



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:47 PM UTC

PDB ID : 3DVL / pdb_00003dvl
Title : Crystal Structure of Full Length Circadian Clock Protein KaiC with Correct Geometry at Phosphorylation Sites
Authors : Pattanayek, R.; Egli, M.
Deposited on : 2008-07-18
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:

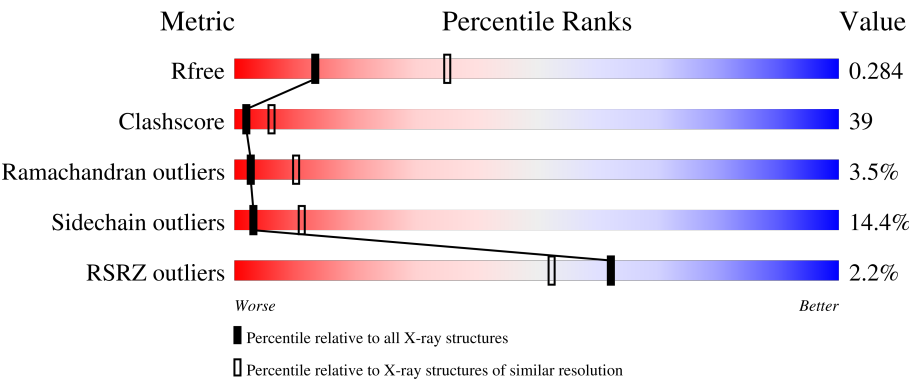
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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



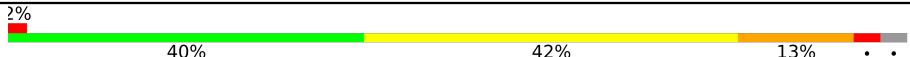
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 37%45%12%••
1	B	519	3% 40%41%13%•5%
1	C	519	2% 41%39%12%•6%
1	D	519	2% 42%39%10%•7%
1	E	519	• 42%36%15%•5%

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Mol	Chain	Length	Quality of chain
1	F	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	-
1	TPO	A	432	-	-	X	-
1	SEP	B	431	-	-	X	-
1	TPO	B	432	X	-	X	-
1	SEP	C	431	-	-	X	-
1	TPO	D	432	X	-	-	-
1	TPO	E	432	X	-	-	-
1	TPO	F	432	X	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23870 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.

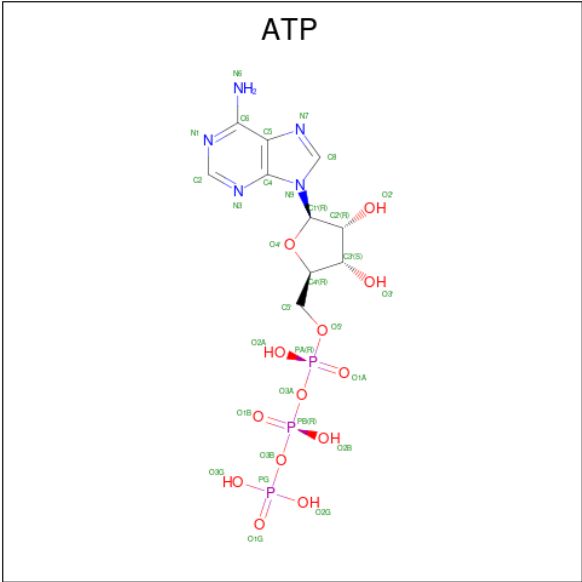
- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3993	2509	701	766	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	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
			3993	2509	701	766	2	15			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

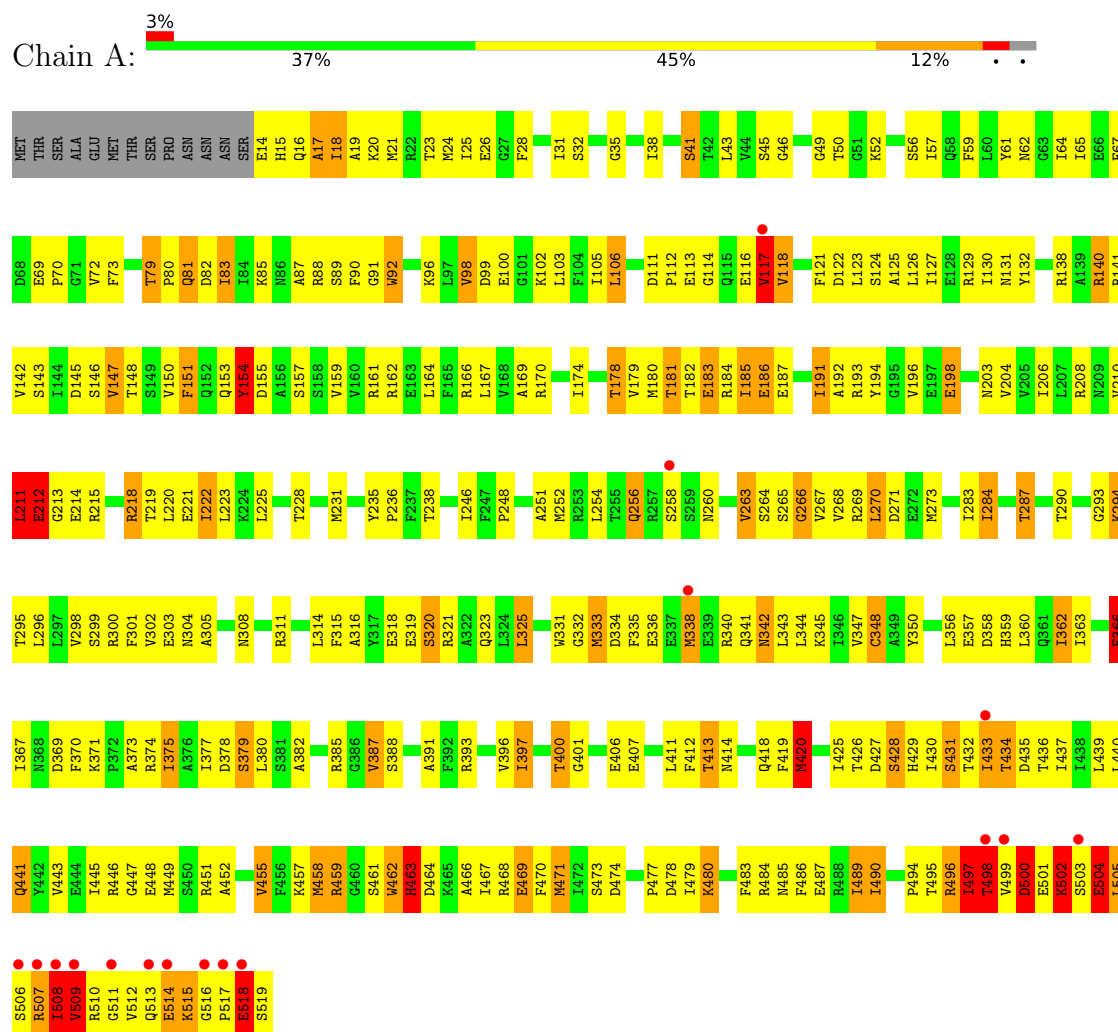
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	5	Total 5	O 5	0	0
4	C	7	Total 7	O 7	0	0
4	D	12	Total 12	O 12	0	0
4	E	10	Total 10	O 10	0	0
4	F	25	Total 25	O 25	0	0

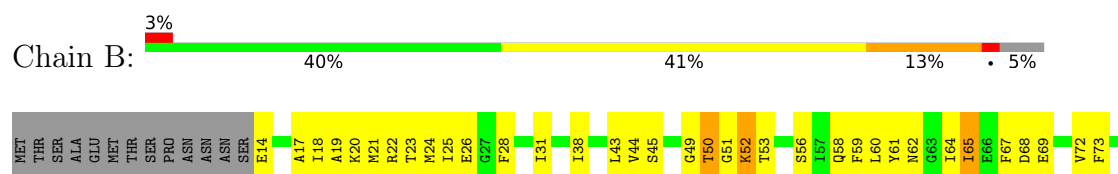
3 Residue-property plots [i](#)

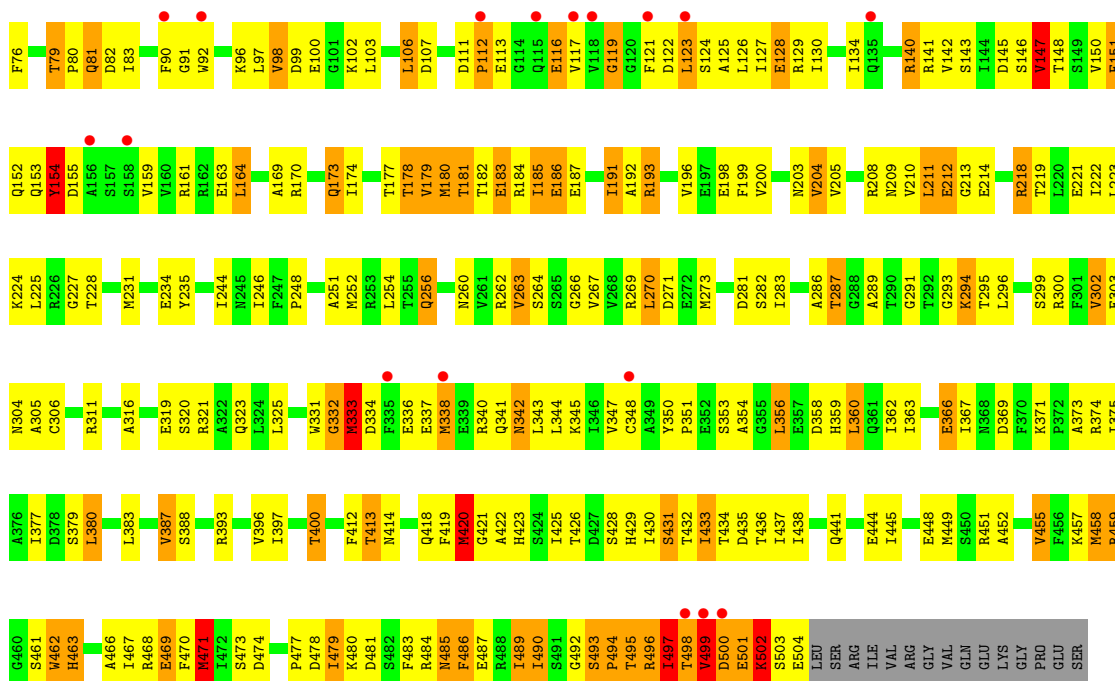
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

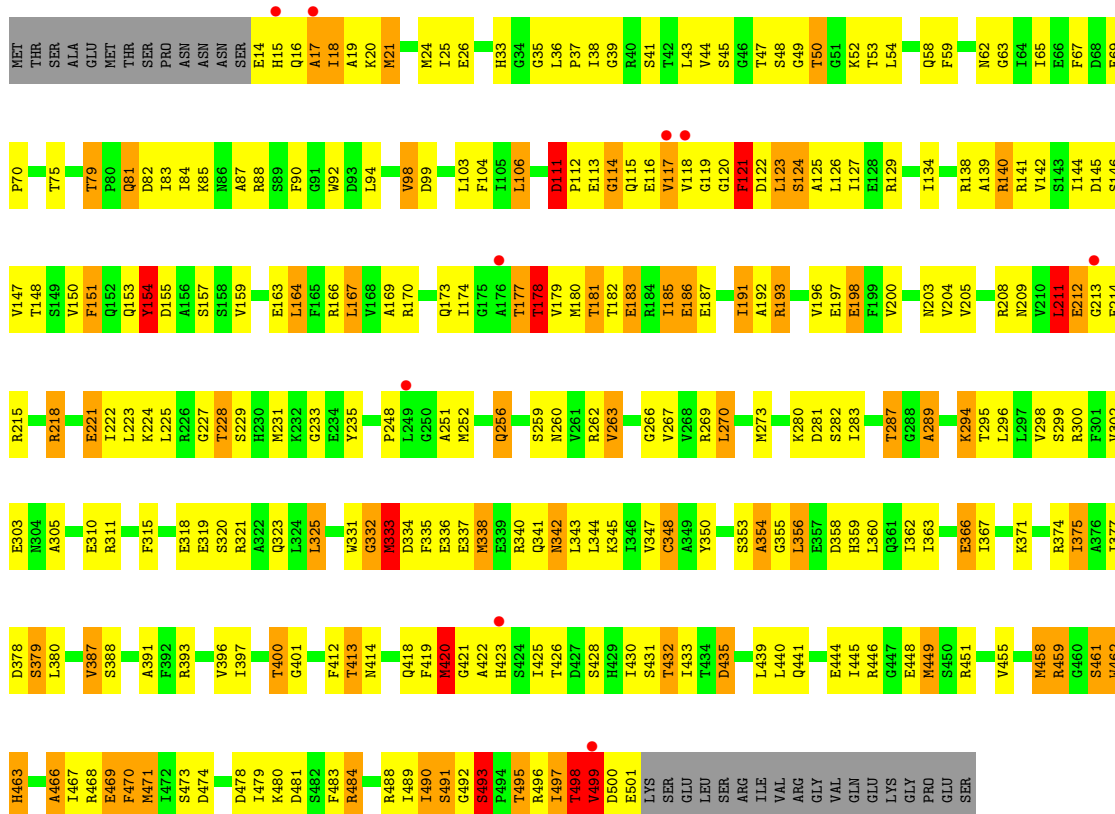


• Molecule 1: Circadian clock protein kinase kaiC

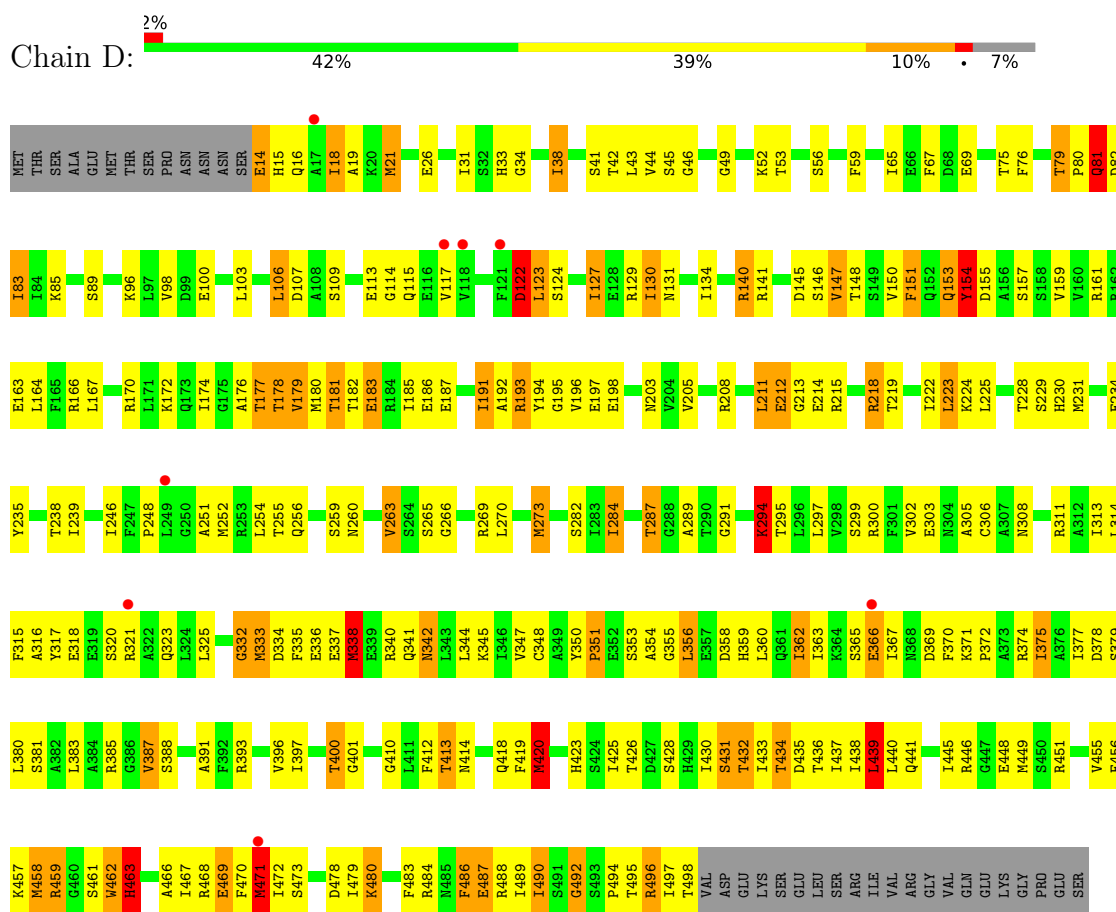




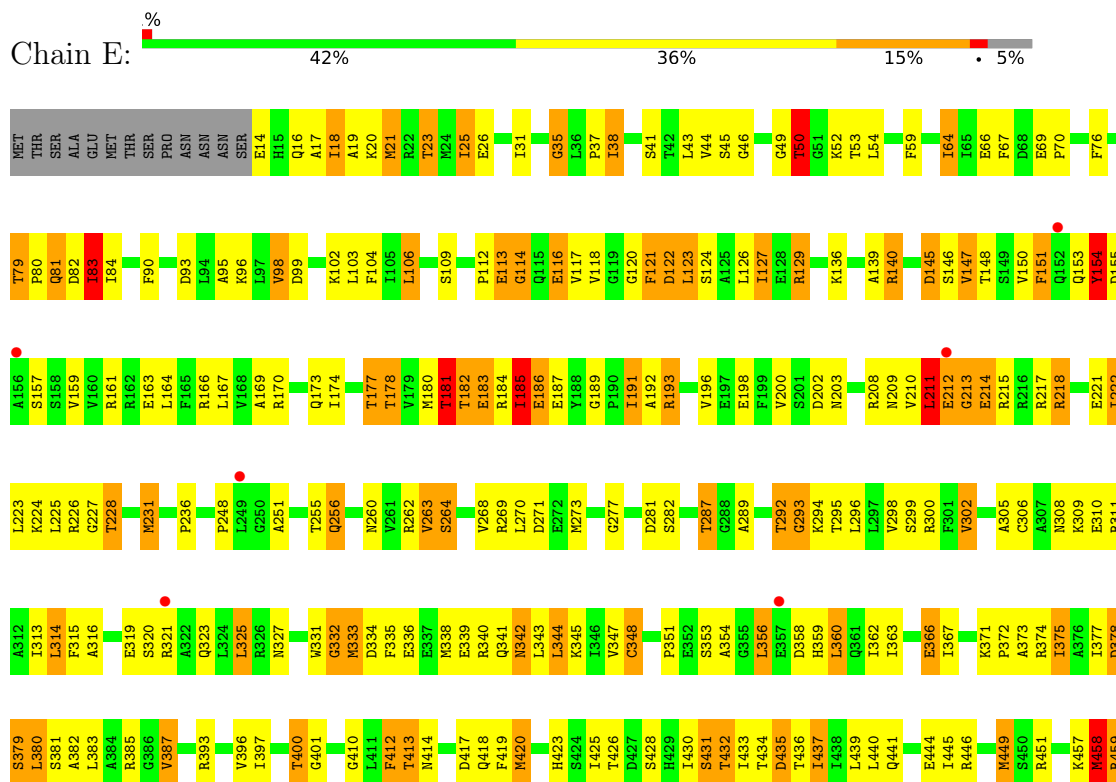
• Molecule 1: Circadian clock protein kinase kaiC



• Molecule 1: Circadian clock protein kinase kaiC

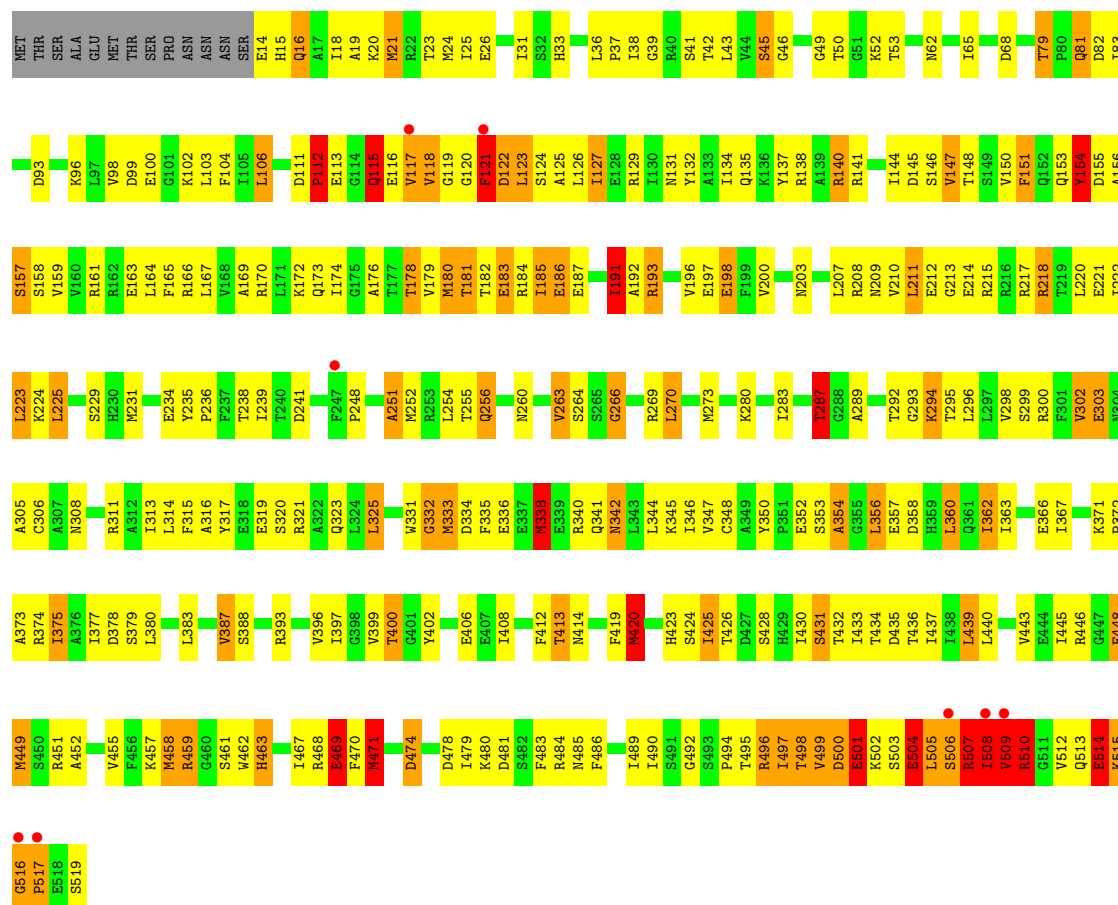


• Molecule 1: Circadian clock protein kinase kaiC





• Molecule 1: 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)	89.6 (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}	0.239 , 0.288 0.237 , 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 , 55.1	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	23870	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: TPO, ATP, SEP, 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	1.17	19/4037 (0.5%)	1.37	37/5437 (0.7%)
1	B	1.03	5/3921 (0.1%)	1.34	35/5282 (0.7%)
1	C	1.09	10/3897 (0.3%)	1.32	32/5251 (0.6%)
1	D	1.29	14/3873 (0.4%)	1.40	34/5218 (0.7%)
1	E	1.29	17/3929 (0.4%)	1.42	38/5293 (0.7%)
1	F	1.27	16/4037 (0.4%)	1.44	48/5437 (0.9%)
All	All	1.20	81/23694 (0.3%)	1.38	224/31918 (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	B	1	0
1	D	1	0
1	E	1	0
1	F	1	0
All	All	4	0

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	21	MET	SD-CE	-10.84	1.52	1.79
1	B	499	VAL	CA-CB	9.66	1.65	1.54
1	B	498	THR	CA-CB	9.03	1.68	1.53
1	B	471	MET	SD-CE	7.69	1.98	1.79
1	A	507	ARG	C-N	7.64	1.44	1.33
1	C	21	MET	SD-CE	-7.26	1.61	1.79
1	C	204	VAL	CA-CB	-6.88	1.45	1.54
1	D	53	THR	CA-C	6.87	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	ILE	CA-CB	6.82	1.62	1.54
1	E	21	MET	SD-CE	-6.81	1.62	1.79
1	C	499	VAL	CA-CB	6.74	1.63	1.54
1	A	517	PRO	CA-C	6.55	1.61	1.52
1	E	458	MET	SD-CE	-6.51	1.63	1.79
1	F	514	GLU	CA-C	6.51	1.60	1.52
1	F	516	GLY	CA-C	6.51	1.56	1.51
1	A	509	VAL	CA-CB	6.43	1.63	1.54
1	C	449	MET	SD-CE	-6.42	1.63	1.79
1	B	333	MET	SD-CE	-6.36	1.63	1.79
1	E	35	GLY	C-O	-6.36	1.17	1.24
1	D	246	ILE	CA-C	-6.32	1.45	1.52
1	A	204	VAL	CA-CB	6.29	1.62	1.54
1	A	507	ARG	CA-C	6.24	1.61	1.52
1	A	498	THR	CA-CB	6.14	1.63	1.53
1	D	56	SER	N-CA	-6.08	1.38	1.46
1	C	498	THR	CA-CB	6.08	1.63	1.53
1	F	41	SER	C-O	-6.07	1.16	1.23
1	A	455	VAL	CA-CB	6.06	1.61	1.53
1	C	87	ALA	CA-CB	-6.04	1.42	1.53
1	E	17	ALA	CA-CB	-6.01	1.43	1.53
1	D	462	TRP	N-CA	-6.01	1.38	1.46
1	F	15	HIS	CA-C	5.99	1.60	1.53
1	A	212	GLU	CA-C	5.98	1.60	1.52
1	C	420	MET	SD-CE	5.96	1.94	1.79
1	D	471	MET	CG-SD	5.90	1.95	1.80
1	D	238	THR	CA-C	-5.87	1.45	1.52
1	A	500	ASP	N-CA	5.86	1.53	1.46
1	A	518	GLU	CA-C	5.84	1.60	1.52
1	F	191	ILE	CA-CB	5.81	1.61	1.54
1	F	180	MET	CA-C	-5.79	1.45	1.52
1	E	231	MET	SD-CE	-5.78	1.65	1.79
1	E	53	THR	CB-OG1	5.71	1.52	1.43
1	E	23	THR	CA-C	-5.70	1.44	1.52
1	D	420	MET	SD-CE	5.69	1.93	1.79
1	F	41	SER	CA-C	-5.69	1.45	1.52
1	D	273	MET	SD-CE	-5.61	1.65	1.79
1	E	83	ILE	CA-CB	5.60	1.60	1.54
1	E	66	GLU	CA-C	-5.59	1.45	1.52
1	E	412	PHE	CA-C	-5.59	1.46	1.52
1	D	434	THR	CA-C	5.56	1.59	1.52
1	F	471	MET	SD-CE	5.54	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	LYS	CA-C	5.53	1.59	1.52
1	A	508	ILE	C-N	5.48	1.41	1.33
1	A	498	THR	CA-C	5.42	1.60	1.52
1	F	420	MET	SD-CE	5.42	1.93	1.79
1	E	471	MET	SD-CE	5.39	1.93	1.79
1	B	180	MET	SD-CE	5.39	1.93	1.79
1	D	81	GLN	CA-C	-5.37	1.45	1.52
1	C	455	VAL	CA-CB	-5.33	1.47	1.53
1	E	50	THR	CA-CB	5.32	1.62	1.53
1	A	92	TRP	NE1-CE2	-5.31	1.31	1.37
1	E	211	LEU	CA-C	-5.31	1.45	1.52
1	F	207	LEU	C-O	-5.30	1.17	1.24
1	D	21	MET	SD-CE	-5.28	1.66	1.79
1	F	225	LEU	CA-C	-5.26	1.47	1.53
1	D	338	MET	SD-CE	5.26	1.92	1.79
1	A	91	GLY	C-N	-5.25	1.26	1.33
1	F	36	LEU	C-O	-5.25	1.17	1.24
1	A	206	ILE	CA-CB	5.21	1.60	1.54
1	F	338	MET	SD-CE	5.18	1.92	1.79
1	E	449	MET	SD-CE	-5.16	1.66	1.79
1	C	466	ALA	CA-CB	-5.12	1.45	1.53
1	C	445	ILE	CA-CB	5.12	1.60	1.54
1	F	134	ILE	CA-CB	5.12	1.60	1.54
1	A	338	MET	SD-CE	5.11	1.92	1.79
1	A	46	GLY	C-N	-5.10	1.26	1.33
1	D	239	ILE	C-O	-5.07	1.18	1.24
1	F	135	GLN	CD-NE2	5.07	1.44	1.33
1	E	46	GLY	C-O	5.06	1.29	1.24
1	E	437	ILE	CA-CB	5.04	1.60	1.54
1	E	17	ALA	C-O	5.03	1.30	1.23
1	A	500	ASP	CA-C	5.01	1.59	1.52

