Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 05:28 PM EST

PDB ID	:	6N8Z
EMDB ID	:	EMD-0377
Title	:	HSP104DWB extended conformation
Authors	:	Lee, S.; Rho, S.H.; Lee, J.; Sung, N.; Liu, J.; Tsai, F.T.F.
Deposited on	:	2018-11-30
Resolution	:	9.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

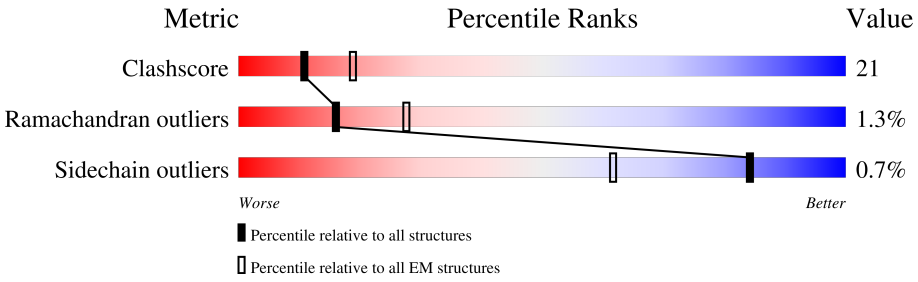
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	879	29% 56% 9% · 34%
1	B	879	24% 69% 12% · 18%
1	C	879	19% 66% 14% · 18%
1	D	879	22% 67% 14% · 18%
1	E	879	24% 66% 14% · 18%
1	F	879	37% 55% 9% · 34%

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
2	ATP	A	1001	-	-	X	-
2	ATP	A	1002	-	-	X	-
2	ATP	D	901	-	-	X	-
2	ATP	E	1003	-	-	X	-

2 Entry composition

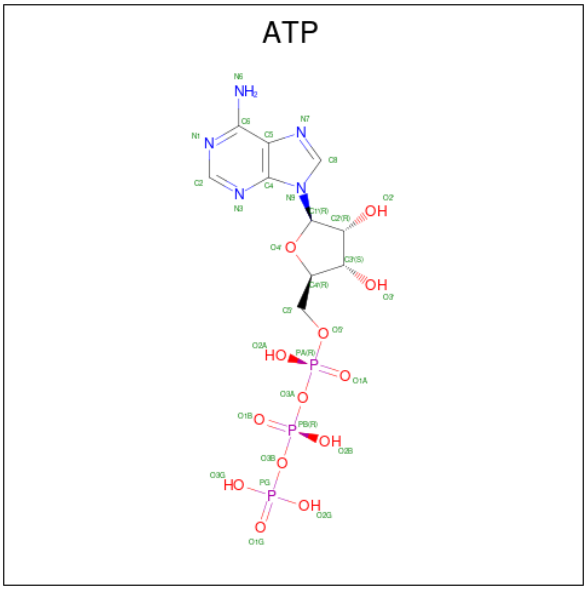
There are 2 unique types of molecules in this entry. The entry contains 32080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	579	Total	C	N	O	S	0	0
			4519	2843	794	864	18		
1	B	723	Total	C	N	O	S	0	0
			5654	3569	988	1079	18		
1	C	723	Total	C	N	O	S	0	0
			5679	3587	994	1080	18		
1	D	723	Total	C	N	O	S	0	0
			5676	3586	994	1078	18		
1	E	723	Total	C	N	O	S	0	0
			5673	3581	994	1080	18		
1	F	579	Total	C	N	O	S	0	0
			4507	2837	788	864	18		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

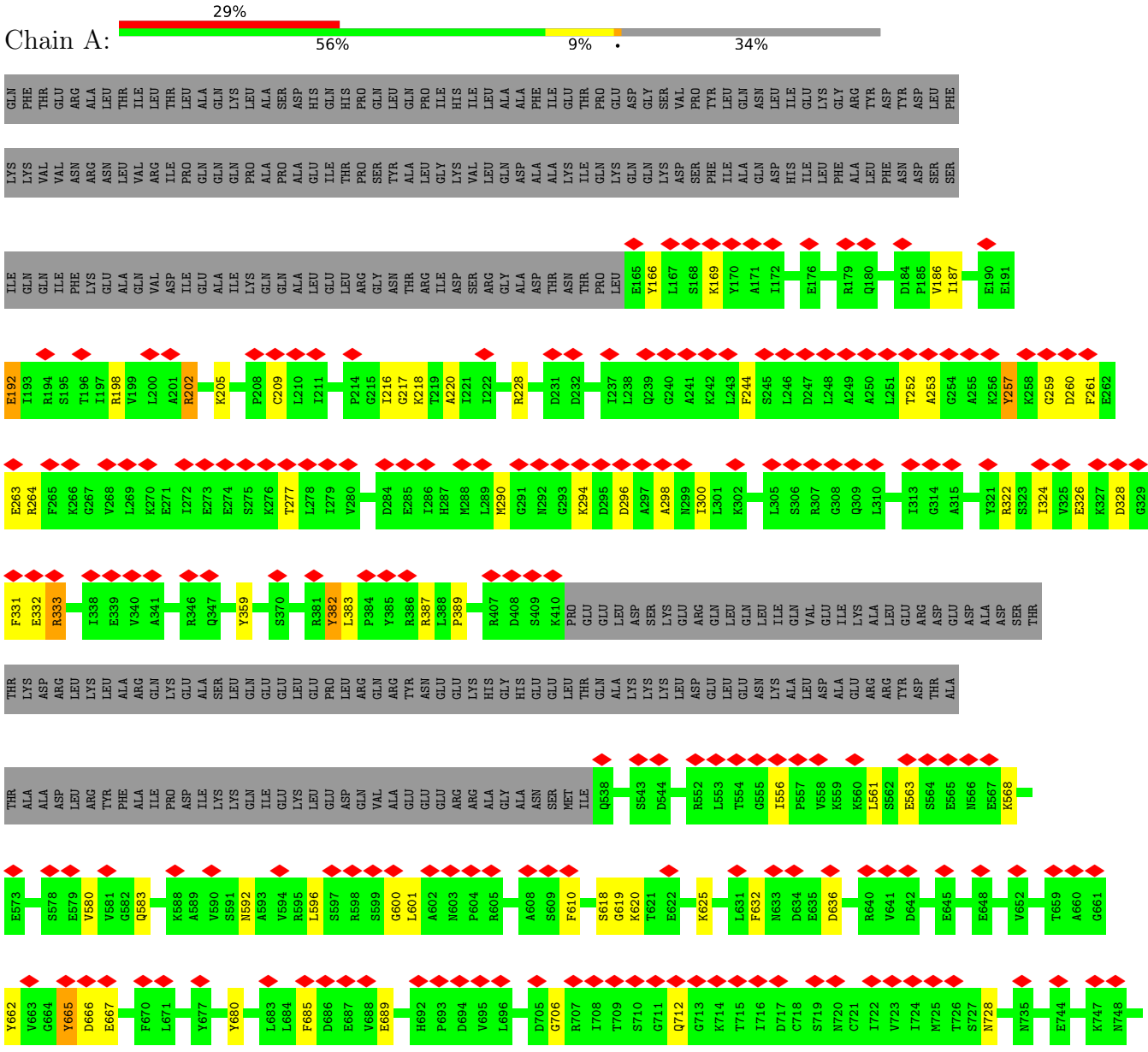


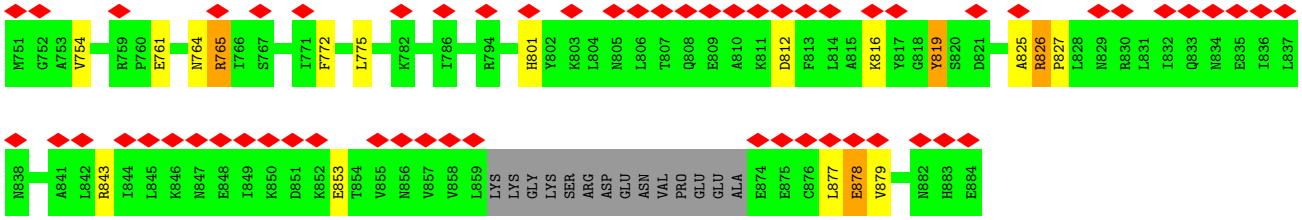
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	E	1	Total	C	N	O	P	0
			93	30	15	39	9	
2	E	1	Total	C	N	O	P	0
			93	30	15	39	9	
2	E	1	Total	C	N	O	P	0
			93	30	15	39	9	
2	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

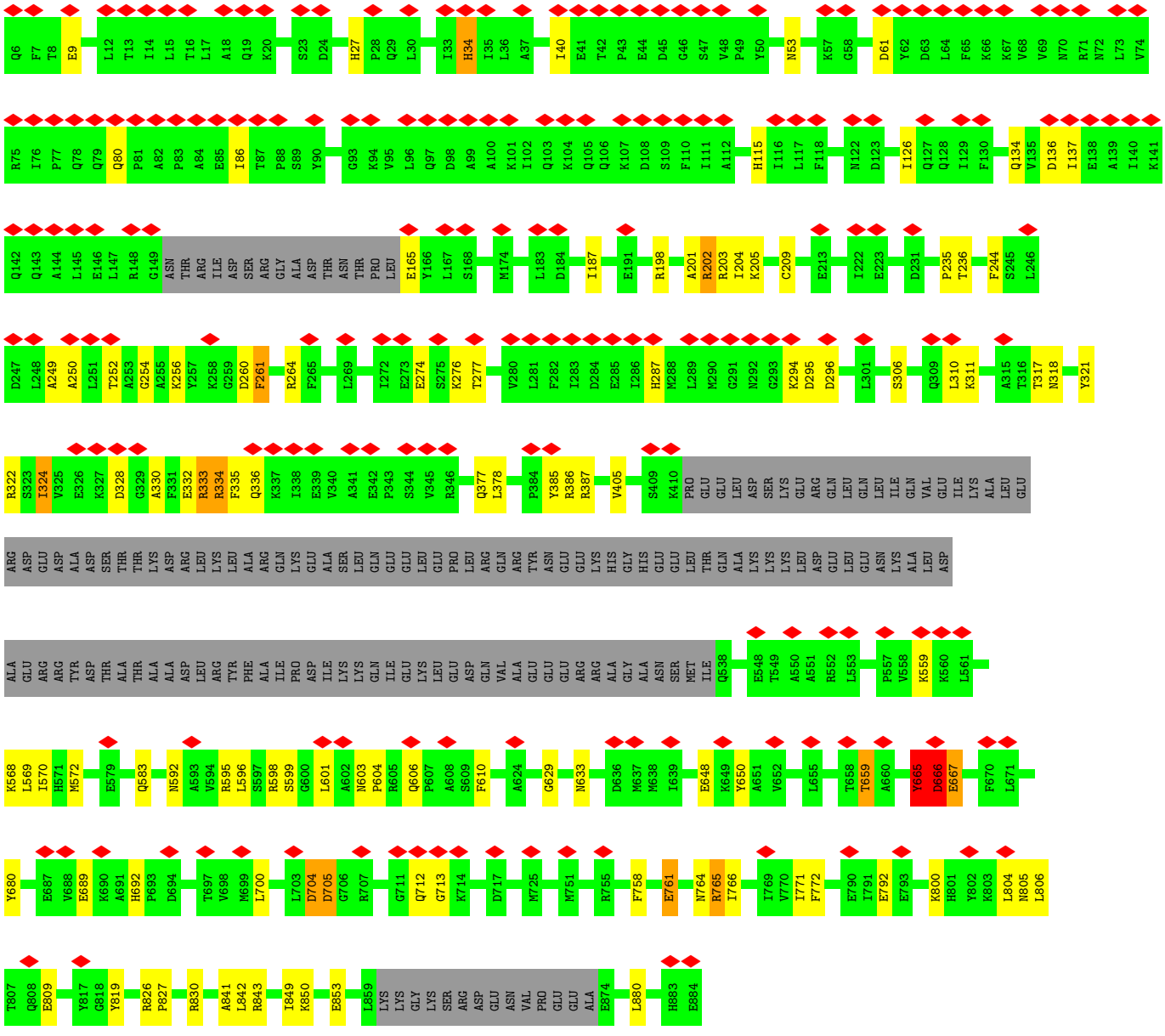
- Molecule 1: Heat shock protein 104





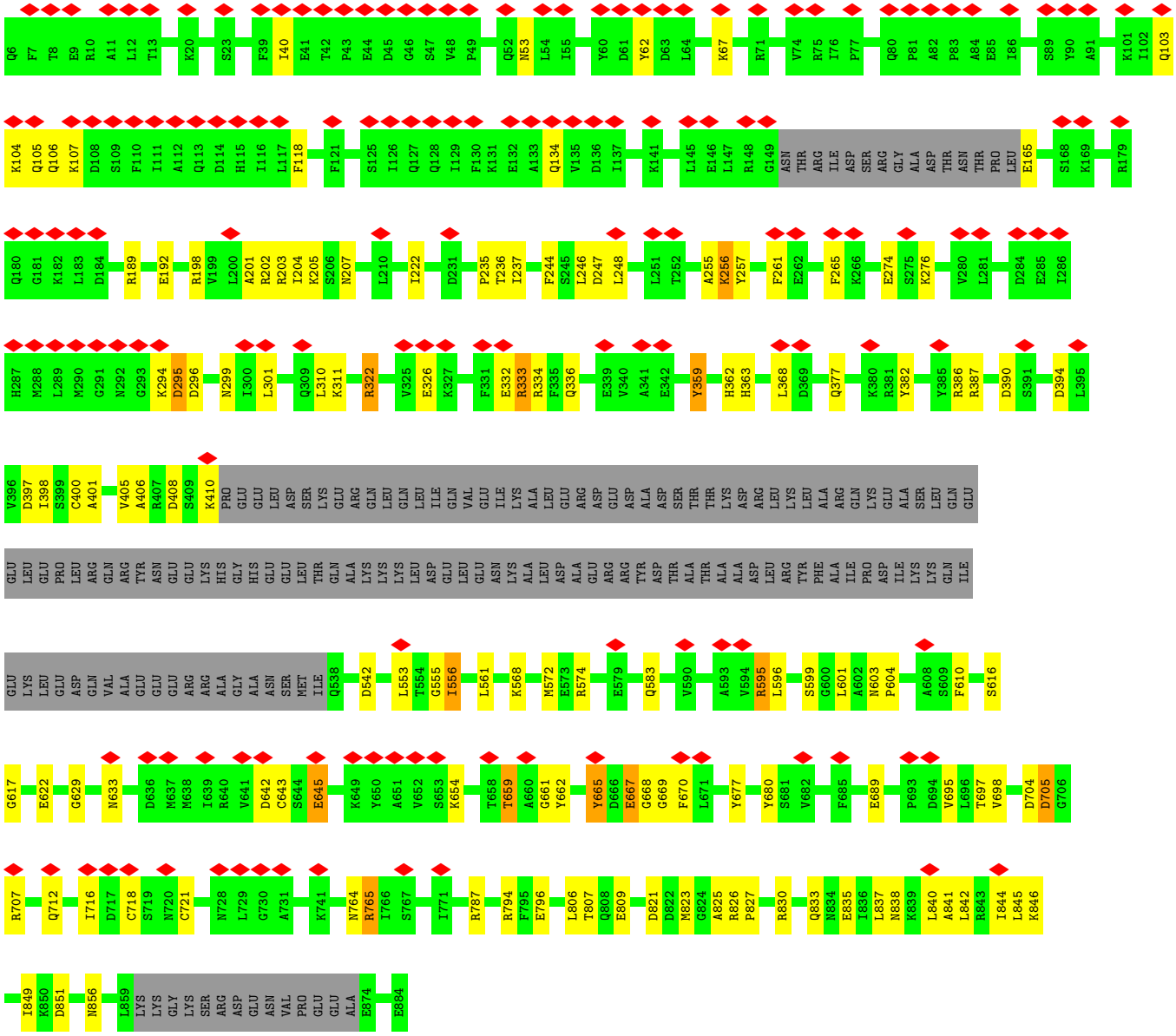
• Molecule 1: Heat shock protein 104

Chain B:



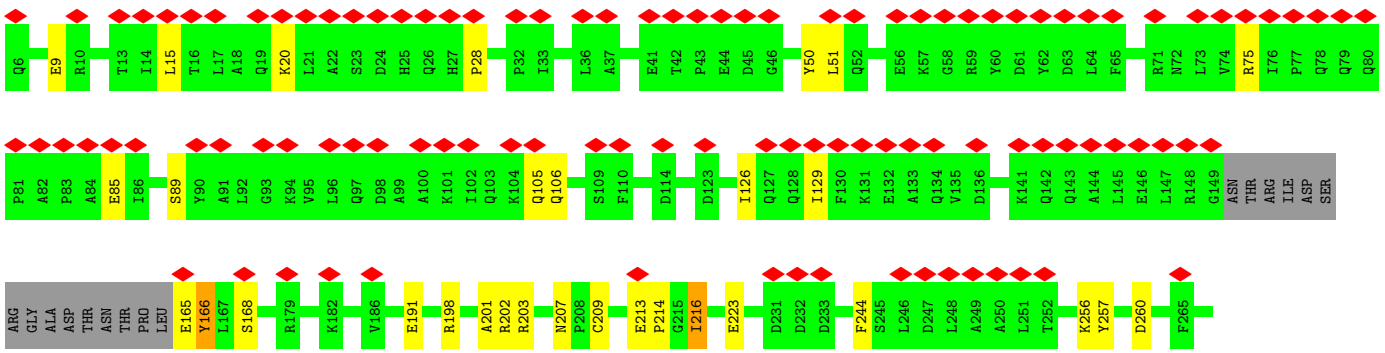
• Molecule 1: Heat shock protein 104

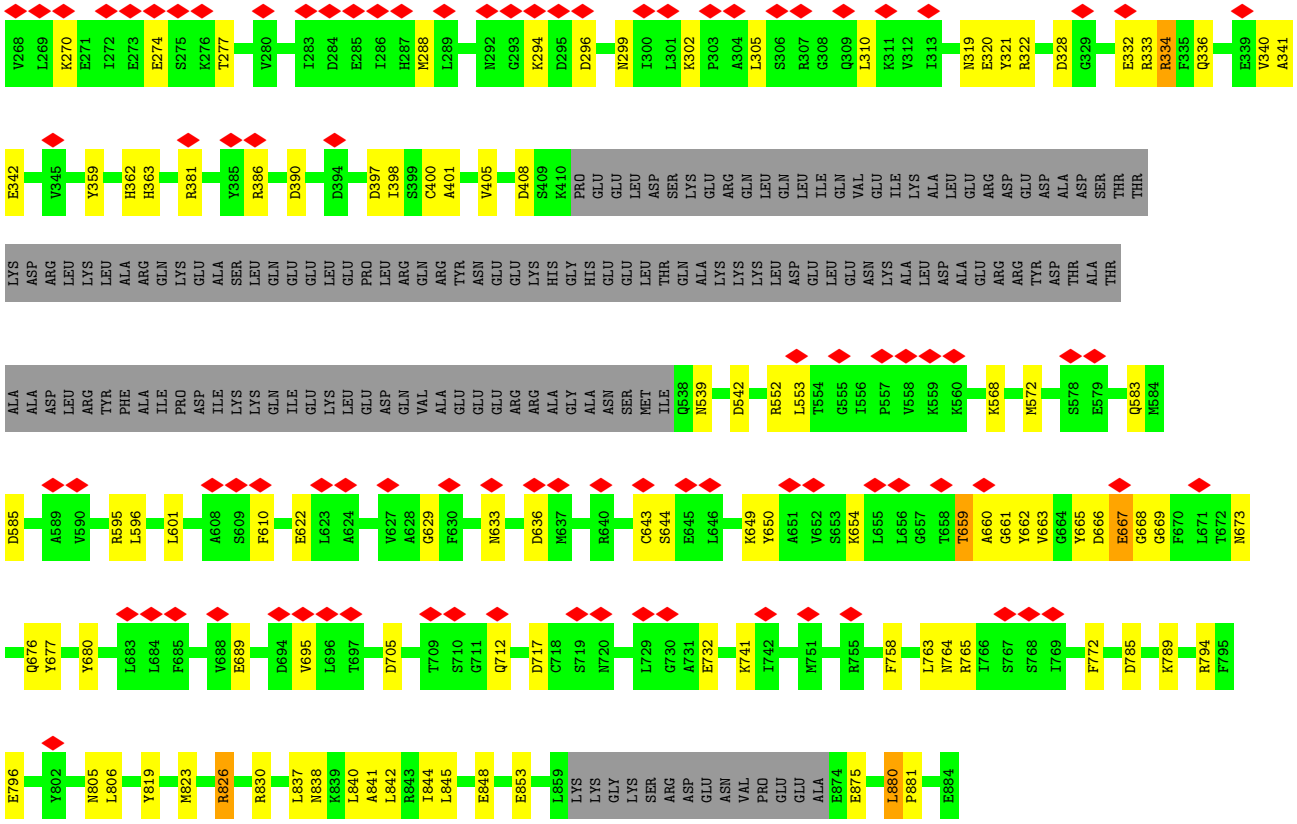
Chain C:



• Molecule 1: Heat shock protein 104

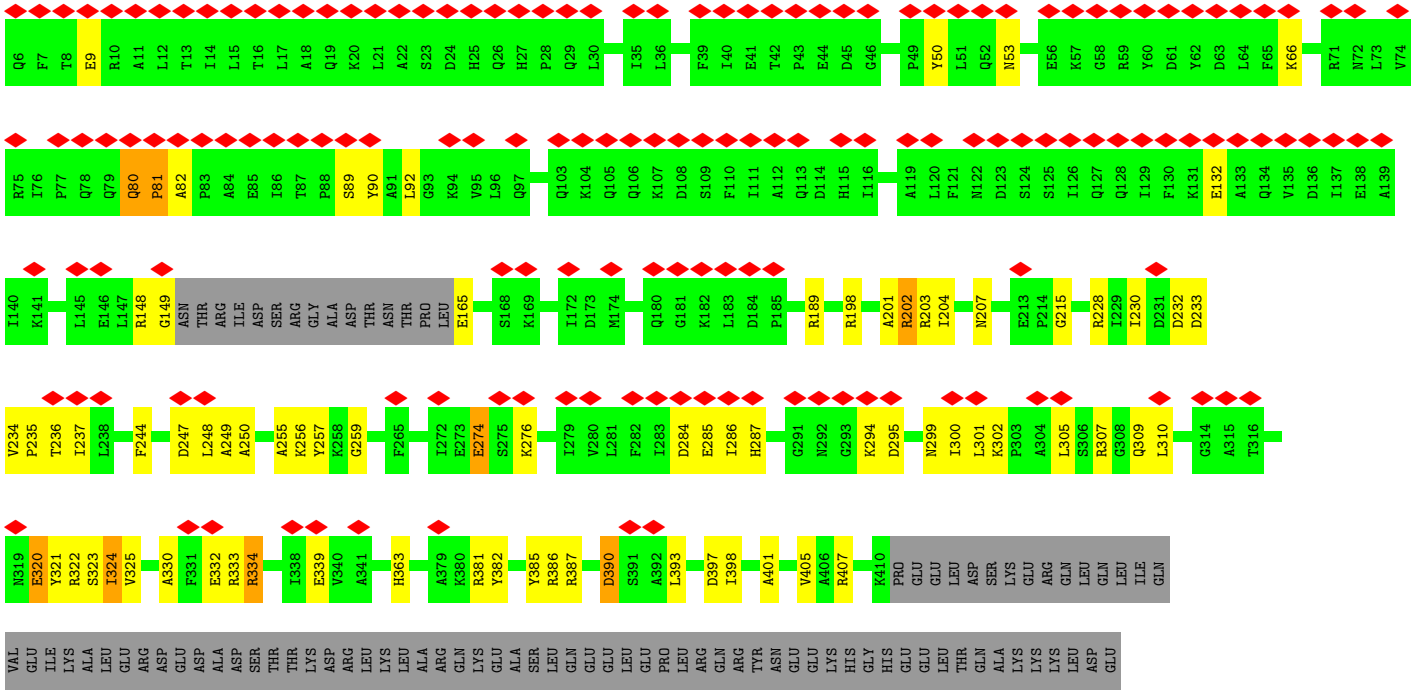
Chain D:

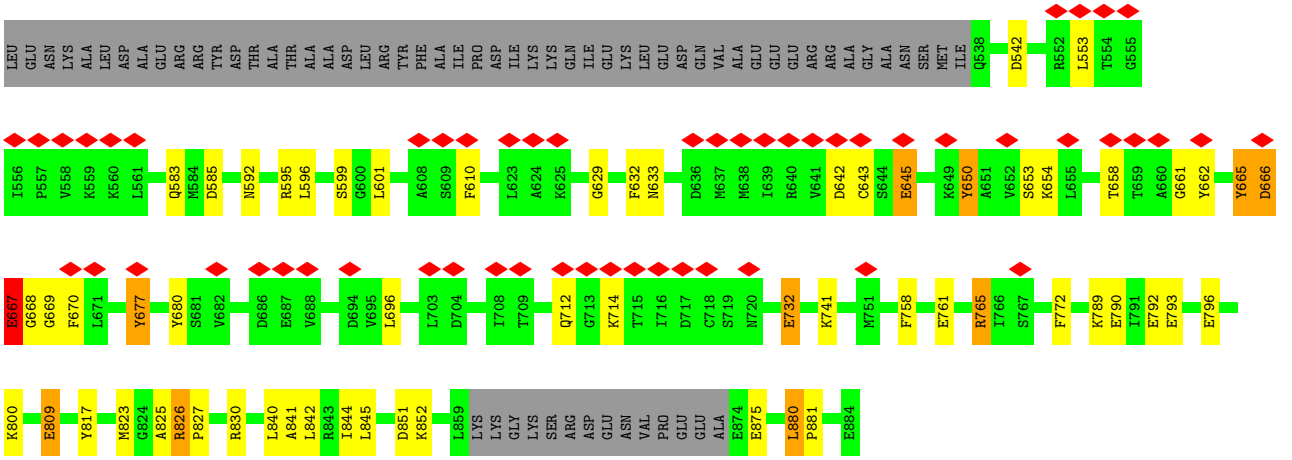




• Molecule 1: Heat shock protein 104

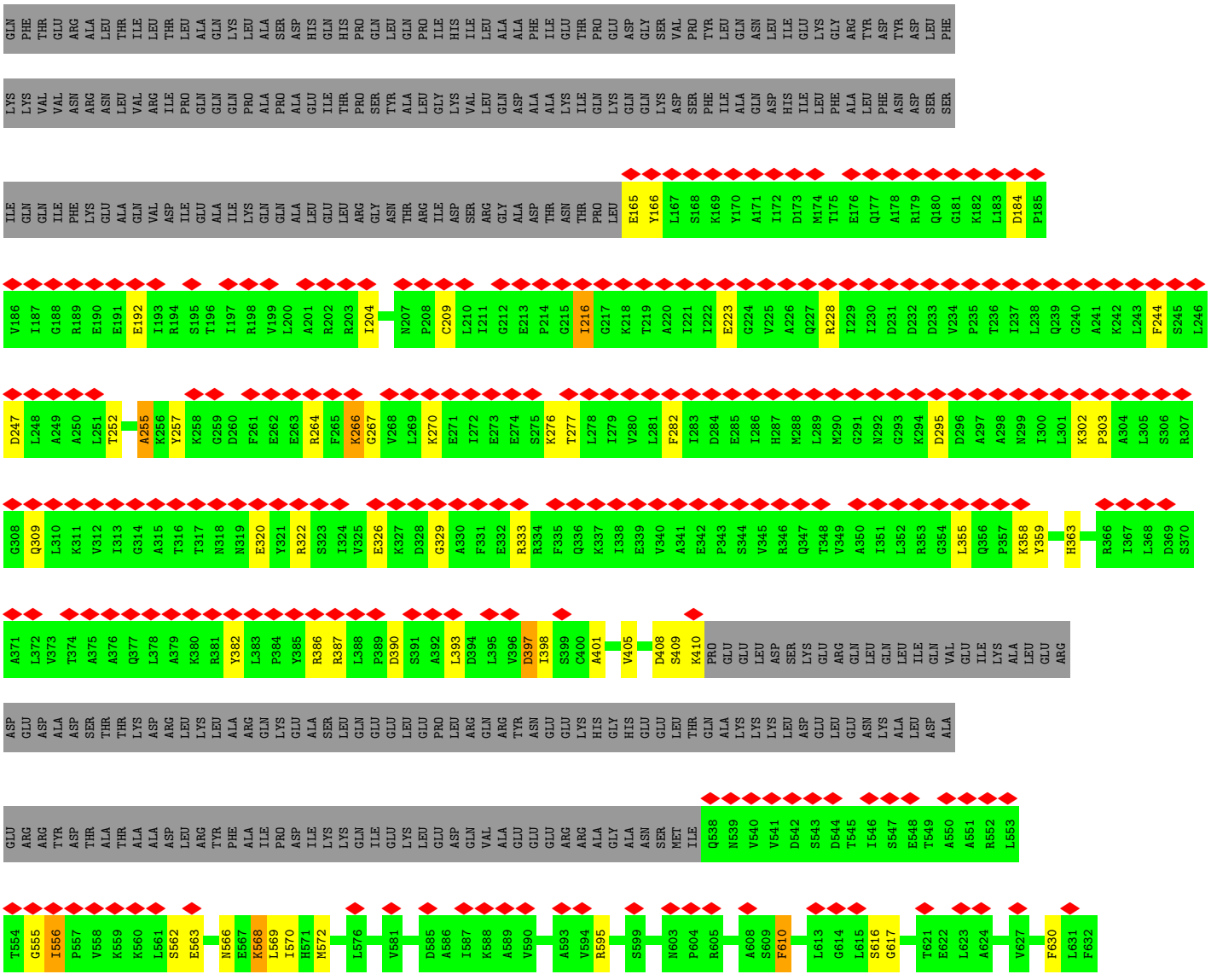
Chain E:

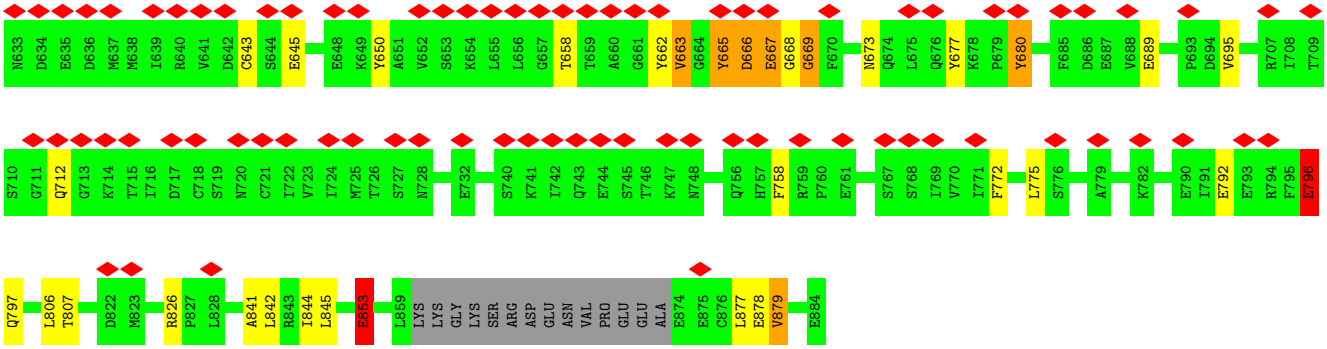




• Molecule 1: Heat shock protein 104

Chain F:




