



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 05:26 PM EST

PDB ID : 6N8T  
EMDB ID : EMD-0375  
Title : Hsp104DWB closed conformation  
Authors : Lee, S.; Rho, S.H.; Lee, J.; Sung, N.; Liu, J.; Tsai, F.T.F.  
Deposited on : 2018-11-30  
Resolution : 7.70 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](mailto: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>.

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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

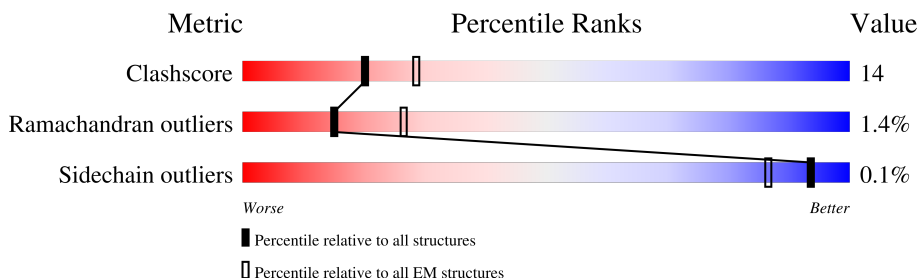
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.70 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	879	<div> <div>40%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	B	879	<div> <div>38%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	C	879	<div> <div>29%</div> <div>67%</div> <div>13%</div> <div>• 18%</div> </div>
1	D	879	<div> <div>27%</div> <div>65%</div> <div>14%</div> <div>• 18%</div> </div>
1	E	879	<div> <div>29%</div> <div>67%</div> <div>13%</div> <div>• 18%</div> </div>
1	F	879	<div> <div>44%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>

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	D	1001	-	-	X	-
2	ATP	D	1002	-	-	X	-

## 2 Entry composition [i](#)

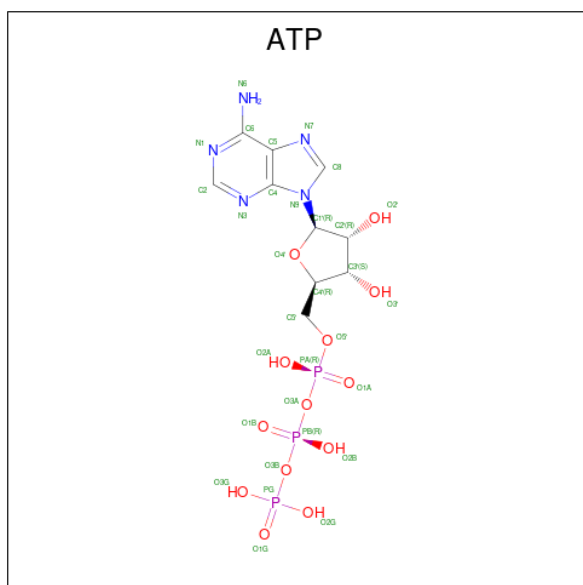
There are 2 unique types of molecules in this entry. The entry contains 37396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	848	Total 6699	4209	1179	1292	19	0	0
1	B	848	Total 6710	4217	1181	1293	19	0	0
1	C	719	Total 5633	3557	986	1072	18	0	0
1	D	720	Total 5657	3574	990	1075	18	0	0
1	E	719	Total 5623	3553	985	1067	18	0	0
1	F	848	Total 6702	4212	1179	1292	19	0	0

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

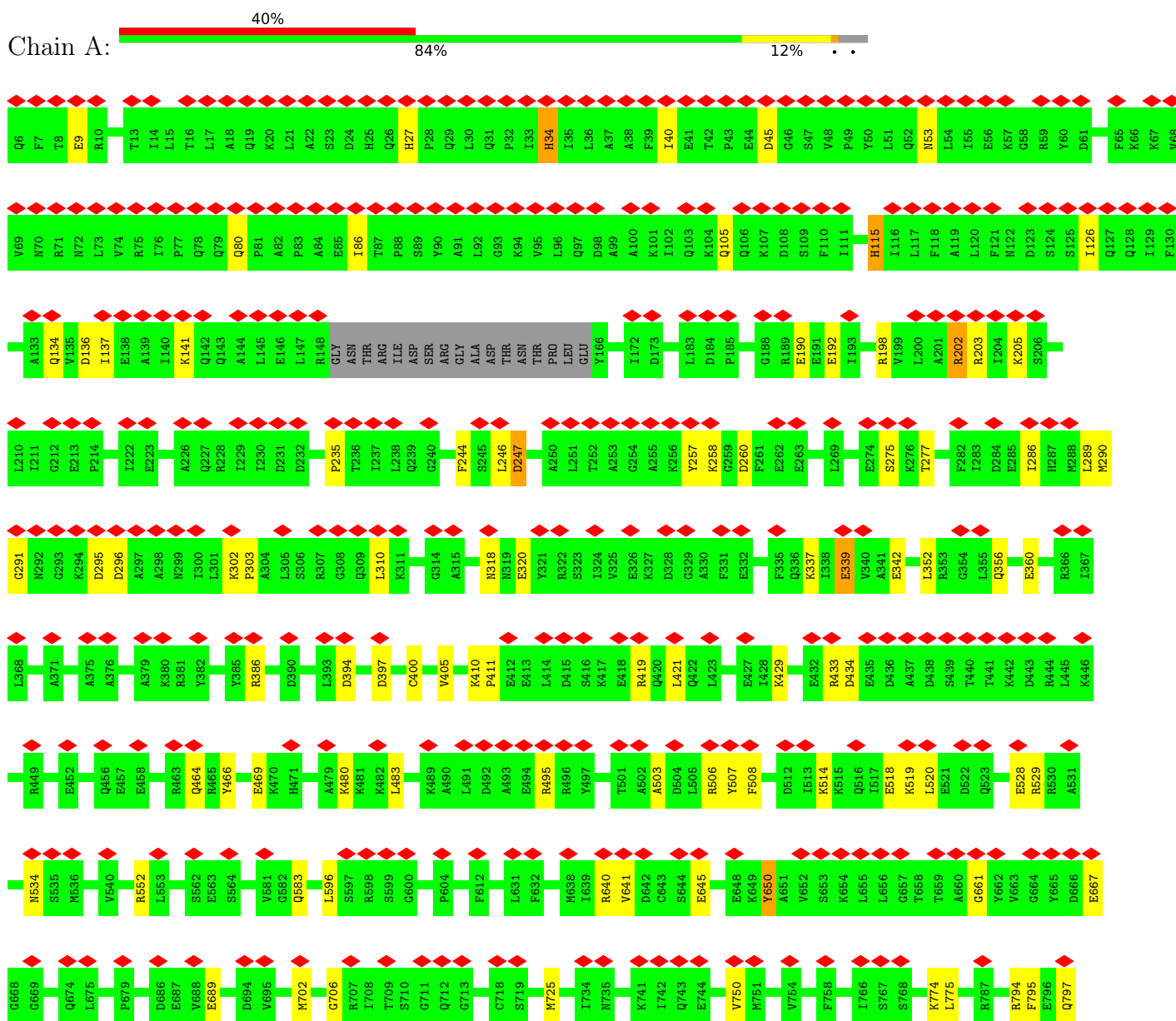


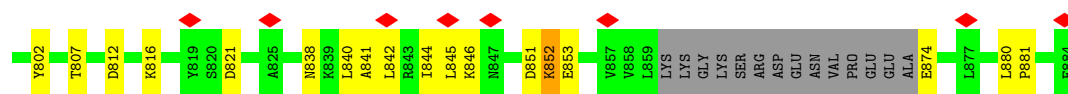
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 62	C 20	N 10	O 26	P 6	0
2	A	1	Total 62	C 20	N 10	O 26	P 6	0
2	B	1	Total 62	C 20	N 10	O 26	P 6	0
2	B	1	Total 62	C 20	N 10	O 26	P 6	0
2	C	1	Total 62	C 20	N 10	O 26	P 6	0
2	C	1	Total 62	C 20	N 10	O 26	P 6	0
2	D	1	Total 62	C 20	N 10	O 26	P 6	0
2	D	1	Total 62	C 20	N 10	O 26	P 6	0
2	E	1	Total 62	C 20	N 10	O 26	P 6	0
2	E	1	Total 62	C 20	N 10	O 26	P 6	0
2	F	1	Total 62	C 20	N 10	O 26	P 6	0
2	F	1	Total 62	C 20	N 10	O 26	P 6	0

### 3 Residue-property plots

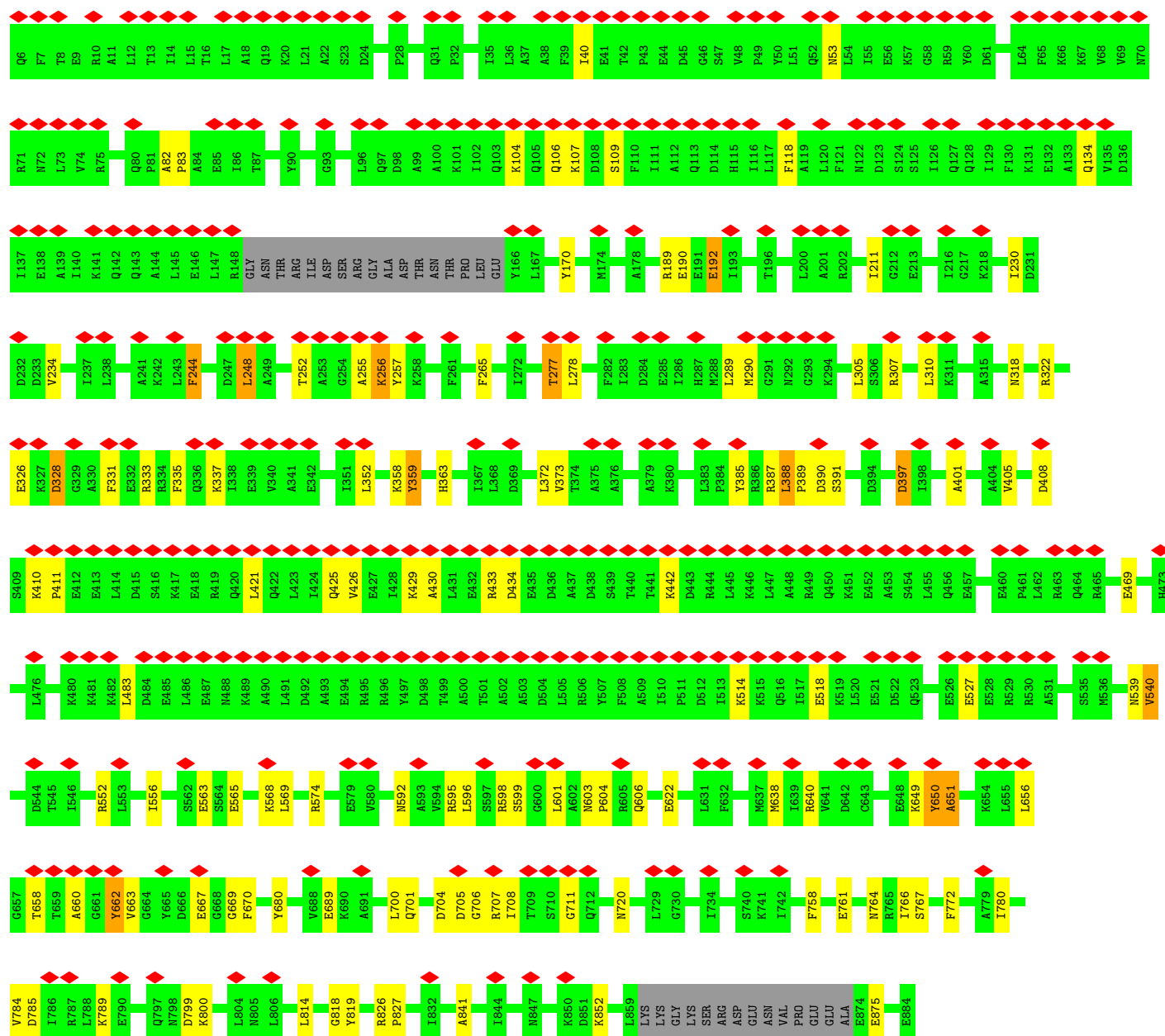
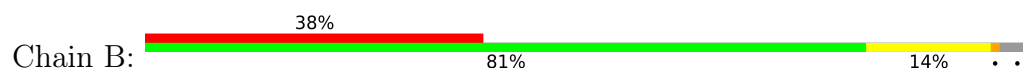
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



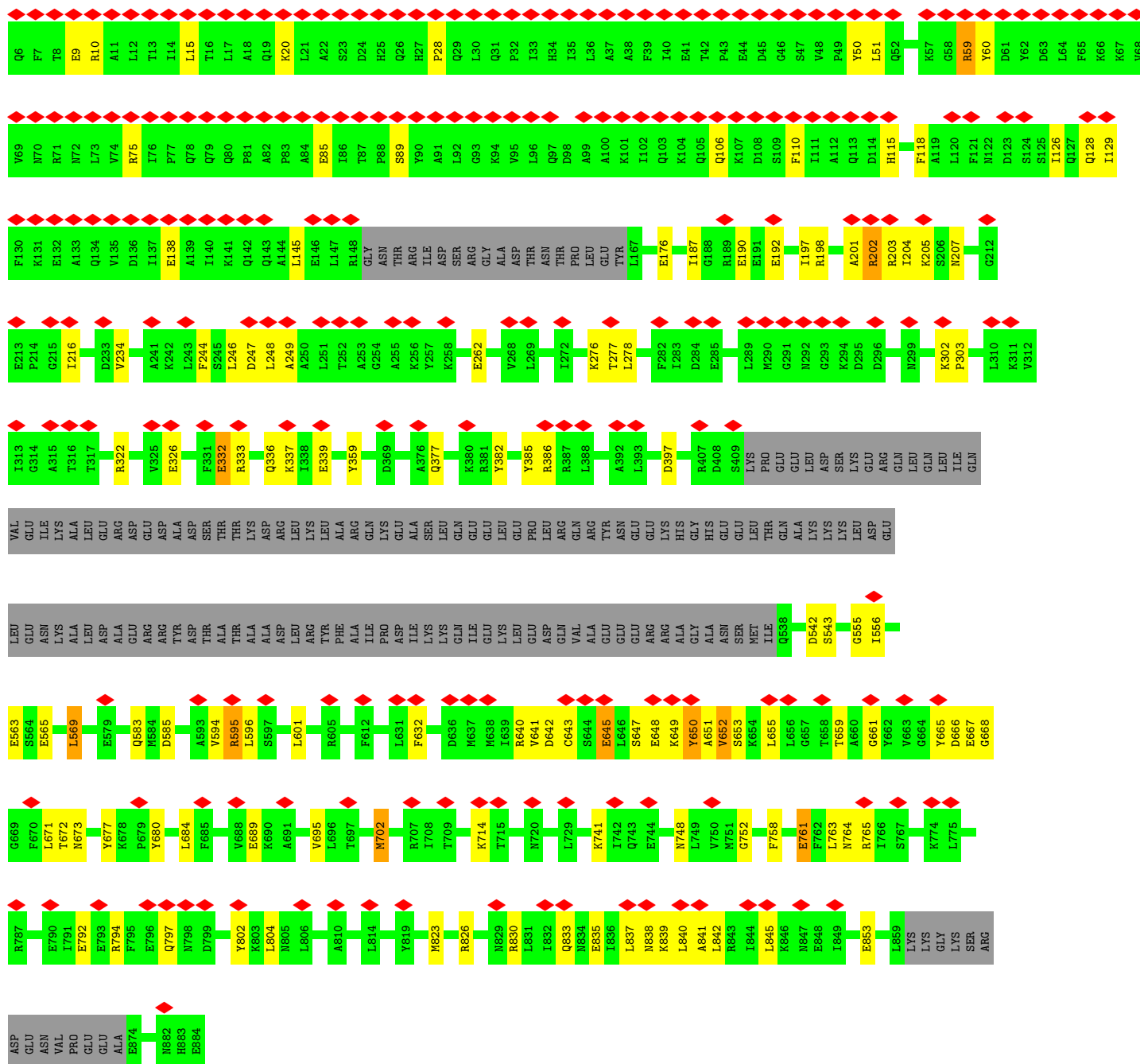


• Molecule 1: Heat shock protein 104

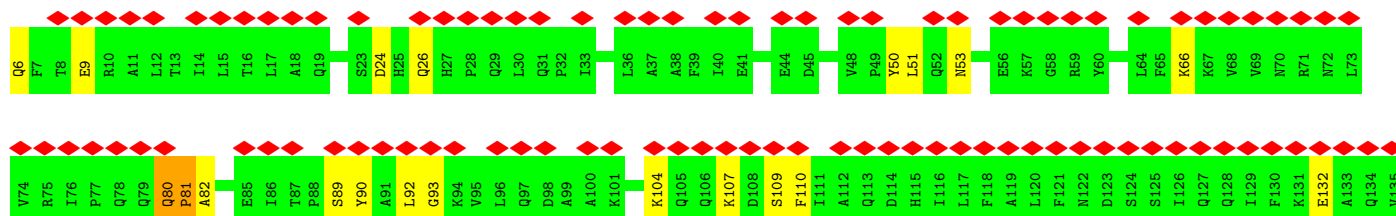


• Molecule 1: Heat shock protein 104





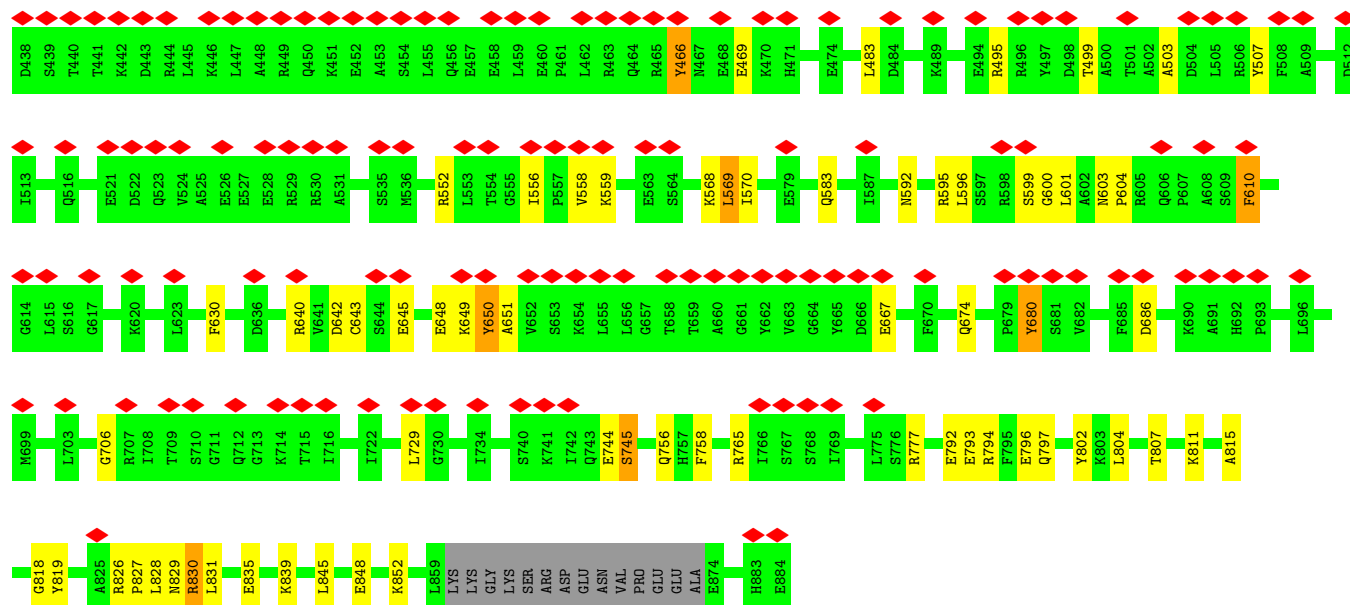
• Molecule 1: Heat shock protein 104











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56859	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 ( $e^-/\text{\AA}^2$ )	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	1.506	Depositor
Minimum map value	-0.838	Depositor
Average map value	-0.339	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.4	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	1.04	17/6787 (0.3%)	0.90	10/9141 (0.1%)
1	B	1.07	19/6798 (0.3%)	0.95	12/9154 (0.1%)
1	C	1.06	19/5710 (0.3%)	0.93	8/7699 (0.1%)
1	D	1.08	19/5735 (0.3%)	0.95	13/7730 (0.2%)
1	E	1.07	16/5700 (0.3%)	0.97	16/7685 (0.2%)
1	F	1.06	19/6790 (0.3%)	0.95	20/9145 (0.2%)
All	All	1.06	109/37520 (0.3%)	0.94	79/50554 (0.2%)

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	652	VAL	CB-CG1	-9.31	1.33	1.52
1	C	652	VAL	CB-CG1	-8.98	1.33	1.52
1	A	400	CYS	CB-SG	-8.12	1.68	1.82
1	F	397	ASP	CB-CG	7.95	1.68	1.51
1	D	802	TYR	CB-CG	-7.91	1.39	1.51
1	E	643	CYS	CB-SG	-7.91	1.68	1.82
1	D	758	PHE	CB-CG	-7.72	1.38	1.51
1	D	670	PHE	CB-CG	-7.71	1.38	1.51
1	A	667	GLU	CG-CD	-7.71	1.40	1.51
1	F	610	PHE	CB-CG	-7.42	1.38	1.51
1	E	397	ASP	CB-CG	7.37	1.67	1.51
1	D	761	GLU	CD-OE1	-7.24	1.17	1.25
1	A	641	VAL	CB-CG2	-7.23	1.37	1.52
1	F	630	PHE	CB-CG	-7.22	1.39	1.51
1	A	397	ASP	CB-CG	7.13	1.66	1.51
1	B	670	PHE	CB-CG	-6.93	1.39	1.51
1	B	265	PHE	CB-CG	-6.91	1.39	1.51
1	C	853	GLU	CD-OE1	-6.86	1.18	1.25
1	A	469	GLU	CD-OE1	-6.78	1.18	1.25
1	D	632	PHE	CB-CG	-6.63	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	802	TYR	CB-CG	-6.48	1.42	1.51
1	C	689	GLU	CD-OE1	-6.47	1.18	1.25
1	B	335	PHE	CG-CD1	-6.41	1.29	1.38
1	C	594	VAL	CB-CG1	-6.35	1.39	1.52
1	C	643	CYS	CB-SG	-6.29	1.71	1.82
1	D	792	GLU	CD-OE2	-6.24	1.18	1.25
1	C	192	GLU	CD-OE1	-6.24	1.18	1.25
1	A	689	GLU	CD-OE1	-6.21	1.18	1.25
1	C	190	GLU	CD-OE2	-6.07	1.19	1.25
1	E	823	MET	CG-SD	-6.07	1.65	1.81
1	E	594	VAL	CB-CG2	-6.05	1.40	1.52
1	B	391	SER	CB-OG	-6.03	1.34	1.42
1	D	397	ASP	CB-CG	5.92	1.64	1.51
1	D	132	GLU	CD-OE1	-5.89	1.19	1.25
1	D	332	GLU	CD-OE1	-5.89	1.19	1.25
1	F	265	PHE	CB-CG	-5.87	1.41	1.51
1	B	234	VAL	CB-CG1	-5.86	1.40	1.52
1	B	469	GLU	CD-OE1	-5.85	1.19	1.25
1	C	332	GLU	CD-OE1	-5.85	1.19	1.25
1	F	667	GLU	CD-OE1	-5.85	1.19	1.25
1	E	718	CYS	CB-SG	-5.84	1.72	1.81
1	C	382	TYR	CB-CG	-5.83	1.42	1.51
1	D	848	GLU	CD-OE1	-5.82	1.19	1.25
1	F	758	PHE	CB-CG	-5.81	1.41	1.51
1	B	244	PHE	CB-CG	-5.73	1.41	1.51
1	D	263	GLU	CD-OE1	-5.73	1.19	1.25
1	B	622	GLU	CD-OE1	-5.68	1.19	1.25
1	D	234	VAL	CB-CG1	-5.67	1.41	1.52
1	C	645	GLU	CD-OE2	-5.66	1.19	1.25
1	F	244	PHE	CB-CG	-5.65	1.41	1.51
1	C	234	VAL	CB-CG1	-5.64	1.41	1.52
1	C	202	ARG	CG-CD	-5.62	1.37	1.51
1	B	328	ASP	CB-CG	-5.59	1.40	1.51
1	D	622	GLU	CD-OE1	-5.58	1.19	1.25
1	B	761	GLU	CD-OE1	-5.58	1.19	1.25
1	C	792	GLU	CD-OE2	-5.55	1.19	1.25
1	E	802	TYR	CB-CG	-5.55	1.43	1.51
1	F	192	GLU	CD-OE1	-5.54	1.19	1.25
1	C	761	GLU	CD-OE1	-5.54	1.19	1.25
1	C	792	GLU	CD-OE1	-5.53	1.19	1.25
1	E	754	VAL	CB-CG1	-5.51	1.41	1.52
1	B	689	GLU	CD-OE1	-5.50	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	GLU	CD-OE1	-5.49	1.19	1.25
1	E	680	TYR	CB-CG	-5.46	1.43	1.51
1	D	643	CYS	CB-SG	-5.44	1.73	1.81
1	D	385	TYR	CB-CG	-5.41	1.43	1.51
1	A	244	PHE	CB-CG	-5.38	1.42	1.51
1	F	792	GLU	CG-CD	-5.36	1.44	1.51
1	E	667	GLU	CD-OE1	-5.34	1.19	1.25
1	F	643	CYS	CB-SG	-5.33	1.73	1.81
1	F	848	GLU	CD-OE1	-5.33	1.19	1.25
1	B	359	TYR	CB-CG	-5.33	1.43	1.51
1	F	469	GLU	CD-OE1	-5.31	1.19	1.25
1	B	397	ASP	CB-CG	5.30	1.62	1.51
1	A	689	GLU	CG-CD	-5.28	1.44	1.51
1	E	56	GLU	CD-OE1	-5.27	1.19	1.25
1	A	34	HIS	CB-CG	-5.25	1.40	1.50
1	D	565	GLU	CD-OE1	-5.24	1.19	1.25
1	A	750	VAL	CB-CG1	-5.24	1.41	1.52
1	F	60	TYR	CB-CG	-5.22	1.43	1.51
1	D	391	SER	CB-OG	-5.21	1.35	1.42
1	B	192	GLU	CD-OE1	-5.18	1.20	1.25
1	F	320	GLU	CG-CD	-5.18	1.44	1.51
1	B	689	GLU	CG-CD	-5.18	1.44	1.51
1	B	758	PHE	CB-CG	-5.17	1.42	1.51
1	E	262	GLU	CD-OE1	-5.16	1.20	1.25
1	D	792	GLU	CG-CD	-5.15	1.44	1.51
1	F	216	ILE	CB-CG1	-5.15	1.39	1.54
1	E	765	ARG	CG-CD	-5.14	1.39	1.51
1	B	680	TYR	CB-CG	-5.14	1.44	1.51
1	E	62	TYR	CE2-CZ	-5.13	1.31	1.38
1	C	326	GLU	CD-OE1	-5.12	1.20	1.25
1	F	645	GLU	CD-OE1	-5.08	1.20	1.25
1	F	793	GLU	CD-OE1	-5.08	1.20	1.25
1	A	853	GLU	CD-OE2	-5.07	1.20	1.25
1	A	802	TYR	CB-CG	-5.07	1.44	1.51
1	A	342	GLU	CD-OE1	-5.04	1.20	1.25
1	E	339	GLU	CD-OE1	-5.04	1.20	1.25
1	F	60	TYR	CG-CD1	-5.04	1.32	1.39
1	E	271	GLU	CD-OE1	-5.03	1.20	1.25
1	A	874	GLU	CD-OE1	-5.03	1.20	1.25
1	C	244	PHE	CB-CG	-5.03	1.42	1.51
1	C	695	VAL	CB-CG2	-5.03	1.42	1.52
1	A	320	GLU	CD-OE1	-5.02	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	853	GLU	CD-OE1	-5.02	1.20	1.25
1	C	758	PHE	CB-CG	-5.01	1.42	1.51
1	E	762	PHE	CB-CG	-5.01	1.42	1.51
1	B	469	GLU	CG-CD	-5.01	1.44	1.51
1	A	339	GLU	CD-OE1	-5.01	1.20	1.25