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	LYS	N-CA-C	-14.01	96.23	114.31
1	E	129	ARG	N-CA-C	-11.85	98.39	111.07
1	A	459	ARG	N-CA-C	11.80	123.69	111.07
1	D	459	ARG	N-CA-C	11.76	124.10	111.28
1	E	214	GLU	N-CA-C	-11.74	94.81	112.54
1	E	459	ARG	N-CA-C	11.68	123.57	111.07
1	E	380	LEU	N-CA-C	-11.34	97.74	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLU	N-CA-C	10.98	126.78	110.52
1	D	380	LEU	N-CA-C	-10.97	99.40	111.36
1	F	380	LEU	N-CA-C	-10.71	99.57	111.14
1	B	380	LEU	N-CA-C	-10.71	99.69	111.36
1	A	512	VAL	N-CA-C	-10.29	98.23	111.09
1	C	380	LEU	N-CA-C	-10.23	100.21	111.36
1	F	459	ARG	N-CA-C	10.00	121.94	111.14
1	C	332	GLY	N-CA-C	-9.73	99.48	111.45
1	A	380	LEU	N-CA-C	-9.47	100.84	111.82
1	B	459	ARG	N-CA-C	9.41	121.30	111.14
1	D	16	GLN	N-CA-C	9.34	122.45	109.18
1	F	121	PHE	N-CA-C	-9.32	101.33	112.89
1	C	459	ARG	N-CA-C	9.19	121.06	111.14
1	F	122	ASP	N-CA-C	-9.00	100.89	112.23
1	A	114	GLY	N-CA-C	8.93	122.19	111.93
1	A	266	GLY	N-CA-C	-8.47	103.33	115.27
1	F	147	VAL	N-CA-C	-8.22	102.42	110.72
1	F	332	GLY	N-CA-C	-8.13	99.12	111.24
1	E	435	ASP	N-CA-C	7.96	119.73	111.14
1	F	373	ALA	N-CA-C	-7.91	104.15	113.88
1	B	497	ILE	N-CA-C	7.83	118.63	110.72
1	F	498	THR	N-CA-C	7.83	124.07	107.70
1	F	513	GLN	N-CA-C	7.77	121.57	110.14
1	D	155	ASP	N-CA-C	7.74	121.65	109.81
1	E	332	GLY	N-CA-C	-7.63	99.87	111.24
1	F	115	GLN	O-C-N	7.50	127.10	121.47
1	D	193	ARG	N-CA-C	7.49	123.74	111.37
1	E	155	ASP	N-CA-C	7.45	121.10	110.14
1	B	489	ILE	CB-CA-C	-7.41	102.55	111.81
1	A	497	ILE	N-CA-C	7.36	124.64	109.34
1	C	493	SER	CA-C-N	7.34	127.26	120.21
1	C	493	SER	C-N-CA	7.34	127.26	120.21
1	F	210	VAL	N-CA-C	7.28	119.11	109.21
1	B	266	GLY	N-CA-C	-7.23	105.08	115.27
1	F	235	TYR	CA-C-N	7.17	126.93	119.76
1	F	235	TYR	C-N-CA	7.17	126.93	119.76
1	A	194	TYR	N-CA-C	7.11	121.79	113.18
1	E	147	VAL	N-CA-C	-7.09	102.22	111.09
1	F	514	GLU	N-CA-C	7.08	122.10	112.68
1	F	474	ASP	N-CA-C	-7.07	103.32	112.23
1	E	178	THR	N-CA-C	7.04	121.14	109.95
1	D	147	VAL	N-CA-C	-6.91	103.74	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	ARG	N-CA-C	6.90	122.69	111.37
1	A	516	GLY	N-CA-C	-6.89	98.29	112.34
1	F	155	ASP	N-CA-C	6.89	120.73	109.85
1	F	509	VAL	N-CA-C	6.87	123.63	109.34
1	B	152	GLN	N-CA-C	-6.85	103.89	113.20
1	B	155	ASP	N-CA-C	6.84	120.28	109.81
1	F	115	GLN	CB-CA-C	-6.84	107.22	117.07
1	B	455	VAL	N-CA-C	-6.80	96.54	106.88
1	A	507	ARG	N-CA-C	-6.77	104.03	112.90
1	D	178	THR	N-CA-C	6.77	120.72	109.95
1	D	480	LYS	N-CA-C	6.77	114.33	108.78
1	C	266	GLY	N-CA-C	-6.63	106.30	114.92
1	C	178	THR	N-CA-C	6.62	120.25	109.59
1	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	E	64	ILE	N-CA-C	6.60	116.73	110.53
1	A	193	ARG	N-CA-C	6.59	122.17	111.37
1	B	500	ASP	N-CA-C	-6.58	100.50	110.70
1	C	155	ASP	N-CA-C	6.56	120.22	109.85
1	A	210	VAL	N-CA-C	6.55	117.53	108.89
1	C	481	ASP	N-CA-C	6.39	119.92	110.46
1	E	210	VAL	N-CA-C	6.37	117.26	109.30
1	A	508	ILE	CA-C-N	6.37	133.43	121.97
1	A	508	ILE	C-N-CA	6.37	133.43	121.97
1	B	178	THR	N-CA-C	6.36	120.00	110.14
1	D	492	GLY	N-CA-C	-6.34	106.00	114.25
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
1	C	111	ASP	CA-C-N	6.30	127.71	119.84
1	C	111	ASP	C-N-CA	6.30	127.71	119.84
1	B	244	ILE	N-CA-C	6.28	117.13	108.84
1	A	155	ASP	N-CA-C	6.28	119.37	110.14
1	F	266	GLY	N-CA-C	-6.27	106.67	115.32
1	B	497	ILE	CB-CA-C	-6.26	103.58	112.22
1	E	373	ALA	N-CA-C	-6.26	105.80	113.50
1	E	114	GLY	N-CA-C	6.25	128.00	113.18
1	B	147	VAL	N-CA-C	-6.24	103.25	111.05
1	F	193	ARG	N-CA-C	6.24	121.60	111.37
1	E	167	LEU	N-CA-C	6.22	117.73	111.07
1	F	439	LEU	N-CA-C	6.20	118.63	108.52
1	B	493	SER	CA-C-N	6.18	127.57	119.84
1	B	493	SER	C-N-CA	6.18	127.57	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	124	SER	N-CA-C	-6.18	105.39	113.12
1	D	235	TYR	O-C-N	6.17	127.30	121.38
1	D	463	HIS	N-CA-C	6.14	123.89	110.80
1	A	391	ALA	N-CA-C	-6.11	104.70	111.36
1	F	499	VAL	N-CA-C	-6.08	103.53	112.04
1	E	136	LYS	N-CA-C	6.05	118.37	111.11
1	B	193	ARG	N-CA-C	6.04	121.34	111.37
1	D	266	GLY	N-CA-C	-6.03	106.77	115.27
1	E	474	ASP	N-CA-C	-6.03	105.76	113.23
1	B	210	VAL	N-CA-C	6.01	116.81	109.30
1	E	504	GLU	CB-CA-C	-5.99	108.66	115.79
1	C	470	PHE	N-CA-C	5.97	118.36	108.99
1	F	516	GLY	N-CA-C	5.96	122.36	115.09
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	B	495	THR	N-CA-C	-5.90	98.20	107.93
1	B	98	VAL	N-CA-C	-5.89	105.00	110.53
1	D	410	GLY	N-CA-C	5.88	119.71	110.71
1	A	98	VAL	N-CA-C	-5.87	104.80	110.72
1	F	280	LYS	N-CA-C	-5.85	104.81	111.07
1	B	332	GLY	N-CA-C	-5.83	99.36	113.18
1	D	332	GLY	N-CA-C	-5.81	99.41	113.18
1	C	204	VAL	N-CA-C	5.80	116.36	107.77
1	E	222	ILE	N-CA-C	-5.79	98.70	107.73
1	C	355	GLY	N-CA-C	-5.76	101.57	112.51
1	C	235	TYR	O-C-N	5.73	128.56	121.79
1	E	503	SER	N-CA-C	5.70	117.93	108.13
1	E	463	HIS	N-CA-C	5.67	122.88	110.80
1	B	28	PHE	N-CA-C	5.64	117.43	111.28
1	E	310	GLU	N-CA-C	-5.64	100.94	109.85
1	F	469	GLU	N-CA-C	-5.64	101.36	110.32
1	D	284	ILE	CB-CA-C	-5.61	103.20	110.84
1	B	65	ILE	N-CA-C	5.61	119.88	112.76
1	F	127	ILE	N-CA-C	-5.61	104.40	110.23
1	A	258	SER	N-CA-C	5.59	117.97	108.02
1	F	115	GLN	CA-C-O	5.58	121.18	117.94
1	B	173	GLN	N-CA-C	-5.57	104.84	111.03
1	C	474	ASP	N-CA-C	-5.56	105.22	112.23
1	D	235	TYR	CA-C-N	-5.56	114.23	119.85
1	D	235	TYR	C-N-CA	-5.56	114.23	119.85
1	F	18	ILE	N-CA-C	5.52	115.84	108.11
1	A	474	ASP	N-CA-C	-5.52	105.41	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ARG	N-CA-C	5.52	122.56	110.80
1	C	435	ASP	N-CA-C	5.50	118.11	111.40
1	E	410	GLY	N-CA-C	5.50	119.12	110.71
1	D	439	LEU	N-CA-C	5.50	117.37	108.41
1	A	362	ILE	CB-CA-C	-5.47	103.67	112.16
1	A	441	GLN	N-CA-C	5.47	118.10	108.75
1	C	222	ILE	N-CA-C	-5.44	99.91	108.23
1	D	176	ALA	N-CA-C	5.43	118.78	110.20
1	B	479	ILE	N-CA-C	5.43	116.20	107.73
1	A	366	GLU	CA-CB-CG	-5.42	103.25	114.10
1	C	167	LEU	N-CA-C	5.42	116.87	111.07
1	C	490	ILE	N-CA-C	-5.42	103.69	111.17
1	B	481	ASP	N-CA-C	5.41	118.47	110.46
1	C	98	VAL	N-CA-C	-5.39	105.27	110.72
1	D	282	SER	N-CA-C	5.38	116.70	108.42
1	D	456	PHE	N-CA-C	5.37	116.82	111.07
1	D	294	LYS	N-CA-C	-5.36	105.34	111.07
1	A	23	THR	N-CA-C	-5.35	106.92	113.50
1	F	198	GLU	CB-CA-C	-5.35	101.58	110.68
1	C	484	ARG	N-CA-C	5.34	117.10	111.28
1	D	362	ILE	CB-CA-C	-5.34	105.05	112.04
1	F	294	LYS	N-CA-C	-5.34	105.46	111.28
1	F	402	TYR	N-CA-C	-5.33	105.16	110.97
1	B	496	ARG	N-CA-C	-5.33	101.78	110.20
1	E	185	ILE	CB-CA-C	-5.33	104.87	110.62
1	F	215	ARG	CA-C-N	-5.32	114.96	122.94
1	F	215	ARG	C-N-CA	-5.32	114.96	122.94
1	D	486	PHE	N-CA-C	5.32	117.91	109.50
1	A	159	VAL	N-CA-C	-5.29	105.37	110.72
1	B	116	GLU	N-CA-C	5.29	115.22	108.24
1	E	298	VAL	CB-CA-C	-5.29	105.20	111.97
1	C	118	VAL	N-CA-C	-5.28	106.72	113.22
1	C	123	LEU	CB-CA-C	-5.26	110.07	117.23
1	D	365	SER	CA-C-N	-5.26	111.93	120.72
1	D	365	SER	C-N-CA	-5.26	111.93	120.72
1	B	486	PHE	N-CA-C	5.26	117.81	109.50
1	C	198	GLU	CB-CA-C	-5.26	101.74	110.68
1	B	373	ALA	N-CA-C	-5.26	107.24	113.97
1	D	459	ARG	CA-C-N	-5.26	111.11	121.41
1	D	459	ARG	C-N-CA	-5.26	111.11	121.41
1	A	147	VAL	N-CA-C	-5.25	104.53	111.09
1	E	98	VAL	O-C-N	5.25	127.06	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	THR	N-CA-C	-5.25	103.21	110.35
1	F	241	ASP	N-CA-C	-5.24	106.84	113.18
1	C	84	ILE	N-CA-C	5.24	115.96	110.62
1	E	264	SER	N-CA-C	5.23	118.64	110.32
1	D	265	SER	N-CA-C	-5.22	106.91	113.28
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	F	16	GLN	N-CA-C	-5.22	99.09	108.48
1	E	38	ILE	N-CA-C	5.21	116.40	109.37
1	D	153	GLN	N-CA-C	-5.21	107.47	113.88
1	E	378	ASP	CA-C-N	5.20	131.46	121.54
1	E	378	ASP	C-N-CA	5.20	131.46	121.54
1	F	481	ASP	N-CA-C	5.19	117.77	110.14
1	E	18	ILE	CB-CA-C	-5.19	102.78	111.29
1	A	308	ASN	N-CA-C	-5.18	105.68	112.41
1	F	176	ALA	N-CA-C	5.18	118.38	110.20
1	D	355	GLY	N-CA-C	-5.17	102.68	112.51
1	F	448	GLU	N-CA-C	5.17	117.67	109.50
1	C	280	LYS	N-CA-C	-5.17	105.54	111.07
1	C	221	GLU	CA-C-N	-5.16	115.92	122.37
1	C	221	GLU	C-N-CA	-5.16	115.92	122.37
1	F	178	THR	N-CA-C	5.16	118.16	109.95
1	B	502	LYS	CA-C-N	5.16	129.51	122.34
1	B	502	LYS	C-N-CA	5.16	129.51	122.34
1	F	287	THR	CB-CA-C	-5.16	98.60	109.38
1	B	437	ILE	N-CA-C	5.15	114.99	107.37
1	F	510	ARG	N-CA-C	5.13	121.74	110.80
1	C	310	GLU	N-CA-C	-5.13	102.60	110.14
1	E	44	VAL	CA-C-N	-5.13	114.53	122.59
1	E	44	VAL	C-N-CA	-5.13	114.53	122.59
1	B	306	CYS	N-CA-C	-5.13	107.15	113.41
1	E	25	ILE	CB-CA-C	-5.13	102.88	111.29
1	A	198	GLU	CB-CA-C	-5.12	102.62	110.81
1	C	227	GLY	N-CA-C	5.11	120.89	114.25
1	A	25	ILE	N-CA-C	-5.11	100.98	108.54
1	E	486	PHE	N-CA-C	5.10	117.89	109.72
1	F	25	ILE	N-CA-C	-5.06	102.21	108.89
1	A	463	HIS	N-CA-C	5.04	121.54	110.80
1	E	145	ASP	N-CA-C	5.04	116.53	108.41
1	F	157	SER	N-CA-C	5.04	121.53	110.80
1	E	484	ARG	N-CA-C	5.04	117.42	111.33
1	D	34	GLY	N-CA-C	5.03	118.96	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	GLY	N-CA-C	5.03	122.06	115.47
1	F	362	ILE	CB-CA-C	-5.02	105.36	112.14
1	F	251	ALA	N-CA-C	-5.02	106.84	113.17
1	E	181	THR	N-CA-CB	-5.02	102.61	110.69
1	F	112	PRO	CA-C-N	5.00	129.24	121.83
1	F	112	PRO	C-N-CA	5.00	129.24	121.83
1	B	204	VAL	N-CA-C	5.00	115.32	108.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	432	TPO	CB
1	D	432	TPO	CB
1	E	432	TPO	CB
1	F	432	TPO	CB

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3993	0	3984	344	0
1	B	3878	0	3862	324	0
1	C	3850	0	3836	303	0
1	D	3826	0	3818	307	0
1	E	3886	0	3872	319	0
1	F	3993	0	3983	340	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	62	0	24	12	0
3	B	62	0	24	9	0
3	C	62	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	62	0	23	6	0
3	E	62	0	24	7	0
3	F	62	0	24	7	0
4	A	7	0	0	0	0
4	B	5	0	0	2	0
4	C	7	0	0	3	0
4	D	12	0	0	2	0
4	E	10	0	0	0	0
4	F	25	0	0	6	0
All	All	23870	0	23498	1831	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 39.