N633 D634 E635 D636 M637 M638 I639 R640 V641 D642 C643 S644 E645 E648 K649 Y650 A651 V652 S653 K654 L655 L656 G657 T658 T659 A660 G661 Y662 V663 G664 Y665 D666 E667 G668 G669 F670 N673 Q674 L675 Q676 Y677 K678 P679 Y680 F685 D686 E687 V688 E689 P693 D694 V695 R707 I708 T709
S710 G711 Q712 G713 K714 T715 I716 D717 C718 S719 N720 C721 I722 V723 I724 M725 T726 S727 N728 E732 S740 K741 I742 Q743 E744 S745 T746 K747 N748 Q756 H757 F758 R759 P760 E761 S767 S768 I769 V770 I771 F772 L775 S776 A779 K782 E790 I791 E792 E793 R794 F795 E796
Q797 L806 T807 D822 M823 R826 P827 L828 A841 L842 R843 I844 L845 B853 L859 LYS LYS GLY LYS SER ARG ASP GLU ASN VAL PRO GLU GLU ALA E874 E875 C876 L877 E878 V879 E884

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.68, 1.68, 1.68	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.11	13/4575 (0.3%)	0.94	12/6157 (0.2%)
1	B	1.15	18/5731 (0.3%)	0.92	6/7725 (0.1%)
1	C	1.19	21/5757 (0.4%)	0.94	9/7758 (0.1%)
1	D	1.16	19/5754 (0.3%)	0.92	4/7754 (0.1%)
1	E	1.18	30/5751 (0.5%)	0.94	9/7750 (0.1%)
1	F	1.17	23/4563 (0.5%)	0.92	8/6143 (0.1%)
All	All	1.16	124/32131 (0.4%)	0.93	48/43287 (0.1%)

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	643	CYS	CB-SG	-9.03	1.67	1.82
1	D	610	PHE	CB-CG	-8.61	1.36	1.51
1	F	673	ASN	CB-CG	-8.52	1.31	1.51
1	F	282	PHE	CB-CG	-8.39	1.37	1.51
1	E	643	CYS	CB-SG	-8.34	1.68	1.82
1	B	792	GLU	CG-CD	-8.11	1.39	1.51
1	E	758	PHE	CB-CG	-7.60	1.38	1.51
1	C	244	PHE	CB-CG	-7.59	1.38	1.51
1	F	689	GLU	CD-OE1	-7.37	1.17	1.25
1	A	209	CYS	CB-SG	-7.33	1.69	1.82
1	E	632	PHE	CB-CG	-7.29	1.39	1.51
1	D	244	PHE	CB-CG	-7.22	1.39	1.51
1	C	645	GLU	CG-CD	-7.21	1.41	1.51
1	E	234	VAL	CB-CG1	-6.99	1.38	1.52
1	F	689	GLU	CG-CD	-6.95	1.41	1.51
1	A	166	TYR	CB-CG	-6.93	1.41	1.51
1	F	792	GLU	CG-CD	-6.79	1.41	1.51
1	A	244	PHE	CB-CG	-6.78	1.39	1.51
1	B	667	GLU	CD-OE2	-6.74	1.18	1.25
1	E	287	HIS	CB-CG	-6.69	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	695	VAL	CB-CG2	-6.65	1.38	1.52
1	F	610	PHE	CB-CG	-6.65	1.40	1.51
1	D	853	GLU	CG-CD	-6.60	1.42	1.51
1	C	610	PHE	CB-CG	-6.54	1.40	1.51
1	C	718	CYS	CB-SG	-6.49	1.71	1.82
1	E	875	GLU	CD-OE2	-6.49	1.18	1.25
1	B	385	TYR	CB-CG	-6.46	1.42	1.51
1	E	792	GLU	CD-OE2	-6.45	1.18	1.25
1	B	689	GLU	CD-OE1	-6.45	1.18	1.25
1	D	643	CYS	CB-SG	-6.37	1.71	1.82
1	B	244	PHE	CB-CG	-6.35	1.40	1.51
1	B	610	PHE	CB-CG	-6.33	1.40	1.51
1	C	643	CYS	CB-SG	-6.33	1.71	1.82
1	E	339	GLU	CD-OE1	-6.27	1.18	1.25
1	D	689	GLU	CD-OE1	-6.25	1.18	1.25
1	F	792	GLU	CD-OE1	-6.24	1.18	1.25
1	D	853	GLU	CD-OE2	-6.20	1.18	1.25
1	F	667	GLU	CG-CD	-6.19	1.42	1.51
1	E	244	PHE	CB-CG	-6.17	1.40	1.51
1	E	670	PHE	CB-CG	-6.16	1.40	1.51
1	E	826	ARG	CG-CD	-6.15	1.36	1.51
1	A	610	PHE	CB-CG	-6.10	1.41	1.51
1	E	653	SER	CB-OG	-6.08	1.34	1.42
1	E	207	ASN	CB-CG	-6.06	1.37	1.51
1	A	382	TYR	CB-CG	-6.03	1.42	1.51
1	B	209	CYS	CB-SG	-6.02	1.72	1.82
1	C	382	TYR	CB-CG	-6.00	1.42	1.51
1	D	207	ASN	CB-CG	-5.98	1.37	1.51
1	B	853	GLU	CD-OE1	-5.97	1.19	1.25
1	E	650	TYR	CB-CG	-5.93	1.42	1.51
1	E	382	TYR	CG-CD2	-5.91	1.31	1.39
1	E	132	GLU	CD-OE1	-5.87	1.19	1.25
1	B	667	GLU	CD-OE1	-5.86	1.19	1.25
1	C	645	GLU	CD-OE2	-5.82	1.19	1.25
1	F	680	TYR	CB-CG	-5.81	1.43	1.51
1	E	645	GLU	CG-CD	-5.76	1.43	1.51
1	B	853	GLU	CG-CD	-5.75	1.43	1.51
1	E	382	TYR	CB-CG	-5.73	1.43	1.51
1	A	878	GLU	CD-OE1	-5.69	1.19	1.25
1	F	667	GLU	CD-OE1	-5.68	1.19	1.25
1	D	191	GLU	CD-OE1	-5.68	1.19	1.25
1	E	610	PHE	CB-CG	-5.66	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	TYR	CB-CG	-5.65	1.43	1.51
1	D	695	VAL	CB-CG1	-5.65	1.41	1.52
1	B	712	GLN	CG-CD	5.63	1.64	1.51
1	D	209	CYS	CB-SG	-5.63	1.72	1.81
1	D	400	CYS	CB-SG	-5.61	1.72	1.81
1	D	321	TYR	CB-CG	-5.58	1.43	1.51
1	C	622	GLU	CD-OE2	-5.57	1.19	1.25
1	F	209	CYS	CB-SG	-5.56	1.72	1.81
1	C	198	ARG	CG-CD	-5.54	1.38	1.51
1	F	689	GLU	CD-OE2	-5.54	1.19	1.25
1	F	320	GLU	CD-OE2	-5.53	1.19	1.25
1	C	359	TYR	CB-CG	-5.52	1.43	1.51
1	B	261	PHE	CB-CG	-5.52	1.42	1.51
1	A	263	GLU	CD-OE1	-5.49	1.19	1.25
1	E	390	ASP	CB-CG	-5.49	1.40	1.51
1	E	875	GLU	CD-OE1	-5.49	1.19	1.25
1	E	645	GLU	CD-OE1	-5.47	1.19	1.25
1	A	754	VAL	CB-CG1	-5.46	1.41	1.52
1	B	335	PHE	CB-CG	-5.42	1.42	1.51
1	E	790	GLU	CD-OE1	-5.40	1.19	1.25
1	D	223	GLU	CD-OE2	-5.39	1.19	1.25
1	D	166	TYR	CB-CG	-5.38	1.43	1.51
1	C	207	ASN	CB-CG	-5.38	1.38	1.51
1	C	265	PHE	CB-CG	-5.36	1.42	1.51
1	A	853	GLU	CD-OE1	-5.34	1.19	1.25
1	F	244	PHE	CB-CG	-5.32	1.42	1.51
1	C	698	VAL	CB-CG2	-5.29	1.41	1.52
1	C	595	ARG	CD-NE	-5.26	1.37	1.46
1	F	796	GLU	CD-OE2	-5.26	1.19	1.25
1	E	667	GLU	CD-OE2	-5.25	1.19	1.25
1	D	667	GLU	CD-OE1	-5.25	1.19	1.25
1	B	34	HIS	CB-CG	-5.24	1.40	1.50
1	F	382	TYR	CG-CD2	-5.23	1.32	1.39
1	D	758	PHE	CB-CG	-5.22	1.42	1.51
1	E	234	VAL	CB-CG2	-5.20	1.42	1.52
1	C	667	GLU	CD-OE1	-5.20	1.20	1.25
1	F	853	GLU	CD-OE2	-5.19	1.20	1.25
1	C	721	CYS	CB-SG	-5.18	1.73	1.81
1	B	287	HIS	CB-CG	-5.16	1.40	1.50
1	E	385	TYR	CB-CG	-5.16	1.44	1.51
1	A	192	GLU	CD-OE1	-5.15	1.20	1.25
1	E	809	GLU	CD-OE2	-5.14	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	875	GLU	CG-CD	-5.14	1.44	1.51
1	E	732	GLU	CD-OE1	-5.14	1.20	1.25
1	C	689	GLU	CD-OE1	-5.13	1.20	1.25
1	F	758	PHE	CB-CG	-5.12	1.42	1.51
1	B	758	PHE	CB-CG	-5.08	1.42	1.51
1	B	761	GLU	CD-OE1	-5.07	1.20	1.25
1	A	689	GLU	CD-OE1	-5.07	1.20	1.25
1	C	809	GLU	CD-OE1	-5.06	1.20	1.25
1	D	848	GLU	CD-OE1	-5.06	1.20	1.25
1	F	192	GLU	CD-OE1	-5.05	1.20	1.25
1	F	695	VAL	CB-CG2	-5.05	1.42	1.52
1	A	359	TYR	CB-CG	-5.05	1.44	1.51
1	F	223	GLU	CG-CD	5.05	1.59	1.51
1	C	103	GLN	CG-CD	-5.04	1.39	1.51
1	E	320	GLU	CD-OE2	-5.04	1.20	1.25
1	A	326	GLU	CD-OE1	-5.03	1.20	1.25
1	D	875	GLU	CD-OE1	-5.02	1.20	1.25
1	D	320	GLU	CD-OE2	-5.02	1.20	1.25
1	F	796	GLU	CG-CD	-5.01	1.44	1.51
1	C	400	CYS	CB-SG	-5.00	1.73	1.81

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	595	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	E	228	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	E	321	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	E	50	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	C	595	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	F	166	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	A	264	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	F	266	LYS	N-CA-C	7.36	130.87	111.00
1	A	826	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	F	267	GLY	N-CA-C	-7.02	95.55	113.10
1	E	202	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	264	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	843	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	552	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	F	680	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	F	397	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	677	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	C	261	PHE	CB-CG-CD1	6.25	125.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	189	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	F	826	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	E	407	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	574	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	202	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	765	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	118	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	F	228	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	261	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	B	324	ILE	CB-CA-C	-5.63	100.33	111.60
1	B	202	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	E	80	GLN	C-N-CD	-5.57	108.36	120.60
1	C	322	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	632	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	D	75	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	843	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	382	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	B	704	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	202	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	115	HIS	CA-CB-CG	-5.33	104.55	113.60
1	D	260	ASP	CB-CG-OD1	5.32	123.09	118.30
1	F	228	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	228	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	307	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	324	ILE	CB-CA-C	-5.23	101.14	111.60
1	C	62	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	E	397	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	322	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	257	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	B	666	ASP	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

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	4519	0	4629	176	0
1	B	5654	0	5763	401	0
1	C	5679	0	5810	547	0
1	D	5676	0	5805	406	0
1	E	5673	0	5789	353	0
1	F	4507	0	4603	210	0
2	A	62	0	24	72	0
2	B	62	0	24	6	0
2	C	62	0	24	8	0
2	D	62	0	24	16	0
2	E	93	0	36	38	0
2	F	31	0	12	7	0
All	All	32080	0	32543	1335	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 21.

