1:A:388:SER:N	2.28	0.48
1:B:264:SER:HA	1:B:271:ASP:OD1	2.13	0.48
1:B:294:LYS:N	4:B:901:ATP:O1B	2.47	0.48
2:D:174:ILE:O	2:D:174:ILE:HG22	2.13	0.48
2:D:323:GLN:NE2	1:E:459:ARG:HD3	2.28	0.48
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.28	0.48
1:B:184:ARG:C	1:B:185:ILE:HD13	2.38	0.48
2:C:120:GLY:C	2:C:122:ASP:N	2.71	0.48
1:E:332:GLY:O	1:E:333:MET:O	2.32	0.48
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.79	0.48
1:A:121:PHE:O	1:A:125:ALA:HB2	2.14	0.48
1:A:151:PHE:C	1:A:153:GLN:N	2.64	0.48
1:B:21:MET:HE3	1:B:141:ARG:CZ	2.43	0.48
1:B:123:LEU:HD13	1:B:127:ILE:HD11	1.96	0.48
2:D:430:ILE:O	2:D:432:TPO:N	2.47	0.48
1:E:18:ILE:CG1	1:E:228:THR:HG23	2.43	0.48
1:E:23:THR:C	1:E:25:ILE:H	2.22	0.48
1:A:164:LEU:CD2	1:A:180:MET:HE1	2.44	0.47
1:B:126:LEU:C	1:B:128:GLU:H	2.21	0.47
1:B:323:GLN:NE2	2:C:459:ARG:HD3	2.29	0.47
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.27	0.47
2:C:340:ARG:C	2:C:342:ASN:N	2.71	0.47
2:D:19:ALA:O	2:D:38:ILE:HD12	2.14	0.47
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.47
1:F:514:GLU:HB3	1:F:519:SER:HB3	1.96	0.47
1:A:89:SER:CB	1:B:227:GLY:O	2.59	0.47
1:A:153:GLN:O	1:A:154:TYR:CB	2.62	0.47
1:A:420:MET:HE3	1:A:420:MET:HB3	1.83	0.47
2:C:300:ARG:N	2:C:333:MET:HE1	2.29	0.47
1:F:426:THR:HG22	1:F:428:SER:N	2.18	0.47
1:A:98:VAL:HA	1:A:103:LEU:O	2.13	0.47
1:A:502:LYS:HG3	1:A:502:LYS:O	2.14	0.47
1:B:111:ASP:O	1:B:113:GLU:N	2.47	0.47
2:C:88:ARG:HD3	2:D:15:HIS:C	2.40	0.47
2:D:21:MET:CE	2:D:59:PHE:CZ	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:GLU:OE1	1:E:336:GLU:HA	2.15	0.47
1:F:504:GLU:HB3	1:F:507:ARG:HH21	1.75	0.47
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.47
1:B:151:PHE:C	1:B:153:GLN:N	2.68	0.47
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.95	0.47
2:D:122:ASP:HB3	2:D:123:LEU:H	1.44	0.47
2:D:213:GLY:O	2:D:214:GLU:HB2	2.14	0.47
1:E:271:ASP:OD1	1:E:277:GLY:HA2	2.14	0.47
1:E:344:LEU:C	1:E:344:LEU:CD1	2.87	0.47
1:E:345:LYS:NZ	1:E:366:GLU:CG	2.77	0.47
1:F:344:LEU:C	1:F:344:LEU:HD13	2.40	0.47
1:A:49:GLY:HA2	4:A:903:ATP:O2B	2.15	0.47
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.30	0.47
1:B:125:ALA:O	1:B:129:ARG:HG3	2.15	0.47
1:B:211:LEU:O	1:B:212:GLU:HB3	2.13	0.47
2:C:320:SER:HA	2:D:254:LEU:HG	1.95	0.47
1:F:111:ASP:CG	1:F:112:PRO:HD2	2.40	0.47
1:A:170:ARG:O	1:A:174:ILE:HG12	2.15	0.47
1:A:332:GLY:O	1:A:333:MET:C	2.58	0.47
1:E:148:THR:HG1	1:E:182:THR:HG23	1.77	0.47
1:E:313:ILE:HD11	1:E:372:PRO:HG3	1.97	0.47
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.49	0.47
1:A:32:SER:HB3	1:A:222:ILE:HD11	1.97	0.47
1:A:45:SER:CB	1:A:182:THR:HB	2.43	0.47
1:A:486:PHE:CD2	1:A:496:ARG:HA	2.50	0.47
1:B:212:GLU:O	1:B:212:GLU:HG2	2.15	0.47
1:B:387:VAL:HG12	1:B:388:SER:N	2.28	0.47
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.79	0.47
2:D:323:GLN:HE22	1:E:459:ARG:HD3	1.79	0.47
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.47
4:D:903:ATP:O3'	1:E:224:LYS:HB2	2.15	0.47
1:E:76:PHE:HZ	1:E:126:LEU:CD2	2.28	0.47
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.50	0.47
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.13	0.47
1:F:117:VAL:HG13	1:F:154:TYR:OH	2.15	0.47
1:F:311:ARG:HD2	1:F:371:LYS:NZ	2.29	0.47
2:D:147:VAL:CG2	2:D:148:THR:N	2.77	0.47
2:D:269:ARG:HB3	2:D:479:ILE:HD12	1.97	0.47
1:F:65:ILE:O	1:F:65:ILE:CG2	2.61	0.47
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.50	0.47
1:A:268:VAL:O	1:A:271:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:LYS:HD3	2:D:182:THR:O	2.15	0.47
1:E:52:LYS:HD3	1:E:182:THR:O	2.14	0.47
1:F:184:ARG:HG2	1:F:191:ILE:O	2.15	0.47
1:A:146:SER:H	1:A:181:THR:CG2	2.27	0.47
1:A:182:THR:HG22	1:A:183:GLU:N	2.30	0.47
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.44	0.47
1:B:60:LEU:HD12	1:B:73:PHE:HB2	1.97	0.47
1:B:182:THR:HG22	1:B:183:GLU:N	2.30	0.47
1:E:79:THR:O	1:E:83:ILE:HD12	2.15	0.47
1:E:344:LEU:HD22	1:E:345:LYS:N	2.30	0.47
1:F:507:ARG:O	1:F:508:ILE:C	2.58	0.47
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.79	0.46
2:C:50:THR:HG22	2:C:209:ASN:HB2	1.97	0.46
2:C:121:PHE:O	2:C:122:ASP:C	2.58	0.46
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.31	0.46
1:A:150:VAL:CG1	1:A:151:PHE:N	2.78	0.46
1:B:150:VAL:HG13	1:B:151:PHE:N	2.29	0.46
1:B:419:PHE:CE2	2:C:425:ILE:HD12	2.49	0.46
1:B:492:GLY:C	1:B:494:PRO:HD3	2.41	0.46
2:C:332:GLY:O	2:C:333:MET:C	2.58	0.46
2:D:150:VAL:HG13	2:D:151:PHE:N	2.29	0.46
1:E:489:ILE:O	1:E:490:ILE:C	2.56	0.46
1:F:306:CYS:C	1:F:308:ASN:N	2.72	0.46
1:F:486:PHE:CE2	1:F:496:ARG:CD	2.80	0.46
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.69	0.46
1:A:186:GLU:OE2	1:A:187:GLU:N	2.49	0.46
1:B:106:LEU:C	1:B:106:LEU:CD1	2.88	0.46
2:C:214:GLU:O	2:C:215:ARG:NH2	2.48	0.46
2:C:344:LEU:C	2:C:344:LEU:HD13	2.40	0.46
2:C:353:SER:O	2:C:354:ALA:HB2	2.14	0.46
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.80	0.46
1:F:165:PHE:O	1:F:166:ARG:C	2.57	0.46
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.97	0.46
1:A:487:GLU:OE1	1:F:496:ARG:HD3	2.16	0.46
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.66	0.46
1:E:345:LYS:HZ3	1:E:366:GLU:CG	2.28	0.46
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.30	0.46
1:F:266:GLY:O	1:F:300:ARG:CG	2.64	0.46
1:F:360:LEU:O	1:F:360:LEU:HD22	2.15	0.46
1:A:430:ILE:O	1:A:431:SEP:C	2.63	0.46
1:A:471:MET:HE1	1:A:473:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.84	0.46
1:B:125:ALA:O	1:B:128:GLU:HB2	2.15	0.46
1:B:300:ARG:CA	1:B:333:MET:HE1	2.42	0.46
2:C:367:ILE:HG12	2:C:375:ILE:CD1	2.46	0.46
2:C:377:ILE:HD12	2:C:412:PHE:HE2	1.79	0.46
2:C:489:ILE:O	2:C:490:ILE:C	2.57	0.46
1:A:518:GLU:HB2	1:A:519:SER:H	1.55	0.46
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.30	0.46
1:B:81:GLN:CD	1:B:81:GLN:N	2.73	0.46
1:B:421:GLY:O	1:B:422:ALA:C	2.56	0.46
2:C:164:LEU:HD21	2:C:180:MET:HE1	1.97	0.46
2:C:471:MET:CG	2:C:478:ASP:HB3	2.46	0.46
2:D:305:ALA:HB2	2:D:374:ARG:CD	2.38	0.46
1:E:49:GLY:O	1:E:218:ARG:NH2	2.49	0.46
1:E:311:ARG:HA	1:E:343:LEU:O	2.16	0.46
1:E:340:ARG:O	1:E:342:ASN:N	2.49	0.46
1:A:191:ILE:HG21	1:A:198:GLU:HG3	1.97	0.46
1:A:497:ILE:CD1	1:A:497:ILE:O	2.64	0.46
1:B:18:ILE:HB	1:B:228:THR:CG2	2.44	0.46
1:B:419:PHE:HD1	1:B:420:MET:HG3	1.80	0.46
1:B:469:GLU:HG3	1:B:470:PHE:N	2.29	0.46
2:C:451:ARG:NH1	2:C:451:ARG:CG	2.78	0.46
2:C:489:ILE:C	2:C:491:SER:N	2.71	0.46
1:E:79:THR:HG23	1:E:81:GLN:NE2	2.30	0.46
1:F:264:SER:O	1:F:374:ARG:NH2	2.47	0.46
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.46
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.96	0.46
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.45	0.46
1:B:429:HIS:HA	1:B:431:SEP:O3P	2.16	0.46
1:F:137:TYR:O	1:F:138:ARG:HB2	2.16	0.46
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.46	0.46
1:B:23:THR:O	1:B:24:MET:HB2	2.16	0.46
1:B:52:LYS:HD3	1:B:182:THR:O	2.16	0.46
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.97	0.46
1:B:323:GLN:HE22	2:C:459:ARG:HD3	1.79	0.46
2:C:47:THR:O	2:C:48:SER:C	2.54	0.46
2:C:82:ASP:O	2:C:83:ILE:C	2.59	0.46
1:E:487:GLU:O	1:E:488:ARG:HB2	2.15	0.46
1:F:38:ILE:HG22	1:F:39:GLY:N	2.30	0.46
1:F:111:ASP:HA	1:F:112:PRO:HD3	1.66	0.46
1:F:256:GLN:H	1:F:256:GLN:HG2	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ASP:O	1:F:362:ILE:HG12	2.16	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.98	0.46
1:B:492:GLY:O	1:B:494:PRO:HD3	2.16	0.46
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.98	0.46
2:D:426:THR:HG21	2:D:430:ILE:HG12	1.97	0.46
1:E:313:ILE:CD1	1:E:372:PRO:HG3	2.46	0.46
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.97	0.46
1:F:469:GLU:HG3	1:F:470:PHE:N	2.31	0.46
1:A:45:SER:HB3	1:A:182:THR:HB	1.97	0.45
1:A:161:ARG:HB2	1:A:196:VAL:CG1	2.47	0.45
2:C:185:ILE:HA	5:D:912:HOH:O	2.15	0.45
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.98	0.45
2:D:396:VAL:HG12	2:D:433:ILE:HG21	1.98	0.45
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.98	0.45
1:A:485:ASN:OD1	1:A:485:ASN:N	2.39	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.45
2:C:187:GLU:O	2:C:208:ARG:HD3	2.16	0.45
1:E:18:ILE:HD13	1:E:227:GLY:HA3	1.96	0.45
1:E:116:GLU:O	1:E:118:VAL:HG23	2.16	0.45
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.94	0.45
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.97	0.45
1:F:509:VAL:CG1	1:F:510:ARG:H	2.08	0.45
1:A:72:VAL:O	1:A:142:VAL:HA	2.16	0.45
1:A:340:ARG:C	1:A:342:ASN:N	2.74	0.45
1:A:455:VAL:HG11	1:A:463:HIS:CB	2.39	0.45
1:A:503:SER:C	1:A:504:GLU:CG	2.88	0.45
1:E:166:ARG:O	1:E:169:ALA:HB3	2.16	0.45
1:E:393:ARG:O	1:E:397:ILE:HG12	2.17	0.45
1:E:483:PHE:HB2	1:E:489:ILE:HD11	1.98	0.45
1:F:446:ARG:H	1:F:496:ARG:NH2	2.15	0.45
1:A:415:THR:HG21	1:B:432:TPO:CG2	2.47	0.45
1:A:436:THR:OG1	1:A:458:MET:HG2	2.17	0.45
1:A:487:GLU:OE1	1:F:495:THR:HA	2.16	0.45
1:B:345:LYS:HZ2	1:B:366:GLU:HG2	1.82	0.45
1:B:471:MET:HE1	1:B:473:SER:CB	2.45	0.45
2:C:14:GLU:CG	2:C:16:GLN:HB2	2.46	0.45
2:C:446:ARG:HA	2:C:496:ARG:NH2	2.31	0.45
2:D:338:MET:H	2:D:338:MET:HG2	1.58	0.45
1:E:344:LEU:HD22	1:E:345:LYS:H	1.82	0.45
1:E:345:LYS:NZ	1:E:366:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:C	1:A:333:MET:CE	2.89	0.45
1:B:186:GLU:OE2	1:B:187:GLU:N	2.49	0.45
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.98	0.45
1:B:296:LEU:HD13	1:B:331:TRP:CD2	2.52	0.45
2:C:497:ILE:O	2:C:498:THR:HG22	2.15	0.45
2:D:21:MET:HE1	2:D:177:THR:HB	1.99	0.45
2:D:52:LYS:N	4:D:903:ATP:O1B	2.50	0.45
1:A:21:MET:HE3	1:A:141:ARG:NE	2.31	0.45
1:A:111:ASP:C	1:A:113:GLU:H	2.24	0.45
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.97	0.45
1:A:455:VAL:CG1	1:A:463:HIS:HB2	2.39	0.45
1:B:19:ALA:C	1:B:38:ILE:HD12	2.41	0.45
1:B:56:SER:HB2	1:B:143:SER:HB3	1.99	0.45
2:C:120:GLY:C	2:C:122:ASP:H	2.24	0.45
2:D:146:SER:CA	2:D:181:THR:HG22	2.45	0.45
2:D:231:MET:HE1	2:D:251:ALA:CB	2.38	0.45
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.62	0.45
1:E:314:LEU:C	1:E:314:LEU:HD12	2.42	0.45
1:B:79:THR:C	1:B:83:ILE:HD12	2.41	0.45
1:B:141:ARG:HB2	5:B:905:HOH:O	2.16	0.45
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.99	0.45
1:E:146:SER:HA	1:E:181:THR:O	2.17	0.45
1:E:147:VAL:CG2	1:E:148:THR:N	2.79	0.45
4:E:901:ATP:H3'	1:F:458:MET:O	2.17	0.45
1:F:79:THR:HG21	1:F:81:GLN:HG2	1.98	0.45
1:A:318:GLU:OE2	1:B:432:TPO:HB	2.16	0.45
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.97	0.45
1:A:496:ARG:O	1:A:497:ILE:HG23	2.16	0.45
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.32	0.45
2:C:433:ILE:O	2:C:433:ILE:CG2	2.64	0.45
2:D:314:LEU:C	2:D:314:LEU:HD12	2.42	0.45
2:D:388:SER:OG	2:D:391:ALA:HB2	2.15	0.45
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.80	0.45
1:E:353:SER:O	1:E:354:ALA:HB2	2.17	0.45
1:F:336:GLU:HA	1:F:336:GLU:OE1	2.17	0.45
1:F:451:ARG:HG2	1:F:451:ARG:NH1	2.32	0.45
1:A:153:GLN:O	1:A:154:TYR:CG	2.70	0.45
1:A:266:GLY:O	1:A:300:ARG:CG	2.65	0.45
1:B:20:LYS:C	1:B:38:ILE:HD11	2.42	0.45
1:B:21:MET:CE	1:B:59:PHE:CZ	3.00	0.45
1:B:379:SER:H	1:B:413:THR:CG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:PHE:HB2	1:B:489:ILE:HD11	1.99	0.45
2:C:387:VAL:HG12	2:C:388:SER:N	2.31	0.45
4:C:903:ATP:O3G	2:D:224:LYS:NZ	2.50	0.45
2:D:371:LYS:CD	2:D:371:LYS:C	2.90	0.45
1:A:504:GLU:O	1:A:506:SER:N	2.49	0.45
2:C:488:ARG:HG3	2:C:488:ARG:NH1	2.31	0.45
2:D:338:MET:HB2	2:D:344:LEU:HB3	1.99	0.45
2:D:448:GLU:HG2	1:E:466:ALA:HA	1.98	0.45
1:E:345:LYS:HZ2	1:E:366:GLU:HG2	1.81	0.45
1:F:186:GLU:OE2	1:F:187:GLU:N	2.50	0.45
1:F:332:GLY:O	1:F:333:MET:O	2.35	0.45
1:A:219:THR:HA	1:A:235:TYR:O	2.17	0.44
1:A:273:MET:O	1:A:463:HIS:CA	2.63	0.44
1:A:432:TPO:O1P	1:A:432:TPO:CG2	2.65	0.44
2:D:153:GLN:C	2:D:154:TYR:CG	2.94	0.44
2:D:379:SER:H	2:D:413:THR:HB	1.82	0.44
1:E:121:PHE:O	1:E:122:ASP:C	2.60	0.44
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.98	0.44
1:F:503:SER:O	1:F:504:GLU:C	2.61	0.44
1:F:504:GLU:CA	1:F:507:ARG:HE	2.30	0.44
1:A:146:SER:HA	1:A:181:THR:O	2.17	0.44
1:A:469:GLU:HG3	1:A:470:PHE:N	2.31	0.44
1:B:22:ARG:NH2	1:B:24:MET:SD	2.90	0.44
1:B:302:VAL:HG13	1:B:344:LEU:HD23	2.00	0.44
1:B:487:GLU:O	1:B:494:PRO:HA	2.17	0.44
1:B:500:ASP:O	1:B:503:SER:HB2	2.17	0.44
2:C:18:ILE:N	2:C:18:ILE:CD1	2.80	0.44
2:C:164:LEU:HD23	2:C:164:LEU:HA	1.70	0.44
2:C:358:ASP:O	2:C:362:ILE:HG12	2.17	0.44
2:D:311:ARG:HG3	2:D:371:LYS:NZ	2.31	0.44
1:E:122:ASP:O	1:E:123:LEU:C	2.60	0.44
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.17	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HD12	1.99	0.44
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.47	0.44
1:B:471:MET:HE2	1:B:478:ASP:CB	2.47	0.44
2:C:497:ILE:C	2:C:498:THR:CG2	2.89	0.44
2:D:318:GLU:OE2	1:E:432:TPO:HB	2.17	0.44
2:D:432:TPO:O1P	2:D:432:TPO:HG21	2.17	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.27	0.44
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.46	0.44
1:E:340:ARG:C	1:E:342:ASN:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.47	0.44
1:B:191:ILE:CB	1:B:198:GLU:CG	2.87	0.44
2:C:94:LEU:O	2:C:98:VAL:HG23	2.17	0.44
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.47	0.44
2:C:345:LYS:HZ3	2:C:366:GLU:CG	2.30	0.44
2:D:170:ARG:O	2:D:174:ILE:HG12	2.17	0.44
2:D:451:ARG:NH1	2:D:472:ILE:HD12	2.32	0.44
1:E:45:SER:HB2	1:E:182:THR:HB	1.99	0.44
1:E:79:THR:O	1:E:80:PRO:C	2.59	0.44
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.48	0.44
1:E:471:MET:HE1	1:E:473:SER:OG	2.17	0.44
1:F:21:MET:HE3	1:F:141:ARG:NE	2.33	0.44
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.99	0.44
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.30	0.44
1:F:311:ARG:HD2	1:F:371:LYS:CD	2.48	0.44
1:A:28:PHE:CD2	1:A:28:PHE:C	2.95	0.44
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.48	0.44
1:A:273:MET:SD	1:A:468:ARG:HD2	2.57	0.44
1:A:467:ILE:HD11	1:F:449:MET:HE3	2.00	0.44
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.16	0.44
1:F:111:ASP:C	1:F:113:GLU:H	2.24	0.44
1:F:116:GLU:C	1:F:117:VAL:HG23	2.43	0.44
1:F:300:ARG:CA	1:F:333:MET:HE1	2.48	0.44
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.00	0.44
1:B:502:LYS:HG3	1:B:504:GLU:C	2.43	0.44
2:C:123:LEU:O	2:C:125:ALA:N	2.50	0.44
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.99	0.44
2:D:420:MET:HE3	2:D:492:GLY:HA3	1.98	0.44
1:E:123:LEU:HD23	1:E:127:ILE:HG13	1.99	0.44
1:E:485:ASN:OD1	1:E:485:ASN:N	2.42	0.44
1:F:20:LYS:O	1:F:38:ILE:HD11	2.17	0.44
1:F:255:THR:O	1:F:255:THR:HG22	2.17	0.44
1:B:51:GLY:O	1:B:54:LEU:N	2.50	0.44
2:C:294:LYS:N	4:C:901:ATP:O1B	2.50	0.44
2:C:426:THR:HG22	2:C:428:SER:N	2.33	0.44
2:D:33:HIS:HD2	2:D:229:SER:OG	2.01	0.44
1:F:33:HIS:HD2	1:F:229:SER:OG	1.99	0.44
1:A:452:ALA:HA	1:A:468:ARG:O	2.17	0.44
1:F:371:LYS:O	1:F:371:LYS:HD2	2.17	0.44
2:C:75:THR:HG23	2:C:75:THR:O	2.18	0.44
2:D:79:THR:HG23	2:D:81:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:THR:HG21	2:D:193:ARG:HD2	2.00	0.44
1:E:164:LEU:HA	1:E:164:LEU:HD23	1.65	0.44
1:F:178:THR:HG22	1:F:179:VAL:N	2.33	0.44
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.17	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG3	2.00	0.44
1:A:153:GLN:C	1:A:154:TYR:CG	2.95	0.43
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.18	0.43
1:A:496:ARG:O	1:A:497:ILE:CG2	2.66	0.43
1:B:359:HIS:O	1:B:363:ILE:HG13	2.18	0.43
1:B:499:VAL:C	1:B:501:GLU:N	2.76	0.43
2:C:116:GLU:O	2:C:117:VAL:HB	2.17	0.43
2:C:439:LEU:HD12	2:C:440:LEU:N	2.32	0.43
2:D:455:VAL:HG11	2:D:463:HIS:HB2	1.99	0.43
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.83	0.43
1:F:120:GLY:C	1:F:123:LEU:H	2.26	0.43