All (1831) 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:F:115:GLN:CG	1:F:116:GLU:H	1.13	1.44
1:B:431:SEP:O	1:B:434:THR:HG22	1.38	1.19
1:D:431:SEP:O	1:D:432:TPO:HB	1.40	1.18
1:F:115:GLN:HG2	1:F:116:GLU:N	1.27	1.14
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.13
1:A:14:GLU:HG3	1:A:15:HIS:H	1.08	1.11
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.31	1.09
1:F:115:GLN:HG3	1:F:116:GLU:H	1.08	1.08
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.16	1.08
1:F:431:SEP:O	1:F:434:THR:HG22	1.54	1.07
1:D:146:SER:H	1:D:181:THR:HG22	1.21	1.04
1:E:146:SER:H	1:E:181:THR:HG22	1.22	1.04
1:A:79:THR:CG2	1:A:81:GLN:HG2	1.87	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	1.93	1.01
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.42	1.01
1:C:123:LEU:HD12	1:C:163:GLU:OE2	1.61	0.99
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.29	0.98
1:E:505:LEU:HG	1:E:505:LEU:O	1.60	0.98
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.46	0.98
1:F:146:SER:H	1:F:181:THR:HG22	1.25	0.97
1:D:446:ARG:N	1:D:496:ARG:HH12	1.60	0.97
1:B:79:THR:HG22	1:B:82:ASP:H	1.29	0.97
1:D:79:THR:HG22	1:D:82:ASP:H	1.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ARG:HH22	1:C:461:SER:HB2	1.32	0.95
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.46	0.95
1:E:501:GLU:O	1:E:502:LYS:HG3	1.67	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	0.95
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.32	0.94
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.48	0.94
1:E:431:SEP:O	1:E:434:THR:HG22	1.69	0.93
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.49	0.93
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.50	0.93
1:D:371:LYS:O	1:D:371:LYS:HD3	1.69	0.93
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.34	0.92
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.00	0.91
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.71	0.90
1:F:115:GLN:CG	1:F:116:GLU:N	1.87	0.90
1:B:379:SER:HA	1:B:413:THR:HG22	1.53	0.90
1:E:123:LEU:HD22	1:E:166:ARG:HD2	1.54	0.89
1:C:140:ARG:HB3	1:C:140:ARG:HH11	1.36	0.89
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.53	0.88
1:D:231:MET:HE1	1:D:251:ALA:HB2	1.53	0.88
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.88	0.87
1:C:123:LEU:HD13	1:C:166:ARG:HD2	1.55	0.87
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.85	0.87
1:C:287:THR:CG2	1:C:414:ASN:HD22	1.87	0.87
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.40	0.87
1:D:147:VAL:HG11	1:D:180:MET:HE3	1.58	0.86
1:A:14:GLU:CG	1:A:15:HIS:H	1.84	0.86
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.54	0.86
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.56	0.86
1:F:45:SER:HB2	1:F:182:THR:HB	1.58	0.86
1:C:146:SER:H	1:C:181:THR:HG22	1.41	0.86
1:D:123:LEU:HD12	1:D:166:ARG:HD2	1.57	0.86
1:A:318:GLU:OE2	1:B:432:TPO:HG21	1.76	0.85
1:F:426:THR:HG22	1:F:428:SER:H	1.38	0.85
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.41	0.85
1:B:471:MET:HE1	1:B:473:SER:OG	1.76	0.85
1:E:147:VAL:HG11	1:E:180:MET:HE3	1.58	0.85
1:F:191:ILE:HB	1:F:198:GLU:CG	2.07	0.85
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.40	0.85
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.58	0.85
1:B:140:ARG:HH11	1:B:140:ARG:CB	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:O	1:B:150:VAL:HG12	1.76	0.85
1:D:147:VAL:HG11	1:D:180:MET:CE	2.07	0.85
1:D:182:THR:HG21	1:D:192:ALA:HB1	1.59	0.85
1:D:191:ILE:HB	1:D:198:GLU:CG	2.07	0.85
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.59	0.84
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.89	0.84
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.57	0.84
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.07	0.84
1:D:106:LEU:C	1:D:106:LEU:HD12	2.01	0.84
1:D:287:THR:CG2	1:D:414:ASN:HD22	1.89	0.84
1:F:509:VAL:O	1:F:512:VAL:HG23	1.76	0.84
1:C:52:LYS:HE3	3:C:903:ATP:O1B	1.78	0.84
1:C:347:VAL:O	1:C:348:CYS:HB2	1.77	0.84
1:A:433:ILE:HG22	1:A:433:ILE:O	1.77	0.83
1:F:145:ASP:OD2	1:F:181:THR:HG21	1.78	0.83
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.61	0.83
1:E:146:SER:N	1:E:181:THR:HG22	1.92	0.83
1:E:432:TPO:OG1	1:E:433:ILE:HD12	1.78	0.83
1:B:191:ILE:HB	1:B:198:GLU:CD	2.04	0.83
1:A:498:THR:HB	1:A:501:GLU:HG3	1.59	0.83
1:E:505:LEU:O	1:E:505:LEU:CG	2.27	0.83
1:F:504:GLU:HB3	1:F:507:ARG:NH2	1.92	0.83
1:D:446:ARG:H	1:D:496:ARG:HH12	1.20	0.82
1:A:14:GLU:HG3	1:A:15:HIS:N	1.91	0.82
1:E:287:THR:CG2	1:E:414:ASN:HD22	1.92	0.82
1:D:344:LEU:HD13	1:D:344:LEU:C	2.04	0.82
1:C:147:VAL:O	1:C:150:VAL:HG12	1.79	0.82
1:A:147:VAL:O	1:A:150:VAL:HG12	1.80	0.82
1:A:379:SER:HA	1:A:413:THR:HG22	1.60	0.82
1:B:191:ILE:HB	1:B:198:GLU:CG	2.10	0.81
1:D:146:SER:N	1:D:181:THR:HG22	1.95	0.81
1:F:515:LYS:HG3	1:F:516:GLY:N	1.95	0.81
1:F:231:MET:HE1	1:F:251:ALA:HB2	1.61	0.81
1:A:79:THR:HG22	1:A:82:ASP:H	1.44	0.81
1:C:262:ARG:NH2	1:C:461:SER:HB2	1.94	0.81
1:E:433:ILE:O	1:E:433:ILE:HG22	1.80	0.80
1:A:252:MET:HE3	1:F:350:TYR:CE1	2.15	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:79:THR:HG21	1:A:81:GLN:HG2	1.62	0.80
1:C:67:PHE:HB2	1:C:69:GLU:HG3	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PHE:C	1:C:153:GLN:H	1.90	0.80
1:D:79:THR:O	1:D:83:ILE:HD12	1.82	0.80
1:F:191:ILE:HB	1:F:198:GLU:CD	2.06	0.80
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.47	0.80
1:B:377:ILE:HD12	1:B:412:PHE:CE2	2.17	0.80
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.64	0.80
1:C:495:THR:HA	1:D:487:GLU:OE2	1.81	0.80
1:D:315:PHE:CZ	1:D:363:ILE:HG23	2.16	0.79
1:E:79:THR:HG22	1:E:82:ASP:H	1.47	0.79
1:E:426:THR:HG22	1:E:428:SER:H	1.47	0.79
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.95	0.79
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.17	0.79
1:A:87:ALA:O	1:A:92:TRP:CD1	2.36	0.79
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.47	0.79
1:D:446:ARG:H	1:D:496:ARG:NH1	1.80	0.79
1:E:147:VAL:O	1:E:150:VAL:HG12	1.82	0.79
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.81	0.79
1:F:502:LYS:NZ	1:F:507:ARG:HB3	1.98	0.79
1:D:311:ARG:HD2	1:D:371:LYS:HD2	1.63	0.78
1:B:471:MET:HB3	1:B:480:LYS:NZ	1.98	0.78
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.65	0.78
1:B:441:GLN:NE2	1:B:490:ILE:HD13	1.98	0.78
1:E:485:ASN:ND2	1:E:496:ARG:HH11	1.82	0.78
1:C:79:THR:HG22	1:C:82:ASP:H	1.49	0.78
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.63	0.78
1:E:371:LYS:HD2	1:E:371:LYS:O	1.84	0.78
1:E:449:MET:HE3	1:F:467:ILE:HD11	1.66	0.78
1:F:486:PHE:HE2	1:F:496:ARG:CD	1.95	0.78
1:E:191:ILE:HB	1:E:198:GLU:CG	2.14	0.77
1:F:218:ARG:HD2	4:F:522:HOH:O	1.85	0.77
1:A:41:SER:HB3	1:A:178:THR:HB	1.67	0.77
1:C:300:ARG:HA	1:C:333:MET:HE1	1.65	0.77
1:B:147:VAL:HG11	1:B:180:MET:CE	2.14	0.77
1:F:509:VAL:O	1:F:512:VAL:CG2	2.32	0.77
1:E:212:GLU:O	1:E:213:GLY:C	2.28	0.77
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.77
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.85	0.77
1:E:504:GLU:OE1	1:E:505:LEU:HD23	1.84	0.76
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.66	0.76
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.67	0.76
3:B:901:ATP:H3'	1:C:458:MET:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:MET:HA	4:F:532:HOH:O	1.83	0.76
1:A:426:THR:HG22	1:A:428:SER:H	1.51	0.76
1:F:146:SER:N	1:F:181:THR:HG22	2.01	0.76
1:F:515:LYS:HG3	1:F:516:GLY:H	1.50	0.76
1:E:14:GLU:HG3	1:E:16:GLN:H	1.50	0.76
1:B:429:HIS:HA	1:B:431:SEP:O1P	1.85	0.76
1:F:439:LEU:HD12	1:F:440:LEU:N	2.01	0.76
1:A:371:LYS:O	1:A:371:LYS:HD3	1.86	0.76
1:B:419:PHE:CD2	1:C:425:ILE:HD12	2.21	0.76
1:E:334:ASP:OD1	1:E:336:GLU:HB2	1.86	0.75
1:A:117:VAL:HA	1:A:154:TYR:OH	1.86	0.75
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.01	0.75
1:E:146:SER:H	1:E:181:THR:CG2	2.00	0.75
1:E:371:LYS:O	1:E:371:LYS:CD	2.35	0.75
1:D:140:ARG:HB3	1:D:140:ARG:HH11	1.50	0.75
1:B:21:MET:HE1	1:B:141:ARG:HG2	1.69	0.75
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.00	0.75
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.51	0.75
1:B:146:SER:H	1:B:181:THR:HG22	1.52	0.75
1:D:419:PHE:CD2	1:E:425:ILE:HD12	2.23	0.74
1:D:431:SEP:O	1:D:432:TPO:CB	2.27	0.74
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.68	0.74
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.85	0.74
1:A:316:ALA:O	1:A:348:CYS:HA	1.88	0.74
1:B:377:ILE:HD12	1:B:412:PHE:HE2	1.52	0.74
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.68	0.74
1:D:151:PHE:C	1:D:153:GLN:H	1.95	0.74
1:D:379:SER:HA	1:D:413:THR:HG22	1.67	0.74
1:D:446:ARG:N	1:D:496:ARG:NH1	2.35	0.74
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.52	0.74
1:E:145:ASP:OD2	1:E:181:THR:HG21	1.87	0.74
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.69	0.74
1:C:81:GLN:NE2	1:C:81:GLN:H	1.85	0.74
1:D:471:MET:HE2	1:D:478:ASP:HB2	1.70	0.74
1:E:419:PHE:CD2	1:F:425:ILE:HD12	2.23	0.74
1:B:363:ILE:O	1:B:367:ILE:HG13	1.88	0.73
1:D:203:ASN:HB3	1:D:225:LEU:HD23	1.70	0.73
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.68	0.73
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.22	0.73
1:D:146:SER:H	1:D:181:THR:CG2	1.99	0.73
1:E:294:LYS:HB2	3:E:901:ATP:O1B	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:SER:OG	1:E:462:TRP:N	2.16	0.73
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.69	0.73
1:D:147:VAL:O	1:D:150:VAL:HG12	1.88	0.73
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.70	0.73
1:E:148:THR:HG21	1:E:183:GLU:HG3	1.68	0.73
1:F:461:SER:OG	1:F:462:TRP:N	2.20	0.73
1:B:21:MET:HE3	1:B:141:ARG:NE	2.03	0.73
1:C:121:PHE:HD1	1:C:121:PHE:H	1.35	0.73
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.54	0.73
1:D:191:ILE:HB	1:D:198:GLU:HG3	1.68	0.73
1:D:287:THR:HG23	1:D:414:ASN:HB3	1.68	0.73
1:F:140:ARG:HB3	1:F:140:ARG:NH1	2.04	0.73
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.19	0.73
1:D:106:LEU:HD12	1:D:107:ASP:N	2.04	0.73
1:F:140:ARG:HH11	1:F:140:ARG:CB	2.02	0.73
1:C:79:THR:CG2	1:C:81:GLN:HG2	2.18	0.72
1:C:123:LEU:HD22	1:C:127:ILE:HD11	1.69	0.72
1:C:451:ARG:HG2	1:C:451:ARG:HH11	1.52	0.72
1:D:148:THR:OG1	1:D:182:THR:HG23	1.89	0.72
1:A:426:THR:HB	1:A:431:SEP:O2P	1.89	0.72
1:C:79:THR:O	1:C:83:ILE:HD12	1.89	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
1:D:299:SER:C	1:D:333:MET:HE1	2.14	0.72
1:E:323:GLN:HE22	1:F:459:ARG:HD3	1.53	0.72
1:A:145:ASP:OD2	1:A:181:THR:HG21	1.89	0.72
1:C:21:MET:HE3	1:C:141:ARG:NE	2.04	0.72
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.71	0.72
1:A:431:SEP:O	1:A:434:THR:HG22	1.89	0.72
1:D:106:LEU:HD11	1:D:129:ARG:NH2	2.04	0.72
1:D:203:ASN:HB3	1:D:225:LEU:CD2	2.19	0.72
1:A:65:ILE:O	1:A:65:ILE:HG22	1.88	0.72
1:B:52:LYS:HB2	3:B:903:ATP:O1B	1.90	0.72
1:E:19:ALA:O	1:E:38:ILE:HD12	1.89	0.72
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.03	0.72
1:C:218:ARG:HB3	4:C:522:HOH:O	1.88	0.72
1:C:140:ARG:HB3	1:C:140:ARG:NH1	2.05	0.72
1:D:486:PHE:HB2	1:D:489:ILE:HD11	1.72	0.72
1:E:497:ILE:O	1:E:498:THR:OG1	2.06	0.72
1:F:182:THR:HG22	1:F:183:GLU:N	2.05	0.72
1:D:426:THR:HG22	1:D:428:SER:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:THR:HG22	1:E:428:SER:N	2.04	0.71
1:C:191:ILE:HB	1:C:198:GLU:CG	2.19	0.71
1:D:263:VAL:HG12	1:D:374:ARG:HH21	1.55	0.71
1:D:497:ILE:HD12	1:D:497:ILE:O	1.90	0.71
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.70	0.71
1:E:418:GLN:HB2	1:F:423:HIS:O	1.89	0.71
1:B:462:TRP:O	1:B:463:HIS:O	2.08	0.71
1:C:123:LEU:HD21	1:C:167:LEU:HB2	1.72	0.71
1:E:396:VAL:O	1:E:400:THR:HB	1.89	0.71
1:C:45:SER:HB2	1:C:182:THR:HB	1.72	0.71
1:D:79:THR:CG2	1:D:81:GLN:HG2	2.19	0.71
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.05	0.71
1:C:315:PHE:CZ	1:C:363:ILE:HG23	2.26	0.71
1:B:497:ILE:HG13	1:B:498:THR:N	2.04	0.71
1:E:344:LEU:C	1:E:344:LEU:HD13	2.15	0.71
1:E:499:VAL:O	1:E:499:VAL:HG12	1.89	0.71
1:C:140:ARG:HH11	1:C:140:ARG:CB	2.04	0.71
1:D:295:THR:HG23	1:D:378:ASP:OD2	1.90	0.71
1:B:119:GLY:C	1:B:121:PHE:H	1.99	0.71
1:C:79:THR:HG23	1:C:81:GLN:HG2	1.71	0.70
1:E:432:TPO:HG21	1:E:432:TPO:O1P	1.88	0.70
1:D:387:VAL:HG12	1:D:388:SER:N	2.05	0.70
1:D:439:LEU:HD12	1:D:440:LEU:N	2.06	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
1:F:379:SER:HA	1:F:413:THR:HG22	1.74	0.70
1:B:397:ILE:HD13	1:B:433:ILE:HG21	1.72	0.70
1:A:425:ILE:HB	1:A:431:SEP:O1P	1.91	0.70
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.73	0.70
1:A:266:GLY:HA3	1:A:300:ARG:O	1.91	0.70
1:B:106:LEU:C	1:B:106:LEU:HD12	2.17	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:F:239:ILE:HB	4:F:533:HOH:O	1.90	0.70
1:A:499:VAL:O	1:A:499:VAL:HG12	1.92	0.70
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.74	0.70
1:B:65:ILE:O	1:B:65:ILE:HG22	1.90	0.70
1:A:151:PHE:C	1:A:153:GLN:H	2.00	0.70
1:B:273:MET:O	1:B:463:HIS:HA	1.91	0.70
1:C:106:LEU:C	1:C:106:LEU:HD12	2.17	0.70
1:D:79:THR:HG23	1:D:81:GLN:H	1.57	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	2.21	0.70
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.91	0.70
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.05	0.69
1:C:379:SER:HA	1:C:413:THR:HG22	1.73	0.69
1:D:451:ARG:HG2	1:D:451:ARG:HH11	1.57	0.69
1:B:18:ILE:HB	1:B:228:THR:HG23	1.73	0.69
1:E:273:MET:O	1:E:463:HIS:HA	1.92	0.69
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.22	0.69
1:B:169:ALA:O	1:B:173:GLN:HG3	1.92	0.69
1:C:14:GLU:HG3	1:C:16:GLN:H	1.58	0.69
1:D:496:ARG:HG2	1:E:487:GLU:OE1	1.92	0.69
1:A:49:GLY:HA2	3:A:903:ATP:O2B	1.93	0.69
1:A:318:GLU:HG2	1:B:432:TPO:O3P	1.92	0.69
1:C:203:ASN:HB3	1:C:225:LEU:HD23	1.74	0.69
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.56	0.69
1:D:345:LYS:NZ	1:D:366:GLU:CG	2.55	0.69
1:F:115:GLN:HG2	1:F:116:GLU:CA	2.21	0.69
1:A:89:SER:HB2	1:B:227:GLY:O	1.93	0.69
1:C:289:ALA:HB2	1:C:419:PHE:HA	1.73	0.69
1:F:502:LYS:HZ1	1:F:507:ARG:HB3	1.55	0.69
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.75	0.69
1:A:377:ILE:HD12	1:A:412:PHE:HE2	1.58	0.69
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.93	0.69
1:B:498:THR:OG1	1:C:499:VAL:HG21	1.92	0.69
1:C:393:ARG:O	1:C:397:ILE:HG12	1.91	0.69
1:D:145:ASP:OD2	1:D:181:THR:HG21	1.93	0.69
1:E:151:PHE:C	1:E:153:GLN:H	2.01	0.69
1:F:151:PHE:C	1:F:153:GLN:H	2.01	0.69
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.23	0.69
1:F:334:ASP:OD1	1:F:336:GLU:HB2	1.93	0.69
1:C:371:LYS:O	1:C:371:LYS:HD3	1.92	0.69
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.75	0.69
1:F:430:ILE:O	1:F:431:SEP:C	2.40	0.69
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.75	0.68
1:C:126:LEU:O	1:C:129:ARG:HB2	1.91	0.68
1:C:146:SER:N	1:C:181:THR:HG22	2.08	0.68
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.23	0.68
1:F:347:VAL:O	1:F:348:CYS:HB2	1.93	0.68
1:C:287:THR:HG23	1:C:414:ASN:HB3	1.74	0.68
1:F:81:GLN:NE2	1:F:81:GLN:H	1.91	0.68
1:F:147:VAL:O	1:F:150:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:TYR:CE1	1:B:252:MET:HE3	2.28	0.68
1:F:14:GLU:HG2	4:F:540:HOH:O	1.93	0.68
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.58	0.68
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.09	0.68
1:A:505:LEU:HD12	1:A:505:LEU:O	1.94	0.68
1:B:300:ARG:HA	1:B:333:MET:HE1	1.76	0.68
1:A:18:ILE:N	1:A:18:ILE:HD12	2.08	0.68
1:B:497:ILE:HD12	1:B:499:VAL:H	1.59	0.68
1:D:106:LEU:CD1	1:D:129:ARG:NH2	2.57	0.68
1:B:295:THR:HG21	1:B:319:GLU:OE2	1.93	0.67
1:C:299:SER:HB3	1:C:333:MET:HE2	1.76	0.67
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.76	0.67
1:D:31:ILE:HG22	1:D:222:ILE:HD12	1.75	0.67
1:D:345:LYS:HZ3	1:D:366:GLU:CD	2.02	0.67
1:A:363:ILE:O	1:A:367:ILE:HG13	1.94	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:A:503:SER:C	1:A:504:GLU:HG3	2.20	0.67
1:F:273:MET:O	1:F:463:HIS:HA	1.94	0.67
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
1:D:367:ILE:HG12	1:D:375:ILE:HD11	1.75	0.67
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.30	0.67
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.07	0.67
1:A:293:GLY:HA2	3:A:901:ATP:O1A	1.95	0.67
1:F:504:GLU:HA	1:F:507:ARG:NE	2.09	0.67
1:A:92:TRP:HD1	1:A:92:TRP:O	1.78	0.67
1:B:151:PHE:C	1:B:153:GLN:H	2.03	0.67
1:C:17:ALA:C	1:C:18:ILE:HD12	2.19	0.67
1:D:14:GLU:CD	1:D:15:HIS:H	2.03	0.67
1:A:273:MET:O	1:A:463:HIS:HA	1.95	0.67
1:C:106:LEU:HD13	1:C:129:ARG:NH2	2.10	0.67
1:E:123:LEU:HD22	1:E:166:ARG:CD	2.24	0.67
1:F:504:GLU:HB3	1:F:507:ARG:CZ	2.24	0.67
1:B:81:GLN:NE2	1:B:81:GLN:H	1.93	0.66
1:F:119:GLY:C	1:F:122:ASP:OD2	2.38	0.66
1:C:182:THR:HG22	1:C:183:GLU:H	1.59	0.66
1:F:371:LYS:O	1:F:371:LYS:CD	2.43	0.66
1:F:471:MET:HB3	1:F:480:LYS:NZ	2.10	0.66
1:D:316:ALA:O	1:D:348:CYS:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ASP:OD1	1:D:336:GLU:HB2	1.95	0.66
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.78	0.66
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.24	0.66
1:C:461:SER:OG	1:C:462:TRP:N	2.25	0.66
1:B:461:SER:OG	1:B:462:TRP:N	2.27	0.66
1:C:21:MET:HE1	1:C:141:ARG:HG2	1.77	0.66
1:D:370:PHE:O	1:D:371:LYS:HD2	1.95	0.66
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.95	0.66
1:C:273:MET:O	1:C:463:HIS:HA	1.96	0.66
1:B:426:THR:HG22	1:B:428:SER:H	1.60	0.66
1:B:497:ILE:HD12	1:B:499:VAL:HB	1.76	0.66
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.09	0.66
1:F:363:ILE:O	1:F:367:ILE:HG13	1.96	0.66
1:D:441:GLN:HE22	1:D:490:ILE:HD12	1.61	0.66
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.77	0.66
1:D:19:ALA:C	1:D:38:ILE:HD12	2.21	0.66
1:D:371:LYS:O	1:D:371:LYS:CD	2.42	0.66
1:B:350:TYR:CE1	1:C:252:MET:HE3	2.31	0.66
1:C:147:VAL:HG11	1:C:180:MET:HE3	1.77	0.66
1:C:334:ASP:OD1	1:C:336:GLU:HB2	1.96	0.66
1:D:182:THR:HG22	1:D:183:GLU:N	2.10	0.66
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.77	0.66
1:C:263:VAL:HG12	1:C:374:ARG:HH21	1.61	0.65
1:D:345:LYS:HZ2	1:D:366:GLU:HG2	1.59	0.65
1:E:439:LEU:HD12	1:E:440:LEU:N	2.11	0.65
1:A:49:GLY:CA	3:A:903:ATP:O2B	2.43	0.65
1:D:191:ILE:CB	1:D:198:GLU:HG3	2.27	0.65
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.76	0.65
1:B:293:GLY:HA2	3:B:901:ATP:O1A	1.96	0.65
1:C:371:LYS:O	1:C:371:LYS:CD	2.43	0.65
1:D:344:LEU:HD13	1:D:345:LYS:N	2.12	0.65
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.78	0.65
1:D:435:ASP:HA	1:D:459:ARG:HD2	1.78	0.65
1:D:345:LYS:NZ	1:D:366:GLU:HG2	2.12	0.65
1:B:79:THR:HG21	1:B:81:GLN:HG2	1.77	0.65
1:E:148:THR:OG1	1:E:182:THR:HG23	1.96	0.65
1:B:45:SER:HB3	1:B:182:THR:HB	1.78	0.65
1:C:470:PHE:HB2	1:C:478:ASP:O	1.97	0.65
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.10	0.65
1:E:359:HIS:O	1:E:363:ILE:HG13	1.97	0.65
1:D:486:PHE:CB	1:D:489:ILE:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:THR:HG23	1:E:81:GLN:HE21	1.60	0.65
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.79	0.65
1:A:146:SER:H	1:A:181:THR:HG22	1.61	0.65
1:A:459:ARG:HD3	1:F:323:GLN:HE22	1.62	0.65
1:C:300:ARG:CA	1:C:333:MET:HE1	2.27	0.65
1:C:419:PHE:O	1:C:420:MET:HB2	1.96	0.65
1:D:385:ARG:NH2	1:E:432:TPO:O3P	2.27	0.65
1:F:471:MET:HB3	1:F:480:LYS:HZ1	1.61	0.65
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.27	0.64
1:B:371:LYS:O	1:B:371:LYS:HD3	1.97	0.64
1:C:182:THR:HG22	1:C:183:GLU:N	2.12	0.64
1:D:299:SER:HB3	1:D:333:MET:HE2	1.79	0.64
1:D:469:GLU:HG3	1:D:470:PHE:N	2.12	0.64
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.27	0.64
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.78	0.64
1:C:41:SER:HB3	1:C:178:THR:HB	1.78	0.64
1:D:191:ILE:HB	1:D:198:GLU:CD	2.21	0.64
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.97	0.64
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.31	0.64
1:E:497:ILE:HG22	1:E:498:THR:H	1.63	0.64
1:C:350:TYR:CE1	1:D:252:MET:HE3	2.32	0.64
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.27	0.64
1:A:79:THR:O	1:A:83:ILE:HD12	1.97	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
1:A:504:GLU:C	1:A:506:SER:H	2.05	0.64
1:D:311:ARG:HD2	1:D:371:LYS:CD	2.28	0.64
1:F:146:SER:H	1:F:181:THR:CG2	2.03	0.64
1:A:396:VAL:O	1:A:400:THR:HB	1.97	0.64
1:B:24:MET:CB	1:B:62:ASN:HD22	2.09	0.64
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.62	0.64
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.97	0.64
1:F:106:LEU:C	1:F:106:LEU:HD12	2.23	0.64
1:F:344:LEU:HD22	1:F:345:LYS:N	2.12	0.64
1:B:21:MET:CE	1:B:141:ARG:HG2	2.27	0.64
1:D:345:LYS:HZ3	1:D:366:GLU:CG	2.11	0.64
1:F:471:MET:HG2	1:F:480:LYS:HE2	1.79	0.64
1:A:419:PHE:CD2	1:B:425:ILE:CD1	2.81	0.64
1:C:311:ARG:HD2	1:C:371:LYS:HD2	1.80	0.64
1:D:313:ILE:CD1	1:D:372:PRO:HG3	2.28	0.64
1:E:462:TRP:O	1:E:463:HIS:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.33	0.64
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.79	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:C:18:ILE:HD12	1:C:18:ILE:N	2.12	0.64
1:C:497:ILE:C	1:C:498:THR:HG22	2.23	0.64
1:D:52:LYS:HE3	3:D:903:ATP:O1B	1.98	0.64
1:D:223:LEU:O	1:D:223:LEU:HD22	1.98	0.64
1:D:471:MET:HE1	1:D:473:SER:OG	1.97	0.64
1:F:299:SER:C	1:F:333:MET:HE1	2.23	0.64
1:C:159:VAL:O	1:C:163:GLU:HG2	1.97	0.63
1:D:311:ARG:HD2	1:D:371:LYS:CE	2.28	0.63
1:A:420:MET:CE	1:B:490:ILE:HG21	2.29	0.63
1:C:231:MET:HE1	1:C:251:ALA:HB2	1.79	0.63
1:D:393:ARG:O	1:D:397:ILE:HG12	1.98	0.63
1:F:122:ASP:O	1:F:126:LEU:N	2.30	0.63
1:B:371:LYS:O	1:B:371:LYS:CD	2.47	0.63
1:C:305:ALA:HB2	1:C:374:ARG:CD	2.29	0.63
1:D:400:THR:HG22	1:D:401:GLY:N	2.13	0.63
1:A:106:LEU:C	1:A:106:LEU:HD12	2.24	0.63
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.81	0.63
1:E:186:GLU:OE2	1:E:187:GLU:N	2.31	0.63
1:E:496:ARG:O	1:E:497:ILE:HD13	1.99	0.63
1:F:120:GLY:HA2	1:F:123:LEU:HB2	1.80	0.63
1:D:340:ARG:O	1:D:342:ASN:N	2.31	0.63
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.34	0.63
1:C:170:ARG:O	1:C:174:ILE:HG12	1.99	0.62
1:C:451:ARG:HG2	1:C:451:ARG:NH1	2.14	0.62
1:D:79:THR:HG23	1:D:81:GLN:HE21	1.64	0.62
1:A:24:MET:CB	1:A:62:ASN:HD22	2.11	0.62
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.62
1:B:170:ARG:O	1:B:174:ILE:HG12	1.99	0.62
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.47	0.62
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.80	0.62
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.80	0.62
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.64	0.62
1:B:19:ALA:O	1:B:38:ILE:HD12	1.99	0.62
1:B:146:SER:H	1:B:181:THR:CG2	2.13	0.62
1:B:444:GLU:OE2	1:C:489:ILE:HG13	1.99	0.62
1:C:419:PHE:CD1	1:C:420:MET:HG3	2.34	0.62
1:D:182:THR:HG22	1:D:183:GLU:H	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:OD2	1:C:181:THR:HG21	1.98	0.62
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.80	0.62
1:A:300:ARG:HA	1:A:333:MET:HE1	1.82	0.62
1:C:19:ALA:O	1:C:38:ILE:HD12	1.99	0.62
1:C:203:ASN:HB3	1:C:225:LEU:CD2	2.29	0.62
1:E:148:THR:OG1	1:E:182:THR:CG2	2.47	0.62
1:E:159:VAL:O	1:E:163:GLU:HG2	2.00	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:B:311:ARG:HD2	1:B:371:LYS:HD2	1.81	0.62
1:C:52:LYS:HD3	1:C:182:THR:O	2.00	0.62
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.80	0.62
1:D:14:GLU:OE1	1:D:14:GLU:HA	1.99	0.62
1:D:377:ILE:HD12	1:D:412:PHE:CE2	2.35	0.62
1:D:486:PHE:CE2	1:D:496:ARG:HB3	2.34	0.62
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.82	0.62
1:B:146:SER:N	1:B:181:THR:HG22	2.14	0.62
1:E:300:ARG:HA	1:E:333:MET:HE1	1.80	0.62
1:F:231:MET:CE	1:F:251:ALA:HB2	2.29	0.62
1:E:148:THR:HG21	1:E:183:GLU:CG	2.30	0.62
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.15	0.62
1:A:441:GLN:HG3	1:A:441:GLN:O	2.00	0.61
1:B:418:GLN:HG3	1:B:418:GLN:O	1.99	0.61
1:A:231:MET:HE1	1:A:251:ALA:HB2	1.82	0.61
1:A:432:TPO:HG21	1:A:432:TPO:O1P	2.00	0.61
1:D:418:GLN:HB2	1:E:423:HIS:O	1.99	0.61
1:E:170:ARG:O	1:E:174:ILE:HG12	2.00	0.61
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.81	0.61
1:F:508:ILE:HG22	1:F:508:ILE:O	2.00	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
1:D:449:MET:HE3	1:E:467:ILE:HD11	1.83	0.61
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.64	0.61
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.82	0.61
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.30	0.61
1:A:85:LYS:NZ	1:B:14:GLU:HG3	2.15	0.61
1:D:49:GLY:O	1:D:218:ARG:NH2	2.34	0.61
1:D:81:GLN:H	1:D:81:GLN:NE2	1.99	0.61
1:E:140:ARG:HB3	1:E:140:ARG:NH1	2.15	0.61
1:A:320:SER:HA	1:B:254:LEU:HG	1.81	0.61
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.82	0.61
1:B:379:SER:CA	1:B:413:THR:HG22	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:H	1:C:81:GLN:CD	2.06	0.61
1:D:41:SER:HB3	1:D:178:THR:HB	1.83	0.61
1:D:140:ARG:HB3	1:D:140:ARG:NH1	2.15	0.61
1:F:21:MET:HE1	1:F:141:ARG:HG2	1.83	0.61
1:F:471:MET:HE2	1:F:478:ASP:HB2	1.82	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:C:150:VAL:O	1:C:153:GLN:HG3	2.01	0.61
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.36	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
1:D:151:PHE:C	1:D:153:GLN:N	2.58	0.61
1:E:14:GLU:HG3	1:E:16:GLN:N	2.15	0.61
1:E:471:MET:HE2	1:E:478:ASP:HB2	1.81	0.61
1:F:19:ALA:O	1:F:38:ILE:HD12	2.01	0.61
1:B:117:VAL:O	1:B:117:VAL:HG12	2.01	0.61
1:E:19:ALA:C	1:E:38:ILE:HD12	2.25	0.61
1:C:340:ARG:O	1:C:342:ASN:N	2.33	0.60
1:D:446:ARG:H	1:D:496:ARG:HH22	1.48	0.60
1:F:340:ARG:O	1:F:342:ASN:N	2.33	0.60
1:F:371:LYS:O	1:F:371:LYS:HD3	2.00	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.31	0.60
1:C:347:VAL:O	1:C:348:CYS:CB	2.45	0.60
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.79	0.60
1:E:347:VAL:HG12	1:E:348:CYS:N	2.15	0.60
1:A:16:GLN:O	1:A:17:ALA:O	2.20	0.60
1:A:347:VAL:O	1:A:348:CYS:HB2	2.01	0.60
1:B:287:THR:HG21	1:B:425:ILE:O	2.01	0.60
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.83	0.60
1:B:91:GLY:O	1:B:92:TRP:HD1	1.84	0.60
1:C:400:THR:HG22	1:C:401:GLY:N	2.16	0.60
1:D:471:MET:HG3	1:D:478:ASP:HB3	1.82	0.60
1:D:347:VAL:O	1:D:348:CYS:HB2	2.01	0.60
1:E:436:THR:HG23	1:E:458:MET:HG3	1.82	0.60
1:F:111:ASP:C	1:F:113:GLU:H	2.07	0.60
1:A:52:LYS:HE3	3:A:903:ATP:O1B	2.02	0.60
1:C:148:THR:OG1	1:C:182:THR:HG23	2.02	0.60
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.32	0.60
1:A:318:GLU:OE2	1:B:432:TPO:CG2	2.48	0.60
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.82	0.60
1:E:345:LYS:HZ3	1:E:366:GLU:CD	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ILE:O	1:E:433:ILE:CG2	2.47	0.60
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.83	0.60
1:F:504:GLU:O	1:F:505:LEU:HB2	1.99	0.60
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.36	0.60
1:C:363:ILE:O	1:C:367:ILE:HG13	2.02	0.60
1:C:21:MET:CE	1:C:141:ARG:HG2	2.32	0.60
1:C:396:VAL:HG11	1:C:430:ILE:HG23	1.84	0.60
1:D:79:THR:HG22	1:D:82:ASP:N	2.07	0.60
1:B:299:SER:HB3	1:B:333:MET:HE2	1.83	0.59
1:D:396:VAL:O	1:D:400:THR:HB	2.02	0.59
1:D:439:LEU:HD12	1:D:439:LEU:C	2.27	0.59
1:F:316:ALA:O	1:F:348:CYS:HA	2.02	0.59
1:F:340:ARG:C	1:F:342:ASN:H	2.10	0.59
1:B:426:THR:HB	1:B:431:SEP:O3P	2.02	0.59
1:C:147:VAL:HG11	1:C:180:MET:CE	2.31	0.59
1:D:446:ARG:H	1:D:496:ARG:NH2	2.00	0.59
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.36	0.59
1:E:382:ALA:O	1:E:385:ARG:HG3	2.01	0.59
1:F:159:VAL:O	1:F:163:GLU:HG2	2.01	0.59
1:E:268:VAL:O	1:E:271:ASP:HB2	2.03	0.59
1:F:218:ARG:HB3	4:F:536:HOH:O	2.02	0.59
1:D:79:THR:HG21	1:D:81:GLN:HG2	1.82	0.59
1:D:130:ILE:O	1:D:134:ILE:HG13	2.02	0.59
1:D:287:THR:HG23	1:D:414:ASN:HD22	1.64	0.59
1:F:123:LEU:O	1:F:127:ILE:HG12	2.01	0.59
1:C:419:PHE:CD2	1:D:425:ILE:HD12	2.37	0.59
1:C:431:SEP:C	1:C:432:TPO:HG22	2.33	0.59
1:C:462:TRP:O	1:C:463:HIS:O	2.20	0.59
1:D:131:ASN:OD1	1:D:174:ILE:HD12	2.02	0.59
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.85	0.59
1:D:79:THR:HG23	1:D:81:GLN:HG2	1.84	0.59
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.67	0.59
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.59
1:C:113:GLU:O	1:C:114:GLY:C	2.45	0.59
1:D:340:ARG:C	1:D:342:ASN:H	2.11	0.59
1:E:316:ALA:O	1:E:348:CYS:HA	2.03	0.59
1:A:379:SER:H	1:A:413:THR:HB	1.67	0.59
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.33	0.59
1:B:340:ARG:C	1:B:342:ASN:H	2.11	0.59
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.66	0.58
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.16	0.58
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.85	0.58
1:B:98:VAL:HA	1:B:103:LEU:O	2.02	0.58
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.38	0.58
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.86	0.58
1:A:420:MET:HE1	1:B:490:ILE:HG21	1.85	0.58
1:A:432:TPO:OG1	1:A:433:ILE:HD12	2.03	0.58
3:A:901:ATP:H3'	1:B:458:MET:O	2.03	0.58
1:D:248:PRO:HB2	1:D:251:ALA:HB3	1.86	0.58
1:D:263:VAL:HG12	1:D:374:ARG:NH2	2.19	0.58
1:D:446:ARG:HG3	1:D:496:ARG:NH1	2.18	0.58
1:F:503:SER:O	1:F:504:GLU:O	2.21	0.58
1:A:166:ARG:HG3	1:F:112:PRO:O	2.02	0.58
1:C:294:LYS:HB2	3:C:901:ATP:O1B	2.04	0.58
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	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:65:ILE:O	1:B:65:ILE:CG2	2.52	0.58
1:E:400:THR:HG22	1:E:401:GLY:N	2.19	0.58
1:F:378:ASP:HB3	4:F:520:HOH:O	2.04	0.58
1:A:19:ALA:C	1:A:38:ILE:HD12	2.29	0.58
1:B:471:MET:HB3	1:B:480:LYS:HZ3	1.69	0.58
1:C:471:MET:HG3	1:C:478:ASP:HB3	1.85	0.58
1:E:485:ASN:HD21	1:E:496:ARG:NH1	2.02	0.58
1:A:400:THR:HG22	1:A:401:GLY:N	2.18	0.58
1:C:344:LEU:HD22	1:C:345:LYS:N	2.19	0.58
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.04	0.58
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.68	0.58
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.86	0.58
1:A:21:MET:CE	1:A:59:PHE:CZ	2.87	0.58
1:A:52:LYS:N	3:A:903:ATP:O1B	2.28	0.58
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.03	0.58
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.86	0.58
1:E:281:ASP:O	1:E:282:SER:HB3	2.04	0.58
1:C:79:THR:CG2	1:C:82:ASP:H	2.16	0.58
1:D:79:THR:CG2	1:D:82:ASP:H	2.10	0.58
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.86	0.58
1:C:33:HIS:HD2	1:C:229:SER:OG	1.87	0.57
1:C:444:GLU:OE2	1:D:489:ILE:HG12	2.03	0.57
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:TRP:O	1:A:463:HIS:O	2.21	0.57
1:C:88:ARG:HD3	1:D:15:HIS:O	2.04	0.57
1:C:426:THR:HG22	1:C:428:SER:H	1.69	0.57
1:E:358:ASP:O	1:E:362:ILE:HG12	2.03	0.57
1:F:182:THR:HG22	1:F:183:GLU:H	1.69	0.57
1:F:300:ARG:HA	1:F:333:MET:HE1	1.86	0.57
1:D:495:THR:HA	1:E:487:GLU:OE2	2.04	0.57
1:B:45:SER:CB	1:B:182:THR:HB	2.34	0.57
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.70	0.57
1:C:449:MET:HE3	1:D:467:ILE:HD11	1.86	0.57
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.87	0.57
1:D:344:LEU:C	1:D:344:LEU:CD1	2.78	0.57
1:E:81:GLN:NE2	1:E:81:GLN:H	2.02	0.57
1:F:79:THR:HG23	1:F:81:GLN:H	1.70	0.57
1:B:119:GLY:C	1:B:121:PHE:N	2.62	0.57
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.86	0.57
1:B:449:MET:HE3	1:C:467:ILE:HD11	1.85	0.57
1:C:248:PRO:HB2	1:C:251:ALA:HB3	1.86	0.57
1:E:41:SER:HB3	1:E:178:THR:HB	1.84	0.57
1:E:191:ILE:HB	1:E:198:GLU:CD	2.30	0.57
1:A:430:ILE:O	1:A:431:SEP:C	2.53	0.57
1:A:513:GLN:HG3	1:A:513:GLN:O	2.04	0.57
1:C:431:SEP:C	1:C:432:TPO:CG2	2.82	0.57
1:E:123:LEU:CD2	1:E:166:ARG:HD2	2.30	0.57
1:E:469:GLU:HB2	1:E:483:PHE:CZ	2.40	0.57
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.86	0.57
1:C:146:SER:H	1:C:181:THR:CG2	2.16	0.57
1:C:419:PHE:O	1:C:420:MET:CB	2.51	0.57
1:F:123:LEU:O	1:F:123:LEU:HD13	2.04	0.57
1:F:295:THR:HG23	1:F:378:ASP:OD2	2.04	0.57
1:A:15:HIS:C	1:A:16:GLN:OE1	2.47	0.57
1:A:61:TYR:CE1	1:A:92:TRP:HB2	2.39	0.57
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.19	0.57
1:D:231:MET:CE	1:D:251:ALA:HB2	2.31	0.57
1:D:471:MET:HB3	1:D:480:LYS:NZ	2.20	0.57
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.40	0.57
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.19	0.57
1:A:252:MET:HE3	1:F:350:TYR:CZ	2.38	0.56
1:D:45:SER:HB2	1:D:182:THR:HB	1.87	0.56
1:D:419:PHE:CD2	1:E:425:ILE:CD1	2.86	0.56
1:D:164:LEU:CD2	1:D:180:MET:HE1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:CD1	1:E:163:GLU:OE2	2.53	0.56
1:F:118:VAL:O	1:F:118:VAL:HG13	2.05	0.56
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.85	0.56
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.86	0.56
1:C:45:SER:CB	1:C:182:THR:HB	2.35	0.56
1:C:79:THR:C	1:C:83:ILE:HD12	2.29	0.56
1:E:231:MET:HE1	1:E:251:ALA:HB2	1.87	0.56
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.88	0.56
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.87	0.56
1:E:471:MET:HE2	1:E:478:ASP:CB	2.34	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:A:211:LEU:HD12	1:A:215:ARG:O	2.06	0.56
1:B:448:GLU:HG2	1:C:466:ALA:HA	1.88	0.56
1:B:497:ILE:HG13	1:B:498:THR:H	1.69	0.56
1:D:96:LYS:O	1:D:100:GLU:HG3	2.05	0.56
1:D:446:ARG:H	1:D:496:ARG:CZ	2.16	0.56
3:A:901:ATP:O3'	1:B:457:LYS:HB2	2.05	0.56
1:B:130:ILE:O	1:B:134:ILE:HG13	2.06	0.56
1:F:436:THR:OG1	1:F:458:MET:HG2	2.05	0.56
1:B:150:VAL:O	1:B:153:GLN:HG3	2.06	0.56
1:B:430:ILE:O	1:B:431:SEP:C	2.53	0.56
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.20	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.69	0.56
1:D:81:GLN:H	1:D:81:GLN:CD	2.14	0.56
1:F:294:LYS:N	3:F:901:ATP:O1B	2.39	0.56
1:D:387:VAL:CG1	1:D:388:SER:N	2.69	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:52:LYS:N	3:B:903:ATP:O1B	2.38	0.56
1:B:79:THR:CG2	1:B:82:ASP:H	2.12	0.56
1:C:49:GLY:O	1:C:218:ARG:NH2	2.39	0.56
1:E:485:ASN:HD21	1:E:496:ARG:HH11	1.50	0.56
1:F:117:VAL:O	1:F:118:VAL:HB	2.06	0.56
1:F:150:VAL:O	1:F:153:GLN:HG3	2.06	0.56
1:A:495:THR:HG22	1:A:497:ILE:CG2	2.36	0.55
1:C:43:LEU:HD11	1:C:182:THR:OG1	2.05	0.55
1:C:104:PHE:CE2	1:C:106:LEU:HB2	2.41	0.55
1:C:340:ARG:C	1:C:342:ASN:H	2.14	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
1:D:147:VAL:HG11	1:D:180:MET:HE2	1.85	0.55
1:D:178:THR:HG22	1:D:179:VAL:N	2.21	0.55
1:F:96:LYS:O	1:F:100:GLU:HG3	2.06	0.55
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.55
1:F:396:VAL:HG11	1:F:430:ILE:CG2	2.36	0.55
1:F:439:LEU:HD12	1:F:439:LEU:C	2.30	0.55
1:A:345:LYS:HZ3	1:A:366:GLU:HG2	1.71	0.55
1:C:356:LEU:HD22	1:C:387:VAL:HG11	1.87	0.55
1:D:469:GLU:HB2	1:D:483:PHE:CZ	2.42	0.55
1:E:49:GLY:CA	3:E:903:ATP:O2B	2.54	0.55
1:B:159:VAL:O	1:B:163:GLU:HG2	2.07	0.55
1:D:140:ARG:HH11	1:D:140:ARG:CB	2.19	0.55
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.36	0.55
1:E:501:GLU:O	1:E:502:LYS:CG	2.49	0.55
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.87	0.55
1:B:294:LYS:HB2	3:B:901:ATP:O1B	2.07	0.55
1:D:67:PHE:HB2	1:D:69:GLU:HG3	1.89	0.55
1:F:151:PHE:C	1:F:153:GLN:N	2.64	0.55
1:A:393:ARG:O	1:A:397:ILE:HG12	2.06	0.55
1:A:433:ILE:O	1:A:433:ILE:CG2	2.50	0.55
1:B:485:ASN:OD1	1:B:485:ASN:N	2.33	0.55
1:D:148:THR:CG2	1:D:193:ARG:HD2	2.37	0.55
1:D:377:ILE:HD12	1:D:412:PHE:HE2	1.72	0.55
1:E:151:PHE:C	1:E:153:GLN:N	2.64	0.55
1:E:496:ARG:HG3	1:E:497:ILE:N	2.21	0.55
1:A:57:ILE:HD13	1:A:73:PHE:CE1	2.42	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.52	0.55
1:A:318:GLU:CD	1:B:432:TPO:CG2	2.80	0.55
1:C:53:THR:HG23	1:C:145:ASP:OD1	2.05	0.55
1:E:123:LEU:HD21	1:E:127:ILE:HD11	1.87	0.55
1:F:49:GLY:HA2	3:F:903:ATP:O2B	2.06	0.55
1:A:439:LEU:HD12	1:A:440:LEU:N	2.21	0.55
1:B:184:ARG:HG2	1:B:191:ILE:O	2.06	0.55
1:C:20:LYS:HE3	1:C:228:THR:HG21	1.89	0.55
1:C:377:ILE:HD12	1:C:412:PHE:CE2	2.42	0.55
1:C:493:SER:HB3	1:D:488:ARG:HG2	1.89	0.55
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.41	0.55
1:A:65:ILE:O	1:A:65:ILE:CG2	2.54	0.54
1:B:148:THR:OG1	1:B:182:THR:HG23	2.07	0.54
1:C:18:ILE:HG21	1:C:37:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASP:HA	1:C:459:ARG:HD2	1.89	0.54
1:E:121:PHE:CD1	1:E:121:PHE:N	2.74	0.54
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.21	0.54
1:B:503:SER:O	1:B:504:GLU:HB2	2.05	0.54
1:D:127:ILE:HD11	1:D:167:LEU:HA	1.87	0.54
1:F:19:ALA:C	1:F:38:ILE:HD12	2.32	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:B:316:ALA:O	1:B:348:CYS:HA	2.07	0.54
1:C:148:THR:HG21	1:C:183:GLU:HG3	1.89	0.54
1:A:340:ARG:C	1:A:342:ASN:H	2.15	0.54
1:B:299:SER:C	1:B:333:MET:HE1	2.32	0.54
1:B:426:THR:HG22	1:B:428:SER:N	2.23	0.54
1:C:169:ALA:O	1:C:173:GLN:HG3	2.08	0.54
1:D:191:ILE:CG2	1:D:198:GLU:HG3	2.37	0.54
1:D:354:ALA:HB3	1:D:359:HIS:NE2	2.23	0.54
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.89	0.54
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.37	0.54
1:F:20:LYS:C	1:F:38:ILE:HD11	2.31	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:C:117:VAL:O	1:C:117:VAL:HG12	2.07	0.54
1:C:208:ARG:NH2	1:C:221:GLU:OE2	2.40	0.54
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.54
1:C:367:ILE:HG12	1:C:375:ILE:HD11	1.89	0.54
1:C:441:GLN:HE22	1:C:490:ILE:HD13	1.72	0.54
1:E:211:LEU:O	1:E:212:GLU:HB3	2.07	0.54
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.08	0.54
1:A:79:THR:HG23	1:A:81:GLN:H	1.73	0.54
1:B:360:LEU:O	1:B:360:LEU:HD22	2.08	0.54
1:C:148:THR:CG2	1:C:193:ARG:HD2	2.38	0.54
1:E:485:ASN:ND2	1:E:496:ARG:NH1	2.52	0.54
1:F:148:THR:HG21	1:F:183:GLU:CG	2.37	0.54
1:B:213:GLY:O	1:B:214:GLU:CB	2.56	0.54
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.38	0.54
1:C:356:LEU:CD2	1:C:387:VAL:HG11	2.38	0.54
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.22	0.54
1:D:489:ILE:HA	1:D:494:PRO:HG3	1.89	0.54
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASP:O	1:B:362:ILE:HG12	2.08	0.54
1:C:150:VAL:HG13	1:C:151:PHE:N	2.22	0.54
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.48	0.54
1:E:471:MET:HB3	1:E:480:LYS:NZ	2.23	0.54
1:A:311:ARG:HA	1:A:343:LEU:O	2.07	0.54
1:B:116:GLU:HG2	1:B:117:VAL:H	1.73	0.54
1:B:213:GLY:O	1:B:214:GLU:HB2	2.06	0.54
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.43	0.54
1:C:359:HIS:O	1:C:363:ILE:HG13	2.07	0.54
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.89	0.54
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.89	0.54
1:F:504:GLU:HA	1:F:507:ARG:HE	1.73	0.54
1:A:17:ALA:C	1:A:18:ILE:HD12	2.33	0.53
1:B:340:ARG:O	1:B:342:ASN:N	2.41	0.53
1:D:150:VAL:O	1:D:153:GLN:HG3	2.07	0.53
1:A:79:THR:HG23	1:A:81:GLN:CG	2.34	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:A:264:SER:HA	1:A:271:ASP:OD1	2.08	0.53
1:B:38:ILE:HA	1:B:177:THR:CG2	2.37	0.53
1:E:118:VAL:O	1:E:118:VAL:HG12	2.09	0.53
1:E:123:LEU:O	1:E:127:ILE:CG1	2.56	0.53
1:E:471:MET:HG2	1:E:480:LYS:HE2	1.90	0.53
1:A:81:GLN:H	1:A:81:GLN:CD	2.16	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:C:164:LEU:HB3	1:C:200:VAL:HG11	1.89	0.53
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.89	0.53
1:B:79:THR:O	1:B:83:ILE:HD12	2.08	0.53
1:E:18:ILE:HD11	1:E:227:GLY:C	2.34	0.53
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.91	0.53
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.90	0.53
1:F:340:ARG:C	1:F:342:ASN:N	2.66	0.53
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.91	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:C:81:GLN:CD	1:C:81:GLN:N	2.66	0.53
1:C:221:GLU:HG3	1:C:233:GLY:O	2.08	0.53
1:C:488:ARG:HG3	1:C:488:ARG:HH11	1.72	0.53
1:D:43:LEU:HD11	1:D:182:THR:OG1	2.08	0.53
1:D:318:GLU:OE2	1:D:379:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:GLY:CA	3:F:903:ATP:O2B	2.56	0.53
1:F:498:THR:HB	1:F:500:ASP:O	2.08	0.53
1:A:457:LYS:HB2	3:F:901:ATP:O3'	2.08	0.53
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.23	0.53
1:C:323:GLN:HE22	1:D:459:ARG:HD3	1.74	0.53
1:C:431:SEP:O	1:C:432:TPO:HG23	2.09	0.53
1:D:21:MET:HE3	1:D:141:ARG:CD	2.38	0.53
1:D:212:GLU:HG2	1:D:212:GLU:O	2.08	0.53
1:F:505:LEU:O	1:F:506:SER:HB3	2.09	0.53
1:A:92:TRP:CD1	1:A:92:TRP:O	2.59	0.53
1:A:426:THR:HG22	1:A:428:SER:N	2.21	0.53
1:A:458:MET:O	3:F:901:ATP:H3'	2.09	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
1:D:294:LYS:HB2	3:D:901:ATP:O1B	2.08	0.53
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.38	0.53
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.24	0.53
1:C:52:LYS:HB2	3:C:903:ATP:O1B	2.09	0.53
1:C:287:THR:HG21	1:C:425:ILE:O	2.08	0.53
1:C:311:ARG:HD2	1:C:371:LYS:CE	2.38	0.53
1:C:430:ILE:O	1:C:432:TPO:N	2.42	0.53
1:E:123:LEU:HD23	1:E:127:ILE:CD1	2.38	0.53
1:E:191:ILE:CB	1:E:198:GLU:CG	2.87	0.53
1:E:437:ILE:HD12	1:E:457:LYS:HE2	1.90	0.53
1:F:122:ASP:OD2	1:F:123:LEU:N	2.42	0.53
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.39	0.53
1:D:359:HIS:O	1:D:363:ILE:HG13	2.08	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
1:E:255:THR:HG22	1:E:255:THR:O	2.08	0.52
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.42	0.52
1:F:379:SER:H	1:F:413:THR:HB	1.74	0.52
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.52
1:A:419:PHE:CE2	1:B:425:ILE:HD12	2.44	0.52
1:C:119:GLY:HA2	1:C:122:ASP:OD1	2.09	0.52
1:C:426:THR:HG21	1:C:430:ILE:HG12	1.90	0.52
1:D:471:MET:HB3	1:D:480:LYS:HZ3	1.75	0.52
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.74	0.52
1:F:500:ASP:O	1:F:501:GLU:HB3	2.09	0.52
1:A:451:ARG:NH1	1:A:451:ARG:CG	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:THR:HG23	1:D:203:ASN:HB2	1.90	0.52
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.91	0.52
1:C:123:LEU:O	1:C:126:LEU:N	2.42	0.52
1:D:255:THR:O	1:D:255:THR:HG22	2.09	0.52
1:F:79:THR:HG23	1:F:81:GLN:HE21	1.74	0.52
1:F:191:ILE:HG21	1:F:198:GLU:HG3	1.92	0.52
1:F:501:GLU:HG3	1:F:502:LYS:N	2.25	0.52
1:B:79:THR:HG23	1:B:81:GLN:HE21	1.74	0.52
1:B:81:GLN:H	1:B:81:GLN:CD	2.15	0.52
1:D:353:SER:O	1:D:354:ALA:HB2	2.10	0.52