All (1335) 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:E:662:TYR:CZ	1:F:650:TYR:HD1	1.08	1.70
1:E:662:TYR:CE2	1:F:650:TYR:CD1	1.78	1.66
1:C:203:ARG:HG3	1:D:362:HIS:CD2	1.13	1.64
1:E:662:TYR:CZ	1:F:650:TYR:CD1	1.80	1.62
1:B:595:ARG:CZ	1:C:842:LEU:HD22	1.20	1.62
1:A:619:GLY:HA2	2:A:1002:ATP:C5'	1.32	1.56
1:C:203:ARG:CG	1:D:362:HIS:CD2	1.86	1.53
1:C:201:ALA:CB	1:D:405:VAL:HG22	1.36	1.52
1:C:201:ALA:CB	1:D:405:VAL:CG2	1.87	1.52
1:D:665:TYR:CE1	1:D:712:GLN:CG	1.87	1.51
1:D:665:TYR:CE1	1:D:712:GLN:HG2	0.98	1.49
1:C:333:ARG:NH1	1:D:390:ASP:CB	1.73	1.48
1:B:601:LEU:HD11	1:C:840:LEU:CG	1.40	1.48
1:B:570:ILE:CG2	1:C:846:LYS:HE2	1.42	1.48
1:C:201:ALA:HB3	1:D:405:VAL:CG2	1.41	1.47
1:C:204:ILE:CG1	1:D:397:ASP:OD2	1.64	1.46
1:B:570:ILE:HG23	1:C:846:LYS:CE	1.43	1.44
1:B:570:ILE:CD1	1:C:846:LYS:HG2	1.42	1.44
1:C:596:LEU:CD2	1:D:841:ALA:HB2	1.44	1.44
1:B:595:ARG:NE	1:C:842:LEU:HD13	1.14	1.43
1:B:601:LEU:CD1	1:C:840:LEU:HG	1.45	1.43
1:D:336:GLN:NE2	1:E:553:LEU:HD22	1.17	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ARG:C	1:C:841:ALA:HB1	1.36	1.43
1:A:618:SER:O	2:A:1002:ATP:C5	1.72	1.43
1:B:601:LEU:CD1	1:C:840:LEU:CG	1.91	1.43
1:A:619:GLY:CA	2:A:1002:ATP:H5'2	1.49	1.41
1:C:203:ARG:HG3	1:D:362:HIS:CG	1.56	1.41
1:E:201:ALA:CB	1:F:405:VAL:HG22	1.48	1.41
1:E:233:ASP:HA	1:F:410:LYS:NZ	1.34	1.40
1:B:596:LEU:HD21	1:C:837:LEU:C	1.39	1.40
1:C:107:LYS:HD3	1:D:106:GLN:NE2	1.10	1.40
1:E:233:ASP:HA	1:F:410:LYS:CE	1.49	1.40
1:B:595:ARG:CZ	1:C:842:LEU:CD2	1.98	1.39
1:B:603:ASN:HA	1:C:794:ARG:CZ	1.49	1.39
1:B:595:ARG:NH1	1:C:842:LEU:HD22	1.12	1.38
1:C:336:GLN:NE2	1:D:553:LEU:HD22	1.33	1.38
1:E:203:ARG:CG	1:F:363:HIS:CE1	2.05	1.38
1:E:232:ASP:O	1:F:410:LYS:CE	1.70	1.38
1:E:662:TYR:OH	1:F:650:TYR:HD1	1.06	1.38
1:D:333:ARG:HG3	1:E:390:ASP:OD2	1.24	1.37
1:A:765:ARG:CZ	1:B:826:ARG:HH12	1.38	1.36
1:B:596:LEU:HA	1:C:841:ALA:CB	1.55	1.35
1:C:764:ASN:OD1	1:D:823:MET:HE3	1.26	1.35
1:E:595:ARG:NH1	1:F:842:LEU:HD11	1.39	1.35
1:B:601:LEU:CD1	1:C:840:LEU:CD2	2.05	1.35
1:A:765:ARG:NH2	1:B:826:ARG:NH1	1.72	1.34
1:E:595:ARG:HH11	1:F:842:LEU:CD1	1.42	1.32
1:C:596:LEU:HD23	1:D:841:ALA:CB	1.58	1.31
1:C:257:TYR:CD1	1:D:256:LYS:HE3	1.64	1.31
1:D:763:LEU:O	1:E:830:ARG:NH2	1.62	1.30
1:B:601:LEU:HD13	1:C:840:LEU:CD2	1.61	1.29
1:A:218:LYS:HB2	2:A:1001:ATP:O1B	1.18	1.29
1:D:596:LEU:CD1	1:E:841:ALA:HB2	1.63	1.28
1:B:764:ASN:OD1	1:C:823:MET:CE	1.80	1.27
1:B:595:ARG:HD3	1:C:842:LEU:CB	1.63	1.27
1:B:596:LEU:CD2	1:C:837:LEU:O	1.82	1.27
1:A:218:LYS:HE3	2:A:1001:ATP:O1G	1.23	1.27
1:B:659:THR:CG2	1:C:654:LYS:HE2	1.65	1.27
1:B:333:ARG:CD	1:C:390:ASP:OD2	1.84	1.26
1:B:595:ARG:O	1:C:841:ALA:HB1	1.35	1.26
1:E:333:ARG:HG3	1:F:390:ASP:OD2	1.35	1.26
1:E:381:ARG:HD2	1:F:796:GLU:OE2	1.27	1.26
1:B:599:SER:HB2	1:C:844:ILE:CD1	1.66	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LYS:CE	1:B:333:ARG:NH2	1.99	1.25
1:C:764:ASN:CA	1:D:830:ARG:NH2	1.96	1.25
1:B:595:ARG:CD	1:C:842:LEU:HD13	1.65	1.25
1:A:765:ARG:CZ	1:B:826:ARG:NH1	1.97	1.25
1:C:333:ARG:HH12	1:D:390:ASP:CB	1.40	1.25
1:C:764:ASN:HA	1:D:830:ARG:NH2	1.50	1.25
1:D:213:GLU:CG	1:D:214:PRO:HD2	1.67	1.25
1:D:665:TYR:CG	1:D:712:GLN:NE2	2.04	1.25
1:A:220:ALA:CB	2:A:1001:ATP:C2	2.21	1.24
1:C:326:GLU:OE2	1:D:676:GLN:NE2	1.69	1.24
1:B:596:LEU:CA	1:C:841:ALA:HB2	1.67	1.23
1:B:595:ARG:NE	1:C:842:LEU:CD1	1.99	1.23
1:B:604:PRO:HD3	1:C:794:ARG:NH1	1.53	1.23
1:B:603:ASN:HA	1:C:794:ARG:NH1	1.51	1.23
1:A:220:ALA:HB1	2:A:1001:ATP:N1	1.52	1.23
1:A:765:ARG:NH2	1:B:826:ARG:HH12	1.32	1.22
1:E:666:ASP:O	1:E:667:GLU:O	1.58	1.22
1:B:596:LEU:HD21	1:C:837:LEU:O	1.32	1.22
1:C:107:LYS:CD	1:D:106:GLN:NE2	2.01	1.22
1:C:765:ARG:NH2	1:D:826:ARG:NH2	1.87	1.22
1:D:202:ARG:HD2	1:E:398:ILE:CD1	1.68	1.21
1:D:601:LEU:CD1	1:E:844:ILE:HD12	1.70	1.21
1:C:204:ILE:HG12	1:D:397:ASP:OD2	1.14	1.21
1:B:204:ILE:HG12	1:C:397:ASP:OD2	1.39	1.20
1:A:596:LEU:HD11	1:B:841:ALA:CB	1.71	1.20
1:E:595:ARG:HB3	1:F:845:LEU:CB	1.71	1.20
1:E:233:ASP:CA	1:F:410:LYS:NZ	2.06	1.19
1:C:203:ARG:HG3	1:D:362:HIS:NE2	1.56	1.19
1:A:198:ARG:HG3	1:B:405:VAL:CG2	1.72	1.18
1:B:601:LEU:CD1	1:C:840:LEU:HD23	1.69	1.18
1:E:201:ALA:HB3	1:F:405:VAL:CG2	1.73	1.18
1:C:333:ARG:CZ	1:D:390:ASP:CB	2.20	1.18
1:E:662:TYR:CE2	1:F:650:TYR:CE1	2.30	1.18
1:A:198:ARG:CG	1:B:405:VAL:HG21	1.73	1.17
1:A:618:SER:O	2:A:1002:ATP:C4	1.97	1.17
1:D:665:TYR:CZ	1:D:712:GLN:HG2	1.79	1.17
1:B:596:LEU:CA	1:C:841:ALA:CB	2.19	1.16
1:D:764:ASN:ND2	1:E:823:MET:HG2	1.60	1.16
1:B:569:LEU:CD1	1:C:845:LEU:HD22	1.76	1.16
2:E:1002:ATP:PG	2:E:1002:ATP:O1G	2.03	1.16
1:B:333:ARG:HD2	1:C:390:ASP:OD2	1.38	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:LEU:HD11	1:C:838:ASN:OD1	1.43	1.16
1:C:765:ARG:NH2	1:D:826:ARG:HH21	1.41	1.16
2:C:1001:ATP:PG	2:C:1001:ATP:O1G	2.04	1.16
2:B:1002:ATP:PG	2:B:1002:ATP:O1G	2.04	1.15
2:D:901:ATP:PG	2:D:901:ATP:O1G	2.03	1.15
1:D:665:TYR:CD1	1:D:712:GLN:NE2	2.14	1.15
2:F:901:ATP:PG	2:F:901:ATP:O1G	2.05	1.15
1:D:336:GLN:CD	1:E:553:LEU:HD22	1.67	1.15
2:D:902:ATP:PG	2:D:902:ATP:O1G	2.05	1.14
1:E:599:SER:HB2	1:F:844:ILE:CG2	1.77	1.14
1:B:665:TYR:O	1:B:666:ASP:C	1.82	1.14
2:C:1002:ATP:O1G	2:C:1002:ATP:PG	2.04	1.14
1:E:381:ARG:CD	1:F:796:GLU:OE2	1.95	1.14
1:A:665:TYR:CD2	1:A:712:GLN:NE2	2.16	1.14
1:B:570:ILE:HG12	1:C:846:LYS:CG	1.78	1.14
1:E:233:ASP:CA	1:F:410:LYS:HZ1	1.57	1.14
2:E:1001:ATP:PG	2:E:1001:ATP:O1G	2.06	1.14
2:A:1001:ATP:O1G	2:A:1001:ATP:PG	2.06	1.13
2:B:1001:ATP:PG	2:B:1001:ATP:O1G	2.05	1.13
1:B:659:THR:HG22	1:C:654:LYS:HE2	1.22	1.13
2:E:1003:ATP:PG	2:E:1003:ATP:O1G	2.05	1.13
1:B:764:ASN:OD1	1:C:823:MET:HE3	0.97	1.13
1:C:601:LEU:HD11	1:D:844:ILE:HD12	1.20	1.13
1:C:601:LEU:HD21	1:D:844:ILE:CD1	1.79	1.13
2:A:1002:ATP:PG	2:A:1002:ATP:O1G	2.06	1.13
1:E:201:ALA:CB	1:F:405:VAL:CG2	2.26	1.13
1:E:233:ASP:OD1	1:F:410:LYS:NZ	1.82	1.13
1:A:198:ARG:NE	1:B:405:VAL:HG11	1.63	1.12
1:C:107:LYS:HE2	1:D:105:GLN:C	1.61	1.12
1:A:218:LYS:CE	2:A:1001:ATP:O1G	1.96	1.12
1:B:205:LYS:HE2	1:B:333:ARG:NH2	1.63	1.12
1:B:604:PRO:HD2	1:C:794:ARG:HD2	1.31	1.12
1:D:596:LEU:HD12	1:E:841:ALA:HB2	1.15	1.12
1:E:232:ASP:O	1:F:410:LYS:HE2	1.30	1.11
1:E:233:ASP:CA	1:F:410:LYS:HE3	1.80	1.11
1:A:198:ARG:HE	1:B:405:VAL:HG11	1.02	1.11
1:B:332:GLU:O	1:C:386:ARG:NH2	1.82	1.11
1:B:596:LEU:N	1:C:841:ALA:CB	2.14	1.11
1:A:198:ARG:HG3	1:B:405:VAL:HG21	1.11	1.11
1:D:826:ARG:NH2	2:D:901:ATP:O3A	1.83	1.11
1:B:570:ILE:HG12	1:C:846:LYS:HG3	1.29	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:GLN:NE2	1:E:553:LEU:CD2	2.13	1.10
1:A:220:ALA:HB2	2:A:1001:ATP:C2	1.86	1.10
1:B:604:PRO:CD	1:C:794:ARG:NH1	2.14	1.10
1:E:203:ARG:CB	1:F:363:HIS:CE1	2.33	1.10
1:A:667:GLU:OE1	1:A:712:GLN:OE1	1.70	1.10
1:A:765:ARG:NH1	1:B:826:ARG:HH12	1.47	1.10
1:C:601:LEU:HD12	1:D:841:ALA:HA	1.23	1.10
1:E:203:ARG:HG2	1:F:363:HIS:CE1	1.76	1.10
1:B:61:ASP:OD2	1:C:67:LYS:NZ	1.84	1.09
1:C:107:LYS:HE2	1:D:105:GLN:O	1.51	1.09
1:B:595:ARG:NH1	1:C:842:LEU:CD2	2.05	1.09
1:D:601:LEU:HD11	1:E:844:ILE:HD12	1.13	1.09
1:A:596:LEU:HD11	1:B:841:ALA:HB1	1.19	1.09
1:C:201:ALA:HB1	1:D:405:VAL:HG22	1.24	1.09
1:C:764:ASN:HA	1:D:830:ARG:CZ	1.81	1.09
1:B:336:GLN:NE2	1:C:553:LEU:HD22	1.68	1.09
1:B:595:ARG:C	1:C:841:ALA:CB	2.21	1.09
1:C:601:LEU:CD1	1:D:844:ILE:HD12	1.82	1.09
1:E:203:ARG:HG3	1:F:363:HIS:ND1	1.68	1.08
1:E:233:ASP:CA	1:F:410:LYS:CE	2.29	1.08
1:B:569:LEU:HD13	1:C:845:LEU:CD2	1.81	1.08
1:B:570:ILE:CD1	1:C:846:LYS:CG	2.30	1.08
1:B:604:PRO:CD	1:C:794:ARG:HH11	1.67	1.08
1:A:665:TYR:CE2	1:A:712:GLN:NE2	2.21	1.08
1:C:667:GLU:OE1	1:C:712:GLN:OE1	1.71	1.08
1:C:203:ARG:HB2	1:D:363:HIS:CE1	1.88	1.07
1:E:203:ARG:CG	1:F:363:HIS:ND1	2.18	1.07
1:B:604:PRO:CD	1:C:794:ARG:HD2	1.84	1.07
1:B:765:ARG:NH2	1:C:826:ARG:HH22	1.52	1.07
1:B:569:LEU:HD13	1:C:845:LEU:HD22	1.14	1.07
1:E:333:ARG:HA	1:F:386:ARG:NH1	1.69	1.07
1:B:595:ARG:CD	1:C:842:LEU:HB2	1.84	1.06
1:B:570:ILE:HD13	1:C:846:LYS:HG2	1.15	1.06
1:E:333:ARG:NH2	2:E:1003:ATP:H8	1.52	1.06
1:E:595:ARG:NH1	1:F:842:LEU:CD1	2.09	1.06
1:B:570:ILE:CG1	1:C:846:LYS:HG2	1.85	1.06
1:C:201:ALA:HB3	1:D:405:VAL:HG21	1.08	1.06
1:E:201:ALA:HB1	1:F:405:VAL:HG22	1.09	1.06
1:B:203:ARG:HG3	1:C:362:HIS:CD2	1.90	1.06
1:D:202:ARG:HD2	1:E:398:ILE:HD13	1.37	1.06
1:C:603:ASN:HA	1:D:794:ARG:NH1	1.69	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ARG:CG	1:E:390:ASP:OD2	2.05	1.05
1:B:569:LEU:CB	1:C:845:LEU:HD13	1.84	1.05
1:B:205:LYS:NZ	1:C:394:ASP:OD1	1.88	1.05
1:C:202:ARG:HA	1:D:401:ALA:CB	1.86	1.05
1:B:766:ILE:O	1:C:830:ARG:NE	1.88	1.05
1:C:203:ARG:CB	1:D:362:HIS:CD2	2.40	1.05
1:D:601:LEU:HD21	1:E:844:ILE:HD11	1.35	1.05
1:D:601:LEU:HD12	1:E:841:ALA:HA	1.32	1.05
1:B:713:GLY:HA2	1:C:670:PHE:CZ	1.92	1.04
1:E:232:ASP:O	1:F:410:LYS:HE3	1.50	1.04
1:E:599:SER:HB2	1:F:844:ILE:HG22	1.37	1.04
1:C:204:ILE:HG13	1:D:397:ASP:OD2	1.56	1.04
1:D:322:ARG:HB2	1:E:677:TYR:OH	1.58	1.04
1:A:619:GLY:HA3	2:A:1002:ATP:C4	1.91	1.04
1:E:333:ARG:CG	1:F:390:ASP:OD2	2.05	1.04
1:B:599:SER:HB2	1:C:844:ILE:HD12	1.09	1.03
1:E:233:ASP:HA	1:F:410:LYS:HE3	1.35	1.03
1:E:333:ARG:HA	1:F:386:ARG:NH2	1.71	1.03
1:C:203:ARG:HD2	1:D:362:HIS:CB	1.89	1.03
1:E:334:ARG:NH2	2:E:1003:ATP:O3A	1.92	1.03
1:B:322:ARG:HB2	1:C:677:TYR:OH	1.56	1.02
1:B:596:LEU:N	1:C:841:ALA:HB1	1.72	1.02
1:B:569:LEU:HB3	1:C:845:LEU:CD1	1.88	1.02
1:B:604:PRO:HD3	1:C:794:ARG:HH11	0.87	1.02
1:D:213:GLU:HG2	1:D:214:PRO:CD	1.88	1.02
1:E:201:ALA:HB3	1:F:405:VAL:HG22	1.34	1.02
1:E:662:TYR:OH	1:F:650:TYR:HA	1.59	1.02
1:C:765:ARG:HH22	1:D:826:ARG:NH2	1.48	1.02
1:D:596:LEU:HA	1:E:841:ALA:HB1	1.38	1.01
1:D:665:TYR:CD2	1:D:712:GLN:NE2	2.27	1.01
1:E:333:ARG:HA	1:F:386:ARG:CZ	1.89	1.01
1:C:105:GLN:O	1:D:105:GLN:OE1	1.76	1.01
1:C:203:ARG:CD	1:D:362:HIS:CG	2.43	1.01
1:E:202:ARG:HA	1:F:401:ALA:CB	1.89	1.01
1:E:662:TYR:OH	1:F:650:TYR:CD1	1.86	1.01
1:A:764:ASN:HB2	1:B:830:ARG:CB	1.90	1.01
1:B:378:LEU:HD23	1:C:796:GLU:OE2	1.59	1.01
1:B:598:ARG:CB	1:C:845:LEU:HD21	1.90	1.01
1:B:601:LEU:HD13	1:C:840:LEU:HD23	1.03	1.01
1:E:333:ARG:HA	1:F:386:ARG:HH12	1.22	1.01
1:A:205:LYS:HD3	1:A:333:ARG:HH11	1.17	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:CD	1:C:553:LEU:HD22	1.81	1.00
1:B:204:ILE:CG1	1:C:397:ASP:OD2	2.10	1.00
1:A:596:LEU:CD1	1:B:841:ALA:HB1	1.90	1.00
1:E:202:ARG:HA	1:F:401:ALA:HB1	1.40	1.00
1:B:570:ILE:CG1	1:C:846:LYS:CG	2.39	0.99
1:D:601:LEU:HD11	1:E:844:ILE:CD1	1.91	0.99
1:E:599:SER:CB	1:F:844:ILE:HG22	1.92	0.99
1:B:603:ASN:CA	1:C:794:ARG:CZ	2.40	0.99
1:A:728:ASN:OD1	2:A:1002:ATP:O1G	1.80	0.99
1:B:306:SER:HB3	1:B:334:ARG:NH2	1.76	0.99
1:C:336:GLN:NE2	1:D:553:LEU:CD2	2.25	0.99
1:B:595:ARG:HD3	1:C:842:LEU:HB2	0.99	0.99
1:C:203:ARG:NH2	1:D:359:TYR:CE1	2.31	0.98
1:A:220:ALA:HB2	2:A:1001:ATP:N3	1.76	0.98
2:A:1001:ATP:O1B	2:A:1001:ATP:O1A	1.66	0.98
1:C:257:TYR:HB3	1:D:256:LYS:HZ2	1.26	0.98
1:C:201:ALA:HB2	1:D:405:VAL:HG22	1.46	0.98
1:B:203:ARG:CG	1:C:362:HIS:CD2	2.46	0.98
1:B:601:LEU:HD11	1:C:840:LEU:CD2	1.83	0.98
1:C:105:GLN:O	1:D:105:GLN:NE2	1.96	0.98
1:E:333:ARG:HA	1:F:386:ARG:HH22	1.24	0.98
1:E:203:ARG:HG3	1:F:363:HIS:CE1	1.93	0.98
1:E:662:TYR:CE2	1:F:650:TYR:CG	2.50	0.98
1:D:601:LEU:CG	1:E:844:ILE:HD12	1.93	0.98
1:E:203:ARG:HB2	1:F:363:HIS:CE1	1.94	0.98
1:A:218:LYS:CB	2:A:1001:ATP:O1B	2.11	0.97
1:B:595:ARG:HE	1:C:842:LEU:HD13	1.16	0.97
1:C:595:ARG:HG2	1:D:845:LEU:CD1	1.94	0.97
1:D:665:TYR:CZ	1:D:712:GLN:CG	2.40	0.97
1:E:381:ARG:NH1	1:F:796:GLU:OE2	1.97	0.97
1:D:202:ARG:HD2	1:E:398:ILE:HD12	1.42	0.97
1:B:592:ASN:HB3	1:C:838:ASN:HB3	1.46	0.97
1:C:595:ARG:HB3	1:D:845:LEU:CD1	1.95	0.97
1:A:596:LEU:HD21	1:B:841:ALA:CA	1.95	0.97
2:E:1003:ATP:C2	1:F:355:LEU:HD11	1.99	0.97
1:B:765:ARG:CZ	1:C:826:ARG:HH12	1.78	0.97
1:C:764:ASN:C	1:D:830:ARG:NH2	2.18	0.96
1:C:601:LEU:HD21	1:D:844:ILE:HD11	1.41	0.96
1:C:601:LEU:HD12	1:D:841:ALA:CA	1.94	0.96
1:B:599:SER:CB	1:C:844:ILE:HD12	1.94	0.96
1:D:596:LEU:HA	1:E:841:ALA:CB	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ASN:HA	1:C:794:ARG:NH2	1.80	0.95
1:C:203:ARG:CD	1:D:362:HIS:CB	2.42	0.95
1:E:333:ARG:CA	1:F:386:ARG:HH22	1.78	0.95
1:E:712:GLN:HG2	1:E:714:LYS:NZ	1.81	0.95
1:A:220:ALA:HB1	2:A:1001:ATP:C6	2.02	0.95
1:C:595:ARG:CB	1:D:845:LEU:HD11	1.97	0.95
1:A:220:ALA:HB1	2:A:1001:ATP:C2	1.93	0.95
1:D:332:GLU:HG2	1:E:386:ARG:NH2	1.81	0.95
1:C:662:TYR:OH	1:D:649:LYS:O	1.85	0.95
1:E:334:ARG:NH2	2:E:1003:ATP:O3B	1.99	0.94
1:A:596:LEU:HD21	1:B:841:ALA:HA	1.48	0.94
1:C:595:ARG:CB	1:D:845:LEU:CD1	2.44	0.94
1:D:601:LEU:HD21	1:E:844:ILE:CD1	1.98	0.94
1:C:764:ASN:CG	1:D:823:MET:HE3	1.88	0.94
1:E:333:ARG:CA	1:F:386:ARG:HH12	1.81	0.94
1:B:596:LEU:HD23	1:C:837:LEU:O	1.68	0.94
1:B:659:THR:HG21	1:C:654:LYS:CE	1.97	0.94
1:E:202:ARG:CZ	1:F:398:ILE:HG12	1.98	0.94
1:C:601:LEU:CG	1:D:844:ILE:HD12	1.98	0.94
1:B:596:LEU:CD2	1:C:837:LEU:C	2.26	0.93
1:A:216:ILE:N	2:A:1001:ATP:O2A	1.97	0.93
1:B:570:ILE:HG21	1:C:846:LYS:HE2	1.46	0.93
1:B:659:THR:CG2	1:C:654:LYS:CE	2.45	0.93
1:B:659:THR:HG21	1:C:654:LYS:HE2	1.49	0.93
1:B:205:LYS:NZ	1:B:333:ARG:HH21	1.66	0.93
1:E:599:SER:CB	1:F:844:ILE:CG2	2.46	0.93
1:A:765:ARG:NH1	1:B:826:ARG:NH1	2.11	0.93
1:C:203:ARG:CD	1:D:362:HIS:HB3	1.99	0.93
1:E:596:LEU:CB	1:F:841:ALA:HB1	1.98	0.93
1:C:601:LEU:HD11	1:D:844:ILE:CD1	1.98	0.92
1:E:333:ARG:HD3	1:E:334:ARG:NH2	1.83	0.92
1:A:765:ARG:HH22	1:B:826:ARG:NH1	1.53	0.92
1:C:203:ARG:HB2	1:D:363:HIS:NE2	1.85	0.92
1:C:257:TYR:CG	1:D:256:LYS:HE3	2.05	0.92
1:E:201:ALA:HB3	1:F:405:VAL:HG21	1.49	0.92
1:E:595:ARG:HH11	1:F:842:LEU:HD13	1.33	0.92
1:E:662:TYR:HE2	1:F:650:TYR:CD1	1.70	0.92
1:C:105:GLN:O	1:D:105:GLN:CD	2.08	0.92
1:B:570:ILE:HG23	1:C:846:LYS:HE3	1.49	0.92
1:D:213:GLU:HG2	1:D:214:PRO:HD2	0.93	0.91
1:E:712:GLN:HG2	1:E:714:LYS:HZ3	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ARG:CD	1:C:842:LEU:CD1	2.45	0.91
1:B:766:ILE:O	1:C:830:ARG:CZ	2.19	0.91
1:E:333:ARG:NH2	2:E:1003:ATP:C8	2.39	0.91
2:C:1001:ATP:O1B	2:C:1001:ATP:O2G	1.85	0.91
1:C:332:GLU:HG2	1:D:386:ARG:NH2	1.85	0.91
1:E:235:PRO:HB3	1:F:409:SER:HA	1.51	0.91
1:D:596:LEU:HD13	1:E:841:ALA:HB2	1.51	0.91
1:C:595:ARG:CA	1:D:845:LEU:HD11	2.02	0.90
1:A:620:LYS:CE	2:A:1002:ATP:O3G	2.20	0.90
1:B:569:LEU:HB3	1:C:845:LEU:HD13	0.93	0.90
1:C:203:ARG:HD3	1:D:362:HIS:HB3	1.51	0.90
1:E:233:ASP:N	1:F:410:LYS:HZ1	1.70	0.90
1:E:809:GLU:N	1:E:809:GLU:OE1	2.05	0.90
1:B:203:ARG:HG3	1:C:362:HIS:CG	2.07	0.90
1:B:598:ARG:HB3	1:C:845:LEU:HD21	1.50	0.89
1:E:662:TYR:HE2	1:F:650:TYR:CG	1.87	0.89
2:E:1003:ATP:C2	1:F:355:LEU:CD1	2.56	0.89
1:C:332:GLU:O	1:D:386:ARG:NH2	2.04	0.89
1:B:205:LYS:CE	1:B:333:ARG:HH21	1.71	0.89
1:C:203:ARG:HG3	1:D:362:HIS:CE1	2.07	0.89
1:C:595:ARG:HB3	1:D:845:LEU:HD12	1.53	0.89
1:C:202:ARG:HA	1:D:401:ALA:HB2	1.53	0.89
1:C:202:ARG:HA	1:D:401:ALA:HB1	1.51	0.89
1:E:202:ARG:NH1	1:F:398:ILE:HG12	1.87	0.88
1:A:765:ARG:HH22	1:B:826:ARG:CZ	1.85	0.88
1:E:203:ARG:HB2	1:F:363:HIS:NE2	1.88	0.88
1:D:201:ALA:CB	1:E:405:VAL:HG22	2.02	0.88
2:E:1003:ATP:O3G	2:E:1003:ATP:O2B	1.84	0.88
1:D:595:ARG:HB3	1:E:845:LEU:HD11	1.54	0.88
1:B:764:ASN:HB3	1:C:826:ARG:HG2	1.55	0.88
1:B:603:ASN:CA	1:C:794:ARG:NH2	2.36	0.88
1:A:198:ARG:HE	1:B:405:VAL:CG1	1.85	0.88
1:A:665:TYR:CG	1:A:712:GLN:NE2	2.40	0.88
1:D:764:ASN:HD21	1:E:823:MET:HG2	1.30	0.88
1:C:105:GLN:C	1:D:105:GLN:HE22	1.78	0.87
1:E:204:ILE:HG13	1:F:359:TYR:HE1	1.39	0.87
1:A:205:LYS:HD3	1:A:333:ARG:NH1	1.89	0.87
1:B:604:PRO:HD2	1:C:794:ARG:CD	2.03	0.87
1:C:107:LYS:CE	1:D:105:GLN:O	2.22	0.87
1:F:216:ILE:HG22	1:F:216:ILE:O	1.74	0.87
1:C:333:ARG:CZ	1:C:333:ARG:HB2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:ARG:CG	1:D:845:LEU:CD1	2.52	0.86
1:B:665:TYR:O	1:B:667:GLU:N	2.09	0.86
1:A:296:ASP:OD1	1:B:252:THR:HG21	1.74	0.86
1:B:198:ARG:HA	1:C:405:VAL:HG21	1.57	0.86
1:C:204:ILE:HG12	1:D:397:ASP:CG	1.96	0.86
1:B:378:LEU:CD2	1:C:796:GLU:OE2	2.23	0.86
1:C:107:LYS:HD3	1:D:106:GLN:CD	1.94	0.86
1:C:595:ARG:HG2	1:D:845:LEU:HD13	1.56	0.86
1:C:665:TYR:CE1	1:C:712:GLN:HG2	2.10	0.86
1:A:620:LYS:HE3	2:A:1002:ATP:O3G	1.76	0.86
1:C:202:ARG:NH1	1:D:398:ILE:HD11	1.91	0.86
1:F:665:TYR:O	1:F:667:GLU:N	2.08	0.86
1:D:665:TYR:CE1	1:D:712:GLN:CD	2.48	0.85
1:D:764:ASN:CG	1:E:823:MET:HG2	1.96	0.85
1:B:601:LEU:CD1	1:C:840:LEU:CB	2.53	0.85
1:A:333:ARG:NE	1:A:333:ARG:O	2.08	0.85
1:C:333:ARG:NH2	1:D:390:ASP:CB	2.38	0.85
1:E:232:ASP:C	1:F:410:LYS:CE	2.44	0.85
2:E:1001:ATP:O2G	2:E:1001:ATP:O1B	1.90	0.85
1:A:601:LEU:HA	1:B:800:LYS:NZ	1.91	0.85
1:B:596:LEU:HD21	1:C:838:ASN:N	1.92	0.85
1:C:192:GLU:OE1	1:C:192:GLU:N	2.08	0.85
1:C:104:LYS:NZ	1:E:81:PRO:HB2	1.92	0.85
1:C:377:GLN:NE2	1:D:796:GLU:O	2.10	0.85
1:C:596:LEU:CD2	1:D:841:ALA:CB	2.30	0.85
1:C:107:LYS:HD3	1:D:106:GLN:HE22	1.02	0.85
1:B:570:ILE:HD11	1:C:846:LYS:HG2	1.55	0.84
1:B:595:ARG:HG2	1:C:845:LEU:HD12	1.58	0.84
1:E:334:ARG:NH2	2:E:1003:ATP:PB	2.51	0.84
1:C:201:ALA:HB1	1:D:405:VAL:CG2	1.82	0.84
1:D:665:TYR:CE1	1:D:712:GLN:NE2	2.46	0.84
1:B:203:ARG:HG3	1:C:362:HIS:CE1	2.13	0.84
1:B:570:ILE:HG23	1:C:846:LYS:HE2	0.86	0.84
1:D:216:ILE:HD11	1:D:340:VAL:HG12	1.59	0.84
1:D:595:ARG:HB3	1:E:845:LEU:CD1	2.06	0.84
1:E:203:ARG:HG2	1:F:363:HIS:ND1	1.90	0.84
1:E:322:ARG:HA	1:F:677:TYR:OH	1.78	0.84
1:E:333:ARG:HH21	2:E:1003:ATP:H8	1.16	0.84
1:C:203:ARG:CG	1:D:362:HIS:CG	2.28	0.84
1:E:202:ARG:CZ	1:F:398:ILE:CG1	2.56	0.84
1:B:595:ARG:NH2	1:C:842:LEU:CD2	2.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:662:TYR:CZ	1:F:650:TYR:CE1	2.57	0.83
1:D:336:GLN:CD	1:E:553:LEU:CD2	2.43	0.83
1:B:330:ALA:O	1:B:334:ARG:HG2	1.78	0.83
1:C:203:ARG:CD	1:D:362:HIS:CD2	2.59	0.83
1:D:665:TYR:O	1:D:712:GLN:NE2	2.12	0.83
1:C:596:LEU:HD21	1:D:837:LEU:O	1.78	0.83
1:A:205:LYS:CD	1:A:333:ARG:HH11	1.90	0.83
1:B:203:ARG:CD	1:C:362:HIS:CG	2.60	0.83
1:C:202:ARG:HD2	1:D:398:ILE:HG12	1.61	0.83
1:D:336:GLN:HE21	1:E:553:LEU:HD22	1.42	0.83
2:E:1003:ATP:C4	1:F:393:LEU:CD1	2.62	0.83
1:C:203:ARG:N	1:D:363:HIS:HE1	1.77	0.83
1:E:198:ARG:HA	1:F:405:VAL:HG11	1.59	0.83
1:F:645:GLU:O	1:F:645:GLU:CD	2.15	0.83
1:E:381:ARG:HH11	1:F:796:GLU:CD	1.81	0.82
1:C:556:ILE:O	1:C:556:ILE:HG13	1.78	0.82
1:D:201:ALA:HB3	1:E:405:VAL:CG2	2.09	0.82
1:C:601:LEU:CD2	1:D:844:ILE:CD1	2.58	0.82
1:B:570:ILE:HD11	1:C:846:LYS:HA	1.60	0.82
1:B:203:ARG:HD3	1:C:362:HIS:CB	2.09	0.82
1:B:203:ARG:HG3	1:C:362:HIS:NE2	1.93	0.82
1:D:601:LEU:CG	1:E:844:ILE:CD1	2.58	0.82
1:D:826:ARG:NH2	2:D:901:ATP:O1G	2.13	0.82
1:C:203:ARG:NH2	1:D:359:TYR:CZ	2.44	0.81
1:C:336:GLN:CD	1:D:553:LEU:HD22	2.00	0.81
1:E:599:SER:HB2	1:F:844:ILE:HG21	1.62	0.81
1:E:601:LEU:CB	1:F:844:ILE:CD1	2.59	0.81
2:D:901:ATP:O1B	2:D:901:ATP:O1A	1.89	0.81
1:B:205:LYS:HZ1	1:B:333:ARG:HH21	1.25	0.81
1:E:661:GLY:HA2	1:F:663:VAL:O	1.80	0.81
1:A:192:GLU:N	1:A:192:GLU:OE1	2.12	0.81
1:C:203:ARG:H	1:D:363:HIS:HE1	1.28	0.81
1:A:619:GLY:CA	2:A:1002:ATP:C5'	2.28	0.80
1:A:596:LEU:HD21	1:B:841:ALA:CB	2.10	0.80
1:A:665:TYR:CZ	1:A:712:GLN:NE2	2.48	0.80
1:B:596:LEU:HA	1:C:841:ALA:HB2	0.81	0.80
1:A:765:ARG:NH2	1:B:826:ARG:CZ	2.42	0.80
1:C:235:PRO:HA	1:D:408:ASP:HB3	1.63	0.80
1:B:203:ARG:CB	1:C:362:HIS:CD2	2.65	0.80
1:C:257:TYR:HB3	1:D:256:LYS:NZ	1.97	0.80
1:D:596:LEU:HD12	1:E:841:ALA:CB	2.05	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ILE:HA	1:C:842:LEU:HD11	1.64	0.79
1:C:202:ARG:CZ	1:D:398:ILE:HG13	2.12	0.79
1:E:333:ARG:HH22	1:F:390:ASP:CA	1.92	0.79
1:E:712:GLN:CG	1:E:714:LYS:HZ3	1.95	0.79
1:D:764:ASN:HA	1:E:830:ARG:NH2	1.97	0.79
1:D:764:ASN:CA	1:E:830:ARG:NH2	2.45	0.79
1:D:332:GLU:O	1:E:386:ARG:NH2	2.14	0.79
1:D:595:ARG:CB	1:E:845:LEU:HD11	2.13	0.79