1:F:217:ARG:HH21	1:F:236:PRO:HB3	1.82	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.33	0.43
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.48	0.43
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.99	0.43
4:A:901:ATP:C5	1:B:461:SER:O	2.71	0.43
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.53	0.43
2:D:21:MET:HE3	2:D:141:ARG:NE	2.33	0.43
2:D:344:LEU:HD22	2:D:345:LYS:H	1.83	0.43
1:E:380:LEU:O	1:E:381:SER:C	2.59	0.43
1:F:123:LEU:HD22	1:F:123:LEU:HA	1.90	0.43
1:A:357:GLU:HG3	1:A:358:ASP:N	2.33	0.43
1:A:499:VAL:O	1:A:499:VAL:CG1	2.64	0.43
1:A:514:GLU:HB3	1:A:515:LYS:HD2	2.00	0.43
2:C:418:GLN:HB2	2:D:423:HIS:O	2.18	0.43
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.99	0.43
1:E:70:PRO:HB2	1:E:139:ALA:HA	2.00	0.43
1:E:79:THR:HG23	1:E:81:GLN:CG	2.36	0.43
1:F:452:ALA:HB1	1:F:467:ILE:HG22	1.99	0.43
1:A:350:TYR:CZ	1:B:252:MET:HE3	2.53	0.43
1:B:52:LYS:N	4:B:903:ATP:O1B	2.51	0.43
1:B:122:ASP:C	1:B:124:SER:N	2.75	0.43
1:B:122:ASP:C	1:B:124:SER:H	2.26	0.43
1:B:164:LEU:HB3	1:B:200:VAL:HG11	2.00	0.43
2:C:121:PHE:HB3	2:C:125:ALA:HB3	2.01	0.43
2:D:426:THR:HG22	2:D:428:SER:N	2.28	0.43
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:ILE:O	1:E:446:ARG:HB2	2.18	0.43
1:A:129:ARG:O	1:A:130:ILE:C	2.59	0.43
1:B:146:SER:HA	1:B:181:THR:HG22	2.01	0.43
1:B:420:MET:HE3	1:B:420:MET:HB3	1.71	0.43
2:C:419:PHE:CD2	2:D:425:ILE:CD1	3.01	0.43
2:D:46:GLY:HA2	5:D:904:HOH:O	2.17	0.43
1:F:191:ILE:HG12	1:F:198:GLU:HG2	2.00	0.43
1:A:49:GLY:O	1:A:218:ARG:NH2	2.52	0.43
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.33	0.43
2:C:471:MET:HE1	2:C:473:SER:OG	2.18	0.43
2:D:153:GLN:O	2:D:154:TYR:CB	2.65	0.43
1:A:265:SER:O	1:A:301:PHE:HA	2.18	0.43
1:A:325:LEU:CD2	1:A:335:PHE:HB2	2.49	0.43
2:C:121:PHE:CD1	2:C:121:PHE:N	2.78	0.43
2:D:65:ILE:O	2:D:65:ILE:CG2	2.67	0.43
2:D:92:TRP:N	2:D:92:TRP:CD1	2.83	0.43
2:D:269:ARG:HG2	2:D:479:ILE:HB	2.01	0.43
1:E:211:LEU:HD12	1:E:215:ARG:O	2.18	0.43
1:E:419:PHE:O	1:E:420:MET:O	2.36	0.43
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.48	0.43
1:F:156:ALA:O	1:F:159:VAL:HG23	2.19	0.43
1:A:57:ILE:CD1	1:A:73:PHE:CE1	3.02	0.43
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.48	0.43
1:B:44:VAL:HG22	1:B:205:VAL:HB	2.01	0.43
2:C:193:ARG:NH2	2:D:195:GLY:O	2.28	0.43
2:C:315:PHE:CE1	2:C:363:ILE:HG23	2.52	0.43
2:C:419:PHE:CE2	2:D:425:ILE:HD12	2.54	0.43
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.34	0.43
2:D:31:ILE:HA	2:D:231:MET:SD	2.59	0.43
1:E:153:GLN:C	1:F:158:SER:HB2	2.44	0.43
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.18	0.43
1:A:118:VAL:C	1:A:122:ASP:OD1	2.62	0.43
1:A:131:ASN:O	1:A:132:TYR:C	2.61	0.43
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.82	0.43
1:F:443:VAL:HG12	1:F:445:ILE:HG12	2.01	0.43
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.54	0.43
1:A:445:ILE:HD12	1:A:486:PHE:CZ	2.54	0.43
1:B:300:ARG:N	1:B:333:MET:HE1	2.34	0.43
1:B:332:GLY:O	1:B:333:MET:O	2.37	0.43
2:C:267:VAL:HB	2:C:270:LEU:HB2	2.01	0.43
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.51	0.43
1:E:302:VAL:HG13	1:E:344:LEU:HD23	2.00	0.43
1:E:433:ILE:O	1:E:433:ILE:HG22	2.18	0.43
1:A:162:ARG:CZ	1:F:116:GLU:HG2	2.49	0.42
1:B:146:SER:CA	1:B:181:THR:HG22	2.48	0.42
2:D:381:SER:HB3	2:D:414:ASN:OD1	2.19	0.42
1:A:88:ARG:O	1:A:89:SER:C	2.61	0.42
1:A:425:ILE:CD1	1:F:419:PHE:CD2	3.01	0.42
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.84	0.42
1:B:350:TYR:O	1:B:351:PRO:C	2.61	0.42
1:B:471:MET:HG3	1:B:478:ASP:HB3	2.01	0.42
2:C:142:VAL:O	2:C:178:THR:HA	2.19	0.42
2:C:151:PHE:O	2:C:153:GLN:N	2.44	0.42
2:C:214:GLU:O	2:C:215:ARG:NE	2.53	0.42
2:C:283:ILE:HD12	2:C:412:PHE:HE1	1.84	0.42
2:C:421:GLY:O	2:C:422:ALA:C	2.62	0.42
2:C:468:ARG:HG2	2:C:468:ARG:NH1	2.33	0.42
2:C:489:ILE:O	2:C:492:GLY:N	2.46	0.42
2:D:191:ILE:HG21	2:D:198:GLU:HG3	2.00	0.42
2:D:299:SER:C	2:D:333:MET:CE	2.88	0.42
1:E:43:LEU:HA	1:E:43:LEU:HD12	1.82	0.42
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.54	0.42
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.84	0.42
1:B:332:GLY:O	1:B:333:MET:C	2.62	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.82	0.42
1:B:490:ILE:HD13	1:B:490:ILE:HA	1.76	0.42
1:B:501:GLU:HB2	1:B:502:LYS:H	1.38	0.42
2:C:191:ILE:CG2	2:C:198:GLU:HG3	2.49	0.42
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.33	0.42
2:C:378:ASP:OD1	2:C:413:THR:HG21	2.18	0.42
2:D:18:ILE:H	2:D:18:ILE:HD12	1.83	0.42
2:D:85:LYS:NZ	1:E:14:GLU:HB3	2.34	0.42
2:D:496:ARG:HE	1:E:487:GLU:HG2	1.84	0.42
1:E:64:ILE:HD13	1:E:102:LYS:HB3	2.01	0.42
1:E:153:GLN:C	1:E:154:TYR:CG	2.97	0.42
1:E:273:MET:O	1:E:463:HIS:CA	2.63	0.42
1:E:340:ARG:C	1:E:342:ASN:N	2.77	0.42
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.33	0.42
1:F:31:ILE:HG22	1:F:222:ILE:CD1	2.48	0.42
1:A:31:ILE:HD11	1:A:246:ILE:HG21	2.01	0.42
1:B:418:GLN:O	1:B:418:GLN:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ALA:HA	1:B:468:ARG:O	2.19	0.42
2:C:111:ASP:CG	2:C:113:GLU:HG2	2.43	0.42
2:C:114:GLY:O	2:C:115:GLN:HB3	2.19	0.42
2:C:337:GLU:OE1	2:C:340:ARG:NH1	2.52	0.42
2:D:140:ARG:HA	2:D:140:ARG:HD2	1.82	0.42
1:E:311:ARG:HD2	1:E:371:LYS:HE3	2.02	0.42
1:F:20:LYS:C	1:F:38:ILE:CD1	2.93	0.42
1:F:338:MET:H	1:F:338:MET:HG2	1.68	0.42
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.55	0.42
1:A:498:THR:HB	1:A:501:GLU:CG	2.41	0.42
1:B:256:GLN:H	1:B:256:GLN:HG2	1.54	0.42
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.50	0.42
1:E:38:ILE:HA	1:E:177:THR:HG23	2.01	0.42
1:E:184:ARG:HG2	1:E:191:ILE:O	2.20	0.42
1:E:501:GLU:O	1:E:502:LYS:CE	2.67	0.42
1:F:462:TRP:CD2	1:F:462:TRP:C	2.96	0.42
1:A:21:MET:CE	1:A:59:PHE:HZ	2.30	0.42
1:B:21:MET:HE3	1:B:141:ARG:CD	2.49	0.42
2:D:370:PHE:O	2:D:371:LYS:CD	2.67	0.42
1:E:147:VAL:HG23	1:E:148:THR:N	2.34	0.42
1:E:256:GLN:H	1:E:256:GLN:HG2	1.52	0.42
1:E:347:VAL:O	1:E:348:CYS:CB	2.65	0.42
1:E:378:ASP:OD1	1:E:413:THR:HG21	2.19	0.42
1:E:419:PHE:CD2	1:F:425:ILE:CD1	3.00	0.42
1:F:292:THR:HB	1:F:440:LEU:HB3	2.02	0.42
1:F:469:GLU:HB2	1:F:483:PHE:CZ	2.54	0.42
1:F:484:ARG:NH1	1:F:484:ARG:CB	2.82	0.42
1:F:506:SER:O	1:F:507:ARG:C	2.62	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42
1:B:337:GLU:O	1:B:338:MET:C	2.59	0.42
2:D:306:CYS:C	2:D:308:ASN:N	2.76	0.42
1:E:76:PHE:O	1:E:109:SER:HA	2.19	0.42
1:E:81:GLN:CD	1:E:81:GLN:N	2.78	0.42
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.50	0.42
1:F:352:GLU:C	1:F:354:ALA:H	2.28	0.42
1:F:367:ILE:HG12	1:F:375:ILE:HD11	2.02	0.42
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.55	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.55	0.42
2:C:211:LEU:HD12	2:C:215:ARG:O	2.20	0.42
2:C:311:ARG:HD2	2:C:371:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:HB2	1:E:227:GLY:O	2.19	0.42
2:D:153:GLN:O	2:D:154:TYR:CG	2.72	0.42
1:E:164:LEU:HB3	1:E:200:VAL:HG11	2.02	0.42
1:F:38:ILE:CG2	1:F:39:GLY:N	2.83	0.42
1:F:98:VAL:HA	1:F:103:LEU:O	2.20	0.42
1:F:302:VAL:HG12	1:F:303:GLU:N	2.35	0.42
1:F:433:ILE:N	1:F:433:ILE:HD12	2.35	0.42
1:F:504:GLU:CA	1:F:507:ARG:NE	2.81	0.42
1:A:70:PRO:HA	1:A:102:LYS:O	2.19	0.42
4:A:901:ATP:O2'	1:B:463:HIS:NE2	2.50	0.42
1:B:119:GLY:O	1:B:121:PHE:N	2.53	0.42
1:B:273:MET:O	1:B:463:HIS:CA	2.63	0.42
2:C:14:GLU:HG3	2:C:16:GLN:HB2	2.01	0.42
2:C:281:ASP:O	2:C:282:SER:HB3	2.20	0.42
2:C:420:MET:HE1	2:D:490:ILE:HG21	2.01	0.42
2:D:219:THR:HB	2:D:234:GLU:HB3	2.02	0.42
1:E:264:SER:O	1:E:374:ARG:NH2	2.51	0.42
1:E:306:CYS:C	1:E:308:ASN:N	2.78	0.42
1:E:379:SER:HA	1:E:413:THR:HG22	2.01	0.42
1:F:23:THR:O	1:F:24:MET:HB2	2.20	0.42
1:F:299:SER:HB3	1:F:333:MET:HE2	2.02	0.42
1:A:14:GLU:CG	1:A:15:HIS:N	2.57	0.42
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.82	0.42
1:A:81:GLN:H	1:A:81:GLN:CD	2.28	0.42
1:A:514:GLU:C	1:A:515:LYS:HD2	2.44	0.42
2:C:123:LEU:HD23	2:C:123:LEU:HA	1.79	0.42
2:C:153:GLN:C	2:C:154:TYR:CG	2.97	0.42
2:C:383:LEU:HA	2:C:383:LEU:HD23	1.85	0.42
2:C:419:PHE:O	2:C:419:PHE:CG	2.72	0.42
2:D:182:THR:CG2	2:D:183:GLU:N	2.80	0.42
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.54	0.42
1:E:21:MET:O	1:E:35:GLY:HA3	2.20	0.42
1:E:106:LEU:HD13	1:E:129:ARG:CZ	2.50	0.42
1:E:130:ILE:O	1:E:134:ILE:HG13	2.19	0.42
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.46	0.42
1:F:213:GLY:O	1:F:214:GLU:HB2	2.19	0.42
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.35	0.41
1:B:53:THR:HG23	1:B:145:ASP:OD1	2.20	0.41
1:B:219:THR:HB	1:B:234:GLU:HB3	2.02	0.41
1:B:291:GLY:C	4:B:901:ATP:O2B	2.63	0.41
1:B:311:ARG:HD2	1:B:371:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:O	1:B:420:MET:O	2.38	0.41
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.54	0.41
2:C:214:GLU:O	2:C:215:ARG:CZ	2.68	0.41
2:D:187:GLU:O	2:D:208:ARG:HD3	2.20	0.41
2:D:194:TYR:O	2:D:196:VAL:HG23	2.19	0.41
2:D:273:MET:O	2:D:463:HIS:HA	2.19	0.41
1:E:345:LYS:NZ	1:E:366:GLU:OE1	2.53	0.41
1:E:382:ALA:O	1:E:385:ARG:HG3	2.20	0.41
1:E:455:VAL:HG11	1:E:463:HIS:HB2	2.01	0.41
1:F:379:SER:CA	1:F:413:THR:HG22	2.46	0.41
1:A:85:LYS:O	1:A:88:ARG:HB2	2.20	0.41
1:A:256:GLN:H	1:A:256:GLN:HG2	1.52	0.41
1:A:486:PHE:CE2	1:A:496:ARG:HA	2.55	0.41
2:C:38:ILE:HG22	2:C:39:GLY:N	2.35	0.41
1:F:238:THR:HG22	1:F:239:ILE:N	2.35	0.41
1:F:367:ILE:HG12	1:F:375:ILE:CD1	2.50	0.41
1:F:387:VAL:HG12	1:F:388:SER:N	2.36	0.41
1:A:510:ARG:N	1:A:510:ARG:HD2	2.35	0.41
1:B:72:VAL:O	1:B:142:VAL:HA	2.21	0.41
1:B:87:ALA:HB1	1:B:92:TRP:HE1	1.85	0.41
2:D:75:THR:HG23	2:D:75:THR:O	2.19	0.41
1:E:371:LYS:O	1:E:371:LYS:HD3	2.17	0.41
1:F:485:ASN:OD1	1:F:485:ASN:N	2.48	0.41
1:A:20:LYS:HD3	1:A:35:GLY:O	2.19	0.41
1:B:180:MET:HE2	1:B:180:MET:HB3	1.92	0.41
2:C:21:MET:O	2:C:35:GLY:HA3	2.20	0.41
2:C:148:THR:HG1	2:C:182:THR:HG23	1.85	0.41
2:C:256:GLN:H	2:C:256:GLN:HG2	1.48	0.41
2:D:33:HIS:CD2	2:D:230:HIS:HA	2.55	0.41
1:F:42:THR:HG23	1:F:203:ASN:HB2	2.02	0.41
1:A:184:ARG:C	1:A:185:ILE:HD13	2.46	0.41
1:B:393:ARG:O	1:B:397:ILE:HG12	2.20	0.41
2:D:300:ARG:CA	2:D:333:MET:HE1	2.51	0.41
2:D:315:PHE:CE2	2:D:363:ILE:HG23	2.53	0.41
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.68	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.01	0.41
1:F:200:VAL:O	1:F:200:VAL:HG12	2.19	0.41
1:F:287:THR:HG23	1:F:414:ASN:CB	2.38	0.41
1:F:396:VAL:HG11	1:F:430:ILE:HG23	2.01	0.41
1:A:296:LEU:HD21	1:A:477:PRO:HD3	2.02	0.41
1:A:345:LYS:NZ	1:A:366:GLU:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:HG11	1:A:430:ILE:HG23	2.03	0.41
2:D:49:GLY:HA2	4:D:903:ATP:O2B	2.20	0.41
2:D:337:GLU:O	2:D:338:MET:C	2.63	0.41
1:F:68:ASP:OD2	1:F:102:LYS:NZ	2.49	0.41
1:F:127:ILE:HD11	1:F:167:LEU:CD1	2.50	0.41
1:A:344:LEU:C	1:A:344:LEU:CD1	2.94	0.41
1:A:426:THR:HG22	1:A:427:ASP:N	2.35	0.41
2:C:65:ILE:HG22	2:C:65:ILE:O	2.20	0.41
2:D:41:SER:HA	2:D:178:THR:O	2.21	0.41
2:D:495:THR:HG23	1:E:487:GLU:OE2	2.21	0.41
1:E:76:PHE:CZ	1:E:126:LEU:CD2	3.03	0.41
1:E:289:ALA:CB	1:E:419:PHE:HA	2.45	0.41
1:E:299:SER:C	1:E:333:MET:HE1	2.45	0.41
1:E:315:PHE:HE1	1:E:375:ILE:CD1	2.34	0.41
1:E:360:LEU:O	1:E:360:LEU:HD22	2.21	0.41
1:E:412:PHE:CD1	1:E:412:PHE:N	2.88	0.41
1:B:68:ASP:OD2	1:B:102:LYS:HE3	2.20	0.41
1:B:153:GLN:O	1:B:154:TYR:CB	2.69	0.41
1:B:153:GLN:C	1:B:154:TYR:CG	2.98	0.41
1:B:252:MET:HE2	1:B:252:MET:HB3	1.96	0.41
2:C:153:GLN:O	2:C:154:TYR:CG	2.74	0.41
2:D:21:MET:CE	2:D:59:PHE:HZ	2.33	0.41
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.49	0.41
1:E:483:PHE:CB	1:E:489:ILE:HD11	2.51	0.41
1:F:140:ARG:HA	1:F:140:ARG:HD2	1.96	0.41
1:F:419:PHE:O	1:F:420:MET:HB2	2.19	0.41
1:A:400:THR:CG2	1:A:401:GLY:N	2.83	0.41
1:A:436:THR:HG23	1:A:458:MET:CG	2.51	0.41
4:A:903:ATP:O3'	1:B:224:LYS:HB2	2.21	0.41
1:B:32:SER:HB3	1:B:222:ILE:HD11	2.02	0.41
1:B:141:ARG:HD2	5:B:905:HOH:O	2.19	0.41
1:B:385:ARG:HG2	2:C:393:ARG:NH1	2.35	0.41
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.35	0.41
4:B:901:ATP:C5	2:C:461:SER:O	2.74	0.41
2:C:182:THR:CG2	2:C:183:GLU:N	2.79	0.41
2:C:338:MET:HB2	2:C:344:LEU:HB3	2.03	0.41
2:C:387:VAL:CG1	2:C:391:ALA:HB3	2.51	0.41
2:D:50:THR:HG22	2:D:209:ASN:HB2	2.03	0.41
2:D:114:GLY:O	2:D:115:GLN:HG3	2.21	0.41
2:D:224:LYS:O	2:D:225:LEU:HD23	2.21	0.41
2:D:445:ILE:C	2:D:496:ARG:HH12	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:MET:HE2	2:D:449:MET:HA	2.03	0.41
1:E:98:VAL:HA	1:E:103:LEU:O	2.21	0.41
1:E:113:GLU:HB3	1:E:114:GLY:H	1.75	0.41
1:E:122:ASP:HB3	1:E:123:LEU:H	1.71	0.41
1:E:150:VAL:HG13	1:E:151:PHE:N	2.36	0.41
1:E:182:THR:HG21	1:E:192:ALA:HB1	2.02	0.41
1:E:336:GLU:O	1:E:339:GLU:HB2	2.21	0.41
1:E:471:MET:HB3	1:E:480:LYS:HZ1	1.84	0.41
1:F:46:GLY:HA2	1:F:184:ARG:CD	2.51	0.41
1:F:126:LEU:O	1:F:127:ILE:C	2.64	0.41
1:F:185:ILE:CD1	1:F:193:ARG:NH1	2.80	0.41
1:F:231:MET:HE1	1:F:251:ALA:CB	2.41	0.41
1:F:506:SER:O	1:F:507:ARG:O	2.39	0.41
1:A:21:MET:CE	1:A:59:PHE:CE1	3.04	0.41
1:A:21:MET:CE	1:A:141:ARG:HG2	2.51	0.41
1:A:484:ARG:CZ	1:A:484:ARG:CB	2.99	0.41
1:A:505:LEU:O	1:A:505:LEU:CD1	2.65	0.41
1:B:406:GLU:O	1:B:407:GLU:HB2	2.20	0.41
2:C:21:MET:HE2	2:C:59:PHE:CE1	2.56	0.41
2:C:79:THR:HG23	2:C:81:GLN:HE21	1.86	0.41
2:D:49:GLY:CA	4:D:903:ATP:O2B	2.69	0.41
2:D:208:ARG:O	2:D:218:ARG:HA	2.21	0.41
1:E:20:LYS:C	1:E:38:ILE:HD11	2.46	0.41
1:E:123:LEU:HD12	1:E:163:GLU:OE2	2.20	0.41
1:F:306:CYS:C	1:F:308:ASN:H	2.29	0.41
1:F:455:VAL:HG11	1:F:463:HIS:CB	2.48	0.41
1:A:183:GLU:CB	1:B:199:PHE:CE1	3.04	0.40
1:A:284:ILE:HB	1:A:411:LEU:HD12	2.02	0.40
1:A:362:ILE:O	1:A:362:ILE:HG22	2.21	0.40
1:B:79:THR:HG23	1:B:81:GLN:CG	2.42	0.40
1:B:441:GLN:O	1:B:441:GLN:HG3	2.21	0.40
1:B:445:ILE:HD12	1:B:486:PHE:CZ	2.56	0.40
2:C:184:ARG:HG2	2:C:191:ILE:O	2.20	0.40
2:D:252:MET:HE2	2:D:252:MET:HB3	1.88	0.40
1:E:344:LEU:HD13	1:E:345:LYS:N	2.35	0.40
1:F:377:ILE:HD11	1:F:399:VAL:HG11	2.03	0.40
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.03	0.40
1:F:484:ARG:CB	1:F:484:ARG:CZ	2.99	0.40
1:F:508:ILE:CD1	1:F:508:ILE:H	2.34	0.40
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.84	0.40
2:D:287:THR:HA	2:D:414:ASN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.56	0.40
2:D:332:GLY:O	2:D:333:MET:C	2.63	0.40
2:D:471:MET:CG	2:D:478:ASP:HB3	2.51	0.40
1:F:266:GLY:HA3	1:F:300:ARG:O	2.22	0.40
1:F:357:GLU:HG3	1:F:358:ASP:N	2.36	0.40
1:F:516:GLY:N	1:F:517:PRO:HD2	2.36	0.40
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.86	0.40
1:B:352:GLU:CD	1:B:352:GLU:H	2.29	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.98	0.40
2:C:269:ARG:NE	5:C:909:HOH:O	2.33	0.40
1:F:429:HIS:HA	1:F:431:SEP:O1P	2.21	0.40
2:D:76:PHE:O	2:D:109:SER:HA	2.21	0.40
2:D:294:LYS:N	4:D:901:ATP:O1B	2.54	0.40
2:D:438:ILE:CD1	2:D:455:VAL:HG22	2.52	0.40
2:D:462:TRP:O	2:D:463:HIS:O	2.40	0.40
1:E:106:LEU:HD12	1:E:106:LEU:C	2.46	0.40
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.22	0.40
1:F:111:ASP:C	1:F:113:GLU:N	2.79	0.40
1:A:140:ARG:HD2	1:A:140:ARG:HA	1.84	0.40
1:A:314:LEU:HD12	1:A:314:LEU:C	2.46	0.40
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.52	0.40
2:C:25:ILE:HG23	2:C:58:GLN:NE2	2.36	0.40
2:C:316:ALA:O	2:C:348:CYS:HA	2.22	0.40
2:D:44:VAL:HA	2:D:205:VAL:O	2.21	0.40
2:D:358:ASP:O	2:D:362:ILE:HG12	2.21	0.40
1:E:306:CYS:O	1:E:309:LYS:N	2.42	0.40
1:F:252:MET:HE2	1:F:252:MET:HB3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	442 (88%)	39 (8%)	21 (4%)	2	7
1	B	487/519 (94%)	431 (88%)	44 (9%)	12 (2%)	4	16
1	E	488/519 (94%)	422 (86%)	49 (10%)	17 (4%)	3	10
1	F	502/519 (97%)	443 (88%)	38 (8%)	21 (4%)	2	7
2	C	485/519 (93%)	436 (90%)	30 (6%)	19 (4%)	2	8
2	D	482/519 (93%)	433 (90%)	37 (8%)	12 (2%)	4	16
All	All	2946/3114 (95%)	2607 (88%)	237 (8%)	102 (4%)	3	10