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	202	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	D	707	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	F	419	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	640	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	386	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	E	397	ASP	CB-CG-OD1	8.33	125.79	118.30
1	F	386	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	D	50	TYR	CB-CG-CD2	-7.92	116.25	121.00
1	F	264	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	F	495	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	189	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	F	802	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	B	552	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	612	PHE	CB-CG-CD2	7.42	126.00	120.80
1	F	179	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	202	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	D	830	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	E	826	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	E	826	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	F	466	TYR	CB-CG-CD1	-7.10	116.74	121.00
1	E	203	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	529	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	F	765	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	F	552	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	F	552	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	F	60	TYR	CB-CG-CD1	-6.86	116.88	121.00
1	A	419	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	662	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	F	777	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	202	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	595	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	E	680	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	466	TYR	CB-CG-CD1	-6.42	117.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	382	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	E	80	GLN	C-N-CD	-6.30	106.75	120.60
1	F	680	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	E	802	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	E	334	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	D	397	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	170	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	B	118	PHE	CB-CG-CD1	-5.79	116.75	120.80
1	F	794	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	359	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	C	75	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	702	MET	CG-SD-CE	5.73	109.37	100.20
1	A	640	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	574	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	495	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	385	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	C	397	ASP	CB-CG-OD1	5.60	123.34	118.30
1	F	385	TYR	CB-CG-CD1	-5.58	117.66	121.00
1	D	574	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	D	80	GLN	C-N-CD	-5.54	108.42	120.60
1	E	552	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	F	830	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	359	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	D	202	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	E	819	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	E	397	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	387	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	552	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	115	HIS	CA-CB-CG	-5.33	104.54	113.60
1	F	495	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	203	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	359	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	598	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	307	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	333	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	E	60	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	F	640	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	E	545	THR	CA-CB-CG2	-5.10	105.26	112.40
1	E	407	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	662	TYR	CB-CG-CD1	5.09	124.05	121.00
1	F	118	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	C	595	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	759	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	409	SER	N-CA-CB	5.07	118.11	110.50
1	D	612	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	C	59	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6699	0	6815	242	0
1	B	6710	0	6840	262	0
1	C	5633	0	5752	351	0
1	D	5657	0	5789	366	0
1	E	5623	0	5745	213	0
1	F	6702	0	6826	218	0
2	A	62	0	24	4	0
2	B	62	0	24	11	0
2	C	62	0	24	5	0
2	D	62	0	24	34	0
2	E	62	0	24	6	0
2	F	62	0	24	5	0
All	All	37396	0	37911	1034	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 14.