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.90	0.52
1:F:52:LYS:HE3	3:F:903:ATP:O1B	2.09	0.52
1:F:191:ILE:CB	1:F:198:GLU:CG	2.80	0.52
1:F:396:VAL:O	1:F:400:THR:HB	2.10	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
1:B:273:MET:HE3	1:B:468:ARG:HD2	1.92	0.52
1:D:106:LEU:C	1:D:106:LEU:CD1	2.75	0.52
1:D:211:LEU:HD12	1:D:215:ARG:O	2.10	0.52
1:E:469:GLU:HG3	1:E:470:PHE:N	2.24	0.52
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.39	0.52
1:C:111:ASP:O	1:C:113:GLU:N	2.39	0.52
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.74	0.52
1:B:96:LYS:O	1:B:100:GLU:HG3	2.09	0.52
1:D:80:PRO:HD2	1:D:81:GLN:NE2	2.25	0.52
1:A:449:MET:HE3	1:B:467:ILE:HD11	1.92	0.52
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.24	0.52
1:B:91:GLY:O	1:B:92:TRP:CD1	2.63	0.52
1:B:178:THR:HG22	1:B:179:VAL:N	2.25	0.52
1:B:436:THR:HG23	1:B:458:MET:HG3	1.92	0.52
1:C:186:GLU:OE2	1:C:187:GLU:N	2.42	0.52
1:D:65:ILE:O	1:D:65:ILE:HG22	2.08	0.52
1:F:509:VAL:HG12	1:F:510:ARG:H	1.75	0.52
1:A:294:LYS:N	3:A:901:ATP:O1B	2.43	0.52
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.44	0.52
1:F:148:THR:OG1	1:F:182:THR:HG23	2.10	0.52
1:F:353:SER:O	1:F:354:ALA:HB2	2.10	0.52
1:C:336:GLU:OE1	1:C:336:GLU:HA	2.10	0.51
1:D:81:GLN:CD	1:D:81:GLN:N	2.68	0.51
1:D:419:PHE:CE2	1:E:425:ILE:HD12	2.44	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:E:433:ILE:HD12	1:E:433:ILE:N	2.25	0.51
1:A:89:SER:CB	1:B:227:GLY:O	2.59	0.51
1:B:52:LYS:HD3	1:B:182:THR:O	2.10	0.51
1:F:81:GLN:CD	1:F:81:GLN:N	2.69	0.51
1:F:502:LYS:HZ2	1:F:507:ARG:HB3	1.74	0.51
1:A:294:LYS:HB2	3:A:901:ATP:O1B	2.10	0.51
1:B:51:GLY:O	1:B:52:LYS:C	2.54	0.51
1:C:191:ILE:HB	1:C:198:GLU:HG3	1.91	0.51
1:D:350:TYR:O	1:D:351:PRO:C	2.51	0.51
1:D:471:MET:HE2	1:D:478:ASP:CB	2.40	0.51
1:E:123:LEU:O	1:E:127:ILE:HG13	2.10	0.51
1:E:262:ARG:NH2	1:E:461:SER:HB2	2.26	0.51
1:F:197:GLU:H	1:F:197:GLU:CD	2.18	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:38:ILE:HA	1:B:177:THR:HG23	1.92	0.51
1:B:286:ALA:HA	1:B:438:ILE:O	2.11	0.51
1:C:151:PHE:C	1:C:153:GLN:N	2.55	0.51
1:D:300:ARG:N	1:D:333:MET:HE1	2.25	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
1:B:191:ILE:CG2	1:B:198:GLU:HG3	2.40	0.51
1:C:164:LEU:CD2	1:C:180:MET:HE1	2.40	0.51
1:D:45:SER:CB	1:D:182:THR:HB	2.41	0.51
1:D:432:TPO:H2	1:D:434:THR:HG22	1.74	0.51
1:E:379:SER:H	1:E:413:THR:HB	1.76	0.51
1:E:471:MET:HG3	1:E:478:ASP:HB3	1.92	0.51
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.41	0.51
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.93	0.51
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.40	0.51
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.46	0.51
1:D:300:ARG:HA	1:D:333:MET:HE1	1.91	0.51
1:D:332:GLY:O	1:D:333:MET:O	2.28	0.51
1:E:49:GLY:HA2	3:E:903:ATP:O2B	2.09	0.51
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.91	0.51
1:F:270:LEU:O	1:F:273:MET:HB2	2.11	0.51
1:A:56:SER:HB2	1:A:143:SER:HB3	1.92	0.51
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.76	0.51
1:B:246:ILE:O	1:B:248:PRO:HD3	2.10	0.51
1:C:134:ILE:HG23	1:C:139:ALA:HB3	1.91	0.51
1:A:425:ILE:HD12	1:F:419:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ALA:C	1:C:38:ILE:HD12	2.36	0.51
1:C:79:THR:HG21	1:C:81:GLN:HG2	1.91	0.51
1:C:295:THR:HG21	1:C:319:GLU:OE2	2.11	0.51
1:D:19:ALA:O	1:D:38:ILE:HD12	2.11	0.51
1:D:335:PHE:HA	1:D:338:MET:HG3	1.93	0.51
1:D:385:ARG:HG2	1:E:393:ARG:NH1	2.26	0.51
1:D:484:ARG:HB3	1:D:484:ARG:NH1	2.25	0.51
1:B:79:THR:HG23	1:B:81:GLN:H	1.75	0.51
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.92	0.51
1:C:123:LEU:HD11	1:C:163:GLU:O	2.10	0.51
1:E:81:GLN:H	1:E:81:GLN:CD	2.19	0.51
1:E:191:ILE:CB	1:E:198:GLU:HG3	2.41	0.51
1:F:81:GLN:NE2	1:F:81:GLN:N	2.59	0.51
1:F:170:ARG:O	1:F:174:ILE:HG12	2.11	0.51
1:A:148:THR:HG1	1:A:182:THR:HG23	1.76	0.50
1:B:49:GLY:O	1:B:218:ARG:NH2	2.44	0.50
1:C:120:GLY:O	1:C:122:ASP:N	2.44	0.50
1:C:191:ILE:HB	1:C:198:GLU:CD	2.35	0.50
1:D:496:ARG:CG	1:E:487:GLU:OE1	2.59	0.50
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.42	0.50
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.11	0.50
1:C:24:MET:HB2	1:C:62:ASN:HD22	1.76	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:C:344:LEU:HD22	1:C:345:LYS:H	1.75	0.50
1:D:340:ARG:C	1:D:342:ASN:N	2.68	0.50
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.94	0.50
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.41	0.50
1:F:462:TRP:O	1:F:463:HIS:O	2.28	0.50
1:A:18:ILE:N	1:A:18:ILE:CD1	2.74	0.50
1:A:436:THR:HG23	1:A:458:MET:HG3	1.93	0.50
1:E:347:VAL:O	1:E:348:CYS:HB2	2.11	0.50
1:C:420:MET:CE	1:D:490:ILE:HG21	2.41	0.50
1:C:431:SEP:O	1:C:432:TPO:CG2	2.59	0.50
1:D:191:ILE:CB	1:D:198:GLU:CG	2.86	0.50
1:D:273:MET:CE	1:D:468:ARG:HD2	2.41	0.50
1:E:169:ALA:O	1:E:173:GLN:HG3	2.11	0.50
1:E:262:ARG:HH22	1:E:461:SER:HB2	1.76	0.50
1:F:120:GLY:O	1:F:123:LEU:HB3	2.11	0.50
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.41	0.50
1:B:91:GLY:C	1:B:92:TRP:CD1	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:HB2	1:C:423:HIS:O	2.11	0.50
1:C:38:ILE:HA	1:C:177:THR:HG23	1.94	0.50
1:D:313:ILE:HD11	1:D:372:PRO:HG3	1.94	0.50
1:B:287:THR:HG23	1:B:414:ASN:HB3	1.94	0.50
1:D:159:VAL:O	1:D:163:GLU:HG2	2.12	0.50
1:E:146:SER:CA	1:E:181:THR:HG22	2.41	0.50
1:E:363:ILE:O	1:E:367:ILE:HG13	2.12	0.50
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.11	0.50
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.76	0.50
1:C:323:GLN:NE2	1:D:459:ARG:HD3	2.27	0.50
1:D:79:THR:HG23	1:D:81:GLN:N	2.26	0.50
1:D:451:ARG:HB3	1:D:470:PHE:CE2	2.47	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.77	0.50
1:F:471:MET:CG	1:F:478:ASP:HB3	2.42	0.50
1:F:509:VAL:HG12	1:F:510:ARG:N	2.27	0.50
1:A:254:LEU:HG	1:F:320:SER:HA	1.94	0.50
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.50
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.94	0.50
1:C:123:LEU:O	1:C:124:SER:C	2.54	0.50
1:C:419:PHE:HD1	1:C:420:MET:HG3	1.75	0.50
1:D:433:ILE:HG22	1:D:433:ILE:O	2.10	0.50
1:A:425:ILE:HD12	1:F:419:PHE:CD2	2.46	0.49
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.94	0.49
1:C:38:ILE:HA	1:C:177:THR:CG2	2.42	0.49
1:C:495:THR:HG22	1:D:487:GLU:OE2	2.11	0.49
1:E:497:ILE:C	1:E:498:THR:HG23	2.37	0.49
1:F:396:VAL:HG11	1:F:430:ILE:HG21	1.92	0.49
1:B:31:ILE:HA	1:B:231:MET:SD	2.52	0.49
1:B:377:ILE:HD12	1:B:412:PHE:CD2	2.46	0.49
1:C:36:LEU:HD12	1:C:59:PHE:CE1	2.46	0.49
1:C:54:LEU:HD13	1:C:90:PHE:CE1	2.47	0.49
1:C:287:THR:HG23	1:C:414:ASN:ND2	2.22	0.49
1:D:396:VAL:HG11	1:D:430:ILE:HG23	1.93	0.49
1:D:468:ARG:NH1	1:D:468:ARG:HG2	2.27	0.49
1:E:496:ARG:C	1:E:497:ILE:HD13	2.37	0.49
1:B:191:ILE:HG21	1:B:198:GLU:HG3	1.94	0.49
1:F:300:ARG:N	1:F:333:MET:HE1	2.26	0.49
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.77	0.49
1:B:126:LEU:C	1:B:128:GLU:N	2.68	0.49
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.93	0.49
1:B:499:VAL:C	1:B:501:GLU:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:N	3:C:903:ATP:O1B	2.42	0.49
1:C:111:ASP:OD1	1:C:113:GLU:HG2	2.12	0.49
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.13	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
1:C:311:ARG:HD2	1:C:371:LYS:CD	2.42	0.49
1:F:79:THR:CG2	1:F:82:ASP:H	2.13	0.49
1:F:406:GLU:HB3	1:F:408:ILE:HG13	1.94	0.49
1:B:68:ASP:CG	1:B:102:LYS:HZ1	2.19	0.49
1:F:121:PHE:O	1:F:125:ALA:N	2.41	0.49
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.94	0.49
1:A:318:GLU:CD	1:B:432:TPO:HG23	2.37	0.49
1:C:54:LEU:HD13	1:C:90:PHE:CZ	2.48	0.49
1:C:318:GLU:CD	1:C:379:SER:HB2	2.38	0.49
1:C:469:GLU:HB2	1:C:483:PHE:CZ	2.47	0.49
1:D:263:VAL:CG1	1:D:374:ARG:HH21	2.21	0.49
1:E:430:ILE:O	1:E:431:SEP:C	2.60	0.49
1:A:267:VAL:O	1:A:271:ASP:OD2	2.31	0.49
1:B:107:ASP:C	1:B:107:ASP:OD1	2.56	0.49
1:C:70:PRO:HG2	1:C:138:ARG:O	2.12	0.49
1:D:197:GLU:H	1:D:197:GLU:CD	2.19	0.49
1:E:21:MET:CE	1:E:59:PHE:CZ	2.96	0.49
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.95	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.93	0.49
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.93	0.49
1:D:148:THR:OG1	1:D:182:THR:CG2	2.60	0.49
1:D:273:MET:HE3	1:D:468:ARG:HD2	1.95	0.49
1:F:220:LEU:HD23	1:F:220:LEU:C	2.38	0.49
1:A:471:MET:HG2	1:A:480:LYS:HE2	1.94	0.49
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.95	0.49
1:B:419:PHE:CD2	1:C:425:ILE:CD1	2.93	0.49
3:B:903:ATP:O3'	1:C:224:LYS:HB2	2.13	0.49
1:C:67:PHE:CB	1:C:69:GLU:HG3	2.40	0.49
1:E:79:THR:HG23	1:E:81:GLN:H	1.76	0.49
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.49
1:A:21:MET:HE1	1:A:141:ARG:HG2	1.95	0.48
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.95	0.48
1:C:325:LEU:CD2	1:C:335:PHE:HB2	2.43	0.48
1:C:332:GLY:O	1:C:333:MET:O	2.30	0.48
1:D:151:PHE:O	1:D:153:GLN:N	2.42	0.48
1:D:347:VAL:O	1:D:348:CYS:CB	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:SER:OG	1:D:462:TRP:N	2.45	0.48
1:E:211:LEU:O	1:E:212:GLU:CB	2.61	0.48
1:E:417:ASP:O	1:F:424:SER:HB3	2.13	0.48
1:F:169:ALA:O	1:F:173:GLN:HG3	2.12	0.48
1:F:501:GLU:HG3	1:F:502:LYS:H	1.78	0.48
1:A:19:ALA:O	1:A:38:ILE:HD12	2.13	0.48
1:A:81:GLN:CD	1:A:81:GLN:N	2.71	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
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.29	0.48
1:B:323:GLN:NE2	1:C:459:ARG:HD3	2.28	0.48
1:B:344:LEU:HD13	1:B:344:LEU:C	2.38	0.48
1:B:431:SEP:O	1:B:434:THR:CG2	2.33	0.48
1:C:471:MET:HB3	1:C:480:LYS:NZ	2.27	0.48
1:D:299:SER:HB3	1:D:333:MET:CE	2.42	0.48
1:E:186:GLU:HB3	1:E:189:GLY:HA3	1.95	0.48
1:B:396:VAL:O	1:B:400:THR:HB	2.13	0.48
1:B:471:MET:HE2	1:B:478:ASP:HB2	1.94	0.48
1:C:21:MET:HE3	1:C:141:ARG:CZ	2.42	0.48
1:F:426:THR:CG2	1:F:428:SER:OG	2.60	0.48
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.47	0.48
1:B:184:ARG:C	1:B:185:ILE:HD13	2.38	0.48
1:C:263:VAL:CG1	1:C:374:ARG:HH21	2.27	0.48
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.48	0.48
1:B:340:ARG:C	1:B:342:ASN:N	2.71	0.48
1:C:58:GLN:HG3	1:C:92:TRP:CH2	2.48	0.48
1:C:350:TYR:CZ	1:D:252:MET:HE3	2.48	0.48
1:D:363:ILE:O	1:D:367:ILE:HG13	2.13	0.48
3:D:903:ATP:O3'	1:E:224:LYS:HB2	2.14	0.48
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.95	0.48
1:F:65:ILE:O	1:F:65:ILE:HG22	2.12	0.48
1:F:311:ARG:HD2	1:F:371:LYS:HD2	1.95	0.48
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.78	0.48
1:A:49:GLY:O	1:A:218:ARG:NH2	2.47	0.48
1:A:433:ILE:HD12	1:A:433:ILE:N	2.29	0.48
1:B:281:ASP:O	1:B:282:SER:HB3	2.13	0.48
1:C:41:SER:HA	1:C:178:THR:O	2.13	0.48
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.48
1:F:344:LEU:C	1:F:344:LEU:HD13	2.39	0.48
1:B:126:LEU:C	1:B:128:GLU:H	2.21	0.48
1:C:44:VAL:HA	1:C:205:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLY:C	1:C:122:ASP:N	2.71	0.48
1:C:340:ARG:C	1:C:342:ASN:N	2.71	0.48
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.44	0.48
1:F:81:GLN:H	1:F:81:GLN:CD	2.19	0.48
1:A:81:GLN:H	1:A:81:GLN:NE2	2.11	0.48
1:A:387:VAL:HG12	1:A:388:SER:N	2.28	0.48
1:C:396:VAL:O	1:C:400:THR:HB	2.14	0.48
1:D:174:ILE:O	1:D:174:ILE:HG22	2.13	0.48
1:D:323:GLN:NE2	1:E:459:ARG:HD3	2.28	0.48
1:E:123:LEU:HD23	1:E:127:ILE:CG1	2.43	0.48
1:F:514:GLU:HB3	1:F:519:SER:HB3	1.96	0.48
1:B:21:MET:HE3	1:B:141:ARG:CZ	2.43	0.48
1:C:49:GLY:CA	3:C:903:ATP:O2B	2.62	0.48
1:F:79:THR:O	1:F:83:ILE:HD12	2.14	0.48
1:A:70:PRO:HA	1:A:102:LYS:O	2.14	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:311:ARG:HA	1:B:343:LEU:O	2.13	0.48
1:E:52:LYS:HD3	1:E:182:THR:O	2.13	0.48
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.29	0.48
1:E:336:GLU:OE1	1:E:336:GLU:HA	2.14	0.48
1:A:164:LEU:CD2	1:A:180:MET:HE1	2.44	0.47
1:B:347:VAL:O	1:B:348:CYS:HB2	2.13	0.47
1:C:98:VAL:HA	1:C:103:LEU:O	2.14	0.47
1:C:305:ALA:CB	1:C:374:ARG:HD2	2.39	0.47
1:D:21:MET:CE	1:D:59:PHE:CZ	2.98	0.47
1:E:79:THR:O	1:E:83:ILE:HD12	2.14	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
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.47	0.47
1:B:396:VAL:HG11	1:B:430:ILE:CG2	2.45	0.47
1:D:388:SER:OG	1:D:391:ALA:CB	2.62	0.47
1:E:344:LEU:C	1:E:344:LEU:CD1	2.86	0.47
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.13	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:61:TYR:CE1	1:B:92:TRP:HB3	2.49	0.47
1:C:354:ALA:HB1	1:C:358:ASP:HB2	1.95	0.47
1:C:367:ILE:HG12	1:C:375:ILE:CD1	2.44	0.47
1:D:98:VAL:HA	1:D:103:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:ILE:O	1:E:498:THR:CB	2.62	0.47
1:F:507:ARG:O	1:F:508:ILE:C	2.57	0.47
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.47
1:B:419:PHE:HD1	1:B:420:MET:HG3	1.79	0.47
1:C:311:ARG:HA	1:C:343:LEU:O	2.14	0.47
1:D:52:LYS:HD3	1:D:182:THR:O	2.14	0.47
1:D:356:LEU:HD21	1:D:387:VAL:HG11	1.96	0.47
1:E:23:THR:C	1:E:25:ILE:H	2.22	0.47
1:E:271:ASP:OD1	1:E:277:GLY:HA2	2.14	0.47
1:E:332:GLY:O	1:E:333:MET:O	2.32	0.47
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.49	0.47
1:A:385:ARG:NE	1:B:432:TPO:O2P	2.47	0.47
1:B:60:LEU:HD12	1:B:73:PHE:HB2	1.96	0.47
1:B:111:ASP:O	1:B:113:GLU:N	2.47	0.47
1:B:123:LEU:HD13	1:B:127:ILE:HD11	1.97	0.47
1:D:150:VAL:HG13	1:D:151:PHE:N	2.28	0.47
1:D:269:ARG:HB3	1:D:479:ILE:HD12	1.97	0.47
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.43	0.47
1:E:344:LEU:HD22	1:E:345:LYS:N	2.29	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:B:431:SEP:C	1:B:434:THR:HG22	2.32	0.47
3:B:901:ATP:C5	1:C:461:SER:O	2.68	0.47
1:C:320:SER:HA	1:D:254:LEU:HG	1.95	0.47
1:D:289:ALA:HB2	1:D:419:PHE:HA	1.94	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:151:PHE:C	1:B:153:GLN:N	2.69	0.47
1:B:264:SER:HA	1:B:271:ASP:OD1	2.14	0.47
1:B:294:LYS:N	3:B:901:ATP:O1B	2.48	0.47
1:C:451:ARG:NH1	1:C:451:ARG:CG	2.77	0.47
1:D:305:ALA:HB2	1:D:374:ARG:CD	2.37	0.47
1:E:18:ILE:HD13	1:E:227:GLY:HA3	1.94	0.47
1:E:76:PHE:HZ	1:E:126:LEU:CD2	2.28	0.47
1:E:79:THR:O	1:E:80:PRO:C	2.57	0.47
1:E:311:ARG:HA	1:E:343:LEU:O	2.15	0.47
1:E:471:MET:HB3	1:E:480:LYS:HZ1	1.78	0.47
1:E:487:GLU:O	1:E:488:ARG:HB2	2.13	0.47
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.80	0.47
1:F:184:ARG:HG2	1:F:191:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ARG:HD2	1:F:371:LYS:NZ	2.29	0.47
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.50	0.47
1:C:88:ARG:HD3	1:D:15:HIS:C	2.40	0.47
1:D:412:PHE:CD1	1:D:412:PHE:N	2.83	0.47
1:E:18:ILE:CG1	1:E:228:THR:HG23	2.44	0.47
1:F:451:ARG:HG2	1:F:451:ARG:NH1	2.30	0.47
1:A:268:VAL:O	1:A:271:ASP:HB2	2.15	0.47
1:B:211:LEU:O	1:B:212:GLU:HB3	2.13	0.47
1:B:421:GLY:O	1:B:422:ALA:C	2.56	0.47
1:C:448:GLU:HG2	1:D:466:ALA:HA	1.97	0.47
1:C:489:ILE:O	1:C:490:ILE:C	2.56	0.47
1:D:468:ARG:HG2	1:D:468:ARG:HH11	1.78	0.47
1:E:148:THR:HG1	1:E:182:THR:HG23	1.78	0.47
1:E:345:LYS:NZ	1:E:366:GLU:CG	2.78	0.47
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.80	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:C:121:PHE:O	1:C:122:ASP:C	2.58	0.47
1:D:213:GLY:O	1:D:214:GLU:HB2	2.15	0.47
1:D:323:GLN:HE22	1:E:459:ARG:HD3	1.79	0.47
1:E:313:ILE:HD11	1:E:372:PRO:HG3	1.97	0.47
1:F:65:ILE:O	1:F:65:ILE:CG2	2.61	0.47
1:A:487:GLU:OE1	1:F:496:ARG:HD3	2.16	0.46
1:B:18:ILE:HB	1:B:228:THR:CG2	2.44	0.46
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.30	0.46
1:B:492:GLY:C	1:B:494:PRO:HD3	2.41	0.46
1:A:150:VAL:CG1	1:A:151:PHE:N	2.78	0.46
1:B:125:ALA:O	1:B:128:GLU:HB2	2.15	0.46
1:B:150:VAL:HG13	1:B:151:PHE:N	2.29	0.46
1:B:182:THR:HG22	1:B:183:GLU:N	2.30	0.46
1:B:219:THR:HA	1:B:235:TYR:O	2.14	0.46
1:B:323:GLN:HE22	1:C:459:ARG:HD3	1.79	0.46
1:C:353:SER:O	1:C:354:ALA:HB2	2.14	0.46
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.97	0.46
1:E:344:LEU:HD22	1:E:345:LYS:H	1.81	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:A:514:GLU:C	1:A:515:LYS:HD2	2.40	0.46
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.44	0.46
1:E:49:GLY:O	1:E:218:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:THR:HG23	1:E:81:GLN:NE2	2.30	0.46
1:F:117:VAL:HG13	1:F:154:TYR:OH	2.16	0.46
1:F:360:LEU:O	1:F:360:LEU:HD22	2.15	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.97	0.46
1:B:90:PHE:O	1:B:92:TRP:NE1	2.48	0.46
1:B:419:PHE:CE2	1:C:425:ILE:HD12	2.49	0.46
1:C:377:ILE:HD12	1:C:412:PHE:HE2	1.79	0.46
1:C:468:ARG:HG2	1:C:468:ARG:HH11	1.80	0.46
1:E:314:LEU:C	1:E:314:LEU:HD12	2.41	0.46
1:F:306:CYS:C	1:F:308:ASN:N	2.72	0.46
1:A:471:MET:HE1	1:A:473:SER:OG	2.15	0.46
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.84	0.46
1:D:231:MET:HE1	1:D:251:ALA:CB	2.37	0.46
1:D:345:LYS:HZ2	1:D:366:GLU:CG	2.23	0.46
1:E:166:ARG:O	1:E:169:ALA:HB3	2.15	0.46
1:E:340:ARG:O	1:E:342:ASN:N	2.49	0.46
1:F:486:PHE:CE2	1:F:496:ARG:CD	2.81	0.46
1:A:82:ASP:O	1:A:83:ILE:C	2.57	0.46
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.96	0.46
1:A:518:GLU:HB2	1:A:519:SER:H	1.55	0.46
1:B:56:SER:HB2	1:B:143:SER:HB3	1.98	0.46
1:B:125:ALA:O	1:B:129:ARG:HG3	2.16	0.46
1:B:387:VAL:HG12	1:B:388:SER:N	2.29	0.46
1:C:300:ARG:N	1:C:333:MET:HE1	2.31	0.46
1:C:332:GLY:O	1:C:333:MET:C	2.58	0.46
1:C:446:ARG:HA	1:C:496:ARG:NH2	2.30	0.46
1:E:483:PHE:HB2	1:E:489:ILE:HD11	1.97	0.46
3:E:901:ATP:H3'	1:F:458:MET:O	2.16	0.46
1:F:115:GLN:HG3	1:F:116:GLU:N	1.94	0.46
1:F:336:GLU:HA	1:F:336:GLU:OE1	2.16	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:23:THR:O	1:B:24:MET:HB2	2.15	0.46
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.66	0.46
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.80	0.46
1:D:21:MET:CE	1:D:141:ARG:HG2	2.46	0.46
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.60	0.46
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.29	0.46
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.46
1:A:429:HIS:O	1:A:432:TPO:O2P	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:CA	1:B:333:MET:HE1	2.43	0.46
1:C:430:ILE:O	1:C:433:ILE:HG12	2.16	0.46
1:D:170:ARG:O	1:D:174:ILE:HG12	2.16	0.46
1:E:489:ILE:O	1:E:490:ILE:C	2.57	0.46
1:F:165:PHE:O	1:F:166:ARG:C	2.58	0.46
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.51	0.46
1:F:504:GLU:HB3	1:F:507:ARG:HH21	1.77	0.46
1:B:397:ILE:HD11	1:B:433:ILE:CD1	2.46	0.46
1:B:432:TPO:C	1:B:434:THR:H	2.29	0.46
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.97	0.46
1:E:313:ILE:CD1	1:E:372:PRO:HG3	2.46	0.46
1:E:499:VAL:O	1:E:499:VAL:CG1	2.61	0.46
1:F:116:GLU:C	1:F:117:VAL:HG23	2.41	0.46
1:F:264:SER:O	1:F:374:ARG:NH2	2.47	0.46
1:F:446:ARG:H	1:F:496:ARG:NH2	2.14	0.46
1:B:81:GLN:CD	1:B:81:GLN:N	2.73	0.46
1:B:379:SER:H	1:B:413:THR:CG2	2.29	0.46
1:C:344:LEU:C	1:C:344:LEU:HD13	2.41	0.46
1:C:489:ILE:C	1:C:491:SER:N	2.71	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
1:B:19:ALA:C	1:B:38:ILE:HD12	2.41	0.45
1:B:20:LYS:C	1:B:38:ILE:HD11	2.41	0.45
1:B:492:GLY:O	1:B:494:PRO:HD3	2.17	0.45
1:C:50:THR:HG22	1:C:209:ASN:HB2	1.98	0.45
1:C:150:VAL:CG1	1:C:151:PHE:N	2.80	0.45
1:C:164:LEU:HD21	1:C:180:MET:HE1	1.98	0.45
1:C:185:ILE:HA	4:D:527:HOH:O	2.15	0.45
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.32	0.45
1:A:485:ASN:OD1	1:A:485:ASN:N	2.39	0.45
1:A:487:GLU:OE1	1:F:495:THR:HA	2.16	0.45
1:B:106:LEU:C	1:B:106:LEU:CD1	2.89	0.45
1:C:197:GLU:H	1:C:197:GLU:CD	2.14	0.45
1:D:338:MET:H	1:D:338:MET:HG2	1.58	0.45
1:E:45:SER:HB2	1:E:182:THR:HB	1.97	0.45
1:F:256:GLN:H	1:F:256:GLN:HG2	1.46	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:B:64:ILE:HG21	1:B:97:LEU:HD13	1.98	0.45
1:B:483:PHE:HB2	1:B:489:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLU:O	1:C:208:ARG:HD3	2.17	0.45
1:C:211:LEU:O	1:C:212:GLU:HB3	2.16	0.45
1:C:325:LEU:HD23	1:C:335:PHE:HB2	1.98	0.45
1:C:471:MET:CG	1:C:478:ASP:HB3	2.47	0.45
1:D:79:THR:HG23	1:D:81:GLN:NE2	2.31	0.45
1:D:106:LEU:HD11	1:D:129:ARG:CZ	2.45	0.45
1:D:455:VAL:HG11	1:D:463:HIS:HB2	1.97	0.45
1:E:353:SER:O	1:E:354:ALA:HB2	2.16	0.45
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.31	0.45
1:F:38:ILE:HG22	1:F:39:GLY:N	2.31	0.45
1:F:433:ILE:O	1:F:433:ILE:HG22	2.15	0.45
1:A:432:TPO:O1P	1:A:432:TPO:CG2	2.65	0.45
1:A:436:THR:OG1	1:A:458:MET:HG2	2.17	0.45
1:C:47:THR:O	1:C:48:SER:C	2.55	0.45
1:C:120:GLY:C	1:C:122:ASP:H	2.24	0.45
1:C:387:VAL:HG12	1:C:388:SER:N	2.31	0.45
1:C:430:ILE:HG23	1:C:433:ILE:HD11	1.98	0.45
1:C:439:LEU:HD12	1:C:440:LEU:N	2.31	0.45
1:D:436:THR:HG23	1:D:458:MET:HG3	1.98	0.45
1:D:448:GLU:HG2	1:E:466:ALA:HA	1.98	0.45
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.97	0.45
1:A:299:SER:C	1:A:333:MET:CE	2.89	0.45
1:B:79:THR:C	1:B:83:ILE:HD12	2.41	0.45
1:C:144:ILE:HG21	1:C:147:VAL:HG12	1.99	0.45
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.69	0.45
1:D:44:VAL:HG22	1:D:205:VAL:HB	1.98	0.45
1:D:122:ASP:HB3	1:D:123:LEU:H	1.44	0.45
1:D:314:LEU:C	1:D:314:LEU:HD12	2.40	0.45
1:E:345:LYS:HZ3	1:E:366:GLU:CG	2.30	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:469:GLU:HG3	1:B:470:PHE:N	2.30	0.45
1:C:14:GLU:CG	1:C:16:GLN:HB2	2.46	0.45
1:D:146:SER:CA	1:D:181:THR:HG22	2.45	0.45
1:D:371:LYS:CD	1:D:371:LYS:C	2.89	0.45
1:D:426:THR:HG21	1:D:430:ILE:HG12	1.98	0.45
1:E:116:GLU:O	1:E:118:VAL:HG23	2.16	0.45
1:E:393:ARG:O	1:E:397:ILE:HG12	2.17	0.45
1:F:79:THR:HG21	1:F:81:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:ARG:HH21	1:F:236:PRO:HB3	1.81	0.45
1:F:469:GLU:HG3	1:F:470:PHE:N	2.32	0.45
1:A:21:MET:CE	1:A:59:PHE:HZ	2.28	0.45
1:A:57:ILE:CD1	1:A:73:PHE:CE1	3.00	0.45
1:A:85:LYS:O	1:A:88:ARG:HB2	2.17	0.45
1:B:296:LEU:HD13	1:B:331:TRP:CD2	2.52	0.45
1:D:379:SER:H	1:D:413:THR:HB	1.82	0.45
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.98	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
1:C:85:LYS:NZ	1:D:14:GLU:HB3	2.32	0.45
1:C:488:ARG:HG3	1:C:488:ARG:NH1	2.31	0.45
1:D:147:VAL:CG2	1:D:148:THR:N	2.79	0.45
1:E:146:SER:HA	1:E:181:THR:O	2.17	0.45
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.95	0.45
1:F:300:ARG:CA	1:F:333:MET:HE1	2.47	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:141:ARG:HB2	4:B:521:HOH:O	2.17	0.45
1:F:137:TYR:O	1:F:138:ARG:HB2	2.17	0.45
1:F:266:GLY:O	1:F:300:ARG:CG	2.65	0.45
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.47	0.45
1:A:504:GLU:O	1:A:506:SER:N	2.49	0.45
1:B:191:ILE:CB	1:B:198:GLU:CG	2.87	0.45
1:B:302:VAL:HG13	1:B:344:LEU:HD23	1.99	0.45
1:B:471:MET:HE1	1:B:473:SER:CB	2.45	0.45
1:D:153:GLN:C	1:D:154:TYR:CG	2.94	0.45
1:F:186:GLU:OE2	1:F:187:GLU:N	2.50	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:B:21:MET:CE	1:B:59:PHE:CZ	3.00	0.44
1:B:186:GLU:OE2	1:B:187:GLU:N	2.50	0.44
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.98	0.44
1:C:358:ASP:O	1:C:362:ILE:HG12	2.17	0.44
1:E:340:ARG:C	1:E:342:ASN:H	2.23	0.44
1:F:68:ASP:OD2	1:F:102:LYS:NZ	2.51	0.44
1:F:371:LYS:O	1:F:371:LYS:HD2	2.16	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:C:144:ILE:CG2	1:C:147:VAL:HG12	2.46	0.44
1:C:215:ARG:HB3	4:C:521:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:N	3:D:903:ATP:O1B	2.50	0.44
1:D:338:MET:HB2	1:D:344:LEU:HB3	1.99	0.44
1:E:211:LEU:HD12	1:E:215:ARG:O	2.16	0.44
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.53	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
1:B:487:GLU:O	1:B:494:PRO:HA	2.17	0.44
1:C:75:THR:HG23	1:C:75:THR:O	2.17	0.44
1:F:503:SER:O	1:F:504:GLU:C	2.61	0.44
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.47	0.44
1:A:467:ILE:HD11	1:F:449:MET:HE3	2.00	0.44
1:B:212:GLU:O	1:B:212:GLU:HG2	2.15	0.44
1:C:116:GLU:O	1:C:117:VAL:HB	2.16	0.44
1:C:426:THR:HG22	1:C:428:SER:N	2.33	0.44
1:D:31:ILE:HA	1:D:231:MET:SD	2.58	0.44
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.99	0.44
1:E:121:PHE:O	1:E:122:ASP:C	2.60	0.44
1:E:164:LEU:HA	1:E:164:LEU:HD23	1.65	0.44
1:A:28:PHE:CD2	1:A:28:PHE:C	2.95	0.44
1:A:273:MET:SD	1:A:468:ARG:HD2	2.57	0.44
1:D:381:SER:HB3	1:D:414:ASN:OD1	2.18	0.44
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.48	0.44
1:E:122:ASP:O	1:E:123:LEU:C	2.60	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:33:HIS:HD2	1:F:229:SER:OG	1.98	0.44
1:B:146:SER:HA	1:B:181:THR:HG22	2.00	0.44
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.82	0.44
1:C:18:ILE:N	1:C:18:ILE:CD1	2.81	0.44
1:C:419:PHE:CD2	1:D:425:ILE:CD1	3.00	0.44
1:D:299:SER:C	1:D:333:MET:CE	2.87	0.44
1:D:344:LEU:HD22	1:D:345:LYS:H	1.82	0.44
1:E:432:TPO:OG1	1:E:433:ILE:CD1	2.56	0.44
1:F:21:MET:HE3	1:F:141:ARG:NE	2.33	0.44
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.17	0.44
1:B:146:SER:CA	1:B:181:THR:HG22	2.47	0.44
1:B:502:LYS:HG3	1:B:504:GLU:C	2.42	0.44
1:C:315:PHE:CE1	1:C:363:ILE:HG23	2.52	0.44
1:E:147:VAL:CG2	1:E:148:THR:N	2.80	0.44
1:E:471:MET:HE1	1:E:473:SER:OG	2.17	0.44
1:F:311:ARG:HD2	1:F:371:LYS:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:GLU:CA	1:F:507:ARG:HE	2.31	0.44
1:A:452:ALA:HA	1:A:468:ARG:O	2.17	0.44
1:B:122:ASP:C	1:B:124:SER:H	2.25	0.44
1:B:499:VAL:C	1:B:501:GLU:N	2.76	0.44
3:C:903:ATP:O3G	1:D:224:LYS:NZ	2.51	0.44
1:D:89:SER:HB2	1:E:227:GLY:O	2.17	0.44
1:E:292:THR:OG1	1:E:294:LYS:HD3	2.18	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HD12	2.00	0.44
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.99	0.44
1:B:122:ASP:C	1:B:124:SER:N	2.75	0.44
1:C:418:GLN:HB2	1:D:423:HIS:O	2.18	0.44
1:C:419:PHE:CE2	1:D:425:ILE:HD12	2.53	0.44
1:C:471:MET:HE1	1:C:473:SER:OG	2.17	0.44
1:D:65:ILE:O	1:D:65:ILE:CG2	2.66	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG3	2.00	0.44
1:F:462:TRP:CD2	1:F:462:TRP:C	2.94	0.44
1:A:153:GLN:C	1:A:154:TYR:CG	2.95	0.43
1:A:350:TYR:CZ	1:B:252:MET:HE3	2.53	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
3:A:901:ATP:C5	1:B:461:SER:O	2.71	0.43
1:C:82:ASP:O	1:C:83:ILE:C	2.61	0.43
1:C:294:LYS:N	3:C:901:ATP:O1B	2.51	0.43
1:D:33:HIS:HD2	1:D:229:SER:OG	2.01	0.43
1:D:311:ARG:HG3	1:D:371:LYS:NZ	2.32	0.43
1:E:212:GLU:CG	1:E:213:GLY:N	2.79	0.43
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.48	0.43
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.17	0.43
1:C:123:LEU:O	1:C:125:ALA:N	2.51	0.43
1:C:433:ILE:HD13	1:C:433:ILE:HG21	1.74	0.43
1:E:293:GLY:HA2	3:E:901:ATP:O1A	2.18	0.43
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.48	0.43
1:F:156:ALA:O	1:F:159:VAL:HG23	2.18	0.43
1:F:452:ALA:HB1	1:F:467:ILE:HG22	1.99	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:B:490:ILE:HD13	1:B:490:ILE:HA	1.75	0.43
1:D:318:GLU:OE2	1:D:379:SER:HB2	2.18	0.43
1:E:123:LEU:HD23	1:E:127:ILE:HG13	1.99	0.43
1:E:497:ILE:O	1:E:498:THR:HG23	2.18	0.43
1:F:120:GLY:C	1:F:123:LEU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:GLY:O	1:F:333:MET:O	2.36	0.43
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.53	0.43
1:B:418:GLN:O	1:B:418:GLN:CG	2.66	0.43
1:C:94:LEU:O	1:C:98:VAL:HG23	2.18	0.43
1:C:121:PHE:HB3	1:C:125:ALA:HB3	2.01	0.43
1:D:21:MET:HE1	1:D:177:THR:HB	2.00	0.43
1:D:46:GLY:HA2	4:D:520:HOH:O	2.17	0.43
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.18	0.43
1:E:445:ILE:O	1:E:446:ARG:HB2	2.18	0.43
1:F:31:ILE:HG22	1:F:222:ILE:CD1	2.47	0.43
1:F:430:ILE:HG22	1:F:433:ILE:HB	2.01	0.43
1:A:129:ARG:O	1:A:130:ILE:C	2.59	0.43
1:A:507:ARG:HG3	1:A:508:ILE:N	2.33	0.43
1:B:164:LEU:HB3	1:B:200:VAL:HG11	2.00	0.43
1:B:420:MET:HE3	1:B:420:MET:HB3	1.72	0.43
1:C:121:PHE:CD1	1:C:121:PHE:N	2.77	0.43
1:D:420:MET:HE3	1:D:492:GLY:HA3	1.99	0.43
1:D:426:THR:HG22	1:D:428:SER:N	2.28	0.43
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.38	0.43
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.33	0.43
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.01	0.43
1:B:359:HIS:O	1:B:363:ILE:HG13	2.19	0.43
1:B:500:ASP:O	1:B:503:SER:HB2	2.18	0.43
1:E:38:ILE:HA	1:E:177:THR:HG23	2.00	0.43
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.54	0.43
1:E:64:ILE:HD13	1:E:102:LYS:HB3	2.00	0.43
1:E:347:VAL:O	1:E:348:CYS:CB	2.64	0.43
1:A:169:ALA:HB3	1:F:112:PRO:HB3	2.00	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
1:B:345:LYS:HZ2	1:B:366:GLU:HG2	1.84	0.43
1:C:484:ARG:HB3	1:C:484:ARG:NH1	2.34	0.43
1:E:70:PRO:HB2	1:E:139:ALA:HA	2.01	0.43
1:E:273:MET:O	1:E:463:HIS:CA	2.62	0.43
1:F:255:THR:O	1:F:255:THR:HG22	2.18	0.43
1:F:358:ASP:O	1:F:362:ILE:HG12	2.19	0.43
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.48	0.43
1:A:87:ALA:O	1:A:92:TRP:NE1	2.51	0.43
1:A:429:HIS:HA	1:A:431:SEP:O2P	2.18	0.43
1:C:151:PHE:O	1:C:153:GLN:N	2.43	0.43
1:E:153:GLN:C	1:F:158:SER:HB2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:THR:O	1:E:451:ARG:NH1	2.52	0.43
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.49	0.43
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.83	0.43
1:F:506:SER:O	1:F:507:ARG:C	2.62	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:A:162:ARG:CZ	1:F:116:GLU:HG2	2.49	0.43
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.48	0.43
1:B:350:TYR:O	1:B:351:PRO:C	2.61	0.43
1:C:142:VAL:O	1:C:178:THR:HA	2.18	0.43
1:D:148:THR:HG21	1:D:193:ARG:HD2	2.01	0.43
1:D:496:ARG:HE	1:E:487:GLU:HG2	1.83	0.43
1:E:79:THR:HG23	1:E:81:GLN:CG	2.36	0.43
1:E:153:GLN:C	1:E:154:TYR:CG	2.97	0.43
1:E:306:CYS:C	1:E:308:ASN:N	2.77	0.43
1:F:367:ILE:HG12	1:F:375:ILE:HD11	2.01	0.43
1:A:425:ILE:CD1	1:F:419:PHE:CD2	3.01	0.43
1:A:445:ILE:HD12	1:A:486:PHE:CZ	2.54	0.43
1:B:53:THR:HG23	1:B:145:ASP:OD1	2.19	0.43
1:C:191:ILE:CG2	1:C:198:GLU:HG3	2.49	0.43
1:C:193:ARG:NH2	1:D:195:GLY:O	2.28	0.43
1:C:396:VAL:HG11	1:C:430:ILE:CG2	2.48	0.43
1:D:317:TYR:CE2	1:D:383:LEU:HD21	2.53	0.43
1:F:178:THR:HG22	1:F:179:VAL:N	2.34	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.34	0.43
1:F:484:ARG:NH1	1:F:484:ARG:CB	2.81	0.43
1:A:514:GLU:OE1	1:A:514:GLU:HA	2.11	0.42
1:B:300:ARG:N	1:B:333:MET:HE1	2.34	0.42
1:C:468:ARG:HG2	1:C:468:ARG:NH1	2.33	0.42
1:D:153:GLN:O	1:D:154:TYR:CB	2.66	0.42
1:E:106:LEU:HD13	1:E:129:ARG:CZ	2.49	0.42
1:E:311:ARG:HD2	1:E:371:LYS:HE3	2.01	0.42
1:E:419:PHE:O	1:E:420:MET:O	2.36	0.42
1:F:123:LEU:HD22	1:F:123:LEU:HA	1.90	0.42
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.84	0.42
1:B:180:MET:HE2	1:B:180:MET:HB3	1.90	0.42
1:C:337:GLU:OE1	1:C:340:ARG:NH1	2.52	0.42
1:C:497:ILE:C	1:C:498:THR:CG2	2.91	0.42
1:D:18:ILE:H	1:D:18:ILE:HD12	1.83	0.42
1:D:85:LYS:NZ	1:E:14:GLU:HB3	2.34	0.42
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ARG:C	1:E:342:ASN:N	2.77	0.42
1:F:46:GLY:HA2	1:F:184:ARG:HD2	2.00	0.42
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.46	0.42
1:F:223:LEU:HD23	1:F:223:LEU:HA	1.81	0.42
1:A:72:VAL:O	1:A:142:VAL:HA	2.19	0.42
1:B:44:VAL:HG22	1:B:205:VAL:HB	2.01	0.42
1:B:311:ARG:HD2	1:B:371:LYS:HE3	2.01	0.42
1:C:111:ASP:CG	1:C:113:GLU:HG2	2.43	0.42
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.18	0.42
3:E:903:ATP:PG	1:F:224:LYS:HZ2	2.40	0.42
1:F:200:VAL:O	1:F:200:VAL:HG12	2.18	0.42
1:F:387:VAL:HG12	1:F:388:SER:N	2.35	0.42
1:F:469:GLU:HB2	1:F:483:PHE:CZ	2.54	0.42
1:A:31:ILE:HD11	1:A:246:ILE:HG21	2.01	0.42
3:A:901:ATP:O2'	1:B:463:HIS:NE2	2.50	0.42
1:C:311:ARG:HD2	1:C:371:LYS:NZ	2.34	0.42
1:D:191:ILE:HG21	1:D:198:GLU:HG3	2.00	0.42
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.51	0.42
1:E:302:VAL:HG13	1:E:344:LEU:HD23	2.01	0.42
1:F:20:LYS:C	1:F:38:ILE:CD1	2.93	0.42
1:F:302:VAL:HG12	1:F:303:GLU:N	2.35	0.42
1:A:169:ALA:CB	1:F:112:PRO:HB3	2.50	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:A:508:ILE:H	1:A:508:ILE:HD13	1.83	0.42
1:A:514:GLU:HB3	1:A:515:LYS:HD2	2.02	0.42
1:B:72:VAL:O	1:B:142:VAL:HA	2.20	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.81	0.42
1:C:211:LEU:HD12	1:C:215:ARG:O	2.19	0.42
1:C:419:PHE:O	1:C:419:PHE:CG	2.72	0.42
1:D:287:THR:HA	1:D:414:ASN:O	2.20	0.42
1:E:43:LEU:HA	1:E:43:LEU:HD12	1.82	0.42
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.48	0.42
1:E:264:SER:O	1:E:374:ARG:NH2	2.51	0.42
1:E:299:SER:C	1:E:333:MET:HE1	2.44	0.42
1:E:379:SER:HA	1:E:413:THR:HG22	2.00	0.42
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.33	0.42
3:E:901:ATP:O2'	1:F:463:HIS:NE2	2.45	0.42
1:F:42:THR:HG23	1:F:203:ASN:HB2	2.02	0.42
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.49	0.42
1:F:338:MET:H	1:F:338:MET:HG2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.02	0.42
1:B:22:ARG:NH2	1:B:24:MET:SD	2.92	0.42
1:C:263:VAL:HG12	1:C:374:ARG:NH2	2.33	0.42
1:D:437:ILE:HD12	1:D:457:LYS:HG2	2.00	0.42
1:D:490:ILE:HD12	1:D:490:ILE:HA	1.91	0.42
1:F:191:ILE:HG12	1:F:198:GLU:HG2	2.01	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.79	0.42
1:D:187:GLU:O	1:D:208:ARG:HD3	2.20	0.42
1:D:388:SER:OG	1:D:391:ALA:HB2	2.18	0.42
1:E:81:GLN:CD	1:E:81:GLN:N	2.78	0.42
1:E:256:GLN:H	1:E:256:GLN:HG2	1.51	0.42
1:F:24:MET:HB2	1:F:62:ASN:ND2	2.33	0.42
1:F:485:ASN:OD1	1:F:485:ASN:N	2.47	0.42
1:F:509:VAL:H	1:F:509:VAL:HG23	1.46	0.42
1:A:70:PRO:HG2	1:A:138:ARG:O	2.19	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:B:332:GLY:O	1:B:333:MET:C	2.63	0.42
1:B:452:ALA:HA	1:B:468:ARG:O	2.19	0.42
1:B:471:MET:HG3	1:B:478:ASP:HB3	2.02	0.42
1:C:21:MET:O	1:C:35:GLY:HA3	2.20	0.42
1:C:38:ILE:HG22	1:C:39:GLY:N	2.34	0.42
1:C:345:LYS:NZ	1:C:366:GLU:CG	2.82	0.42
1:D:153:GLN:O	1:D:154:TYR:CG	2.72	0.42
1:D:306:CYS:C	1:D:308:ASN:N	2.77	0.42
1:D:451:ARG:NH1	1:D:472:ILE:HD12	2.34	0.42
1:E:360:LEU:O	1:E:360:LEU:HD22	2.20	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:238:THR:HG22	1:F:239:ILE:N	2.34	0.42
1:F:287:THR:HG23	1:F:414:ASN:CB	2.37	0.42
1:F:367:ILE:HG12	1:F:375:ILE:CD1	2.49	0.42
1:B:256:GLN:H	1:B:256:GLN:HG2	1.55	0.42
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.34	0.42
1:C:153:GLN:C	1:C:154:TYR:CG	2.97	0.42
1:C:421:GLY:O	1:C:422:ALA:C	2.63	0.42
1:D:33:HIS:CD2	1:D:230:HIS:HA	2.55	0.42
1:D:140:ARG:HA	1:D:140:ARG:HD2	1.82	0.42
1:D:194:TYR:O	1:D:196:VAL:HG23	2.19	0.42
1:E:164:LEU:HB3	1:E:200:VAL:HG11	2.02	0.42
1:E:315:PHE:HE1	1:E:375:ILE:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.68	0.42
1:A:14:GLU:CG	1:A:15:HIS:N	2.57	0.42
1:B:21:MET:HE3	1:B:141:ARG:CD	2.49	0.42
1:B:68:ASP:OD2	1:B:102:LYS:HE3	2.19	0.42
1:B:119:GLY:O	1:B:121:PHE:N	2.53	0.42
1:C:283:ILE:HD12	1:C:412:PHE:HE1	1.85	0.42
1:C:497:ILE:O	1:C:498:THR:HG22	2.19	0.42
1:D:114:GLY:O	1:D:115:GLN:HG3	2.20	0.42
1:D:208:ARG:O	1:D:218:ARG:HA	2.20	0.42
1:E:345:LYS:NZ	1:E:366:GLU:HG2	2.35	0.42
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.35	0.41
1:D:52:LYS:HB2	3:D:903:ATP:O1B	2.20	0.41
1:E:106:LEU:HD13	1:E:129:ARG:NH2	2.35	0.41
1:F:443:VAL:HG12	1:F:445:ILE:HG12	2.02	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
1:B:332:GLY:O	1:B:333:MET:O	2.38	0.41
1:B:337:GLU:O	1:B:338:MET:C	2.59	0.41
1:B:445:ILE:HD12	1:B:486:PHE:CZ	2.55	0.41
1:D:300:ARG:CA	1:D:333:MET:HE1	2.50	0.41
1:E:76:PHE:O	1:E:109:SER:HA	2.19	0.41
1:E:150:VAL:HG13	1:E:151:PHE:N	2.35	0.41
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.48	0.41
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.50	0.41
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.56	0.41
1:A:430:ILE:O	1:A:432:TPO:N	2.53	0.41
1:A:510:ARG:N	1:A:510:ARG:HD2	2.35	0.41
1:B:153:GLN:O	1:B:154:TYR:CB	2.68	0.41
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.55	0.41
1:C:114:GLY:O	1:C:115:GLN:HB3	2.20	0.41
1:C:378:ASP:OD1	1:C:413:THR:HG21	2.20	0.41
1:C:489:ILE:O	1:C:492:GLY:N	2.47	0.41
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.82	0.41
1:D:370:PHE:O	1:D:371:LYS:CD	2.67	0.41
1:E:182:THR:HG21	1:E:192:ALA:HB1	2.01	0.41
1:E:336:GLU:O	1:E:339:GLU:HB2	2.21	0.41
1:E:505:LEU:O	1:E:505:LEU:CD1	2.69	0.41
1:F:140:ARG:HA	1:F:140:ARG:HD2	1.95	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.01	0.41
1:F:185:ILE:CD1	1:F:193:ARG:NH1	2.79	0.41
1:A:20:LYS:HD3	1:A:35:GLY:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:H	1:C:256:GLN:HG2	1.47	0.41
1:C:420:MET:HE1	1:D:490:ILE:HG21	2.02	0.41
1:D:224:LYS:O	1:D:225:LEU:HD23	2.20	0.41
1:E:21:MET:O	1:E:35:GLY:HA3	2.20	0.41
1:E:76:PHE:CZ	1:E:126:LEU:CD2	3.02	0.41
1:E:122:ASP:HB3	1:E:123:LEU:H	1.70	0.41
1:E:412:PHE:CD1	1:E:412:PHE:N	2.88	0.41
1:F:213:GLY:O	1:F:214:GLU:HB2	2.20	0.41
1:F:292:THR:HB	1:F:440:LEU:HB3	2.02	0.41
1:F:352:GLU:C	1:F:354:ALA:H	2.28	0.41
1:F:419:PHE:O	1:F:420:MET:HB2	2.19	0.41
1:F:504:GLU:CA	1:F:507:ARG:NE	2.81	0.41
1:A:184:ARG:C	1:A:185:ILE:HD13	2.46	0.41
1:B:153:GLN:C	1:B:154:TYR:CG	2.97	0.41
1:C:153:GLN:O	1:C:154:TYR:CG	2.74	0.41
1:C:387:VAL:CG1	1:C:391:ALA:HB3	2.50	0.41
1:D:21:MET:HE3	1:D:141:ARG:NE	2.35	0.41
1:D:21:MET:CE	1:D:59:PHE:HZ	2.33	0.41
1:D:438:ILE:CD1	1:D:455:VAL:HG22	2.51	0.41
1:E:289:ALA:CB	1:E:419:PHE:HA	2.45	0.41
1:E:344:LEU:HD13	1:E:345:LYS:N	2.34	0.41
1:F:126:LEU:O	1:F:127:ILE:C	2.63	0.41
1:F:484:ARG:CB	1:F:484:ARG:CZ	2.98	0.41
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.86	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
1:B:273:MET:O	1:B:463:HIS:CA	2.63	0.41
1:B:501:GLU:HB2	1:B:502:LYS:H	1.39	0.41
1:C:14:GLU:HG3	1:C:16:GLN:HB2	2.01	0.41
1:C:65:ILE:HG22	1:C:65:ILE:O	2.20	0.41
1:C:267:VAL:HB	1:C:270:LEU:HB2	2.03	0.41
1:C:281:ASP:O	1:C:282:SER:HB3	2.21	0.41
1:D:273:MET:SD	1:D:468:ARG:HD2	2.61	0.41
1:E:147:VAL:HG23	1:E:148:THR:N	2.35	0.41
1:E:446:ARG:CZ	1:E:496:ARG:NH2	2.84	0.41
1:F:23:THR:O	1:F:24:MET:HB2	2.20	0.41
1:F:299:SER:HB3	1:F:333:MET:HE2	2.03	0.41
1:F:516:GLY:N	1:F:517:PRO:HD2	2.36	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
1:A:430:ILE:O	1:A:433:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HD2	4:B:521:HOH:O	2.19	0.41
1:D:75:THR:HG23	1:D:75:THR:O	2.19	0.41
1:D:337:GLU:O	1:D:338:MET:C	2.63	0.41
1:E:345:LYS:HZ2	1:E:366:GLU:HG2	1.85	0.41
1:E:432:TPO:O2P	1:E:433:ILE:HD11	2.20	0.41
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.21	0.41
1:A:382:ALA:HB2	1:B:432:TPO:O3P	2.21	0.41
1:C:338:MET:HB2	1:C:344:LEU:HB3	2.03	0.41
1:D:273:MET:O	1:D:463:HIS:HA	2.20	0.41
1:E:483:PHE:CB	1:E:489:ILE:HD11	2.51	0.41
1:F:379:SER:CA	1:F:413:THR:HG22	2.47	0.41
1:A:21:MET:CE	1:A:59:PHE:CE1	3.04	0.41
1:A:400:THR:CG2	1:A:401:GLY:N	2.83	0.41
1:A:432:TPO:P	1:A:433:ILE:CD1	3.09	0.41
1:A:436:THR:HG23	1:A:458:MET:CG	2.51	0.41
1:B:252:MET:HE2	1:B:252:MET:HB3	1.96	0.41
1:C:21:MET:HE2	1:C:59:PHE:CE1	2.56	0.41
1:C:81:GLN:NE2	1:C:81:GLN:N	2.63	0.41
1:D:252:MET:HE2	1:D:252:MET:HB3	1.89	0.41
1:D:315:PHE:CE2	1:D:363:ILE:HG23	2.54	0.41
1:D:358:ASP:O	1:D:362:ILE:HG12	2.20	0.41
1:D:445:ILE:C	1:D:496:ARG:HH12	2.25	0.41
1:E:113:GLU:HB3	1:E:114:GLY:H	1.75	0.41
1:F:357:GLU:HG3	1:F:358:ASP:N	2.36	0.41
1:F:377:ILE:HD11	1:F:399:VAL:HG11	2.02	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:C:79:THR:HG23	1:C:81:GLN:H	1.86	0.41
1:E:148:THR:OG1	1:E:182:THR:HG22	2.21	0.41
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.51	0.41
1:E:306:CYS:O	1:E:309:LYS:N	2.41	0.41
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
3:A:903:ATP:O3'	1:B:224:LYS:HB2	2.21	0.40
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.84	0.40
1:B:79:THR:HG23	1:B:81:GLN:CG	2.42	0.40
1:B:219:THR:HB	1:B:234:GLU:HB3	2.03	0.40
1:B:291:GLY:C	3:B:901:ATP:O2B	2.64	0.40
1:C:79:THR:HG23	1:C:81:GLN:HE21	1.87	0.40
1:C:269:ARG:NE	4:C:525:HOH:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:SER:HA	1:D:178:THR:O	2.21	0.40
1:D:76:PHE:O	1:D:109:SER:HA	2.21	0.40
1:D:150:VAL:CG1	1:D:151:PHE:N	2.84	0.40
1:D:182:THR:CG2	1:D:183:GLU:N	2.81	0.40
1:E:380:LEU:O	1:E:381:SER:C	2.62	0.40
1:C:44:VAL:HG22	1:C:205:VAL:HB	2.03	0.40
1:D:49:GLY:HA2	3:D:903:ATP:O2B	2.21	0.40
1:D:383:LEU:HD23	1:D:383:LEU:HA	1.81	0.40
1:D:471:MET:CG	1:D:478:ASP:HB3	2.51	0.40
1:D:495:THR:HG23	1:E:487:GLU:OE2	2.21	0.40
1:E:20:LYS:C	1:E:38:ILE:HD11	2.46	0.40
1:E:345:LYS:NZ	1:E:366:GLU:OE1	2.55	0.40
1:F:98:VAL:HA	1:F:103:LEU:O	2.21	0.40
1:F:127:ILE:HD11	1:F:167:LEU:CD1	2.51	0.40
1:F:203:ASN:CB	1:F:225:LEU:HD23	2.39	0.40
1:F:252:MET:HE2	1:F:252:MET:HB3	1.90	0.40
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.86	0.40
1:B:60:LEU:CD1	1:B:73:PHE:HB2	2.50	0.40
1:C:18:ILE:CG2	1:C:37:PRO:HB3	2.51	0.40
1:C:20:LYS:C	1:C:38:ILE:HD11	2.46	0.40
1:D:315:PHE:CE1	1:D:363:ILE:HG23	2.56	0.40
1:D:396:VAL:HG11	1:D:430:ILE:CG2	2.50	0.40
1:D:462:TRP:O	1:D:463:HIS:O	2.39	0.40
1:E:184:ARG:HG2	1:E:191:ILE:O	2.22	0.40
1:F:21:MET:HE3	1:F:141:ARG:CZ	2.51	0.40
1:F:306:CYS:C	1:F:308:ASN:H	2.29	0.40
1:B:393:ARG:O	1:B:397:ILE:HG12	2.21	0.40
1:C:25:ILE:HG23	1:C:58:GLN:NE2	2.36	0.40
1:D:497:ILE:H	1:D:497:ILE:HG13	1.78	0.40
1:E:356:LEU:HD21	1:E:387:VAL:HG11	2.02	0.40
1:F:129:ARG:O	1:F:132:TYR:HB3	2.21	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
1:B:148:THR:HG1	1:B:182:THR:HG23	1.86	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.98	0.40
1:B:441:GLN:O	1:B:441:GLN:HG3	2.21	0.40
1:C:62:ASN:O	1:C:63:GLY:C	2.64	0.40
1:C:148:THR:HG21	1:C:193:ARG:HD2	2.02	0.40
1:D:219:THR:HB	1:D:234:GLU:HB3	2.03	0.40
1:D:344:LEU:HD22	1:D:345:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:VAL:HA	1:E:103:LEU:O	2.22	0.40
1:E:193:ARG:HH11	1:E:193:ARG:HG2	1.86	0.40
1:E:371:LYS:O	1:E:371:LYS:HD3	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	445 (89%)	35 (7%)	22 (4%)	2	7
1	B	487/519 (94%)	430 (88%)	45 (9%)	12 (2%)	4	16
1	C	484/519 (93%)	433 (90%)	32 (7%)	19 (4%)	2	8
1	D	481/519 (93%)	433 (90%)	37 (8%)	11 (2%)	5	18
1	E	488/519 (94%)	416 (85%)	53 (11%)	19 (4%)	2	8
1	F	502/519 (97%)	442 (88%)	39 (8%)	21 (4%)	2	7
All	All	2944/3114 (94%)	2599 (88%)	241 (8%)	104 (4%)	3	10