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	387	VAL
1	A	463	HIS
1	A	502	LYS
1	A	509	VAL
1	B	52	LYS
1	B	154	TYR
1	B	333	MET
1	B	341	GLN
1	B	387	VAL
1	B	463	HIS
2	C	17	ALA
2	C	112	PRO
2	C	117	VAL
2	C	124	SER
2	C	154	TYR
2	C	333	MET
2	C	341	GLN
2	C	431	SER
2	C	463	HIS
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
2	D	387	VAL
2	D	431	SER
2	D	463	HIS
1	E	122	ASP

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Mol	Chain	Res	Type
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	420	MET
1	E	463	HIS
1	E	502	LYS
1	F	118	VAL
1	F	154	TYR
1	F	333	MET
1	F	463	HIS
1	F	501	GLU
1	F	504	GLU
1	F	506	SER
1	F	507	ARG
1	F	508	ILE
1	F	509	VAL
1	A	117	VAL
1	A	157	SER
1	A	341	GLN
1	A	500	ASP
1	A	505	LEU
1	B	17	ALA
1	B	119	GLY
1	B	211	LEU
1	B	420	MET
2	C	121	PHE
2	C	379	SER
2	C	387	VAL
2	D	18	ILE
2	D	113	GLU
2	D	341	GLN
2	D	420	MET
1	E	117	VAL
1	E	120	GLY
1	E	341	GLN
1	E	387	VAL
1	F	114	GLY
1	F	117	VAL
1	F	211	LEU
1	F	341	GLN
1	F	510	ARG
1	A	379	SER

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Mol	Chain	Res	Type
1	A	420	MET
1	B	112	PRO
2	C	114	GLY
2	C	211	LEU
2	C	289	ALA
1	E	157	SER
1	F	157	SER
1	F	420	MET
1	A	480	LYS
1	A	504	GLU
2	C	354	ALA
2	C	499	VAL
2	D	211	LEU
1	E	379	SER
1	B	494	PRO
2	C	157	SER
1	E	348	CYS
1	F	354	ALA
1	F	500	ASP
1	F	517	PRO
1	A	212	GLU
1	A	348	CYS
2	C	348	CYS
2	D	157	SER
1	E	212	GLU
1	E	494	PRO
1	A	112	PRO
1	A	497	ILE
1	F	387	VAL
1	E	112	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	430/442 (97%)	366 (85%)	64 (15%)	3 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	417/442 (94%)	360 (86%)	57 (14%)	3	13
1	E	418/442 (95%)	360 (86%)	58 (14%)	3	12
1	F	430/442 (97%)	374 (87%)	56 (13%)	4	14
2	C	415/443 (94%)	351 (85%)	64 (15%)	2	10
2	D	412/443 (93%)	351 (85%)	61 (15%)	3	10
All	All	2522/2654 (95%)	2162 (86%)	360 (14%)	3	11

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	26	GLU
1	A	41	SER
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	123	LEU
1	A	124	SER
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	179	VAL
1	A	181	THR
1	A	183	GLU
1	A	185	ILE
1	A	186	GLU
1	A	191	ILE
1	A	211	LEU
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	228	THR
1	A	238	THR
1	A	256	GLN
1	A	260	ASN
1	A	263	VAL
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	284	ILE
1	A	287	THR
1	A	294	LYS
1	A	298	VAL
1	A	302	VAL
1	A	303	GLU
1	A	320	SER
1	A	321	ARG
1	A	325	LEU
1	A	338	MET
1	A	342	ASN
1	A	360	LEU
1	A	366	GLU
1	A	369	ASP
1	A	375	ILE
1	A	400	THR
1	A	413	THR
1	A	420	MET
1	A	428	SER
1	A	434	THR
1	A	458	MET
1	A	462	TRP
1	A	469	GLU
1	A	471	MET
1	A	489	ILE
1	A	490	ILE
1	A	496	ARG
1	A	498	THR
1	A	500	ASP
1	A	504	GLU
1	A	508	ILE
1	A	509	VAL
1	A	514	GLU
1	A	518	GLU
1	B	26	GLU
1	B	50	THR
1	B	79	THR
1	B	81	GLN
1	B	99	ASP
1	B	106	LEU
1	B	112	PRO
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	128	GLU
1	B	140	ARG
1	B	147	VAL
1	B	151	PHE
1	B	154	TYR
1	B	164	LEU
1	B	179	VAL
1	B	181	THR
1	B	183	GLU
1	B	185	ILE
1	B	186	GLU
1	B	191	ILE
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	256	GLN
1	B	260	ASN
1	B	263	VAL
1	B	270	LEU
1	B	287	THR
1	B	294	LYS
1	B	302	VAL
1	B	303	GLU
1	B	320	SER
1	B	321	ARG
1	B	325	LEU
1	B	333	MET
1	B	338	MET
1	B	342	ASN
1	B	356	LEU
1	B	360	LEU
1	B	366	GLU
1	B	369	ASP
1	B	375	ILE
1	B	400	THR
1	B	413	THR
1	B	420	MET
1	B	458	MET
1	B	462	TRP
1	B	469	GLU
1	B	471	MET
1	B	474	ASP

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Mol	Chain	Res	Type
1	B	485	ASN
1	B	490	ILE
1	B	495	THR
1	B	497	ILE
1	B	499	VAL
1	B	501	GLU
1	B	502	LYS
2	C	15	HIS
2	C	18	ILE
2	C	26	GLU
2	C	50	THR
2	C	79	THR
2	C	81	GLN
2	C	83	ILE
2	C	99	ASP
2	C	106	LEU
2	C	111	ASP
2	C	121	PHE
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	164	LEU
2	C	177	THR
2	C	178	THR
2	C	179	VAL
2	C	181	THR
2	C	183	GLU
2	C	185	ILE
2	C	186	GLU
2	C	191	ILE
2	C	196	VAL
2	C	211	LEU
2	C	212	GLU
2	C	218	ARG
2	C	223	LEU
2	C	228	THR
2	C	256	GLN
2	C	259	SER
2	C	260	ASN
2	C	263	VAL
2	C	270	LEU
2	C	287	THR

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Mol	Chain	Res	Type
2	C	294	LYS
2	C	298	VAL
2	C	302	VAL
2	C	303	GLU
2	C	321	ARG
2	C	325	LEU
2	C	333	MET
2	C	338	MET
2	C	342	ASN
2	C	356	LEU
2	C	360	LEU
2	C	366	GLU
2	C	375	ILE
2	C	400	THR
2	C	413	THR
2	C	420	MET
2	C	428	SER
2	C	458	MET
2	C	461	SER
2	C	462	TRP
2	C	469	GLU
2	C	471	MET
2	C	491	SER
2	C	493	SER
2	C	495	THR
2	C	497	ILE
2	C	498	THR
2	C	500	ASP
2	C	501	GLU
2	D	14	GLU
2	D	26	GLU
2	D	38	ILE
2	D	79	THR
2	D	81	GLN
2	D	83	ILE
2	D	106	LEU
2	D	117	VAL
2	D	122	ASP
2	D	123	LEU
2	D	124	SER
2	D	127	ILE
2	D	140	ARG

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Mol	Chain	Res	Type
2	D	151	PHE
2	D	154	TYR
2	D	172	LYS
2	D	177	THR
2	D	179	VAL
2	D	181	THR
2	D	183	GLU
2	D	185	ILE
2	D	186	GLU
2	D	191	ILE
2	D	212	GLU
2	D	218	ARG
2	D	223	LEU
2	D	256	GLN
2	D	259	SER
2	D	260	ASN
2	D	263	VAL
2	D	270	LEU
2	D	284	ILE
2	D	287	THR
2	D	294	LYS
2	D	302	VAL
2	D	303	GLU
2	D	320	SER
2	D	321	ARG
2	D	325	LEU
2	D	338	MET
2	D	342	ASN
2	D	351	PRO
2	D	356	LEU
2	D	360	LEU
2	D	366	GLU
2	D	369	ASP
2	D	371	LYS
2	D	375	ILE
2	D	400	THR
2	D	413	THR
2	D	420	MET
2	D	431	SER
2	D	439	LEU
2	D	458	MET
2	D	463	HIS

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Mol	Chain	Res	Type
2	D	469	GLU
2	D	471	MET
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
1	E	26	GLU
1	E	37	PRO
1	E	50	THR
1	E	79	THR
1	E	81	GLN
1	E	83	ILE
1	E	99	ASP
1	E	106	LEU
1	E	113	GLU
1	E	116	GLU
1	E	121	PHE
1	E	123	LEU
1	E	124	SER
1	E	127	ILE
1	E	140	ARG
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	181	THR
1	E	182	THR
1	E	183	GLU
1	E	185	ILE
1	E	186	GLU
1	E	191	ILE
1	E	211	LEU
1	E	212	GLU
1	E	218	ARG
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	260	ASN
1	E	263	VAL
1	E	270	LEU
1	E	287	THR
1	E	302	VAL
1	E	314	LEU

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Mol	Chain	Res	Type
1	E	321	ARG
1	E	325	LEU
1	E	338	MET
1	E	342	ASN
1	E	344	LEU
1	E	351	PRO
1	E	360	LEU
1	E	366	GLU
1	E	375	ILE
1	E	400	THR
1	E	413	THR
1	E	458	MET
1	E	461	SER
1	E	469	GLU
1	E	471	MET
1	E	474	ASP
1	E	495	THR
1	E	496	ARG
1	E	501	GLU
1	E	503	SER
1	E	504	GLU
1	E	505	LEU
1	F	26	GLU
1	F	45	SER
1	F	79	THR
1	F	81	GLN
1	F	99	ASP
1	F	106	LEU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	151	PHE
1	F	154	TYR
1	F	172	LYS
1	F	181	THR
1	F	183	GLU
1	F	185	ILE
1	F	186	GLU
1	F	191	ILE
1	F	211	LEU
1	F	212	GLU
1	F	218	ARG

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Mol	Chain	Res	Type
1	F	223	LEU
1	F	256	GLN
1	F	260	ASN
1	F	263	VAL
1	F	270	LEU
1	F	287	THR
1	F	298	VAL
1	F	302	VAL
1	F	303	GLU
1	F	314	LEU
1	F	321	ARG
1	F	325	LEU
1	F	338	MET
1	F	342	ASN
1	F	356	LEU
1	F	360	LEU
1	F	366	GLU
1	F	375	ILE
1	F	400	THR
1	F	413	THR
1	F	425	ILE
1	F	428	SER
1	F	449	MET
1	F	458	MET
1	F	469	GLU
1	F	471	MET
1	F	496	ARG
1	F	497	ILE
1	F	499	VAL
1	F	501	GLU
1	F	504	GLU
1	F	505	LEU
1	F	507	ARG
1	F	509	VAL
1	F	514	GLU
1	F	515	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	81	GLN
1	A	256	GLN
1	A	304	ASN
1	A	323	GLN
1	A	414	ASN
1	A	429	HIS
1	A	441	GLN
1	B	62	ASN
1	B	81	GLN
1	B	209	ASN
1	B	245	ASN
1	B	256	GLN
1	B	260	ASN
1	B	304	ASN
1	B	361	GLN
1	B	414	ASN
1	B	441	GLN
2	C	33	HIS
2	C	81	GLN
2	C	209	ASN
2	C	245	ASN
2	C	256	GLN
2	C	304	ASN
2	C	323	GLN
2	C	342	ASN
2	C	368	ASN
2	C	389	ASN
2	C	414	ASN
2	C	441	GLN
2	D	16	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	256	GLN
2	D	304	ASN
2	D	414	ASN
2	D	441	GLN
2	D	454	ASN
1	E	33	HIS
1	E	81	GLN
1	E	153	GLN

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Mol	Chain	Res	Type
1	E	209	ASN
1	E	256	GLN
1	E	304	ASN
1	E	323	GLN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	33	HIS
1	F	62	ASN
1	F	81	GLN
1	F	115	GLN
1	F	152	GLN
1	F	153	GLN
1	F	209	ASN
1	F	256	GLN
1	F	260	ASN
1	F	323	GLN
1	F	414	ASN
1	F	429	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	SEP	B	431	1	8,9,10	5.77	4 (50%)	7,12,14	3.81	4 (57%)
1	TPO	F	432	1	8,10,11	6.78	6 (75%)	10,14,16	2.76	5 (50%)
2	TPO	C	432	2	8,10,11	7.54	5 (62%)	10,14,16	2.54	4 (40%)
1	TPO	A	432	1	8,10,11	6.94	5 (62%)	10,14,16	2.45	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	E	431	1	8,9,10	5.98	5 (62%)	7,12,14	2.17	3 (42%)
1	TPO	E	432	1	8,10,11	5.84	7 (87%)	10,14,16	2.74	4 (40%)
2	TPO	D	432	2	8,10,11	6.91	6 (75%)	10,14,16	2.60	3 (30%)
1	SEP	A	431	1	8,9,10	5.82	4 (50%)	7,12,14	4.33	4 (57%)
1	SEP	F	431	1	8,9,10	6.03	5 (62%)	7,12,14	2.85	2 (28%)
1	TPO	B	432	1	8,10,11	6.94	5 (62%)	10,14,16	2.52	4 (40%)