All (1034) 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:A:141:LYS:HE3	1:F:107:LYS:CA	1.18	1.63
1:A:842:LEU:HD13	1:F:595:ARG:CZ	1.22	1.60
1:B:107:LYS:HD2	1:C:118:PHE:CE2	1.40	1.57
1:D:662:TYR:CD2	1:E:649:LYS:HD2	1.36	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:SER:HB3	1:E:137:ILE:CB	1.34	1.56
1:A:141:LYS:NZ	1:F:107:LYS:CG	1.68	1.55
1:A:141:LYS:CE	1:F:107:LYS:HA	1.10	1.54
1:D:662:TYR:CE1	1:E:649:LYS:HB3	1.43	1.49
1:C:59:ARG:NH2	1:D:26:GLN:HG2	1.21	1.44
1:C:59:ARG:NH2	1:D:26:GLN:CG	1.78	1.43
1:D:104:LYS:NZ	1:E:122:ASN:HA	1.33	1.42
1:D:266:LYS:HE3	1:E:249:ALA:CB	1.50	1.41
1:B:766:ILE:O	1:C:830:ARG:CZ	1.68	1.41
1:C:59:ARG:HH21	1:D:26:GLN:CG	1.32	1.41
1:D:301:LEU:HD13	1:E:248:LEU:CD2	1.48	1.41
1:B:107:LYS:CD	1:C:118:PHE:CD2	2.04	1.39
1:A:141:LYS:NZ	1:F:107:LYS:HG2	1.28	1.35
1:C:59:ARG:HG3	1:D:24:ASP:CA	1.56	1.35
1:D:601:LEU:HD11	1:E:844:ILE:CD1	1.55	1.35
1:D:109:SER:CB	1:E:137:ILE:CB	2.05	1.35
1:B:107:LYS:HD3	1:C:118:PHE:CD2	1.59	1.33
1:B:596:LEU:CG	1:C:838:ASN:OD1	1.76	1.33
1:A:845:LEU:CD1	1:F:595:ARG:HA	1.56	1.33
1:A:141:LYS:CE	1:F:107:LYS:CA	1.79	1.33
1:A:842:LEU:HD13	1:F:595:ARG:NE	1.42	1.32
1:D:662:TYR:OH	1:E:649:LYS:HA	1.29	1.30
1:B:322:ARG:NH2	1:C:666:ASP:HA	1.47	1.29
1:B:766:ILE:O	1:C:830:ARG:NH2	1.64	1.28
1:C:59:ARG:HH12	1:D:81:PRO:CG	1.45	1.28
1:D:662:TYR:CZ	1:E:649:LYS:HA	1.68	1.28
1:D:186:VAL:HG12	2:D:1001:ATP:C2	1.67	1.27
1:D:662:TYR:CE2	1:E:649:LYS:HD2	1.69	1.27
1:B:704:ASP:OD2	1:C:826:ARG:NH1	1.65	1.27
1:D:662:TYR:CE2	1:E:649:LYS:CD	2.17	1.26
1:A:842:LEU:CD1	1:F:595:ARG:CZ	2.14	1.25
1:C:203:ARG:NH2	1:D:362:HIS:O	1.69	1.25
1:A:845:LEU:HD11	1:F:595:ARG:CA	1.66	1.24
1:B:599:SER:CB	1:C:841:ALA:CB	2.15	1.24
1:D:596:LEU:CD2	1:E:841:ALA:HB2	1.65	1.22
1:B:599:SER:OG	1:C:841:ALA:HB2	1.37	1.21
1:D:266:LYS:CE	1:E:249:ALA:HB1	1.71	1.21
1:C:322:ARG:HD3	1:D:677:TYR:OH	1.40	1.20
1:D:595:ARG:HG2	1:E:845:LEU:CD1	1.70	1.20
1:B:596:LEU:HG	1:C:838:ASN:OD1	1.06	1.20
1:B:704:ASP:OD2	1:C:826:ARG:NH2	1.75	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:NH1	1:D:398:ILE:HG12	1.57	1.19
1:D:662:TYR:CD2	1:E:649:LYS:CD	2.25	1.19
1:A:506:ARG:HB2	1:B:426:VAL:HG11	1.24	1.19
1:C:202:ARG:NH1	1:D:398:ILE:CG1	2.06	1.19
1:A:115:HIS:NE2	1:F:107:LYS:CE	2.06	1.17
1:A:844:ILE:CG2	1:F:599:SER:HB2	1.74	1.17
1:B:660:ALA:HB3	1:C:652:VAL:HG11	1.18	1.17
1:C:201:ALA:CB	1:D:405:VAL:HG23	1.72	1.16
1:C:59:ARG:HG2	1:D:24:ASP:O	1.46	1.16
1:D:662:TYR:CZ	1:E:649:LYS:CA	2.28	1.16
1:C:59:ARG:NH1	1:D:81:PRO:HG3	1.60	1.16
1:A:506:ARG:CB	1:B:426:VAL:HG11	1.75	1.15
1:C:201:ALA:CB	1:D:405:VAL:CG2	2.25	1.15
1:C:661:GLY:HA2	1:D:663:VAL:O	1.46	1.15
1:A:844:ILE:CD1	1:F:601:LEU:HD11	1.76	1.15
1:B:107:LYS:CD	1:C:118:PHE:CE2	2.23	1.15
1:D:662:TYR:CE1	1:E:649:LYS:CB	2.28	1.15
1:B:599:SER:HB2	1:C:841:ALA:HA	1.18	1.15
1:B:601:LEU:HD22	1:C:837:LEU:HD22	1.17	1.14
2:D:1001:ATP:PG	2:D:1001:ATP:O1G	2.06	1.14
2:A:1002:ATP:PG	2:A:1002:ATP:O1G	2.06	1.14
1:A:795:PHE:HA	1:F:603:ASN:ND2	1.62	1.13
1:C:59:ARG:HH21	1:D:26:GLN:HG3	1.04	1.13
1:C:60:TYR:OH	1:D:26:GLN:OE1	1.62	1.13
1:C:595:ARG:HG2	1:D:845:LEU:CD2	1.78	1.13
2:E:1002:ATP:PG	2:E:1002:ATP:O1G	2.06	1.13
2:F:1001:ATP:PG	2:F:1001:ATP:O1G	2.06	1.13
1:B:662:TYR:OH	1:C:649:LYS:HA	1.49	1.13
2:C:1001:ATP:PG	2:C:1001:ATP:O1G	2.07	1.13
1:E:204:ILE:HB	1:F:397:ASP:OD2	1.47	1.13
1:B:599:SER:CB	1:C:841:ALA:HA	1.78	1.13
2:B:1001:ATP:PG	2:B:1001:ATP:O1G	2.06	1.13
2:E:1001:ATP:PG	2:E:1001:ATP:O1G	2.07	1.13
2:B:1002:ATP:PG	2:B:1002:ATP:O1G	2.06	1.12
2:C:1002:ATP:O1G	2:C:1002:ATP:PG	2.06	1.12
1:B:704:ASP:OD2	1:C:826:ARG:CZ	1.97	1.12
1:C:202:ARG:HG2	1:D:401:ALA:CB	1.79	1.12
1:D:601:LEU:CD1	1:E:844:ILE:HD12	1.78	1.12
2:F:1002:ATP:PG	2:F:1002:ATP:O1G	2.06	1.12
2:A:1001:ATP:PG	2:A:1001:ATP:O1G	2.07	1.11
1:A:141:LYS:CE	1:F:107:LYS:N	2.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:CG	1:D:401:ALA:CB	2.29	1.11
1:B:599:SER:HB3	1:C:841:ALA:HB1	1.28	1.11
1:C:201:ALA:HB2	1:D:405:VAL:CG2	1.81	1.11
1:D:104:LYS:HZ1	1:E:136:ASP:HA	1.08	1.10
1:C:764:ASN:HA	1:D:830:ARG:NH2	1.65	1.10
1:D:104:LYS:NZ	1:E:122:ASN:CA	2.13	1.10
1:A:844:ILE:HD12	1:F:601:LEU:CD1	1.81	1.10
1:C:202:ARG:HG2	1:D:401:ALA:HB3	1.31	1.10
1:D:662:TYR:OH	1:E:649:LYS:CA	1.98	1.10
1:B:599:SER:OG	1:C:841:ALA:CB	1.98	1.10
1:C:595:ARG:HG2	1:D:845:LEU:HD22	1.17	1.10
1:C:202:ARG:HA	1:D:401:ALA:HB2	1.11	1.09
1:A:844:ILE:HG21	1:F:599:SER:HB2	1.17	1.09
1:B:107:LYS:HD2	1:C:118:PHE:CD2	1.77	1.09
1:A:141:LYS:NZ	1:F:107:LYS:HG3	1.64	1.09
1:B:601:LEU:CB	1:C:837:LEU:HB3	1.80	1.09
1:B:601:LEU:HD21	1:C:840:LEU:HD23	1.32	1.08
1:E:201:ALA:CB	1:F:405:VAL:HG22	1.83	1.08
1:D:595:ARG:HG2	1:E:845:LEU:HD13	1.25	1.08
1:C:59:ARG:CG	1:D:24:ASP:O	2.02	1.08
1:A:844:ILE:CD1	1:F:601:LEU:CD1	2.31	1.07
1:A:507:TYR:OH	1:B:433:ARG:CB	2.02	1.07
1:B:599:SER:HB3	1:C:841:ALA:CB	1.81	1.07
1:D:595:ARG:CG	1:E:845:LEU:CD1	2.32	1.07
1:C:59:ARG:HH12	1:D:81:PRO:HG3	1.03	1.07
1:C:595:ARG:CG	1:D:845:LEU:HD22	1.84	1.07
1:E:109:SER:OG	1:E:276:LYS:HD3	1.54	1.07
1:C:601:LEU:HD11	1:D:844:ILE:HD12	1.36	1.07
1:D:301:LEU:CD1	1:E:248:LEU:CD2	2.33	1.07
1:A:260:ASP:OD1	1:B:256:LYS:NZ	1.87	1.06
1:B:767:SER:C	1:C:830:ARG:HH21	1.57	1.06
1:D:709:THR:OG1	1:E:645:GLU:OE1	1.72	1.06
1:A:506:ARG:HB2	1:B:426:VAL:CG1	1.85	1.05
1:B:599:SER:CB	1:C:841:ALA:CA	2.33	1.05
1:C:596:LEU:HD12	1:D:841:ALA:CB	1.84	1.05
1:D:662:TYR:CE2	1:E:649:LYS:HD3	1.87	1.05
1:D:662:TYR:CG	1:E:649:LYS:HD2	1.90	1.05
1:A:844:ILE:HD11	1:F:601:LEU:HD11	1.35	1.05
1:C:202:ARG:CA	1:D:401:ALA:HB2	1.85	1.05
1:C:204:ILE:HB	1:D:397:ASP:OD2	1.57	1.05
1:D:6:GLN:HG2	1:E:138:GLU:OE2	1.52	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:LYS:HA	1:F:570:ILE:HD11	1.35	1.04
1:C:202:ARG:HA	1:D:401:ALA:CB	1.86	1.04
1:A:115:HIS:NE2	1:F:107:LYS:HE3	1.71	1.04
1:B:601:LEU:HD11	1:C:840:LEU:HB3	1.33	1.04
1:D:301:LEU:HD13	1:E:248:LEU:HD22	1.40	1.04
1:D:595:ARG:CB	1:E:845:LEU:HD11	1.87	1.04
1:B:662:TYR:CD1	1:C:649:LYS:HE3	1.92	1.03
1:C:59:ARG:HG3	1:D:24:ASP:HA	1.04	1.03
1:D:596:LEU:HD23	1:E:841:ALA:HB2	1.04	1.03
1:E:794:ARG:O	1:E:794:ARG:NE	1.89	1.03
1:A:845:LEU:HD12	1:F:595:ARG:CB	1.88	1.02
1:A:433:ARG:NH2	1:F:503:ALA:HB1	1.72	1.02
1:B:107:LYS:HB2	1:C:106:GLN:NE2	1.73	1.02
1:D:601:LEU:HD11	1:E:844:ILE:HD12	1.05	1.02
1:B:601:LEU:HB3	1:C:837:LEU:CB	1.89	1.01
1:A:141:LYS:HE2	1:F:107:LYS:H	1.16	1.01
1:A:141:LYS:HE2	1:F:107:LYS:N	1.70	1.01
1:E:381:ARG:CZ	1:F:796:GLU:HA	1.90	1.01
1:A:842:LEU:HA	1:F:595:ARG:HD3	1.42	1.01
1:B:106:GLN:O	1:C:106:GLN:NE2	1.93	1.00
1:A:507:TYR:CD1	1:B:429:LYS:HG2	1.96	1.00
1:A:842:LEU:CD1	1:F:595:ARG:NE	2.23	1.00
1:D:218:LYS:NZ	2:D:1001:ATP:O2G	1.93	0.99
1:D:662:TYR:CD1	1:E:649:LYS:HB3	1.96	0.99
1:A:794:ARG:O	1:F:603:ASN:ND2	1.94	0.99
1:A:845:LEU:HD12	1:F:595:ARG:HG2	1.45	0.98
1:D:595:ARG:CB	1:E:845:LEU:CD1	2.41	0.98
1:C:201:ALA:HB2	1:D:405:VAL:HG22	1.41	0.98
1:C:202:ARG:CG	1:D:401:ALA:HB3	1.91	0.98
1:E:204:ILE:HD12	1:F:397:ASP:CG	1.83	0.98
1:B:601:LEU:HB3	1:C:837:LEU:HB3	0.98	0.98
1:A:842:LEU:HD22	1:F:595:ARG:NH1	1.79	0.97
1:D:301:LEU:HD13	1:E:248:LEU:HD21	1.45	0.97
1:B:322:ARG:NH2	1:C:666:ASP:CA	2.27	0.97
1:C:203:ARG:HG2	1:D:362:HIS:CG	1.98	0.97
1:E:381:ARG:NH2	1:F:796:GLU:HA	1.78	0.97
1:B:767:SER:O	1:C:830:ARG:NH2	1.96	0.97
1:C:377:GLN:NE2	1:D:796:GLU:O	1.97	0.97
1:D:662:TYR:CZ	1:E:649:LYS:CB	2.47	0.97
1:A:507:TYR:OH	1:B:433:ARG:HB3	1.65	0.97
1:C:201:ALA:HB3	1:D:405:VAL:HG23	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:VAL:HB	2:D:1001:ATP:N1	1.78	0.96
1:A:845:LEU:CD1	1:F:595:ARG:CA	2.32	0.96
1:A:845:LEU:HD12	1:F:595:ARG:CG	1.95	0.96
1:A:507:TYR:OH	1:B:433:ARG:HB2	1.63	0.96
1:D:595:ARG:CZ	1:E:842:LEU:HD13	1.96	0.95
1:D:104:LYS:HZ3	1:E:122:ASN:HA	0.85	0.95
1:C:59:ARG:CG	1:D:24:ASP:HA	1.97	0.95
1:C:59:ARG:O	1:D:24:ASP:HB3	1.67	0.95
1:C:59:ARG:CZ	1:D:81:PRO:HG3	1.97	0.94
1:A:141:LYS:NZ	1:F:107:LYS:CB	2.29	0.94
1:B:322:ARG:HB2	1:C:677:TYR:OH	1.68	0.94
1:D:595:ARG:HB3	1:E:845:LEU:CD1	1.97	0.94
1:D:217:GLY:HA2	2:D:1001:ATP:O2A	1.66	0.94
1:B:704:ASP:CG	1:C:826:ARG:HH22	1.70	0.94
1:D:301:LEU:CD1	1:E:248:LEU:HD22	1.94	0.94
1:C:650:TYR:O	1:C:650:TYR:CD1	2.21	0.93
1:D:104:LYS:HZ3	1:E:122:ASN:CA	1.78	0.93
1:D:186:VAL:CG1	2:D:1001:ATP:C2	2.50	0.93
1:D:616:SER:HA	2:D:1002:ATP:O2B	1.69	0.93
1:D:596:LEU:HD23	1:E:841:ALA:CB	1.97	0.93
1:B:322:ARG:CZ	1:C:666:ASP:HA	1.99	0.93
1:A:797:GLN:HG2	1:F:604:PRO:HG2	1.51	0.92
1:B:596:LEU:CD2	1:C:838:ASN:OD1	2.17	0.92
1:A:141:LYS:HE2	1:F:107:LYS:CA	1.97	0.92
1:A:846:LYS:HA	1:F:570:ILE:CD1	1.98	0.92
1:B:107:LYS:HD2	1:C:118:PHE:HE2	1.18	0.92
1:A:141:LYS:NZ	1:F:107:LYS:CA	2.31	0.91
1:A:433:ARG:NH2	1:F:503:ALA:CB	2.32	0.91
1:D:104:LYS:HZ2	1:E:122:ASN:CA	1.78	0.91
1:E:45:ASP:OD2	1:F:24:ASP:HB3	1.71	0.91
1:C:650:TYR:O	1:C:650:TYR:HD1	1.50	0.91
1:B:322:ARG:HH22	1:C:666:ASP:HA	1.26	0.90
1:C:202:ARG:HH11	1:D:398:ILE:HG12	1.31	0.90
1:B:662:TYR:CE1	1:C:649:LYS:HG2	2.05	0.90
1:B:104:LYS:HG2	1:C:138:GLU:HG3	1.54	0.90
1:B:603:ASN:N	1:C:833:GLN:OE1	2.05	0.90
1:C:202:ARG:NH1	1:D:398:ILE:HG13	1.83	0.90
1:C:59:ARG:NH1	1:D:81:PRO:CG	2.25	0.90
1:E:201:ALA:CB	1:F:405:VAL:CG2	2.49	0.90
1:A:433:ARG:HH21	1:F:503:ALA:HB1	1.30	0.89
1:C:203:ARG:HE	1:D:362:HIS:HB3	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:CZ	1:D:398:ILE:HG13	2.02	0.89
1:E:201:ALA:HB3	1:F:405:VAL:CG2	2.01	0.89
1:B:107:LYS:HD3	1:C:118:PHE:HD2	1.12	0.89
1:A:844:ILE:CD1	1:F:601:LEU:HG	2.02	0.89
1:A:507:TYR:CZ	1:B:433:ARG:HB2	2.06	0.89
1:C:59:ARG:NH2	1:D:26:GLN:HG3	1.66	0.88
1:D:104:LYS:HZ1	1:E:136:ASP:CA	1.85	0.88
1:A:844:ILE:CD1	1:F:601:LEU:CG	2.51	0.88
1:A:105:GLN:HG2	1:F:141:LYS:HZ3	1.37	0.88
1:C:202:ARG:CA	1:D:401:ALA:CB	2.46	0.88
1:D:266:LYS:HD3	1:E:253:ALA:CB	2.04	0.88
1:B:599:SER:CB	1:C:841:ALA:HB1	1.90	0.88
1:B:596:LEU:HD13	1:C:833:GLN:HG2	1.56	0.88
1:B:322:ARG:HH22	1:C:666:ASP:CA	1.87	0.87
1:B:601:LEU:CD2	1:C:840:LEU:HD23	2.04	0.87
1:B:601:LEU:O	1:C:837:LEU:HD13	1.73	0.87
1:C:336:GLN:NE2	1:D:553:LEU:HB3	1.90	0.87
1:A:844:ILE:HG21	1:F:599:SER:CB	2.03	0.87
1:C:59:ARG:NH2	1:D:81:PRO:HG3	1.90	0.86
1:C:332:GLU:OE1	1:C:332:GLU:N	2.07	0.86
1:B:601:LEU:HD22	1:C:837:LEU:CD2	2.04	0.86
1:A:795:PHE:HA	1:F:603:ASN:HD22	1.38	0.86
2:B:1001:ATP:O1A	2:B:1001:ATP:O2G	1.93	0.86
1:D:266:LYS:CE	1:E:249:ALA:CB	2.43	0.86
1:D:104:LYS:HZ2	1:E:122:ASN:HA	1.33	0.86
1:E:192:GLU:N	1:E:192:GLU:OE1	2.09	0.86
1:D:186:VAL:CB	2:D:1001:ATP:N1	2.39	0.86
1:D:595:ARG:HB3	1:E:845:LEU:HD11	1.54	0.86
1:D:761:GLU:N	1:D:761:GLU:OE1	2.09	0.86
1:D:104:LYS:NZ	1:E:136:ASP:HA	1.90	0.85
1:B:705:ASP:OD2	1:C:640:ARG:NH1	2.09	0.85
1:C:204:ILE:CB	1:D:397:ASP:OD2	2.24	0.85
1:C:10:ARG:HD3	1:C:276:LYS:NZ	1.92	0.85
1:B:660:ALA:CB	1:C:652:VAL:HG11	2.03	0.85
1:C:59:ARG:HH12	1:D:81:PRO:HG2	1.38	0.85
1:C:377:GLN:OE1	1:D:797:GLN:HG3	1.76	0.85
1:D:109:SER:HB2	1:E:137:ILE:CB	2.02	0.85
1:C:59:ARG:CG	1:D:24:ASP:CA	2.50	0.85
1:A:842:LEU:HD22	1:F:595:ARG:HH12	1.42	0.85
1:A:842:LEU:HD13	1:F:595:ARG:NH1	1.90	0.85
1:B:599:SER:HB3	1:C:841:ALA:CA	2.02	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLN:CD	1:D:553:LEU:HD13	1.98	0.84
2:F:1002:ATP:O1B	2:F:1002:ATP:O3G	1.89	0.84
1:A:795:PHE:CZ	1:F:600:GLY:O	2.30	0.84
1:C:59:ARG:HH22	1:D:26:GLN:HG2	1.02	0.83
1:B:599:SER:HB2	1:C:841:ALA:CA	2.01	0.83
1:A:845:LEU:CD1	1:F:595:ARG:CB	2.53	0.83
1:C:596:LEU:HD12	1:D:841:ALA:HB2	1.61	0.83
1:A:45:ASP:HB3	1:A:275:SER:HA	1.59	0.83
1:B:662:TYR:OH	1:C:649:LYS:CA	2.26	0.83
1:C:59:ARG:HG3	1:D:24:ASP:C	1.99	0.82
1:D:266:LYS:HD3	1:E:253:ALA:HB2	1.61	0.82
1:E:202:ARG:HG2	1:F:401:ALA:CB	2.09	0.82
1:D:662:TYR:OH	1:E:649:LYS:O	1.97	0.82
1:A:137:ILE:HG12	1:F:104:LYS:CB	2.09	0.81
1:A:235:PRO:HA	1:B:408:ASP:OD2	1.79	0.81
1:D:301:LEU:HD13	1:E:248:LEU:HD23	1.57	0.81
1:A:840:LEU:HG	1:F:601:LEU:HD11	1.61	0.81
1:A:844:ILE:CG2	1:F:599:SER:CB	2.55	0.81
1:C:202:ARG:CZ	1:D:398:ILE:CG1	2.58	0.81
1:D:263:GLU:OE1	1:E:256:LYS:CD	2.29	0.81
1:A:795:PHE:HE1	1:F:604:PRO:HD3	1.46	0.81
1:A:845:LEU:HD11	1:F:595:ARG:HA	0.83	0.81
1:C:59:ARG:HA	1:D:24:ASP:HB3	1.63	0.81
1:B:767:SER:C	1:C:830:ARG:NH2	2.32	0.81
1:D:192:GLU:N	1:D:192:GLU:OE1	2.14	0.81
1:A:844:ILE:HD13	1:F:601:LEU:HG	1.62	0.81
1:A:845:LEU:CD1	1:F:595:ARG:HG2	2.11	0.81
1:B:601:LEU:CD1	1:C:840:LEU:HB3	2.10	0.81
1:C:59:ARG:HA	1:D:24:ASP:CG	2.01	0.81
1:B:322:ARG:NH2	1:C:666:ASP:OD1	2.13	0.80
1:A:257:TYR:HB2	1:B:256:LYS:HG3	1.63	0.80
1:A:507:TYR:CE1	1:B:433:ARG:HB2	2.16	0.80
1:D:595:ARG:NE	1:E:842:LEU:HD13	1.95	0.80
1:B:109:SER:HB3	1:C:145:LEU:CD1	2.11	0.80
1:E:381:ARG:CD	1:F:796:GLU:HG2	2.11	0.80
1:D:596:LEU:CD2	1:E:841:ALA:CB	2.56	0.80
1:A:842:LEU:CA	1:F:595:ARG:HD3	2.10	0.80
1:A:141:LYS:HE3	1:F:107:LYS:CB	2.12	0.79
1:B:660:ALA:HB3	1:C:652:VAL:CG1	2.09	0.79
1:A:503:ALA:HA	1:B:426:VAL:HG22	1.63	0.79
1:D:595:ARG:CA	1:E:845:LEU:HD11	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ARG:N	1:D:363:HIS:CE1	2.50	0.79
1:C:322:ARG:CD	1:D:677:TYR:OH	2.28	0.79
1:D:214:PRO:HA	2:D:1001:ATP:O3G	1.82	0.79
1:D:217:GLY:CA	2:D:1001:ATP:O2A	2.29	0.79
1:B:701:GLN:CD	1:C:645:GLU:OE2	2.21	0.79
1:A:115:HIS:NE2	1:F:107:LYS:NZ	2.30	0.79
1:B:650:TYR:CD2	1:B:650:TYR:O	2.36	0.79
1:C:59:ARG:HA	1:D:24:ASP:CB	2.12	0.78
1:C:202:ARG:HG2	1:D:401:ALA:HB2	1.65	0.78
1:B:662:TYR:CG	1:C:649:LYS:HE3	2.17	0.78
1:A:257:TYR:CB	1:B:256:LYS:CG	2.62	0.78
1:D:601:LEU:CD1	1:E:844:ILE:CD1	2.47	0.78
1:C:59:ARG:HH22	1:D:81:PRO:HG3	1.46	0.78
2:C:1001:ATP:O2G	2:C:1001:ATP:O1A	2.01	0.78
1:D:662:TYR:OH	1:E:649:LYS:C	2.22	0.78
1:A:257:TYR:CB	1:B:256:LYS:HG3	2.14	0.77
1:A:141:LYS:CE	1:F:107:LYS:CB	2.62	0.77
2:B:1001:ATP:H5'1	2:B:1001:ATP:H8	1.50	0.77
1:C:10:ARG:HD3	1:C:276:LYS:HZ1	1.47	0.77
1:C:595:ARG:CG	1:D:845:LEU:CD2	2.51	0.77
1:C:202:ARG:N	1:D:401:ALA:HB1	2.00	0.76
1:A:257:TYR:HB2	1:B:256:LYS:CG	2.15	0.76
1:C:764:ASN:CA	1:D:830:ARG:NH2	2.47	0.76
1:A:434:ASP:OD2	1:F:507:TYR:OH	2.04	0.76
1:C:59:ARG:CA	1:D:24:ASP:HB3	2.16	0.76
1:E:204:ILE:CB	1:F:397:ASP:OD2	2.31	0.76
1:D:322:ARG:NH2	1:E:666:ASP:HA	2.01	0.75
1:A:506:ARG:CB	1:B:426:VAL:CG1	2.52	0.75
1:C:202:ARG:CG	1:D:401:ALA:HB2	2.16	0.75
1:C:764:ASN:HA	1:D:830:ARG:HH22	1.50	0.75
1:D:266:LYS:HE3	1:E:249:ALA:HB2	1.67	0.75
1:B:109:SER:HB3	1:C:145:LEU:HD12	1.68	0.75
1:D:322:ARG:CD	1:E:673:ASN:ND2	2.50	0.75
1:C:202:ARG:HG3	1:D:401:ALA:CB	2.16	0.75
1:C:10:ARG:CG	1:C:276:LYS:HZ2	1.99	0.75
1:B:107:LYS:HE3	1:C:106:GLN:CG	2.17	0.75
1:B:192:GLU:N	1:B:192:GLU:OE1	2.16	0.75
1:D:595:ARG:CG	1:E:845:LEU:HD12	2.14	0.75
1:C:596:LEU:CD1	1:D:841:ALA:CB	2.64	0.75
1:D:266:LYS:HE3	1:E:249:ALA:HB1	0.78	0.75
1:E:201:ALA:HB1	1:F:405:VAL:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:CD	1:C:118:PHE:HD2	1.69	0.74
1:D:595:ARG:HB3	1:E:845:LEU:HD12	1.70	0.74
1:F:674:GLN:N	1:F:674:GLN:OE1	2.20	0.74
1:A:845:LEU:HD12	1:F:595:ARG:HB3	1.70	0.73
1:B:310:LEU:HG	1:B:310:LEU:O	1.87	0.73
1:A:141:LYS:HZ3	1:F:107:LYS:HG3	1.53	0.73
1:A:507:TYR:HE1	1:B:429:LYS:O	1.70	0.73
1:A:795:PHE:CE1	1:F:604:PRO:HD3	2.24	0.73
1:C:203:ARG:N	1:D:363:HIS:HE1	1.84	0.73
1:D:662:TYR:CZ	1:E:649:LYS:CD	2.72	0.73
1:C:59:ARG:CG	1:D:24:ASP:C	2.55	0.73
1:C:565:GLU:OE1	1:C:565:GLU:N	2.22	0.73
1:C:202:ARG:CD	1:D:398:ILE:HA	2.19	0.73
1:D:601:LEU:HD11	1:E:844:ILE:HD13	1.69	0.72
1:C:203:ARG:H	1:D:363:HIS:CE1	2.07	0.72
1:E:563:GLU:OE1	1:E:563:GLU:N	2.20	0.72
1:B:662:TYR:CE2	1:C:649:LYS:HB3	2.24	0.72
1:A:795:PHE:HA	1:F:603:ASN:HD21	1.55	0.72
1:A:844:ILE:HD12	1:F:601:LEU:HD12	1.67	0.72
2:A:1002:ATP:O1A	2:A:1002:ATP:O1B	2.06	0.72
1:A:508:PHE:HZ	1:B:430:ALA:O	1.73	0.72
1:B:662:TYR:CG	1:C:649:LYS:CE	2.73	0.72
1:C:10:ARG:CD	1:C:276:LYS:HZ1	2.03	0.72
1:B:601:LEU:CD2	1:C:837:LEU:HD22	2.09	0.71
1:C:203:ARG:NE	1:D:362:HIS:HB3	2.04	0.71
1:B:322:ARG:HD3	1:C:673:ASN:CG	2.11	0.71
1:A:506:ARG:HB3	1:B:426:VAL:HG11	1.68	0.71
1:B:104:LYS:HE3	1:C:138:GLU:OE2	1.91	0.71
1:E:763:LEU:O	1:F:830:ARG:NH2	2.23	0.71
1:C:10:ARG:CG	1:C:276:LYS:NZ	2.54	0.71
1:C:59:ARG:C	1:D:24:ASP:HB3	2.11	0.71
1:B:107:LYS:HE3	1:C:106:GLN:HG3	1.72	0.71
1:A:141:LYS:NZ	1:F:107:LYS:N	2.38	0.70
1:D:322:ARG:HH22	1:E:666:ASP:HA	1.56	0.70
1:A:842:LEU:HD13	1:F:595:ARG:NH2	2.02	0.70
1:A:137:ILE:CG1	1:F:104:LYS:CB	2.70	0.70
1:A:429:LYS:HG3	1:F:499:THR:HG21	1.74	0.70
1:C:595:ARG:CD	1:D:845:LEU:CD2	2.69	0.70
1:D:662:TYR:CE1	1:E:649:LYS:CA	2.70	0.70
1:A:115:HIS:NE2	1:F:107:LYS:HE2	2.02	0.69
1:D:556:ILE:O	1:D:556:ILE:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:SER:O	1:E:834:ASN:ND2	2.25	0.69
1:C:10:ARG:CD	1:C:276:LYS:NZ	2.55	0.69
1:D:601:LEU:HD23	1:E:795:PHE:CE1	2.27	0.69
1:C:377:GLN:CD	1:D:797:GLN:HE21	1.96	0.69
1:E:204:ILE:HD12	1:F:397:ASP:OD1	1.92	0.69
1:B:662:TYR:CZ	1:C:649:LYS:HB3	2.27	0.69
1:A:105:GLN:HG2	1:F:141:LYS:NZ	2.07	0.69
1:D:110:PHE:CZ	1:E:138:GLU:HG2	2.28	0.69
1:B:662:TYR:CZ	1:C:649:LYS:CB	2.76	0.69
1:C:204:ILE:N	1:D:397:ASP:OD2	2.24	0.69
1:D:263:GLU:OE1	1:E:256:LYS:HD3	1.93	0.69
1:A:795:PHE:CA	1:F:603:ASN:ND2	2.49	0.69
1:C:596:LEU:CD1	1:D:841:ALA:HB2	2.23	0.69
1:E:648:GLU:OE1	1:E:648:GLU:N	2.20	0.69
1:A:310:LEU:O	1:A:310:LEU:HG	1.93	0.68
1:A:844:ILE:CB	1:F:599:SER:HB2	2.22	0.68
1:C:764:ASN:ND2	1:D:826:ARG:HG2	2.08	0.68
1:C:10:ARG:HG2	1:C:276:LYS:NZ	2.09	0.68
1:B:322:ARG:NH2	1:C:666:ASP:CB	2.57	0.68
1:E:795:PHE:CG	1:E:795:PHE:O	2.46	0.68
1:C:665:TYR:OH	1:D:663:VAL:HG12	1.93	0.68
1:D:262:GLU:HG2	1:E:252:THR:OG1	1.94	0.68
1:D:805:ASN:OD1	1:D:805:ASN:N	2.27	0.68
1:A:507:TYR:CE1	1:B:429:LYS:O	2.46	0.68
1:B:563:GLU:N	1:B:563:GLU:OE1	2.27	0.68
1:C:201:ALA:HB3	1:D:405:VAL:CG2	2.11	0.68
1:E:381:ARG:CZ	1:F:796:GLU:CA	2.72	0.68
1:A:257:TYR:HB3	1:B:256:LYS:CB	2.24	0.67
1:D:300:ILE:HG21	1:E:287:HIS:NE2	2.09	0.67
1:D:104:LYS:HZ2	1:E:121:PHE:C	1.97	0.67
2:B:1001:ATP:O2G	2:B:1001:ATP:O1B	2.13	0.67
1:A:841:ALA:HB2	1:F:596:LEU:CD2	2.25	0.67
1:E:381:ARG:NH1	1:F:796:GLU:H	1.92	0.67
1:A:235:PRO:CA	1:B:408:ASP:OD2	2.42	0.67
1:A:45:ASP:CB	1:A:275:SER:HA	2.25	0.66
1:C:203:ARG:HG2	1:D:362:HIS:CB	2.24	0.66
1:E:109:SER:HG	1:E:276:LYS:HD3	1.58	0.66
1:A:203:ARG:HD3	1:B:359:TYR:CE1	2.30	0.66
1:D:301:LEU:HB2	1:E:248:LEU:HD21	1.75	0.66
1:E:377:GLN:HE22	1:F:797:GLN:CG	2.09	0.66
1:B:104:LYS:HG2	1:C:138:GLU:CG	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:ARG:HA	1:E:387:ARG:NE	2.11	0.66
1:C:202:ARG:NE	1:D:398:ILE:HA	2.11	0.65
1:B:701:GLN:NE2	1:C:645:GLU:OE2	2.30	0.65
1:A:842:LEU:CD2	1:F:595:ARG:NH1	2.59	0.65
1:C:764:ASN:HD21	1:D:826:ARG:HG2	1.61	0.65
1:A:258:LYS:HB3	1:B:255:ALA:O	1.97	0.65
1:A:838:ASN:CG	1:F:592:ASN:HB3	2.16	0.65
1:F:650:TYR:O	1:F:650:TYR:CD1	2.49	0.65
1:C:110:PHE:HZ	1:C:176:GLU:HG2	1.62	0.65
1:B:107:LYS:NZ	1:C:115:HIS:CD2	2.65	0.64
1:A:845:LEU:HD13	1:F:569:LEU:HB3	1.79	0.64
1:B:707:ARG:NH2	1:C:640:ARG:HD2	2.11	0.64
1:D:217:GLY:N	2:D:1001:ATP:O2A	2.30	0.64
1:D:852:LYS:HD2	1:D:852:LYS:N	2.11	0.64
1:E:204:ILE:HD12	1:F:397:ASP:OD2	1.96	0.64
1:E:381:ARG:NE	1:F:796:GLU:HG2	2.12	0.64
1:C:203:ARG:HB2	1:D:363:HIS:CE1	2.32	0.64
1:C:563:GLU:OE1	1:C:563:GLU:N	2.27	0.64
1:B:556:ILE:HG13	1:B:556:ILE:O	1.95	0.64
1:B:662:TYR:CD1	1:C:649:LYS:CE	2.77	0.64
1:E:718:CYS:O	1:E:718:CYS:SG	2.55	0.64
1:C:202:ARG:CB	1:D:401:ALA:HB2	2.28	0.64
1:A:844:ILE:HD11	1:F:601:LEU:CD1	2.11	0.64
2:B:1002:ATP:O2G	2:B:1002:ATP:O2B	2.15	0.63
1:C:203:ARG:HG2	1:D:362:HIS:HB3	1.80	0.63
1:C:203:ARG:CZ	1:D:362:HIS:O	2.45	0.63
1:E:794:ARG:HE	1:E:794:ARG:C	1.97	0.63
1:F:386:ARG:HA	1:F:386:ARG:NE	2.14	0.63
1:A:842:LEU:CD1	1:F:595:ARG:NH2	2.62	0.63
1:C:198:ARG:HA	1:D:405:VAL:HG21	1.80	0.63
1:C:203:ARG:HB2	1:D:363:HIS:NE2	2.13	0.63
1:D:322:ARG:HD2	1:E:673:ASN:ND2	2.14	0.63
2:F:1001:ATP:O1B	2:F:1001:ATP:O2G	2.17	0.63
1:A:845:LEU:HD22	1:F:569:LEU:HD13	1.81	0.63
1:E:381:ARG:HD3	1:F:796:GLU:HG2	1.81	0.63
1:E:67:LYS:NZ	1:F:80:GLN:HG2	2.14	0.63
1:D:596:LEU:HD21	1:E:841:ALA:HB2	1.76	0.62
1:E:109:SER:OG	1:E:276:LYS:CD	2.41	0.62
1:C:203:ARG:CG	1:D:362:HIS:HB3	2.28	0.62
1:D:581:VAL:H	2:D:1002:ATP:HN62	1.48	0.62
1:A:645:GLU:CD	1:F:756:GLN:HG2	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:ILE:O	1:C:556:ILE:HG13	1.98	0.62
1:D:186:VAL:HA	2:D:1001:ATP:C2	2.35	0.62
1:C:59:ARG:HG3	1:D:24:ASP:CB	2.27	0.62
1:C:595:ARG:HG2	1:D:845:LEU:HD21	1.77	0.62
1:B:875:GLU:HG3	1:B:875:GLU:O	1.99	0.62
1:A:115:HIS:CE1	1:F:107:LYS:NZ	2.68	0.62
1:A:508:PHE:CE1	1:B:430:ALA:HB1	2.35	0.62
1:A:845:LEU:CD1	1:F:595:ARG:CG	2.68	0.62
1:A:192:GLU:OE1	1:A:192:GLU:N	2.29	0.61
1:A:645:GLU:CD	1:F:756:GLN:HE21	2.02	0.61
1:A:842:LEU:HD13	1:F:595:ARG:CD	2.28	0.61
1:C:332:GLU:HB3	1:D:386:ARG:CZ	2.29	0.61
2:C:1002:ATP:H5'2	2:C:1002:ATP:C8	2.35	0.61
1:D:186:VAL:CB	2:D:1001:ATP:C2	2.82	0.61
1:D:595:ARG:HA	1:E:845:LEU:HD11	1.82	0.61
1:B:601:LEU:HD21	1:C:840:LEU:CD2	2.19	0.61
1:D:652:VAL:O	1:D:652:VAL:HG22	1.98	0.61
1:C:204:ILE:H	1:D:397:ASP:CG	2.04	0.61
2:E:1001:ATP:O1A	2:E:1001:ATP:O1B	2.13	0.61
1:A:508:PHE:CZ	1:B:430:ALA:O	2.52	0.61
1:B:596:LEU:HD21	1:C:838:ASN:N	2.16	0.61
1:C:202:ARG:HG3	1:D:401:ALA:HB3	1.79	0.61
1:A:80:GLN:OE1	1:A:80:GLN:N	2.27	0.61
1:B:53:ASN:OD1	1:B:53:ASN:C	2.32	0.61
1:D:595:ARG:CD	1:E:842:LEU:HD13	2.31	0.61
1:C:202:ARG:CA	1:D:401:ALA:HB1	2.30	0.61
1:A:841:ALA:HB2	1:F:596:LEU:HD23	1.81	0.60
1:B:601:LEU:HD11	1:C:840:LEU:CB	2.21	0.60
1:B:662:TYR:CZ	1:C:649:LYS:HA	2.36	0.60
2:C:1001:ATP:O1A	2:C:1001:ATP:O1B	2.18	0.60
1:A:507:TYR:O	1:A:507:TYR:CD2	2.54	0.60
1:B:599:SER:HG	1:C:841:ALA:CB	2.14	0.60
1:A:797:GLN:HG2	1:F:604:PRO:CG	2.28	0.60
1:A:840:LEU:HG	1:F:601:LEU:CD1	2.32	0.60
1:A:842:LEU:HB2	1:F:595:ARG:NH1	2.16	0.60
1:D:322:ARG:HD2	1:E:673:ASN:HD21	1.66	0.60
1:D:595:ARG:CZ	1:E:842:LEU:CD1	2.76	0.60
1:C:207:ASN:OD1	1:C:207:ASN:C	2.40	0.60
1:C:601:LEU:HD11	1:D:844:ILE:CD1	2.22	0.60
1:D:301:LEU:HD12	1:E:248:LEU:HD22	1.81	0.60
1:A:105:GLN:OE1	1:F:105:GLN:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HB3	1:B:408:ASP:OD2	2.01	0.60
1:C:59:ARG:NE	1:D:24:ASP:O	2.34	0.60
1:C:601:LEU:CD1	1:D:844:ILE:HD12	2.24	0.60
1:A:795:PHE:HZ	1:F:600:GLY:O	1.82	0.60
1:D:617:GLY:O	2:D:1002:ATP:H8	1.84	0.60
1:D:831:LEU:C	1:D:831:LEU:HD13	2.22	0.60
2:B:1002:ATP:O2A	2:B:1002:ATP:O1B	2.18	0.59
1:B:322:ARG:HB2	1:C:677:TYR:HH	1.65	0.59
1:B:596:LEU:HD13	1:C:833:GLN:CG	2.31	0.59
1:A:838:ASN:HB3	1:F:592:ASN:CG	2.22	0.59
1:E:819:TYR:CD1	1:E:819:TYR:C	2.69	0.59
1:B:322:ARG:CD	1:C:673:ASN:CG	2.71	0.59
1:D:263:GLU:OE1	1:E:256:LYS:HD2	2.00	0.59
1:A:40:ILE:HG22	1:A:40:ILE:O	2.03	0.59
1:A:844:ILE:HD12	1:F:601:LEU:HD11	1.51	0.59
1:D:387:ARG:NE	1:D:387:ARG:HA	2.18	0.59
1:A:842:LEU:HB2	1:F:595:ARG:HH11	1.67	0.59
1:C:202:ARG:HD2	1:D:398:ILE:HA	1.83	0.59
1:A:257:TYR:HB3	1:B:256:LYS:CG	2.33	0.58
1:B:596:LEU:CD1	1:C:833:GLN:HG2	2.31	0.58
1:B:711:GLY:O	1:C:653:SER:HB3	2.03	0.58