1:E:334:ARG:HH22	2:E:1003:ATP:PA	2.04	0.79
1:C:765:ARG:HH21	1:D:826:ARG:HH21	1.30	0.79
1:E:201:ALA:HB1	1:F:405:VAL:CG2	2.03	0.79
1:E:666:ASP:O	1:E:667:GLU:C	2.21	0.79
1:B:333:ARG:NE	1:C:390:ASP:OD2	2.16	0.79
1:C:665:TYR:CZ	1:C:712:GLN:HG2	2.18	0.78
1:A:618:SER:O	2:A:1002:ATP:N7	2.15	0.78
1:A:619:GLY:HA3	2:A:1002:ATP:N3	1.97	0.78
1:B:205:LYS:HE2	1:B:333:ARG:CZ	2.12	0.78
1:C:203:ARG:H	1:D:363:HIS:CE1	2.01	0.78
1:B:205:LYS:HE3	1:B:333:ARG:NH2	1.96	0.78
1:B:202:ARG:HD2	1:C:398:ILE:HG12	1.65	0.78
1:B:306:SER:HB3	1:B:334:ARG:HH22	1.47	0.78
2:B:1002:ATP:O1B	2:B:1002:ATP:O3G	1.99	0.78
1:C:107:LYS:CD	1:D:106:GLN:CD	2.52	0.78
1:B:203:ARG:HD3	1:C:362:HIS:HB3	1.63	0.78
1:C:595:ARG:HA	1:D:845:LEU:HD11	1.65	0.78
1:A:257:TYR:HB3	1:B:256:LYS:HG2	1.65	0.78
1:B:592:ASN:CB	1:C:838:ASN:HB3	2.14	0.78
1:E:601:LEU:CB	1:F:844:ILE:HD13	2.14	0.78
1:D:322:ARG:CB	1:E:677:TYR:OH	2.31	0.78
1:D:665:TYR:CZ	1:D:712:GLN:CD	2.57	0.78
1:C:203:ARG:CB	1:D:363:HIS:CE1	2.66	0.78
1:E:235:PRO:CB	1:F:409:SER:HA	2.14	0.78
1:E:203:ARG:H	1:F:363:HIS:HE1	1.33	0.77
1:E:662:TYR:OH	1:F:650:TYR:CA	2.31	0.77
1:B:764:ASN:O	1:C:826:ARG:CG	2.33	0.77
1:B:592:ASN:HB3	1:C:838:ASN:CB	2.15	0.77
1:C:601:LEU:CD1	1:D:841:ALA:HA	2.10	0.77
1:D:601:LEU:CD1	1:E:841:ALA:HA	2.14	0.77
1:F:563:GLU:N	1:F:563:GLU:OE1	2.17	0.77
1:A:296:ASP:CG	1:B:252:THR:HG22	2.05	0.77
1:A:220:ALA:CB	2:A:1001:ATP:N1	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASP:CG	1:B:252:THR:CG2	2.53	0.77
1:D:332:GLU:HG2	1:E:386:ARG:HH21	1.50	0.77
1:B:333:ARG:NE	1:C:390:ASP:CG	2.38	0.76
1:C:203:ARG:HD2	1:D:362:HIS:CG	2.15	0.76
1:B:601:LEU:HD13	1:C:840:LEU:CB	2.14	0.76
1:D:662:TYR:OH	1:E:650:TYR:HA	1.84	0.76
1:E:333:ARG:HH22	1:F:390:ASP:HA	1.50	0.76
1:A:296:ASP:OD2	1:B:252:THR:HG22	1.84	0.76
1:E:381:ARG:CZ	1:F:796:GLU:OE2	2.33	0.76
1:B:601:LEU:HD13	1:C:840:LEU:CG	1.84	0.76
1:E:386:ARG:HD3	1:E:390:ASP:OD2	1.85	0.76
1:E:595:ARG:CB	1:F:845:LEU:CB	2.61	0.76
1:E:666:ASP:C	1:E:667:GLU:O	2.21	0.76
1:E:645:GLU:O	1:E:645:GLU:HG3	1.84	0.76
1:C:203:ARG:HB2	1:D:362:HIS:HD2	1.50	0.76
1:D:764:ASN:C	1:E:830:ARG:NH2	2.39	0.76
1:A:257:TYR:HB2	1:B:256:LYS:HE2	1.66	0.76
1:B:205:LYS:NZ	1:B:333:ARG:NH2	2.30	0.76
1:B:766:ILE:O	1:C:830:ARG:NH2	2.19	0.76
1:D:202:ARG:CD	1:E:398:ILE:HD12	2.15	0.76
1:D:601:LEU:CD2	1:E:844:ILE:CD1	2.64	0.76
1:B:596:LEU:HD13	1:C:833:GLN:NE2	2.01	0.75
1:B:203:ARG:CG	1:C:362:HIS:CG	2.67	0.75
1:C:583:GLN:HA	1:C:583:GLN:OE1	1.86	0.75
1:B:603:ASN:CA	1:C:794:ARG:NH1	2.42	0.75
1:C:595:ARG:HD3	1:D:842:LEU:HD13	1.68	0.75
1:F:645:GLU:O	1:F:645:GLU:OE1	2.02	0.75
2:C:1002:ATP:O1B	2:C:1002:ATP:O3G	1.98	0.75
1:A:592:ASN:ND2	1:B:842:LEU:HD21	2.01	0.75
1:B:203:ARG:HB2	1:C:362:HIS:CD2	2.22	0.75
1:E:333:ARG:N	1:F:386:ARG:HH12	1.85	0.75
1:E:665:TYR:C	1:E:667:GLU:H	1.90	0.75
1:A:220:ALA:HB2	2:A:1001:ATP:C4	2.21	0.74
1:B:595:ARG:NH2	1:C:842:LEU:HD21	2.02	0.74
1:B:765:ARG:HH22	1:C:826:ARG:HH22	1.30	0.74
1:E:381:ARG:NH1	1:F:796:GLU:CD	2.40	0.74
1:C:203:ARG:HD2	1:D:362:HIS:HB2	1.69	0.74
1:C:596:LEU:CG	1:D:841:ALA:HB2	2.17	0.74
1:E:203:ARG:HG3	1:F:363:HIS:CG	2.21	0.74
1:E:333:ARG:CD	1:F:390:ASP:OD2	2.35	0.74
1:A:765:ARG:HH12	1:B:826:ARG:HH12	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:CZ	1:D:398:ILE:CG1	2.65	0.74
1:C:707:ARG:NH2	1:D:636:ASP:OD1	2.20	0.74
1:F:665:TYR:O	1:F:666:ASP:C	2.26	0.74
1:C:235:PRO:HB3	1:D:408:ASP:HB2	1.69	0.74
1:D:763:LEU:C	1:E:830:ARG:HH22	1.88	0.74
1:A:601:LEU:HA	1:B:800:LYS:HZ1	1.52	0.74
1:A:764:ASN:OD1	1:A:765:ARG:HG2	1.87	0.74
1:B:665:TYR:O	1:B:666:ASP:O	2.06	0.74
1:A:218:LYS:NZ	2:A:1001:ATP:O1G	2.21	0.74
1:A:819:TYR:O	1:A:819:TYR:CD2	2.41	0.74
1:A:619:GLY:HA2	2:A:1002:ATP:C4'	2.17	0.73
2:E:1003:ATP:H2	1:F:355:LEU:CD1	1.99	0.73
2:E:1002:ATP:O1A	2:E:1002:ATP:O1B	1.89	0.73
1:D:665:TYR:CD1	1:D:712:GLN:CG	2.69	0.73
1:E:324:ILE:HG13	1:E:325:VAL:H	1.51	0.73
1:B:601:LEU:HD11	1:C:840:LEU:HG	0.75	0.73
1:D:601:LEU:HD12	1:E:841:ALA:CA	2.13	0.73
1:A:296:ASP:OD2	1:B:252:THR:CG2	2.37	0.73
1:A:257:TYR:CB	1:B:256:LYS:HE2	2.17	0.73
1:C:203:ARG:N	1:D:363:HIS:CE1	2.56	0.73
1:E:202:ARG:HA	1:F:401:ALA:HB2	1.70	0.73
1:A:596:LEU:HD11	1:B:841:ALA:HB2	1.68	0.73
1:B:765:ARG:NH2	1:C:826:ARG:NH2	2.34	0.72
1:A:596:LEU:CG	1:B:841:ALA:HB1	2.19	0.72
1:B:330:ALA:O	1:B:334:ARG:CD	2.36	0.72
1:C:332:GLU:HG2	1:D:386:ARG:HH21	1.51	0.72
1:C:601:LEU:HD13	1:D:840:LEU:HG	1.72	0.72
1:C:257:TYR:CG	1:D:256:LYS:CE	2.72	0.72
1:E:305:LEU:HB2	1:E:334:ARG:HG2	1.70	0.72
1:F:797:GLN:OE1	1:F:797:GLN:O	2.06	0.72
1:B:203:ARG:CD	1:C:362:HIS:CB	2.66	0.72
1:C:203:ARG:CB	1:D:363:HIS:NE2	2.52	0.72
1:C:257:TYR:CD1	1:D:256:LYS:CE	2.59	0.72
1:E:203:ARG:N	1:F:363:HIS:HE1	1.86	0.72
1:C:104:LYS:HZ1	1:E:81:PRO:HB2	1.52	0.72
1:D:665:TYR:CE2	1:D:712:GLN:NE2	2.58	0.72
1:C:596:LEU:HA	1:D:841:ALA:HB1	1.71	0.71
1:A:596:LEU:HD21	1:B:841:ALA:HB1	1.73	0.71
1:A:620:LYS:HE2	2:A:1002:ATP:O3G	1.89	0.71
1:B:595:ARG:CZ	1:C:842:LEU:CD1	2.67	0.71
1:B:598:ARG:HB2	1:C:845:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HD3	1:F:329:GLY:HA3	1.72	0.71
1:D:662:TYR:CZ	1:E:650:TYR:HA	2.26	0.71
1:D:764:ASN:HB3	1:E:823:MET:HE2	1.70	0.71
1:B:261:PHE:CD1	1:B:261:PHE:C	2.64	0.71
1:B:333:ARG:CD	1:C:390:ASP:CG	2.59	0.71
1:B:599:SER:HB3	1:C:841:ALA:HA	1.72	0.71
1:B:570:ILE:CG1	1:C:846:LYS:HG3	2.12	0.71
1:C:387:ARG:HA	1:C:387:ARG:NE	2.06	0.71
1:B:377:GLN:NE2	1:C:796:GLU:O	2.24	0.71
1:E:592:ASN:OD1	1:F:842:LEU:HD13	1.90	0.71
1:B:595:ARG:CZ	1:C:842:LEU:HD21	2.17	0.71
1:B:599:SER:HB2	1:C:844:ILE:HD13	1.71	0.71
1:A:596:LEU:CD1	1:B:841:ALA:CB	2.57	0.70
1:A:198:ARG:CD	1:B:405:VAL:HG11	2.22	0.70
1:C:596:LEU:HA	1:D:841:ALA:CB	2.20	0.70
1:C:599:SER:OG	1:D:845:LEU:HG	1.90	0.70
1:E:232:ASP:C	1:F:410:LYS:HE3	2.07	0.70
1:B:601:LEU:CD2	1:C:840:LEU:CD2	2.69	0.70
1:E:233:ASP:HA	1:F:410:LYS:HZ2	1.48	0.70
1:B:203:ARG:HD3	1:C:362:HIS:CG	2.26	0.70
1:B:599:SER:CB	1:C:841:ALA:HA	2.21	0.70
1:D:201:ALA:CB	1:E:405:VAL:CG2	2.69	0.70
2:E:1003:ATP:C4	1:F:393:LEU:HD12	2.25	0.70
2:E:1003:ATP:H2	1:F:355:LEU:HD11	1.50	0.70
1:B:570:ILE:CG2	1:C:846:LYS:CE	2.27	0.70
1:D:381:ARG:HD2	1:E:796:GLU:OE2	1.91	0.70
1:E:334:ARG:CZ	2:E:1003:ATP:O3B	2.40	0.70
1:E:662:TYR:HH	1:F:650:TYR:HA	1.55	0.70
2:E:1003:ATP:C8	2:E:1003:ATP:H5'2	2.27	0.70
1:C:201:ALA:CB	1:D:405:VAL:HG23	2.14	0.69
2:D:901:ATP:O1G	2:D:901:ATP:PB	2.50	0.69
1:B:659:THR:HG21	1:C:654:LYS:HE3	1.72	0.69
1:C:107:LYS:HG3	1:D:105:GLN:HE21	1.57	0.69
1:C:764:ASN:OD1	1:D:823:MET:CE	2.22	0.69
1:E:202:ARG:NH2	1:F:398:ILE:HG13	2.08	0.69
1:A:619:GLY:C	2:A:1002:ATP:N3	2.46	0.69
1:D:662:TYR:CE2	1:E:650:TYR:HA	2.27	0.69
1:B:601:LEU:HD13	1:C:840:LEU:HB3	1.72	0.69
1:C:595:ARG:CD	1:D:842:LEU:HD13	2.22	0.69
1:B:764:ASN:HB3	1:C:826:ARG:CG	2.23	0.69
1:E:599:SER:CB	1:F:844:ILE:HG21	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ILE:HD11	1:C:846:LYS:CG	2.18	0.69
1:B:596:LEU:CA	1:C:841:ALA:HB1	2.07	0.69
1:C:601:LEU:CD1	1:D:840:LEU:HG	2.22	0.69
1:B:604:PRO:CG	1:C:794:ARG:HD2	2.23	0.69
1:E:387:ARG:HA	1:E:387:ARG:NE	2.08	0.69
1:B:569:LEU:HD12	1:C:845:LEU:HD22	1.73	0.68
1:C:645:GLU:OE1	1:C:645:GLU:O	2.11	0.68
1:A:217:GLY:HA2	2:A:1001:ATP:O5'	1.93	0.68
1:B:330:ALA:O	1:B:334:ARG:CG	2.41	0.68
1:C:661:GLY:HA2	1:D:663:VAL:O	1.94	0.68
1:D:601:LEU:HG	1:E:844:ILE:HD12	1.76	0.68
1:D:583:GLN:OE1	1:D:583:GLN:HA	1.91	0.68
2:D:902:ATP:O1A	2:D:902:ATP:O1B	2.05	0.68
1:E:761:GLU:N	1:E:761:GLU:OE1	2.21	0.68
1:E:596:LEU:CB	1:F:841:ALA:CB	2.71	0.68
1:E:202:ARG:NH1	1:F:398:ILE:CG1	2.57	0.68
1:B:202:ARG:HA	1:C:401:ALA:HB2	1.76	0.68
1:D:595:ARG:HD3	1:E:842:LEU:HD13	1.75	0.68
2:E:1002:ATP:O1G	2:E:1002:ATP:PB	2.50	0.68
1:B:334:ARG:HD2	1:B:334:ARG:N	2.08	0.67
1:C:764:ASN:CG	1:D:823:MET:CE	2.63	0.67
1:A:260:ASP:OD1	1:B:256:LYS:NZ	2.26	0.67
1:A:775:LEU:HD11	2:A:1002:ATP:C8	2.29	0.67
1:B:322:ARG:CB	1:C:677:TYR:OH	2.37	0.67
1:A:583:GLN:HG2	2:A:1002:ATP:HN62	1.60	0.67
1:B:595:ARG:HD3	1:C:842:LEU:CG	2.23	0.67
1:B:595:ARG:HD3	1:C:842:LEU:CA	2.24	0.67
1:D:216:ILE:HD12	1:D:341:ALA:C	2.15	0.67
2:A:1002:ATP:O1B	2:A:1002:ATP:O2A	2.10	0.67
1:C:386:ARG:HD3	1:C:390:ASP:OD2	1.94	0.67
1:A:619:GLY:CA	2:A:1002:ATP:N3	2.58	0.67
1:B:570:ILE:HD11	1:C:846:LYS:CA	2.25	0.67
1:C:596:LEU:CG	1:D:841:ALA:CB	2.73	0.67
1:C:603:ASN:OD1	1:D:794:ARG:HD2	1.95	0.67
1:A:220:ALA:CB	2:A:1001:ATP:C6	2.75	0.67
1:D:202:ARG:HA	1:E:401:ALA:CB	2.25	0.66
1:C:235:PRO:CB	1:D:408:ASP:HB2	2.25	0.66
1:C:203:ARG:HG3	1:D:362:HIS:ND1	2.07	0.66
1:C:764:ASN:O	1:D:830:ARG:NE	2.28	0.66
1:D:764:ASN:ND2	1:E:823:MET:CG	2.48	0.66
1:C:106:GLN:CA	1:D:105:GLN:HE22	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:ARG:CB	1:D:845:LEU:HD12	2.20	0.66
1:E:381:ARG:NE	1:F:796:GLU:OE2	2.29	0.66
1:B:583:GLN:OE1	1:B:583:GLN:HA	1.96	0.66
1:B:604:PRO:HD2	1:C:794:ARG:NH1	2.10	0.66
1:E:662:TYR:OH	1:F:650:TYR:CG	2.47	0.66
1:D:622:GLU:HG3	2:D:901:ATP:H2'	1.77	0.66
1:A:618:SER:O	2:A:1002:ATP:C8	2.49	0.65
1:C:659:THR:HG21	1:D:654:LYS:HG3	1.78	0.65
1:A:765:ARG:HH22	1:B:826:ARG:NH2	1.94	0.65
1:B:306:SER:HB3	1:B:334:ARG:HH21	1.58	0.65
1:A:583:GLN:HG3	1:A:583:GLN:O	1.96	0.65
1:B:596:LEU:HD22	1:C:837:LEU:HB3	1.78	0.65
1:C:645:GLU:O	1:C:645:GLU:CD	2.34	0.65
1:D:216:ILE:CD1	1:D:340:VAL:HG12	2.25	0.65
1:E:595:ARG:HH12	1:F:842:LEU:HD11	1.57	0.65
1:A:667:GLU:CD	1:A:712:GLN:OE1	2.35	0.65
1:B:596:LEU:CD1	1:C:838:ASN:OD1	2.33	0.65
1:C:336:GLN:HE21	1:D:553:LEU:HD22	1.52	0.65
1:A:198:ARG:HG2	1:B:405:VAL:HG21	1.76	0.65
1:A:619:GLY:CA	2:A:1002:ATP:C4	2.75	0.65
1:A:217:GLY:CA	2:A:1001:ATP:O5'	2.43	0.65
1:C:595:ARG:HD3	1:D:842:LEU:CD1	2.26	0.65
1:A:619:GLY:HA2	2:A:1002:ATP:H5'2	0.67	0.65
1:B:595:ARG:CZ	1:C:842:LEU:CG	2.74	0.65
1:B:601:LEU:CD1	1:C:840:LEU:HB3	2.24	0.65
1:C:256:LYS:HD2	1:C:256:LYS:N	2.12	0.65
1:A:252:THR:OG1	1:F:322:ARG:NH2	2.30	0.65
1:A:618:SER:O	2:A:1002:ATP:C6	2.47	0.64
1:D:826:ARG:CZ	2:D:901:ATP:O3A	2.44	0.64
1:E:204:ILE:HG13	1:F:359:TYR:CE1	2.29	0.64
1:A:619:GLY:HA3	2:A:1002:ATP:N9	2.11	0.64
1:B:601:LEU:CD2	1:C:840:LEU:HD23	2.26	0.64
1:C:202:ARG:CD	1:D:398:ILE:HG12	2.26	0.64
1:A:296:ASP:OD1	1:B:252:THR:CG2	2.43	0.64
1:D:665:TYR:CZ	1:D:712:GLN:NE2	2.66	0.64
1:E:601:LEU:CB	1:F:844:ILE:HD12	2.28	0.64
1:B:604:PRO:HD2	1:C:794:ARG:CZ	2.27	0.63
1:A:205:LYS:CD	1:A:333:ARG:NH1	2.57	0.63
1:C:595:ARG:CG	1:D:845:LEU:HD12	2.28	0.63
1:A:619:GLY:C	2:A:1002:ATP:H5'2	2.18	0.63
1:C:205:LYS:NZ	1:C:333:ARG:HE	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLN:OE1	1:B:80:GLN:N	2.27	0.63
1:E:712:GLN:HG2	1:E:714:LYS:HZ2	1.63	0.63
1:C:601:LEU:CD2	1:D:844:ILE:HD12	2.27	0.63
1:E:202:ARG:HG2	1:F:401:ALA:HB3	1.81	0.63
1:D:764:ASN:HB3	1:E:826:ARG:HD2	1.80	0.63
1:A:619:GLY:HA2	2:A:1002:ATP:O5'	1.96	0.63
1:C:53:ASN:C	1:C:53:ASN:OD1	2.32	0.63
1:A:596:LEU:CD2	1:B:841:ALA:HB1	2.29	0.62
1:B:596:LEU:HG	1:C:838:ASN:HA	1.79	0.62
1:C:336:GLN:HE22	1:D:553:LEU:HD22	1.56	0.62
1:E:662:TYR:OH	1:F:650:TYR:CB	2.46	0.62
1:B:601:LEU:HB3	1:C:837:LEU:HD22	1.81	0.62
1:C:107:LYS:CE	1:D:106:GLN:NE2	2.62	0.62
1:E:233:ASP:C	1:F:410:LYS:HE3	2.19	0.62
1:E:204:ILE:HG12	1:F:397:ASP:OD1	2.00	0.62
1:E:233:ASP:CG	1:F:410:LYS:NZ	2.52	0.62
1:B:601:LEU:HD22	1:C:840:LEU:HD23	1.81	0.62
1:D:763:LEU:C	1:E:830:ARG:NH2	2.50	0.62
2:A:1001:ATP:O1G	2:A:1001:ATP:PB	2.58	0.62
1:C:237:ILE:CD1	1:C:237:ILE:N	2.62	0.62
1:D:601:LEU:CD1	1:E:840:LEU:HG	2.29	0.62
1:C:202:ARG:NH1	1:D:398:ILE:CG1	2.63	0.62
1:C:237:ILE:CD1	1:C:237:ILE:H	2.12	0.62
1:B:601:LEU:CD2	1:C:840:LEU:HD21	2.30	0.62
1:D:764:ASN:CB	1:E:823:MET:HE2	2.30	0.62
1:E:333:ARG:HG3	1:F:386:ARG:NH2	2.15	0.62
1:B:596:LEU:HD23	1:C:841:ALA:HB2	1.80	0.61
1:B:601:LEU:CG	1:C:840:LEU:HD23	2.28	0.61
1:C:237:ILE:N	1:C:237:ILE:HD12	2.14	0.61
1:D:665:TYR:HE1	1:D:712:GLN:HG2	0.80	0.61
1:D:202:ARG:HG2	1:E:401:ALA:CB	2.30	0.61
1:D:216:ILE:HG13	1:D:216:ILE:O	1.99	0.61
1:B:333:ARG:HE	1:C:390:ASP:CG	2.02	0.61
1:B:596:LEU:N	1:C:841:ALA:HB3	2.14	0.61
1:C:603:ASN:HA	1:D:794:ARG:HH12	1.57	0.61
1:B:595:ARG:HD3	1:C:842:LEU:CD1	2.20	0.61
1:B:596:LEU:CG	1:C:838:ASN:HA	2.30	0.61
1:E:203:ARG:HG2	1:F:363:HIS:HE1	1.58	0.61
1:D:601:LEU:HD11	1:E:840:LEU:HG	1.83	0.61
1:B:595:ARG:O	1:C:841:ALA:CB	2.30	0.61
1:C:257:TYR:CB	1:D:256:LYS:NZ	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:LEU:CA	1:E:841:ALA:HB1	2.24	0.61
1:F:853:GLU:OE1	1:F:853:GLU:O	2.17	0.61
1:C:202:ARG:NH1	1:D:398:ILE:CD1	2.62	0.61
1:D:310:LEU:HG	1:D:310:LEU:O	2.00	0.61
1:D:596:LEU:CD1	1:E:841:ALA:CB	2.59	0.61
1:D:764:ASN:HB3	1:E:823:MET:CE	2.30	0.61
1:E:334:ARG:NH1	2:E:1003:ATP:O1A	2.34	0.61
1:F:680:TYR:O	1:F:680:TYR:CD2	2.54	0.61
1:B:333:ARG:CG	1:B:333:ARG:HH11	2.13	0.60
1:B:596:LEU:CD1	1:C:833:GLN:NE2	2.64	0.60
1:B:205:LYS:O	1:B:205:LYS:HG2	2.01	0.60
1:B:333:ARG:HD3	1:C:390:ASP:OD2	1.96	0.60
1:C:235:PRO:CA	1:D:408:ASP:HB3	2.32	0.60
1:D:764:ASN:HA	1:E:830:ARG:CZ	2.31	0.60
1:E:765:ARG:HH11	1:E:765:ARG:CG	2.14	0.60
1:B:595:ARG:NE	1:C:842:LEU:CG	2.64	0.60
1:B:603:ASN:CB	1:C:794:ARG:NH2	2.65	0.60
1:C:107:LYS:CD	1:D:106:GLN:HE22	1.93	0.60
1:C:595:ARG:HB3	1:D:845:LEU:HD11	1.66	0.60
1:E:712:GLN:CD	1:E:714:LYS:HZ3	2.05	0.60
1:D:595:ARG:CB	1:E:845:LEU:CD1	2.75	0.60
1:E:203:ARG:H	1:F:363:HIS:CE1	2.18	0.60
1:E:202:ARG:CZ	1:F:398:ILE:HG13	2.30	0.59
1:C:603:ASN:CA	1:D:794:ARG:NH1	2.58	0.59
1:C:333:ARG:HB2	1:C:333:ARG:NH2	2.17	0.59
1:D:659:THR:HB	1:E:654:LYS:HG2	1.85	0.59
2:E:1003:ATP:C2	1:F:355:LEU:HD13	2.38	0.59
1:D:203:ARG:HB2	1:E:363:HIS:CE1	2.37	0.59
1:F:556:ILE:O	1:F:556:ILE:HG22	2.03	0.59
1:D:764:ASN:CB	1:E:823:MET:CE	2.81	0.59
1:A:333:ARG:HA	1:B:386:ARG:NH2	2.18	0.59
1:E:662:TYR:CD2	1:F:650:TYR:CE1	2.89	0.59
1:C:642:ASP:OD1	1:C:642:ASP:C	2.38	0.59
1:C:704:ASP:CB	1:C:765:ARG:HG2	2.33	0.59
1:B:596:LEU:HD21	1:C:838:ASN:CA	2.33	0.58
1:D:9:GLU:OE1	1:D:9:GLU:N	2.29	0.58
2:D:901:ATP:O1G	2:D:901:ATP:O2B	2.21	0.58
1:B:596:LEU:HD13	1:C:833:GLN:HE22	1.69	0.58
1:B:599:SER:CB	1:C:844:ILE:HB	2.33	0.58
1:B:604:PRO:CD	1:C:794:ARG:CD	2.69	0.58
1:B:205:LYS:CE	1:B:333:ARG:CZ	2.78	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:PRO:CD	1:C:794:ARG:CZ	2.80	0.58
1:A:619:GLY:C	2:A:1002:ATP:C2	2.77	0.58
1:C:596:LEU:CA	1:D:841:ALA:HB1	2.33	0.58
1:E:583:GLN:HA	1:E:583:GLN:OE1	2.04	0.58
1:D:665:TYR:OH	1:D:712:GLN:HB3	2.04	0.58
1:F:266:LYS:O	1:F:270:LYS:HG3	2.03	0.58
1:C:336:GLN:CD	1:C:336:GLN:C	2.62	0.58
1:A:198:ARG:HG3	1:B:405:VAL:CG1	2.34	0.58
1:C:322:ARG:HB2	1:D:677:TYR:OH	2.04	0.58
1:C:106:GLN:N	1:D:105:GLN:HE22	2.02	0.57
2:B:1001:ATP:PA	2:B:1001:ATP:H3'	2.43	0.57
1:C:202:ARG:CA	1:D:401:ALA:CB	2.74	0.57
1:B:40:ILE:HG22	1:B:40:ILE:O	2.03	0.57
1:D:165:GLU:N	1:D:168:SER:HG	2.01	0.57
2:E:1002:ATP:O1G	2:E:1002:ATP:O2B	2.21	0.57
2:E:1003:ATP:N3	1:F:393:LEU:CD1	2.68	0.57
1:D:595:ARG:HB3	1:E:845:LEU:HD12	1.87	0.57
1:D:601:LEU:HG	1:E:844:ILE:CD1	2.29	0.57
1:B:203:ARG:HG3	1:C:362:HIS:ND1	2.19	0.57
1:B:601:LEU:HD21	1:C:840:LEU:HD21	1.87	0.57
1:B:764:ASN:O	1:C:826:ARG:HG2	2.04	0.57
1:D:213:GLU:CG	1:D:214:PRO:CD	2.62	0.57
1:D:333:ARG:HA	1:E:386:ARG:HE	1.69	0.57
2:E:1003:ATP:N1	1:F:355:LEU:HD11	2.18	0.57
1:D:202:ARG:HA	1:E:401:ALA:HB2	1.86	0.57
2:D:902:ATP:O1B	2:D:902:ATP:O2G	2.23	0.57
1:E:189:ARG:HG2	1:E:189:ARG:HH11	1.69	0.57
1:E:665:TYR:C	1:E:667:GLU:N	2.58	0.57
1:C:333:ARG:HH22	1:D:390:ASP:CB	2.15	0.57
1:D:202:ARG:CD	1:E:398:ILE:CD1	2.62	0.57
1:D:202:ARG:HA	1:E:401:ALA:HB1	1.87	0.57
1:A:389:PRO:HB3	2:A:1001:ATP:H8	1.68	0.56
1:B:9:GLU:OE1	1:B:9:GLU:N	2.32	0.56
1:C:202:ARG:CA	1:D:401:ALA:HB1	2.30	0.56
1:E:305:LEU:CB	1:E:334:ARG:HG2	2.35	0.56
1:A:220:ALA:CA	2:A:1001:ATP:C2	2.87	0.56
1:B:601:LEU:HD12	1:C:840:LEU:HG	1.72	0.56
1:A:600:GLY:O	1:B:800:LYS:NZ	2.38	0.56
1:A:665:TYR:O	1:A:667:GLU:N	2.36	0.56
1:C:256:LYS:HD2	1:C:256:LYS:H	1.70	0.56
1:C:601:LEU:CG	1:D:844:ILE:CD1	2.76	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ILE:CD1	1:D:341:ALA:C	2.73	0.56
1:E:257:TYR:HB3	1:F:255:ALA:HB1	1.86	0.56
1:E:662:TYR:HH	1:F:650:TYR:CA	2.16	0.56
1:A:387:ARG:HA	1:A:387:ARG:NE	2.20	0.56
1:E:233:ASP:N	1:F:410:LYS:CE	2.68	0.56
1:C:294:LYS:O	1:C:296:ASP:N	2.39	0.56
1:D:333:ARG:HE	1:E:390:ASP:HB2	1.71	0.56
1:D:596:LEU:CA	1:E:841:ALA:CB	2.80	0.56
1:A:583:GLN:CG	2:A:1002:ATP:HN62	2.19	0.56
1:B:704:ASP:HB2	1:B:765:ARG:HE	1.70	0.56
1:E:233:ASP:N	1:F:410:LYS:HE3	2.20	0.56
1:B:606:GLN:OE1	1:B:606:GLN:HA	2.06	0.56
1:B:665:TYR:O	1:B:667:GLU:CA	2.53	0.56
1:A:619:GLY:HA3	2:A:1002:ATP:C1'	2.35	0.55
1:A:775:LEU:HD11	2:A:1002:ATP:N7	2.21	0.55
1:D:202:ARG:CG	1:E:398:ILE:HD12	2.36	0.55
1:E:233:ASP:CB	1:F:410:LYS:NZ	2.69	0.55
1:E:286:ILE:O	1:E:286:ILE:HD12	2.05	0.55
1:E:333:ARG:NE	1:F:390:ASP:OD2	2.24	0.55
1:E:599:SER:HB3	1:F:844:ILE:HG22	1.85	0.55
1:E:233:ASP:CB	1:F:410:LYS:HZ1	2.15	0.55
1:D:666:ASP:O	1:D:667:GLU:C	2.45	0.55
2:F:901:ATP:O1G	2:F:901:ATP:O1B	2.25	0.55
1:C:104:LYS:HZ1	1:E:81:PRO:CB	2.20	0.55
1:D:785:ASP:OD2	1:D:789:LYS:NZ	2.38	0.55
1:E:202:ARG:HG2	1:F:401:ALA:CB	2.37	0.55
1:B:595:ARG:CG	1:C:842:LEU:HD13	2.32	0.55
1:B:764:ASN:O	1:C:826:ARG:HG3	2.05	0.55
1:C:645:GLU:OE1	1:C:654:LYS:NZ	2.40	0.55
1:D:880:LEU:HB2	1:D:881:PRO:HD2	1.87	0.55
1:F:264:ARG:HA	1:F:264:ARG:NE	2.22	0.55
1:B:333:ARG:NE	1:C:390:ASP:OD1	2.37	0.55
1:B:599:SER:HA	1:C:844:ILE:HG21	1.87	0.55
1:E:330:ALA:CB	2:E:1003:ATP:PG	2.94	0.55
1:E:332:GLU:C	1:F:386:ARG:HH12	2.09	0.55
1:D:126:ILE:H	1:D:126:ILE:HD12	1.70	0.55
2:F:901:ATP:H5'1	2:F:901:ATP:C8	2.42	0.55
1:B:595:ARG:HA	1:C:845:LEU:HD11	1.89	0.55
1:C:204:ILE:CD1	1:D:397:ASP:OD2	2.50	0.55
1:C:235:PRO:CB	1:D:408:ASP:CB	2.85	0.55
1:D:305:LEU:HB3	1:D:334:ARG:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:TYR:HE1	1:D:712:GLN:CG	1.70	0.55
1:E:235:PRO:CA	1:F:409:SER:HA	2.36	0.55
1:B:601:LEU:HD22	1:C:840:LEU:CD2	2.35	0.55
1:C:659:THR:HB	1:D:654:LYS:HG2	1.89	0.54
1:A:202:ARG:CZ	1:A:205:LYS:HB2	2.37	0.54
1:B:598:ARG:HB3	1:C:845:LEU:CD2	2.30	0.54
1:F:645:GLU:CD	1:F:645:GLU:C	2.65	0.54
1:C:201:ALA:HB1	1:D:405:VAL:HG23	1.81	0.54
1:D:662:TYR:CD1	1:D:662:TYR:N	2.73	0.54
1:E:305:LEU:HD13	1:E:334:ARG:HB3	1.89	0.54
1:E:765:ARG:HH11	1:E:765:ARG:HG2	1.73	0.54
1:F:562:SER:HB2	1:F:568:LYS:HE2	1.88	0.54
1:A:257:TYR:HB3	1:B:256:LYS:HE2	1.90	0.54
1:E:662:TYR:CD1	1:E:662:TYR:N	2.73	0.54
1:B:333:ARG:NH1	1:B:333:ARG:HG3	2.22	0.54
1:A:186:VAL:HG13	2:A:1001:ATP:HN62	1.72	0.54
1:B:680:TYR:CD2	1:B:680:TYR:N	2.71	0.54
1:B:765:ARG:HG2	1:C:826:ARG:NH1	2.23	0.54
1:E:235:PRO:HB3	1:F:409:SER:CA	2.32	0.54
1:D:764:ASN:CG	1:E:823:MET:CE	2.76	0.53
1:B:136:ASP:OD1	1:B:136:ASP:C	2.46	0.53
2:F:901:ATP:C8	2:F:901:ATP:C5'	2.90	0.53
1:A:765:ARG:HH22	1:B:826:ARG:HH12	1.18	0.53
1:D:332:GLU:CG	1:E:386:ARG:NH2	2.66	0.53
1:D:333:ARG:HE	1:E:215:GLY:HA2	1.73	0.53
2:E:1001:ATP:C5'	2:E:1001:ATP:C8	2.92	0.53
1:A:198:ARG:CG	1:B:405:VAL:HG11	2.39	0.53
1:B:603:ASN:HB2	1:C:794:ARG:NH2	2.23	0.53
1:B:604:PRO:HD2	1:C:794:ARG:NE	2.23	0.53
1:C:716:ILE:HD12	1:C:716:ILE:N	2.23	0.53
1:E:204:ILE:CG1	1:F:397:ASP:OD1	2.53	0.53
1:A:332:GLU:O	1:B:386:ARG:NH2	2.41	0.53
1:B:665:TYR:HD1	1:B:667:GLU:OE2	1.91	0.53
1:B:387:ARG:HA	1:B:387:ARG:NE	2.24	0.53
1:C:542:ASP:C	1:C:542:ASP:OD1	2.42	0.53
1:C:601:LEU:HG	1:D:844:ILE:HD12	1.89	0.53
1:C:595:ARG:CZ	1:D:842:LEU:HD13	2.39	0.53
1:C:601:LEU:HD12	1:D:841:ALA:N	2.22	0.53
1:A:596:LEU:CD2	1:B:841:ALA:CB	2.85	0.53
1:A:601:LEU:HA	1:B:800:LYS:HZ3	1.70	0.53
1:F:387:ARG:HA	1:F:387:ARG:NE	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLN:CD	1:D:553:LEU:CD2	2.69	0.53
1:F:184:ASP:OD1	1:F:358:LYS:NZ	2.42	0.53
1:B:306:SER:CB	1:B:334:ARG:NH2	2.63	0.52