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
1	SEP	B	431	1	-	4/6/8/10	-
1	TPO	F	432	1	-	4/9/11/13	-
2	TPO	C	432	2	-	0/9/11/13	-
1	TPO	A	432	1	-	2/9/11/13	-
1	SEP	E	431	1	-	2/6/8/10	-
1	TPO	E	432	1	-	1/9/11/13	-
2	TPO	D	432	2	-	1/9/11/13	-
1	SEP	A	431	1	-	4/6/8/10	-
1	SEP	F	431	1	-	5/6/8/10	-
1	TPO	B	432	1	-	1/9/11/13	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	432	TPO	P-OG1	14.81	1.85	1.59
2	C	432	TPO	P-OG1	14.40	1.84	1.59
1	A	432	TPO	P-OG1	12.52	1.81	1.59
1	F	432	TPO	P-O1P	12.23	1.88	1.50
1	F	431	SEP	P-O1P	12.11	1.88	1.50
1	F	432	TPO	P-OG1	11.81	1.80	1.59
1	B	432	TPO	P-OG1	11.42	1.79	1.59
2	C	432	TPO	P-O1P	11.33	1.85	1.50
1	B	432	TPO	P-O1P	11.31	1.85	1.50
1	A	432	TPO	P-O1P	10.96	1.84	1.50
1	B	431	SEP	P-O1P	10.48	1.83	1.50
1	A	431	SEP	P-O3P	10.33	1.93	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	TPO	P-OG1	9.80	1.76	1.59
2	D	432	TPO	P-O1P	9.39	1.79	1.50
1	E	432	TPO	P-O1P	9.03	1.78	1.50
1	E	431	SEP	P-O1P	8.99	1.78	1.50
1	F	431	SEP	P-O2P	8.72	1.87	1.54
1	E	431	SEP	P-OG	8.49	1.87	1.60
1	A	431	SEP	P-O1P	8.44	1.76	1.50
1	B	432	TPO	P-O3P	8.14	1.85	1.54
1	A	432	TPO	P-O3P	8.05	1.84	1.54
1	E	431	SEP	P-O2P	7.95	1.84	1.54
2	C	432	TPO	P-O3P	7.70	1.83	1.54
1	E	431	SEP	P-O3P	7.51	1.82	1.54
1	A	431	SEP	P-O2P	7.50	1.82	1.54
1	B	431	SEP	P-O3P	7.49	1.82	1.54
1	B	431	SEP	P-O2P	7.29	1.81	1.54
1	B	432	TPO	P-O2P	7.26	1.81	1.54
2	C	432	TPO	P-O2P	7.16	1.81	1.54
1	B	431	SEP	P-OG	6.49	1.80	1.60
1	E	432	TPO	P-O2P	6.28	1.78	1.54
1	F	432	TPO	P-O2P	5.87	1.76	1.54
1	A	431	SEP	P-OG	5.64	1.78	1.60
2	D	432	TPO	P-O2P	5.63	1.75	1.54
1	F	431	SEP	P-O3P	5.56	1.75	1.54
1	F	432	TPO	P-O3P	5.55	1.75	1.54
1	F	431	SEP	P-OG	5.33	1.77	1.60
1	A	432	TPO	P-O2P	5.25	1.74	1.54
1	E	432	TPO	P-O3P	5.00	1.73	1.54
2	D	432	TPO	P-O3P	4.84	1.72	1.54
1	E	432	TPO	CB-CA	-4.29	1.44	1.53
1	A	432	TPO	CA-N	3.78	1.58	1.47
2	D	432	TPO	CA-N	3.28	1.57	1.47
1	E	431	SEP	CB-CA	3.20	1.61	1.52
1	E	432	TPO	CA-N	2.78	1.55	1.47
1	B	432	TPO	CA-N	2.55	1.55	1.47
2	C	432	TPO	CA-N	2.51	1.55	1.47
1	F	431	SEP	CB-CA	2.45	1.59	1.52
1	F	432	TPO	CA-N	2.26	1.54	1.47
1	F	432	TPO	CB-CA	-2.10	1.49	1.53
1	E	432	TPO	CG2-CB	-2.01	1.46	1.51
2	D	432	TPO	CB-CA	2.01	1.58	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	SEP	OG-CB-CA	9.61	117.50	108.14
1	B	431	SEP	O3P-P-OG	7.05	125.06	106.67
1	F	431	SEP	OG-CB-CA	6.66	114.62	108.14
2	D	432	TPO	P-OG1-CB	-6.59	105.42	123.33
1	B	431	SEP	OG-CB-CA	5.44	113.44	108.14
2	C	432	TPO	O-C-CA	-5.39	110.90	124.77
1	F	432	TPO	CG2-CB-CA	-5.37	102.79	113.26
1	A	431	SEP	O2P-P-OG	4.86	119.34	106.67
1	E	432	TPO	CG2-CB-CA	-4.85	103.82	113.26
1	E	432	TPO	P-OG1-CB	-4.63	110.75	123.33
1	E	432	TPO	O-C-CA	-4.58	112.98	124.77
1	A	432	TPO	O-C-CA	-4.56	113.05	124.77
1	B	432	TPO	P-OG1-CB	-4.39	111.39	123.33
1	B	432	TPO	O-C-CA	-4.36	113.56	124.77
1	A	432	TPO	CG2-CB-CA	-4.03	105.42	113.26
1	F	432	TPO	P-OG1-CB	-3.86	112.84	123.33
2	D	432	TPO	O-C-CA	-3.84	114.89	124.77
1	F	432	TPO	O-C-CA	-3.82	114.95	124.77
2	C	432	TPO	P-OG1-CB	-3.80	112.99	123.33
1	B	431	SEP	O3P-P-O1P	-3.39	97.62	110.83
1	B	432	TPO	O2P-P-OG1	3.14	118.08	105.85
1	A	432	TPO	P-OG1-CB	-3.12	114.85	123.33
1	E	431	SEP	OG-CB-CA	3.03	111.09	108.14
2	C	432	TPO	O3P-P-O1P	2.93	122.27	110.83
1	B	432	TPO	O3P-P-OG1	-2.93	94.44	105.85
1	B	431	SEP	OG-P-O1P	-2.85	98.74	106.44
1	E	431	SEP	O2P-P-OG	2.72	113.76	106.67
1	F	431	SEP	O3P-P-OG	2.68	113.67	106.67
1	E	431	SEP	O3P-P-OG	2.59	113.42	106.67
1	A	431	SEP	O3P-P-OG	-2.42	100.37	106.67
1	A	431	SEP	OG-P-O1P	2.32	112.71	106.44
1	A	432	TPO	O3P-P-OG1	-2.29	96.93	105.85
2	C	432	TPO	CG2-CB-CA	2.25	117.65	113.26
1	F	432	TPO	O3P-P-O1P	2.15	119.20	110.83
2	D	432	TPO	OG1-P-O1P	-2.10	101.85	109.33
1	F	432	TPO	O2P-P-O1P	-2.03	102.91	110.83
1	E	432	TPO	O3P-P-O1P	2.01	118.65	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	A	431	SEP	CB-OG-P-O2P
1	A	431	SEP	CB-OG-P-O3P
1	A	432	TPO	CG2-CB-OG1-P
1	B	431	SEP	CA-CB-OG-P
1	B	431	SEP	CB-OG-P-O2P
1	E	431	SEP	CB-OG-P-O3P
1	F	431	SEP	N-CA-CB-OG
1	F	431	SEP	C-CA-CB-OG
1	F	431	SEP	CA-CB-OG-P
1	F	431	SEP	CB-OG-P-O3P
1	F	432	TPO	N-CA-CB-CG2
1	F	432	TPO	N-CA-CB-OG1
1	F	432	TPO	O-C-CA-CB
1	F	432	TPO	CG2-CB-OG1-P
1	B	431	SEP	CB-OG-P-O1P
1	F	431	SEP	CB-OG-P-O2P
1	A	431	SEP	CA-CB-OG-P
1	E	431	SEP	CB-OG-P-O1P
1	B	431	SEP	CB-OG-P-O3P
1	A	432	TPO	O-C-CA-CB
1	B	432	TPO	O-C-CA-CB
2	D	432	TPO	O-C-CA-CB
1	E	432	TPO	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	431	SEP	5	0
1	F	432	TPO	1	0
2	C	432	TPO	2	0
1	A	432	TPO	3	0
1	E	431	SEP	1	0
1	E	432	TPO	1	0
2	D	432	TPO	3	0
1	A	431	SEP	4	0
1	F	431	SEP	2	0
1	B	432	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	903	-	32,33,33	1.97	11 (34%)	48,52,52	2.07	15 (31%)
4	ATP	A	901	3	32,33,33	1.61	7 (21%)	48,52,52	2.03	15 (31%)
4	ATP	D	901	3	32,33,33	2.27	8 (25%)	48,52,52	2.07	12 (25%)
4	ATP	F	901	3	32,33,33	1.72	7 (21%)	48,52,52	2.09	14 (29%)
4	ATP	E	901	3	32,33,33	1.60	5 (15%)	48,52,52	2.10	14 (29%)
4	ATP	B	901	3	32,33,33	1.47	5 (15%)	48,52,52	1.99	16 (33%)
4	ATP	F	903	-	32,33,33	2.04	7 (21%)	48,52,52	2.14	15 (31%)
4	ATP	D	903	-	32,33,33	2.64	8 (25%)	48,52,52	2.33	13 (27%)
4	ATP	C	903	-	32,33,33	1.98	5 (15%)	48,52,52	2.17	14 (29%)
4	ATP	C	901	3	32,33,33	2.22	8 (25%)	48,52,52	2.18	13 (27%)
4	ATP	E	903	-	32,33,33	2.42	9 (28%)	48,52,52	2.13	13 (27%)
4	ATP	B	903	-	32,33,33	1.94	7 (21%)	48,52,52	2.34	17 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	903	-	-	7/22/38/38	0/3/3/3
4	ATP	A	901	3	-	7/22/38/38	0/3/3/3
4	ATP	D	901	3	-	7/22/38/38	0/3/3/3
4	ATP	F	901	3	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	E	901	3	-	7/22/38/38	0/3/3/3
4	ATP	B	901	3	-	6/22/38/38	0/3/3/3
4	ATP	F	903	-	-	8/22/38/38	0/3/3/3
4	ATP	D	903	-	-	8/22/38/38	0/3/3/3
4	ATP	C	903	-	-	8/22/38/38	0/3/3/3
4	ATP	C	901	3	-	7/22/38/38	0/3/3/3
4	ATP	E	903	-	-	11/22/38/38	0/3/3/3
4	ATP	B	903	-	-	9/22/38/38	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	ATP	PB-O3B	-9.64	1.49	1.59
4	D	903	ATP	PB-O3B	-8.80	1.50	1.59
4	C	901	ATP	PB-O3A	-8.54	1.50	1.59
4	D	903	ATP	PB-O3A	-7.74	1.51	1.59
4	D	901	ATP	PB-O3B	-7.74	1.51	1.59
4	C	903	ATP	PB-O3A	-7.45	1.51	1.59
4	A	903	ATP	PB-O3B	-6.80	1.52	1.59
4	D	901	ATP	PB-O3A	-6.52	1.52	1.59
4	F	903	ATP	PB-O3B	-6.44	1.52	1.59
4	F	903	ATP	PB-O3A	-6.39	1.52	1.59
4	B	903	ATP	PB-O3A	-5.78	1.53	1.59
4	F	901	ATP	PB-O3A	-5.45	1.53	1.59
4	A	901	ATP	PB-O3B	-4.63	1.54	1.59
4	E	901	ATP	PB-O3B	-4.16	1.55	1.59
4	D	903	ATP	O4'-C4'	-4.10	1.35	1.45
4	C	903	ATP	PA-O3A	-3.86	1.55	1.59
4	C	901	ATP	PA-O3A	-3.84	1.55	1.59
4	E	903	ATP	C5-N7	-3.73	1.32	1.39
4	B	903	ATP	C1'-N9	3.64	1.56	1.46
4	B	901	ATP	C2-N1	3.63	1.40	1.33
4	B	903	ATP	C8-N9	3.54	1.43	1.37
4	A	903	ATP	C2-N1	3.52	1.40	1.33
4	C	901	ATP	PB-O1B	-3.43	1.38	1.50
4	C	903	ATP	O4'-C4'	-3.40	1.37	1.45
4	F	901	ATP	PA-O3A	-3.34	1.55	1.59
4	E	901	ATP	C2-N3	3.28	1.39	1.33
4	E	903	ATP	PB-O3A	-3.27	1.56	1.59
4	C	901	ATP	C5-N7	-3.23	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	ATP	C2-N3	3.23	1.39	1.33
4	C	901	ATP	PB-O3B	-3.20	1.56	1.59
4	D	903	ATP	PB-O1B	-3.17	1.39	1.50
4	E	901	ATP	C4-N3	3.06	1.40	1.34
4	D	903	ATP	PB-O2B	-2.96	1.41	1.55
4	B	903	ATP	C4-N3	2.94	1.39	1.34
4	C	901	ATP	C2-N3	2.91	1.39	1.33
4	F	901	ATP	C4-N3	2.87	1.39	1.34
4	B	901	ATP	C4-N3	2.86	1.39	1.34
4	E	903	ATP	PB-O1B	-2.85	1.40	1.50
4	A	901	ATP	PB-O3A	-2.81	1.56	1.59
4	E	901	ATP	PB-O3A	-2.75	1.56	1.59
4	D	903	ATP	C2'-C1'	-2.74	1.44	1.53
4	C	903	ATP	C8-N7	2.73	1.36	1.31
4	F	901	ATP	C2-N1	2.69	1.38	1.33
4	B	901	ATP	C1'-N9	2.66	1.53	1.46
4	F	901	ATP	C2-N3	2.62	1.38	1.33
4	F	903	ATP	PB-O1B	-2.62	1.41	1.50
4	C	903	ATP	C6-N1	2.62	1.43	1.35
4	D	901	ATP	C4-N9	-2.59	1.32	1.37
4	B	901	ATP	PB-O1B	-2.58	1.41	1.50
4	F	903	ATP	C2-N1	2.58	1.38	1.33
4	F	903	ATP	C2-N3	2.53	1.38	1.33
4	D	901	ATP	O2'-C2'	-2.52	1.36	1.43
4	A	901	ATP	C2-N3	2.52	1.38	1.33
4	D	901	ATP	C3'-C4'	2.51	1.59	1.53
4	D	903	ATP	C2-N3	2.50	1.38	1.33
4	E	901	ATP	PB-O1B	-2.50	1.42	1.50
4	F	901	ATP	PB-O1B	-2.50	1.42	1.50
4	E	903	ATP	O4'-C4'	-2.45	1.39	1.45
4	D	901	ATP	C5-N7	-2.44	1.34	1.39
4	B	903	ATP	O4'-C1'	2.44	1.47	1.42
4	E	903	ATP	PA-O1A	-2.39	1.42	1.50
4	E	903	ATP	C2'-C3'	-2.37	1.46	1.53
4	B	903	ATP	PB-O3B	-2.37	1.56	1.59
4	A	901	ATP	PB-O1B	-2.34	1.42	1.50
4	A	903	ATP	C8-N7	2.32	1.36	1.31
4	F	903	ATP	C6-N6	-2.31	1.28	1.34
4	A	903	ATP	C5-C4	2.30	1.43	1.39
4	E	903	ATP	PG-O1G	2.30	1.57	1.50
4	A	901	ATP	C2-N1	2.26	1.38	1.33
4	F	903	ATP	C4-N9	-2.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	ATP	C2-N3	2.19	1.37	1.33
4	F	901	ATP	C5'-C4'	2.17	1.58	1.51
4	A	901	ATP	C1'-N9	2.16	1.52	1.46
4	E	903	ATP	C4-N9	-2.15	1.33	1.37
4	A	901	ATP	C5'-C4'	2.14	1.58	1.51
4	A	903	ATP	PB-O1B	-2.13	1.43	1.50
4	A	903	ATP	C4-N3	2.12	1.38	1.34
4	A	903	ATP	PG-O1G	2.11	1.57	1.50
4	D	903	ATP	PA-O1A	-2.07	1.43	1.50
4	C	901	ATP	O4'-C4'	-2.07	1.40	1.45
4	D	901	ATP	PB-O1B	-2.07	1.43	1.50
4	A	903	ATP	PB-O2B	-2.06	1.45	1.55
4	D	901	ATP	PA-O3A	-2.03	1.57	1.59
4	A	903	ATP	PB-O3A	-2.03	1.57	1.59
4	B	901	ATP	C5-C4	2.02	1.42	1.39
4	C	901	ATP	PB-O2B	-2.01	1.46	1.55
4	A	903	ATP	C3'-C4'	2.00	1.58	1.53