1:F:386:ARG:HA	1:F:386:ARG:HE	1.68	0.58
1:C:595:ARG:NH1	1:D:842:LEU:HD13	2.18	0.58
1:C:60:TYR:OH	1:D:26:GLN:CD	2.37	0.58
1:D:700:LEU:O	1:D:700:LEU:HD23	2.03	0.58
1:A:650:TYR:O	1:A:650:TYR:CD2	2.56	0.58
1:B:333:ARG:HD3	1:C:386:ARG:NH1	2.18	0.58
2:D:1002:ATP:N3	2:D:1002:ATP:H2'	2.18	0.58
1:A:503:ALA:HB2	1:B:425:GLN:HE22	1.68	0.58
1:A:246:LEU:N	1:A:246:LEU:HD12	2.19	0.58
1:C:197:ILE:HG22	1:D:405:VAL:HG11	1.84	0.58
1:A:296:ASP:OD1	1:B:248:LEU:HD23	2.03	0.58
1:B:322:ARG:CD	1:C:673:ASN:OD1	2.52	0.58
1:B:322:ARG:HD2	1:C:673:ASN:OD1	2.04	0.57
1:D:104:LYS:NZ	1:E:121:PHE:O	2.35	0.57
1:D:772:PHE:CD1	1:D:772:PHE:N	2.71	0.57
1:D:619:GLY:N	2:D:1002:ATP:O2A	2.28	0.57
1:E:595:ARG:HG2	1:F:845:LEU:CD1	2.35	0.57
1:C:642:ASP:OD1	1:C:642:ASP:N	2.33	0.57
1:C:702:MET:SD	1:C:702:MET:N	2.78	0.57
1:B:601:LEU:O	1:C:837:LEU:CD1	2.49	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD22	1:F:569:LEU:CD1	2.35	0.57
1:E:377:GLN:HE22	1:F:797:GLN:HG2	1.69	0.57
1:C:377:GLN:OE1	1:D:797:GLN:NE2	2.35	0.56
1:C:126:ILE:HD12	1:C:126:ILE:H	1.70	0.56
1:D:186:VAL:HG12	2:D:1001:ATP:H2	1.58	0.56
1:D:240:GLY:O	1:D:277:THR:OG1	2.22	0.56
1:D:729:LEU:C	1:D:729:LEU:HD23	2.26	0.56
1:B:649:LYS:O	1:B:651:ALA:N	2.39	0.56
1:C:203:ARG:HG2	1:D:362:HIS:CD2	2.39	0.56
1:A:838:ASN:OD1	1:F:592:ASN:HB3	2.05	0.56
1:B:596:LEU:HD21	1:C:838:ASN:OD1	2.03	0.56
1:C:202:ARG:CB	1:D:401:ALA:CB	2.82	0.56
1:C:204:ILE:CA	1:D:397:ASP:OD2	2.54	0.56
1:B:662:TYR:CZ	1:C:649:LYS:CA	2.89	0.56
1:C:9:GLU:OE1	1:C:9:GLU:N	2.29	0.56
1:C:650:TYR:CD1	1:C:650:TYR:C	2.79	0.56
2:E:1001:ATP:O1G	2:E:1001:ATP:O1B	2.23	0.56
2:D:1001:ATP:O1A	2:D:1001:ATP:O1B	2.24	0.55
1:D:6:GLN:N	1:E:138:GLU:OE2	2.39	0.55
1:B:109:SER:HB3	1:C:145:LEU:HD13	1.89	0.55
1:C:202:ARG:HH21	1:D:397:ASP:HB3	1.70	0.55
1:A:257:TYR:CG	1:B:256:LYS:HB3	2.41	0.55
1:B:708:ILE:O	1:B:708:ILE:CG2	2.54	0.55
1:C:262:GLU:OE1	1:C:262:GLU:N	2.31	0.55
1:D:621:THR:OG1	2:D:1002:ATP:O3G	2.25	0.55
1:A:429:LYS:HG3	1:F:499:THR:CG2	2.36	0.55
1:C:336:GLN:OE1	1:D:553:LEU:HD13	2.05	0.55
1:D:322:ARG:HB2	1:E:677:TYR:OH	2.07	0.55
1:F:831:LEU:HD23	1:F:831:LEU:C	2.27	0.55
1:C:203:ARG:CB	1:D:363:HIS:NE2	2.70	0.55
1:C:641:VAL:N	1:C:684:LEU:O	2.40	0.55
1:A:507:TYR:HB2	1:B:429:LYS:HD3	1.88	0.54
1:F:337:LYS:NZ	1:F:339:GLU:OE2	2.40	0.54
1:A:134:GLN:OE1	1:A:134:GLN:N	2.27	0.54
1:A:203:ARG:NH2	1:B:358:LYS:HB3	2.23	0.54
1:A:203:ARG:HD3	1:B:359:TYR:CD1	2.42	0.54
1:B:328:ASP:OD2	1:B:331:PHE:N	2.40	0.54
1:E:583:GLN:HA	1:E:583:GLN:OE1	2.07	0.54
1:B:565:GLU:HB3	1:C:845:LEU:HD11	1.89	0.54
1:C:336:GLN:CG	1:D:553:LEU:HD22	2.38	0.54
1:D:257:TYR:HB3	1:E:256:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LYS:NZ	1:C:339:GLU:OE2	2.40	0.54
1:A:257:TYR:CE1	1:B:257:TYR:CZ	2.95	0.54
2:E:1002:ATP:O1A	2:E:1002:ATP:O1B	2.24	0.54
1:A:257:TYR:HB3	1:B:256:LYS:HG3	1.87	0.54
1:A:258:LYS:HE3	1:B:252:THR:CG2	2.38	0.54
1:D:262:GLU:OE1	1:D:262:GLU:N	2.41	0.54
1:F:649:LYS:O	1:F:651:ALA:N	2.41	0.54
1:A:136:ASP:C	1:A:136:ASP:OD1	2.45	0.54
1:D:104:LYS:NZ	1:E:122:ASN:C	2.60	0.54
1:A:9:GLU:OE1	1:A:9:GLU:N	2.32	0.53
1:A:483:LEU:C	1:A:483:LEU:HD23	2.29	0.53
1:C:765:ARG:HA	1:D:826:ARG:HH21	1.72	0.53
1:F:278:LEU:C	1:F:278:LEU:HD23	2.28	0.53
1:D:772:PHE:N	1:D:772:PHE:HD1	2.05	0.53
1:C:59:ARG:HH22	1:D:81:PRO:CG	2.20	0.53
1:D:378:LEU:C	1:D:378:LEU:HD23	2.29	0.53
1:D:403:VAL:O	1:D:407:ARG:N	2.42	0.53
1:D:650:TYR:CD1	1:D:650:TYR:C	2.82	0.53
1:B:662:TYR:CG	1:C:649:LYS:HE2	2.44	0.53
1:A:507:TYR:CE1	1:B:429:LYS:HG2	2.41	0.53
1:B:337:LYS:NZ	1:C:677:TYR:O	2.42	0.53
1:A:126:ILE:HG22	1:A:126:ILE:O	2.08	0.53
1:C:763:LEU:O	1:D:830:ARG:NH2	2.41	0.53
1:C:333:ARG:NH2	1:D:386:ARG:HA	2.23	0.53
1:D:301:LEU:CD1	1:E:248:LEU:HD21	2.17	0.53
1:F:466:TYR:CD1	1:F:466:TYR:N	2.75	0.53
1:C:596:LEU:HD12	1:D:841:ALA:HB3	1.83	0.53
1:C:655:LEU:N	1:C:655:LEU:HD23	2.24	0.53
1:A:433:ARG:HH22	1:F:503:ALA:CB	2.22	0.53
1:D:365:VAL:HG23	1:D:365:VAL:O	2.09	0.53
1:A:202:ARG:HA	1:B:363:HIS:CE1	2.44	0.52
1:A:257:TYR:CD1	1:B:256:LYS:HB3	2.44	0.52
1:A:508:PHE:CZ	1:B:430:ALA:HB1	2.42	0.52
1:F:50:TYR:C	1:F:50:TYR:CD1	2.81	0.52
1:A:235:PRO:CB	1:B:408:ASP:OD2	2.57	0.52
1:C:377:GLN:NE2	1:D:796:GLU:C	2.62	0.52
1:B:595:ARG:HD3	1:C:842:LEU:HD21	1.91	0.52
1:B:322:ARG:CD	1:C:673:ASN:ND2	2.72	0.52
1:B:764:ASN:HB3	1:C:823:MET:HE2	1.92	0.52
1:B:322:ARG:NH2	1:C:666:ASP:CG	2.63	0.52
1:D:831:LEU:HD13	1:D:831:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:O	1:A:291:GLY:N	2.43	0.52
1:A:433:ARG:NH2	1:F:503:ALA:HB3	2.19	0.52
1:B:107:LYS:NZ	1:C:118:PHE:CD2	2.78	0.52
1:B:764:ASN:ND2	1:C:823:MET:HG2	2.25	0.52
1:A:797:GLN:CG	1:F:604:PRO:HG2	2.32	0.52
1:B:322:ARG:NE	1:C:673:ASN:ND2	2.58	0.52
1:A:506:ARG:HB2	1:B:426:VAL:HG13	1.83	0.52
1:B:107:LYS:CE	1:C:118:PHE:HD2	2.23	0.52
1:F:130:PHE:O	1:F:130:PHE:CD1	2.63	0.52
2:B:1002:ATP:H3'	2:B:1002:ATP:N3	2.25	0.52
1:D:618:SER:C	2:D:1002:ATP:N7	2.63	0.52
1:B:107:LYS:CE	1:C:118:PHE:CD2	2.90	0.51
1:D:700:LEU:HD23	1:D:700:LEU:C	2.31	0.51
1:E:309:GLN:N	1:E:309:GLN:OE1	2.42	0.51
1:B:107:LYS:NZ	1:C:118:PHE:HD2	2.08	0.51
1:D:184:ASP:OD1	1:D:358:LYS:NZ	2.42	0.51
1:A:844:ILE:HD11	1:F:601:LEU:CG	2.36	0.51
1:B:766:ILE:O	1:C:830:ARG:NE	2.36	0.51
1:D:332:GLU:O	1:E:386:ARG:NH2	2.43	0.51
1:F:831:LEU:HD23	1:F:831:LEU:O	2.10	0.51
1:C:601:LEU:HD12	1:D:841:ALA:HA	1.92	0.51
1:D:852:LYS:HD2	1:D:852:LYS:H	1.75	0.51
1:E:381:ARG:HH12	1:F:796:GLU:H	1.57	0.51
1:C:595:ARG:CD	1:D:845:LEU:HD23	2.41	0.51
1:D:202:ARG:HD3	1:E:398:ILE:HG12	1.93	0.51
1:C:595:ARG:HD3	1:D:845:LEU:HD23	1.92	0.51
1:B:104:LYS:CG	1:C:138:GLU:HG3	2.33	0.51
1:A:725:MET:SD	1:A:725:MET:N	2.84	0.51
1:B:289:LEU:O	1:B:290:MET:HB2	2.10	0.51
1:A:318:ASN:OD1	1:A:318:ASN:N	2.44	0.50
1:B:606:GLN:HG3	1:C:826:ARG:NH2	2.27	0.50
1:B:766:ILE:O	1:C:830:ARG:NH1	2.33	0.50
1:D:215:GLY:N	2:D:1001:ATP:O2B	2.43	0.50
1:D:107:LYS:HE3	1:E:123:ASP:OD2	2.11	0.50
1:E:819:TYR:C	1:E:819:TYR:HD1	2.12	0.50
1:D:186:VAL:CA	2:D:1001:ATP:N1	2.74	0.50
1:F:410:LYS:O	1:F:410:LYS:HG3	2.11	0.50
1:A:846:LYS:CA	1:F:570:ILE:HD11	2.25	0.50
1:B:662:TYR:CZ	1:C:649:LYS:HG2	2.46	0.50
1:D:322:ARG:HD3	1:E:673:ASN:ND2	2.24	0.50
1:F:294:LYS:HG3	1:F:295:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:NH1	1:C:666:ASP:HA	2.26	0.50
1:B:704:ASP:CB	1:C:826:ARG:HH22	2.25	0.50
1:C:205:LYS:NZ	1:D:394:ASP:OD2	2.40	0.50
1:A:302:LYS:N	1:A:303:PRO:HD2	2.26	0.50
1:B:599:SER:CB	1:C:841:ALA:HB2	2.10	0.50
1:D:662:TYR:CZ	1:E:649:LYS:HD3	2.42	0.50
1:D:301:LEU:CB	1:E:248:LEU:HD21	2.40	0.50
1:E:211:ILE:HD12	1:E:211:ILE:N	2.27	0.50
1:F:58:GLY:O	1:F:59:ARG:HB3	2.10	0.50
1:F:556:ILE:O	1:F:680:TYR:OH	2.29	0.50
1:A:794:ARG:C	1:F:603:ASN:ND2	2.64	0.49
1:F:483:LEU:C	1:F:483:LEU:HD23	2.32	0.49
1:A:115:HIS:CE1	1:F:107:LYS:HZ1	2.30	0.49
1:A:257:TYR:HB3	1:B:256:LYS:CA	2.42	0.49
1:B:40:ILE:HG22	1:B:40:ILE:O	2.10	0.49
1:D:104:LYS:HZ2	1:E:122:ASN:N	2.10	0.49
1:D:393:LEU:CD1	2:D:1001:ATP:H1'	2.42	0.49
1:B:704:ASP:HB2	1:C:826:ARG:NH2	2.27	0.49
1:F:134:GLN:HA	1:F:134:GLN:OE1	2.11	0.49
1:E:794:ARG:O	1:E:796:GLU:N	2.45	0.49
1:A:115:HIS:CE1	1:F:107:LYS:HE3	2.44	0.49
1:C:187:ILE:C	1:C:187:ILE:HD12	2.33	0.49
1:C:595:ARG:HD3	1:D:845:LEU:CD2	2.43	0.49
1:E:67:LYS:HZ3	1:F:80:GLN:HG2	1.76	0.49
1:B:539:ASN:O	1:B:540:VAL:C	2.50	0.49
1:C:197:ILE:HG22	1:D:405:VAL:CG1	2.42	0.49
1:E:794:ARG:O	1:E:794:ARG:HG3	2.12	0.49
1:C:10:ARG:HD3	1:C:276:LYS:CE	2.42	0.49
1:A:27:HIS:ND1	1:A:34:HIS:NE2	2.54	0.49
1:A:842:LEU:CD1	1:F:595:ARG:CD	2.90	0.49
1:B:819:TYR:CD1	1:B:819:TYR:N	2.81	0.49
1:F:365:VAL:HG13	1:F:365:VAL:O	2.13	0.49
1:E:120:LEU:O	1:E:124:SER:N	2.45	0.49
1:E:705:ASP:O	1:E:707:ARG:N	2.46	0.49
1:D:257:TYR:CD2	1:E:256:LYS:O	2.66	0.49
1:D:266:LYS:CD	1:E:253:ALA:HB2	2.39	0.49
1:D:616:SER:CA	2:D:1002:ATP:O2B	2.52	0.49
1:E:852:LYS:N	1:E:852:LYS:HD2	2.28	0.49
1:A:105:GLN:NE2	1:F:105:GLN:OE1	2.46	0.48
1:C:647:SER:OG	1:C:648:GLU:N	2.46	0.48
1:A:257:TYR:CB	1:B:256:LYS:CB	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.36	0.48
1:D:595:ARG:HD3	1:E:842:LEU:HD13	1.95	0.48
1:F:31:GLN:HB2	1:F:32:PRO:HD2	1.95	0.48
1:C:10:ARG:HG2	1:C:276:LYS:HZ2	1.69	0.48
1:C:665:TYR:CZ	1:D:663:VAL:HG12	2.48	0.48
1:C:668:GLY:O	1:C:672:THR:N	2.47	0.48
1:D:186:VAL:HB	2:D:1001:ATP:C6	2.47	0.48
1:B:720:ASN:OD1	1:B:720:ASN:N	2.45	0.48
1:C:761:GLU:OE1	1:C:761:GLU:N	2.35	0.48
1:E:794:ARG:O	1:E:794:ARG:CG	2.61	0.48
1:F:58:GLY:O	1:F:59:ARG:CB	2.60	0.48
1:F:276:LYS:O	1:F:277:THR:OG1	2.28	0.48
1:F:278:LEU:HD23	1:F:278:LEU:O	2.14	0.48
1:C:187:ILE:HD12	1:C:187:ILE:O	2.14	0.48
1:E:45:ASP:CG	1:F:24:ASP:HB3	2.34	0.48
1:B:107:LYS:HB2	1:C:106:GLN:HE22	1.66	0.48
1:B:651:ALA:HA	1:B:656:LEU:HB3	1.95	0.48
1:D:378:LEU:HD23	1:D:378:LEU:O	2.14	0.48
1:A:795:PHE:CE1	1:F:604:PRO:CD	2.94	0.48
1:B:650:TYR:O	1:B:650:TYR:CG	2.60	0.48
1:A:842:LEU:CB	1:F:595:ARG:HD3	2.43	0.48
1:A:105:GLN:HE21	1:F:141:LYS:NZ	2.11	0.48
1:A:840:LEU:HD23	1:F:601:LEU:HD13	1.95	0.48
1:F:50:TYR:CD1	1:F:50:TYR:O	2.67	0.48
1:B:388:LEU:O	1:B:389:PRO:C	2.53	0.47
1:B:785:ASP:OD1	1:B:789:LYS:NZ	2.44	0.47
2:B:1001:ATP:H5'1	2:B:1001:ATP:C8	2.42	0.47
1:A:246:LEU:O	1:A:247:ASP:CB	2.62	0.47
1:C:649:LYS:O	1:C:651:ALA:N	2.47	0.47
1:D:670:PHE:C	1:D:670:PHE:CD2	2.87	0.47
1:B:772:PHE:CD1	1:B:772:PHE:N	2.81	0.47
1:C:655:LEU:HD23	1:C:655:LEU:H	1.79	0.47
1:D:765:ARG:CD	1:E:826:ARG:NE	2.78	0.47
1:B:322:ARG:HH22	1:C:666:ASP:CG	2.17	0.47
1:B:322:ARG:NE	1:C:673:ASN:HD21	2.12	0.47
1:F:211:ILE:HD12	1:F:211:ILE:N	2.30	0.47
1:C:15:LEU:C	1:C:15:LEU:HD13	2.34	0.47
1:E:246:LEU:N	1:E:246:LEU:HD12	2.30	0.47
1:B:373:VAL:HG11	1:C:797:GLN:OE1	2.14	0.47
1:C:203:ARG:HE	1:D:362:HIS:CB	2.18	0.47
1:D:186:VAL:HA	2:D:1001:ATP:H2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ILE:HG21	1:E:287:HIS:CE1	2.49	0.47
1:D:322:ARG:HD3	1:E:673:ASN:CG	2.34	0.47
1:E:854:THR:OG1	1:E:855:VAL:N	2.47	0.47
1:B:599:SER:HG	1:C:841:ALA:HB2	1.67	0.47
1:D:186:VAL:CG1	2:D:1001:ATP:N1	2.72	0.47
1:E:283:ILE:N	1:E:283:ILE:HD12	2.30	0.47
1:A:507:TYR:CD1	1:B:429:LYS:C	2.89	0.47
1:B:421:LEU:C	1:B:421:LEU:HD23	2.35	0.47
1:D:6:GLN:CG	1:E:138:GLU:OE2	2.43	0.47
1:D:650:TYR:O	1:D:651:ALA:C	2.53	0.47
1:D:668:GLY:O	1:D:672:THR:N	2.48	0.47
1:A:257:TYR:CZ	1:B:257:TYR:CZ	3.02	0.47
1:A:795:PHE:CA	1:F:603:ASN:HD21	2.20	0.47
1:C:246:LEU:HD22	1:C:246:LEU:N	2.30	0.47
1:E:725:MET:N	1:E:725:MET:SD	2.88	0.47
1:F:89:SER:OG	1:F:90:TYR:N	2.48	0.47
2:A:1001:ATP:O1B	2:A:1001:ATP:O2G	2.33	0.46
1:C:377:GLN:OE1	1:D:797:GLN:CG	2.57	0.46
1:D:333:ARG:HG3	1:E:214:PRO:HB2	1.97	0.46
1:E:595:ARG:HG2	1:F:845:LEU:HD11	1.96	0.46
1:B:53:ASN:OD1	1:B:53:ASN:O	2.32	0.46
1:B:799:ASP:OD2	1:B:800:LYS:NZ	2.47	0.46
1:D:377:GLN:HE22	1:E:797:GLN:HG2	1.80	0.46
1:D:542:ASP:OD1	1:D:543:SER:N	2.48	0.46
1:A:53:ASN:OD1	1:A:53:ASN:C	2.53	0.46
1:A:203:ARG:CD	1:B:359:TYR:CD1	2.97	0.46
1:B:410:LYS:N	1:B:411:PRO:CD	2.78	0.46
1:C:204:ILE:HG12	1:D:359:TYR:HE1	1.79	0.46
1:C:632:PHE:CD1	1:C:632:PHE:N	2.84	0.46
1:D:618:SER:O	2:D:1002:ATP:N7	2.49	0.46
1:D:880:LEU:CB	1:D:881:PRO:CD	2.94	0.46
1:E:823:MET:HG3	1:E:824:GLY:O	2.15	0.46
1:A:507:TYR:CZ	1:B:433:ARG:CB	2.83	0.46
1:D:186:VAL:CA	2:D:1001:ATP:C2	2.98	0.46
1:D:652:VAL:O	1:D:652:VAL:CG2	2.62	0.46
1:E:764:ASN:HB3	1:F:826:ARG:HD3	1.97	0.46
1:A:508:PHE:CE2	1:B:430:ALA:HA	2.51	0.46
1:E:289:LEU:O	1:E:290:MET:HB2	2.15	0.46
1:A:506:ARG:HB3	1:B:426:VAL:CG1	2.36	0.46
1:C:201:ALA:HB1	1:D:405:VAL:HG23	1.84	0.46
1:C:569:LEU:HB2	1:D:845:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:LEU:O	1:F:278:LEU:CD2	2.64	0.46
1:A:141:LYS:HZ3	1:F:107:LYS:N	2.12	0.46
1:B:704:ASP:CB	1:C:826:ARG:NH2	2.79	0.46
1:D:665:TYR:CD2	1:D:665:TYR:O	2.68	0.46
1:E:365:VAL:HG13	1:E:365:VAL:O	2.16	0.46
2:E:1001:ATP:O1G	2:E:1001:ATP:O2A	2.33	0.46
1:B:107:LYS:HE3	1:C:106:GLN:CD	2.36	0.46
1:D:211:ILE:N	1:D:211:ILE:HD12	2.30	0.46
1:E:685:PHE:CD1	1:E:685:PHE:N	2.83	0.46
1:D:289:LEU:HD22	1:D:289:LEU:N	2.31	0.46
1:F:40:ILE:HG22	1:F:40:ILE:O	2.16	0.46
1:B:708:ILE:O	1:B:708:ILE:HG23	2.14	0.45
2:B:1001:ATP:O1B	2:B:1001:ATP:O2A	2.34	0.45
1:C:332:GLU:CG	1:D:386:ARG:NH2	2.79	0.45
1:C:596:LEU:HD12	1:D:841:ALA:HB1	1.88	0.45
1:D:583:GLN:HG2	1:D:773:ASN:H	1.81	0.45
1:F:130:PHE:O	1:F:130:PHE:HD1	1.97	0.45
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.65	0.45
1:C:336:GLN:CG	1:D:553:LEU:HD13	2.47	0.45
1:D:80:GLN:O	1:D:82:ALA:N	2.50	0.45
1:D:377:GLN:HE22	1:E:797:GLN:CG	2.29	0.45
1:D:596:LEU:HD11	1:E:838:ASN:HA	1.98	0.45
1:E:202:ARG:HG2	1:F:401:ALA:HB2	1.96	0.45
1:E:204:ILE:CD1	1:F:397:ASP:OD2	2.63	0.45
1:E:337:LYS:NZ	1:E:339:GLU:OE2	2.49	0.45
1:F:352:LEU:O	1:F:356:GLN:N	2.50	0.45
1:A:203:ARG:HD2	1:B:359:TYR:HA	1.98	0.45
1:A:812:ASP:O	1:A:816:LYS:N	2.49	0.45
1:B:596:LEU:CD2	1:C:838:ASN:N	2.80	0.45
2:B:1001:ATP:H8	2:B:1001:ATP:C5'	2.26	0.45
1:D:110:PHE:CE2	1:E:138:GLU:HG2	2.51	0.45
1:D:662:TYR:CZ	1:E:649:LYS:HD2	2.37	0.45
1:F:213:GLU:O	1:F:218:LYS:NZ	2.47	0.45
1:A:257:TYR:HB2	1:B:256:LYS:HG2	1.97	0.45
1:D:262:GLU:CG	1:E:252:THR:OG1	2.62	0.45
1:F:610:PHE:CD1	1:F:610:PHE:N	2.83	0.45
1:B:603:ASN:H	1:C:833:GLN:CD	2.19	0.45
1:C:555:GLY:O	1:C:556:ILE:C	2.55	0.45
1:D:705:ASP:O	1:D:707:ARG:N	2.50	0.45
1:D:104:LYS:HZ2	1:E:122:ASN:C	2.20	0.45
1:E:201:ALA:HB3	1:F:405:VAL:HG21	1.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LEU:O	1:E:290:MET:CB	2.65	0.45
1:F:559:LYS:O	1:F:559:LYS:HG2	2.16	0.45
1:D:247:ASP:OD1	1:D:248:LEU:N	2.49	0.45
1:D:880:LEU:HB2	1:D:881:PRO:HD2	1.98	0.45
1:B:107:LYS:NZ	1:C:115:HIS:HD2	2.12	0.45
1:B:638:MET:O	1:B:638:MET:HG3	2.16	0.45
1:D:798:ASN:OD1	1:D:798:ASN:N	2.50	0.45
1:F:51:LEU:HA	1:F:51:LEU:HD23	1.78	0.45
1:A:203:ARG:N	1:B:397:ASP:OD1	2.45	0.45
1:B:326:GLU:OE2	1:C:714:LYS:NZ	2.49	0.45
1:C:652:VAL:HG22	1:C:652:VAL:O	2.17	0.45
1:D:296:ASP:O	1:D:296:ASP:CG	2.53	0.45
1:B:819:TYR:N	1:B:819:TYR:HD1	2.13	0.44
1:E:183:LEU:N	1:E:183:LEU:HD12	2.32	0.44
1:E:352:LEU:O	1:E:356:GLN:N	2.50	0.44
1:E:678:LYS:O	1:E:679:PRO:C	2.55	0.44
1:A:337:LYS:NZ	1:A:339:GLU:OE2	2.50	0.44
1:A:841:ALA:HB2	1:F:596:LEU:HG	1.99	0.44
1:D:601:LEU:HD12	1:E:841:ALA:HA	1.99	0.44
1:A:596:LEU:HD13	1:B:841:ALA:CB	2.48	0.44
1:B:211:ILE:N	1:B:211:ILE:HD12	2.32	0.44
1:D:246:LEU:O	1:D:247:ASP:CB	2.65	0.44
1:D:331:PHE:CG	1:D:332:GLU:N	2.85	0.44
1:D:595:ARG:CD	1:E:845:LEU:HD12	2.46	0.44
1:E:67:LYS:HZ1	1:F:80:GLN:HG2	1.80	0.44
1:A:360:GLU:OE1	1:A:480:LYS:NZ	2.50	0.44
1:B:601:LEU:HD13	1:C:837:LEU:CB	2.24	0.44
1:C:659:THR:CG2	1:D:652:VAL:CG1	2.94	0.44
1:E:143:GLN:OE1	1:E:143:GLN:HA	2.16	0.44
1:B:326:GLU:HG3	1:C:714:LYS:HE2	1.99	0.44
1:D:104:LYS:CE	1:E:136:ASP:HA	2.48	0.44
1:F:729:LEU:HD23	1:F:729:LEU:C	2.38	0.44
2:F:1001:ATP:O1B	2:F:1001:ATP:O2A	2.34	0.44
1:A:583:GLN:OE1	1:A:583:GLN:HA	2.17	0.44
1:B:601:LEU:CD1	1:C:837:LEU:HB3	2.47	0.44
1:B:604:PRO:HD3	1:C:794:ARG:CZ	2.48	0.44
1:C:671:LEU:HD23	1:C:671:LEU:HA	1.68	0.44
1:D:595:ARG:NE	1:E:842:LEU:CD1	2.75	0.44
1:A:508:PHE:CZ	1:B:430:ALA:CA	3.01	0.44
1:B:134:GLN:O	1:B:134:GLN:HG2	2.17	0.44
1:C:332:GLU:HB3	1:D:386:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:ASP:CG	1:D:543:SER:H	2.20	0.44
1:E:201:ALA:HB2	1:F:405:VAL:HG22	1.88	0.44
1:E:202:ARG:HG2	1:F:401:ALA:HB3	1.95	0.44
1:A:137:ILE:HG13	1:A:137:ILE:O	2.17	0.43
1:A:352:LEU:O	1:A:356:GLN:N	2.51	0.43
1:A:507:TYR:CG	1:B:429:LYS:HG2	2.48	0.43
1:B:277:THR:OG1	1:B:278:LEU:N	2.50	0.43
1:C:276:LYS:O	1:C:278:LEU:N	2.51	0.43
1:C:655:LEU:H	1:C:655:LEU:CD2	2.31	0.43
1:E:15:LEU:C	1:E:15:LEU:HD23	2.39	0.43
1:A:528:GLU:H	1:A:528:GLU:CD	2.21	0.43
1:E:597:SER:OG	1:E:598:ARG:N	2.51	0.43
1:B:352:LEU:HB3	1:B:372:LEU:HD22	1.99	0.43
1:B:662:TYR:CD2	1:C:649:LYS:HE2	2.54	0.43
1:A:661:GLY:N	1:B:663:VAL:O	2.49	0.43
1:B:658:THR:H	1:B:667:GLU:HB2	1.83	0.43
1:B:780:ILE:O	1:B:780:ILE:HG22	2.17	0.43
1:F:804:LEU:O	1:F:804:LEU:HG	2.17	0.43
1:A:507:TYR:CD1	1:B:430:ALA:HA	2.52	0.43
1:A:774:LYS:NZ	1:A:821:ASP:OD2	2.50	0.43
1:B:107:LYS:HB2	1:C:106:GLN:CD	2.36	0.43
1:E:204:ILE:CG1	1:F:397:ASP:OD2	2.66	0.43
1:A:507:TYR:CD2	1:B:429:LYS:HE2	2.53	0.43
1:B:190:GLU:H	1:B:190:GLU:CD	2.22	0.43
1:D:612:PHE:CD1	1:D:724:ILE:HG23	2.54	0.43
1:D:620:LYS:HB2	2:D:1002:ATP:O1B	2.18	0.43
1:F:558:VAL:O	1:F:558:VAL:HG22	2.18	0.43
1:A:421:LEU:HD23	1:A:421:LEU:C	2.39	0.43
1:B:826:ARG:N	1:B:827:PRO:CD	2.82	0.43
1:C:601:LEU:HD12	1:D:841:ALA:CA	2.49	0.43
1:A:507:TYR:CE1	1:B:430:ALA:HA	2.53	0.43
1:A:841:ALA:HB2	1:F:596:LEU:CG	2.48	0.43
1:A:845:LEU:CD2	1:F:569:LEU:HD13	2.47	0.43
1:F:835:GLU:OE1	1:F:839:LYS:NZ	2.51	0.43
1:A:286:ILE:O	1:A:286:ILE:HG22	2.17	0.43
1:A:503:ALA:HA	1:B:426:VAL:CG2	2.43	0.43
1:C:246:LEU:N	1:C:246:LEU:CD2	2.82	0.43
1:D:263:GLU:OE1	1:E:256:LYS:NZ	2.50	0.43
1:D:595:ARG:HD3	1:E:845:LEU:HD12	2.01	0.43
1:A:198:ARG:HA	1:B:405:VAL:HG21	2.01	0.43
1:A:507:TYR:HD1	1:B:430:ALA:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ILE:HB	1:F:599:SER:HB2	1.97	0.43
1:B:483:LEU:HD23	1:B:483:LEU:C	2.39	0.43
1:C:20:LYS:HD3	1:C:20:LYS:HA	1.78	0.43
1:C:595:ARG:CB	1:D:845:LEU:HD22	2.45	0.43
1:D:368:LEU:HD12	1:D:368:LEU:N	2.34	0.43
1:D:565:GLU:O	1:D:568:LYS:N	2.52	0.43
1:F:826:ARG:N	1:F:827:PRO:CD	2.82	0.43
1:A:841:ALA:HB1	1:F:596:LEU:N	2.34	0.42
1:B:662:TYR:CE1	1:C:649:LYS:CG	2.91	0.42
1:D:565:GLU:O	1:D:566:ASN:C	2.58	0.42
1:D:595:ARG:CB	1:E:845:LEU:HD12	2.26	0.42
1:D:641:VAL:HG13	1:D:641:VAL:O	2.18	0.42
1:A:410:LYS:HB3	1:A:411:PRO:CD	2.50	0.42
1:A:842:LEU:CG	1:F:595:ARG:NH1	2.82	0.42
1:B:700:LEU:HD12	1:B:700:LEU:C	2.40	0.42
1:C:835:GLU:OE1	1:C:839:LYS:NZ	2.51	0.42
1:D:758:PHE:O	1:D:759:ARG:C	2.58	0.42
1:F:568:LYS:O	1:F:569:LEU:HB2	2.19	0.42
1:D:236:THR:HA	1:D:239:GLN:HB2	2.00	0.42
1:E:67:LYS:NZ	1:F:80:GLN:CG	2.82	0.42
1:F:285:GLU:O	1:F:287:HIS:N	2.52	0.42
1:B:104:LYS:HE2	1:C:138:GLU:HG3	2.01	0.42
1:C:59:ARG:CD	1:D:24:ASP:O	2.65	0.42
1:C:333:ARG:HD2	1:C:333:ARG:N	2.35	0.42
1:A:105:GLN:NE2	1:F:141:LYS:NZ	2.67	0.42
1:A:507:TYR:CD1	1:B:429:LYS:CG	2.85	0.42
1:C:50:TYR:CD2	1:C:51:LEU:HG	2.54	0.42
1:D:581:VAL:N	2:D:1002:ATP:HN62	2.14	0.42
1:E:80:GLN:O	1:E:82:ALA:N	2.52	0.42
1:A:429:LYS:HD3	1:A:429:LYS:HA	1.74	0.42
1:B:434:ASP:OD2	1:B:442:LYS:NZ	2.49	0.42
1:C:129:ILE:HG13	1:C:129:ILE:O	2.18	0.42
1:C:542:ASP:OD1	1:C:543:SER:N	2.51	0.42
1:C:748:ASN:O	1:C:752:GLY:N	2.53	0.42
1:D:612:PHE:CD1	1:D:612:PHE:N	2.87	0.42
1:F:811:LYS:HB3	1:F:811:LYS:HE3	1.87	0.42
1:A:405:VAL:HG21	1:F:198:ARG:HG3	2.02	0.42
1:A:464:GLN:OE1	1:A:464:GLN:HA	2.19	0.42
1:A:519:LYS:HD2	1:A:519:LYS:HA	1.87	0.42
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.88	0.42
1:C:336:GLN:HG2	1:D:553:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:TYR:CD2	1:E:51:LEU:HG	2.55	0.42
1:A:203:ARG:CD	1:B:359:TYR:CE1	3.02	0.42
1:A:795:PHE:HE1	1:F:604:PRO:CD	2.22	0.42
1:C:596:LEU:CD1	1:D:841:ALA:HB3	2.44	0.42
1:D:825:ALA:HB3	2:D:1002:ATP:H1'	2.01	0.42
1:E:107:LYS:HG3	1:E:170:TYR:HE2	1.84	0.42
1:F:583:GLN:OE1	1:F:583:GLN:HA	2.19	0.42
1:A:514:LYS:NZ	1:A:518:GLU:OE2	2.50	0.42
1:A:880:LEU:HB3	1:A:881:PRO:HD3	2.00	0.42
1:B:565:GLU:CB	1:C:845:LEU:HD11	2.41	0.42
1:C:247:ASP:O	1:C:249:ALA:N	2.52	0.42
1:F:648:GLU:OE1	1:F:648:GLU:N	2.41	0.42
1:A:235:PRO:HA	1:B:408:ASP:CG	2.37	0.42
1:A:507:TYR:O	1:A:507:TYR:CG	2.70	0.42
1:F:744:GLU:O	1:F:745:SER:CB	2.68	0.42
1:A:394:ASP:OD2	1:F:205:LYS:NZ	2.47	0.41
1:A:852:LYS:HD2	1:A:852:LYS:N	2.35	0.41
1:D:337:LYS:NZ	1:D:339:GLU:OE1	2.53	0.41
1:D:831:LEU:C	1:D:831:LEU:CD1	2.88	0.41
1:C:203:ARG:HB3	1:D:397:ASP:OD1	2.19	0.41
1:D:662:TYR:CE1	1:E:649:LYS:C	2.93	0.41
1:E:761:GLU:O	1:E:765:ARG:HD3	2.20	0.41
1:F:409:SER:O	1:F:410:LYS:C	2.57	0.41
1:B:305:LEU:HB3	1:B:310:LEU:HB2	2.02	0.41
1:B:322:ARG:HD3	1:C:673:ASN:OD1	2.16	0.41
1:E:725:MET:HE2	1:E:725:MET:HB2	1.95	0.41
1:F:60:TYR:CD1	1:F:60:TYR:C	2.93	0.41
1:B:592:ASN:HB3	1:C:838:ASN:ND2	2.36	0.41
1:E:260:ASP:OD1	1:E:261:PHE:N	2.51	0.41
1:A:205:LYS:NZ	1:B:390:ASP:OD2	2.53	0.41
1:A:851:ASP:OD2	1:A:852:LYS:NZ	2.45	0.41
1:D:53:ASN:OD1	1:D:53:ASN:C	2.57	0.41
1:D:277:THR:OG1	1:D:278:LEU:N	2.53	0.41
1:B:244:PHE:CD1	1:B:244:PHE:N	2.87	0.41
1:B:814:LEU:O	1:B:818:GLY:N	2.53	0.41
1:C:204:ILE:CG1	1:D:359:TYR:HE1	2.32	0.41
1:C:601:LEU:CD1	1:D:841:ALA:HA	2.50	0.41
1:E:62:TYR:HA	1:E:65:PHE:HB3	2.03	0.41
1:E:373:VAL:HG11	1:F:797:GLN:OE1	2.20	0.41
1:A:105:GLN:CG	1:F:141:LYS:HZ3	2.20	0.41
1:A:141:LYS:HG2	1:F:104:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ALA:CA	1:B:426:VAL:HG22	2.42	0.41
1:B:514:LYS:NZ	1:B:518:GLU:OE2	2.51	0.41
1:D:278:LEU:N	1:D:278:LEU:HD22	2.36	0.41
1:D:556:ILE:O	1:D:556:ILE:CG2	2.62	0.41
1:E:203:ARG:HG2	1:F:363:HIS:CE1	2.56	0.41
1:E:794:ARG:NE	1:E:794:ARG:CA	2.83	0.41
1:E:876:CYS:SG	1:E:877:LEU:N	2.94	0.41
1:B:568:LYS:O	1:B:569:LEU:HB2	2.21	0.41
1:B:784:VAL:O	1:B:785:ASP:HB3	2.21	0.41
1:C:680:TYR:CD1	1:C:680:TYR:N	2.89	0.41
1:A:190:GLU:H	1:A:190:GLU:CD	2.23	0.41
1:A:844:ILE:HD12	1:F:601:LEU:CG	2.34	0.41
1:B:322:ARG:HD3	1:C:673:ASN:ND2	2.36	0.41
1:B:596:LEU:HD21	1:C:833:GLN:O	2.21	0.41
1:B:662:TYR:CZ	1:C:649:LYS:CG	3.03	0.41
1:C:667:GLU:O	1:C:667:GLU:HG3	2.21	0.41
1:D:333:ARG:NE	1:D:333:ARG:HA	2.36	0.41
1:E:700:LEU:HD23	1:E:700:LEU:HA	1.89	0.41
1:E:794:ARG:NE	1:E:794:ARG:C	2.66	0.41
1:F:247:ASP:O	1:F:249:ALA:N	2.54	0.41
1:F:650:TYR:O	1:F:650:TYR:HD1	2.00	0.41
1:F:828:LEU:O	1:F:829:ASN:C	2.59	0.41
1:D:51:LEU:HD23	1:D:51:LEU:HA	1.86	0.41
1:E:297:ALA:O	1:E:298:ALA:HB3	2.21	0.41
1:E:629:GLY:O	1:E:633:ASN:N	2.54	0.41
1:B:82:ALA:HB3	1:B:83:PRO:HD3	2.03	0.40
1:C:302:LYS:HB2	1:C:303:PRO:HD3	2.03	0.40
1:D:9:GLU:H	1:D:9:GLU:CD	2.14	0.40
1:D:66:LYS:HB3	1:D:66:LYS:HE2	1.80	0.40
1:D:92:LEU:O	1:D:93:GLY:C	2.59	0.40
1:A:198:ARG:O	1:B:401:ALA:HB1	2.21	0.40
1:A:202:ARG:HB3	1:B:397:ASP:OD2	2.20	0.40
1:D:216:ILE:HD12	1:D:216:ILE:HA	1.77	0.40
1:D:235:PRO:O	1:D:239:GLN:N	2.54	0.40
1:F:359:TYR:CD1	1:F:359:TYR:N	2.83	0.40
1:C:583:GLN:O	1:C:583:GLN:HG3	2.21	0.40
1:C:802:TYR:HB3	1:C:804:LEU:H	1.86	0.40
1:F:642:ASP:C	1:F:642:ASP:OD1	2.59	0.40
1:A:534:ASN:OD1	1:A:534:ASN:C	2.59	0.40
1:C:126:ILE:HG22	1:C:128:GLN:H	1.87	0.40
1:D:89:SER:OG	1:D:90:TYR:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:GLY:O	2:D:1002:ATP:C8	2.72	0.40
1:E:823:MET:HG3	1:E:824:GLY:N	2.36	0.40
1:C:216:ILE:HD13	1:C:216:ILE:HA	1.90	0.40
1:E:387:ARG:HA	1:E:387:ARG:HE	1.81	0.40
1:F:815:ALA:HA	1:F:819:TYR:CD1	2.56	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	842/879 (96%)	795 (94%)	38 (4%)	9 (1%)	14	52
1	B	842/879 (96%)	784 (93%)	47 (6%)	11 (1%)	12	48
1	C	711/879 (81%)	669 (94%)	35 (5%)	7 (1%)	15	55
1	D	712/879 (81%)	665 (93%)	33 (5%)	14 (2%)	7	38
1	E	711/879 (81%)	661 (93%)	36 (5%)	14 (2%)	7	38
1	F	842/879 (96%)	788 (94%)	42 (5%)	12 (1%)	11	46
All	All	4660/5274 (88%)	4362 (94%)	231 (5%)	67 (1%)	15	46