All (104) 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	154	TYR

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Mol	Chain	Res	Type
1	B	333	MET
1	B	341	GLN
1	B	387	VAL
1	B	463	HIS
1	C	17	ALA
1	C	112	PRO
1	C	117	VAL
1	C	124	SER
1	C	154	TYR
1	C	333	MET
1	C	341	GLN
1	C	463	HIS
1	D	122	ASP
1	D	154	TYR
1	D	333	MET
1	D	387	VAL
1	D	463	HIS
1	E	122	ASP
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	420	MET
1	E	463	HIS
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	F	510	ARG
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

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Mol	Chain	Res	Type
1	B	420	MET
1	C	121	PHE
1	C	379	SER
1	C	387	VAL
1	D	18	ILE
1	D	113	GLU
1	D	341	GLN
1	D	420	MET
1	E	117	VAL
1	E	120	GLY
1	E	213	GLY
1	E	341	GLN
1	E	387	VAL
1	E	502	LYS
1	F	117	VAL
1	F	157	SER
1	F	211	LEU
1	F	341	GLN
1	A	379	SER
1	A	420	MET
1	B	112	PRO
1	C	114	GLY
1	C	211	LEU
1	C	499	VAL
1	E	157	SER
1	E	498	THR
1	F	420	MET
1	A	480	LYS
1	A	504	GLU
1	B	52	LYS
1	C	289	ALA
1	C	354	ALA
1	D	211	LEU
1	E	293	GLY
1	A	433	ILE
1	B	494	PRO
1	C	157	SER
1	E	348	CYS
1	E	379	SER
1	F	354	ALA
1	F	500	ASP
1	F	517	PRO

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Mol	Chain	Res	Type
1	A	212	GLU
1	A	348	CYS
1	C	213	GLY
1	C	348	CYS
1	D	157	SER
1	E	494	PRO
1	F	112	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%)	365 (85%)	65 (15%)	3	10
1	B	417/442 (94%)	359 (86%)	58 (14%)	3	12
1	C	414/442 (94%)	351 (85%)	63 (15%)	3	10
1	D	411/442 (93%)	351 (85%)	60 (15%)	3	11
1	E	418/442 (95%)	359 (86%)	59 (14%)	3	12
1	F	430/442 (97%)	371 (86%)	59 (14%)	3	13
All	All	2520/2652 (95%)	2156 (86%)	364 (14%)	3	11

All (364) 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	50	THR
1	A	79	THR
1	A	81	GLN
1	A	83	ILE

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	433	ILE
1	B	458	MET
1	B	462	TRP
1	B	469	GLU
1	B	471	MET
1	B	474	ASP
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
1	C	15	HIS
1	C	18	ILE
1	C	26	GLU
1	C	50	THR
1	C	79	THR
1	C	81	GLN
1	C	99	ASP
1	C	106	LEU
1	C	111	ASP
1	C	121	PHE

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Mol	Chain	Res	Type
1	C	140	ARG
1	C	151	PHE
1	C	154	TYR
1	C	164	LEU
1	C	177	THR
1	C	178	THR
1	C	179	VAL
1	C	181	THR
1	C	183	GLU
1	C	185	ILE
1	C	186	GLU
1	C	191	ILE
1	C	196	VAL
1	C	211	LEU
1	C	212	GLU
1	C	214	GLU
1	C	218	ARG
1	C	223	LEU
1	C	228	THR
1	C	256	GLN
1	C	259	SER
1	C	260	ASN
1	C	263	VAL
1	C	270	LEU
1	C	287	THR
1	C	294	LYS
1	C	298	VAL
1	C	302	VAL
1	C	303	GLU
1	C	321	ARG
1	C	325	LEU
1	C	333	MET
1	C	338	MET
1	C	342	ASN
1	C	356	LEU
1	C	360	LEU
1	C	366	GLU
1	C	375	ILE
1	C	400	THR
1	C	413	THR
1	C	420	MET
1	C	458	MET

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Mol	Chain	Res	Type
1	C	461	SER
1	C	462	TRP
1	C	469	GLU
1	C	471	MET
1	C	491	SER
1	C	493	SER
1	C	495	THR
1	C	497	ILE
1	C	498	THR
1	C	500	ASP
1	C	501	GLU
1	D	14	GLU
1	D	26	GLU
1	D	38	ILE
1	D	79	THR
1	D	81	GLN
1	D	83	ILE
1	D	106	LEU
1	D	117	VAL
1	D	122	ASP
1	D	123	LEU
1	D	124	SER
1	D	127	ILE
1	D	140	ARG
1	D	151	PHE
1	D	154	TYR
1	D	172	LYS
1	D	177	THR
1	D	179	VAL
1	D	181	THR
1	D	183	GLU
1	D	185	ILE
1	D	186	GLU
1	D	191	ILE
1	D	212	GLU
1	D	218	ARG
1	D	223	LEU
1	D	228	THR
1	D	256	GLN
1	D	259	SER
1	D	260	ASN
1	D	263	VAL