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	ATP	N3-C2-N1	-6.34	118.98	128.58
4	B	901	ATP	N3-C2-N1	-6.08	119.38	128.58
4	C	903	ATP	N3-C2-N1	-6.07	119.40	128.58
4	E	901	ATP	N3-C2-N1	-6.00	119.50	128.58
4	D	901	ATP	N3-C2-N1	-5.96	119.56	128.58
4	D	903	ATP	N3-C2-N1	-5.88	119.68	128.58
4	F	901	ATP	N3-C2-N1	-5.79	119.81	128.58
4	C	901	ATP	C5-N7-C8	5.78	112.53	103.45
4	E	903	ATP	N3-C2-N1	-5.73	119.91	128.58
4	D	903	ATP	C5-N7-C8	5.60	112.24	103.45
4	A	901	ATP	N3-C2-N1	-5.56	120.17	128.58
4	D	903	ATP	C4-C5-N7	-5.53	104.26	110.58
4	D	903	ATP	N9-C8-N7	-5.28	106.44	113.94
4	C	903	ATP	N9-C8-N7	-5.26	106.48	113.94
4	C	901	ATP	N3-C2-N1	-5.22	120.67	128.58
4	C	901	ATP	N9-C8-N7	-5.16	106.61	113.94
4	A	903	ATP	N3-C2-N1	-5.16	120.78	128.58
4	F	903	ATP	N3-C2-N1	-5.15	120.78	128.58
4	B	903	ATP	N9-C8-N7	-5.15	106.63	113.94
4	A	901	ATP	C5-N7-C8	5.10	111.47	103.45
4	E	901	ATP	C5-N7-C8	5.09	111.45	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	903	ATP	C5-N7-C8	5.09	111.45	103.45
4	F	901	ATP	C5-N7-C8	5.04	111.38	103.45
4	E	901	ATP	N9-C8-N7	-5.03	106.81	113.94
4	E	903	ATP	N9-C8-N7	-5.00	106.84	113.94
4	F	903	ATP	C4-C5-N7	-4.99	104.88	110.58
4	A	903	ATP	N9-C8-N7	-4.93	106.95	113.94
4	C	901	ATP	C4-C5-N7	-4.91	104.97	110.58
4	F	903	ATP	C5-N7-C8	4.89	111.14	103.45
4	F	903	ATP	N9-C8-N7	-4.85	107.05	113.94
4	B	901	ATP	C5-N7-C8	4.81	111.01	103.45
4	D	901	ATP	O2B-PB-O3B	4.78	120.21	107.27
4	A	903	ATP	C4-C5-N7	-4.78	105.12	110.58
4	F	901	ATP	N9-C8-N7	-4.77	107.17	113.94
4	B	903	ATP	C5-N7-C8	4.76	110.93	103.45
4	A	901	ATP	C4-C5-N7	-4.61	105.31	110.58
4	B	901	ATP	N9-C8-N7	-4.54	107.49	113.94
4	A	903	ATP	C5-N7-C8	4.52	110.55	103.45
4	A	901	ATP	N9-C8-N7	-4.51	107.53	113.94
4	F	901	ATP	C4-C5-N7	-4.50	105.44	110.58
4	E	901	ATP	C4-C5-N7	-4.46	105.48	110.58
4	C	901	ATP	O2B-PB-O3B	4.45	119.30	107.27
4	D	901	ATP	N9-C8-N7	-4.32	107.81	113.94
4	B	903	ATP	O2B-PB-O3B	4.29	118.86	107.27
4	C	903	ATP	C5-N7-C8	4.27	110.16	103.45
4	B	903	ATP	C4-C5-N7	-4.25	105.73	110.58
4	C	903	ATP	C4-C5-N7	-4.22	105.76	110.58
4	B	901	ATP	O2B-PB-O3B	4.21	118.66	107.27
4	E	903	ATP	C4-C5-N7	-4.12	105.88	110.58
4	D	901	ATP	C5-N7-C8	4.07	109.85	103.45
4	D	903	ATP	C2'-C1'-N9	3.97	123.17	113.30
4	B	903	ATP	O3A-PA-O1A	-3.74	99.45	110.70
4	B	903	ATP	C6-C5-N7	3.72	139.27	132.09
4	E	903	ATP	O3A-PB-O1B	-3.70	99.56	110.70
4	D	903	ATP	O2B-PB-O3B	3.69	117.25	107.27
4	B	901	ATP	C4-C5-N7	-3.67	106.39	110.58
4	A	903	ATP	O3A-PB-O1B	-3.66	99.70	110.70
4	C	903	ATP	C2-N3-C4	3.64	120.72	111.83
4	D	901	ATP	C4-C5-N7	-3.60	106.46	110.58
4	D	901	ATP	O3B-PB-O1B	-3.58	99.94	110.70
4	C	903	ATP	O2B-PB-O3B	3.57	116.93	107.27
4	F	903	ATP	O3A-PB-O1B	-3.55	100.03	110.70
4	D	901	ATP	O3A-PB-O1B	-3.54	100.04	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	C4-N9-C8	3.50	109.41	105.74
4	F	901	ATP	O2B-PB-O3B	3.49	116.70	107.27
4	C	903	ATP	O3B-PB-O1B	-3.46	100.31	110.70
4	A	901	ATP	O2B-PB-O3B	3.42	116.53	107.27
4	A	903	ATP	C6-C5-N7	3.41	138.66	132.09
4	D	903	ATP	C2-N3-C4	3.40	120.13	111.83
4	C	901	ATP	O2B-PB-O3A	3.39	116.42	107.27
4	B	903	ATP	C2-N3-C4	3.32	119.94	111.83
4	D	903	ATP	C6-C5-N7	3.31	138.47	132.09
4	D	901	ATP	O2B-PB-O3A	3.31	116.21	107.27
4	E	901	ATP	C6-C5-N7	3.23	138.31	132.09
4	C	901	ATP	C5-C4-N3	-3.20	122.31	126.72
4	F	903	ATP	C4-N9-C8	3.18	109.08	105.74
4	E	903	ATP	C2'-C1'-N9	3.17	121.19	113.30
4	E	901	ATP	C2-N3-C4	3.17	119.57	111.83
4	D	903	ATP	C5-C4-N3	-3.17	122.36	126.72
4	E	901	ATP	O3A-PB-O1B	-3.14	101.25	110.70
4	E	903	ATP	O2B-PB-O3B	3.13	115.74	107.27
4	F	903	ATP	C2'-C1'-N9	3.10	121.01	113.30
4	C	901	ATP	O3B-PB-O1B	-3.09	101.40	110.70
4	E	903	ATP	C5-C4-N3	-3.07	122.48	126.72
4	F	903	ATP	O2B-PB-O3B	3.07	115.56	107.27
4	D	903	ATP	O3A-PB-O1B	-3.06	101.51	110.70
4	E	901	ATP	C4-N9-C8	3.05	108.94	105.74
4	C	903	ATP	C4-N9-C8	3.04	108.93	105.74
4	F	901	ATP	C6-C5-N7	3.01	137.90	132.09
4	F	901	ATP	C2-N3-C4	3.00	119.15	111.83
4	A	901	ATP	C5-C4-N3	-2.99	122.59	126.72
4	F	903	ATP	C6-C5-N7	2.97	137.82	132.09
4	E	903	ATP	C2-N3-C4	2.97	119.08	111.83
4	E	901	ATP	C5-C4-N3	-2.96	122.64	126.72
4	F	901	ATP	C5-C4-N3	-2.95	122.66	126.72
4	C	903	ATP	C6-C5-N7	2.94	137.76	132.09
4	A	901	ATP	C2-N3-C4	2.92	118.97	111.83
4	D	901	ATP	C2-N3-C4	2.92	118.95	111.83
4	D	903	ATP	O3B-PB-O1B	-2.89	102.01	110.70
4	F	901	ATP	O2'-C2'-C3'	2.87	121.01	111.82
4	F	903	ATP	C5-C4-N3	-2.86	122.77	126.72
4	A	903	ATP	C4-N9-C8	2.86	108.74	105.74
4	B	901	ATP	O2B-PB-O3A	2.83	114.94	107.27
4	F	901	ATP	C4-N9-C8	2.83	108.71	105.74
4	B	903	ATP	O2B-PB-O3A	2.82	114.91	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	ATP	C5-C4-N3	-2.82	122.84	126.72
4	A	901	ATP	C6-C5-N7	2.80	137.48	132.09
4	A	903	ATP	C2-N3-C4	2.79	118.66	111.83
4	B	903	ATP	O2'-C2'-C3'	2.79	120.77	111.82
4	F	903	ATP	C2-N3-C4	2.77	118.59	111.83
4	F	901	ATP	O3A-PB-O1B	-2.74	102.45	110.70
4	B	903	ATP	O3A-PB-O1B	-2.73	102.48	110.70
4	C	901	ATP	O3A-PB-O1B	-2.71	102.56	110.70
4	C	903	ATP	O3A-PB-O1B	-2.71	102.56	110.70
4	B	903	ATP	O3B-PB-O1B	-2.69	102.62	110.70
4	E	903	ATP	O2B-PB-O3A	2.67	114.49	107.27
4	B	901	ATP	C2-N3-C4	2.66	118.32	111.83
4	D	901	ATP	C4-N9-C8	2.65	108.52	105.74
4	A	903	ATP	O2B-PB-O3B	2.65	114.42	107.27
4	B	903	ATP	N6-C6-N1	-2.63	112.51	118.38
4	C	903	ATP	C5-C4-N9	2.63	108.67	105.81
4	C	901	ATP	O2'-C2'-C3'	2.62	120.22	111.82
4	C	901	ATP	C2-N3-C4	2.61	118.22	111.83
4	A	903	ATP	C5-C4-N9	2.60	108.65	105.81
4	B	901	ATP	O3B-PB-O1B	-2.59	102.91	110.70
4	B	903	ATP	C5-C4-N3	-2.59	123.16	126.72
4	B	903	ATP	O4'-C1'-N9	2.59	113.05	108.09
4	E	903	ATP	C6-C5-N7	2.57	137.05	132.09
4	D	901	ATP	C6-C5-N7	2.55	137.01	132.09
4	F	903	ATP	O3B-PB-O1B	-2.55	103.05	110.70
4	F	901	ATP	O2B-PB-O3A	2.54	114.13	107.27
4	C	901	ATP	C6-C5-N7	2.53	136.97	132.09
4	B	903	ATP	C4-N9-C8	2.49	108.35	105.74
4	C	901	ATP	C4-N9-C8	2.49	108.35	105.74
4	D	903	ATP	O3A-PA-O1A	-2.48	103.24	110.70
4	E	901	ATP	O2B-PB-O3B	2.48	113.97	107.27
4	D	901	ATP	C5-C4-N3	-2.47	123.32	126.72
4	A	901	ATP	O2B-PB-O3A	2.44	113.88	107.27
4	A	903	ATP	O2B-PB-O3A	2.42	113.82	107.27
4	B	901	ATP	C6-C5-N7	2.42	136.75	132.09
4	A	901	ATP	C4-N9-C8	2.41	108.27	105.74
4	C	903	ATP	C2'-C1'-N9	2.41	119.28	113.30
4	B	901	ATP	C4-N9-C8	2.40	108.25	105.74
4	E	901	ATP	N6-C6-N1	-2.39	113.06	118.38
4	E	901	ATP	C2'-C1'-N9	2.39	119.23	113.30
4	B	903	ATP	C5-C4-N9	2.33	108.36	105.81
4	A	901	ATP	C2'-C1'-N9	2.32	119.06	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	ATP	N6-C6-N1	-2.31	113.23	118.38
4	C	903	ATP	O5'-PA-O1A	-2.31	99.79	108.94
4	E	903	ATP	C4-N9-C8	2.29	108.14	105.74
4	F	903	ATP	N6-C6-N1	-2.28	113.31	118.38
4	A	901	ATP	O3A-PB-O1B	-2.26	103.89	110.70
4	F	903	ATP	O2B-PB-O3A	2.26	113.39	107.27
4	B	901	ATP	O3A-PA-O1A	-2.24	103.97	110.70
4	E	901	ATP	O2'-C2'-C3'	2.22	118.93	111.82
4	B	901	ATP	O2'-C2'-C3'	2.22	118.92	111.82
4	A	903	ATP	C2'-C1'-N9	2.21	118.79	113.30
4	B	901	ATP	C5-C4-N3	-2.20	123.68	126.72
4	A	901	ATP	O2'-C2'-C3'	2.20	118.86	111.82
4	B	901	ATP	O2G-PG-O3B	2.11	111.71	104.64
4	A	903	ATP	C5-C4-N3	-2.10	123.82	126.72
4	B	901	ATP	C2-N1-C6	2.10	122.18	118.73
4	A	901	ATP	O3B-PB-O1B	-2.09	104.42	110.70
4	E	901	ATP	O2B-PB-O3A	2.09	112.91	107.27
4	F	901	ATP	C2'-C1'-N9	2.07	118.44	113.30
4	B	901	ATP	C2'-C1'-N9	2.05	118.40	113.30
4	A	903	ATP	O3A-PA-O1A	-2.05	104.53	110.70
4	E	903	ATP	O2G-PG-O1G	2.03	118.75	110.83
4	F	901	ATP	N6-C6-N1	-2.02	113.89	118.38
4	F	903	ATP	O2G-PG-O1G	2.01	118.68	110.83
4	A	901	ATP	O3A-PA-O1A	-2.01	104.67	110.70

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	ATP	C5'-O5'-PA-O3A
4	A	903	ATP	PB-O3B-PG-O3G
4	A	903	ATP	C5'-O5'-PA-O1A
4	A	903	ATP	C3'-C4'-C5'-O5'
4	B	901	ATP	C5'-O5'-PA-O3A
4	B	903	ATP	PB-O3B-PG-O3G
4	B	903	ATP	PB-O3A-PA-O5'
4	B	903	ATP	C5'-O5'-PA-O1A
4	B	903	ATP	O4'-C4'-C5'-O5'
4	C	901	ATP	C5'-O5'-PA-O3A
4	C	903	ATP	PB-O3B-PG-O3G
4	C	903	ATP	C5'-O5'-PA-O1A
4	C	903	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	D	901	ATP	C5'-O5'-PA-O3A
4	D	903	ATP	PB-O3B-PG-O3G
4	D	903	ATP	C5'-O5'-PA-O1A
4	D	903	ATP	C5'-O5'-PA-O3A
4	D	903	ATP	O4'-C4'-C5'-O5'
4	E	901	ATP	C5'-O5'-PA-O3A
4	E	903	ATP	PB-O3B-PG-O3G
4	E	903	ATP	PB-O3A-PA-O5'
4	E	903	ATP	C5'-O5'-PA-O1A
4	E	903	ATP	C5'-O5'-PA-O3A
4	E	903	ATP	C3'-C4'-C5'-O5'
4	F	901	ATP	C5'-O5'-PA-O3A
4	F	903	ATP	PB-O3B-PG-O3G
4	F	903	ATP	PB-O3A-PA-O5'
4	F	903	ATP	C5'-O5'-PA-O1A
4	F	903	ATP	O4'-C4'-C5'-O5'
4	A	901	ATP	C3'-C4'-C5'-O5'
4	B	901	ATP	C3'-C4'-C5'-O5'
4	B	903	ATP	C3'-C4'-C5'-O5'
4	C	901	ATP	C3'-C4'-C5'-O5'
4	D	901	ATP	C3'-C4'-C5'-O5'
4	D	903	ATP	C3'-C4'-C5'-O5'
4	E	901	ATP	C3'-C4'-C5'-O5'
4	F	901	ATP	C3'-C4'-C5'-O5'
4	A	901	ATP	O4'-C4'-C5'-O5'
4	A	903	ATP	O4'-C4'-C5'-O5'
4	B	901	ATP	O4'-C4'-C5'-O5'
4	C	901	ATP	O4'-C4'-C5'-O5'
4	C	903	ATP	C3'-C4'-C5'-O5'
4	D	901	ATP	O4'-C4'-C5'-O5'
4	E	901	ATP	O4'-C4'-C5'-O5'
4	E	903	ATP	O4'-C4'-C5'-O5'
4	F	903	ATP	C3'-C4'-C5'-O5'
4	F	901	ATP	O4'-C4'-C5'-O5'
4	A	901	ATP	PB-O3A-PA-O5'
4	A	903	ATP	PB-O3A-PA-O5'
4	B	901	ATP	PB-O3A-PA-O5'
4	C	901	ATP	PB-O3A-PA-O5'
4	C	903	ATP	PB-O3A-PA-O5'
4	D	901	ATP	PB-O3A-PA-O5'
4	D	903	ATP	PB-O3A-PA-O5'
4	E	901	ATP	PB-O3A-PA-O5'

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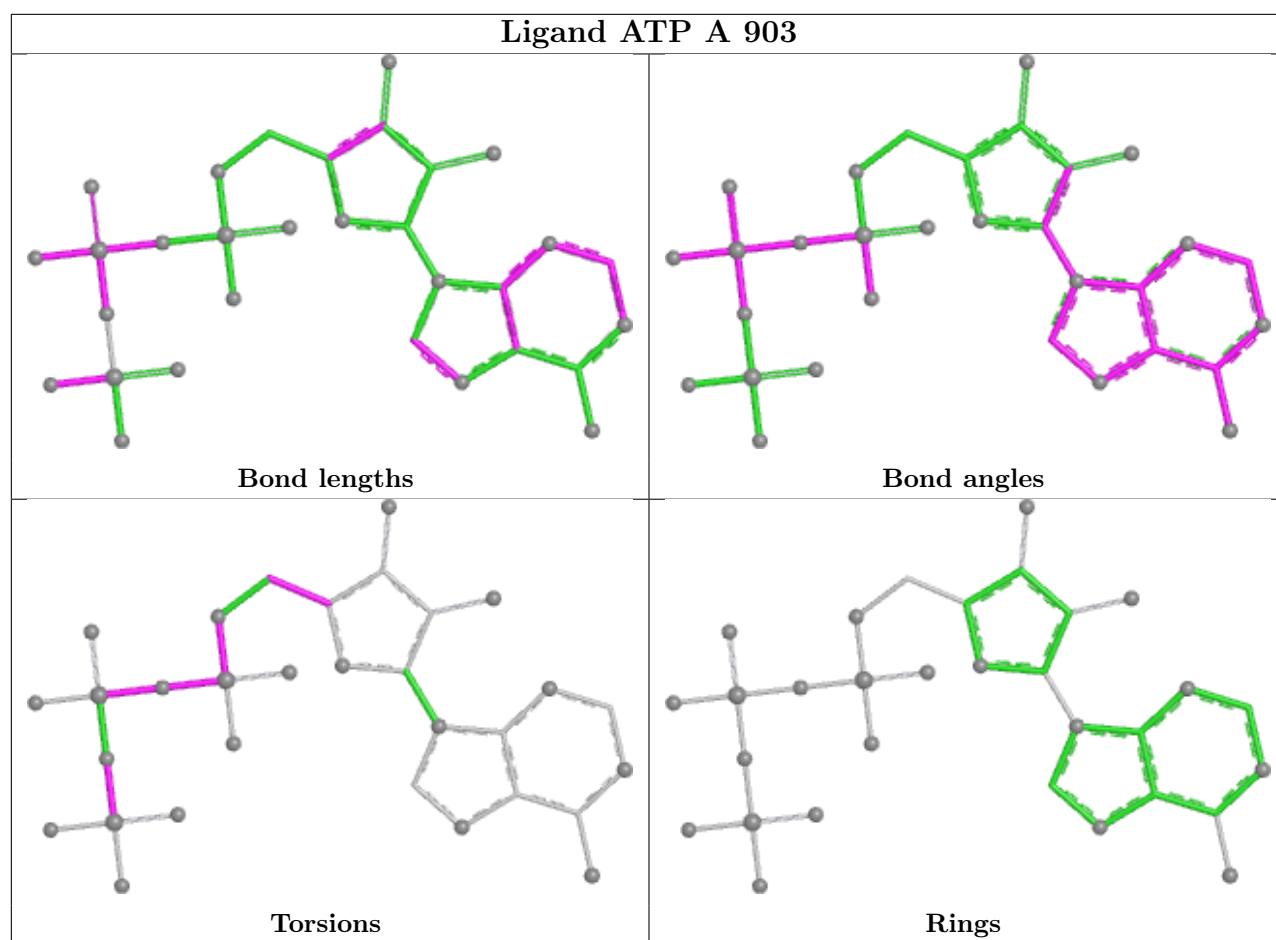
Mol	Chain	Res	Type	Atoms
4	F	901	ATP	PB-O3A-PA-O5'
4	A	901	ATP	PA-O3A-PB-O2B
4	A	903	ATP	PA-O3A-PB-O2B
4	B	901	ATP	PA-O3A-PB-O2B
4	B	903	ATP	PA-O3A-PB-O2B
4	C	901	ATP	PA-O3A-PB-O2B
4	C	903	ATP	PA-O3A-PB-O2B
4	D	901	ATP	PA-O3A-PB-O2B
4	D	903	ATP	PA-O3A-PB-O2B
4	E	901	ATP	PA-O3A-PB-O2B
4	E	903	ATP	PA-O3A-PB-O2B
4	F	901	ATP	PA-O3A-PB-O2B
4	F	903	ATP	PA-O3A-PB-O2B
4	A	901	ATP	C5'-O5'-PA-O1A
4	B	901	ATP	C5'-O5'-PA-O1A
4	C	901	ATP	C5'-O5'-PA-O1A
4	C	901	ATP	C5'-O5'-PA-O2A
4	D	901	ATP	C5'-O5'-PA-O1A
4	E	901	ATP	C5'-O5'-PA-O1A
4	F	901	ATP	C5'-O5'-PA-O1A
4	E	903	ATP	PB-O3B-PG-O1G
4	B	903	ATP	PB-O3B-PG-O2G
4	C	903	ATP	PB-O3B-PG-O2G
4	E	903	ATP	PB-O3B-PG-O2G
4	A	903	ATP	PB-O3A-PA-O1A
4	B	903	ATP	PA-O3A-PB-O1B
4	D	901	ATP	PA-O3A-PB-O1B
4	F	903	ATP	PA-O3A-PB-O1B
4	B	903	ATP	PB-O3B-PG-O1G
4	A	901	ATP	PB-O3A-PA-O2A
4	C	903	ATP	PB-O3A-PA-O2A
4	D	903	ATP	PA-O3A-PB-O1B
4	E	901	ATP	PB-O3A-PA-O2A
4	E	903	ATP	PA-O3A-PB-O1B
4	E	903	ATP	PB-O3A-PA-O2A
4	F	901	ATP	PB-O3A-PA-O2A
4	F	903	ATP	PB-O3A-PA-O2A

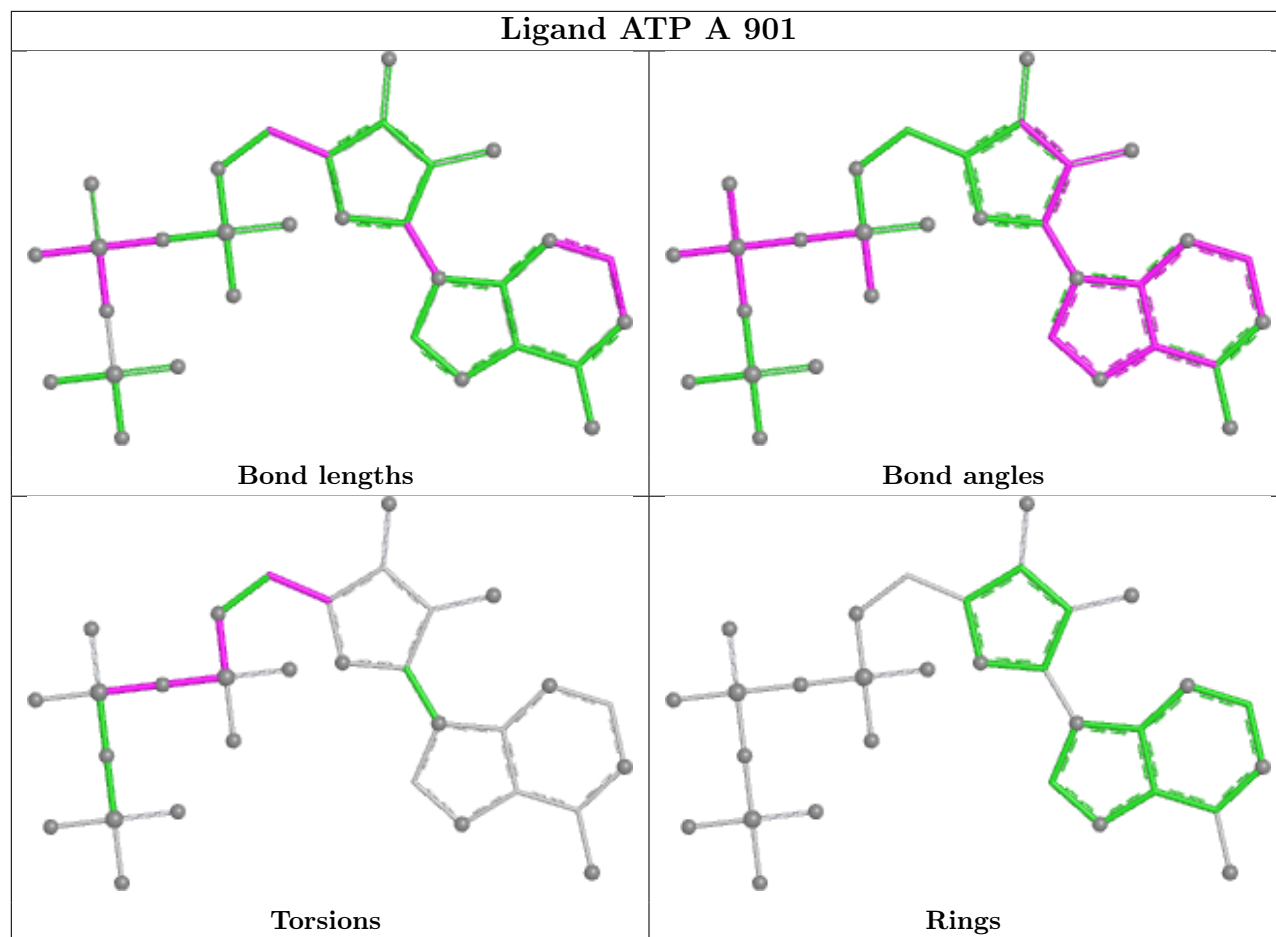
There are no ring outliers.