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	THR
1	A	290	MET
1	A	807	THR
1	B	318	ASN
1	B	540	VAL
1	B	650	TYR
1	B	706	GLY

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Mol	Chain	Res	Type
1	C	28	PRO
1	C	85	GLU
1	C	650	TYR
1	D	81	PRO
1	D	247	ASP
1	D	277	THR
1	D	542	ASP
1	D	566	ASN
1	D	807	THR
1	E	81	PRO
1	E	277	THR
1	E	290	MET
1	E	569	LEU
1	E	650	TYR
1	E	651	ALA
1	E	706	GLY
1	E	795	PHE
1	E	807	THR
1	F	286	ILE
1	F	569	LEU
1	F	650	TYR
1	F	745	SER
1	F	807	THR
1	A	247	ASP
1	A	852	LYS
1	B	277	THR
1	B	388	LEU
1	B	669	GLY
1	B	852	LYS
1	C	248	LEU
1	C	277	THR
1	C	569	LEU
1	D	706	GLY
1	D	852	LYS
1	E	137	ILE
1	F	59	ARG
1	F	248	LEU
1	F	706	GLY
1	D	651	ALA
1	E	852	LYS
1	F	686	ASP
1	A	295	ASP

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Mol	Chain	Res	Type
1	A	650	TYR
1	B	248	LEU
1	D	249	ALA
1	D	294	LYS
1	D	880	LEU
1	E	298	ALA
1	E	299	ASN
1	F	267	GLY
1	F	818	GLY
1	F	852	LYS
1	B	385	TYR
1	E	679	PRO
1	B	651	ALA
1	C	89	SER
1	D	561	LEU
1	A	86	ILE
1	D	556	ILE
1	A	706	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	727/758 (96%)	726 (100%)	1 (0%)	93	97
1	B	730/758 (96%)	729 (100%)	1 (0%)	93	97
1	C	614/758 (81%)	613 (100%)	1 (0%)	93	96
1	D	618/758 (82%)	618 (100%)	0	100	100
1	E	611/758 (81%)	610 (100%)	1 (0%)	93	96
1	F	728/758 (96%)	728 (100%)	0	100	100
All	All	4028/4548 (89%)	4024 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	775	LEU
1	B	256	LYS
1	C	702	MET
1	E	819	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	523	GLN
1	B	606	GLN
1	C	106	GLN
1	C	115	HIS
1	C	829	ASN
1	D	128	GLN
1	D	377	GLN
1	D	720	ASN
1	D	797	GLN
1	E	377	GLN
1	E	883	HIS
1	F	523	GLN

### 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	B	1002	-	26,33,33	3.65	5 (19%)	31,52,52	2.19	9 (29%)
2	ATP	D	1002	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
2	ATP	E	1002	-	26,33,33	3.60	4 (15%)	31,52,52	2.48	13 (41%)
2	ATP	F	1002	-	26,33,33	3.63	4 (15%)	31,52,52	2.05	9 (29%)
2	ATP	A	1001	-	26,33,33	3.66	5 (19%)	31,52,52	2.22	8 (25%)
2	ATP	E	1001	-	26,33,33	3.63	3 (11%)	31,52,52	2.20	9 (29%)
2	ATP	F	1001	-	26,33,33	3.56	4 (15%)	31,52,52	2.22	9 (29%)
2	ATP	C	1002	-	26,33,33	3.60	4 (15%)	31,52,52	2.24	9 (29%)
2	ATP	A	1002	-	26,33,33	3.62	6 (23%)	31,52,52	2.23	10 (32%)
2	ATP	D	1001	-	26,33,33	3.59	4 (15%)	31,52,52	2.49	12 (38%)
2	ATP	C	1001	-	26,33,33	3.62	3 (11%)	31,52,52	2.28	7 (22%)
2	ATP	B	1001	-	26,33,33	3.58	2 (7%)	31,52,52	2.31	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	B	1002	-	-	8/18/38/38	0/3/3/3
2	ATP	D	1002	-	-	3/18/38/38	0/3/3/3
2	ATP	E	1002	-	-	2/18/38/38	0/3/3/3
2	ATP	F	1002	-	-	6/18/38/38	0/3/3/3
2	ATP	A	1001	-	-	2/18/38/38	0/3/3/3
2	ATP	E	1001	-	-	7/18/38/38	0/3/3/3
2	ATP	F	1001	-	-	10/18/38/38	0/3/3/3
2	ATP	C	1002	-	-	4/18/38/38	0/3/3/3
2	ATP	A	1002	-	-	1/18/38/38	0/3/3/3
2	ATP	D	1001	-	-	2/18/38/38	0/3/3/3
2	ATP	C	1001	-	-	5/18/38/38	0/3/3/3
2	ATP	B	1001	-	-	8/18/38/38	0/3/3/3



All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ATP	PG-O1G	17.58	2.07	1.50
2	E	1001	ATP	PG-O1G	17.50	2.07	1.50
2	C	1001	ATP	PG-O1G	17.48	2.07	1.50
2	B	1002	ATP	PG-O1G	17.44	2.06	1.50
2	F	1002	ATP	PG-O1G	17.44	2.06	1.50
2	B	1001	ATP	PG-O1G	17.39	2.06	1.50
2	C	1002	ATP	PG-O1G	17.37	2.06	1.50
2	A	1002	ATP	PG-O1G	17.32	2.06	1.50
2	E	1002	ATP	PG-O1G	17.26	2.06	1.50
2	D	1001	ATP	PG-O1G	17.23	2.06	1.50
2	F	1001	ATP	PG-O1G	17.19	2.06	1.50
2	E	1002	ATP	C5-C4	2.79	1.48	1.40
2	B	1002	ATP	O4'-C1'	2.78	1.45	1.41
2	D	1001	ATP	C5-C4	2.78	1.48	1.40
2	A	1002	ATP	C2'-C1'	-2.78	1.49	1.53
2	B	1002	ATP	C5-C4	2.77	1.48	1.40
2	E	1001	ATP	C5-C4	2.70	1.48	1.40
2	F	1002	ATP	C5-C4	2.55	1.47	1.40
2	F	1002	ATP	O4'-C1'	2.54	1.44	1.41
2	D	1002	ATP	C5-C4	2.51	1.47	1.40
2	A	1002	ATP	C5-C4	2.49	1.47	1.40
2	C	1002	ATP	O4'-C1'	2.45	1.44	1.41
2	A	1001	ATP	C2-N3	2.44	1.36	1.32
2	C	1001	ATP	C5-C4	2.43	1.47	1.40
2	A	1001	ATP	C5-C4	2.43	1.47	1.40
2	F	1001	ATP	C5-C4	2.36	1.47	1.40
2	B	1001	ATP	C5-C4	2.35	1.47	1.40
2	C	1002	ATP	C5-C4	2.34	1.47	1.40
2	A	1001	ATP	PG-O2G	2.30	1.63	1.54
2	C	1001	ATP	O4'-C1'	2.25	1.44	1.41
2	C	1002	ATP	C2-N3	2.22	1.35	1.32
2	A	1002	ATP	O4'-C1'	2.14	1.44	1.41
2	D	1001	ATP	C5-N7	-2.11	1.32	1.39
2	E	1002	ATP	C5-N7	-2.11	1.32	1.39
2	F	1001	ATP	C2-N3	2.11	1.35	1.32
2	B	1002	ATP	PG-O2G	2.08	1.62	1.54
2	A	1001	ATP	O4'-C1'	2.08	1.44	1.41
2	A	1002	ATP	C2-N3	2.07	1.35	1.32
2	F	1001	ATP	C2'-C1'	-2.06	1.50	1.53
2	E	1002	ATP	O4'-C1'	2.05	1.43	1.41
2	D	1001	ATP	O4'-C1'	2.05	1.43	1.41
2	A	1002	ATP	PG-O2G	2.04	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1002	ATP	C2'-C1'	-2.04	1.50	1.53
2	E	1001	ATP	C2-N3	2.03	1.35	1.32
2	B	1002	ATP	C2-N3	2.02	1.35	1.32