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Mol	Chain	Res	Type
1	D	270	LEU
1	D	284	ILE
1	D	287	THR
1	D	294	LYS
1	D	302	VAL
1	D	303	GLU
1	D	320	SER
1	D	321	ARG
1	D	325	LEU
1	D	338	MET
1	D	342	ASN
1	D	351	PRO
1	D	356	LEU
1	D	360	LEU
1	D	366	GLU
1	D	369	ASP
1	D	375	ILE
1	D	400	THR
1	D	413	THR
1	D	420	MET
1	D	439	LEU
1	D	458	MET
1	D	463	HIS
1	D	469	GLU
1	D	471	MET
1	D	487	GLU
1	D	490	ILE
1	D	496	ARG
1	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

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Mol	Chain	Res	Type
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	292	THR
1	E	302	VAL
1	E	314	LEU
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	356	LEU
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

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Mol	Chain	Res	Type
1	E	501	GLU
1	E	503	SER
1	E	504	GLU
1	E	505	LEU
1	F	26	GLU
1	F	37	PRO
1	F	45	SER
1	F	79	THR
1	F	81	GLN
1	F	99	ASP
1	F	106	LEU
1	F	115	GLN
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
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

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Mol	Chain	Res	Type
1	F	366	GLU
1	F	375	ILE
1	F	400	THR
1	F	413	THR
1	F	425	ILE
1	F	449	MET
1	F	458	MET
1	F	469	GLU
1	F	471	MET
1	F	474	ASP
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	508	ILE
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 (66) such sidechains are listed below:

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

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

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Mol	Chain	Res	Type
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 ⓘ

12 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	C	431	1	4,5,10	0.87	0	1,5,14	0.65	0
1	TPO	C	432	1	8,10,11	1.43	1 (12%)	10,14,16	1.44	2 (20%)
1	SEP	B	431	1	8,9,10	2.07	1 (12%)	7,12,14	2.46	2 (28%)
1	TPO	D	432	1	8,10,11	1.60	3 (37%)	10,14,16	1.66	2 (20%)
1	SEP	F	431	1	8,9,10	2.03	2 (25%)	7,12,14	1.03	0
1	TPO	E	432	1	8,10,11	1.07	0	10,14,16	1.29	2 (20%)
1	SEP	D	431	1	4,5,10	1.81	1 (25%)	1,5,14	0.81	0
1	SEP	E	431	1	8,9,10	2.53	3 (37%)	7,12,14	2.72	3 (42%)
1	SEP	A	431	1	8,9,10	2.03	3 (37%)	7,12,14	3.53	2 (28%)
1	TPO	F	432	1	8,10,11	3.59	7 (87%)	10,14,16	3.80	5 (50%)
1	TPO	B	432	1	8,10,11	0.59	0	10,14,16	1.13	0
1	TPO	A	432	1	8,10,11	0.68	0	10,14,16	1.22	0

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	C	431	1	-	2/2/4/10	-
1	TPO	C	432	1	-	1/9/11/13	-
1	SEP	B	431	1	-	4/6/8/10	-
1	TPO	D	432	1	1/1/3/4	6/9/11/13	-
1	SEP	F	431	1	-	0/6/8/10	-
1	TPO	E	432	1	1/1/3/4	4/9/11/13	-
1	SEP	D	431	1	-	2/2/4/10	-
1	SEP	E	431	1	-	2/6/8/10	-
1	SEP	A	431	1	-	1/6/8/10	-
1	TPO	F	432	1	1/1/3/4	2/9/11/13	-
1	TPO	B	432	1	1/1/3/4	6/9/11/13	-
1	TPO	A	432	1	-	1/9/11/13	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	432	TPO	P-O2P	-5.84	1.33	1.54
1	E	431	SEP	P-O1P	5.68	1.68	1.50
1	B	431	SEP	P-O1P	5.28	1.66	1.50
1	F	431	SEP	P-O1P	4.63	1.64	1.50
1	F	432	TPO	P-OG1	-4.59	1.51	1.59
1	A	431	SEP	P-O2P	3.70	1.68	1.54
1	F	432	TPO	CG2-CB	-3.68	1.42	1.51
1	F	432	TPO	P-O1P	-3.62	1.39	1.50
1	D	431	SEP	O-C	3.47	1.33	1.20
1	E	431	SEP	P-O2P	3.36	1.67	1.54
1	A	431	SEP	CB-CA	3.07	1.60	1.52
1	C	432	TPO	P-O1P	3.05	1.60	1.50
1	F	432	TPO	O-C	-3.04	1.08	1.20
1	A	431	SEP	P-O3P	2.72	1.64	1.54
1	D	432	TPO	P-OG1	2.49	1.63	1.59
1	D	432	TPO	CG2-CB	2.47	1.57	1.51
1	F	432	TPO	P-O3P	-2.28	1.46	1.54
1	F	431	SEP	P-O3P	2.26	1.63	1.54
1	E	431	SEP	CB-CA	2.21	1.58	1.52
1	D	432	TPO	P-O1P	2.18	1.57	1.50
1	F	432	TPO	CB-CA	-2.09	1.49	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	432	TPO	CG2-CB-CA	-9.73	94.31	113.26
1	A	431	SEP	OG-CB-CA	-6.76	101.57	108.14
1	A	431	SEP	OG-P-O1P	5.72	121.90	106.44
1	B	431	SEP	OG-CB-CA	5.70	113.69	108.14
1	E	431	SEP	OG-CB-CA	-4.76	103.52	108.14
1	E	431	SEP	O3P-P-OG	4.60	118.66	106.67
1	F	432	TPO	CB-CA-N	-4.07	87.56	114.17
1	F	432	TPO	O3P-P-O1P	3.62	124.93	110.83
1	D	432	TPO	CG2-CB-CA	-2.84	107.73	113.26
1	D	432	TPO	O3P-P-O2P	2.77	118.19	107.80
1	F	432	TPO	P-OG1-CB	-2.61	116.23	123.33
1	C	432	TPO	P-OG1-CB	-2.57	116.34	123.33
1	C	432	TPO	O3P-P-O2P	2.53	117.28	107.80
1	F	432	TPO	OG1-P-O1P	-2.50	100.42	109.33
1	E	432	TPO	P-OG1-CB	-2.27	117.17	123.33
1	B	431	SEP	O3P-P-OG	2.08	112.10	106.67
1	E	432	TPO	O-C-CA	-2.07	119.44	124.77
1	E	431	SEP	O2P-P-O1P	-2.01	102.99	110.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	432	TPO	CB
1	D	432	TPO	CB
1	E	432	TPO	CB
1	F	432	TPO	CB

All (31) torsion outliers are listed below:

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

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

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	431	SEP	4	0
1	C	432	TPO	5	0
1	B	431	SEP	6	0
1	D	432	TPO	3	0
1	F	431	SEP	2	0
1	E	432	TPO	5	0
1	D	431	SEP	2	0
1	E	431	SEP	2	0
1	A	431	SEP	5	0
1	B	432	TPO	8	0
1	A	432	TPO	6	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	ATP	D	901	-	32,33,33	2.54	8 (25%)	48,52,52	2.10	13 (27%)
3	ATP	C	903	-	32,33,33	2.03	5 (15%)	48,52,52	2.18	14 (29%)
3	ATP	F	903	-	32,33,33	2.09	7 (21%)	48,52,52	2.13	15 (31%)
3	ATP	B	903	-	32,33,33	1.92	6 (18%)	48,52,52	2.23	18 (37%)
3	ATP	B	901	-	32,33,33	1.61	6 (18%)	48,52,52	1.96	15 (31%)
3	ATP	A	903	-	32,33,33	1.97	11 (34%)	48,52,52	2.07	15 (31%)
3	ATP	C	901	-	32,33,33	2.53	8 (25%)	48,52,52	2.10	12 (25%)
3	ATP	E	901	-	32,33,33	1.62	6 (18%)	48,52,52	2.06	14 (29%)
3	ATP	A	901	-	32,33,33	1.61	7 (21%)	48,52,52	2.03	15 (31%)
3	ATP	E	903	-	32,33,33	2.43	10 (31%)	48,52,52	1.99	12 (25%)
3	ATP	D	903	-	32,33,33	2.62	8 (25%)	48,52,52	2.27	13 (27%)
3	ATP	F	901	-	32,33,33	2.01	7 (21%)	48,52,52	2.07	13 (27%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	901	-	-	7/22/38/38	0/3/3/3
3	ATP	E	903	-	-	11/22/38/38	0/3/3/3
3	ATP	D	903	-	-	8/22/38/38	0/3/3/3
3	ATP	F	901	-	-	7/22/38/38	0/3/3/3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ATP	PB-O3A	-10.39	1.48	1.59
3	E	903	ATP	PB-O3B	-9.98	1.48	1.59
3	D	901	ATP	PB-O3B	-8.85	1.49	1.59
3	D	903	ATP	PB-O3B	-8.57	1.50	1.59
3	D	903	ATP	PB-O3A	-7.97	1.50	1.59
3	C	903	ATP	PB-O3A	-7.80	1.51	1.59
3	D	901	ATP	PB-O3A	-7.79	1.51	1.59
3	A	903	ATP	PB-O3B	-6.80	1.52	1.59
3	F	901	ATP	PB-O3A	-6.77	1.52	1.59
3	F	903	ATP	PB-O3B	-6.38	1.52	1.59
3	F	903	ATP	PB-O3A	-6.16	1.52	1.59
3	B	903	ATP	PB-O3A	-5.29	1.53	1.59
3	C	901	ATP	PA-O3A	-4.69	1.54	1.59
3	A	901	ATP	PB-O3B	-4.63	1.54	1.59
3	F	901	ATP	PA-O3A	-4.16	1.55	1.59
3	C	903	ATP	PA-O3A	-4.04	1.55	1.59
3	E	901	ATP	PB-O3B	-4.00	1.55	1.59
3	B	903	ATP	C4-N3	3.97	1.41	1.34
3	C	901	ATP	PB-O3B	-3.95	1.55	1.59
3	D	903	ATP	O4'-C4'	-3.94	1.36	1.45
3	B	903	ATP	C2-N3	3.65	1.40	1.33
3	F	901	ATP	C4-N3	3.55	1.41	1.34
3	A	903	ATP	C2-N1	3.52	1.40	1.33
3	B	901	ATP	C4-N3	3.49	1.40	1.34
3	C	903	ATP	O4'-C4'	-3.48	1.37	1.45
3	B	901	ATP	C2-N1	3.31	1.39	1.33
3	B	903	ATP	C1'-N9	3.24	1.55	1.46
3	C	901	ATP	PB-O1B	-3.23	1.39	1.50
3	E	901	ATP	C2-N3	3.22	1.39	1.33
3	E	903	ATP	C5-N7	-3.16	1.33	1.39
3	D	903	ATP	PB-O1B	-3.14	1.39	1.50
3	B	903	ATP	C8-N9	3.11	1.42	1.37
3	C	901	ATP	C2-N3	3.11	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	ATP	PB-O3A	-3.09	1.56	1.59
3	E	901	ATP	C4-N3	3.03	1.40	1.34
3	E	903	ATP	PB-O1B	-2.99	1.40	1.50
3	F	901	ATP	C2-N3	2.95	1.39	1.33
3	F	903	ATP	C2-N3	2.90	1.39	1.33
3	D	903	ATP	PB-O2B	-2.89	1.41	1.55
3	F	903	ATP	C2-N1	2.84	1.39	1.33
3	A	901	ATP	PB-O3A	-2.81	1.56	1.59
3	C	901	ATP	C5-N7	-2.76	1.34	1.39
3	B	901	ATP	PB-O3A	-2.74	1.56	1.59
3	D	901	ATP	C5-N7	-2.74	1.34	1.39
3	E	903	ATP	C6-N6	-2.74	1.27	1.34
3	D	901	ATP	PA-O3A	-2.73	1.56	1.59
3	F	901	ATP	C2-N1	2.71	1.38	1.33
3	F	903	ATP	C6-N6	-2.70	1.27	1.34
3	B	901	ATP	PB-O1B	-2.66	1.41	1.50
3	F	903	ATP	PB-O1B	-2.65	1.41	1.50
3	D	901	ATP	C4-N9	-2.62	1.32	1.37
3	C	903	ATP	C6-N1	2.60	1.43	1.35
3	D	901	ATP	C3'-C4'	2.58	1.59	1.53
3	B	901	ATP	C1'-N9	2.58	1.53	1.46
3	D	903	ATP	C2-N3	2.57	1.38	1.33
3	E	901	ATP	PB-O1B	-2.56	1.41	1.50
3	D	903	ATP	C2'-C1'	-2.56	1.45	1.53
3	A	901	ATP	C2-N3	2.52	1.38	1.33
3	E	903	ATP	PA-O1A	-2.49	1.42	1.50
3	D	901	ATP	O2'-C2'	-2.47	1.36	1.43
3	E	903	ATP	O4'-C4'	-2.46	1.39	1.45
3	C	903	ATP	C8-N7	2.39	1.36	1.31
3	A	901	ATP	PB-O1B	-2.34	1.42	1.50
3	F	903	ATP	C4-N9	-2.33	1.32	1.37
3	E	903	ATP	PB-O3A	-2.32	1.57	1.59
3	A	903	ATP	C8-N7	2.32	1.36	1.31
3	A	903	ATP	C5-C4	2.30	1.43	1.39
3	E	903	ATP	C2'-C3'	-2.26	1.47	1.53
3	A	901	ATP	C2-N1	2.26	1.38	1.33
3	E	903	ATP	PG-O1G	2.24	1.57	1.50
3	C	901	ATP	O4'-C4'	-2.21	1.40	1.45
3	A	903	ATP	C2-N3	2.19	1.37	1.33
3	E	903	ATP	PB-O2B	-2.18	1.45	1.55
3	B	901	ATP	C5-C4	2.18	1.43	1.39
3	A	901	ATP	C1'-N9	2.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	ATP	C5'-C4'	2.15	1.58	1.51
3	A	901	ATP	C5'-C4'	2.14	1.58	1.51
3	A	903	ATP	PB-O1B	-2.13	1.43	1.50
3	A	903	ATP	C4-N3	2.12	1.38	1.34
3	A	903	ATP	PG-O1G	2.11	1.57	1.50
3	E	901	ATP	C2-N1	2.08	1.37	1.33
3	D	901	ATP	C4-N3	2.08	1.38	1.34
3	A	903	ATP	PB-O2B	-2.06	1.45	1.55
3	C	901	ATP	C4-N3	2.05	1.38	1.34
3	D	903	ATP	C4-N3	2.04	1.38	1.34
3	A	903	ATP	PB-O3A	-2.03	1.57	1.59
3	F	901	ATP	PB-O1B	-2.03	1.43	1.50
3	B	903	ATP	C2-N1	2.01	1.37	1.33
3	A	903	ATP	C3'-C4'	2.00	1.58	1.53

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	ATP	N3-C2-N1	-6.16	119.26	128.58
3	D	901	ATP	N3-C2-N1	-6.04	119.44	128.58
3	B	901	ATP	N3-C2-N1	-6.03	119.45	128.58
3	B	903	ATP	N3-C2-N1	-6.03	119.46	128.58
3	D	903	ATP	N3-C2-N1	-5.97	119.55	128.58
3	E	901	ATP	N3-C2-N1	-5.80	119.81	128.58
3	A	901	ATP	N3-C2-N1	-5.56	120.17	128.58
3	F	901	ATP	N3-C2-N1	-5.54	120.20	128.58
3	C	901	ATP	C5-N7-C8	5.47	112.05	103.45
3	D	903	ATP	C4-C5-N7	-5.45	104.35	110.58
3	D	903	ATP	C5-N7-C8	5.35	111.86	103.45
3	C	903	ATP	N9-C8-N7	-5.34	106.36	113.94
3	E	903	ATP	N3-C2-N1	-5.29	120.57	128.58
3	F	903	ATP	N3-C2-N1	-5.16	120.77	128.58
3	A	903	ATP	N3-C2-N1	-5.16	120.78	128.58
3	F	903	ATP	C4-C5-N7	-5.13	104.72	110.58
3	A	901	ATP	C5-N7-C8	5.10	111.47	103.45
3	C	901	ATP	N9-C8-N7	-5.04	106.78	113.94
3	D	901	ATP	O2B-PB-O3B	5.00	120.78	107.27
3	E	901	ATP	C5-N7-C8	4.97	111.26	103.45
3	D	903	ATP	N9-C8-N7	-4.95	106.91	113.94
3	E	901	ATP	N9-C8-N7	-4.95	106.92	113.94
3	A	903	ATP	N9-C8-N7	-4.93	106.95	113.94
3	C	901	ATP	N3-C2-N1	-4.90	121.16	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	ATP	C4-C5-N7	-4.78	105.12	110.58
3	F	903	ATP	C5-N7-C8	4.77	110.94	103.45
3	C	901	ATP	C4-C5-N7	-4.77	105.13	110.58
3	F	901	ATP	C5-N7-C8	4.72	110.88	103.45
3	C	901	ATP	O2B-PB-O3B	4.70	119.97	107.27
3	A	901	ATP	C4-C5-N7	-4.61	105.31	110.58
3	F	903	ATP	N9-C8-N7	-4.58	107.44	113.94
3	B	903	ATP	N9-C8-N7	-4.57	107.45	113.94
3	F	901	ATP	C4-C5-N7	-4.57	105.36	110.58
3	A	903	ATP	C5-N7-C8	4.52	110.55	103.45
3	E	903	ATP	C5-N7-C8	4.51	110.55	103.45
3	A	901	ATP	N9-C8-N7	-4.51	107.53	113.94
3	B	901	ATP	C5-N7-C8	4.51	110.54	103.45
3	F	901	ATP	N9-C8-N7	-4.50	107.55	113.94
3	B	901	ATP	N9-C8-N7	-4.39	107.70	113.94
3	D	901	ATP	N9-C8-N7	-4.39	107.70	113.94
3	B	901	ATP	O2B-PB-O3B	4.37	119.09	107.27
3	E	903	ATP	N9-C8-N7	-4.34	107.77	113.94
3	E	901	ATP	C4-C5-N7	-4.33	105.63	110.58
3	C	903	ATP	C5-N7-C8	4.31	110.23	103.45
3	C	903	ATP	C4-C5-N7	-4.31	105.65	110.58
3	E	903	ATP	C4-C5-N7	-4.21	105.77	110.58
3	D	901	ATP	C5-N7-C8	4.18	110.02	103.45
3	B	903	ATP	C4-C5-N7	-4.15	105.84	110.58
3	B	903	ATP	C5-N7-C8	4.14	109.96	103.45
3	D	901	ATP	O3A-PB-O1B	-4.12	98.32	110.70
3	B	903	ATP	O2B-PB-O3B	4.09	118.34	107.27
3	E	903	ATP	C5-C4-N3	-4.03	121.17	126.72
3	B	903	ATP	O3A-PA-O1A	-3.78	99.34	110.70
3	F	901	ATP	O2B-PB-O3B	3.76	117.45	107.27
3	B	901	ATP	C4-C5-N7	-3.69	106.36	110.58
3	A	903	ATP	O3A-PB-O1B	-3.66	99.70	110.70
3	D	903	ATP	C2'-C1'-N9	3.64	122.34	113.30
3	E	903	ATP	O3A-PB-O1B	-3.61	99.84	110.70
3	C	903	ATP	O2B-PB-O3B	3.58	116.95	107.27
3	D	903	ATP	O2B-PB-O3B	3.58	116.95	107.27
3	D	901	ATP	C4-C5-N7	-3.58	106.49	110.58
3	C	903	ATP	C2-N3-C4	3.55	120.50	111.83
3	C	901	ATP	O2B-PB-O3A	3.49	116.69	107.27
3	C	901	ATP	C5-C4-N3	-3.48	121.92	126.72
3	F	903	ATP	O3A-PB-O1B	-3.48	100.24	110.70
3	D	901	ATP	O3B-PB-O1B	-3.47	100.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ATP	O2B-PB-O3B	3.42	116.53	107.27
3	A	903	ATP	C6-C5-N7	3.41	138.66	132.09
3	C	903	ATP	O3B-PB-O1B	-3.41	100.46	110.70
3	D	903	ATP	C2-N3-C4	3.35	120.02	111.83
3	F	901	ATP	C5-C4-N3	-3.35	122.10	126.72
3	D	903	ATP	C5-C4-N3	-3.35	122.10	126.72
3	B	903	ATP	C5-C4-N3	-3.26	122.23	126.72
3	D	903	ATP	C6-C5-N7	3.23	138.32	132.09
3	F	903	ATP	O2B-PB-O3B	3.21	115.95	107.27
3	D	901	ATP	O2B-PB-O3A	3.21	115.94	107.27
3	C	901	ATP	O3B-PB-O1B	-3.17	101.16	110.70
3	D	903	ATP	C4-N9-C8	3.16	109.05	105.74
3	C	903	ATP	C4-N9-C8	3.15	109.05	105.74
3	E	903	ATP	O2B-PB-O3B	3.14	115.77	107.27
3	B	903	ATP	O4'-C1'-N9	3.14	114.12	108.09
3	F	901	ATP	O3A-PB-O1B	-3.14	101.26	110.70
3	F	903	ATP	C2'-C1'-N9	3.12	121.05	113.30
3	E	901	ATP	C2-N3-C4	3.08	119.35	111.83
3	C	901	ATP	O3A-PB-O1B	-3.08	101.44	110.70
3	E	901	ATP	C6-C5-N7	3.07	138.00	132.09
3	D	903	ATP	O3A-PB-O1B	-3.03	101.59	110.70
3	E	901	ATP	O3A-PB-O1B	-3.01	101.65	110.70
3	F	903	ATP	C4-N9-C8	3.01	108.89	105.74
3	E	901	ATP	C4-N9-C8	3.00	108.89	105.74
3	B	901	ATP	O2B-PB-O3A	2.99	115.37	107.27
3	A	901	ATP	C5-C4-N3	-2.99	122.59	126.72
3	C	903	ATP	C5-C4-N3	-2.98	122.61	126.72
3	E	901	ATP	C5-C4-N3	-2.97	122.63	126.72
3	F	903	ATP	C6-C5-N7	2.96	137.79	132.09
3	F	903	ATP	C5-C4-N3	-2.95	122.65	126.72
3	D	901	ATP	C2-N3-C4	2.93	118.98	111.83
3	A	901	ATP	C2-N3-C4	2.92	118.97	111.83
3	F	901	ATP	O2'-C2'-C3'	2.91	121.15	111.82
3	B	903	ATP	O2'-C2'-C3'	2.89	121.07	111.82
3	A	903	ATP	C4-N9-C8	2.86	108.74	105.74
3	D	903	ATP	O3B-PB-O1B	-2.86	102.11	110.70
3	B	903	ATP	C2-N3-C4	2.84	118.77	111.83
3	B	903	ATP	C6-C5-N7	2.83	137.54	132.09
3	C	903	ATP	C6-C5-N7	2.83	137.54	132.09
3	A	901	ATP	C6-C5-N7	2.80	137.48	132.09
3	A	903	ATP	C2-N3-C4	2.79	118.66	111.83
3	B	901	ATP	C5-C4-N3	-2.77	122.90	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	ATP	C2'-C1'-N9	2.75	120.13	113.30
3	F	903	ATP	C2-N3-C4	2.74	118.52	111.83
3	C	903	ATP	C2'-C1'-N9	2.73	120.09	113.30
3	B	903	ATP	O2B-PB-O3A	2.68	114.53	107.27
3	B	903	ATP	O3A-PB-O1B	-2.68	102.64	110.70
3	F	901	ATP	O2B-PB-O3A	2.66	114.46	107.27
3	F	901	ATP	C2-N3-C4	2.65	118.31	111.83
3	A	903	ATP	O2B-PB-O3B	2.65	114.42	107.27
3	C	903	ATP	O3A-PB-O1B	-2.64	102.76	110.70
3	F	901	ATP	C4-N9-C8	2.63	108.50	105.74
3	E	903	ATP	O2B-PB-O3A	2.63	114.37	107.27
3	F	901	ATP	C6-C5-N7	2.61	137.12	132.09
3	A	903	ATP	C5-C4-N9	2.60	108.65	105.81
3	E	901	ATP	O2B-PB-O3B	2.60	114.29	107.27
3	D	901	ATP	C6-C5-N7	2.56	137.03	132.09
3	D	903	ATP	O3A-PA-O1A	-2.56	103.02	110.70
3	D	901	ATP	C4-N9-C8	2.55	108.42	105.74
3	F	903	ATP	O3B-PB-O1B	-2.55	103.05	110.70
3	B	901	ATP	O3B-PB-O1B	-2.54	103.06	110.70
3	C	901	ATP	O2'-C2'-C3'	2.52	119.91	111.82
3	B	901	ATP	C2-N3-C4	2.52	117.98	111.83
3	D	901	ATP	C5-C4-N3	-2.46	123.32	126.72
3	A	901	ATP	O2B-PB-O3A	2.44	113.88	107.27
3	A	903	ATP	O2B-PB-O3A	2.42	113.82	107.27
3	A	901	ATP	C4-N9-C8	2.41	108.27	105.74
3	B	903	ATP	O3B-PB-O1B	-2.41	103.47	110.70
3	C	901	ATP	C4-N9-C8	2.39	108.25	105.74
3	A	901	ATP	C2'-C1'-N9	2.32	119.06	113.30
3	B	903	ATP	C4-N9-C8	2.32	108.17	105.74
3	A	903	ATP	N6-C6-N1	-2.31	113.23	118.38
3	E	901	ATP	N6-C6-N1	-2.29	113.29	118.38
3	E	901	ATP	C2'-C1'-N9	2.27	118.95	113.30
3	A	901	ATP	O3A-PB-O1B	-2.26	103.89	110.70
3	F	903	ATP	N6-C6-N1	-2.24	113.39	118.38
3	B	901	ATP	O2'-C2'-C3'	2.23	118.97	111.82
3	E	903	ATP	C2-N3-C4	2.23	117.28	111.83
3	C	903	ATP	O5'-PA-O1A	-2.22	100.13	108.94
3	B	901	ATP	C4-N9-C8	2.21	108.06	105.74
3	A	903	ATP	C2'-C1'-N9	2.21	118.79	113.30
3	A	901	ATP	O2'-C2'-C3'	2.20	118.86	111.82
3	C	903	ATP	C5-C4-N9	2.18	108.19	105.81
3	E	901	ATP	O2'-C2'-C3'	2.18	118.80	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	903	ATP	O2B-PB-O3A	2.17	113.14	107.27
3	B	901	ATP	C2-N1-C6	2.16	122.27	118.73
3	C	901	ATP	C2-N3-C4	2.15	117.09	111.83
3	B	903	ATP	N6-C6-N1	-2.14	113.61	118.38
3	B	901	ATP	O3A-PB-O1B	-2.14	104.26	110.70
3	D	901	ATP	C2'-C1'-N9	2.11	118.54	113.30
3	A	903	ATP	C5-C4-N3	-2.10	123.82	126.72
3	B	901	ATP	O2G-PG-O3B	2.10	111.67	104.64
3	B	903	ATP	C6-C5-C4	-2.10	114.31	117.18
3	A	901	ATP	O3B-PB-O1B	-2.09	104.42	110.70
3	E	903	ATP	O2G-PG-O1G	2.08	118.96	110.83
3	E	901	ATP	O2B-PB-O3A	2.08	112.91	107.27
3	B	901	ATP	C6-C5-N7	2.07	136.08	132.09
3	A	903	ATP	O3A-PA-O1A	-2.05	104.53	110.70
3	E	903	ATP	O3B-PB-O1B	-2.04	104.57	110.70
3	E	903	ATP	O3A-PA-O1A	-2.04	104.58	110.70
3	B	903	ATP	C4-N9-C1'	-2.01	121.93	126.63
3	F	903	ATP	C5-C4-N9	2.01	108.00	105.81
3	A	901	ATP	O3A-PA-O1A	-2.01	104.67	110.70

There are no chirality outliers.

All (94) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	903	ATP	PB-O3B-PG-O3G
3	E	903	ATP	PB-O3A-PA-O5'
3	E	903	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C5'-O5'-PA-O3A
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C5'-O5'-PA-O3A
3	F	903	ATP	PB-O3B-PG-O3G
3	F	903	ATP	PB-O3A-PA-O5'
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PB-O3A-PA-O5'
3	A	903	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3A-PA-O5'
3	C	901	ATP	PB-O3A-PA-O5'
3	C	903	ATP	PB-O3A-PA-O5'
3	D	901	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3A-PA-O5'
3	E	901	ATP	PB-O3A-PA-O5'
3	F	901	ATP	PB-O3A-PA-O5'
3	A	901	ATP	PA-O3A-PB-O2B
3	A	903	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	B	903	ATP	PA-O3A-PB-O2B

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

There are no ring outliers.

12 monomers are involved in 48 short contacts:

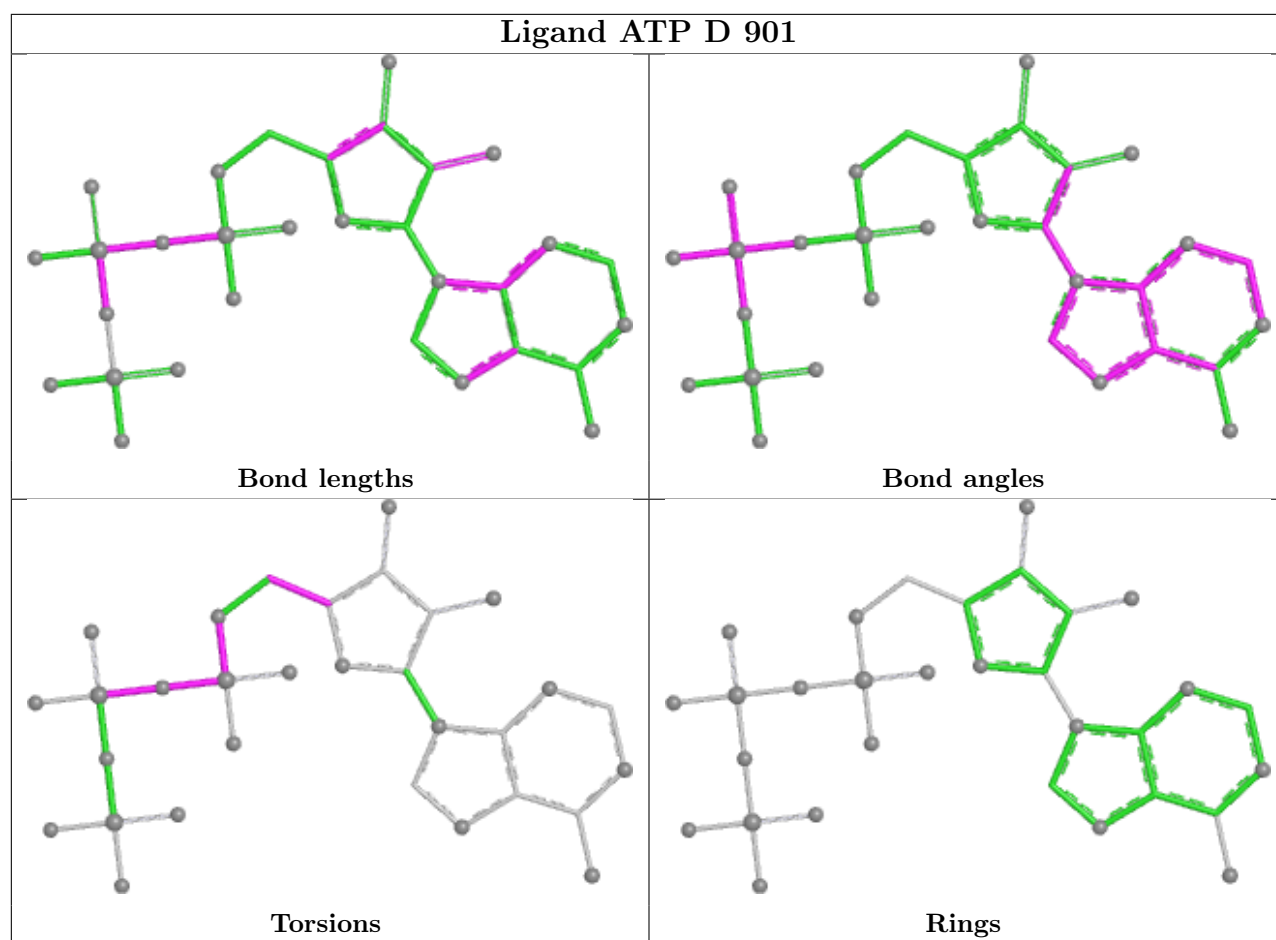
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	901	ATP	1	0
3	C	903	ATP	5	0
3	F	903	ATP	3	0