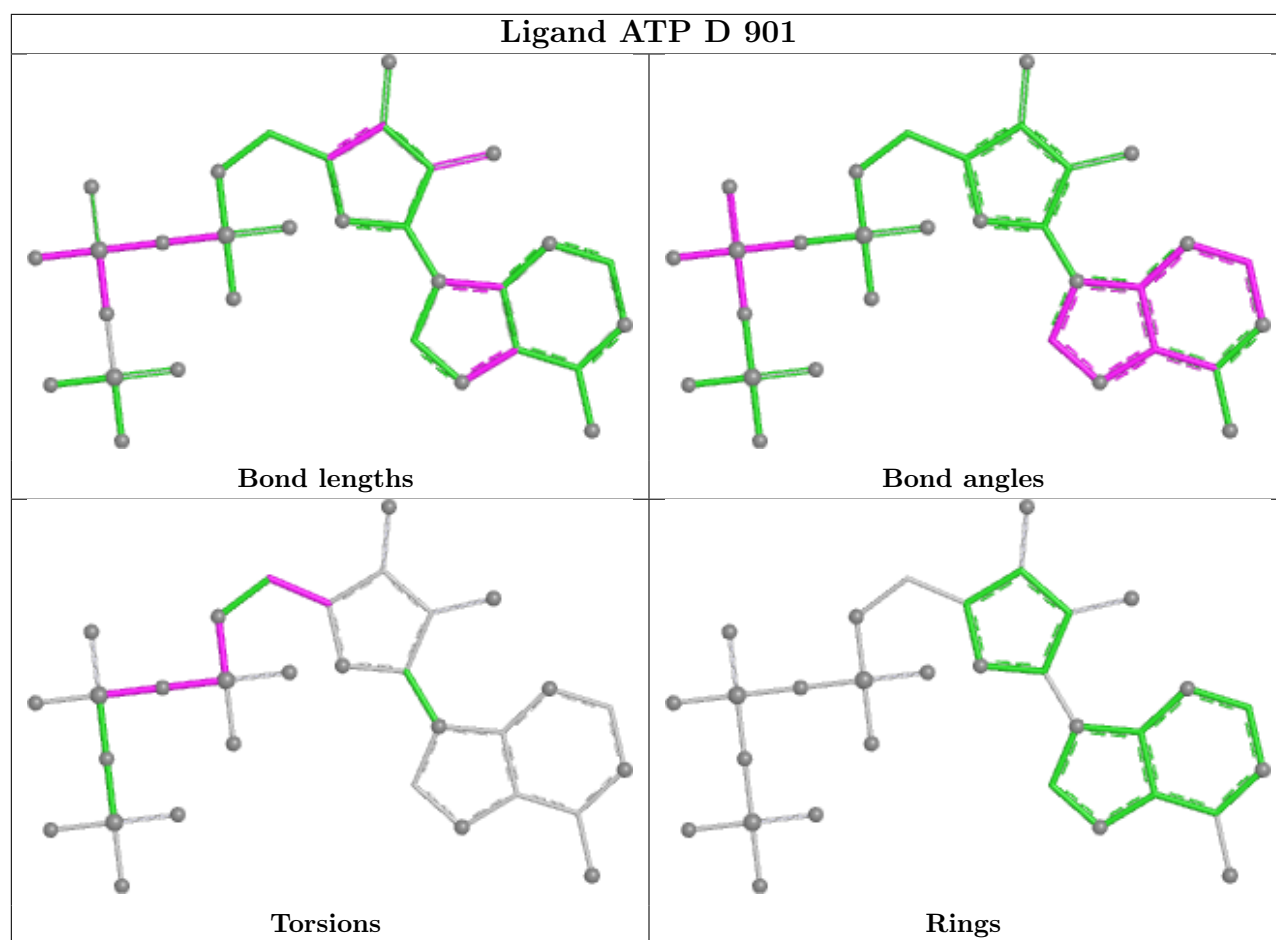
12 monomers are involved in 48 short contacts:

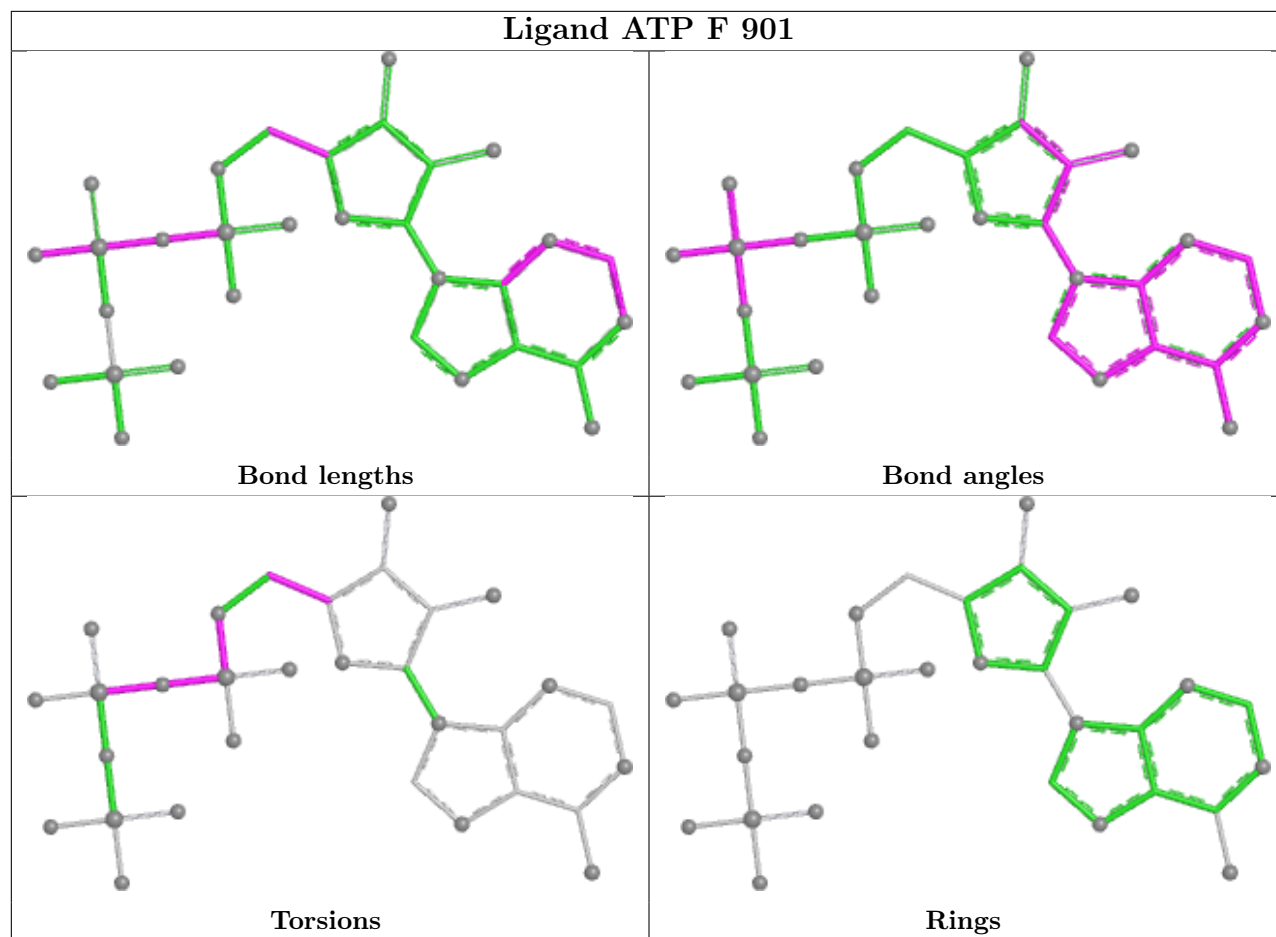
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	ATP	5	0
4	A	901	ATP	7	0
4	D	901	ATP	2	0
4	F	901	ATP	4	0
4	E	901	ATP	4	0
4	B	901	ATP	6	0
4	F	903	ATP	3	0
4	D	903	ATP	5	0
4	C	903	ATP	5	0
4	C	901	ATP	2	0
4	E	903	ATP	2	0
4	B	903	ATP	3	0

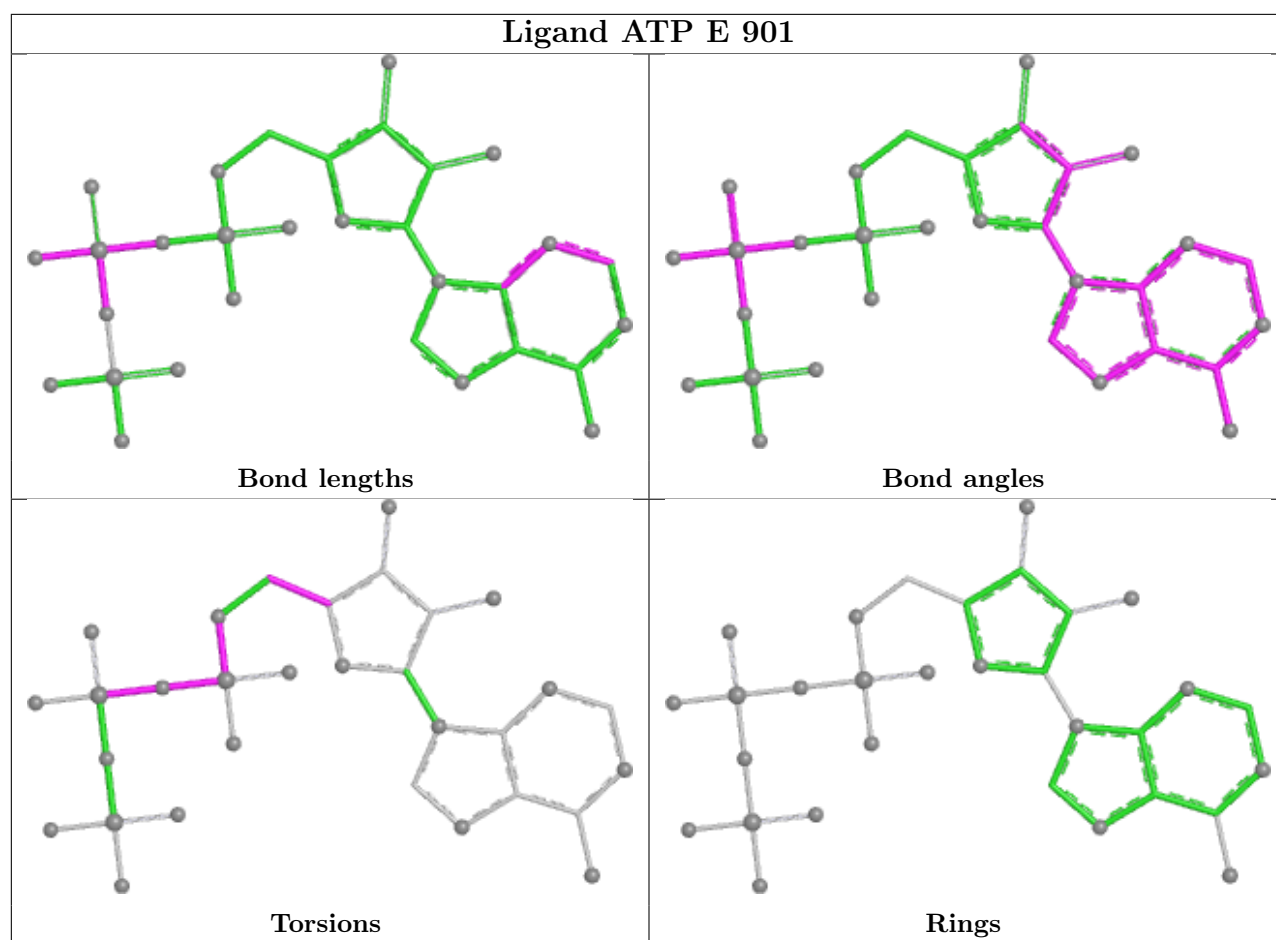
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