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	ATP	PA-O3A-PB	-7.94	105.58	132.83
2	E	1002	ATP	PA-O3A-PB	-7.93	105.61	132.83
2	A	1002	ATP	PA-O3A-PB	-7.28	107.84	132.83
2	C	1001	ATP	PA-O3A-PB	-7.09	108.49	132.83
2	B	1001	ATP	PA-O3A-PB	-6.99	108.85	132.83
2	F	1001	ATP	PA-O3A-PB	-6.78	109.57	132.83
2	B	1001	ATP	PB-O3B-PG	-6.64	110.04	132.83
2	B	1002	ATP	PB-O3B-PG	-6.60	110.17	132.83
2	C	1002	ATP	PB-O3B-PG	-6.57	110.27	132.83
2	E	1001	ATP	PA-O3A-PB	-6.54	110.38	132.83
2	A	1001	ATP	PA-O3A-PB	-6.40	110.86	132.83
2	C	1001	ATP	PB-O3B-PG	-6.39	110.89	132.83
2	E	1001	ATP	PB-O3B-PG	-6.04	112.11	132.83
2	B	1002	ATP	PA-O3A-PB	-5.97	112.36	132.83
2	E	1002	ATP	PB-O3B-PG	-5.94	112.44	132.83
2	D	1001	ATP	PB-O3B-PG	-5.94	112.44	132.83
2	C	1002	ATP	PA-O3A-PB	-5.70	113.28	132.83
2	A	1001	ATP	PB-O3B-PG	-5.45	114.14	132.83
2	F	1002	ATP	PB-O3B-PG	-5.33	114.55	132.83
2	F	1002	ATP	PA-O3A-PB	-5.16	115.14	132.83
2	F	1001	ATP	PB-O3B-PG	-5.01	115.63	132.83
2	A	1002	ATP	PB-O3B-PG	-4.52	117.33	132.83
2	D	1002	ATP	PB-O3B-PG	-3.61	120.43	132.83
2	D	1002	ATP	PA-O3A-PB	-3.60	120.47	132.83
2	C	1002	ATP	N6-C6-N1	3.59	126.02	118.57
2	F	1001	ATP	N6-C6-N1	3.57	125.99	118.57
2	A	1001	ATP	N6-C6-N1	3.55	125.95	118.57
2	A	1001	ATP	O2G-PG-O3B	3.45	116.20	104.64
2	B	1001	ATP	N6-C6-N1	3.43	125.69	118.57
2	D	1002	ATP	C3'-C2'-C1'	3.42	106.12	100.98
2	A	1002	ATP	N6-C6-N1	3.38	125.59	118.57
2	A	1002	ATP	O2G-PG-O3B	3.32	115.78	104.64
2	B	1002	ATP	N6-C6-N1	3.31	125.45	118.57
2	D	1001	ATP	N6-C6-N1	3.22	125.26	118.57
2	E	1002	ATP	N6-C6-N1	3.22	125.25	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1002	ATP	O2G-PG-O3B	3.14	115.17	104.64
2	D	1002	ATP	N3-C2-N1	-3.14	123.77	128.68
2	F	1001	ATP	O2G-PG-O3B	3.14	115.15	104.64
2	D	1001	ATP	O2G-PG-O3B	3.13	115.13	104.64
2	C	1002	ATP	O2G-PG-O3B	3.07	114.94	104.64
2	F	1002	ATP	O3B-PG-O1G	-3.03	94.39	111.19
2	F	1001	ATP	O3B-PG-O1G	-2.99	94.63	111.19
2	F	1002	ATP	O2G-PG-O3B	2.95	114.52	104.64
2	E	1001	ATP	C3'-C2'-C1'	2.85	105.27	100.98
2	E	1001	ATP	O2G-PG-O3B	2.82	114.08	104.64
2	B	1001	ATP	O3B-PG-O1G	-2.80	95.66	111.19
2	E	1002	ATP	O3B-PG-O1G	-2.77	95.83	111.19
2	F	1002	ATP	N6-C6-N1	2.77	124.31	118.57
2	D	1001	ATP	O3B-PG-O1G	-2.76	95.87	111.19
2	D	1002	ATP	C4-C5-N7	-2.72	106.56	109.40
2	F	1001	ATP	C5-C6-N6	-2.72	116.22	120.35
2	A	1002	ATP	O3B-PG-O1G	-2.69	96.26	111.19
2	C	1001	ATP	O3B-PG-O1G	-2.66	96.42	111.19
2	A	1001	ATP	O3B-PG-O1G	-2.64	96.52	111.19
2	C	1001	ATP	O2G-PG-O3B	2.63	113.45	104.64
2	E	1002	ATP	O2B-PB-O1B	2.62	125.19	112.24
2	D	1001	ATP	O2B-PB-O1B	2.62	125.17	112.24
2	C	1002	ATP	C5'-C4'-C3'	-2.61	105.40	115.18
2	A	1002	ATP	N3-C2-N1	-2.59	124.64	128.68
2	A	1001	ATP	O2B-PB-O1B	2.58	124.99	112.24
2	C	1002	ATP	O3B-PG-O1G	-2.58	96.90	111.19
2	B	1002	ATP	O3B-PG-O1G	-2.57	96.95	111.19
2	A	1002	ATP	C3'-C2'-C1'	2.57	104.84	100.98
2	B	1002	ATP	O2G-PG-O3B	2.57	113.24	104.64
2	E	1001	ATP	N6-C6-N1	2.56	123.88	118.57
2	C	1001	ATP	C4-C5-N7	-2.55	106.74	109.40
2	F	1002	ATP	N3-C2-N1	-2.55	124.70	128.68
2	B	1001	ATP	N3-C2-N1	-2.54	124.70	128.68
2	B	1001	ATP	O2G-PG-O3B	2.53	113.12	104.64
2	A	1001	ATP	C5-C6-N6	-2.52	116.53	120.35
2	C	1001	ATP	N3-C2-N1	-2.51	124.75	128.68
2	E	1001	ATP	O3B-PG-O1G	-2.50	97.32	111.19
2	C	1002	ATP	C5-C6-N6	-2.50	116.56	120.35
2	D	1001	ATP	C1'-N9-C4	2.44	130.92	126.64
2	A	1001	ATP	N3-C2-N1	-2.43	124.88	128.68
2	D	1001	ATP	O5'-C5'-C4'	-2.43	100.64	108.99
2	E	1002	ATP	C1'-N9-C4	2.42	130.88	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	ATP	N3-C2-N1	-2.41	124.91	128.68
2	E	1001	ATP	C2'-C3'-C4'	2.41	107.32	102.64
2	E	1002	ATP	O5'-C5'-C4'	-2.40	100.73	108.99
2	B	1002	ATP	C5'-C4'-C3'	-2.40	106.19	115.18
2	B	1002	ATP	C4-C5-N7	-2.39	106.91	109.40
2	C	1002	ATP	C3'-C2'-C1'	2.38	104.56	100.98
2	B	1001	ATP	O3'-C3'-C4'	-2.31	104.36	111.05
2	A	1002	ATP	O2B-PB-O1B	2.31	123.66	112.24
2	F	1001	ATP	N3-C2-N1	-2.29	125.10	128.68
2	F	1002	ATP	O2B-PB-O1B	2.28	123.51	112.24
2	E	1002	ATP	N3-C2-N1	-2.26	125.14	128.68
2	E	1001	ATP	C4-C5-N7	-2.24	107.06	109.40
2	D	1001	ATP	N3-C2-N1	-2.21	125.22	128.68
2	B	1002	ATP	N3-C2-N1	-2.21	125.23	128.68
2	D	1001	ATP	O5'-PA-O1A	2.20	117.64	109.07
2	E	1001	ATP	N3-C2-N1	-2.18	125.27	128.68
2	E	1002	ATP	O5'-PA-O1A	2.17	117.56	109.07
2	D	1001	ATP	C4-C5-N7	-2.16	107.15	109.40
2	A	1002	ATP	C4-C5-N7	-2.15	107.16	109.40
2	C	1001	ATP	O2B-PB-O1B	2.14	122.83	112.24
2	F	1002	ATP	C5'-C4'-C3'	-2.12	107.22	115.18
2	A	1002	ATP	C5-C6-N6	-2.11	117.15	120.35
2	F	1001	ATP	O2A-PA-O1A	2.08	122.55	112.24
2	E	1002	ATP	C4-C5-N7	-2.08	107.23	109.40
2	B	1002	ATP	O2B-PB-O1B	2.08	122.52	112.24
2	F	1002	ATP	C4-C5-N7	-2.08	107.24	109.40
2	F	1001	ATP	O2B-PB-O1B	2.07	122.49	112.24
2	E	1002	ATP	C3'-C2'-C1'	2.07	104.09	100.98
2	D	1001	ATP	C3'-C2'-C1'	2.06	104.08	100.98
2	B	1001	ATP	O2A-PA-O1A	2.05	122.40	112.24
2	E	1002	ATP	C2'-C3'-C4'	2.02	106.56	102.64

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	PB-O3B-PG-O2G
2	B	1001	ATP	C5'-O5'-PA-O2A
2	B	1001	ATP	C5'-O5'-PA-O3A
2	B	1002	ATP	PB-O3B-PG-O2G
2	B	1002	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	1002	ATP	C5'-O5'-PA-O3A
2	C	1001	ATP	C5'-O5'-PA-O2A
2	C	1002	ATP	C3'-C4'-C5'-O5'
2	D	1002	ATP	C5'-O5'-PA-O2A
2	D	1002	ATP	C5'-O5'-PA-O3A
2	E	1001	ATP	C5'-O5'-PA-O2A
2	E	1001	ATP	C5'-O5'-PA-O3A
2	F	1001	ATP	PB-O3B-PG-O2G
2	F	1001	ATP	C5'-O5'-PA-O3A
2	F	1002	ATP	PB-O3B-PG-O3G
2	A	1001	ATP	C3'-C4'-C5'-O5'
2	D	1001	ATP	O4'-C4'-C5'-O5'
2	D	1001	ATP	C3'-C4'-C5'-O5'
2	E	1001	ATP	O4'-C4'-C5'-O5'
2	E	1002	ATP	O4'-C4'-C5'-O5'
2	E	1002	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	C3'-C4'-C5'-O5'
2	C	1002	ATP	O4'-C4'-C5'-O5'
2	B	1002	ATP	C3'-C4'-C5'-O5'
2	E	1001	ATP	C3'-C4'-C5'-O5'
2	F	1002	ATP	C3'-C4'-C5'-O5'
2	F	1001	ATP	O4'-C4'-C5'-O5'
2	F	1001	ATP	C3'-C4'-C5'-O5'
2	C	1001	ATP	PB-O3B-PG-O1G
2	F	1002	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	PB-O3B-PG-O3G
2	F	1001	ATP	PB-O3B-PG-O3G
2	F	1002	ATP	PB-O3B-PG-O2G
2	C	1001	ATP	C5'-O5'-PA-O3A
2	C	1002	ATP	PB-O3A-PA-O2A
2	E	1001	ATP	PG-O3B-PB-O1B
2	B	1001	ATP	C5'-O5'-PA-O1A
2	C	1001	ATP	C5'-O5'-PA-O1A
2	E	1001	ATP	C5'-O5'-PA-O1A
2	F	1001	ATP	C5'-O5'-PA-O2A
2	B	1002	ATP	O4'-C4'-C5'-O5'
2	F	1002	ATP	PB-O3A-PA-O2A
2	D	1002	ATP	PG-O3B-PB-O1B
2	B	1001	ATP	PB-O3B-PG-O1G
2	B	1002	ATP	PB-O3B-PG-O1G
2	F	1001	ATP	PB-O3B-PG-O1G

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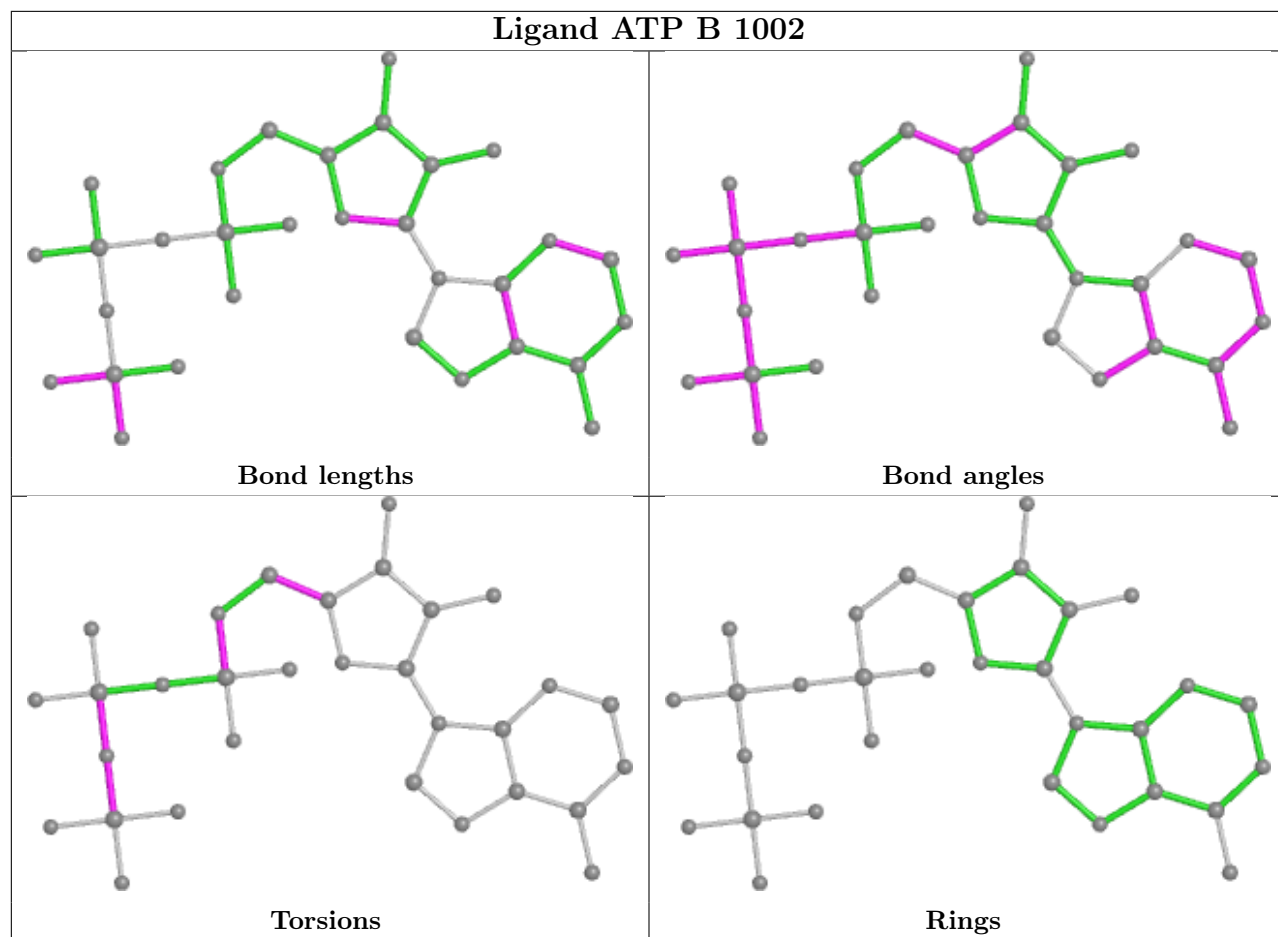
Mol	Chain	Res	Type	Atoms
2	F	1002	ATP	PB-O3B-PG-O1G
2	B	1002	ATP	PB-O3B-PG-O3G
2	A	1002	ATP	O4'-C4'-C5'-O5'
2	C	1001	ATP	O4'-C4'-C5'-O5'
2	B	1002	ATP	PG-O3B-PB-O1B
2	E	1001	ATP	PG-O3B-PB-O2B
2	F	1001	ATP	PG-O3B-PB-O1B
2	F	1001	ATP	PA-O3A-PB-O1B
2	C	1002	ATP	C5'-O5'-PA-O1A
2	F	1001	ATP	C5'-O5'-PA-O1A

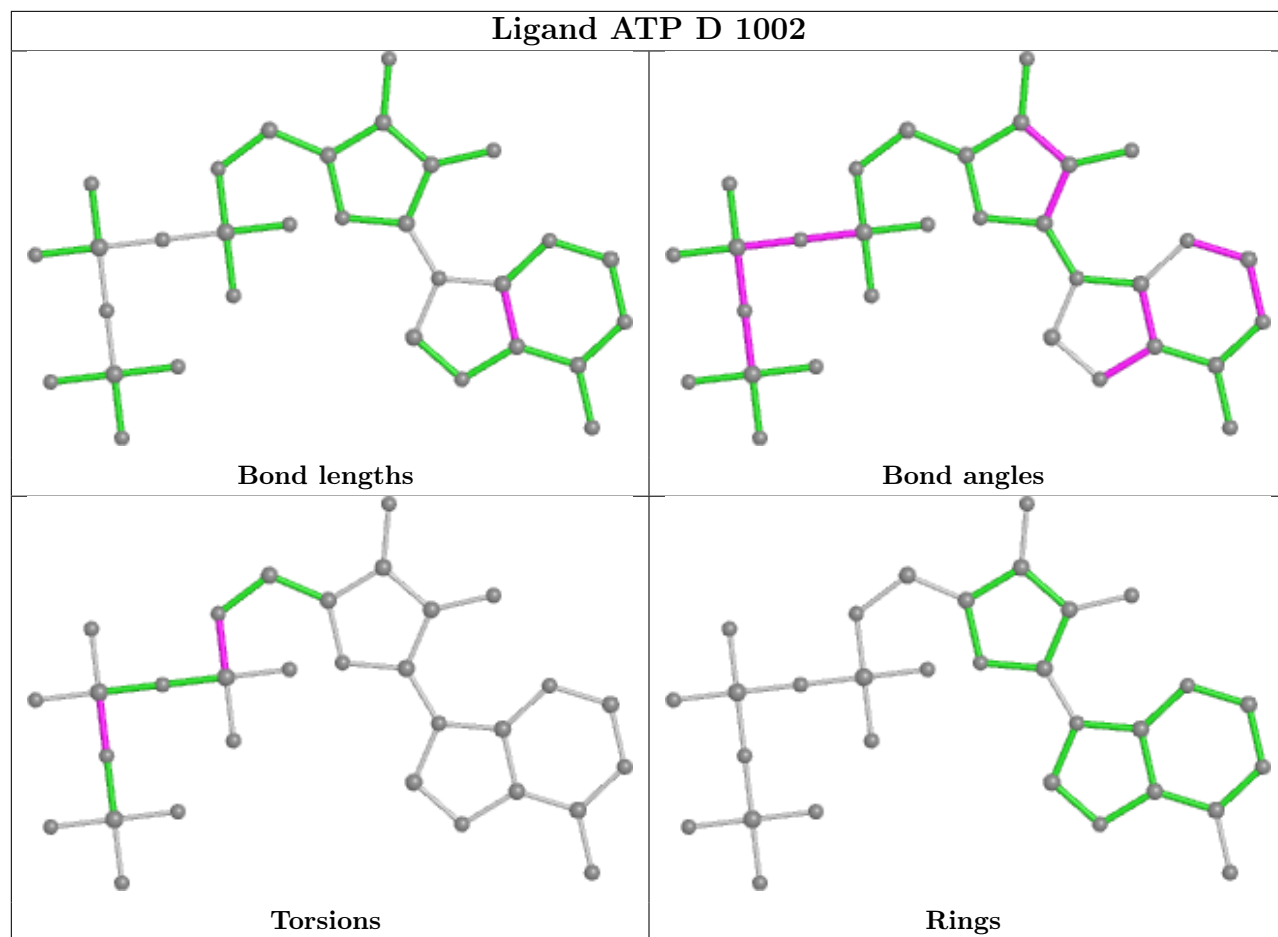
There are no ring outliers.

12 monomers are involved in 65 short contacts:

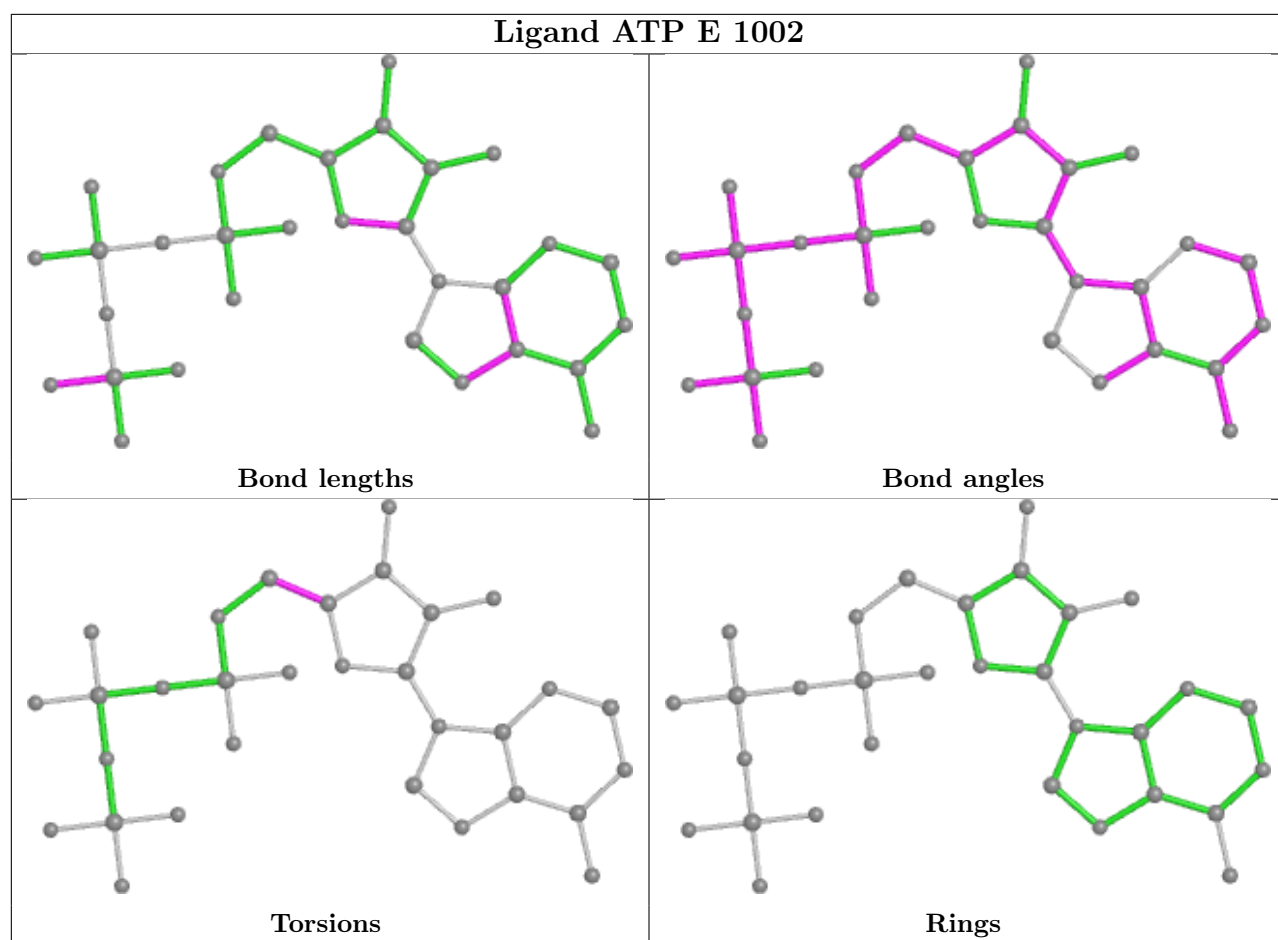
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	ATP	4	0
2	D	1002	ATP	13	0
2	E	1002	ATP	2	0
2	F	1002	ATP	2	0
2	A	1001	ATP	2	0
2	E	1001	ATP	4	0
2	F	1001	ATP	3	0
2	C	1002	ATP	2	0
2	A	1002	ATP	2	0
2	D	1001	ATP	21	0
2	C	1001	ATP	3	0
2	B	1001	ATP	7	0