1:E:247:ASP:OD1	1:E:248:LEU:N	2.42	0.52
1:D:764:ASN:CG	1:E:823:MET:HE2	2.30	0.52
1:E:332:GLU:HG3	1:F:386:ARG:HH11	1.73	0.52
1:E:645:GLU:O	1:E:645:GLU:CG	2.53	0.52
1:C:203:ARG:HA	1:D:362:HIS:NE2	2.24	0.52
1:C:617:GLY:CA	2:C:1002:ATP:O2A	2.57	0.52
1:C:617:GLY:HA2	2:C:1002:ATP:O2A	2.10	0.52
1:D:732:GLU:HA	1:D:732:GLU:OE1	2.09	0.52
1:E:235:PRO:HA	1:F:409:SER:HA	1.91	0.52
1:E:286:ILE:HD12	1:E:286:ILE:C	2.29	0.52
1:E:333:ARG:NH2	1:F:390:ASP:HA	2.21	0.52
1:B:126:ILE:O	1:B:126:ILE:HG22	2.08	0.52
1:B:805:ASN:O	1:B:806:LEU:C	2.47	0.52
1:C:322:ARG:NH1	1:D:673:ASN:OD1	2.42	0.52
1:C:596:LEU:HD23	1:D:841:ALA:HB2	0.62	0.52
1:C:336:GLN:O	1:C:336:GLN:OE1	2.26	0.52
1:A:665:TYR:CZ	1:A:712:GLN:HG2	2.44	0.52
1:A:765:ARG:CZ	1:B:826:ARG:HH11	2.13	0.52
1:D:680:TYR:CD1	1:D:680:TYR:C	2.82	0.52
1:E:333:ARG:HD3	1:E:334:ARG:HH22	1.70	0.52
1:A:198:ARG:HG3	1:B:405:VAL:HG11	1.92	0.52
1:B:599:SER:HB3	1:C:844:ILE:HB	1.91	0.52
1:C:203:ARG:CG	1:D:362:HIS:NE2	2.40	0.52
1:C:333:ARG:NH2	1:C:333:ARG:CB	2.73	0.52
1:C:617:GLY:N	2:C:1002:ATP:O2B	2.33	0.52
1:E:680:TYR:CD1	1:E:680:TYR:C	2.83	0.52
2:A:1002:ATP:O3G	2:A:1002:ATP:O1B	2.28	0.52
1:E:761:GLU:H	1:E:761:GLU:CD	2.11	0.52
1:B:202:ARG:NH1	1:C:398:ILE:HD11	2.25	0.51
1:D:583:GLN:OE1	1:D:583:GLN:CA	2.57	0.51
1:A:592:ASN:HD21	1:B:842:LEU:HD21	1.74	0.51
1:C:205:LYS:HZ2	1:C:333:ARG:HE	1.57	0.51
1:C:568:LYS:O	1:C:572:MET:N	2.43	0.51
1:C:680:TYR:CD1	1:C:680:TYR:C	2.84	0.51
1:B:203:ARG:HA	1:C:362:HIS:NE2	2.26	0.51
1:B:765:ARG:NH1	1:C:826:ARG:HH12	2.07	0.51
1:C:40:ILE:O	1:C:40:ILE:HG22	2.10	0.51
1:E:333:ARG:NH2	1:F:390:ASP:CA	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NH1	1:A:205:LYS:HB2	2.26	0.51
1:A:825:ALA:HB3	2:A:1002:ATP:O4'	2.10	0.51
1:D:302:LYS:C	1:D:302:LYS:HD3	2.31	0.51
2:F:901:ATP:C5'	2:F:901:ATP:H8	2.23	0.51
1:C:246:LEU:N	1:C:246:LEU:HD12	2.25	0.51
1:D:319:ASN:OD1	1:D:319:ASN:N	2.42	0.51
2:E:1003:ATP:C2	1:F:393:LEU:HD11	2.46	0.51
1:B:595:ARG:NE	1:C:842:LEU:HD22	2.07	0.51
1:B:761:GLU:HG3	1:C:616:SER:HB3	1.93	0.51
1:E:765:ARG:CG	1:E:765:ARG:NH1	2.73	0.51
1:C:583:GLN:OE1	1:C:583:GLN:CA	2.51	0.51
1:F:797:GLN:CD	1:F:797:GLN:C	2.70	0.51
1:A:625:LYS:NZ	1:A:636:ASP:OD1	2.44	0.51
1:E:189:ARG:HG2	1:E:189:ARG:NH1	2.26	0.51
1:B:596:LEU:CD1	1:C:833:GLN:HE21	2.23	0.50
1:B:765:ARG:CZ	1:C:826:ARG:NH1	2.61	0.50
1:D:299:ASN:C	1:D:299:ASN:OD1	2.48	0.50
1:D:595:ARG:HG2	1:E:845:LEU:CD1	2.40	0.50
1:C:856:ASN:OD1	1:C:856:ASN:C	2.49	0.50
1:E:233:ASP:CG	1:F:410:LYS:HZ1	2.13	0.50
1:F:569:LEU:O	1:F:572:MET:HB3	2.11	0.50
1:B:764:ASN:CB	1:C:826:ARG:HG2	2.35	0.50
1:E:333:ARG:C	1:F:386:ARG:HH22	2.15	0.50
1:A:186:VAL:HA	2:A:1001:ATP:HN62	1.76	0.50
1:B:134:GLN:OE1	1:B:134:GLN:N	2.27	0.50
1:B:700:LEU:HD22	1:B:765:ARG:HD2	1.92	0.50
1:C:704:ASP:O	1:C:705:ASP:CB	2.59	0.50
2:E:1003:ATP:H8	2:E:1003:ATP:H5'2	1.72	0.50
2:D:901:ATP:O1G	2:D:901:ATP:O3A	2.29	0.50
1:A:218:LYS:HE3	2:A:1001:ATP:PB	2.51	0.50
1:B:260:ASP:OD2	1:B:264:ARG:NH1	2.44	0.50
1:B:666:ASP:OD1	1:B:666:ASP:N	2.45	0.50
1:E:165:GLU:OE2	1:E:276:LYS:NZ	2.44	0.50
1:B:569:LEU:HD13	1:C:845:LEU:HD21	1.86	0.50
2:E:1001:ATP:H8	2:E:1001:ATP:H5'2	1.77	0.50
2:E:1002:ATP:O1G	2:E:1002:ATP:O3A	2.29	0.50
1:C:825:ALA:HB3	2:C:1002:ATP:C8	2.47	0.50
1:C:561:LEU:O	1:C:561:LEU:HG	2.11	0.49
1:C:596:LEU:HG	1:D:841:ALA:CB	2.43	0.49
1:C:601:LEU:HD13	1:D:840:LEU:CG	2.39	0.49
1:D:764:ASN:OD1	1:E:823:MET:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ASP:N	1:F:410:LYS:NZ	2.44	0.49
1:C:406:ALA:O	1:C:410:LYS:N	2.45	0.49
1:E:202:ARG:CA	1:F:401:ALA:HB1	2.28	0.49
1:B:203:ARG:HD2	1:C:362:HIS:CB	2.43	0.49
1:C:596:LEU:HA	1:D:841:ALA:HB2	1.95	0.49
1:D:601:LEU:HD23	1:E:800:LYS:HG2	1.94	0.49
1:A:812:ASP:O	1:A:816:LYS:N	2.46	0.49
1:B:202:ARG:CD	1:C:398:ILE:HG12	2.38	0.49
1:D:764:ASN:O	1:E:830:ARG:CZ	2.61	0.49
1:E:542:ASP:OD1	1:E:542:ASP:C	2.45	0.49
1:B:294:LYS:O	1:B:296:ASP:N	2.45	0.49
1:B:595:ARG:HB3	1:C:842:LEU:N	2.26	0.49
1:D:596:LEU:HD13	1:E:841:ALA:CB	2.32	0.49
1:D:805:ASN:O	1:D:806:LEU:C	2.49	0.49
1:A:662:TYR:CE1	1:B:650:TYR:HD2	2.30	0.49
1:B:201:ALA:CB	1:C:405:VAL:HG22	2.43	0.49
1:B:334:ARG:CD	1:B:334:ARG:N	2.73	0.49
1:D:595:ARG:CG	1:E:845:LEU:CD1	2.90	0.49
1:E:232:ASP:C	1:F:410:LYS:NZ	2.66	0.49
1:A:680:TYR:CD2	1:A:680:TYR:N	2.81	0.49
1:B:761:GLU:O	1:B:765:ARG:HG3	2.12	0.49
1:C:596:LEU:CA	1:D:841:ALA:CB	2.88	0.49
1:D:826:ARG:NH2	2:D:901:ATP:PA	2.84	0.49
1:C:595:ARG:NE	1:D:842:LEU:HD13	2.28	0.49
1:B:603:ASN:HA	1:C:794:ARG:HH12	1.63	0.48
1:C:237:ILE:HD13	1:D:408:ASP:OD2	2.13	0.48
1:C:806:LEU:O	1:C:807:THR:C	2.50	0.48
1:D:213:GLU:CB	1:D:214:PRO:HD2	2.35	0.48
1:F:216:ILE:O	1:F:216:ILE:CG2	2.49	0.48
1:A:764:ASN:ND2	1:B:826:ARG:HG2	2.27	0.48
1:A:775:LEU:CD1	2:A:1002:ATP:C8	2.97	0.48
1:B:205:LYS:NZ	1:C:394:ASP:CG	2.64	0.48
1:C:332:GLU:C	1:D:386:ARG:HH21	2.14	0.48
1:F:568:LYS:O	1:F:630:PHE:HE2	1.95	0.48
1:B:203:ARG:NH2	1:C:359:TYR:CE1	2.72	0.48
1:E:789:LYS:NZ	1:E:793:GLU:OE2	2.46	0.48
1:B:595:ARG:HE	1:C:842:LEU:CD1	1.95	0.48
1:B:629:GLY:O	1:B:633:ASN:N	2.45	0.48
1:E:202:ARG:CA	1:F:401:ALA:CB	2.78	0.48
1:F:797:GLN:OE1	1:F:797:GLN:C	2.51	0.48
1:B:333:ARG:CG	1:B:333:ARG:NH1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:CZ	1:C:333:ARG:CB	2.86	0.48
1:C:764:ASN:CA	1:D:830:ARG:CZ	2.62	0.48
1:D:201:ALA:HB3	1:E:405:VAL:HG22	1.72	0.48
1:D:660:ALA:HB2	1:D:665:TYR:CZ	2.48	0.48
1:D:662:TYR:CE2	1:E:650:TYR:CA	2.92	0.48
1:E:817:TYR:N	1:E:817:TYR:CD1	2.81	0.48
1:A:300:ILE:HG13	1:A:300:ILE:O	2.13	0.48
1:A:819:TYR:O	1:A:819:TYR:CG	2.65	0.48
1:B:187:ILE:H	2:B:1001:ATP:HN62	1.62	0.48
1:B:603:ASN:N	1:C:794:ARG:HH22	2.11	0.48
1:B:659:THR:HG21	1:C:654:LYS:HB2	1.95	0.48
1:B:665:TYR:O	1:B:667:GLU:HA	2.14	0.48
1:B:665:TYR:C	1:B:666:ASP:OD1	2.52	0.48
1:C:165:GLU:OE2	1:C:276:LYS:NZ	2.45	0.48
1:B:203:ARG:HD2	1:C:362:HIS:HB2	1.95	0.48
1:C:322:ARG:CB	1:D:677:TYR:OH	2.62	0.48
1:E:324:ILE:HG13	1:E:325:VAL:N	2.26	0.48
1:F:568:LYS:O	1:F:630:PHE:CE2	2.67	0.48
1:A:665:TYR:CD1	1:A:712:GLN:NE2	2.64	0.48
1:E:880:LEU:CB	1:E:881:PRO:CD	2.91	0.48
1:B:205:LYS:HZ3	1:B:333:ARG:HE	1.62	0.47
1:B:294:LYS:NZ	1:B:328:ASP:OD1	2.46	0.47
1:A:220:ALA:HA	2:A:1001:ATP:C2	2.50	0.47
1:A:592:ASN:CG	1:B:842:LEU:HD21	2.34	0.47
1:B:378:LEU:HD21	1:C:796:GLU:OE2	2.13	0.47
1:C:203:ARG:NE	1:D:359:TYR:CD1	2.82	0.47
1:C:764:ASN:C	1:D:830:ARG:CZ	2.81	0.47
1:D:15:LEU:HD13	1:D:15:LEU:C	2.34	0.47
1:B:592:ASN:CG	1:C:838:ASN:HB3	2.35	0.47
1:C:53:ASN:OD1	1:C:53:ASN:O	2.32	0.47
1:C:601:LEU:CD1	1:D:841:ALA:N	2.77	0.47
1:D:819:TYR:O	1:D:819:TYR:CG	2.64	0.47
1:B:205:LYS:HE3	1:B:333:ARG:HH21	1.64	0.47
1:B:235:PRO:HG3	1:C:405:VAL:HG13	1.95	0.47
1:B:317:THR:O	1:B:318:ASN:C	2.53	0.47
1:C:202:ARG:HG2	1:D:401:ALA:CB	2.45	0.47
1:C:203:ARG:HB2	1:D:362:HIS:CD2	2.24	0.47
1:D:333:ARG:NE	1:E:215:GLY:HA2	2.30	0.47
1:E:333:ARG:NE	2:E:1003:ATP:O5'	2.47	0.47
1:E:642:ASP:OD1	1:E:642:ASP:C	2.53	0.47
1:F:610:PHE:CD1	1:F:610:PHE:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLN:CA	1:D:105:GLN:NE2	2.77	0.47
1:C:662:TYR:CZ	1:D:649:LYS:O	2.68	0.47
1:C:697:THR:HG22	1:D:644:SER:HB2	1.97	0.47
1:F:775:LEU:N	1:F:775:LEU:HD22	2.30	0.47
1:B:53:ASN:OD1	1:B:53:ASN:C	2.53	0.47
1:D:294:LYS:NZ	1:D:328:ASP:OD1	2.47	0.47
1:E:387:ARG:NE	1:E:387:ARG:CA	2.77	0.47
1:C:107:LYS:CE	1:D:106:GLN:CD	2.63	0.46
1:C:202:ARG:CZ	1:D:398:ILE:HG12	2.43	0.46
1:C:668:GLY:O	1:C:669:GLY:C	2.50	0.46
1:D:332:GLU:C	1:E:386:ARG:HH21	2.15	0.46
1:D:333:ARG:NE	1:E:390:ASP:HB2	2.30	0.46
1:D:661:GLY:HA3	1:E:658:THR:HG21	1.97	0.46
2:E:1003:ATP:H2	1:F:355:LEU:HD13	1.77	0.46
1:C:295:ASP:HA	1:D:288:MET:SD	2.54	0.46
1:C:256:LYS:H	1:C:256:LYS:CD	2.27	0.46
1:D:305:LEU:CD1	1:D:334:ARG:HG2	2.45	0.46
1:E:148:ARG:O	1:E:149:GLY:C	2.53	0.46
2:E:1001:ATP:C8	2:E:1001:ATP:H5'2	2.50	0.46
1:F:555:GLY:O	1:F:556:ILE:HB	2.16	0.46
1:F:877:LEU:O	1:F:879:VAL:N	2.49	0.46
1:A:169:LYS:CD	1:F:329:GLY:HA3	2.44	0.46
1:C:659:THR:HG21	1:D:654:LYS:CG	2.44	0.46
1:C:765:ARG:NH2	1:D:826:ARG:CZ	2.70	0.46
1:D:595:ARG:CD	1:E:842:LEU:HD13	2.43	0.46
1:D:667:GLU:OE2	1:D:712:GLN:OE1	2.34	0.46
1:F:566:ASN:HA	1:F:570:ILE:HB	1.97	0.46
1:B:601:LEU:CG	1:C:840:LEU:CD2	2.86	0.46
1:B:804:LEU:C	1:B:805:ASN:O	2.51	0.46
1:D:764:ASN:O	1:E:830:ARG:NE	2.48	0.46
1:E:9:GLU:H	1:E:9:GLU:CD	2.14	0.46
1:E:323:SER:O	1:E:324:ILE:C	2.54	0.46
1:E:629:GLY:O	1:E:633:ASN:N	2.47	0.46
1:B:826:ARG:N	1:B:827:PRO:HD2	2.31	0.46
1:E:274:GLU:O	1:E:274:GLU:HG3	2.14	0.46
1:D:216:ILE:CD1	1:D:341:ALA:O	2.64	0.46
1:A:198:ARG:HG3	1:B:405:VAL:HG22	1.85	0.46
1:E:332:GLU:HG3	1:F:386:ARG:NH1	2.30	0.46
1:E:381:ARG:NH1	1:F:796:GLU:OE1	2.46	0.46
1:E:585:ASP:OD2	1:E:741:LYS:NZ	2.49	0.46
1:A:220:ALA:CB	2:A:1001:ATP:C4	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LYS:HE2	2:A:1001:ATP:O2B	2.15	0.46
1:D:216:ILE:HD12	1:D:342:GLU:N	2.31	0.46
1:D:595:ARG:CA	1:E:845:LEU:HD11	2.46	0.46
1:A:618:SER:O	2:A:1002:ATP:N9	2.42	0.45
1:B:771:ILE:HD12	1:B:771:ILE:N	2.32	0.45
2:B:1001:ATP:O2G	2:B:1001:ATP:O3A	2.33	0.45
1:E:257:TYR:HB3	1:F:255:ALA:CB	2.45	0.45
1:E:825:ALA:C	1:E:827:PRO:HD2	2.36	0.45
1:F:665:TYR:CZ	1:F:712:GLN:OE1	2.69	0.45
1:F:806:LEU:O	1:F:807:THR:OG1	2.28	0.45
1:B:596:LEU:HD21	1:C:838:ASN:HA	1.97	0.45
1:C:104:LYS:NZ	1:E:81:PRO:CB	2.74	0.45
1:D:665:TYR:CD1	1:D:712:GLN:CD	2.80	0.45
1:B:203:ARG:HB2	1:C:362:HIS:HD2	1.73	0.45
1:C:107:LYS:HG3	1:D:105:GLN:HG3	1.98	0.45
1:C:601:LEU:HD11	1:D:840:LEU:HG	1.98	0.45
1:E:333:ARG:CG	1:F:386:ARG:HH22	2.28	0.45
1:B:203:ARG:HB2	1:C:363:HIS:NE2	2.31	0.45
1:C:256:LYS:N	1:C:256:LYS:CD	2.80	0.45
1:D:213:GLU:HB3	1:D:216:ILE:HG22	1.98	0.45
1:D:198:ARG:HA	1:E:405:VAL:HG21	1.99	0.45
1:D:585:ASP:OD2	1:D:741:LYS:NZ	2.49	0.45
1:A:257:TYR:CD1	1:A:257:TYR:N	2.79	0.45
1:A:764:ASN:HD21	1:B:826:ARG:HG2	1.82	0.45
1:B:205:LYS:HZ3	1:B:333:ARG:NE	2.15	0.45
1:B:603:ASN:CB	1:C:794:ARG:CZ	2.95	0.45
1:A:187:ILE:H	2:A:1001:ATP:N6	2.14	0.45
1:C:237:ILE:H	1:C:237:ILE:HD13	1.81	0.45
1:C:387:ARG:NE	1:C:387:ARG:CA	2.77	0.45
1:E:817:TYR:N	1:E:817:TYR:HD1	2.15	0.45
1:B:764:ASN:OD1	1:C:823:MET:HE2	2.00	0.45
1:B:843:ARG:HB3	1:B:849:ILE:HG12	1.99	0.45
1:C:134:GLN:O	1:C:134:GLN:HG2	2.17	0.45
1:C:665:TYR:CE2	1:C:712:GLN:NE2	2.84	0.45
1:C:667:GLU:HB2	1:C:712:GLN:CD	2.37	0.45
1:A:259:GLY:HA3	1:B:254:GLY:HA2	1.99	0.45
1:B:596:LEU:HD11	1:C:833:GLN:HE21	1.80	0.45
1:C:295:ASP:H	1:D:288:MET:HE1	1.81	0.45
1:C:555:GLY:O	1:C:556:ILE:C	2.56	0.45
1:A:596:LEU:CD2	1:B:841:ALA:HA	2.34	0.45
1:B:203:ARG:CD	1:C:362:HIS:CD2	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLN:C	1:D:105:GLN:NE2	2.53	0.45
1:C:556:ILE:O	1:C:556:ILE:CG1	2.50	0.45
1:E:80:GLN:O	1:E:82:ALA:N	2.50	0.45
1:E:732:GLU:OE1	1:E:732:GLU:N	2.49	0.45
1:A:331:PHE:N	1:A:331:PHE:CD1	2.84	0.44
1:B:336:GLN:CG	1:C:553:LEU:HD22	2.44	0.44
1:B:809:GLU:H	1:B:809:GLU:CD	2.19	0.44
1:B:819:TYR:C	1:B:819:TYR:CD1	2.90	0.44
1:C:765:ARG:NH2	2:D:901:ATP:O1G	2.50	0.44
1:E:712:GLN:HG2	1:E:712:GLN:O	2.17	0.44
1:F:562:SER:CB	1:F:568:LYS:HE2	2.47	0.44
1:A:169:LYS:HD3	1:F:329:GLY:CA	2.44	0.44
1:C:299:ASN:OD1	1:C:299:ASN:C	2.54	0.44
1:D:202:ARG:HG2	1:E:401:ALA:HB3	1.98	0.44
1:B:204:ILE:HG13	1:C:397:ASP:OD2	2.07	0.44
1:B:583:GLN:OE1	1:B:583:GLN:CA	2.64	0.44
1:C:202:ARG:CA	1:D:401:ALA:HB2	2.37	0.44
1:C:247:ASP:OD1	1:C:248:LEU:N	2.50	0.44
1:D:336:GLN:HE22	1:E:553:LEU:HB3	1.82	0.44
1:D:764:ASN:HA	1:E:823:MET:HE3	1.99	0.44
1:D:880:LEU:CB	1:D:881:PRO:CD	2.95	0.44
1:C:629:GLY:O	1:C:633:ASN:N	2.51	0.44
1:C:851:ASP:OD1	1:C:851:ASP:C	2.54	0.44
1:D:305:LEU:HB3	1:D:334:ARG:CG	2.47	0.44
1:E:236:THR:N	1:F:408:ASP:O	2.50	0.44
1:A:580:VAL:O	1:A:580:VAL:HG12	2.17	0.44
1:B:310:LEU:O	1:B:311:LYS:C	2.53	0.44
1:C:604:PRO:HD2	1:D:794:ARG:HH11	1.83	0.44
1:C:665:TYR:CD2	1:C:712:GLN:NE2	2.86	0.44
1:A:775:LEU:HD21	2:A:1002:ATP:N7	2.32	0.44
1:B:665:TYR:HD1	1:B:665:TYR:HA	1.66	0.44
1:C:596:LEU:HD11	1:D:838:ASN:HA	1.98	0.44
1:D:201:ALA:HB1	1:E:405:VAL:HG22	1.92	0.44
1:E:237:ILE:CD1	1:F:408:ASP:HB2	2.48	0.44
1:B:201:ALA:HB3	1:C:405:VAL:CG2	2.47	0.44
1:B:849:ILE:HD13	1:B:880:LEU:H	1.83	0.44
1:C:203:ARG:CZ	1:D:359:TYR:CE1	3.00	0.44
1:C:826:ARG:N	1:C:827:PRO:CD	2.81	0.44
1:F:204:ILE:O	1:F:204:ILE:HG13	2.17	0.44
1:F:665:TYR:CE1	1:F:712:GLN:NE2	2.86	0.44
1:B:137:ILE:HG13	1:B:137:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:LEU:CD2	1:C:838:ASN:HA	2.48	0.43
1:B:764:ASN:O	1:C:830:ARG:HD2	2.17	0.43
1:D:214:PRO:O	2:D:902:ATP:O3B	2.35	0.43
1:E:696:LEU:HD23	1:E:696:LEU:HA	1.76	0.43
1:C:106:GLN:HA	1:D:105:GLN:HE22	1.82	0.43
1:A:186:VAL:HG13	2:A:1001:ATP:N6	2.33	0.43
1:A:765:ARG:HH12	1:B:826:ARG:NH1	1.96	0.43
1:B:261:PHE:CD1	1:B:261:PHE:O	2.72	0.43
1:D:203:ARG:N	1:E:363:HIS:HE1	2.16	0.43
1:D:294:LYS:O	1:D:296:ASP:N	2.50	0.43
1:E:645:GLU:OE2	1:E:654:LYS:NZ	2.51	0.43
1:E:714:LYS:N	1:E:714:LYS:HD2	2.33	0.43
1:F:616:SER:HA	2:F:901:ATP:O2B	2.18	0.43
1:A:218:LYS:HE3	2:A:1001:ATP:O1B	2.19	0.43
1:B:713:GLY:HA2	1:C:670:PHE:CE1	2.46	0.43
1:B:850:LYS:HD2	1:B:850:LYS:HA	1.81	0.43
1:C:202:ARG:NE	1:D:398:ILE:HG12	2.32	0.43
1:E:299:ASN:O	1:E:301:LEU:N	2.51	0.43
1:F:668:GLY:O	1:F:669:GLY:C	2.57	0.43
1:C:599:SER:HG	1:D:845:LEU:HG	1.82	0.43
1:D:764:ASN:CB	1:E:823:MET:HE3	2.48	0.43
1:A:685:PHE:CD1	1:A:685:PHE:N	2.86	0.43
1:D:601:LEU:HD13	1:E:840:LEU:HG	1.98	0.43
1:B:198:ARG:HA	1:C:405:VAL:CG2	2.39	0.43
1:B:205:LYS:HZ2	1:C:394:ASP:CG	2.22	0.43
1:C:222:ILE:HD13	1:C:222:ILE:HA	1.58	0.43
1:C:235:PRO:HB3	1:D:408:ASP:CB	2.42	0.43
1:E:299:ASN:O	1:E:300:ILE:C	2.53	0.43
1:F:302:LYS:HB2	1:F:303:PRO:HD3	2.01	0.43
1:B:27:HIS:ND1	1:B:34:HIS:NE2	2.54	0.43
1:C:106:GLN:C	1:D:105:GLN:NE2	2.72	0.43
1:C:386:ARG:HD3	1:C:390:ASP:CG	2.39	0.43
1:E:53:ASN:C	1:E:53:ASN:OD1	2.57	0.43
1:E:324:ILE:CG1	1:E:325:VAL:H	2.26	0.43
1:E:599:SER:OG	1:F:844:ILE:HG21	2.18	0.43
1:E:662:TYR:HH	1:F:650:TYR:HD1	1.00	0.43
1:E:668:GLY:O	1:E:669:GLY:C	2.55	0.43
1:A:169:LYS:CD	1:F:329:GLY:CA	2.97	0.43
1:A:218:LYS:CE	2:A:1001:ATP:O2B	2.67	0.43
1:C:295:ASP:H	1:D:288:MET:CE	2.32	0.43
1:D:216:ILE:HD12	1:D:341:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ARG:N	1:A:827:PRO:HD2	2.34	0.42
1:E:66:LYS:HB3	1:E:66:LYS:HE2	1.80	0.42
1:E:233:ASP:HA	1:F:410:LYS:CD	2.38	0.42
1:A:583:GLN:CB	2:A:1002:ATP:N6	2.83	0.42
1:A:761:GLU:O	1:A:765:ARG:HG3	2.19	0.42
1:C:246:LEU:N	1:C:246:LEU:CD1	2.82	0.42
1:C:255:ALA:O	1:C:256:LYS:C	2.54	0.42
1:D:772:PHE:N	1:D:772:PHE:CD1	2.85	0.42
1:E:772:PHE:N	1:E:772:PHE:CD1	2.85	0.42
1:F:569:LEU:HD13	1:F:595:ARG:HG3	2.00	0.42
1:B:202:ARG:HA	1:C:401:ALA:CB	2.48	0.42
1:B:599:SER:HB2	1:C:844:ILE:CB	2.49	0.42
1:C:236:THR:HB	1:D:408:ASP:OD2	2.19	0.42
1:D:129:ILE:HG13	1:D:129:ILE:O	2.18	0.42
1:D:764:ASN:C	1:E:830:ARG:HH21	2.16	0.42
1:E:851:ASP:OD2	1:E:852:LYS:NZ	2.44	0.42
1:F:658:THR:HG21	1:F:662:TYR:HB2	2.01	0.42
1:A:253:ALA:HA	1:F:326:GLU:OE1	2.19	0.42
1:A:331:PHE:N	1:A:331:PHE:HD1	2.17	0.42
1:C:332:GLU:CG	1:D:386:ARG:HH21	2.27	0.42
1:D:764:ASN:CG	1:E:823:MET:CG	2.79	0.42
1:E:294:LYS:O	1:E:295:ASP:C	2.57	0.42
1:B:772:PHE:N	1:B:772:PHE:CD1	2.87	0.42
1:D:50:TYR:CD2	1:D:51:LEU:HG	2.54	0.42
1:E:320:GLU:O	1:E:324:ILE:HG12	2.20	0.42
1:F:772:PHE:HD1	1:F:772:PHE:N	2.18	0.42
1:A:619:GLY:CA	2:A:1002:ATP:C4'	2.87	0.42
1:B:599:SER:OG	1:C:841:ALA:HA	2.19	0.42
1:C:662:TYR:CE2	1:D:650:TYR:HD1	2.38	0.42
1:C:764:ASN:O	1:D:830:ARG:CZ	2.67	0.42
1:E:259:GLY:HA3	1:F:252:THR:HB	2.01	0.42
1:E:330:ALA:HB2	2:E:1003:ATP:PG	2.59	0.42
1:B:665:TYR:CD1	1:B:667:GLU:OE2	2.72	0.42
1:C:387:ARG:HA	1:C:387:ARG:HE	1.82	0.42
1:C:849:ILE:O	1:C:849:ILE:HG23	2.20	0.42
1:D:336:GLN:OE1	1:E:553:LEU:HD13	2.20	0.42
1:D:764:ASN:CA	1:E:823:MET:HE3	2.50	0.42
1:A:619:GLY:CA	2:A:1002:ATP:O4'	2.68	0.42
1:B:603:ASN:CA	1:C:794:ARG:HH22	2.28	0.42
1:C:368:LEU:HD12	1:C:368:LEU:N	2.35	0.42
1:C:596:LEU:N	1:D:841:ALA:HB1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LYS:HA	1:D:20:LYS:HD3	1.78	0.42
1:E:230:ILE:HD13	1:E:230:ILE:HA	1.89	0.42
1:F:772:PHE:N	1:F:772:PHE:CD1	2.86	0.42
1:B:570:ILE:HD13	1:C:846:LYS:CG	2.11	0.42
1:D:668:GLY:O	1:D:669:GLY:C	2.58	0.42
1:D:764:ASN:CA	1:E:830:ARG:HH22	2.32	0.42
1:A:764:ASN:OD1	1:A:765:ARG:CG	2.63	0.42
1:C:333:ARG:HD3	1:C:334:ARG:NH1	2.35	0.42
1:C:659:THR:CB	1:D:654:LYS:HG2	2.49	0.42
1:D:126:ILE:HD12	1:D:126:ILE:N	2.35	0.42
1:D:216:ILE:HD12	1:D:342:GLU:HA	2.01	0.42
1:F:617:GLY:O	2:F:901:ATP:C8	2.73	0.42
1:B:236:THR:OG1	1:C:408:ASP:OD2	2.37	0.41
1:B:333:ARG:HH11	1:B:333:ARG:HG3	1.79	0.41
1:B:704:ASP:O	1:B:705:ASP:CB	2.68	0.41
1:C:764:ASN:HD21	1:D:823:MET:HG2	1.85	0.41
1:C:787:ARG:HD2	1:C:787:ARG:HA	1.82	0.41
1:D:333:ARG:HG2	1:D:333:ARG:O	2.20	0.41
1:C:601:LEU:CD1	1:D:840:LEU:C	2.88	0.41
1:F:165:GLU:OE2	1:F:276:LYS:NZ	2.53	0.41
1:F:216:ILE:HA	1:F:216:ILE:HD13	1.86	0.41
1:A:662:TYR:CE1	1:B:650:TYR:CD2	3.09	0.41
1:B:595:ARG:CD	1:C:842:LEU:CG	2.85	0.41
1:D:539:ASN:OD1	1:D:539:ASN:N	2.44	0.41
1:E:203:ARG:N	1:F:363:HIS:CE1	2.74	0.41
2:E:1001:ATP:O2B	2:E:1001:ATP:O2A	2.37	0.41
1:A:198:ARG:HG3	1:B:405:VAL:CB	2.44	0.41
1:A:772:PHE:CD2	2:A:1002:ATP:N1	2.89	0.41
1:C:310:LEU:O	1:C:311:LYS:C	2.56	0.41
2:D:901:ATP:O2B	2:D:901:ATP:O3G	2.37	0.41
1:A:294:LYS:NZ	1:A:328:ASP:OD1	2.48	0.41
1:C:202:ARG:HG2	1:D:401:ALA:HB3	2.02	0.41
1:C:299:ASN:O	1:C:301:LEU:N	2.54	0.41
1:C:336:GLN:C	1:C:336:GLN:OE1	2.59	0.41
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.82	0.41
1:E:255:ALA:O	1:E:256:LYS:C	2.58	0.41
1:E:665:TYR:O	1:E:667:GLU:N	2.54	0.41
1:B:205:LYS:NZ	1:B:333:ARG:HE	2.19	0.41
1:C:821:ASP:N	1:C:821:ASP:OD1	2.51	0.41
1:D:629:GLY:O	1:D:633:ASN:N	2.53	0.41
1:E:237:ILE:HG13	1:F:408:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ARG:HG3	1:F:386:ARG:HH22	1.85	0.41
1:B:249:ALA:O	1:B:250:ALA:C	2.59	0.41
1:B:570:ILE:HD11	1:C:846:LYS:CB	2.51	0.41
1:B:592:ASN:HB3	1:C:838:ASN:CG	2.41	0.41
1:B:595:ARG:HG2	1:C:845:LEU:CD1	2.40	0.41
1:C:835:GLU:OE1	1:C:835:GLU:HA	2.20	0.41
1:D:270:LYS:NZ	1:D:274:GLU:OE1	2.54	0.41
1:B:205:LYS:NZ	1:B:333:ARG:CZ	2.82	0.41
1:B:330:ALA:O	1:B:334:ARG:HD2	2.15	0.41
1:B:599:SER:HB2	1:C:844:ILE:HB	2.02	0.41
1:C:665:TYR:HD1	1:C:665:TYR:HA	1.78	0.41
1:A:382:TYR:CD2	1:A:383:LEU:HG	2.56	0.41
1:B:596:LEU:CD2	1:C:837:LEU:HB3	2.48	0.41
1:B:601:LEU:HG	1:C:844:ILE:CD1	2.51	0.41
1:C:203:ARG:CA	1:D:363:HIS:CE1	3.04	0.41
1:E:237:ILE:HD12	1:F:405:VAL:HA	2.03	0.41
1:E:284:ASP:O	1:E:285:GLU:C	2.60	0.41
1:E:393:LEU:HD23	1:E:393:LEU:HA	1.92	0.41
1:A:563:GLU:OE1	1:A:563:GLU:N	2.27	0.40
1:D:322:ARG:CA	1:E:677:TYR:OH	2.69	0.40
1:E:309:GLN:O	1:E:310:LEU:C	2.59	0.40
1:F:555:GLY:O	1:F:556:ILE:CB	2.69	0.40
1:B:203:ARG:HD3	1:C:362:HIS:CD2	2.56	0.40
1:B:324:ILE:HG21	1:B:324:ILE:HD13	1.89	0.40
1:E:89:SER:OG	1:E:90:TYR:N	2.53	0.40
1:A:568:LYS:HD3	1:A:568:LYS:HA	1.91	0.40
1:B:568:LYS:O	1:B:572:MET:N	2.54	0.40
1:B:648:GLU:HB3	1:B:692:HIS:HB3	2.04	0.40
1:D:880:LEU:CB	1:D:881:PRO:HD2	2.52	0.40
1:E:249:ALA:O	1:E:250:ALA:C	2.59	0.40
1:E:595:ARG:HD3	1:F:845:LEU:CB	2.51	0.40
2:A:1001:ATP:N3	2:A:1001:ATP:H3'	2.35	0.40
1:B:201:ALA:CB	1:C:405:VAL:CG2	2.99	0.40
1:B:665:TYR:HA	1:B:667:GLU:OE2	2.22	0.40
1:B:764:ASN:HD21	1:C:823:MET:HG2	1.86	0.40
1:D:305:LEU:HD13	1:D:334:ARG:HG2	2.03	0.40
1:D:542:ASP:C	1:D:542:ASP:OD1	2.59	0.40
1:D:568:LYS:O	1:D:572:MET:N	2.54	0.40
1:A:261:PHE:CD1	1:A:261:PHE:C	2.93	0.40
1:B:165:GLU:OE2	1:B:276:LYS:NZ	2.51	0.40
1:B:559:LYS:HD3	1:B:559:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LYS:O	1:D:257:TYR:HB2	2.22	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 PDB entries followed by that with respect to all EM entries.