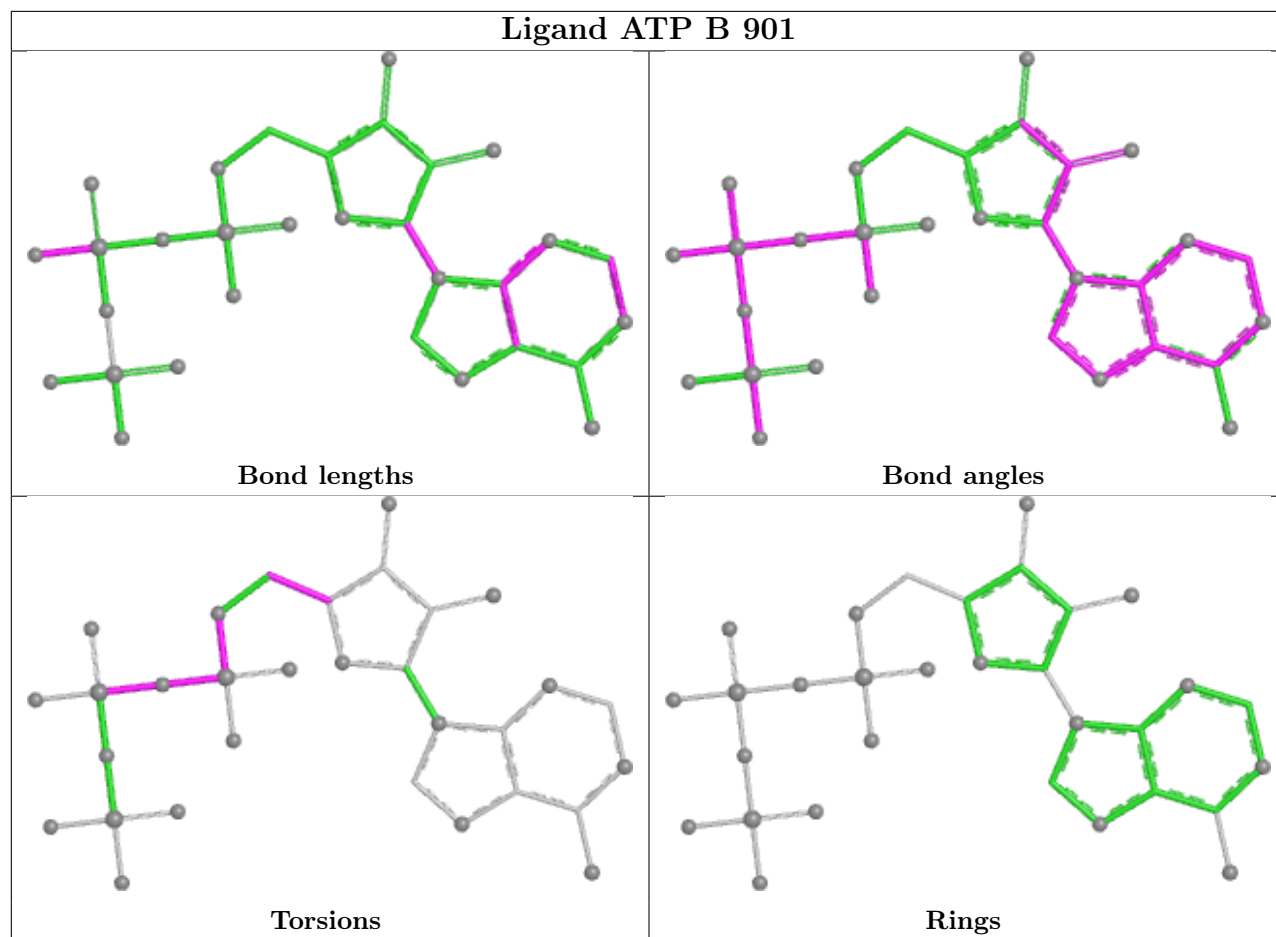




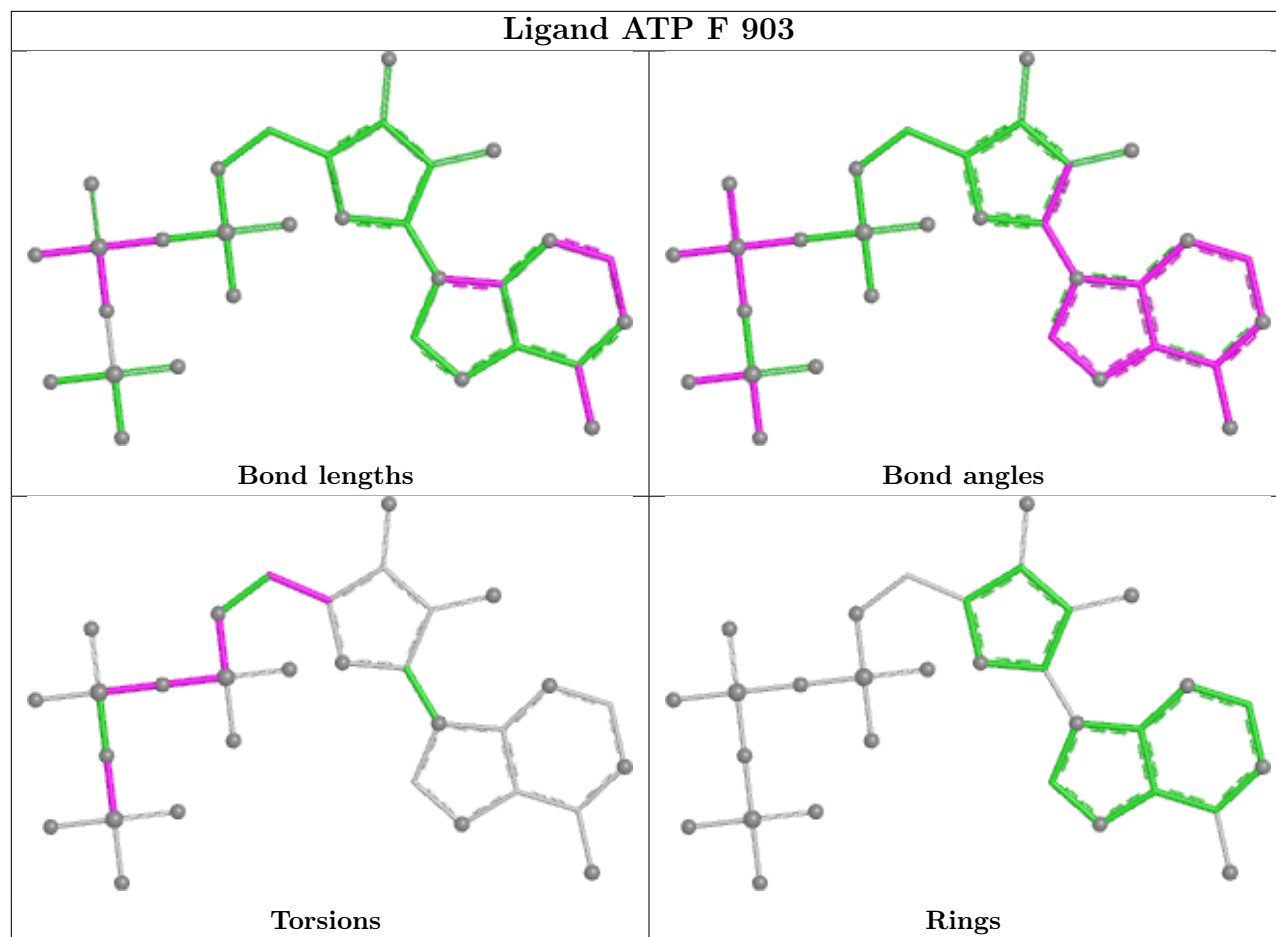


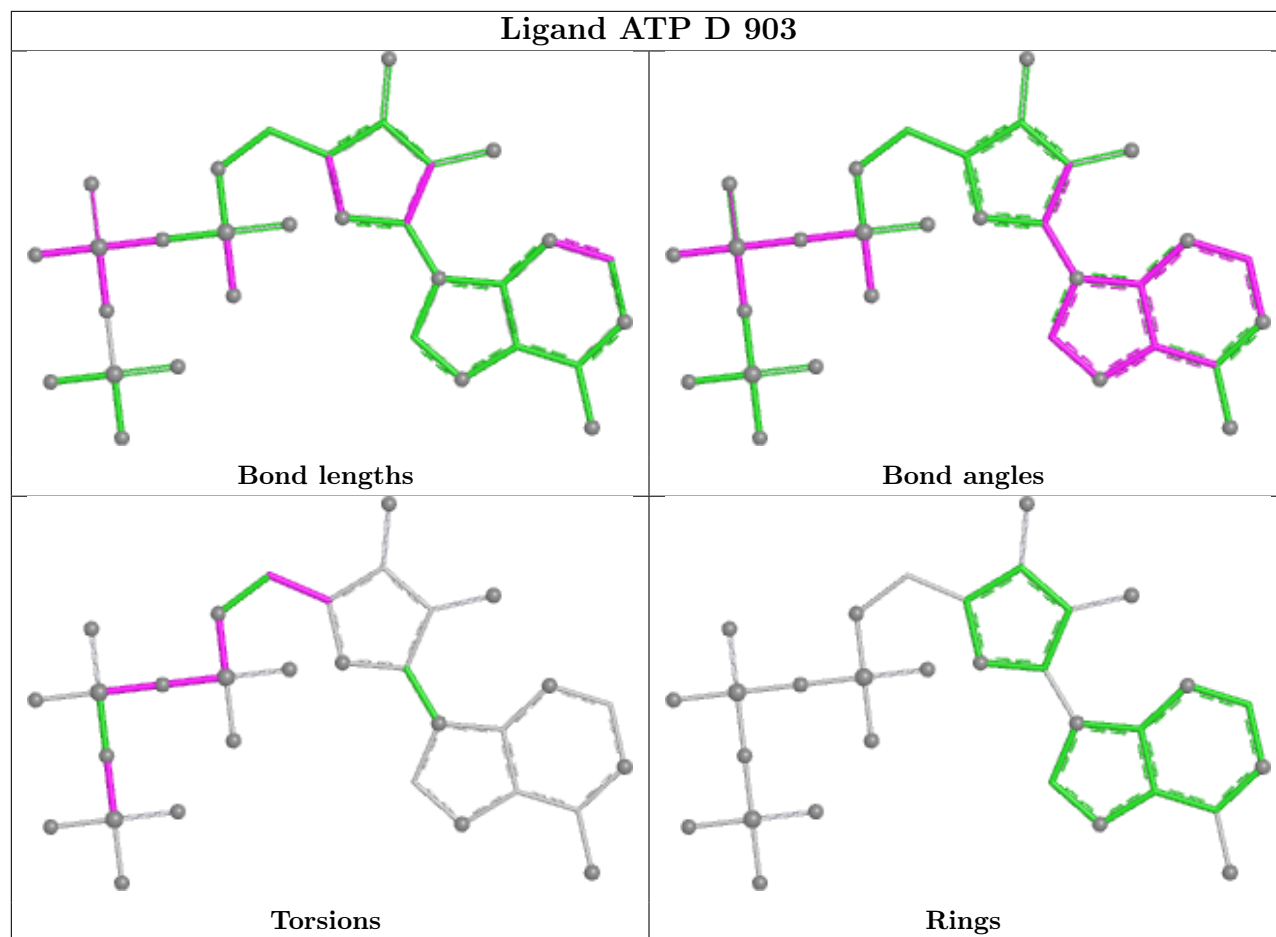




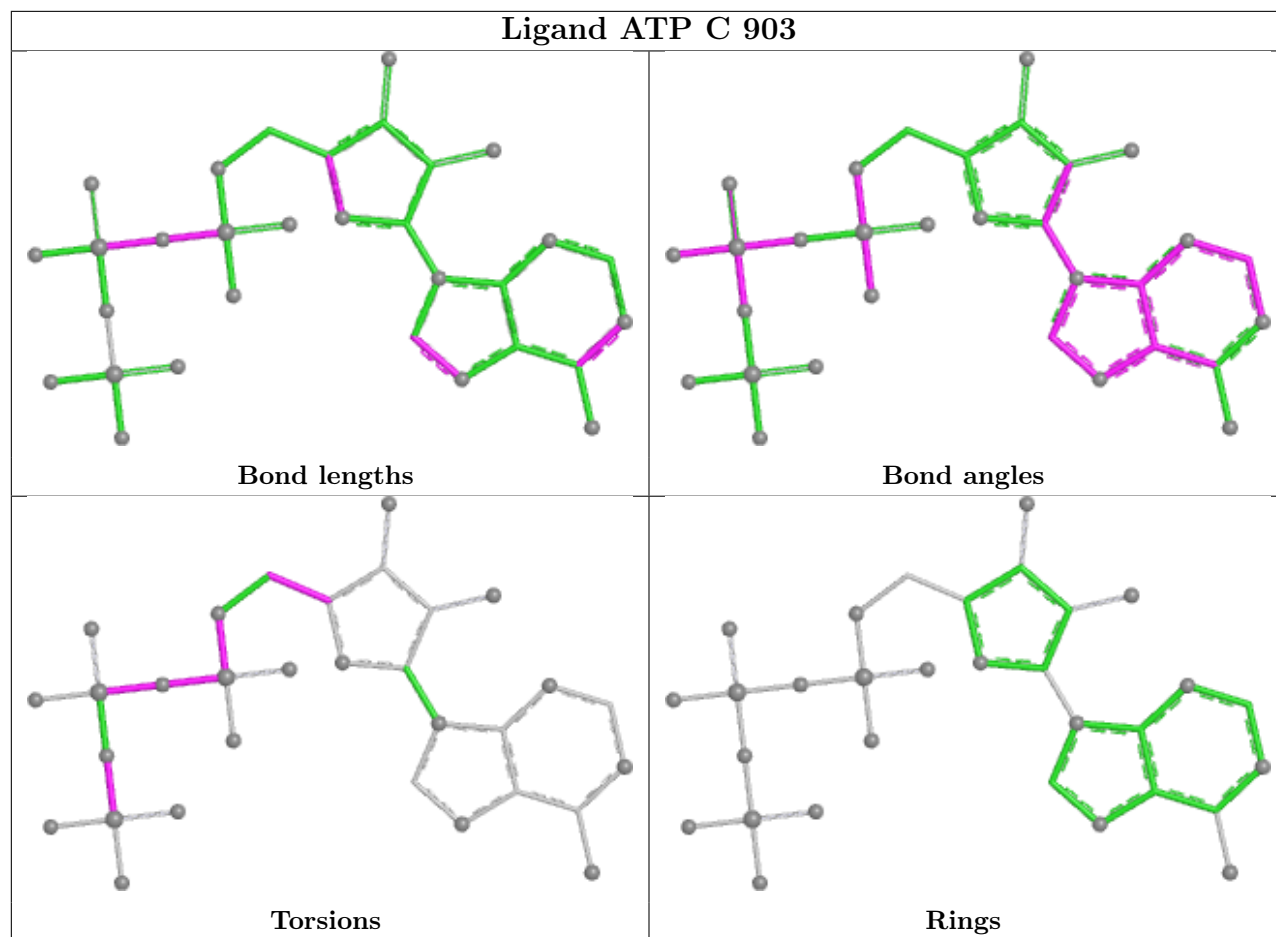


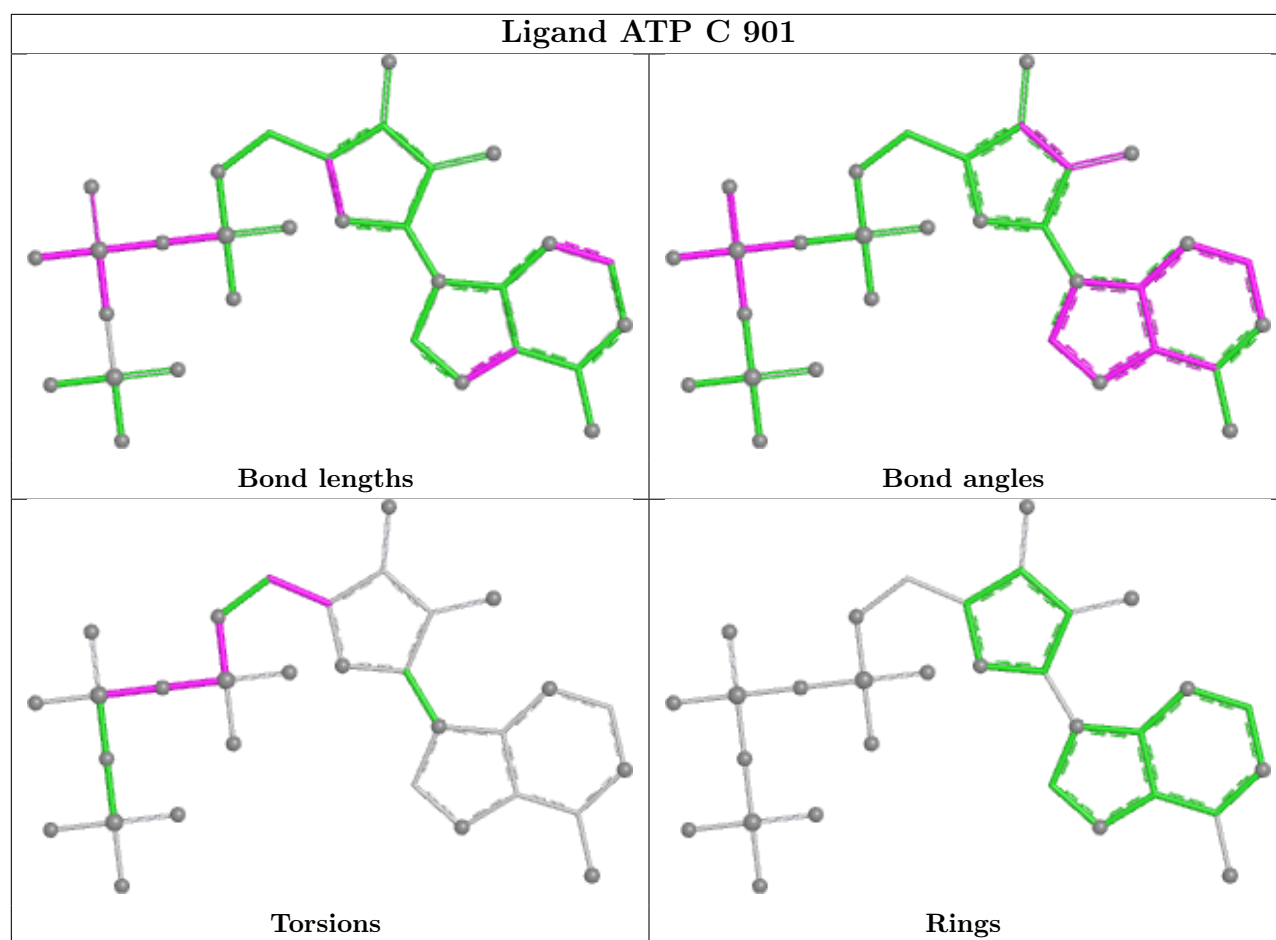
Ligand ATP F 903



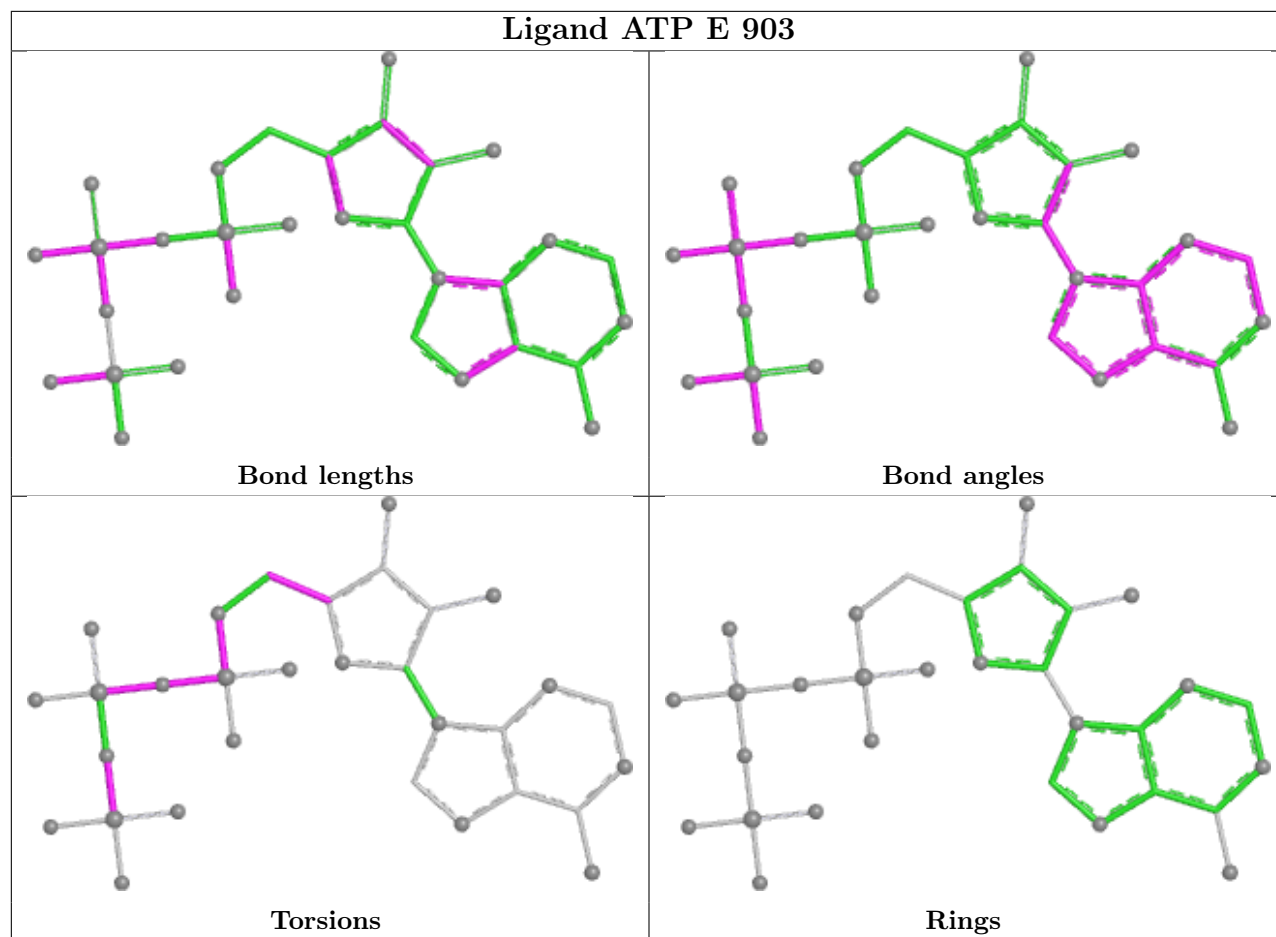


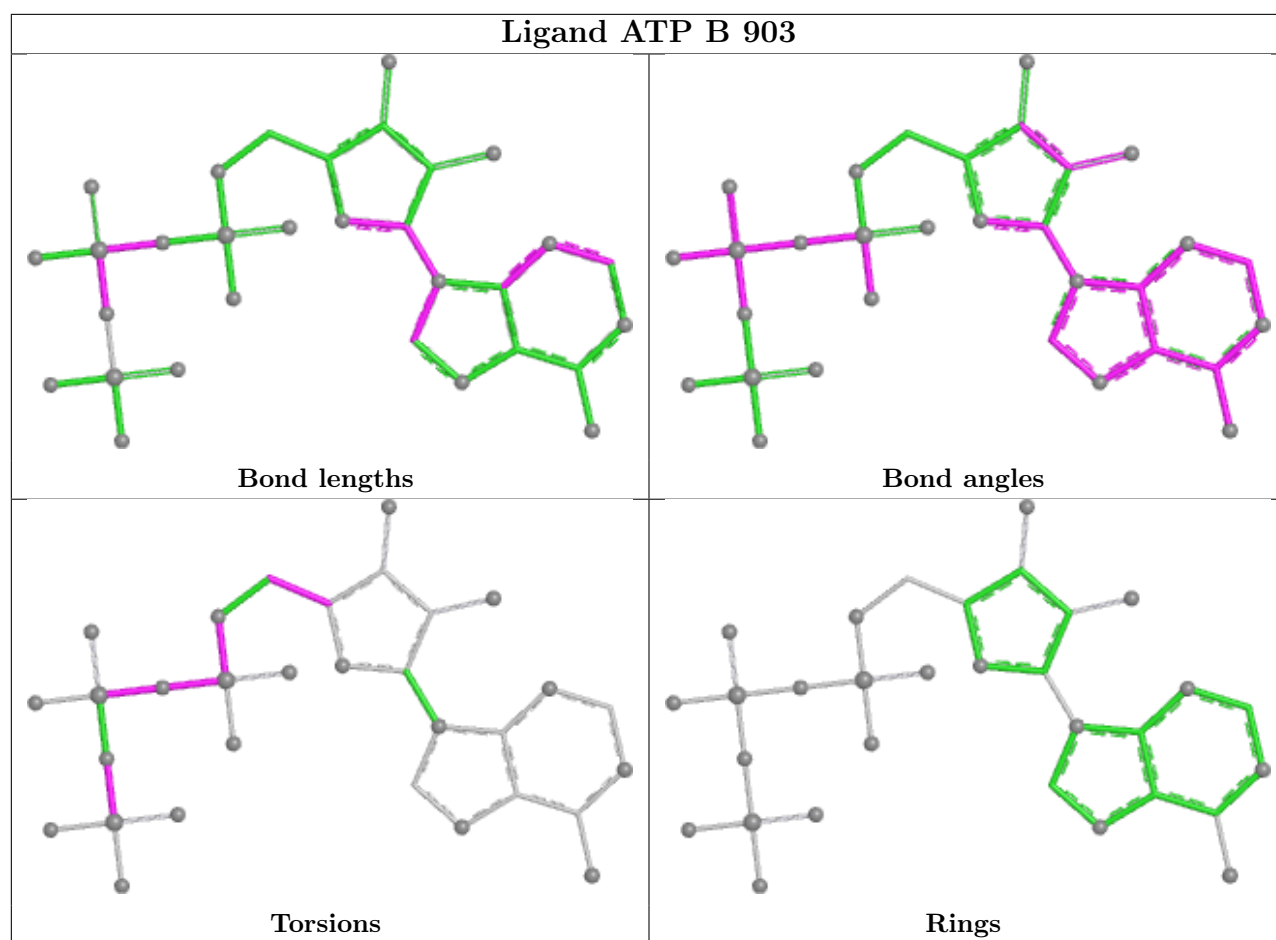
Ligand ATP C 903





Ligand ATP E 903





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	504/519 (97%)	0.13	15 (2%)	52 42	30, 77, 128, 155	0
1	B	489/519 (94%)	0.23	13 (2%)	56 46	41, 83, 129, 161	0
1	E	490/519 (94%)	-0.23	6 (1%)	76 68	21, 61, 107, 156	0
1	F	504/519 (97%)	-0.08	8 (1%)	70 61	21, 69, 115, 159	0
2	C	487/519 (93%)	-0.01	11 (2%)	61 51	34, 73, 124, 161	0
2	D	484/519 (93%)	-0.23	9 (1%)	66 57	27, 59, 110, 161	0
All	All	2958/3114 (94%)	-0.03	62 (2%)	63 54	21, 71, 122, 161	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	117	VAL	3.6
1	A	258	SER	3.5
1	A	517	PRO	3.3
1	A	509	VAL	3.3
1	F	508	ILE	3.2
2	D	121	PHE	3.1
1	F	121	PHE	2.9
1	E	249	LEU	2.9
1	A	117	VAL	2.9
2	C	249	LEU	2.9
2	C	17	ALA	2.8
1	A	506	SER	2.8
2	D	17	ALA	2.8
1	A	511	GLY	2.8
2	C	118	VAL	2.7
1	B	90	PHE	2.7
1	B	117	VAL	2.7
1	E	152	GLN	2.6
1	B	499	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	498	THR	2.5
1	B	338	MET	2.5
1	E	505	LEU	2.5
1	A	508	ILE	2.5
1	B	500	ASP	2.5
1	A	503	SER	2.5
1	F	509	VAL	2.5
2	C	423	HIS	2.5
1	B	498	THR	2.4
1	A	499	VAL	2.4
1	A	507	ARG	2.4
1	A	518	GLU	2.4
2	C	176	ALA	2.4
1	E	156	ALA	2.4
2	C	117	VAL	2.3
1	A	514	GLU	2.3
1	B	112	PRO	2.3
1	B	335	PHE	2.3
1	A	516	GLY	2.3
1	F	516	GLY	2.3
1	F	517	PRO	2.3
1	A	338	MET	2.3
1	B	118	VAL	2.3
1	F	247	PHE	2.2
1	B	123	LEU	2.2
1	E	153	GLN	2.2
2	C	431	SER	2.2
1	B	135	GLN	2.2
1	B	115	GLN	2.1
1	B	121	PHE	2.1
1	E	357	GLU	2.1
1	F	506	SER	2.1
2	D	249	LEU	2.1
2	D	357	GLU	2.1
2	D	321	ARG	2.1
2	D	338	MET	2.0
2	D	471	MET	2.0
2	C	123	LEU	2.0
2	C	92	TRP	2.0
2	C	15	HIS	2.0
2	C	499	VAL	2.0
2	D	118	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	156	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	D	432	11/12	0.80	0.22	3,9,61,64	0
1	SEP	F	431	10/11	0.80	0.27	4,80,83,83	0
1	SEP	E	431	10/11	0.81	0.23	4,57,60,61	0
1	TPO	F	432	11/12	0.83	0.23	3,10,75,76	0
1	SEP	B	431	10/11	0.85	0.24	4,82,87,88	0
2	TPO	C	432	11/12	0.87	0.21	3,10,78,79	0
1	SEP	A	431	10/11	0.88	0.23	4,79,81,84	0
1	TPO	E	432	11/12	0.88	0.17	3,10,59,61	0
1	TPO	A	432	11/12	0.90	0.20	3,19,82,83	0
1	TPO	B	432	11/12	0.90	0.21	3,19,83,84	0

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	MG	B	802	1/1	0.75	0.09	73,73,73,73	0
4	ATP	F	901	31/31	0.87	0.12	74,90,114,121	0
4	ATP	B	903	31/31	0.90	0.09	43,54,77,81	0
3	MG	E	805	1/1	0.90	0.11	19,19,19,19	0
4	ATP	A	901	31/31	0.91	0.10	75,89,103,112	0
4	ATP	A	903	31/31	0.92	0.09	42,54,76,81	0
3	MG	A	801	1/1	0.93	0.18	19,19,19,19	0

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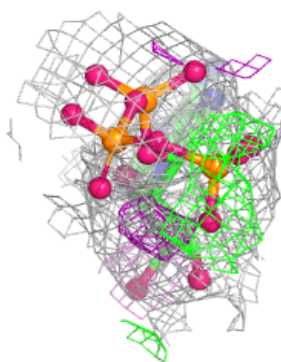
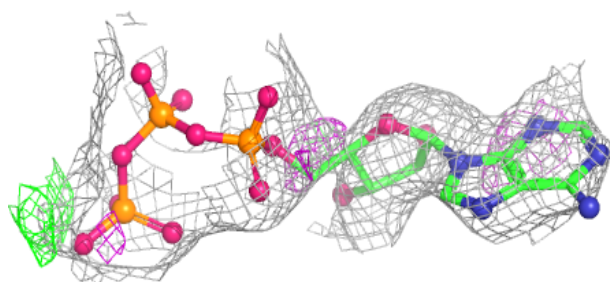
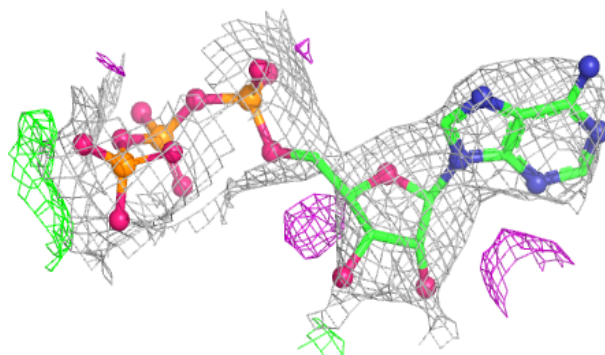
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	B	901	31/31	0.93	0.08	62,73,109,116	0
3	MG	C	803	1/1	0.94	0.08	19,19,19,19	0
4	ATP	C	903	31/31	0.94	0.08	43,54,77,81	0
4	ATP	D	901	31/31	0.94	0.09	53,66,89,104	0
4	ATP	D	903	31/31	0.94	0.10	42,54,77,81	0
4	ATP	E	901	31/31	0.94	0.08	61,77,101,113	0
4	ATP	E	903	31/31	0.94	0.11	42,54,77,80	0
3	MG	D	804	1/1	0.94	0.05	19,19,19,19	0
4	ATP	F	903	31/31	0.94	0.10	42,54,76,80	0
4	ATP	C	901	31/31	0.95	0.09	48,55,97,110	0
3	MG	F	806	1/1	0.96	0.16	19,19,19,19	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.