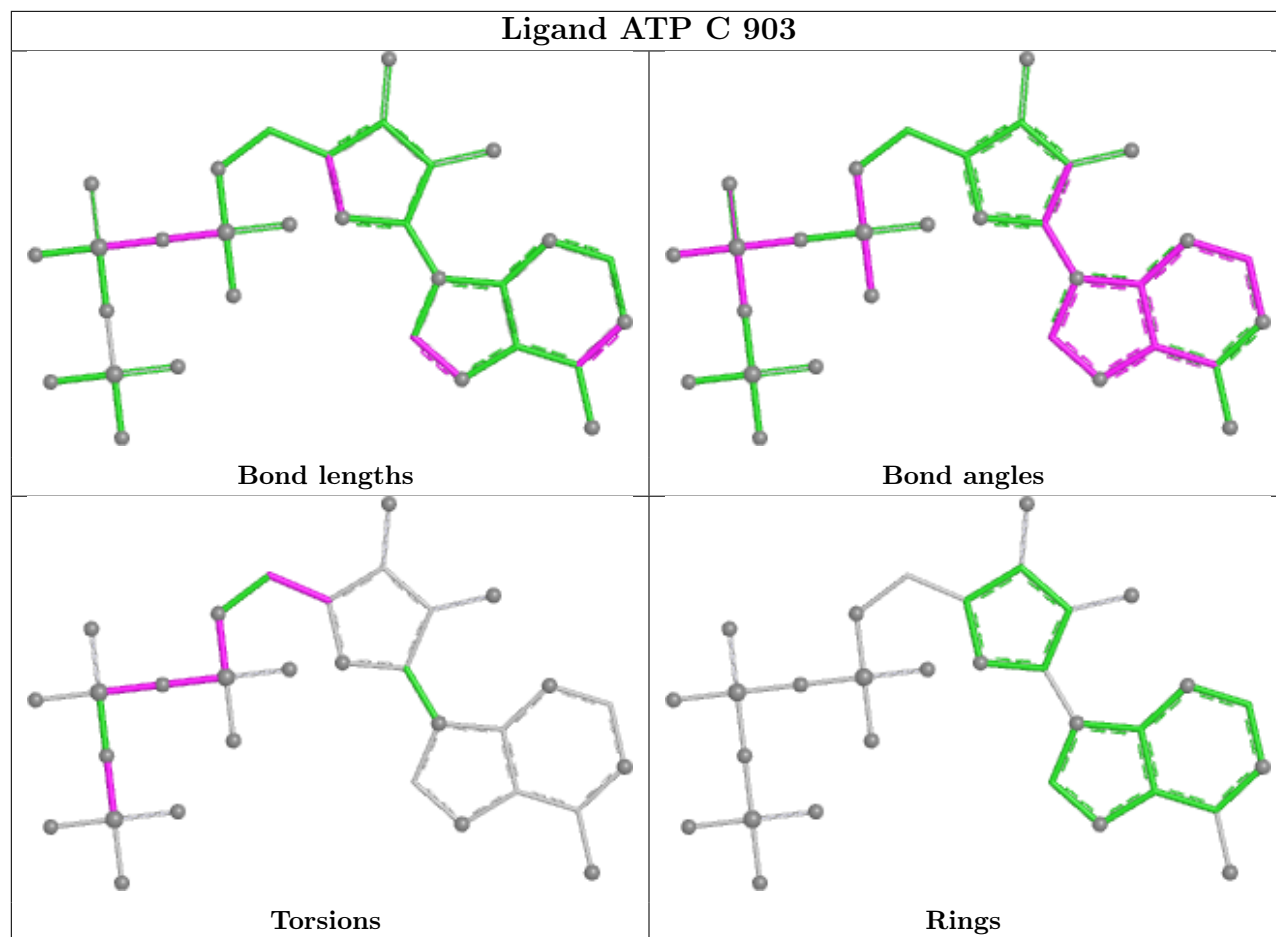
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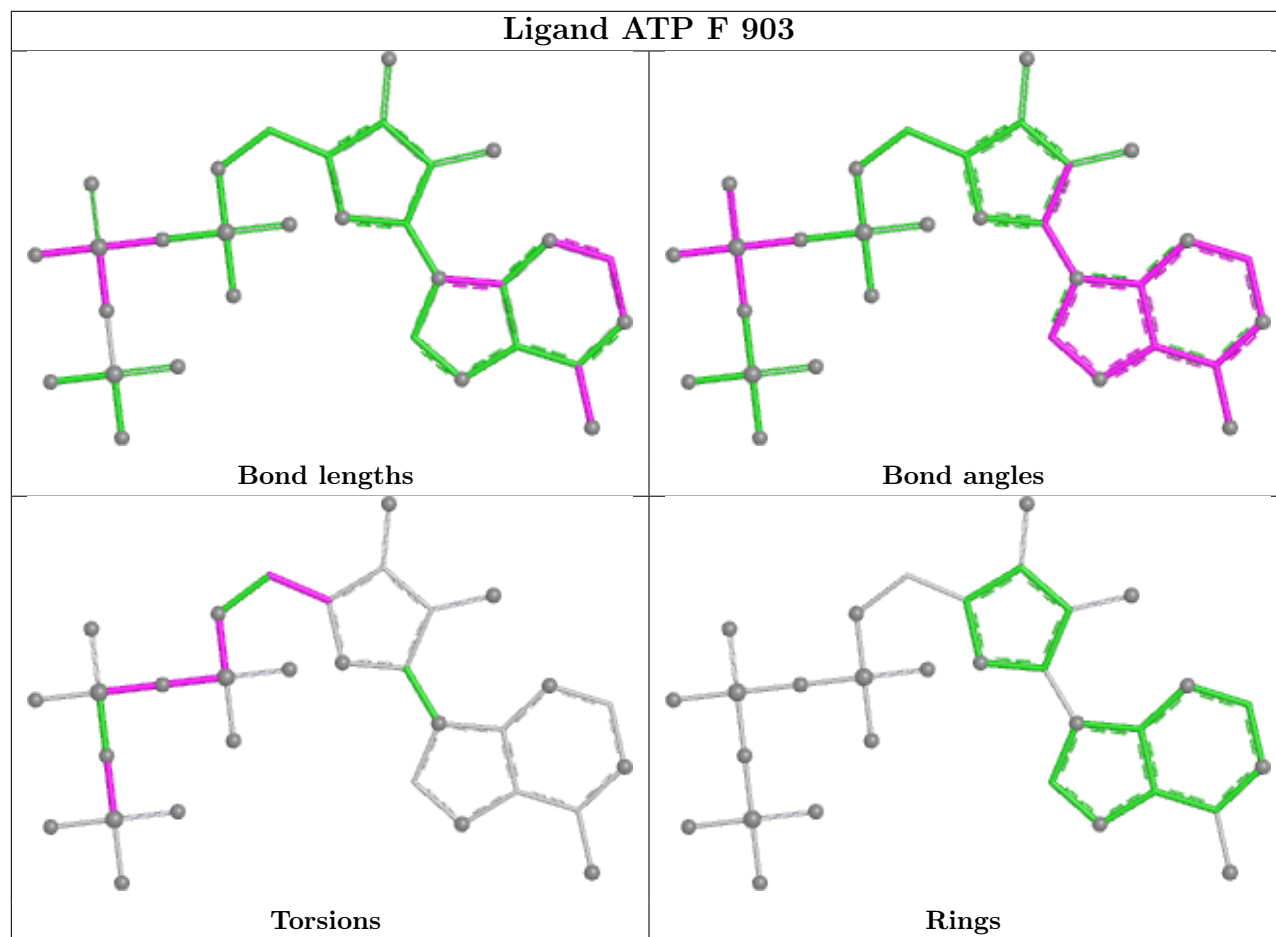
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	ATP	3	0
3	B	901	ATP	6	0
3	A	903	ATP	5	0
3	C	901	ATP	2	0
3	E	901	ATP	4	0
3	A	901	ATP	7	0
3	E	903	ATP	3	0
3	D	903	ATP	5	0
3	F	901	ATP	4	0

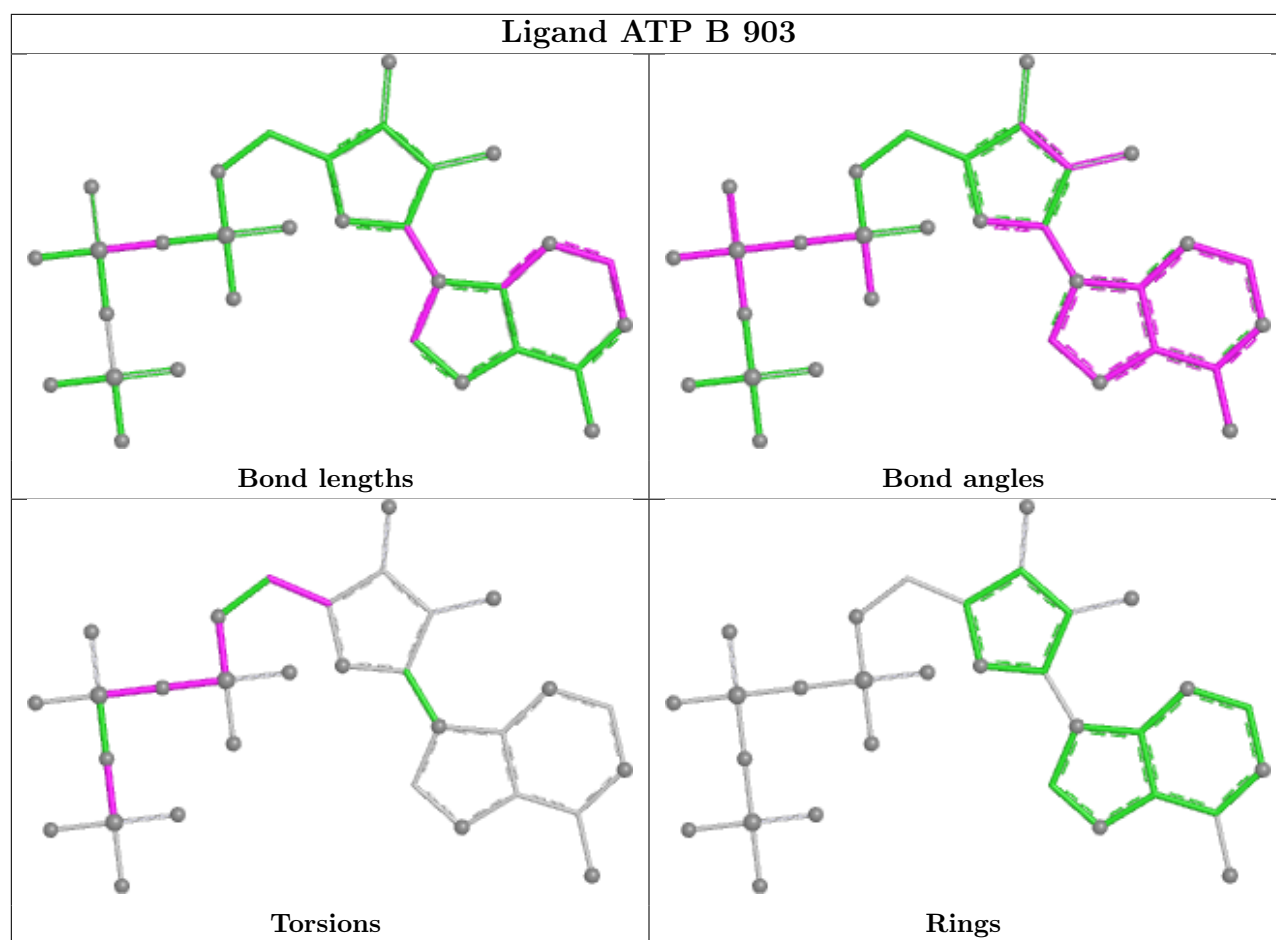
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