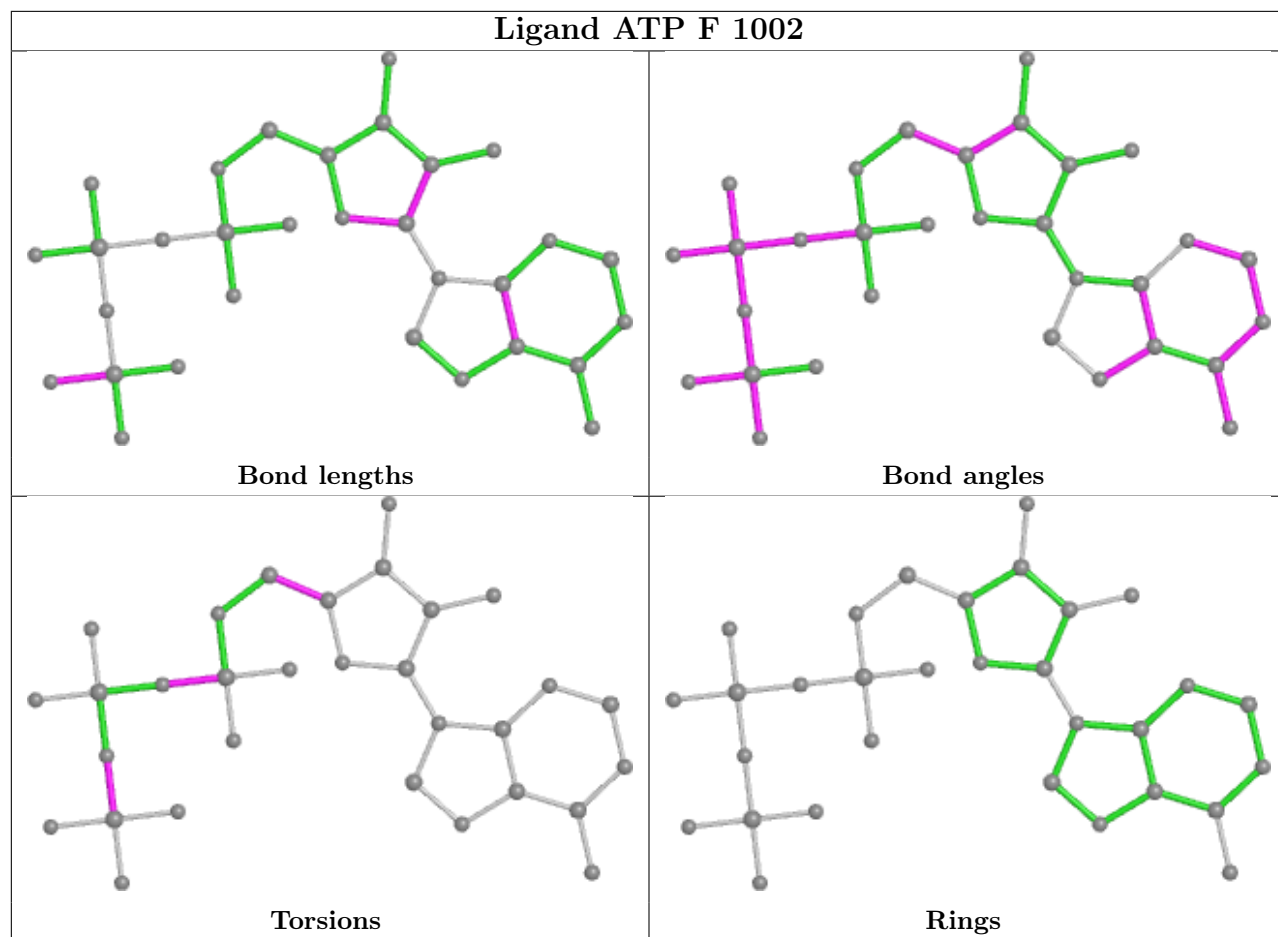
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