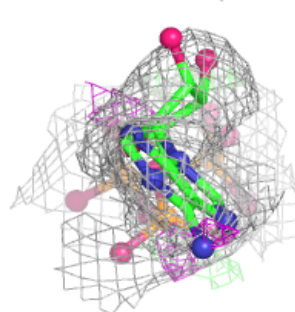
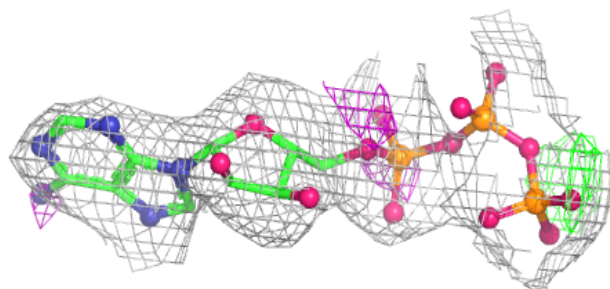
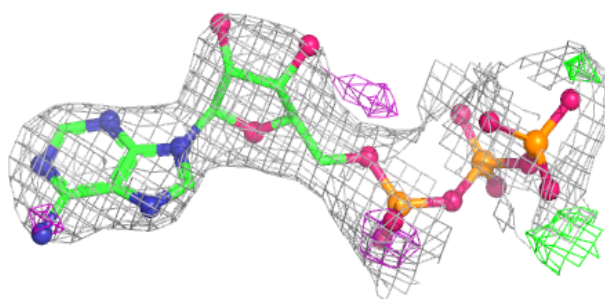
Electron density around ATP F 901:

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

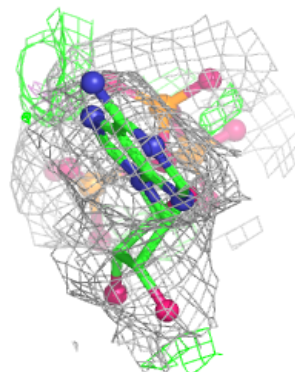
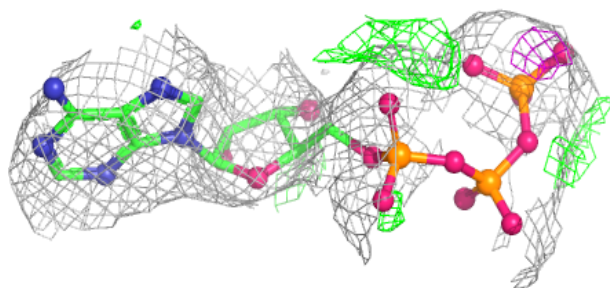
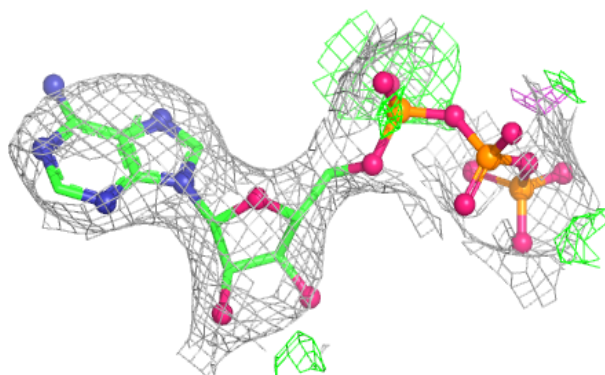


Electron density around ATP B 903:

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and green (positive)

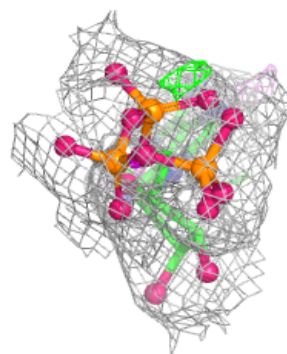
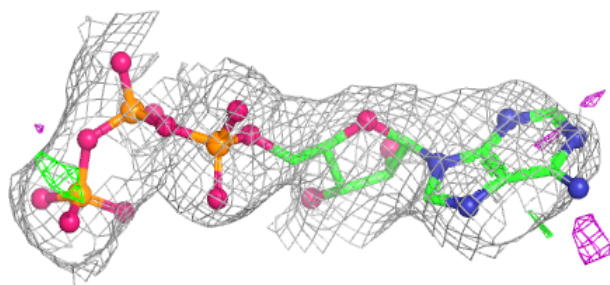
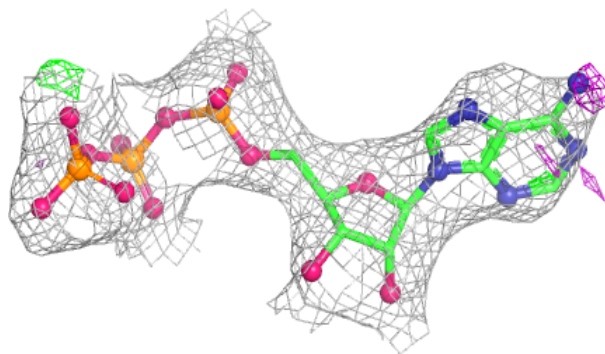
**Electron density around ATP A 901:**

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and green (positive)

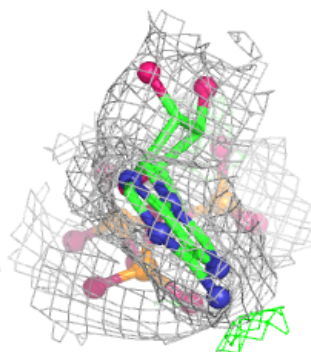
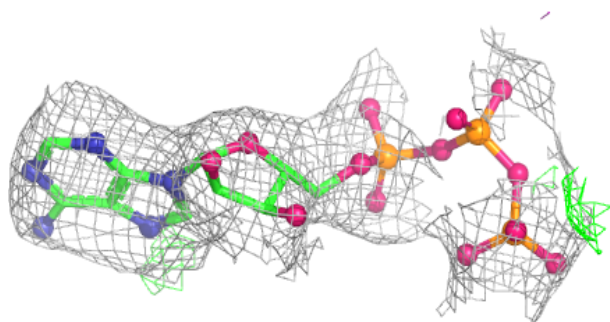
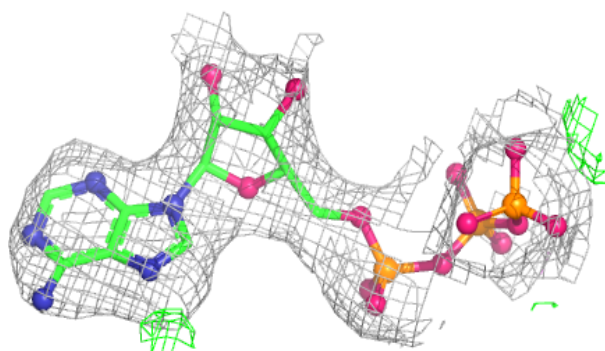


Electron density around ATP A 903:

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and green (positive)

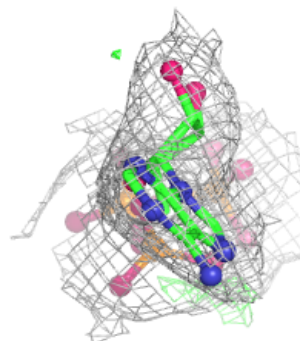
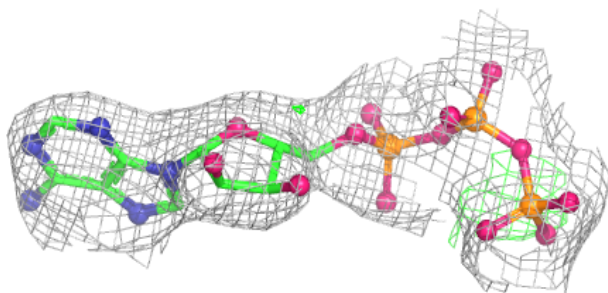
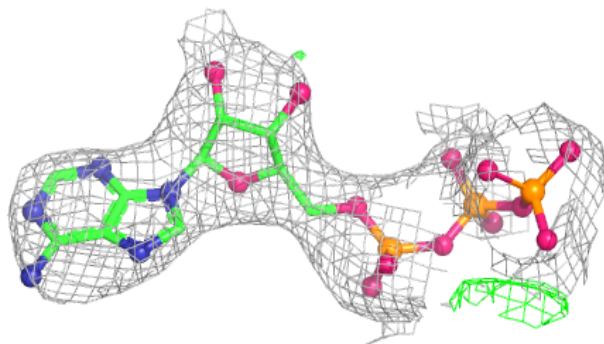
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and green (positive)

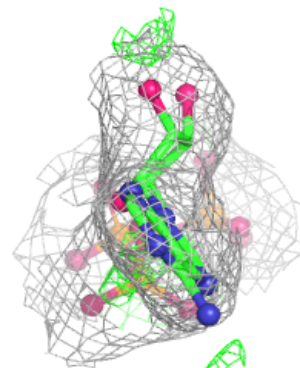
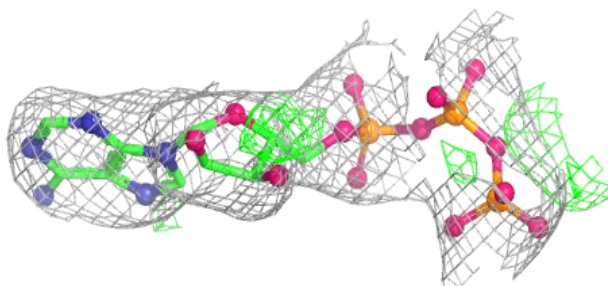
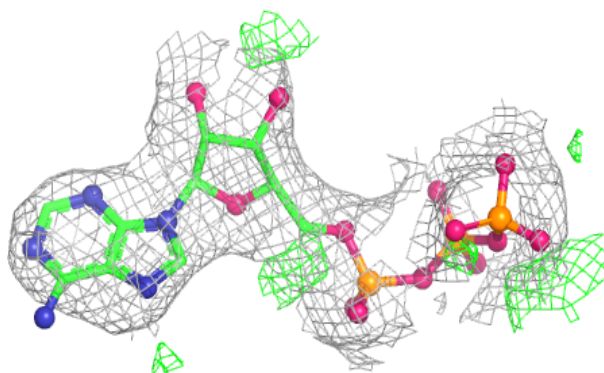


Electron density around ATP C 903:

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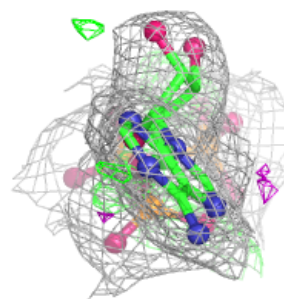
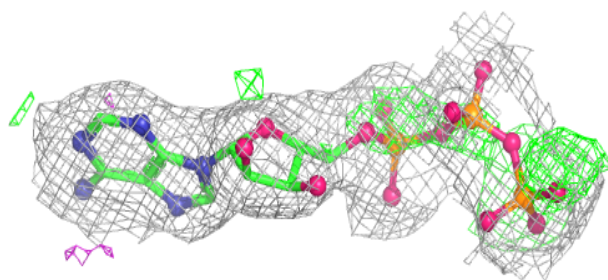
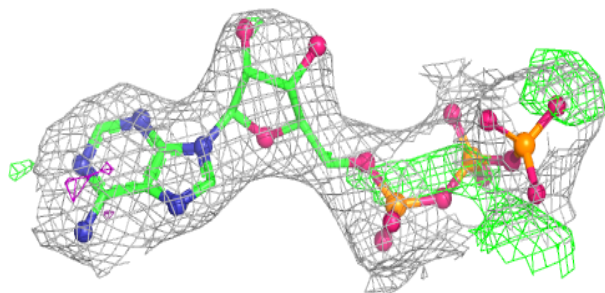
**Electron density around ATP D 901:**

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and green (positive)

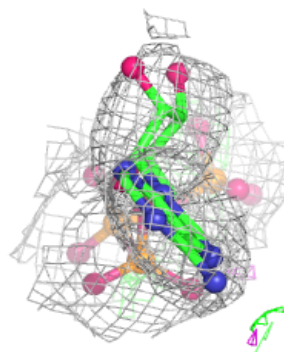
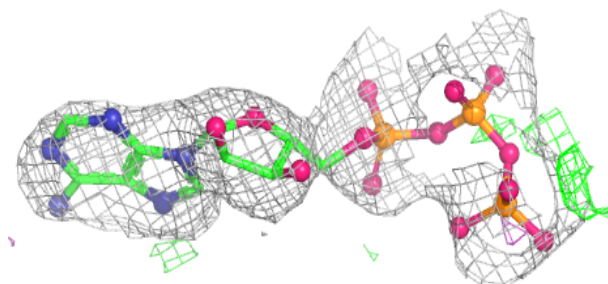
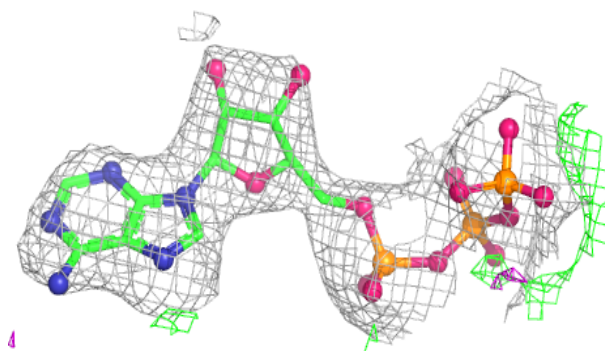


Electron density around ATP D 903:

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and green (positive)

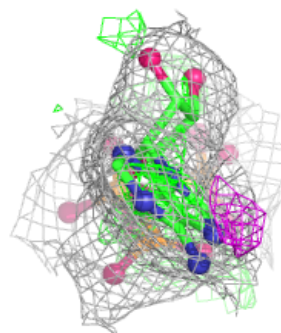
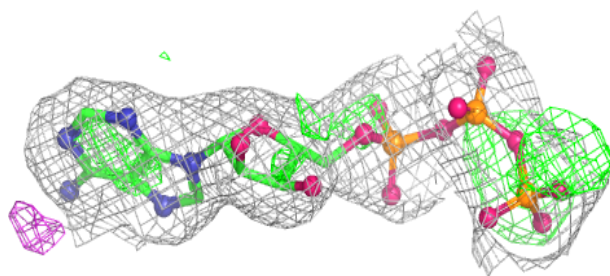
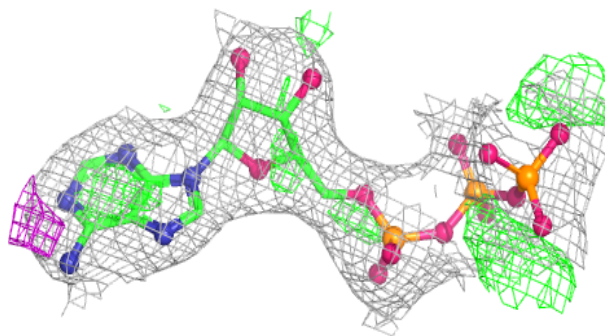
**Electron density around ATP E 901:**

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

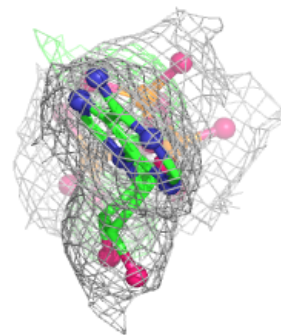
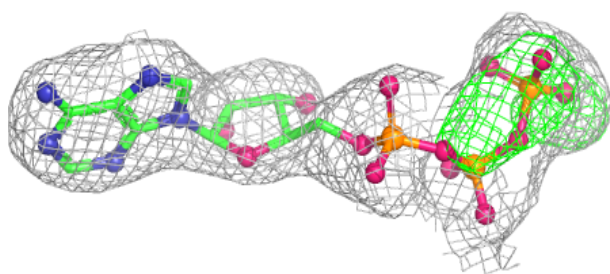
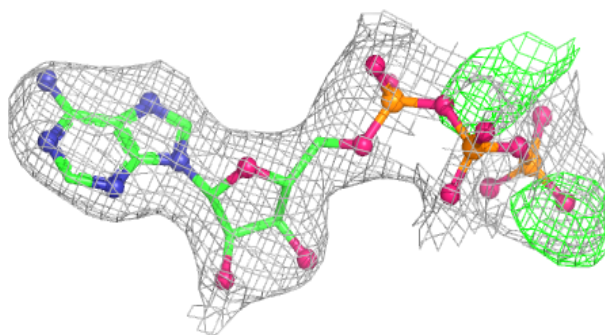


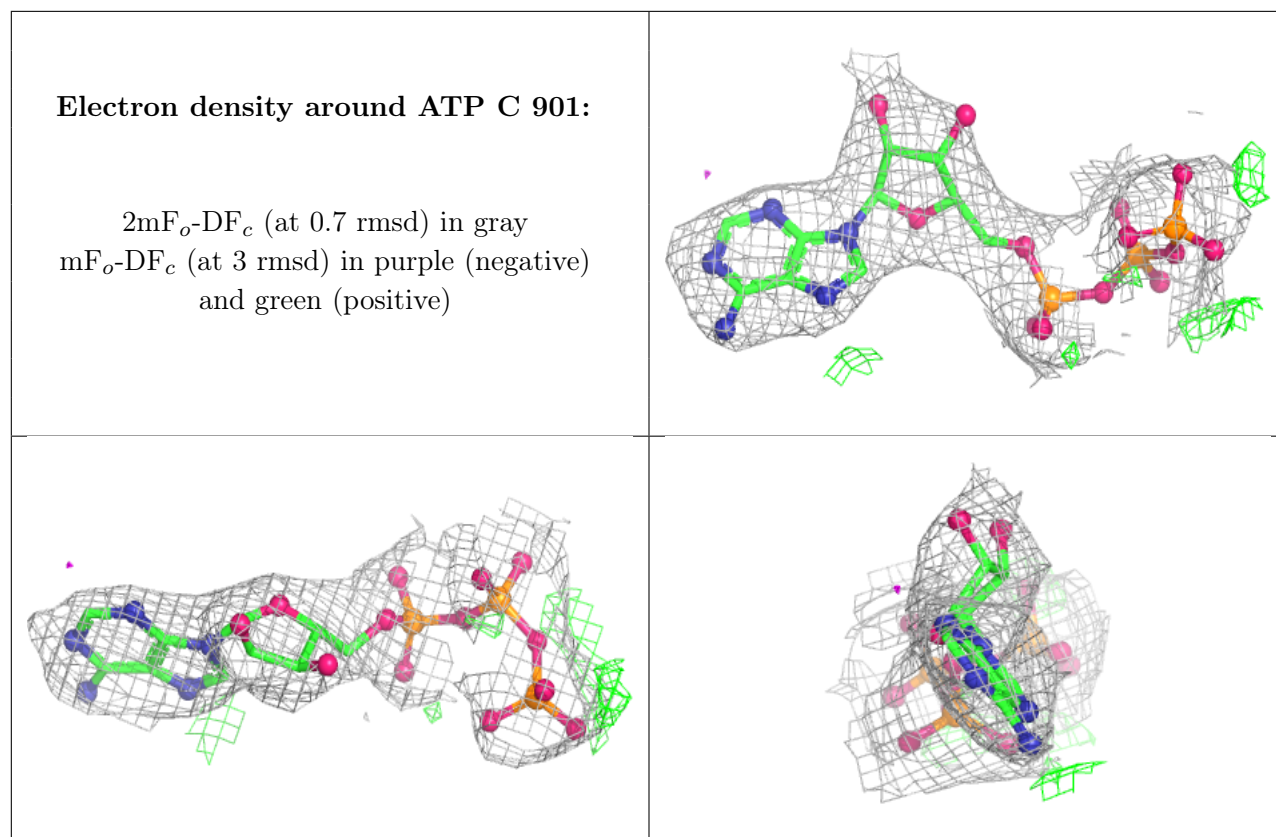
Electron density around ATP E 903:

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

**Electron density around ATP F 903:**

$2mF_o-DF_c$ (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.