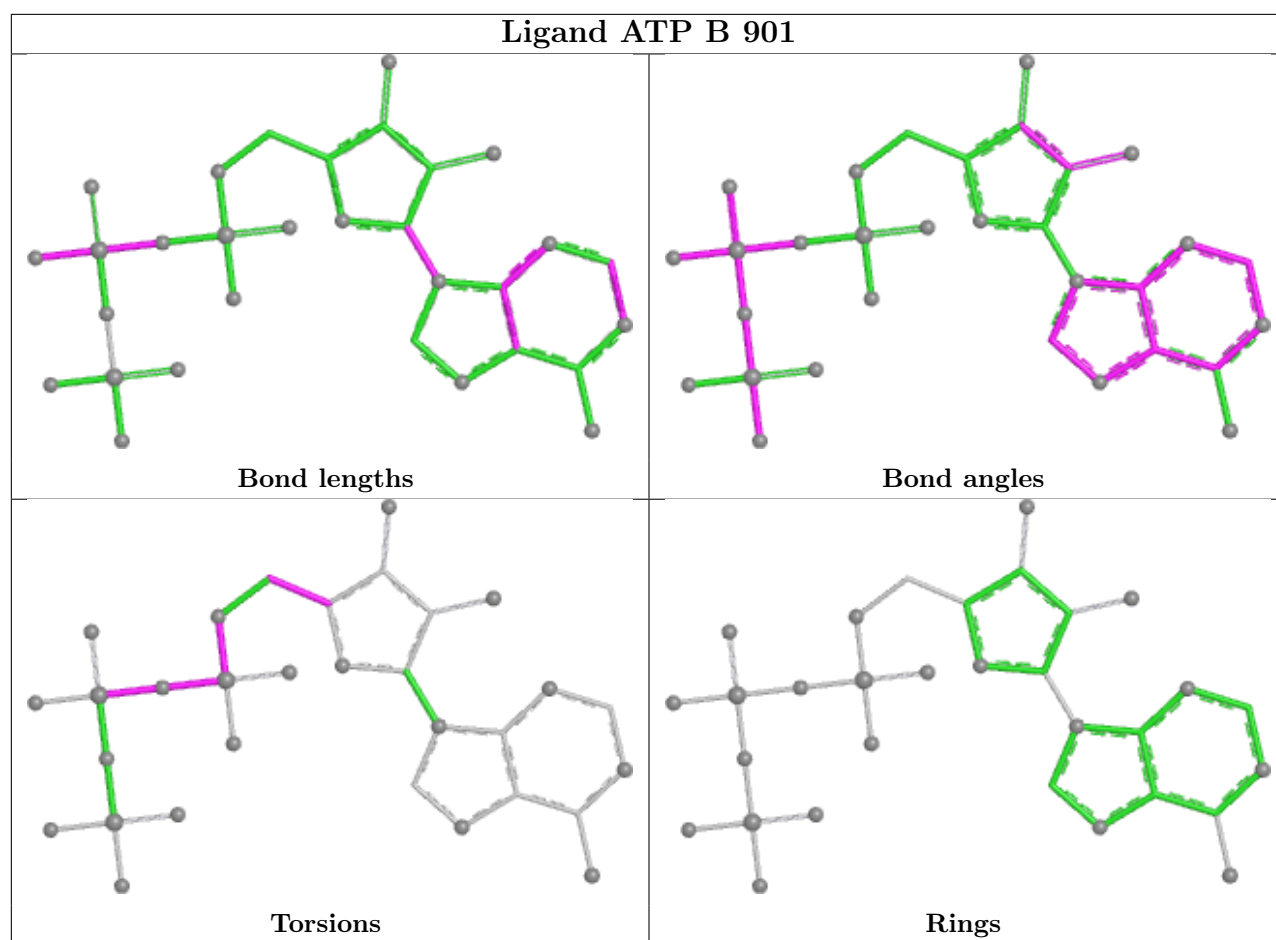


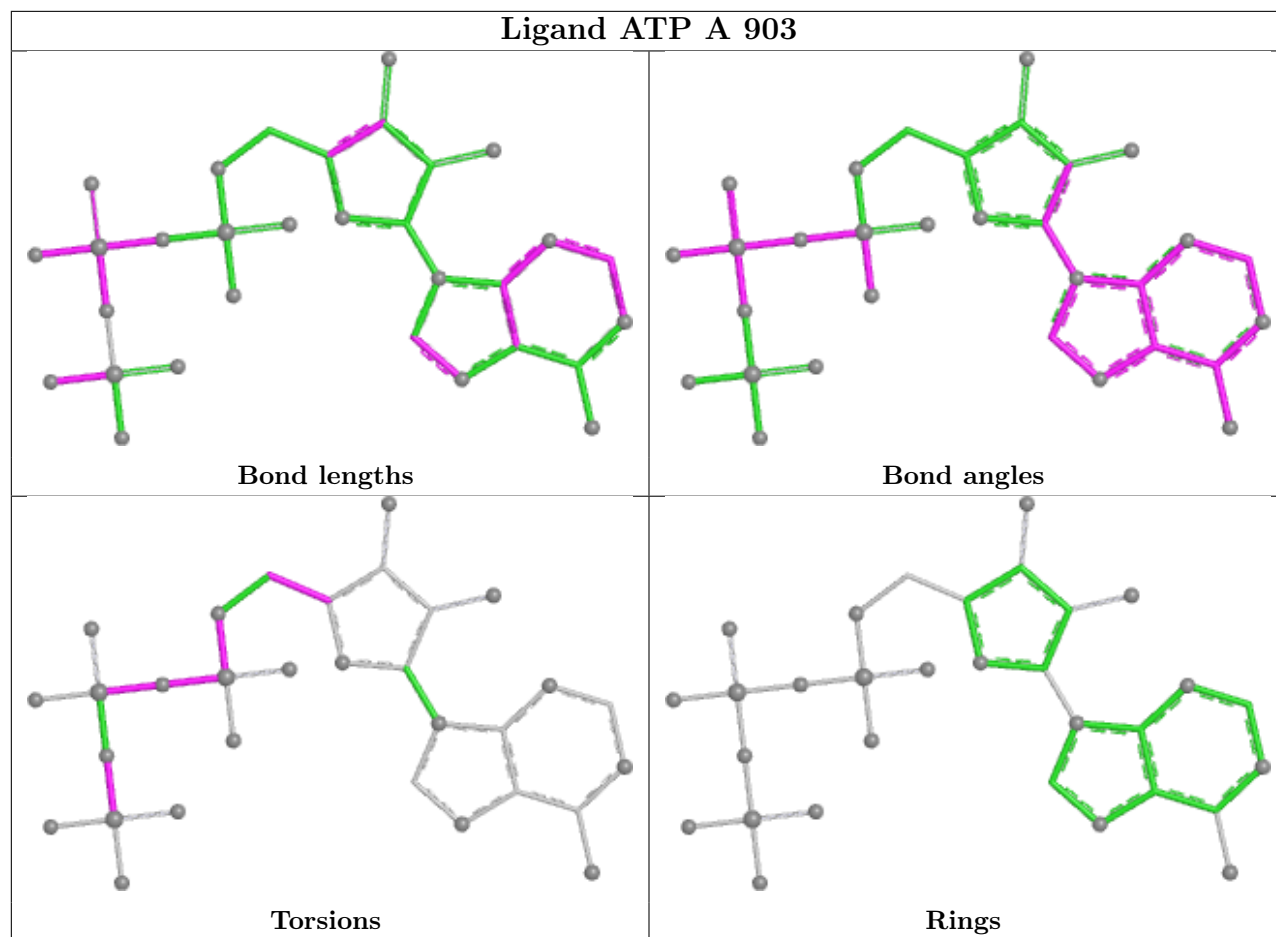


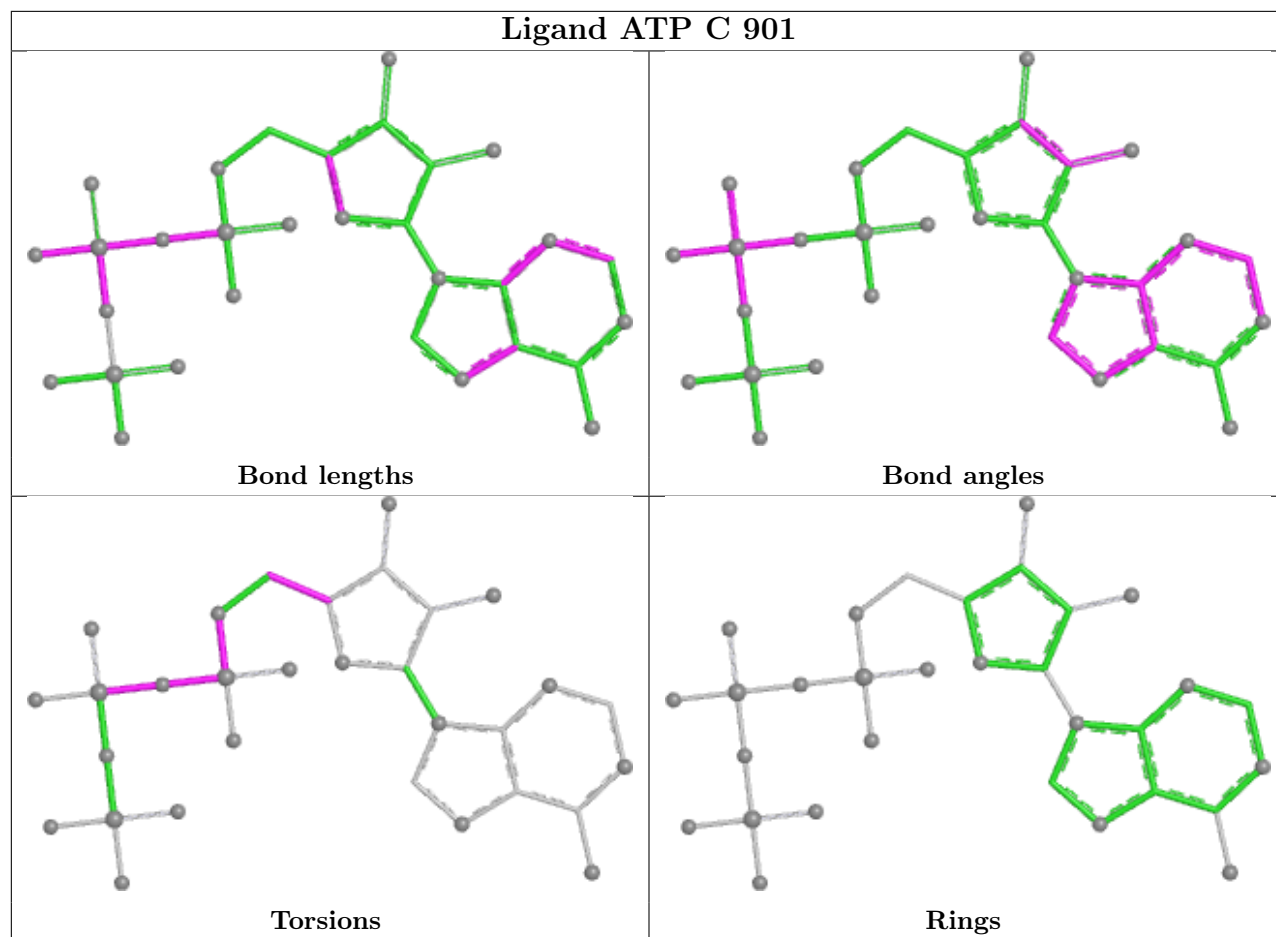
Ligand ATP F 903

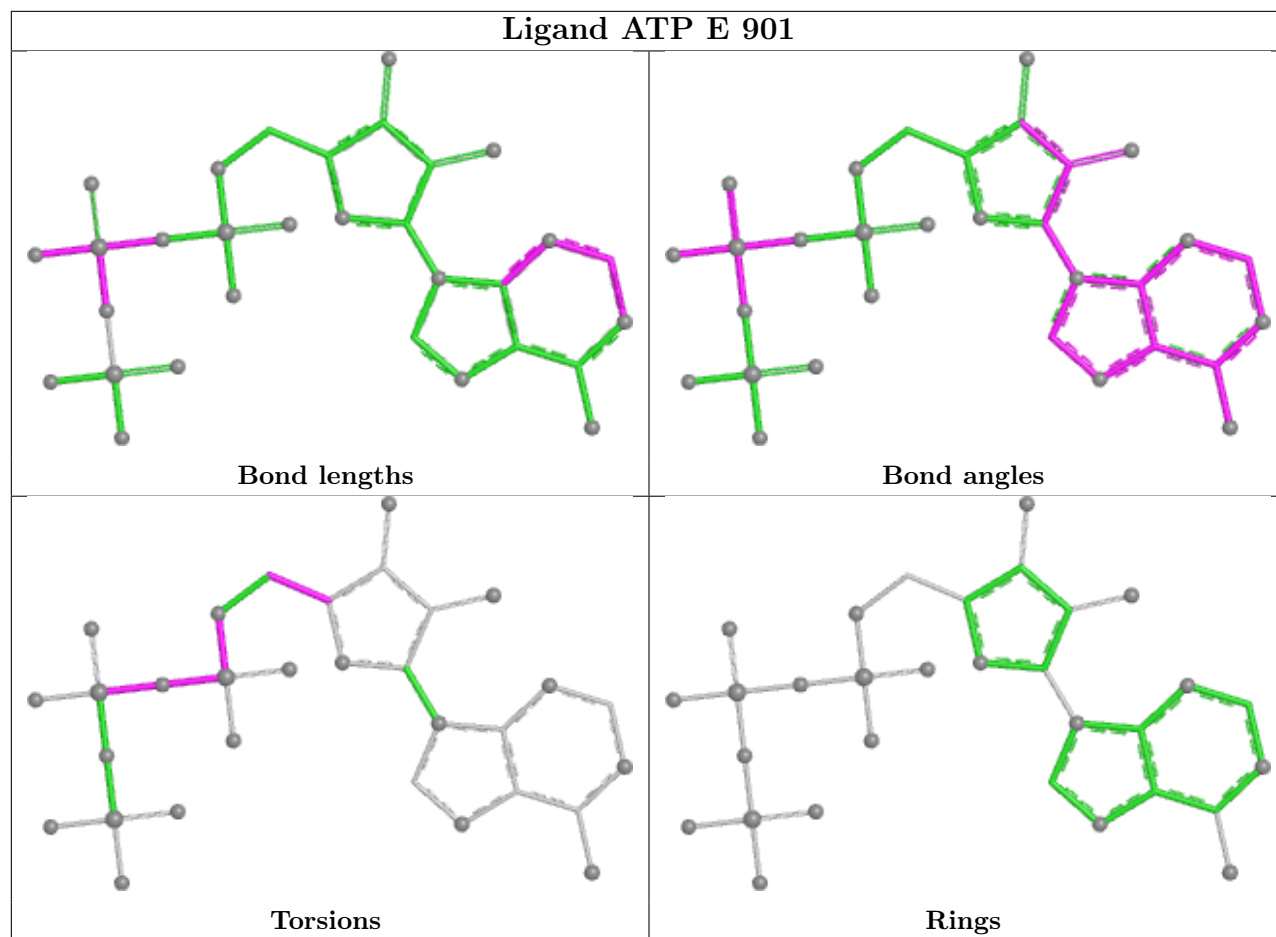


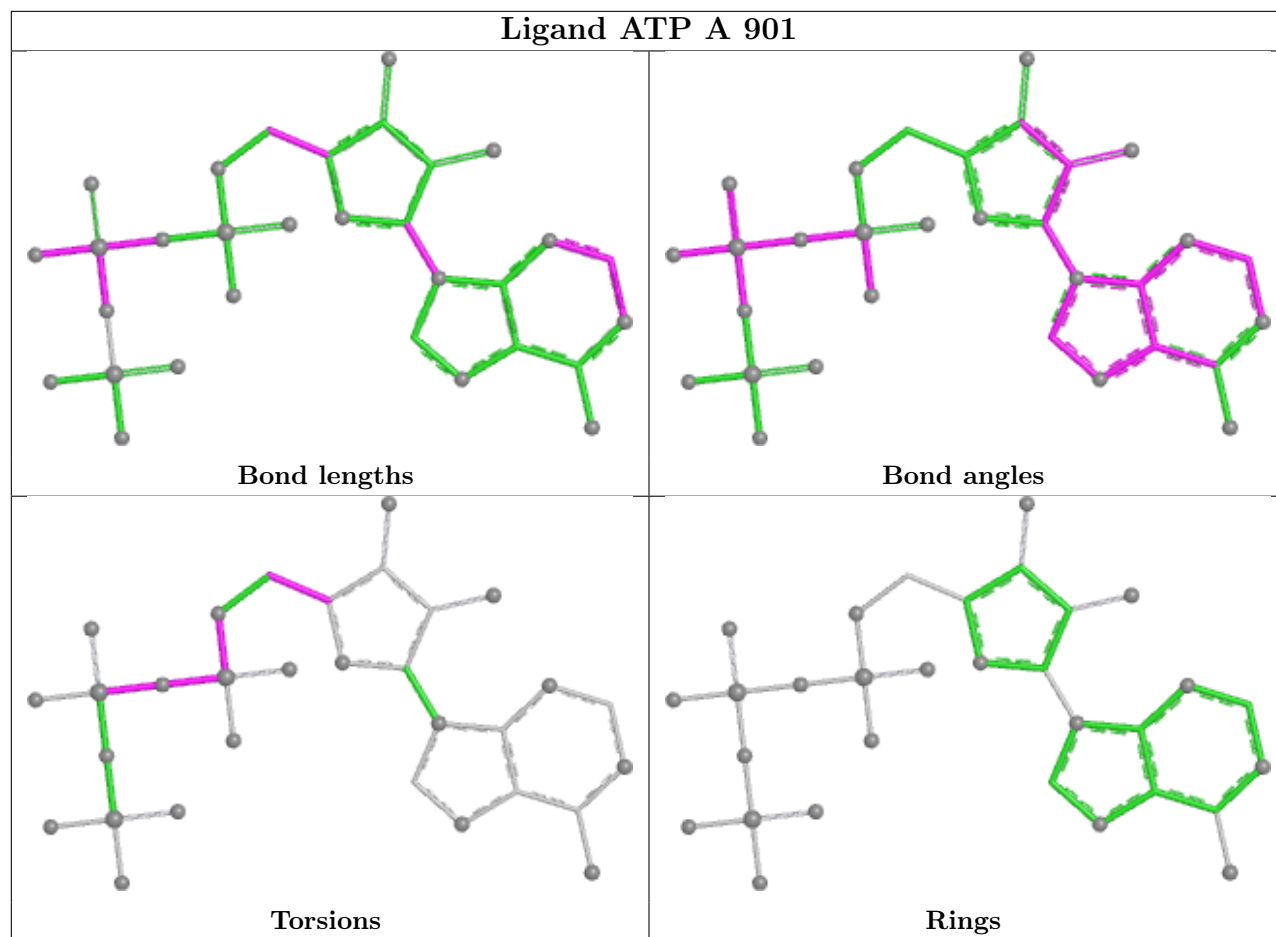


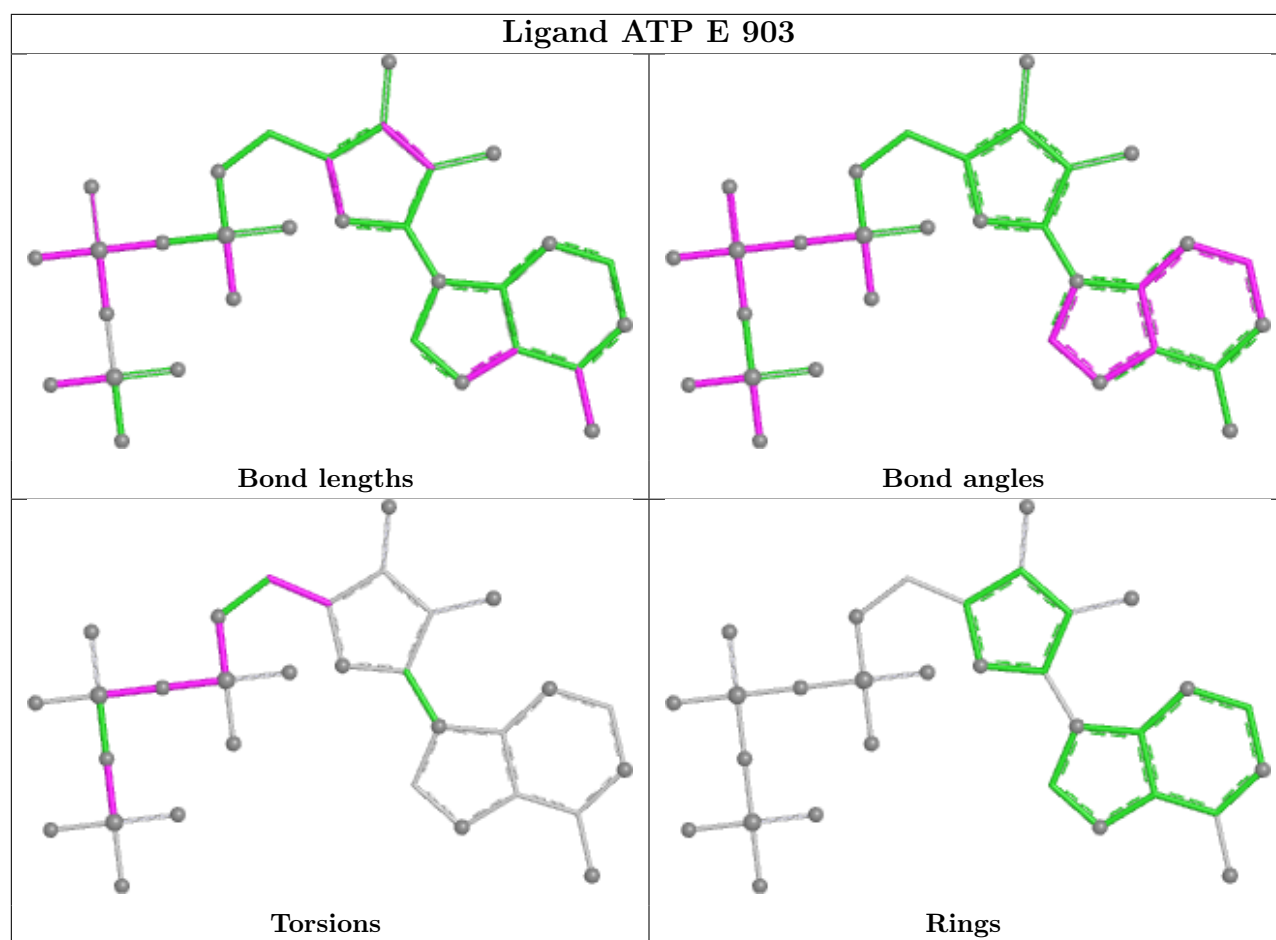


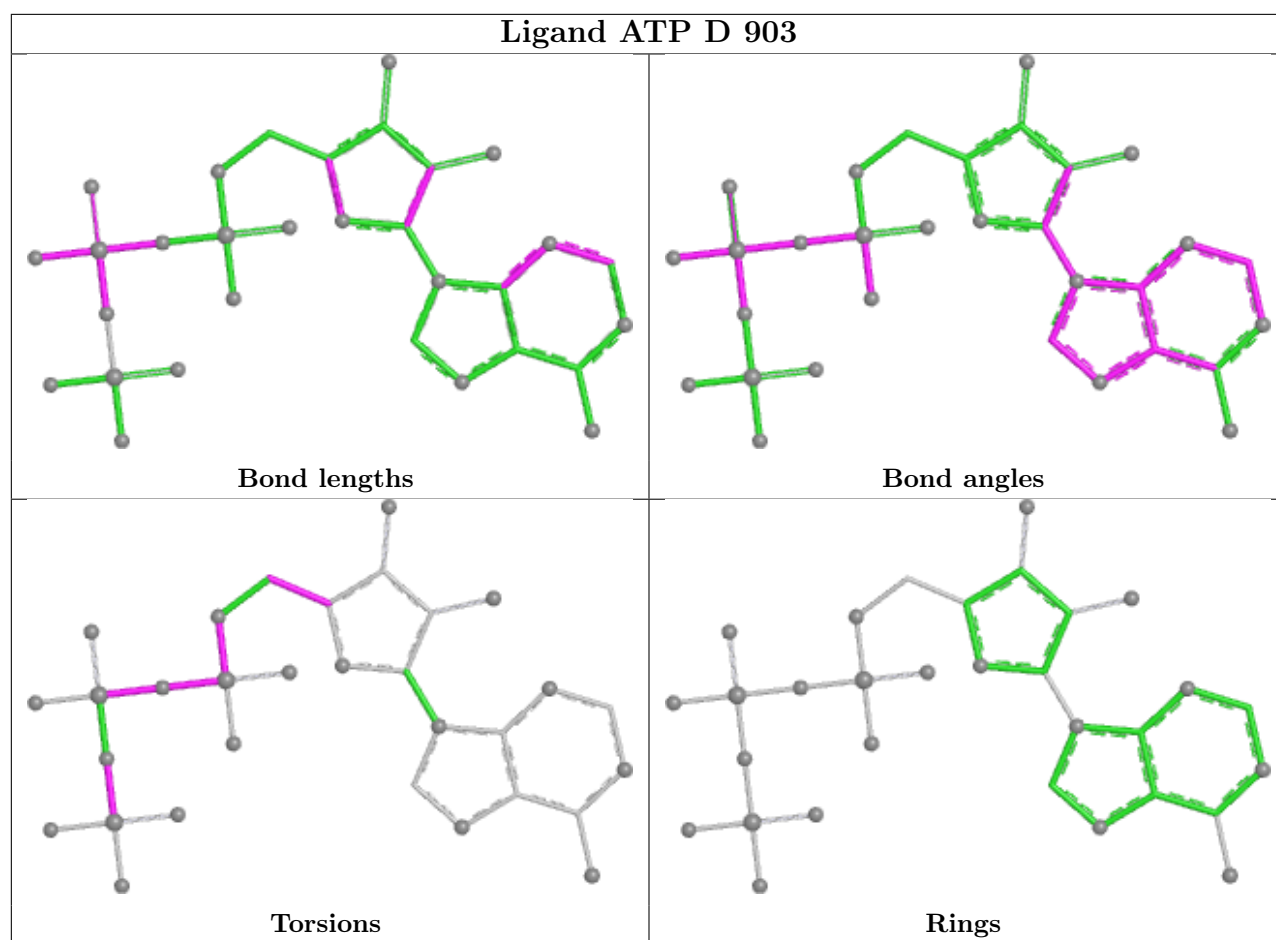


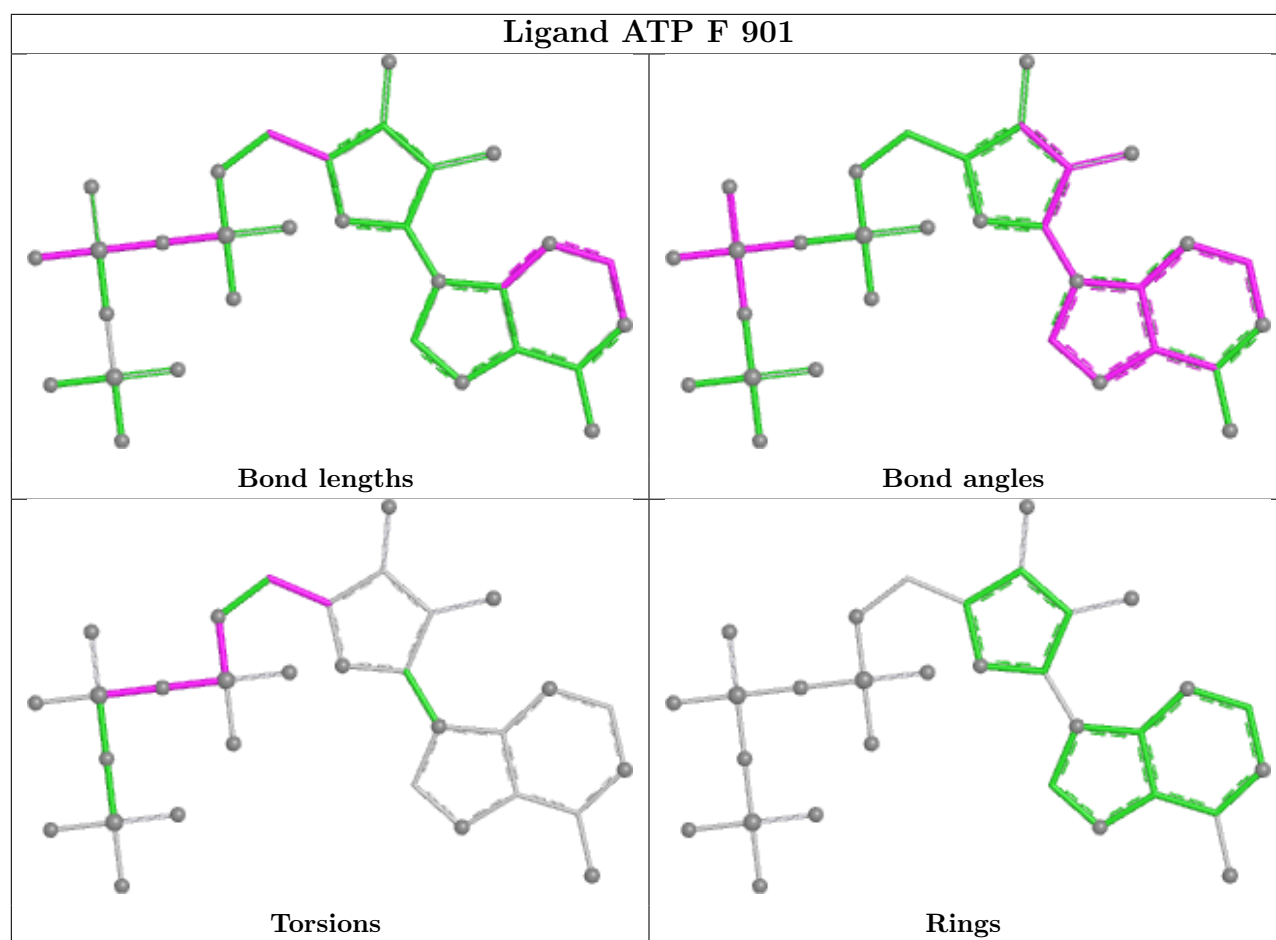












5.7 Other polymers [i](#)

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%)	0.17	17 (3%)	48 39	29, 76, 127, 154	0
1	B	489/519 (94%)	0.27	17 (3%)	47 38	24, 82, 128, 160	0
1	C	486/519 (93%)	0.02	9 (1%)	66 57	33, 73, 124, 160	0
1	D	483/519 (93%)	-0.20	8 (1%)	69 60	27, 58, 109, 160	0
1	E	490/519 (94%)	-0.18	7 (1%)	73 64	20, 60, 107, 155	0
1	F	504/519 (97%)	-0.05	8 (1%)	70 61	20, 69, 114, 158	0
All	All	2956/3114 (94%)	0.01	66 (2%)	62 52	20, 71, 121, 160	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	VAL	3.7
1	A	258	SER	3.7
1	B	92	TRP	3.6
1	B	117	VAL	3.4
1	A	509	VAL	3.3
1	F	508	ILE	3.2
1	D	121	PHE	3.1
1	A	506	SER	3.0
1	C	249	LEU	3.0
1	E	249	LEU	2.9
1	A	517	PRO	2.9
1	F	121	PHE	2.9
1	A	117	VAL	2.9
1	E	505	LEU	2.8
1	C	213	GLY	2.8
1	D	17	ALA	2.8
1	A	503	SER	2.8
1	B	499	VAL	2.7
1	A	508	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	511	GLY	2.6
1	C	118	VAL	2.6
1	E	152	GLN	2.6
1	B	335	PHE	2.6
1	B	500	ASP	2.6
1	C	17	ALA	2.6
1	B	90	PHE	2.6
1	B	338	MET	2.5
1	A	499	VAL	2.5
1	A	514	GLU	2.5
1	B	498	THR	2.5
1	C	423	HIS	2.5
1	E	212	GLU	2.5
1	A	498	THR	2.5
1	B	121	PHE	2.4
1	D	366	GLU	2.4
1	F	509	VAL	2.4
1	F	506	SER	2.4
1	E	156	ALA	2.4
1	B	112	PRO	2.4
1	D	118	VAL	2.4
1	A	518	GLU	2.4
1	F	516	GLY	2.3
1	B	118	VAL	2.3
1	C	117	VAL	2.3
1	A	507	ARG	2.3
1	D	321	ARG	2.3
1	F	517	PRO	2.3
1	B	115	GLN	2.3
1	D	249	LEU	2.3
1	B	158	SER	2.3
1	A	338	MET	2.2
1	C	499	VAL	2.2
1	F	247	PHE	2.2
1	C	176	ALA	2.2
1	E	321	ARG	2.2
1	A	516	GLY	2.2
1	E	357	GLU	2.2
1	B	135	GLN	2.1
1	A	433	ILE	2.1
1	C	15	HIS	2.1
1	B	156	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	471	MET	2.1
1	B	123	LEU	2.0
1	A	513	GLN	2.0
1	F	117	VAL	2.0
1	B	348	CYS	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
1	SEP	E	431	10/11	0.61	0.26	13,56,60,60	0
1	TPO	B	432	11/12	0.67	0.27	29,29,29,29	0
1	TPO	A	432	11/12	0.69	0.27	19,19,19,19	0
1	TPO	C	432	11/12	0.72	0.25	10,19,77,79	0
1	TPO	E	432	11/12	0.72	0.20	17,18,22,23	0
1	SEP	F	431	10/11	0.75	0.29	13,79,83,83	0
1	TPO	D	432	11/12	0.76	0.24	19,19,19,19	0
1	SEP	B	431	10/11	0.79	0.23	29,81,86,88	0
1	SEP	D	431	6/11	0.79	0.17	57,63,68,70	0
1	SEP	C	431	6/11	0.80	0.18	75,79,81,84	0
1	TPO	F	432	11/12	0.82	0.23	16,20,74,75	0
1	SEP	A	431	10/11	0.84	0.23	17,78,80,83	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
2	MG	B	802	1/1	0.77	0.08	73,73,73,73	0

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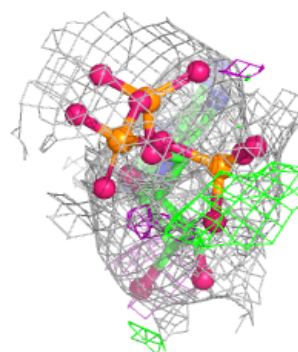
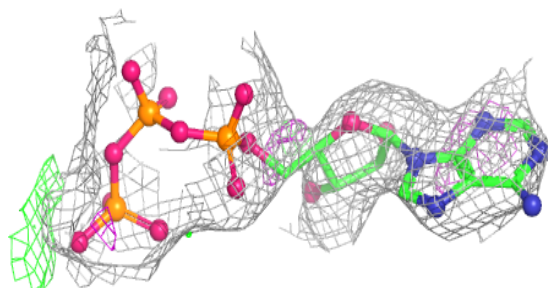
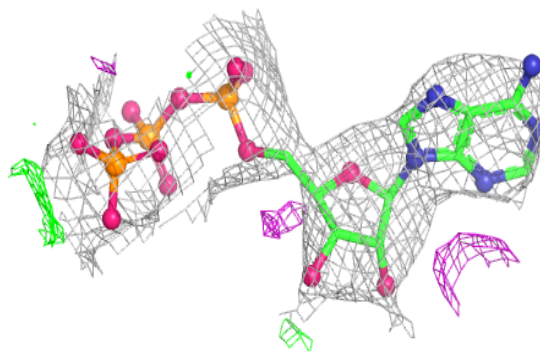
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	F	901	31/31	0.87	0.11	74,89,113,120	0
3	ATP	B	903	31/31	0.90	0.09	43,54,76,80	0
2	MG	E	805	1/1	0.90	0.09	18,18,18,18	0
3	ATP	A	901	31/31	0.91	0.10	75,88,102,112	0
3	ATP	A	903	31/31	0.93	0.09	42,54,76,80	0
3	ATP	E	901	31/31	0.93	0.09	61,76,100,113	0
3	ATP	B	901	31/31	0.93	0.08	61,73,109,115	0
3	ATP	C	903	31/31	0.94	0.08	42,54,76,80	0
3	ATP	D	901	31/31	0.94	0.09	53,65,88,104	0
2	MG	A	801	1/1	0.94	0.18	18,18,18,18	0
3	ATP	E	903	31/31	0.94	0.11	42,53,76,80	0
3	ATP	C	901	31/31	0.94	0.09	47,55,96,109	0
3	ATP	F	903	31/31	0.94	0.10	42,53,76,79	0
2	MG	C	803	1/1	0.95	0.08	18,18,18,18	0
2	MG	F	806	1/1	0.95	0.15	18,18,18,18	0
2	MG	D	804	1/1	0.95	0.04	18,18,18,18	0
3	ATP	D	903	31/31	0.95	0.10	42,53,76,80	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.

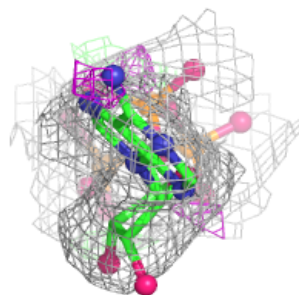
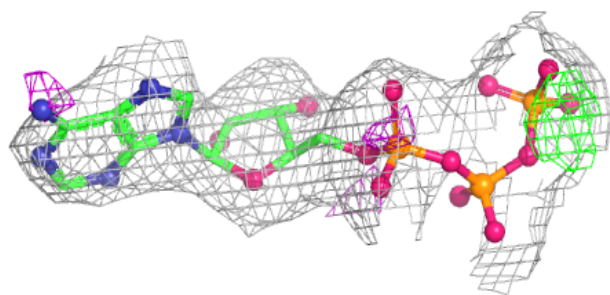
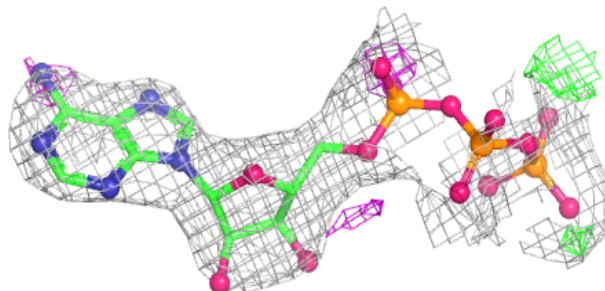
Electron density around ATP F 901:

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

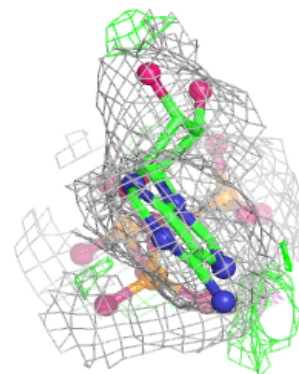
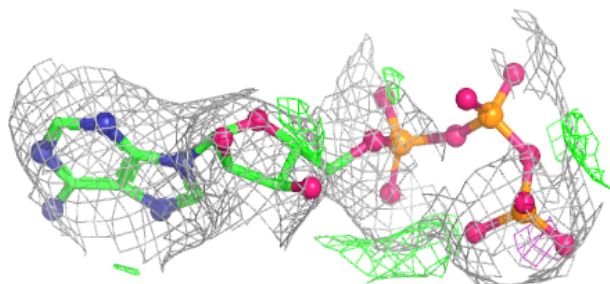
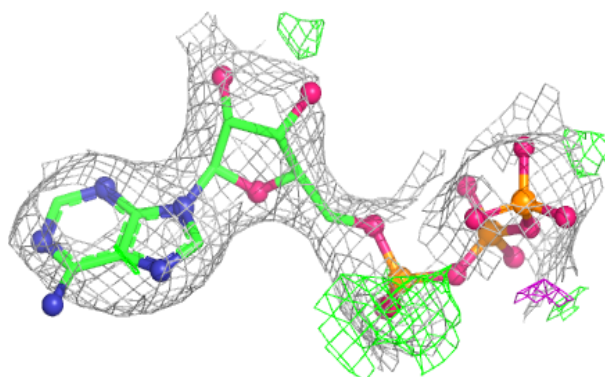


Electron density around ATP B 903:

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and green (positive)

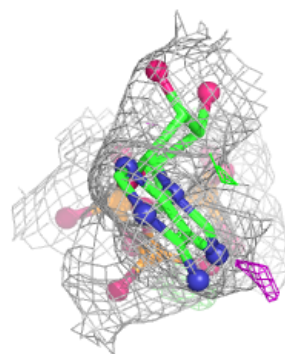
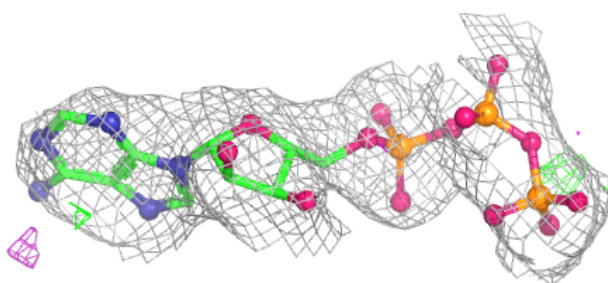
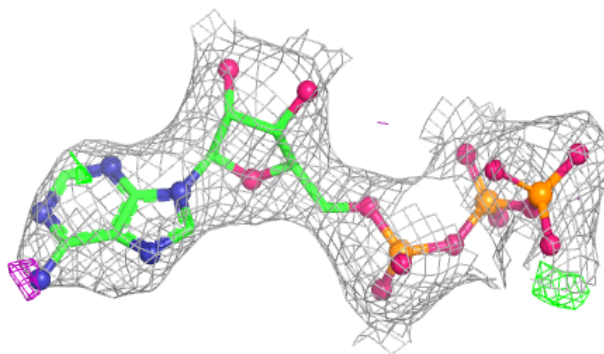
**Electron density around ATP A 901:**

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

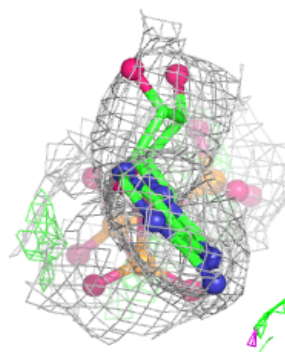
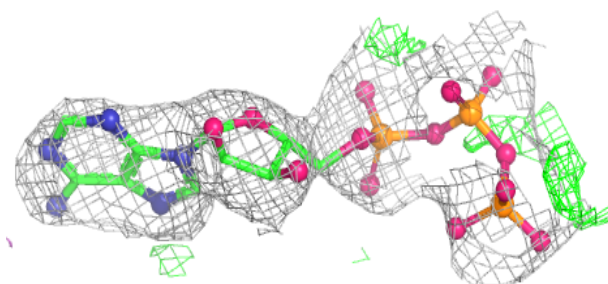
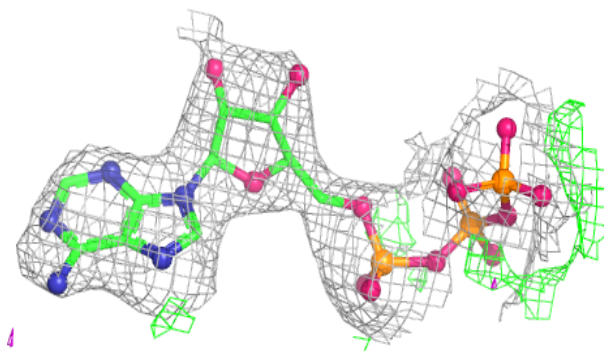


Electron density around ATP A 903:

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and green (positive)

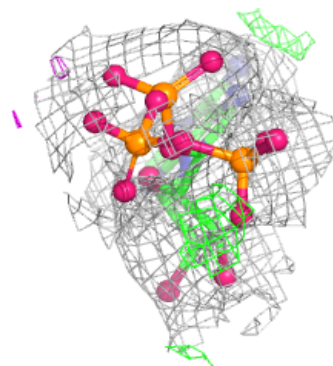
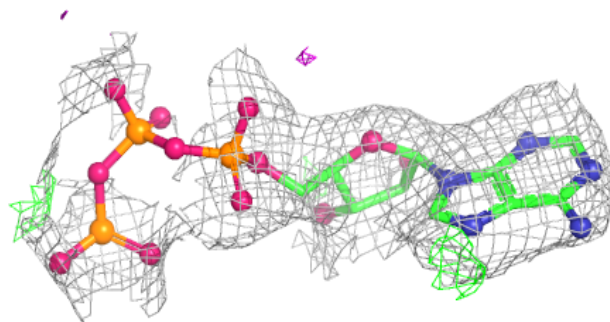
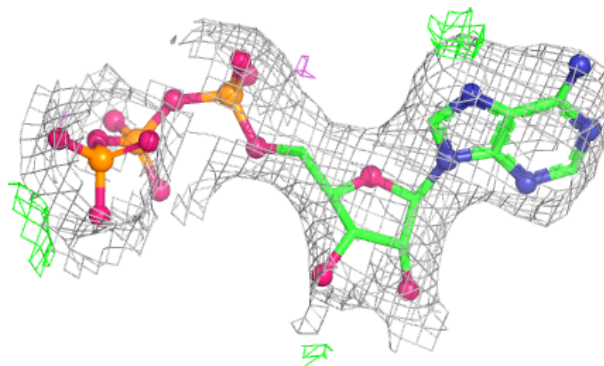
**Electron density around ATP E 901:**

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and green (positive)

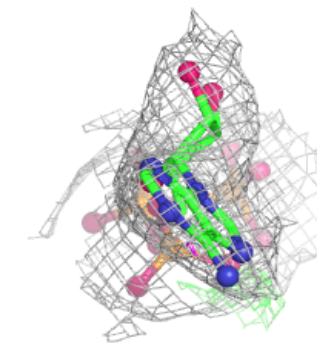
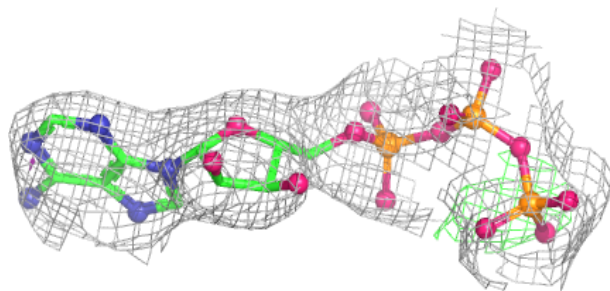
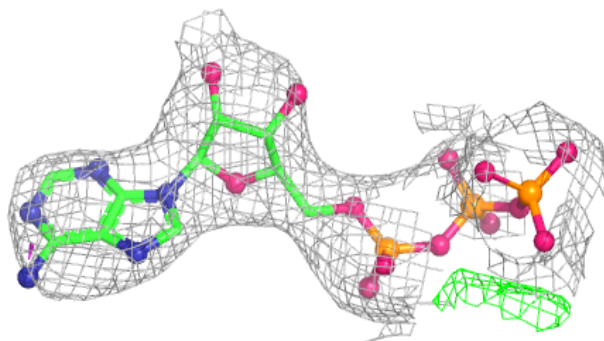


Electron density around ATP B 901:

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and green (positive)

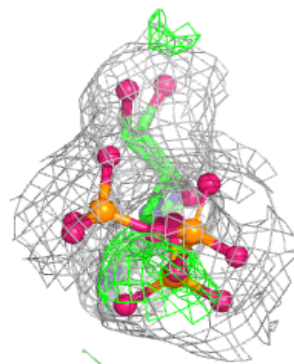
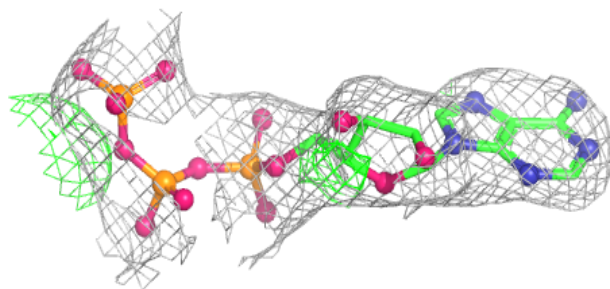
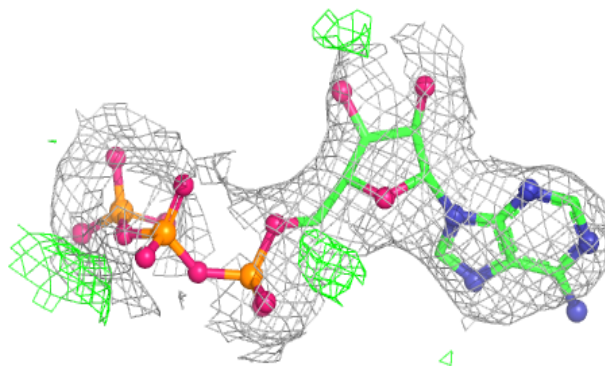
**Electron density around ATP C 903:**

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and green (positive)

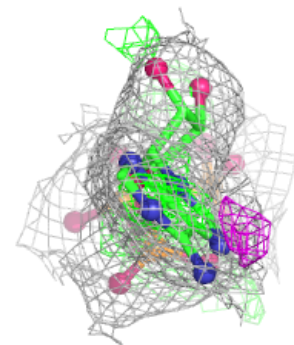
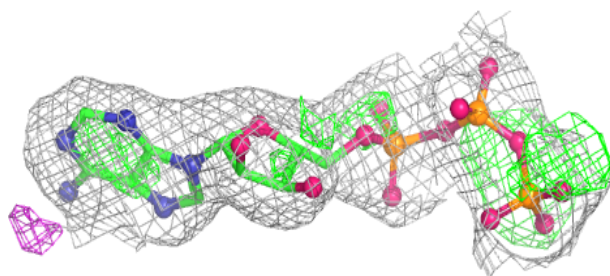
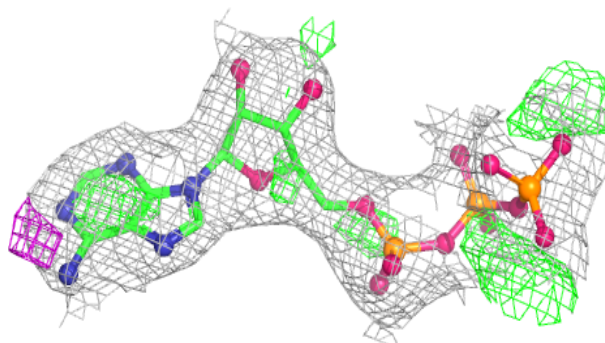


Electron density around ATP D 901:

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and green (positive)

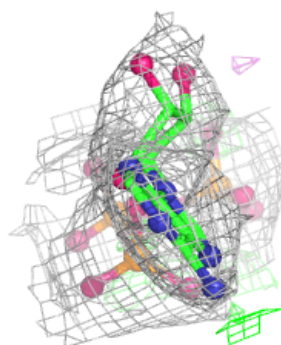
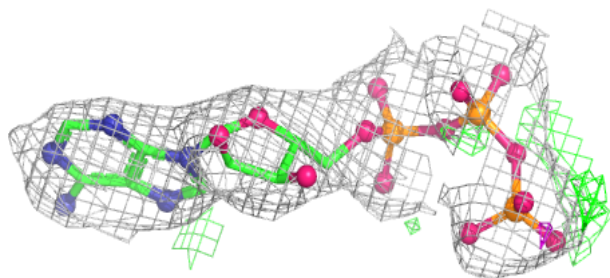
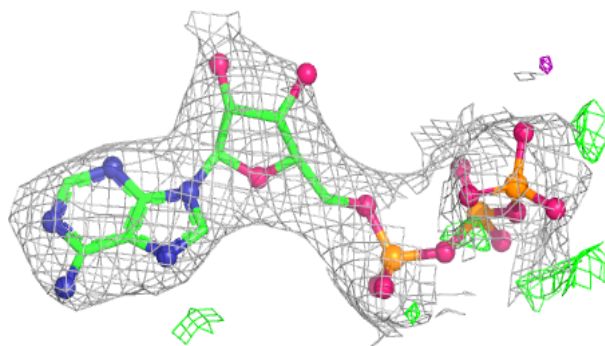
**Electron density around ATP E 903:**

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

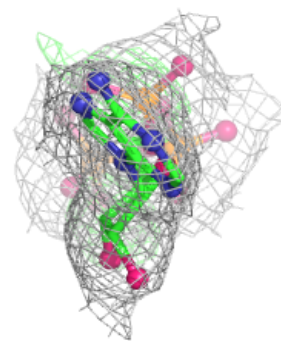
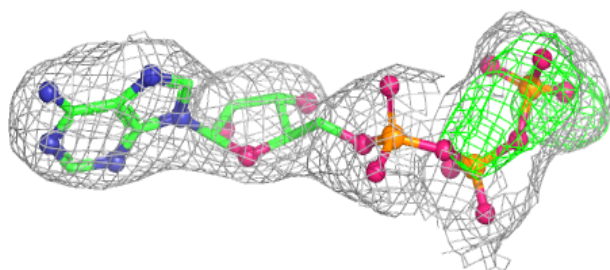
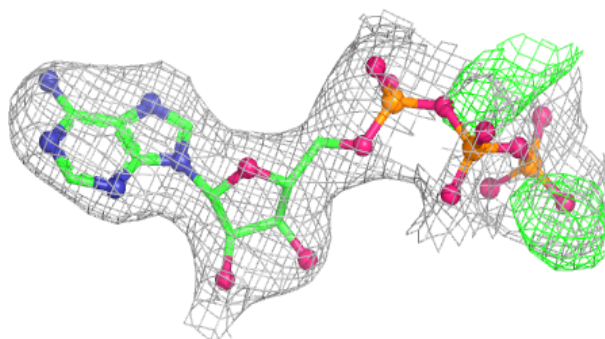


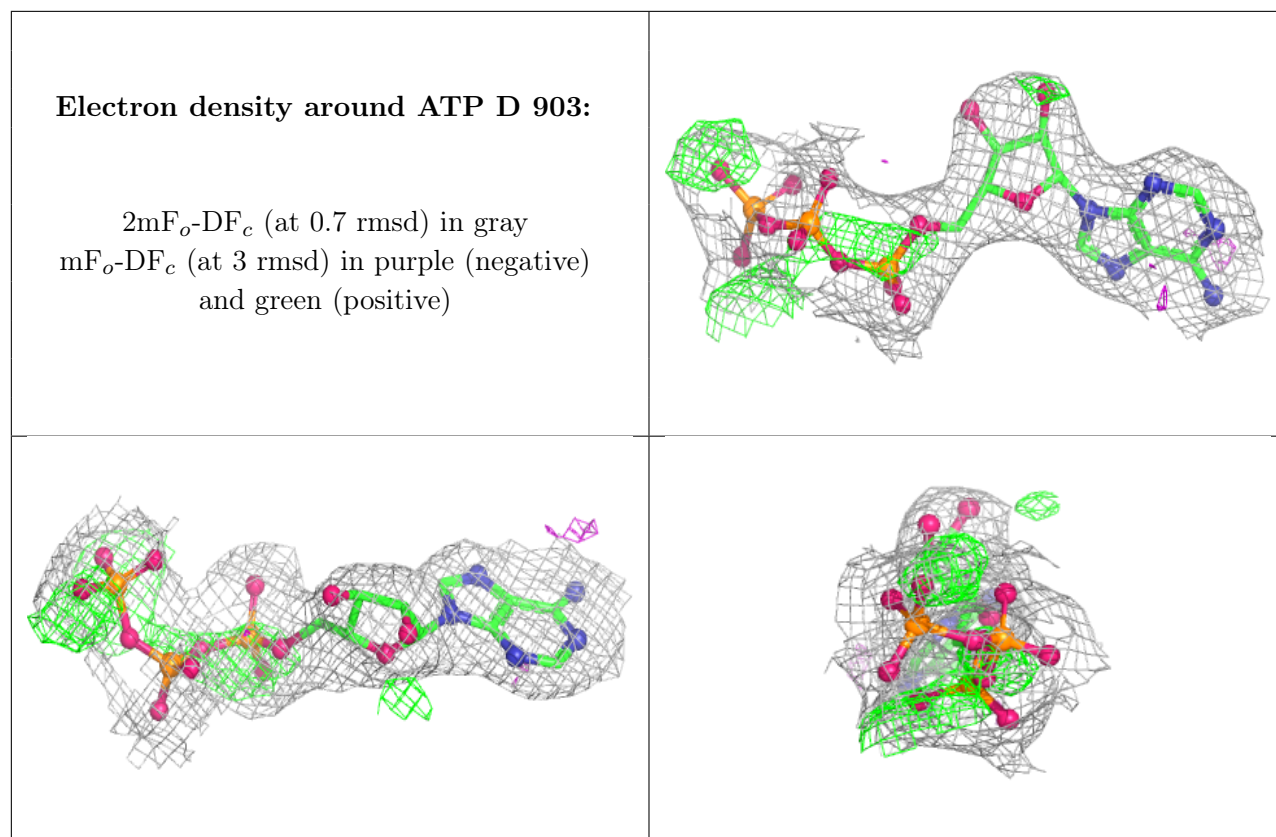
Electron density around ATP C 901:

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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.