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	573/879 (65%)	530 (92%)	31 (5%)	12 (2%)	7 36
1	B	715/879 (81%)	675 (94%)	33 (5%)	7 (1%)	15 55
1	C	715/879 (81%)	680 (95%)	31 (4%)	4 (1%)	25 66
1	D	715/879 (81%)	672 (94%)	35 (5%)	8 (1%)	14 52
1	E	715/879 (81%)	677 (95%)	32 (4%)	6 (1%)	19 60
1	F	573/879 (65%)	529 (92%)	29 (5%)	15 (3%)	5 31
All	All	4006/5274 (76%)	3763 (94%)	191 (5%)	52 (1%)	16 48

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	MET
1	B	295	ASP
1	B	666	ASP
1	C	295	ASP
1	C	705	ASP
1	D	28	PRO
1	D	85	GLU
1	E	81	PRO
1	E	324	ILE
1	E	667	GLU
1	F	247	ASP

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Mol	Chain	Res	Type
1	F	666	ASP
1	F	853	GLU
1	A	277	THR
1	A	561	LEU
1	A	706	GLY
1	A	819	TYR
1	B	274	GLU
1	B	277	THR
1	C	274	GLU
1	D	277	THR
1	D	717	ASP
1	D	880	LEU
1	E	274	GLU
1	F	277	THR
1	F	669	GLY
1	F	796	GLU
1	F	878	GLU
1	A	801	HIS
1	D	705	ASP
1	F	255	ALA
1	F	257	TYR
1	F	309	GLN
1	A	666	ASP
1	A	877	LEU
1	A	878	GLU
1	D	166	TYR
1	F	556	ILE
1	F	663	VAL
1	A	298	ALA
1	A	556	ILE
1	B	665	TYR
1	E	880	LEU
1	F	879	VAL
1	A	879	VAL
1	B	705	ASP
1	D	89	SER
1	F	295	ASP
1	C	556	ILE
1	E	302	LYS
1	F	216	ILE
1	B	86	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	494/758 (65%)	491 (99%)	3 (1%)	86 92
1	B	615/758 (81%)	610 (99%)	5 (1%)	81 89
1	C	620/758 (82%)	615 (99%)	5 (1%)	81 89
1	D	619/758 (82%)	615 (99%)	4 (1%)	86 92
1	E	618/758 (82%)	614 (99%)	4 (1%)	86 92
1	F	492/758 (65%)	489 (99%)	3 (1%)	86 92
All	All	3458/4548 (76%)	3434 (99%)	24 (1%)	84 90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ARG
1	A	665	TYR
1	A	765	ARG
1	B	333	ARG
1	B	334	ARG
1	B	659	THR
1	B	665	TYR
1	B	765	ARG
1	C	256	LYS
1	C	333	ARG
1	C	659	THR
1	C	665	TYR
1	C	765	ARG
1	D	216	ILE
1	D	334	ARG
1	D	659	THR
1	D	826	ARG
1	E	334	ARG
1	E	665	TYR
1	E	666	ASP
1	E	765	ARG
1	F	333	ARG

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Mol	Chain	Res	Type
1	F	568	LYS
1	F	665	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	C	362	HIS
1	C	833	GLN
1	D	105	GLN
1	D	106	GLN
1	D	362	HIS
1	D	363	HIS
1	D	712	GLN
1	E	128	GLN
1	E	712	GLN
1	F	363	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands 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	$\#\|Z\| > 2$
2	ATP	C	1001	-	26,33,33	3.47	4 (15%)	31,52,52	2.81	7 (22%)
2	ATP	E	1001	-	26,33,33	3.60	5 (19%)	31,52,52	2.33	8 (25%)
2	ATP	E	1002	-	26,33,33	3.47	6 (23%)	31,52,52	2.66	8 (25%)
2	ATP	B	1002	-	26,33,33	3.53	5 (19%)	31,52,52	2.55	11 (35%)
2	ATP	F	901	-	26,33,33	3.52	4 (15%)	31,52,52	2.69	9 (29%)
2	ATP	A	1001	-	26,33,33	3.59	2 (7%)	31,52,52	2.18	7 (22%)
2	ATP	C	1002	-	26,33,33	3.51	5 (19%)	31,52,52	2.54	12 (38%)
2	ATP	D	902	-	26,33,33	3.51	3 (11%)	31,52,52	2.44	10 (32%)
2	ATP	D	901	-	26,33,33	3.48	5 (19%)	31,52,52	2.66	8 (25%)
2	ATP	A	1002	-	26,33,33	3.66	5 (19%)	31,52,52	2.08	8 (25%)
2	ATP	B	1001	-	26,33,33	3.56	3 (11%)	31,52,52	2.36	8 (25%)
2	ATP	E	1003	-	26,33,33	3.54	3 (11%)	31,52,52	2.43	8 (25%)

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
2	ATP	C	1001	-	-	2/18/38/38	0/3/3/3
2	ATP	E	1001	-	-	7/18/38/38	0/3/3/3
2	ATP	E	1002	-	-	5/18/38/38	0/3/3/3
2	ATP	B	1002	-	-	2/18/38/38	0/3/3/3
2	ATP	F	901	-	-	3/18/38/38	0/3/3/3
2	ATP	A	1001	-	-	6/18/38/38	0/3/3/3
2	ATP	C	1002	-	-	2/18/38/38	0/3/3/3
2	ATP	D	902	-	-	6/18/38/38	0/3/3/3
2	ATP	D	901	-	-	5/18/38/38	0/3/3/3
2	ATP	A	1002	-	-	5/18/38/38	0/3/3/3
2	ATP	B	1001	-	-	9/18/38/38	0/3/3/3
2	ATP	E	1003	-	-	6/18/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ATP	PG-O1G	17.44	2.06	1.50
2	A	1002	ATP	PG-O1G	17.43	2.06	1.50
2	E	1001	ATP	PG-O1G	17.31	2.06	1.50
2	B	1001	ATP	PG-O1G	17.15	2.05	1.50
2	E	1003	ATP	PG-O1G	17.04	2.05	1.50
2	D	902	ATP	PG-O1G	16.91	2.05	1.50
2	F	901	ATP	PG-O1G	16.88	2.05	1.50
2	B	1002	ATP	PG-O1G	16.77	2.04	1.50
2	C	1002	ATP	PG-O1G	16.72	2.04	1.50
2	C	1001	ATP	PG-O1G	16.61	2.04	1.50
2	D	901	ATP	PG-O1G	16.51	2.03	1.50
2	E	1002	ATP	PG-O1G	16.44	2.03	1.50
2	A	1002	ATP	O4'-C1'	3.31	1.45	1.41
2	B	1001	ATP	C2'-C1'	-3.00	1.49	1.53
2	E	1002	ATP	C2'-C1'	-2.91	1.49	1.53
2	D	901	ATP	C2'-C1'	-2.82	1.49	1.53
2	C	1001	ATP	C2'-C1'	-2.74	1.49	1.53
2	B	1002	ATP	C2'-C1'	-2.71	1.49	1.53
2	A	1002	ATP	C5-C4	2.70	1.48	1.40
2	C	1002	ATP	C2'-C1'	-2.67	1.49	1.53
2	F	901	ATP	C5-C4	2.47	1.47	1.40
2	C	1002	ATP	C5-C4	2.46	1.47	1.40
2	E	1001	ATP	C2'-C1'	-2.44	1.50	1.53
2	A	1001	ATP	C5-C4	2.42	1.47	1.40
2	E	1003	ATP	C2'-C1'	-2.41	1.50	1.53
2	D	901	ATP	C5-N7	-2.39	1.31	1.39
2	B	1002	ATP	C5-C4	2.38	1.47	1.40
2	C	1002	ATP	C5-N7	-2.34	1.31	1.39
2	E	1002	ATP	C5-N7	-2.33	1.31	1.39
2	E	1002	ATP	C5-C4	2.33	1.47	1.40
2	B	1002	ATP	C5-N7	-2.30	1.31	1.39
2	A	1002	ATP	C2'-C1'	-2.29	1.50	1.53
2	E	1003	ATP	C5-C4	2.28	1.47	1.40
2	D	901	ATP	C5-C4	2.26	1.46	1.40
2	E	1001	ATP	C5-C4	2.22	1.46	1.40
2	B	1002	ATP	O4'-C1'	2.22	1.44	1.41
2	C	1002	ATP	O4'-C1'	2.19	1.44	1.41
2	D	902	ATP	C2'-C1'	-2.13	1.50	1.53
2	E	1002	ATP	O4'-C1'	2.12	1.44	1.41
2	C	1001	ATP	C4-N3	-2.10	1.32	1.35
2	A	1002	ATP	C2-N3	2.08	1.35	1.32
2	F	901	ATP	C5-N7	-2.07	1.32	1.39
2	D	901	ATP	O4'-C1'	2.07	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	ATP	C5-C4	2.06	1.46	1.40
2	F	901	ATP	C2'-C1'	-2.03	1.50	1.53
2	B	1001	ATP	PG-O3G	-2.02	1.47	1.54
2	E	1001	ATP	C4-N3	-2.01	1.32	1.35
2	E	1001	ATP	PG-O3G	-2.01	1.47	1.54
2	E	1002	ATP	PG-O3G	-2.01	1.47	1.54
2	C	1001	ATP	PG-O3G	-2.01	1.47	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	ATP	PA-O3A-PB	-10.47	96.90	132.83
2	F	901	ATP	PA-O3A-PB	-8.84	102.50	132.83
2	D	901	ATP	PB-O3B-PG	-8.54	103.51	132.83
2	E	1002	ATP	PB-O3B-PG	-8.54	103.53	132.83
2	C	1001	ATP	PB-O3B-PG	-8.36	104.13	132.83
2	D	902	ATP	PA-O3A-PB	-8.22	104.60	132.83
2	F	901	ATP	PB-O3B-PG	-7.93	105.63	132.83
2	B	1002	ATP	PB-O3B-PG	-7.93	105.63	132.83
2	C	1002	ATP	PB-O3B-PG	-7.92	105.66	132.83
2	D	901	ATP	PA-O3A-PB	-7.83	105.97	132.83
2	E	1002	ATP	PA-O3A-PB	-7.82	105.98	132.83
2	E	1003	ATP	PB-O3B-PG	-7.76	106.21	132.83
2	B	1001	ATP	PA-O3A-PB	-7.38	107.50	132.83
2	E	1003	ATP	PA-O3A-PB	-7.27	107.86	132.83
2	B	1002	ATP	PA-O3A-PB	-7.27	107.87	132.83
2	C	1002	ATP	PA-O3A-PB	-7.27	107.88	132.83
2	E	1001	ATP	PB-O3B-PG	-7.05	108.63	132.83
2	A	1001	ATP	PA-O3A-PB	-6.92	109.09	132.83
2	B	1001	ATP	PB-O3B-PG	-6.89	109.17	132.83
2	E	1001	ATP	PA-O3A-PB	-6.61	110.14	132.83
2	D	902	ATP	PB-O3B-PG	-6.20	111.55	132.83
2	A	1001	ATP	PB-O3B-PG	-5.93	112.49	132.83
2	A	1002	ATP	PB-O3B-PG	-5.53	113.85	132.83
2	A	1002	ATP	PA-O3A-PB	-5.27	114.74	132.83
2	E	1002	ATP	N6-C6-N1	3.84	126.55	118.57
2	D	901	ATP	N6-C6-N1	3.84	126.55	118.57
2	D	902	ATP	O3B-PG-O1G	-3.31	92.85	111.19
2	D	901	ATP	O2G-PG-O3B	3.27	115.60	104.64
2	E	1002	ATP	O2G-PG-O3B	3.26	115.58	104.64
2	B	1002	ATP	N6-C6-N1	3.24	125.30	118.57
2	C	1002	ATP	N6-C6-N1	3.22	125.27	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	ATP	N6-C6-N1	3.17	125.16	118.57
2	E	1001	ATP	O3B-PG-O1G	-3.11	93.94	111.19
2	C	1001	ATP	N6-C6-N1	3.08	124.97	118.57
2	E	1003	ATP	O3B-PG-O1G	-3.08	94.12	111.19
2	E	1001	ATP	O2G-PG-O3B	3.04	114.82	104.64
2	F	901	ATP	O3B-PG-O1G	-3.02	94.44	111.19
2	A	1002	ATP	O2G-PG-O3B	2.98	114.62	104.64
2	F	901	ATP	O2G-PG-O3B	2.97	114.60	104.64
2	D	901	ATP	O3B-PG-O1G	-2.97	94.73	111.19
2	B	1001	ATP	O3B-PG-O1G	-2.97	94.74	111.19
2	E	1002	ATP	O3B-PG-O1G	-2.96	94.78	111.19
2	C	1002	ATP	O2G-PG-O3B	2.93	114.46	104.64
2	B	1002	ATP	O2G-PG-O3B	2.90	114.37	104.64
2	F	901	ATP	N6-C6-N1	2.90	124.59	118.57
2	E	1001	ATP	N6-C6-N1	2.88	124.56	118.57
2	D	902	ATP	N6-C6-N1	2.86	124.50	118.57
2	B	1002	ATP	O3B-PG-O1G	-2.85	95.37	111.19
2	C	1002	ATP	O3B-PG-O1G	-2.84	95.41	111.19
2	C	1001	ATP	O2G-PG-O3B	2.84	114.17	104.64
2	F	901	ATP	C3'-C2'-C1'	2.82	105.22	100.98
2	D	902	ATP	O2G-PG-O3B	2.81	114.07	104.64
2	B	1001	ATP	N6-C6-N1	2.81	124.41	118.57
2	E	1003	ATP	O2G-PG-O3B	2.80	114.03	104.64
2	E	1003	ATP	O2B-PB-O1B	2.79	126.02	112.24
2	A	1001	ATP	O3B-PG-O1G	-2.78	95.75	111.19
2	A	1001	ATP	O2G-PG-O3B	2.74	113.84	104.64
2	A	1001	ATP	O5'-C5'-C4'	-2.74	99.55	108.99
2	F	901	ATP	O2B-PB-O1B	2.74	125.79	112.24
2	B	1001	ATP	N3-C2-N1	-2.72	124.43	128.68
2	D	901	ATP	O2B-PB-O1B	2.71	125.63	112.24
2	E	1002	ATP	O2B-PB-O1B	2.69	125.53	112.24
2	B	1001	ATP	O2G-PG-O3B	2.68	113.61	104.64
2	A	1002	ATP	C5'-C4'-C3'	-2.64	105.28	115.18
2	A	1001	ATP	N3-C2-N1	-2.63	124.56	128.68
2	D	902	ATP	O2B-PB-O1B	2.53	124.76	112.24
2	C	1001	ATP	O3B-PG-O1G	-2.51	97.27	111.19
2	C	1002	ATP	C2'-C3'-C4'	2.50	107.51	102.64
2	B	1002	ATP	C2'-C3'-C4'	2.50	107.49	102.64
2	A	1002	ATP	O4'-C4'-C5'	2.49	117.57	109.37
2	B	1001	ATP	O2B-PB-O1B	2.45	124.37	112.24
2	D	902	ATP	C5'-C4'-C3'	-2.45	106.01	115.18
2	E	1003	ATP	N3-C2-N1	-2.42	124.89	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	ATP	O3B-PG-O1G	-2.39	97.91	111.19
2	E	1003	ATP	N6-C6-N1	2.39	123.53	118.57
2	E	1003	ATP	C4-C5-N7	-2.39	106.91	109.40
2	E	1002	ATP	N3-C2-N1	-2.39	124.95	128.68
2	D	901	ATP	N3-C2-N1	-2.36	124.98	128.68
2	B	1002	ATP	O5'-C5'-C4'	-2.36	100.86	108.99
2	C	1002	ATP	O5'-C5'-C4'	-2.35	100.91	108.99
2	A	1002	ATP	N3-C2-N1	-2.33	125.03	128.68
2	F	901	ATP	N3-C2-N1	-2.33	125.04	128.68
2	A	1001	ATP	N6-C6-N1	2.31	123.38	118.57
2	B	1002	ATP	N3-C2-N1	-2.29	125.10	128.68
2	C	1001	ATP	N3-C2-N1	-2.28	125.12	128.68
2	C	1002	ATP	N3-C2-N1	-2.26	125.15	128.68
2	E	1001	ATP	C5'-C4'-C3'	-2.21	106.89	115.18
2	D	902	ATP	N3-C2-N1	-2.20	125.24	128.68
2	E	1001	ATP	O2A-PA-O1A	2.20	123.10	112.24
2	B	1002	ATP	C3'-C2'-C1'	2.19	104.27	100.98
2	C	1002	ATP	C3'-C2'-C1'	2.17	104.24	100.98
2	C	1001	ATP	O5'-C5'-C4'	-2.16	101.56	108.99
2	F	901	ATP	C5'-C4'-C3'	-2.15	107.12	115.18
2	D	901	ATP	C5-C6-N6	-2.07	117.20	120.35
2	B	1002	ATP	C5-C6-N1	-2.04	115.72	120.35
2	B	1001	ATP	O2A-PA-O1A	2.04	122.32	112.24
2	B	1002	ATP	O2B-PB-O1B	2.04	122.31	112.24
2	C	1002	ATP	O2B-PB-O1B	2.03	122.29	112.24
2	D	902	ATP	C4-C5-N7	-2.03	107.29	109.40
2	E	1001	ATP	C4-C5-N7	-2.02	107.30	109.40
2	C	1002	ATP	C5-C6-N1	-2.01	115.78	120.35
2	E	1002	ATP	C5-C6-N6	-2.01	117.29	120.35
2	D	902	ATP	O5'-C5'-C4'	-2.01	102.06	108.99
2	C	1002	ATP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C5'-O5'-PA-O2A
2	A	1001	ATP	C5'-O5'-PA-O3A
2	A	1001	ATP	O4'-C4'-C5'-O5'
2	A	1001	ATP	C3'-C4'-C5'-O5'
2	A	1002	ATP	C5'-O5'-PA-O3A
2	B	1001	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	1001	ATP	C5'-O5'-PA-O2A
2	B	1002	ATP	O4'-C4'-C5'-O5'
2	B	1002	ATP	C3'-C4'-C5'-O5'
2	C	1002	ATP	O4'-C4'-C5'-O5'
2	C	1002	ATP	C3'-C4'-C5'-O5'
2	D	901	ATP	C5'-O5'-PA-O3A
2	D	902	ATP	C5'-O5'-PA-O3A
2	E	1001	ATP	PB-O3B-PG-O2G
2	E	1001	ATP	C5'-O5'-PA-O1A
2	E	1002	ATP	C5'-O5'-PA-O3A
2	E	1003	ATP	C5'-O5'-PA-O3A
2	E	1003	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	O4'-C4'-C5'-O5'
2	C	1001	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	C3'-C4'-C5'-O5'
2	E	1003	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	C3'-C4'-C5'-O5'
2	D	902	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	PB-O3B-PG-O1G
2	C	1001	ATP	C3'-C4'-C5'-O5'
2	A	1001	ATP	C4'-C5'-O5'-PA
2	E	1001	ATP	C4'-C5'-O5'-PA
2	B	1001	ATP	PB-O3B-PG-O2G
2	A	1002	ATP	PA-O3A-PB-O1B
2	D	901	ATP	PA-O3A-PB-O1B
2	E	1002	ATP	PA-O3A-PB-O1B
2	E	1003	ATP	PA-O3A-PB-O1B
2	F	901	ATP	PA-O3A-PB-O1B
2	A	1001	ATP	C5'-O5'-PA-O1A
2	A	1002	ATP	C5'-O5'-PA-O1A
2	D	901	ATP	C5'-O5'-PA-O2A
2	D	902	ATP	C5'-O5'-PA-O2A
2	E	1002	ATP	C5'-O5'-PA-O2A
2	E	1003	ATP	C5'-O5'-PA-O1A
2	D	902	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	PB-O3A-PA-O2A
2	D	901	ATP	C4'-C5'-O5'-PA
2	E	1002	ATP	C4'-C5'-O5'-PA
2	B	1001	ATP	C4'-C5'-O5'-PA
2	F	901	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	A	1002	ATP	PA-O3A-PB-O2B
2	A	1002	ATP	PB-O3A-PA-O1A
2	B	1001	ATP	PB-O3A-PA-O2A
2	D	901	ATP	PG-O3B-PB-O2B
2	D	902	ATP	PG-O3B-PB-O1B
2	D	902	ATP	PG-O3B-PB-O2B
2	E	1002	ATP	PG-O3B-PB-O2B
2	E	1003	ATP	C4'-C5'-O5'-PA
2	F	901	ATP	O4'-C4'-C5'-O5'
2	E	1001	ATP	PB-O3B-PG-O1G

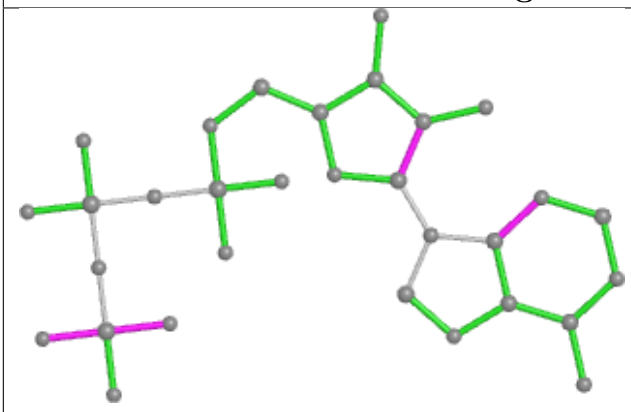
There are no ring outliers.

12 monomers are involved in 147 short contacts:

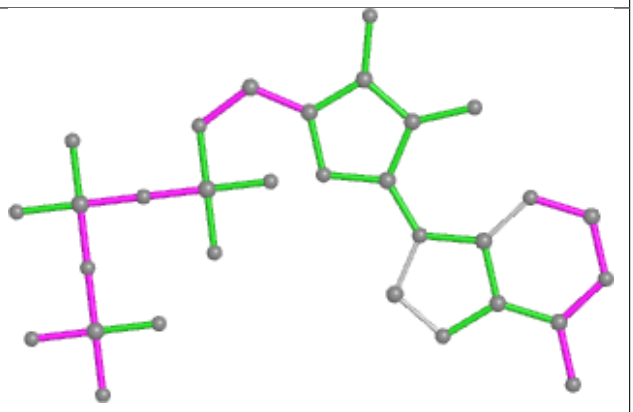
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	ATP	2	0
2	E	1001	ATP	6	0
2	E	1002	ATP	5	0
2	B	1002	ATP	2	0
2	F	901	ATP	7	0
2	A	1001	ATP	33	0
2	C	1002	ATP	6	0
2	D	902	ATP	4	0
2	D	901	ATP	12	0
2	A	1002	ATP	39	0
2	B	1001	ATP	4	0
2	E	1003	ATP	27	0

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 then 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.

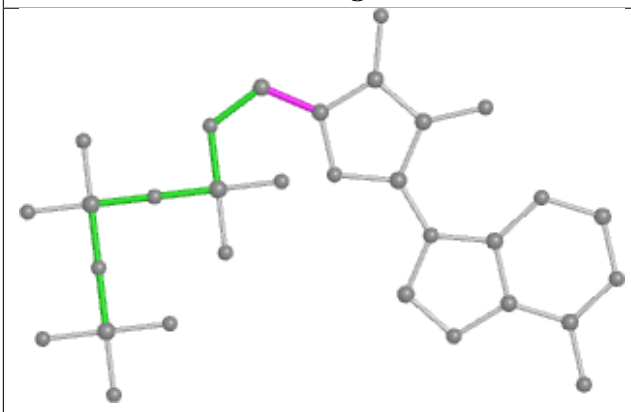
Ligand ATP C 1001



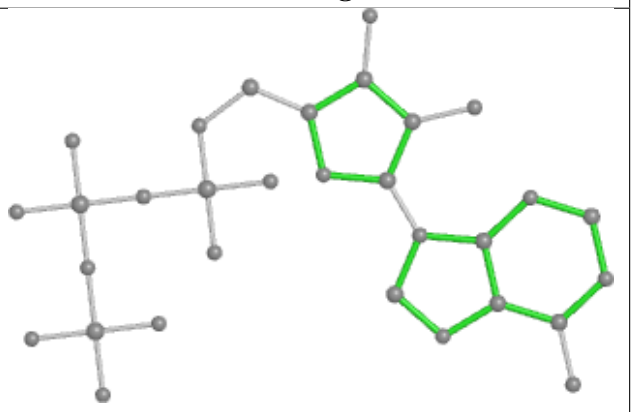
Bond lengths



Bond angles

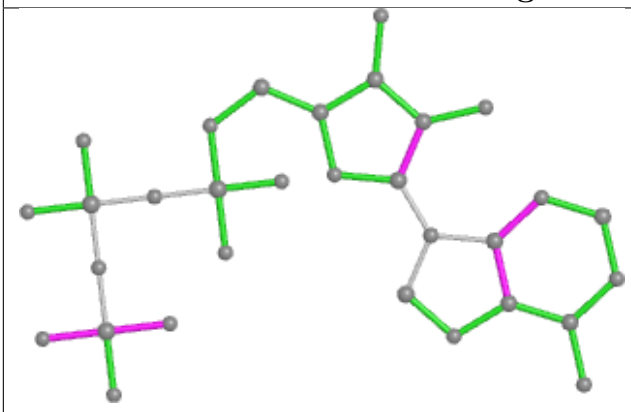


Torsions

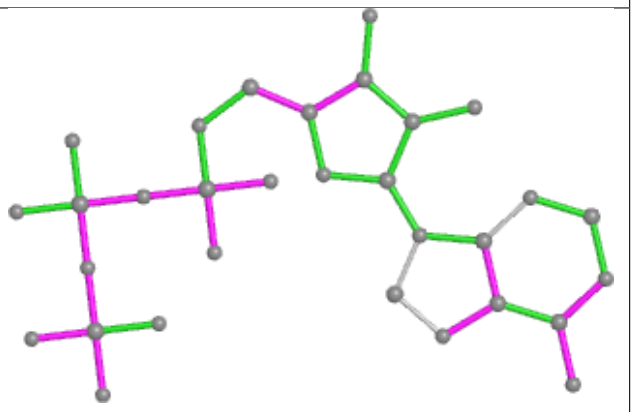


Rings

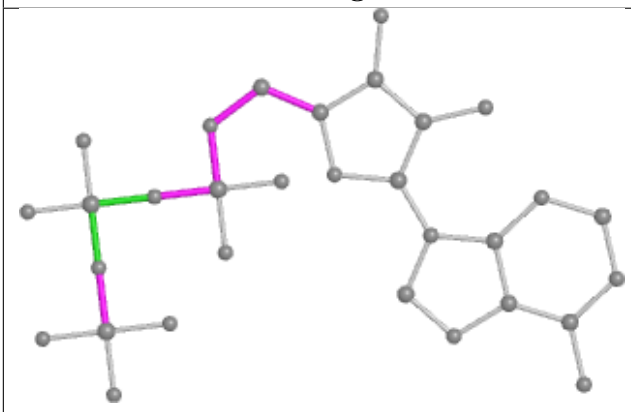
Ligand ATP E 1001



Bond lengths



Bond angles



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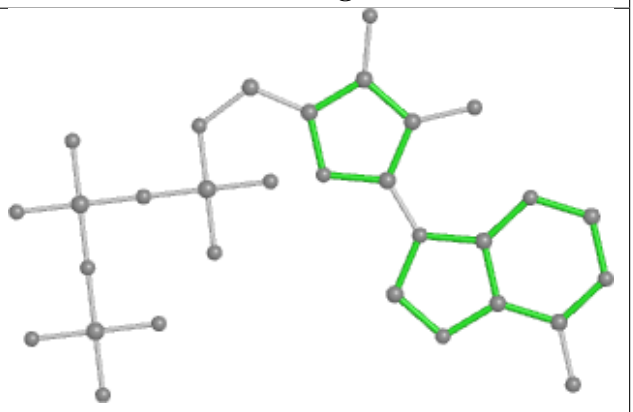
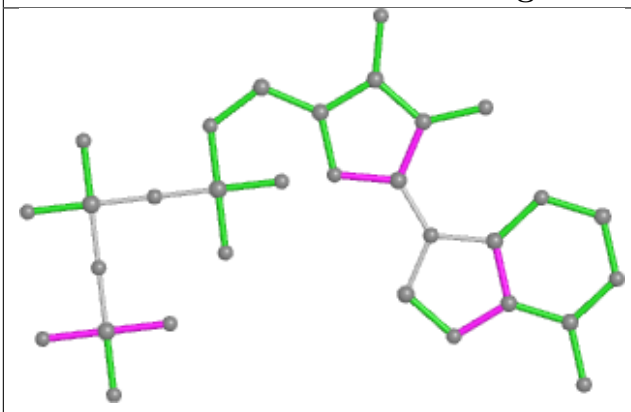
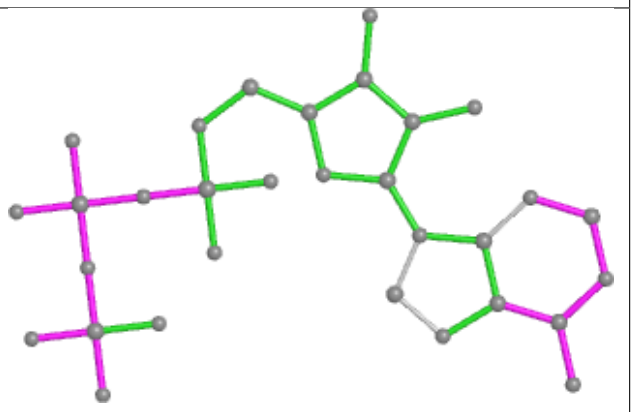


Rings

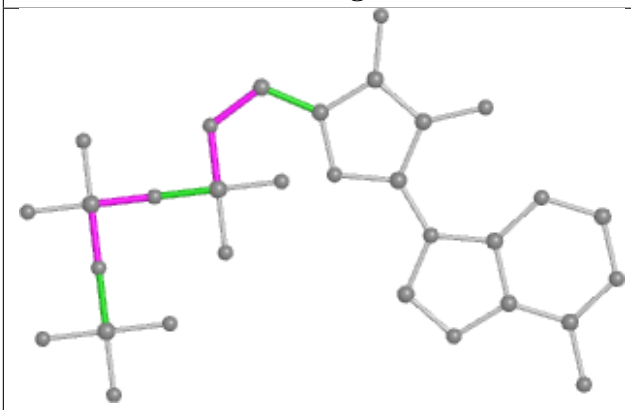
Ligand ATP E 1002



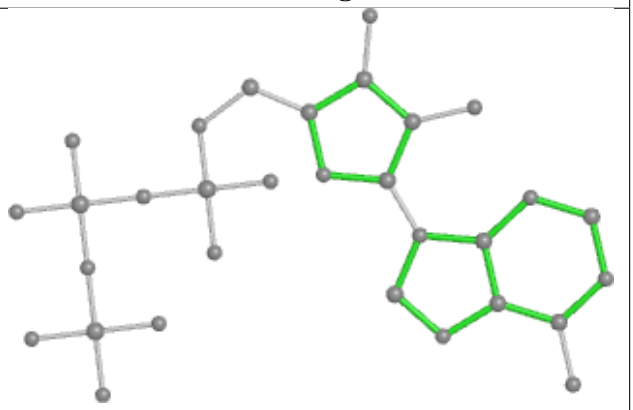
Bond lengths



Bond angles

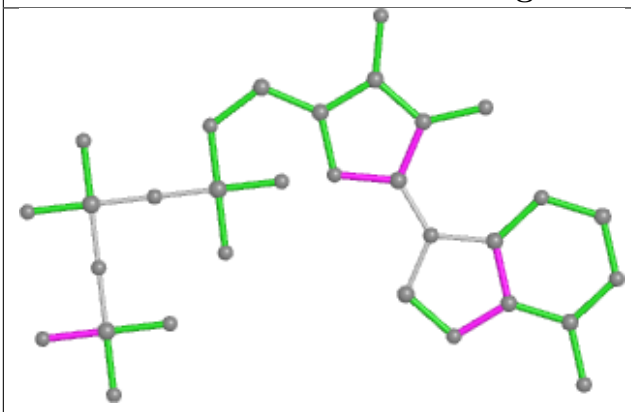


Torsions

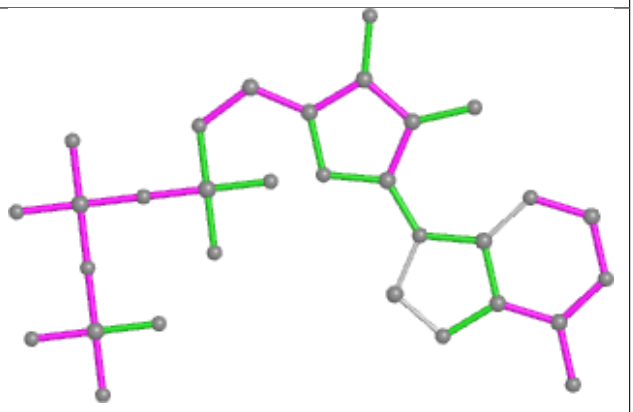


Rings

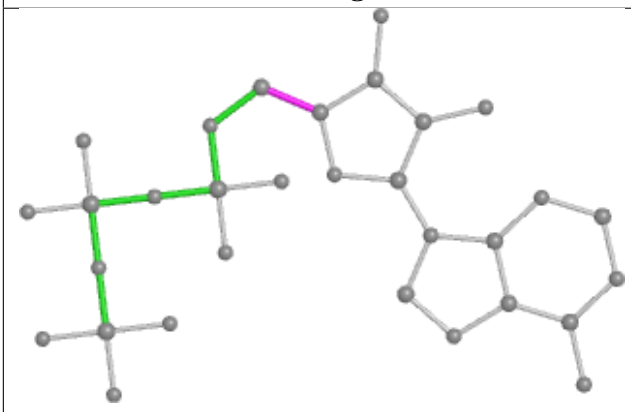
Ligand ATP B 1002



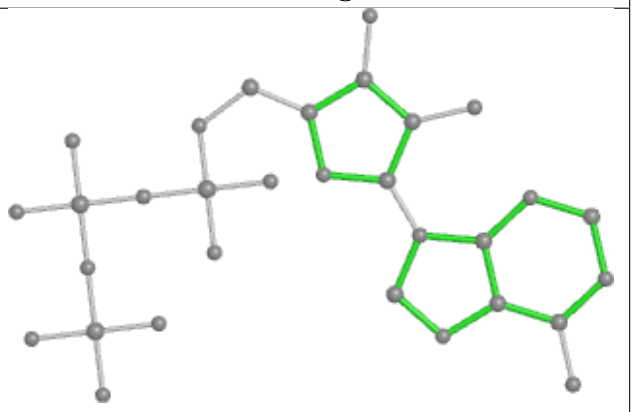
Bond lengths



Bond angles

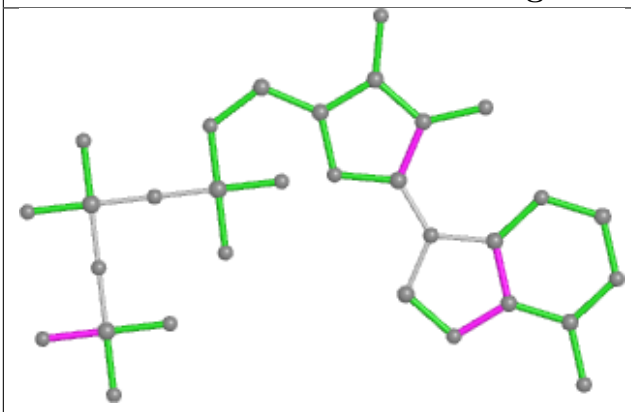


Torsions

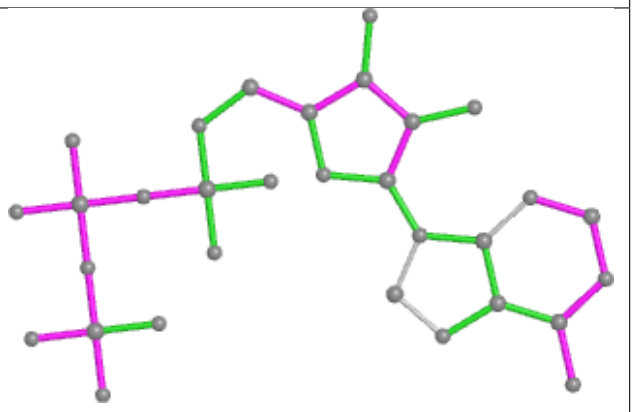


Rings

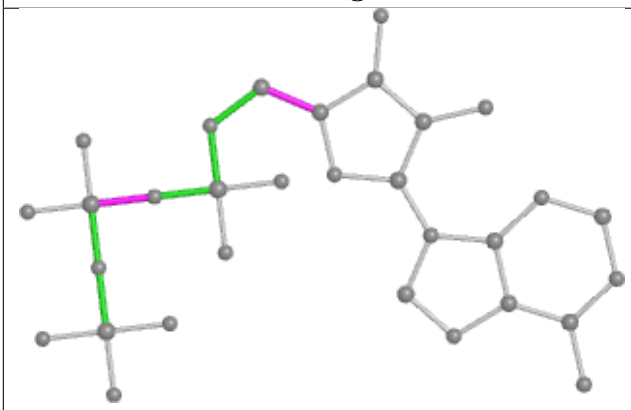
Ligand ATP F 901



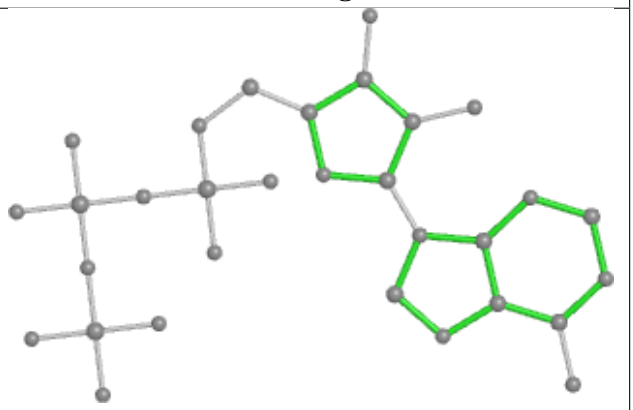
Bond lengths



Bond angles

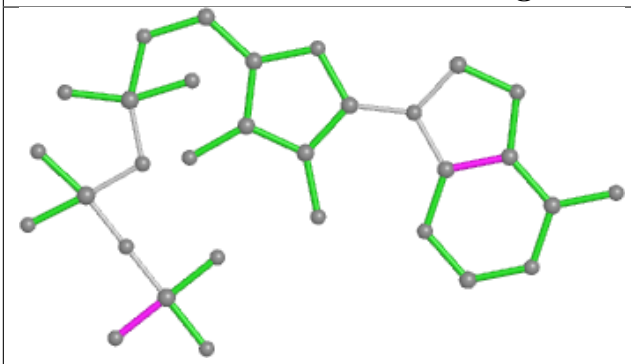


Torsions

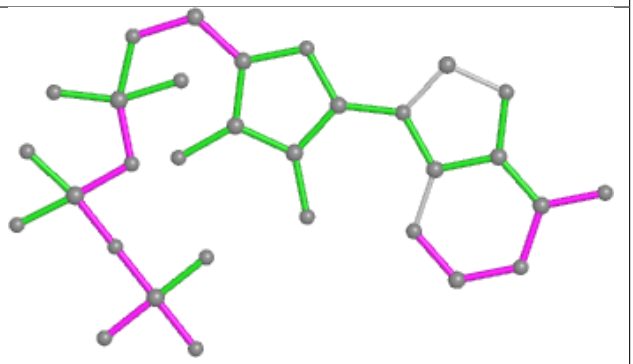


Rings

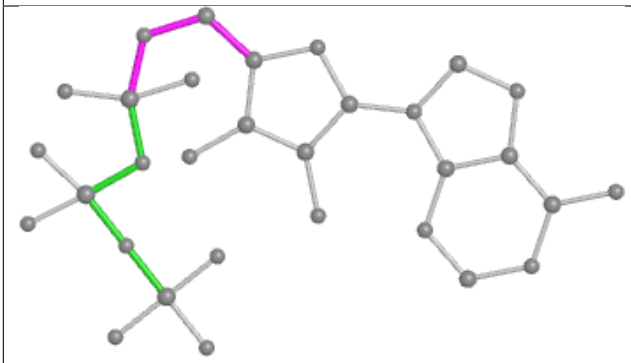
Ligand ATP A 1001



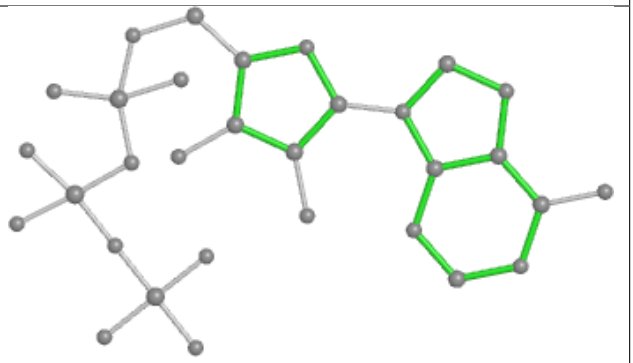
Bond lengths



Bond angles

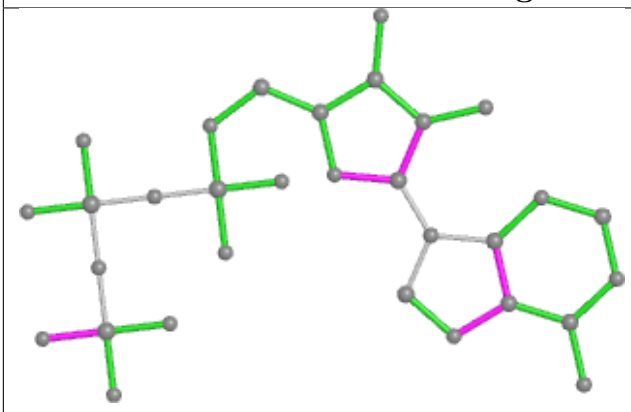


Torsions

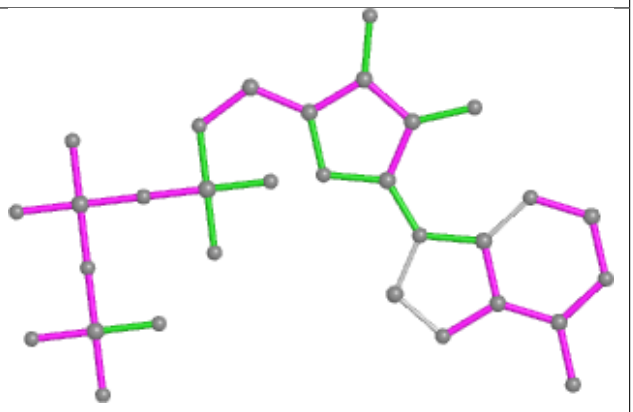


Rings

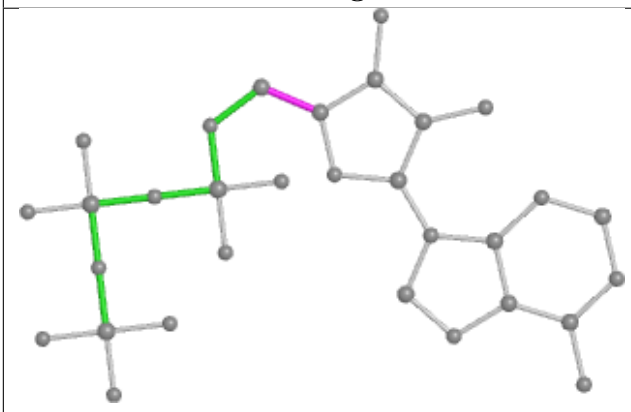
Ligand ATP C 1002



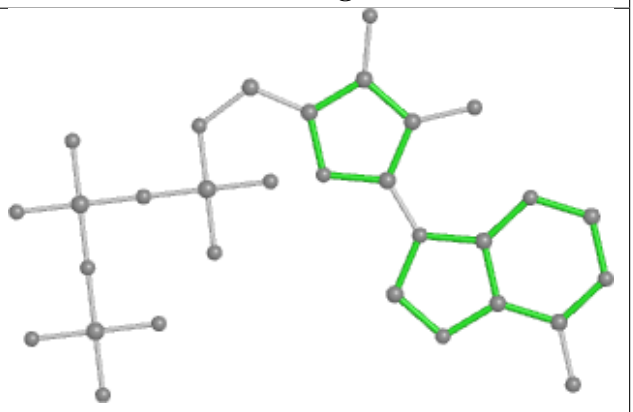
Bond lengths



Bond angles

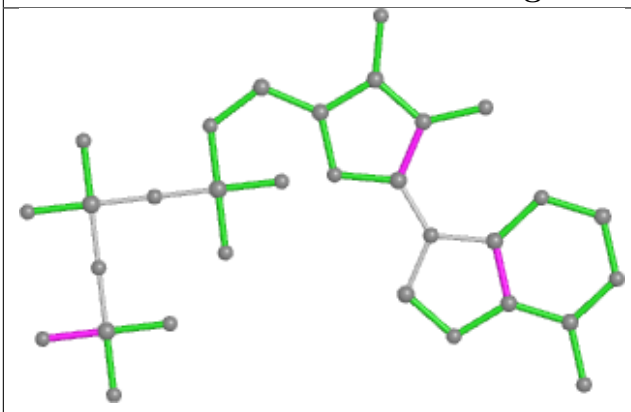


Torsions

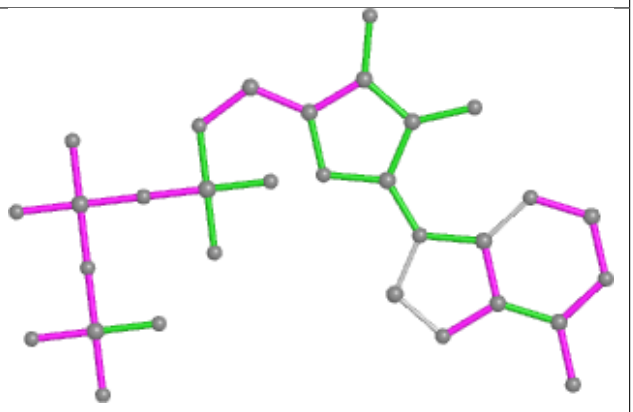


Rings

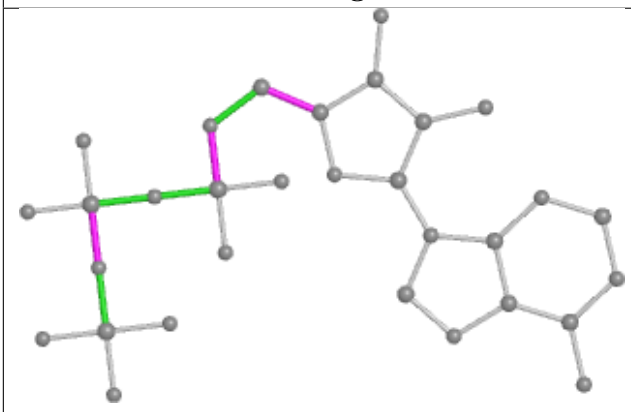
Ligand ATP D 902



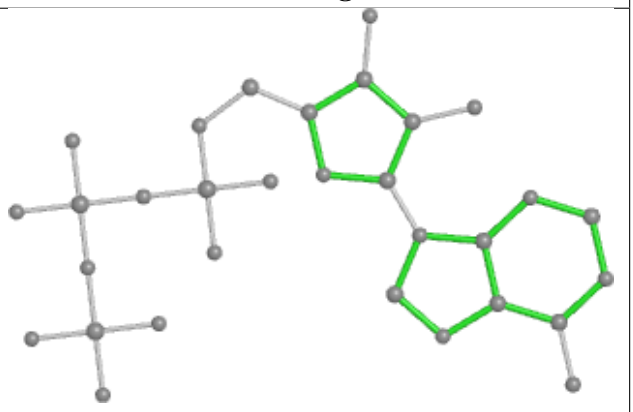
Bond lengths



Bond angles

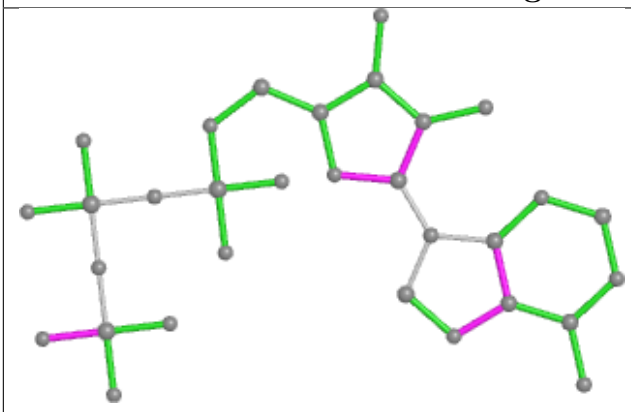


Torsions

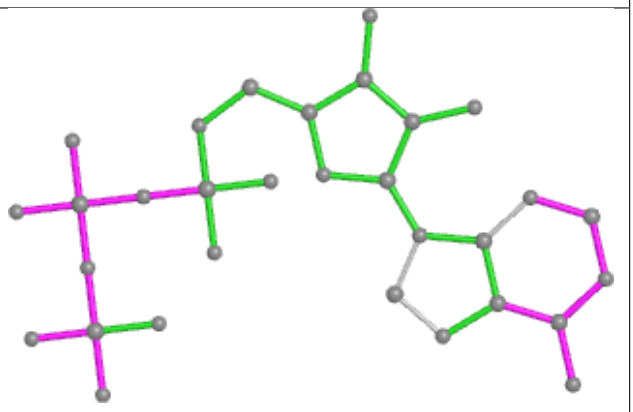


Rings

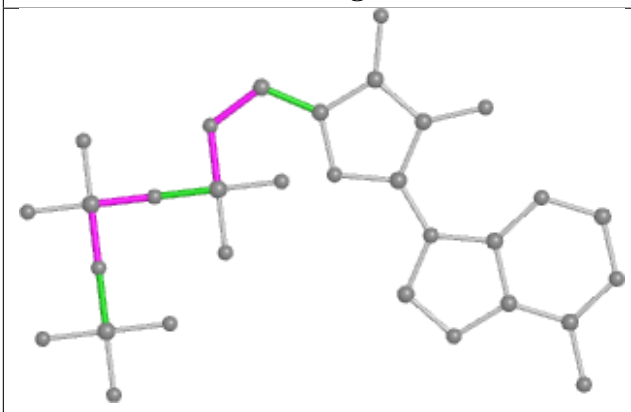
Ligand ATP D 901



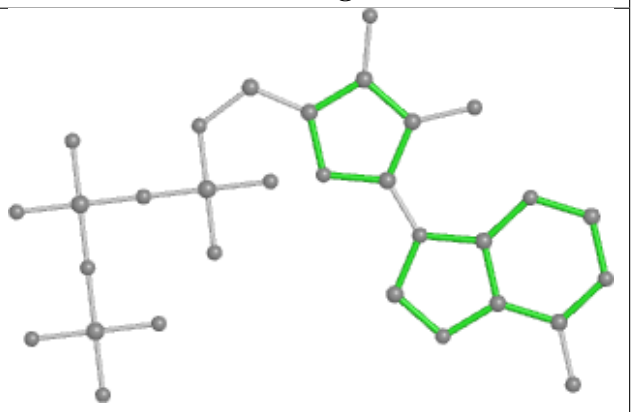
Bond lengths



Bond angles

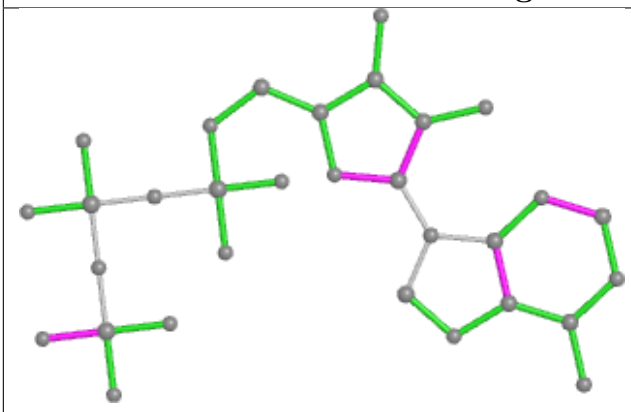


Torsions

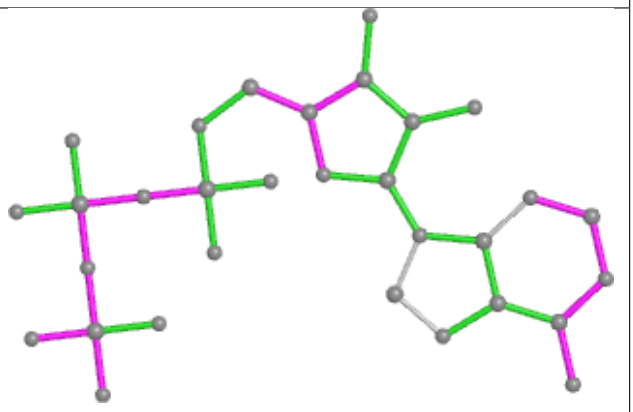


Rings

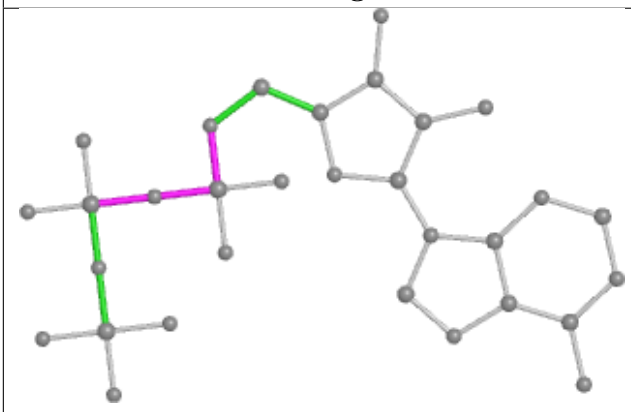
Ligand ATP A 1002



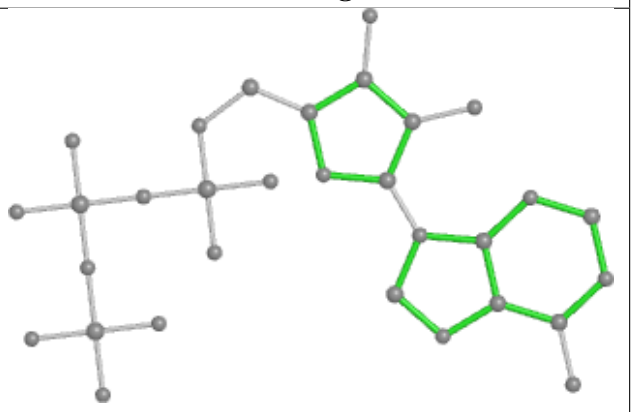
Bond lengths



Bond angles

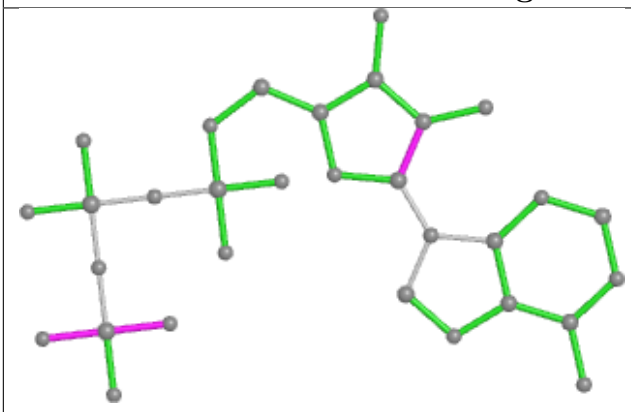


Torsions

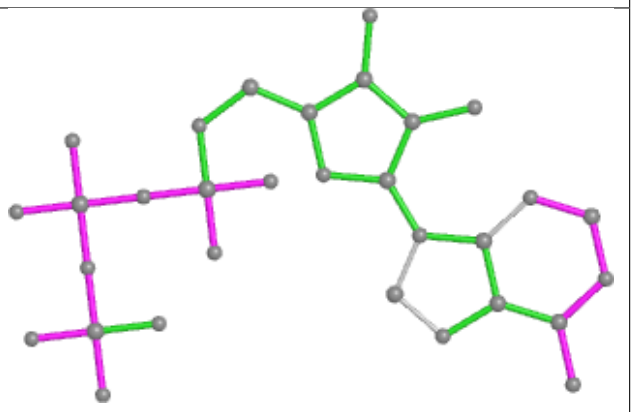


Rings

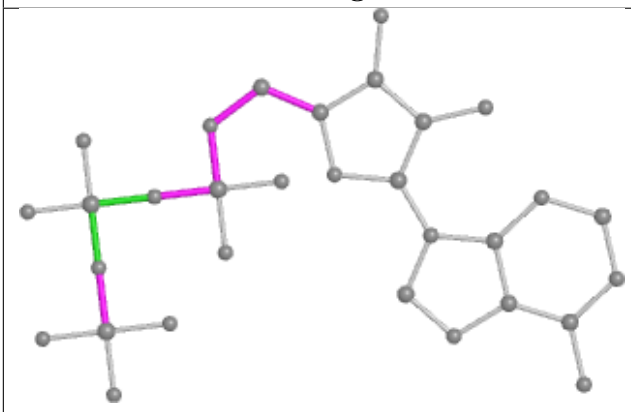
Ligand ATP B 1001



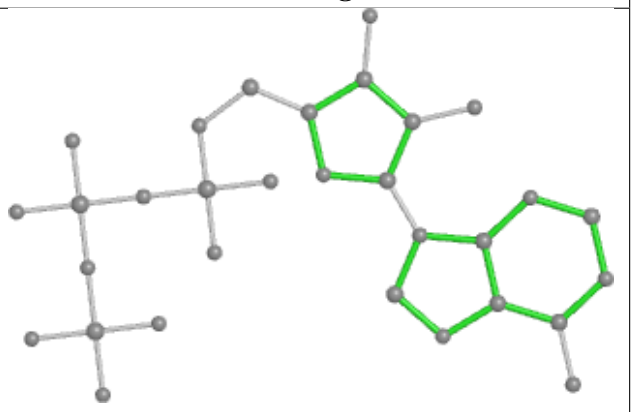
Bond lengths



Bond angles

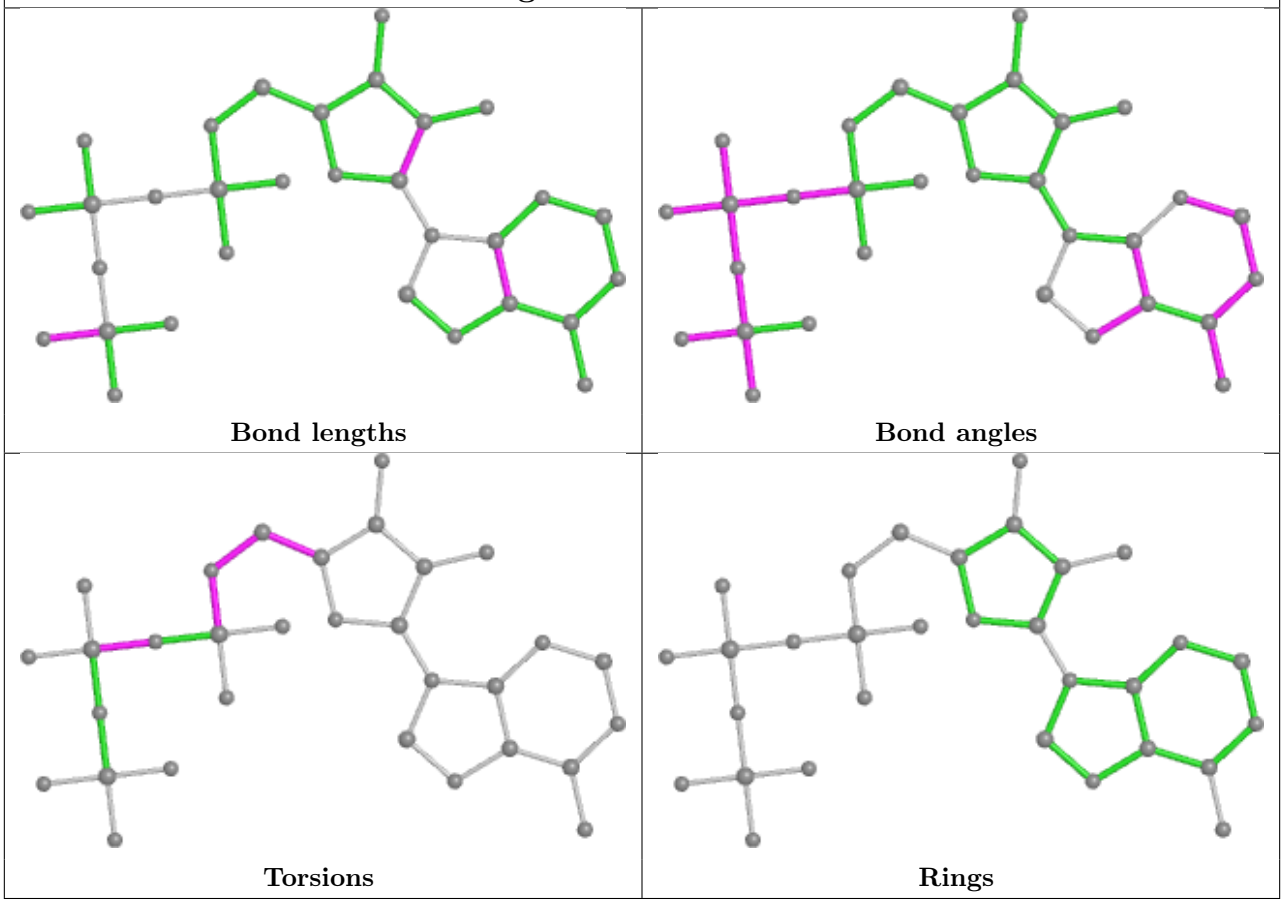


Torsions



Rings

Ligand ATP E 1003



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.

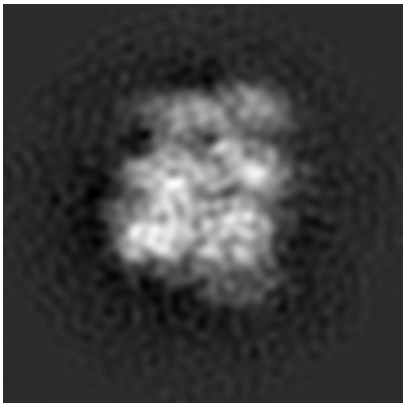
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0377. These allow visual inspection of the internal detail of the map and identification of artifacts.

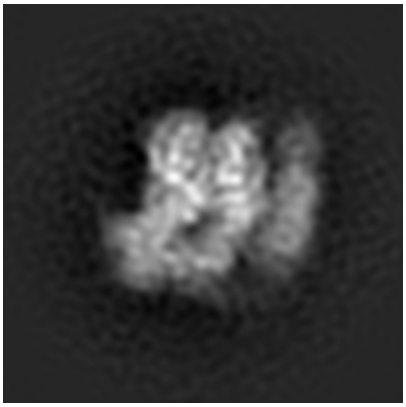
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

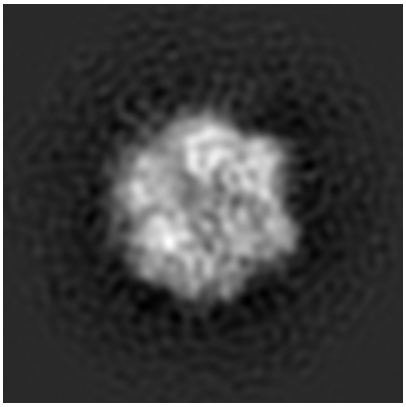
6.1.1 Primary map



X



Y

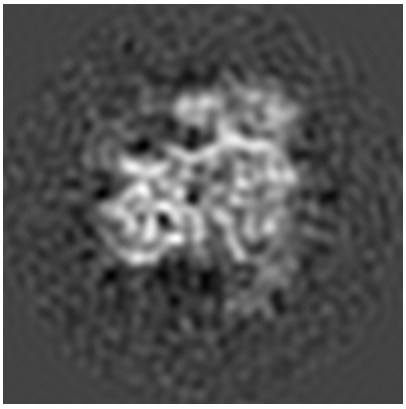


Z

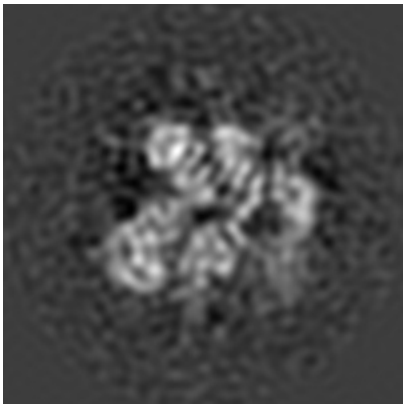
The images above show the map projected in three orthogonal directions.

6.2 Central slices

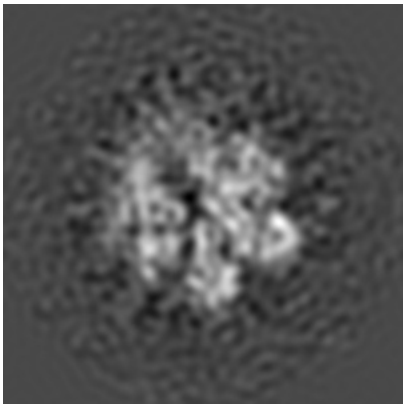
6.2.1 Primary map



X Index: 80



Y Index: 80

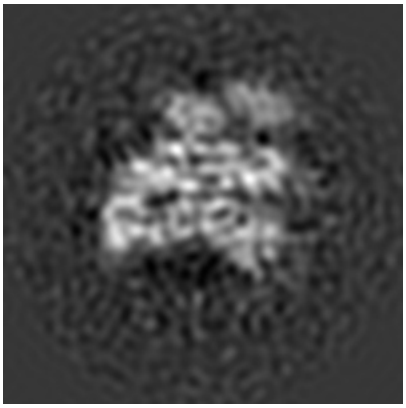


Z Index: 80

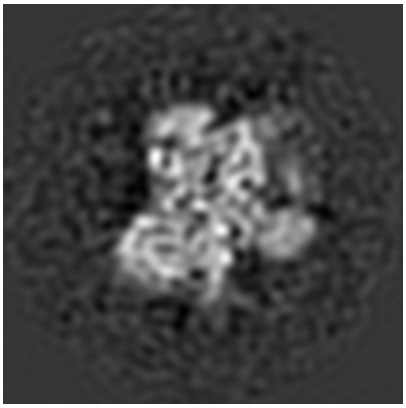
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

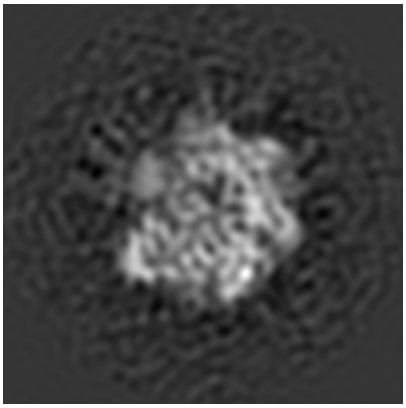
6.3.1 Primary map



X Index: 89



Y Index: 66

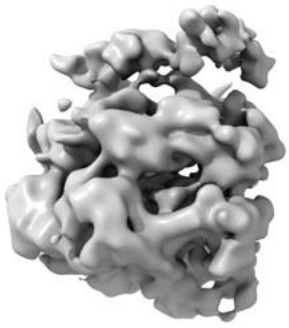


Z Index: 68

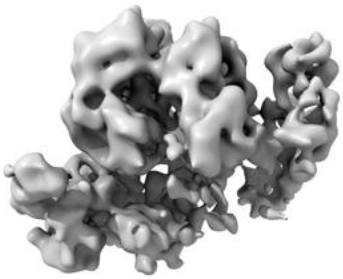
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

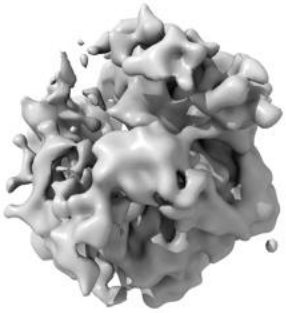
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

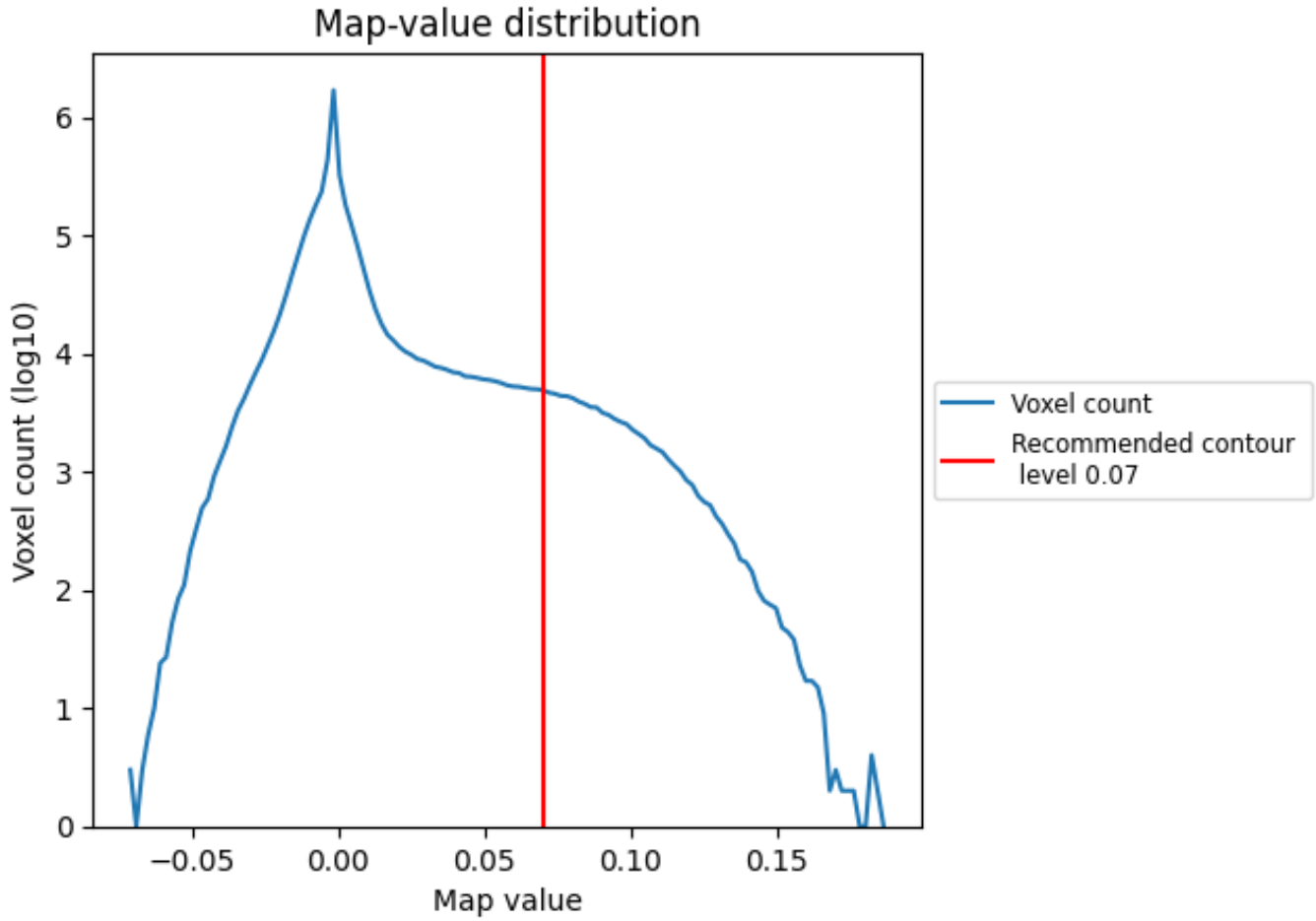
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

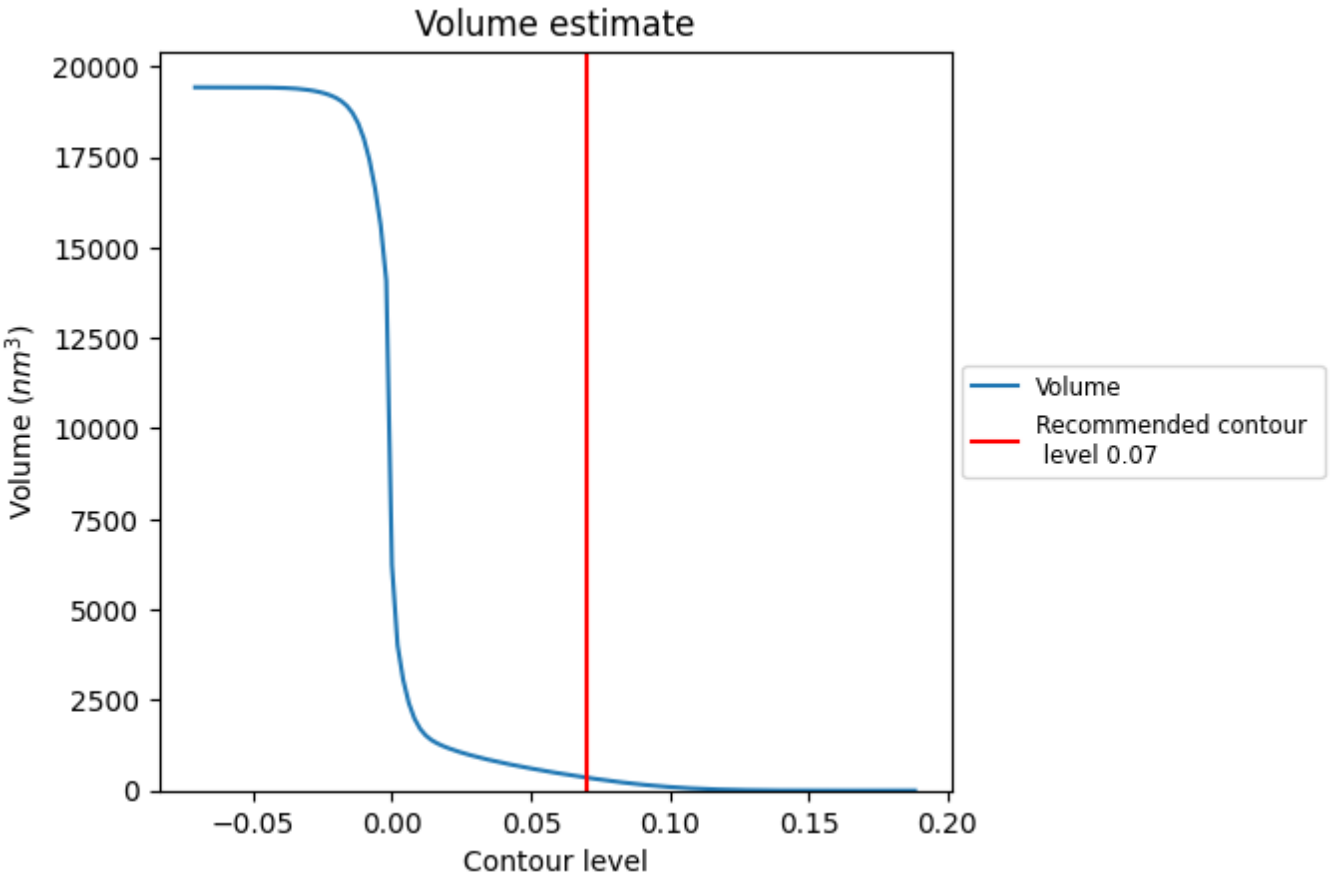
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

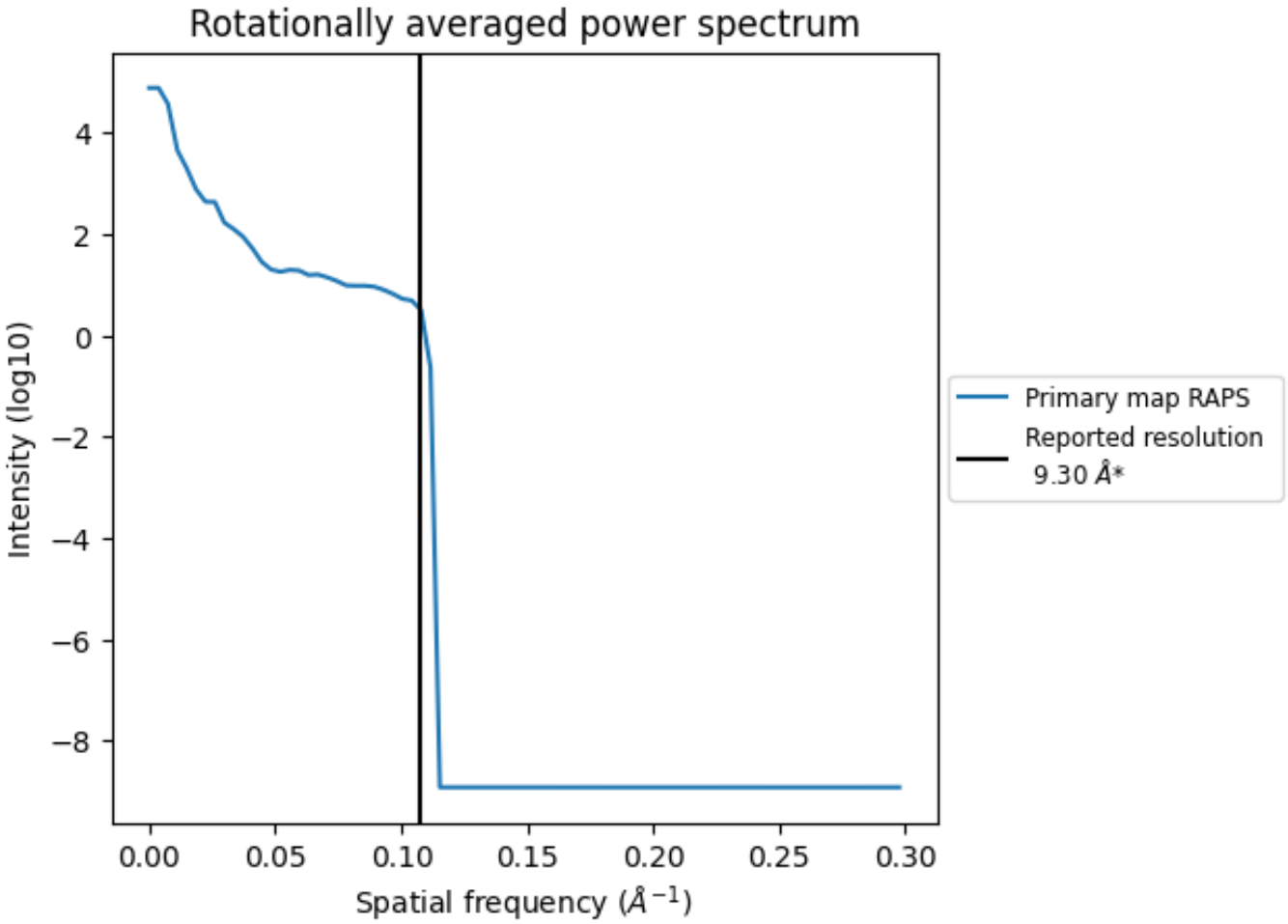
7.2 Volume estimate



The volume at the recommended contour level is 360 nm^3; this corresponds to an approximate mass of 325 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

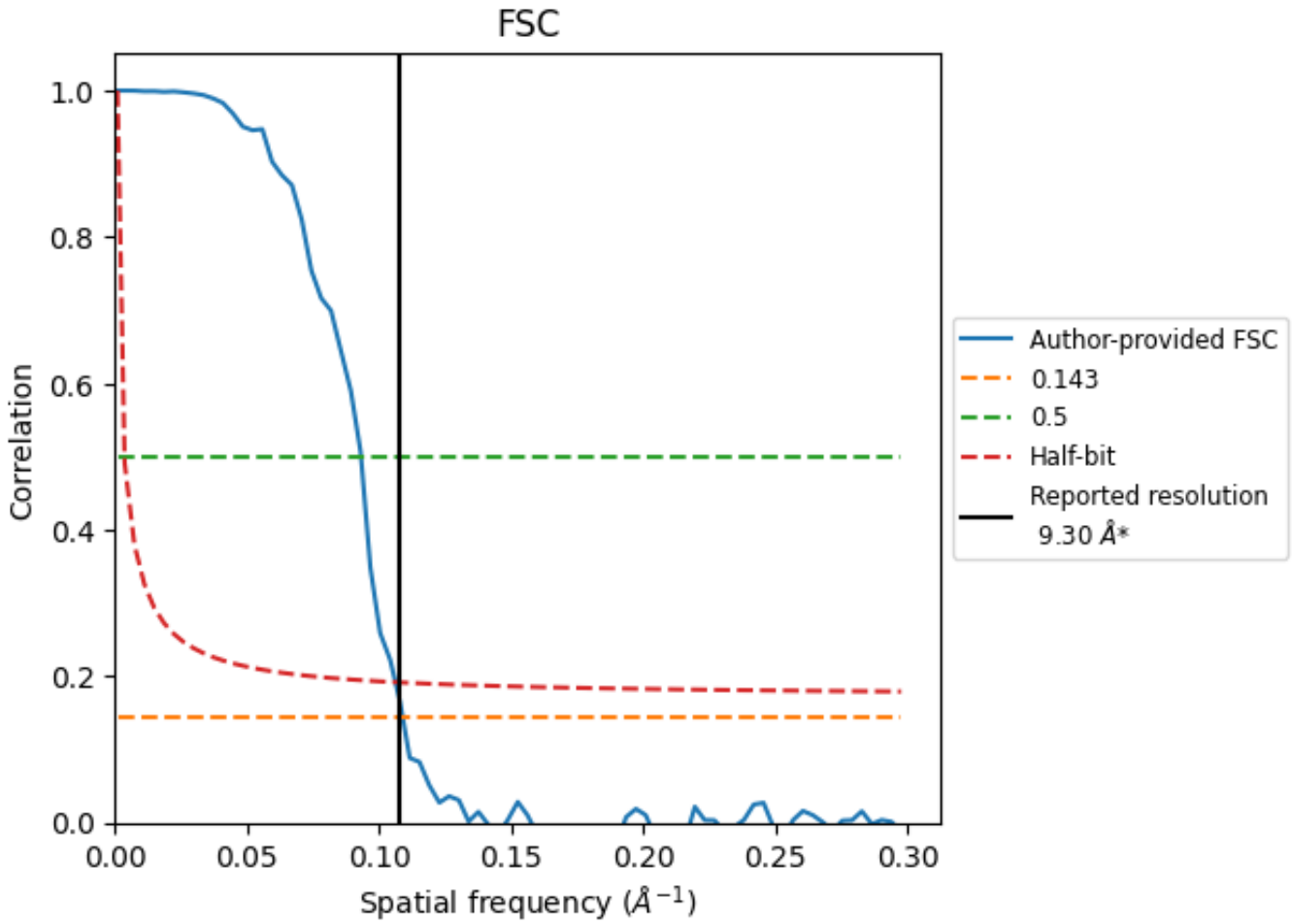


*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

8.2 Resolution estimates (i)

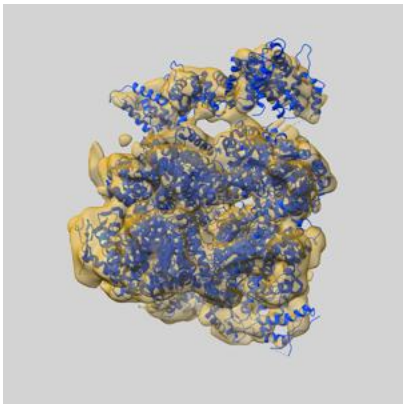
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.30	-	-
Author-provided FSC curve	9.17	10.73	9.42
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

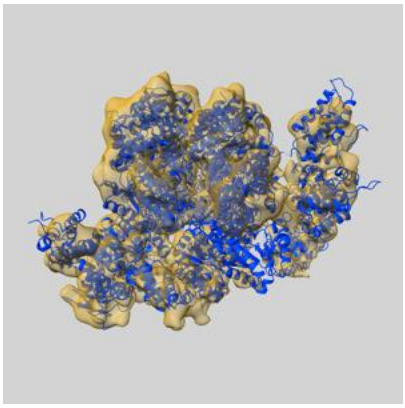
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0377 and PDB model 6N8Z. Per-residue inclusion information can be found in section 3 on page 6.

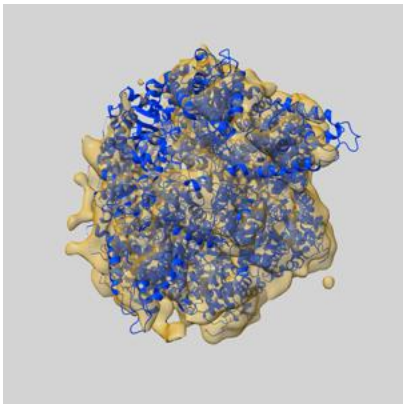
9.1 Map-model overlay



X



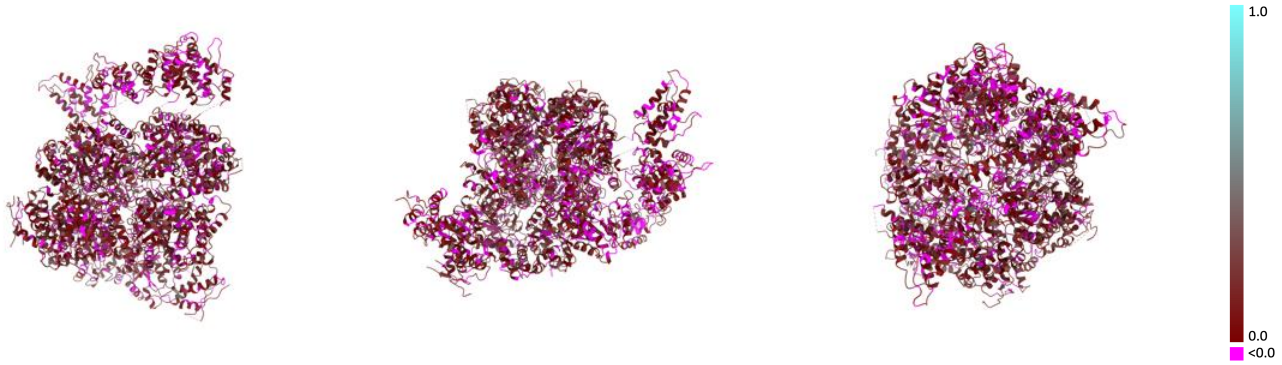
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

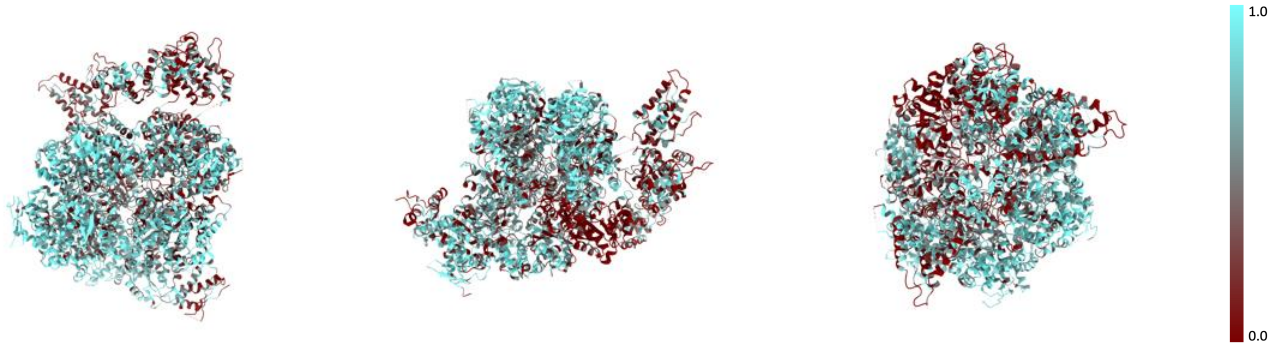
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

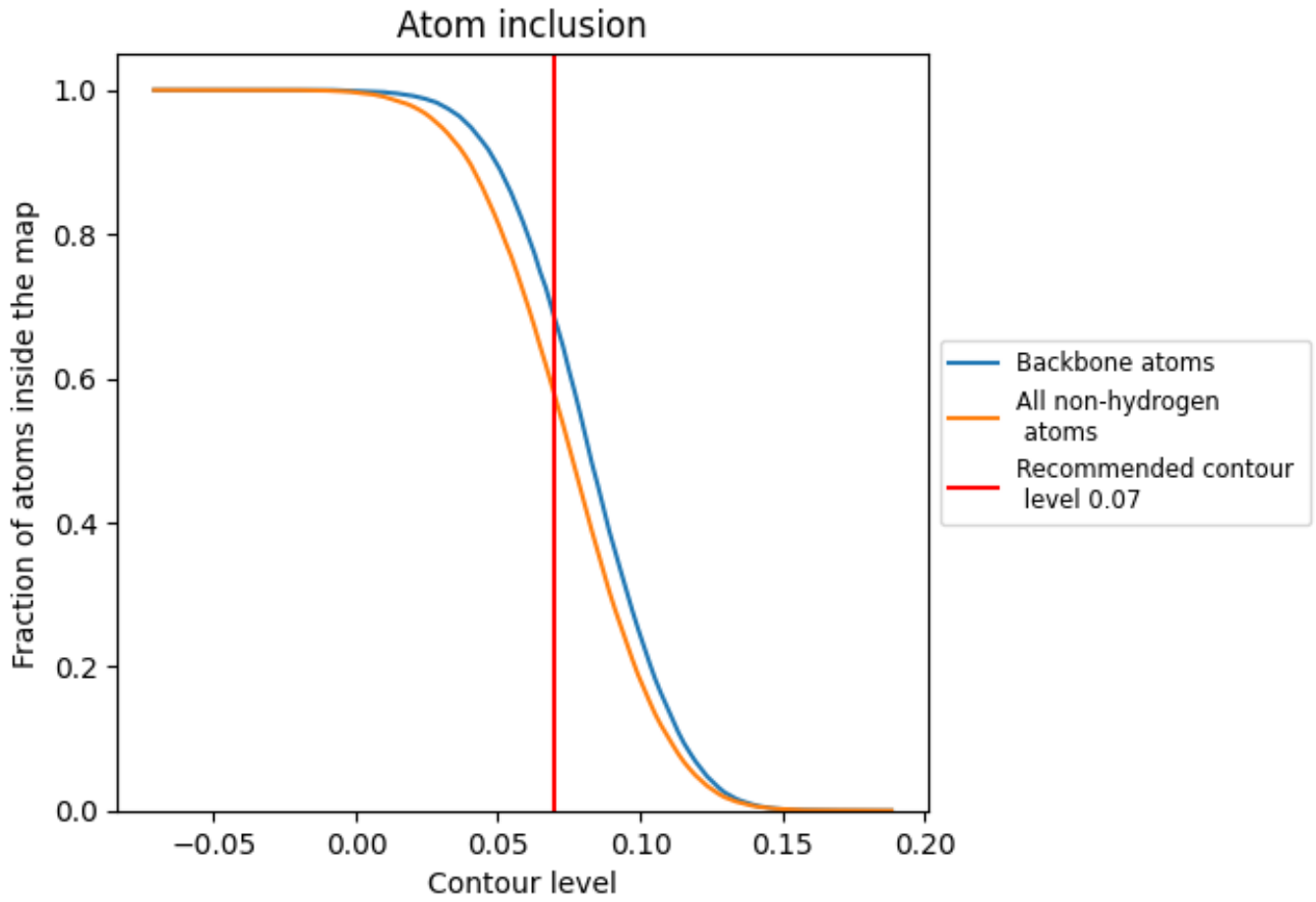
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5759	0.0970
A	0.5000	0.0890
B	0.6224	0.1020
C	0.6677	0.1060
D	0.6226	0.1000
E	0.6012	0.0940
F	0.3864	0.0850