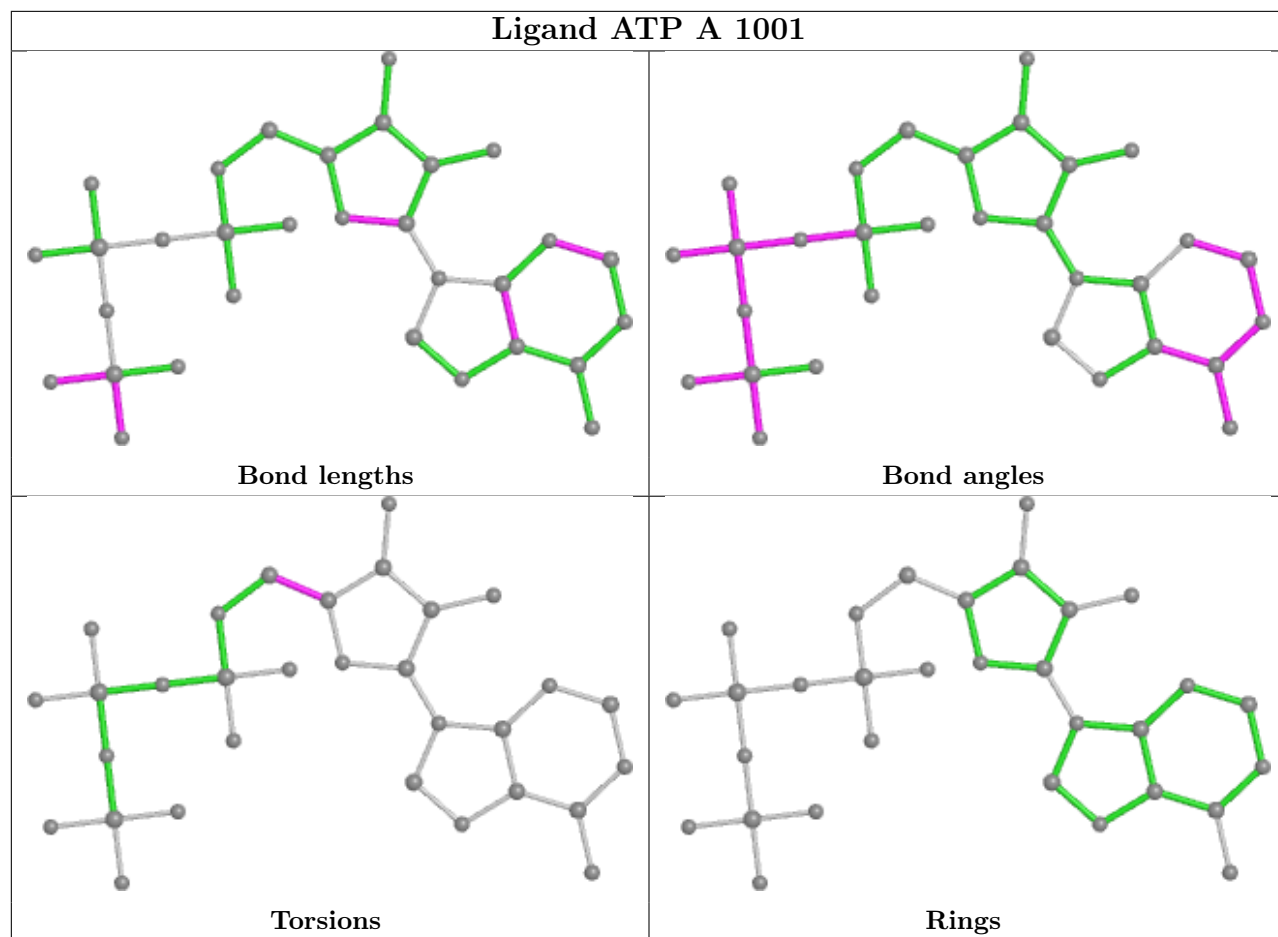


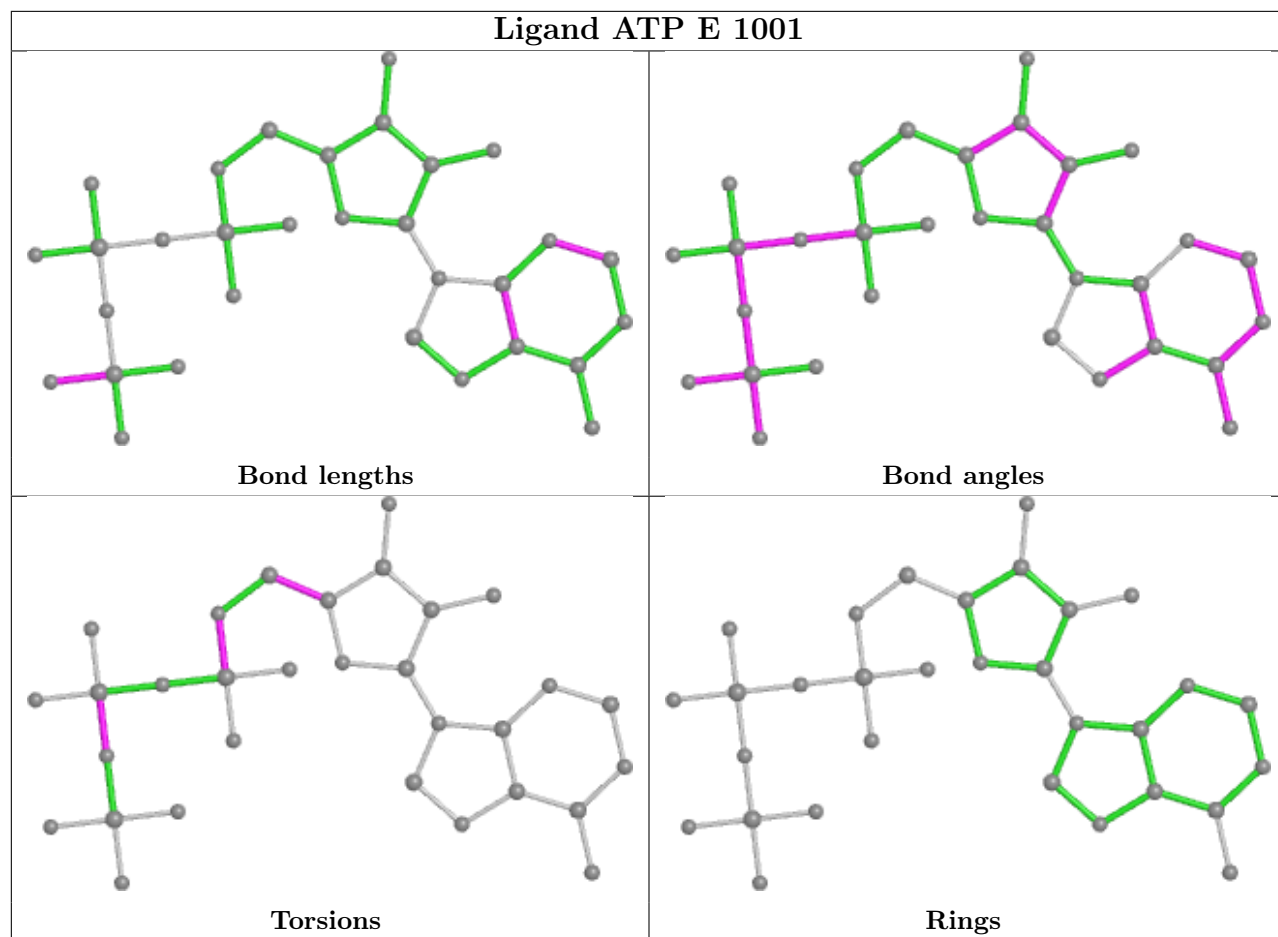


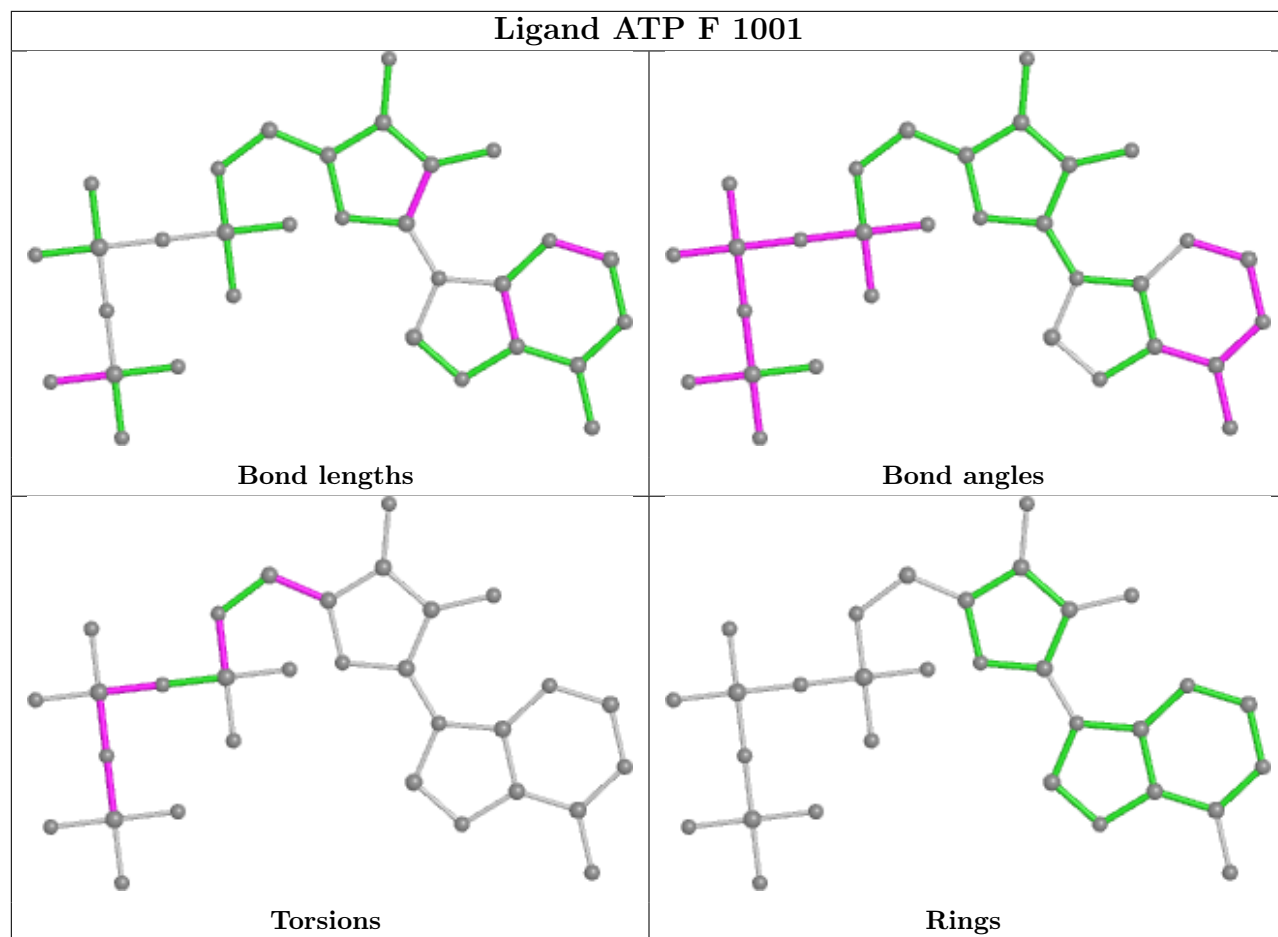


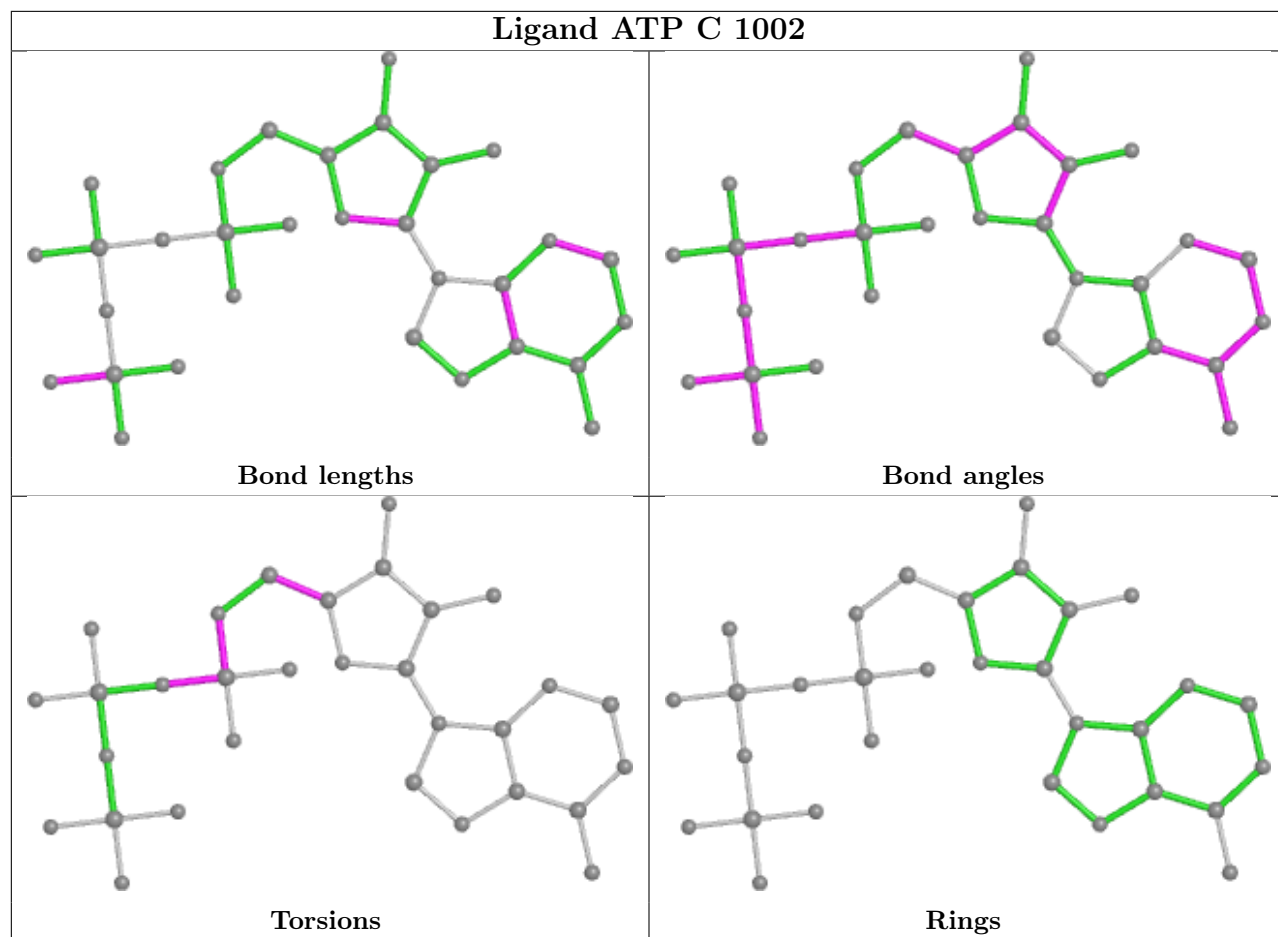


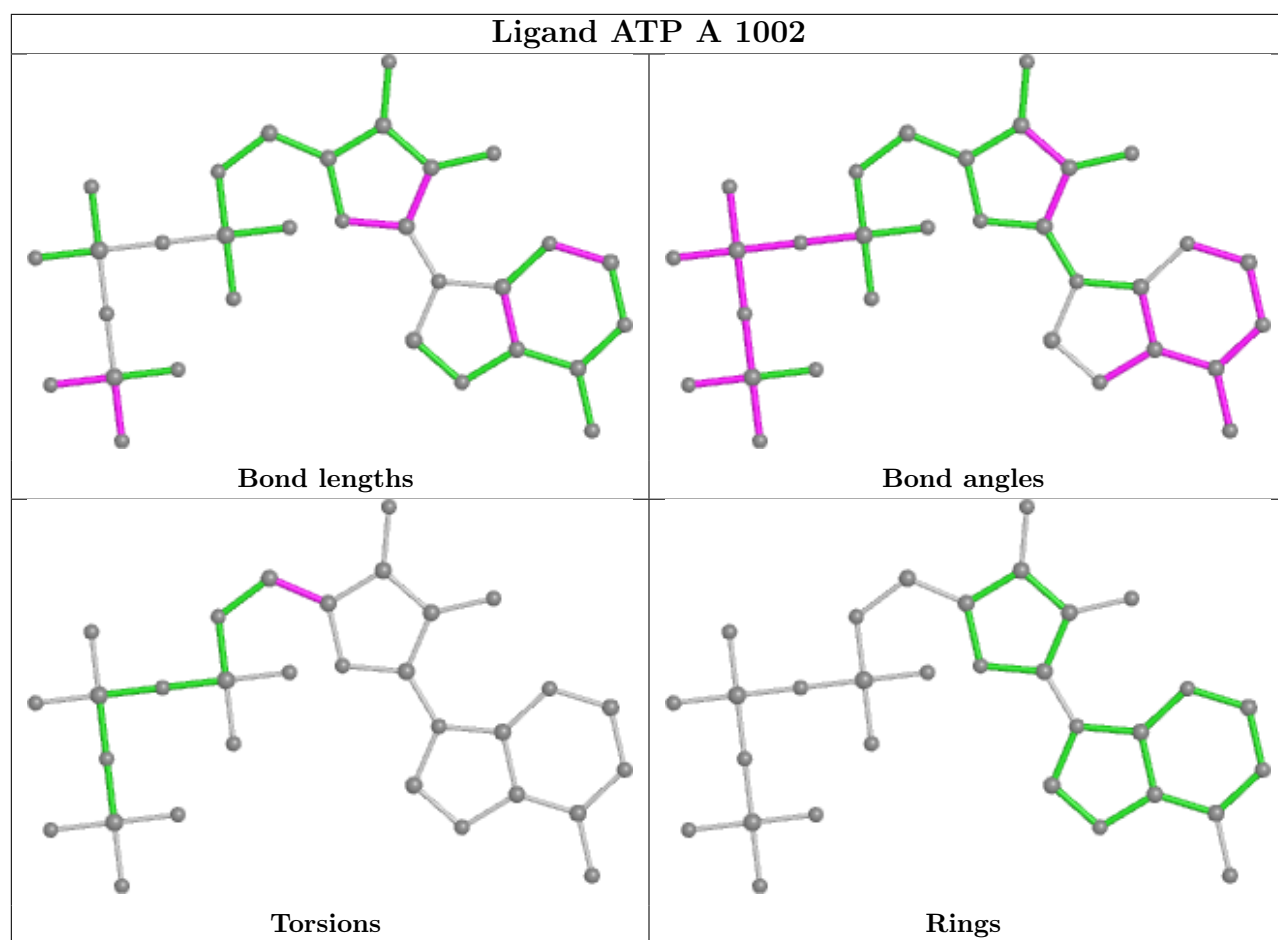


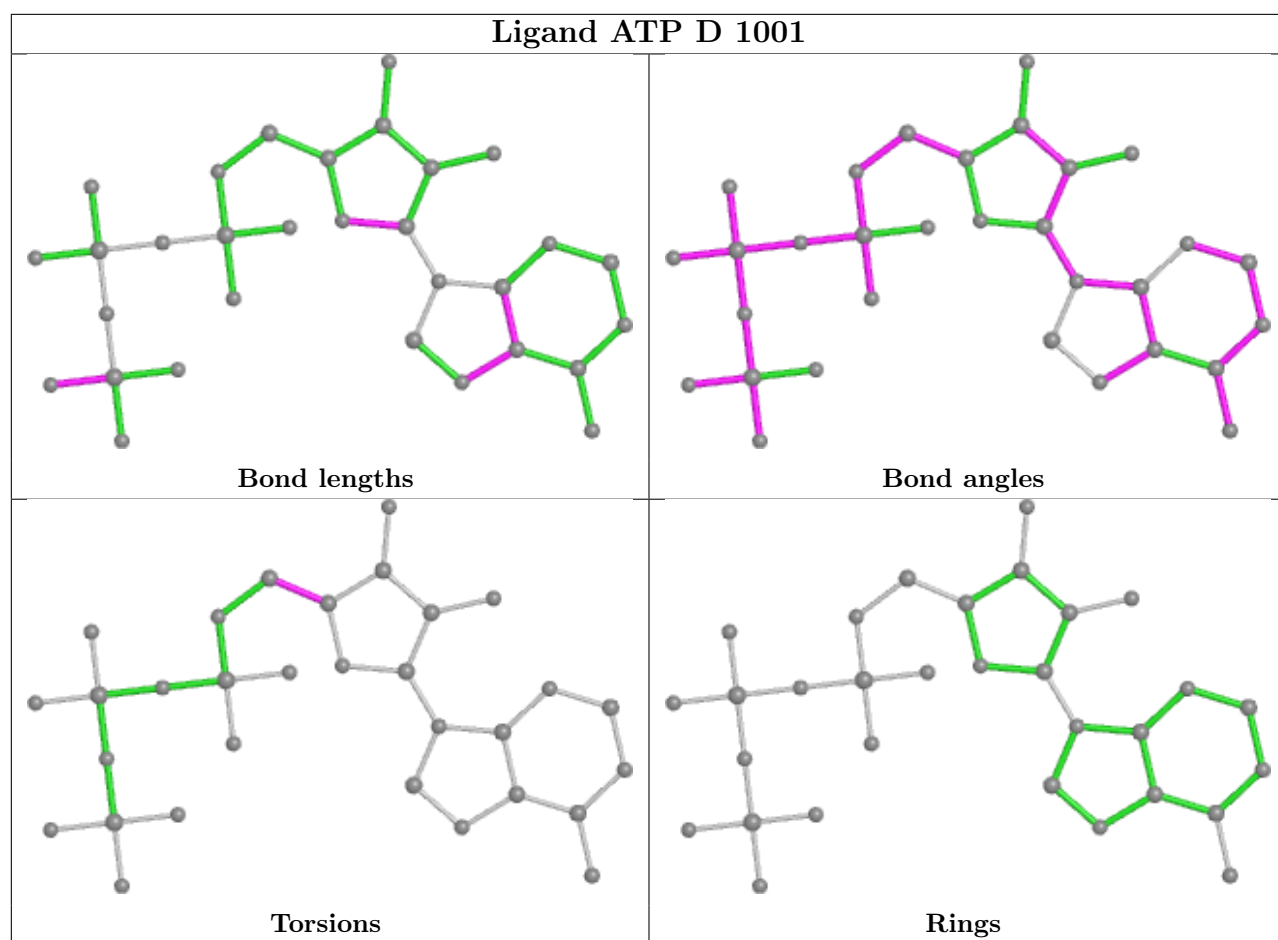




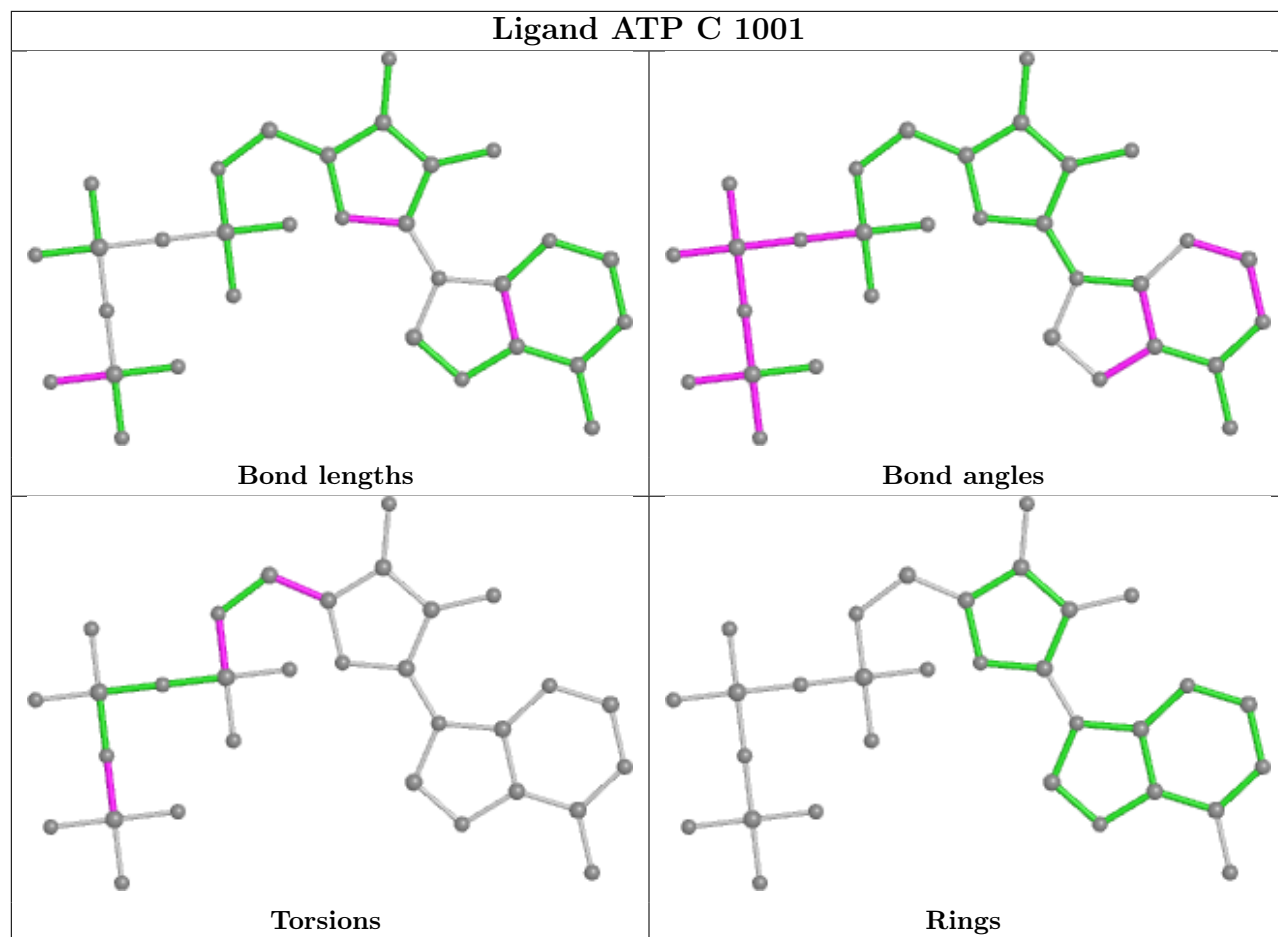


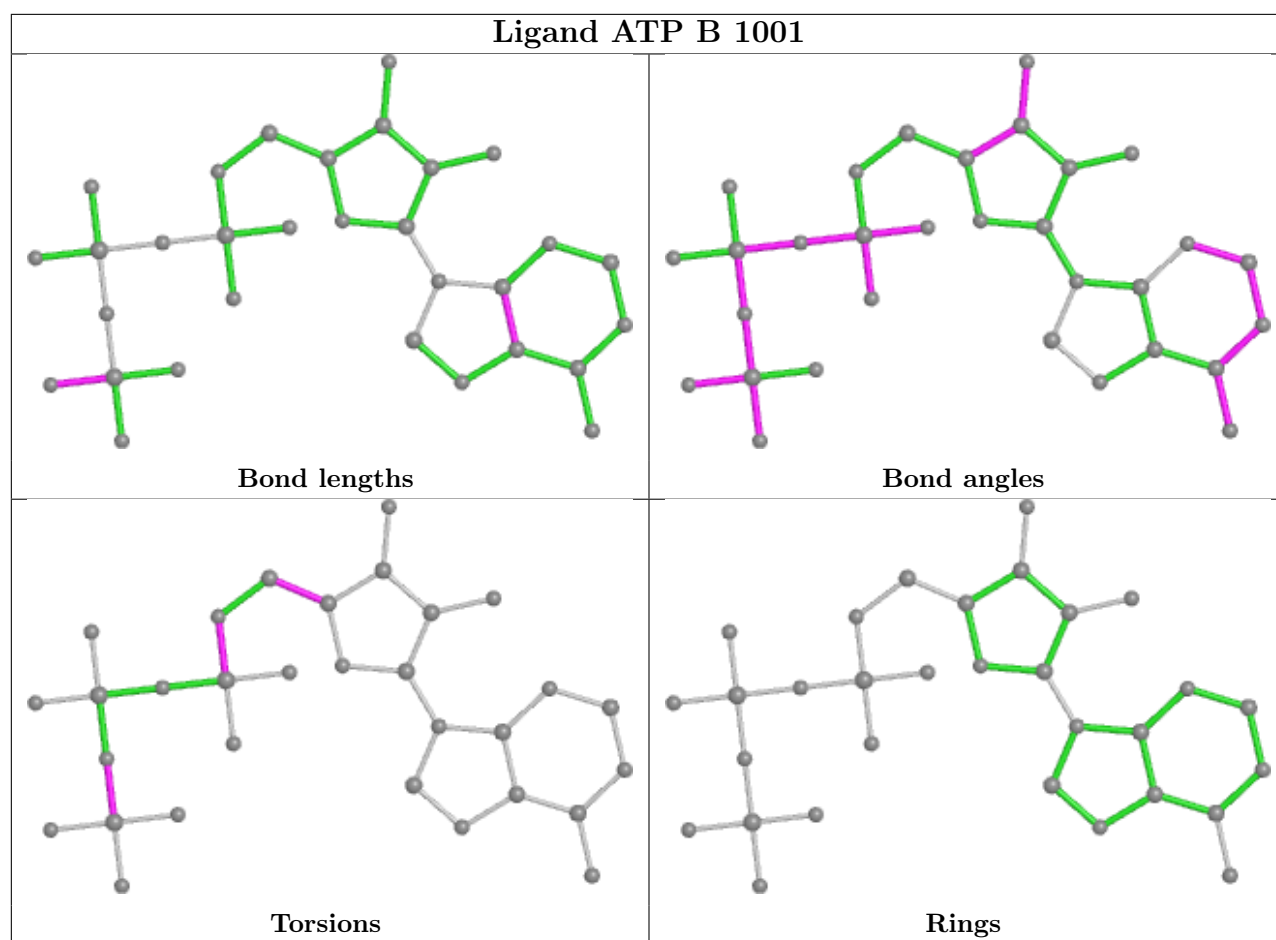












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

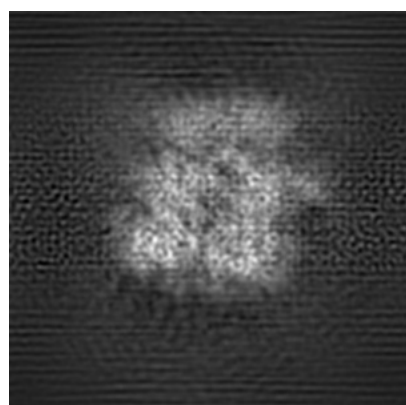
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0375. These allow visual inspection of the internal detail of the map and identification of artifacts.

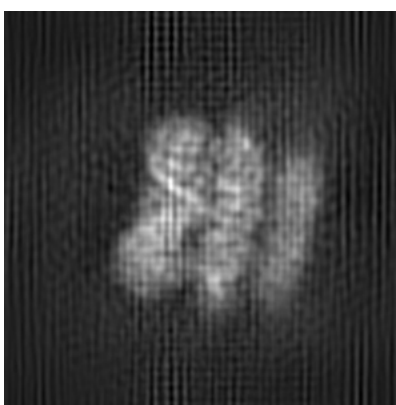
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

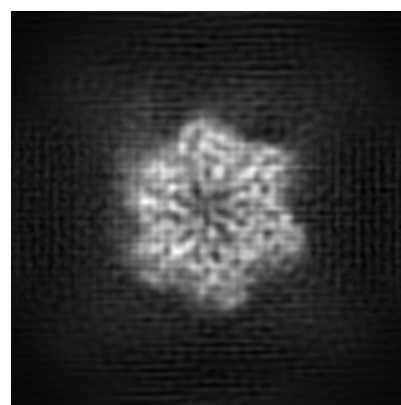
#### 6.1.1 Primary map



X



Y

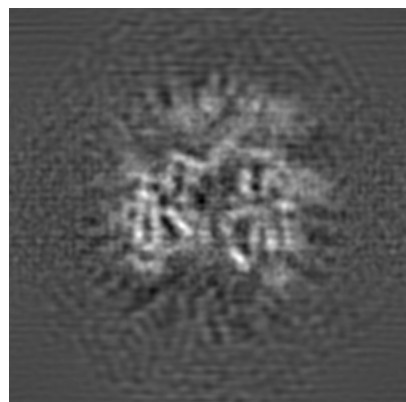


Z

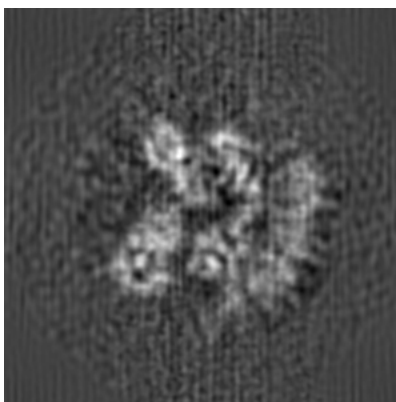
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

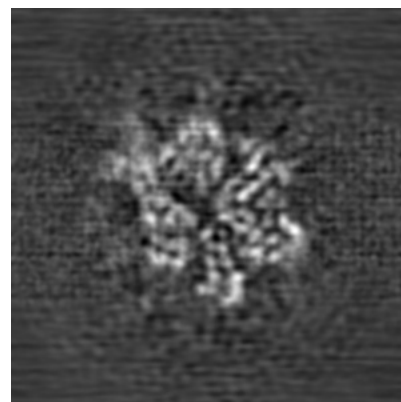
#### 6.2.1 Primary map



X Index: 80



Y Index: 80

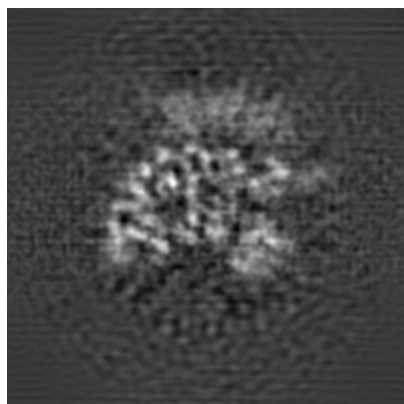


Z Index: 80

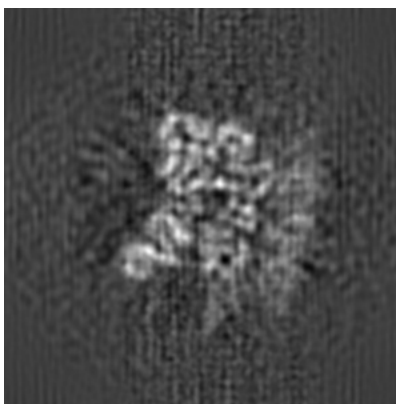
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

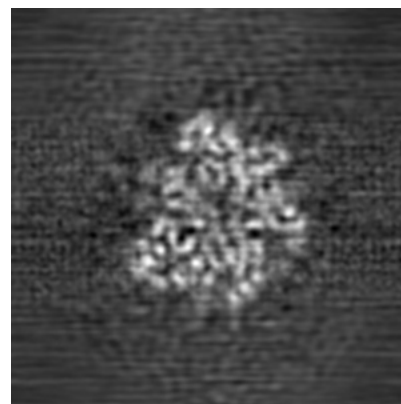
### 6.3.1 Primary map



X Index: 88



Y Index: 73

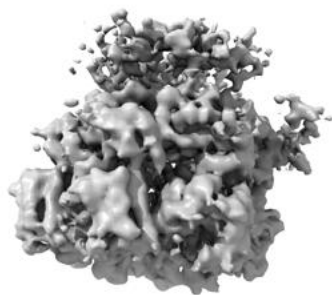


Z Index: 66

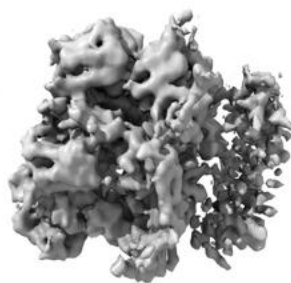
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

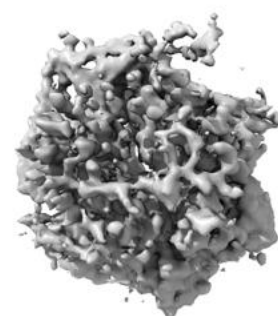
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

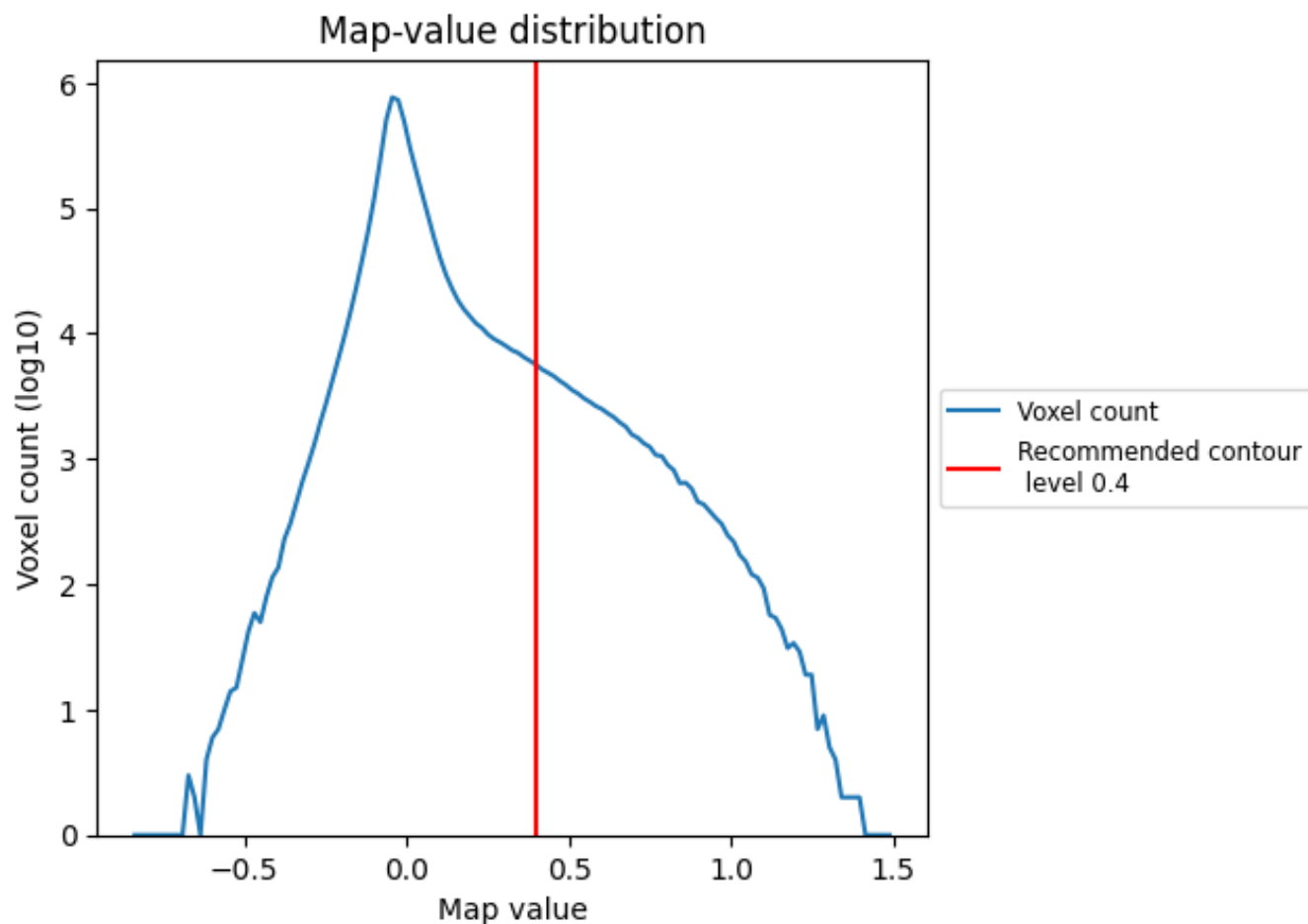
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

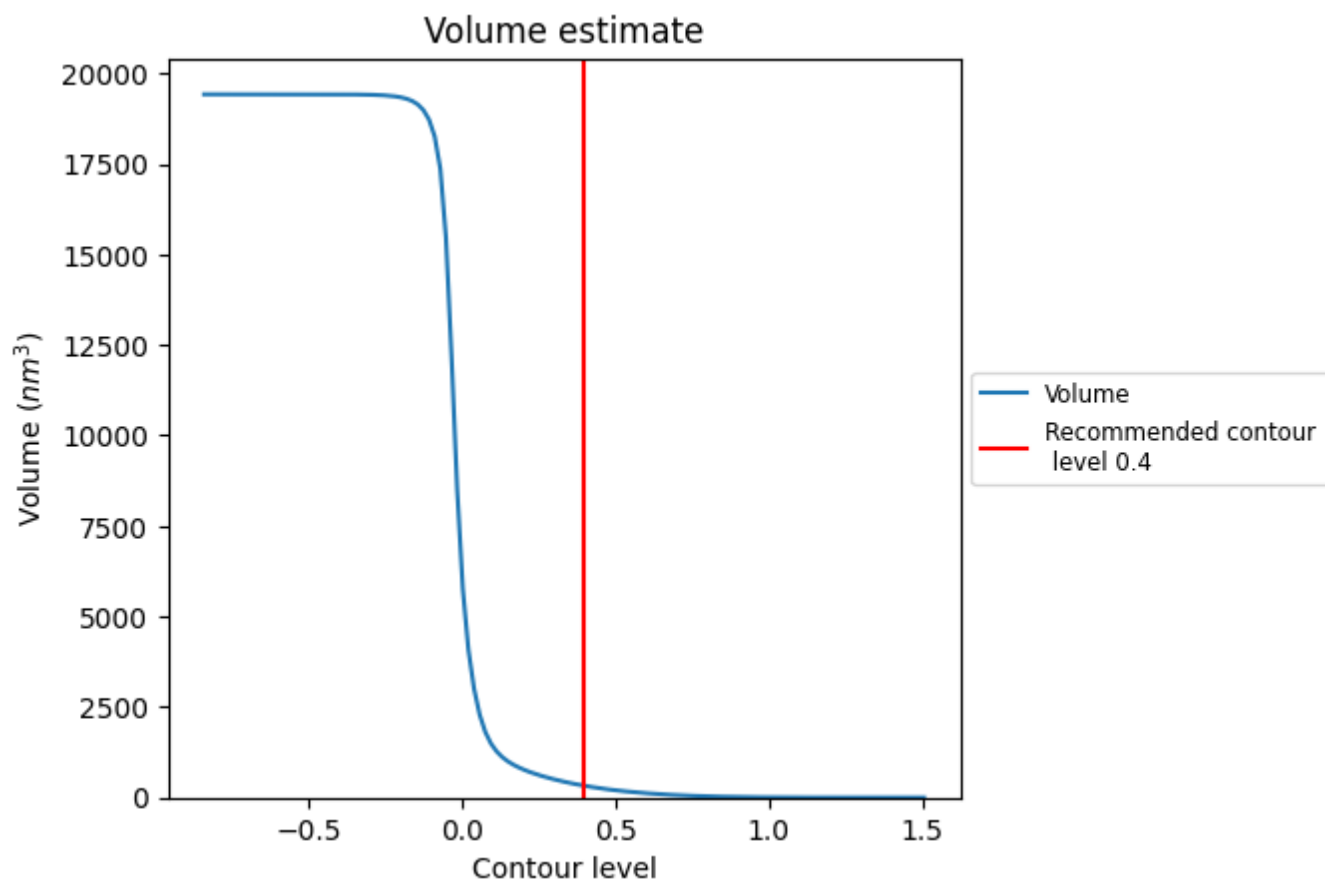
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

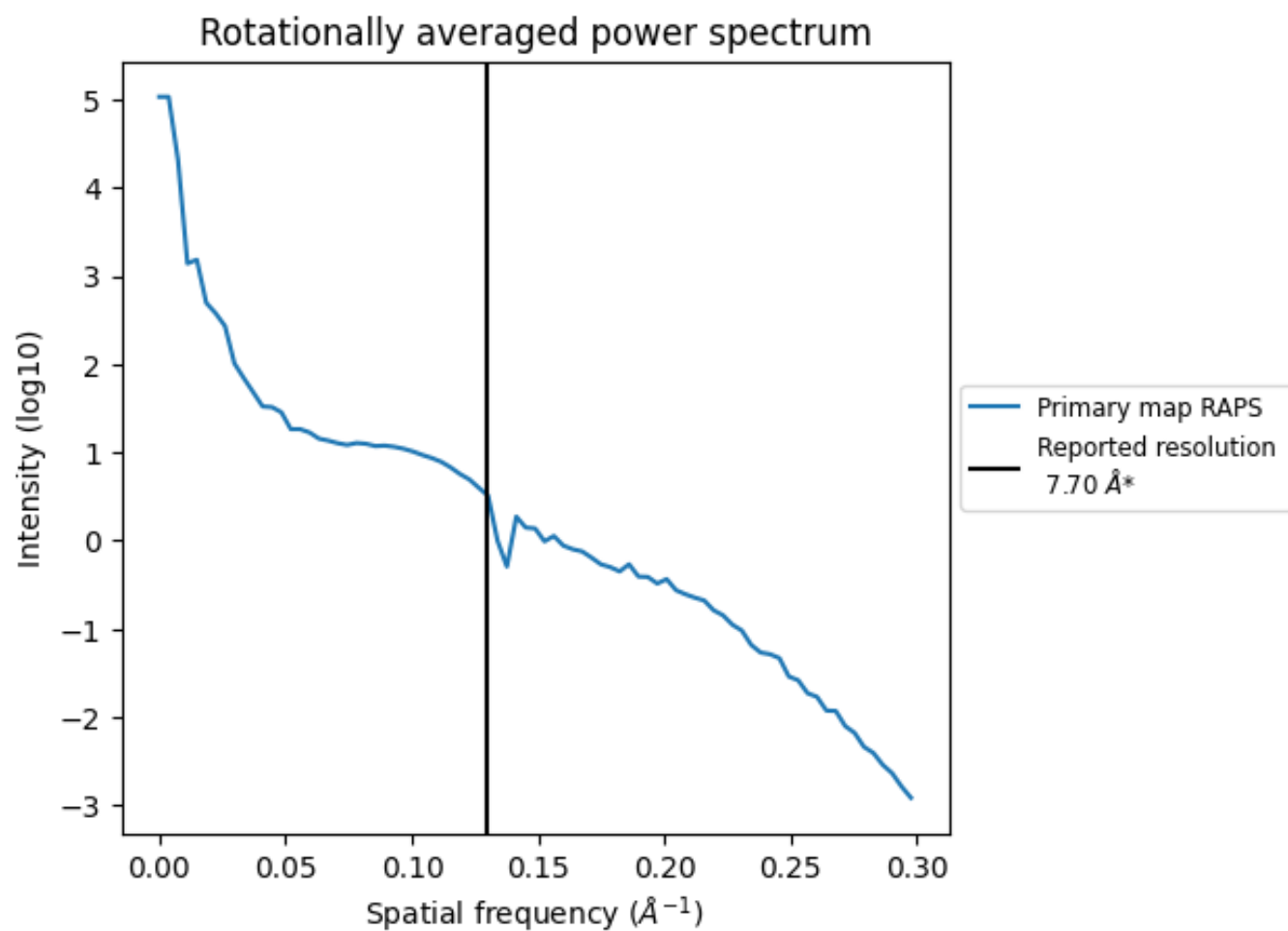
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm<sup>3</sup>; this corresponds to an approximate mass of 294 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 ⓘ



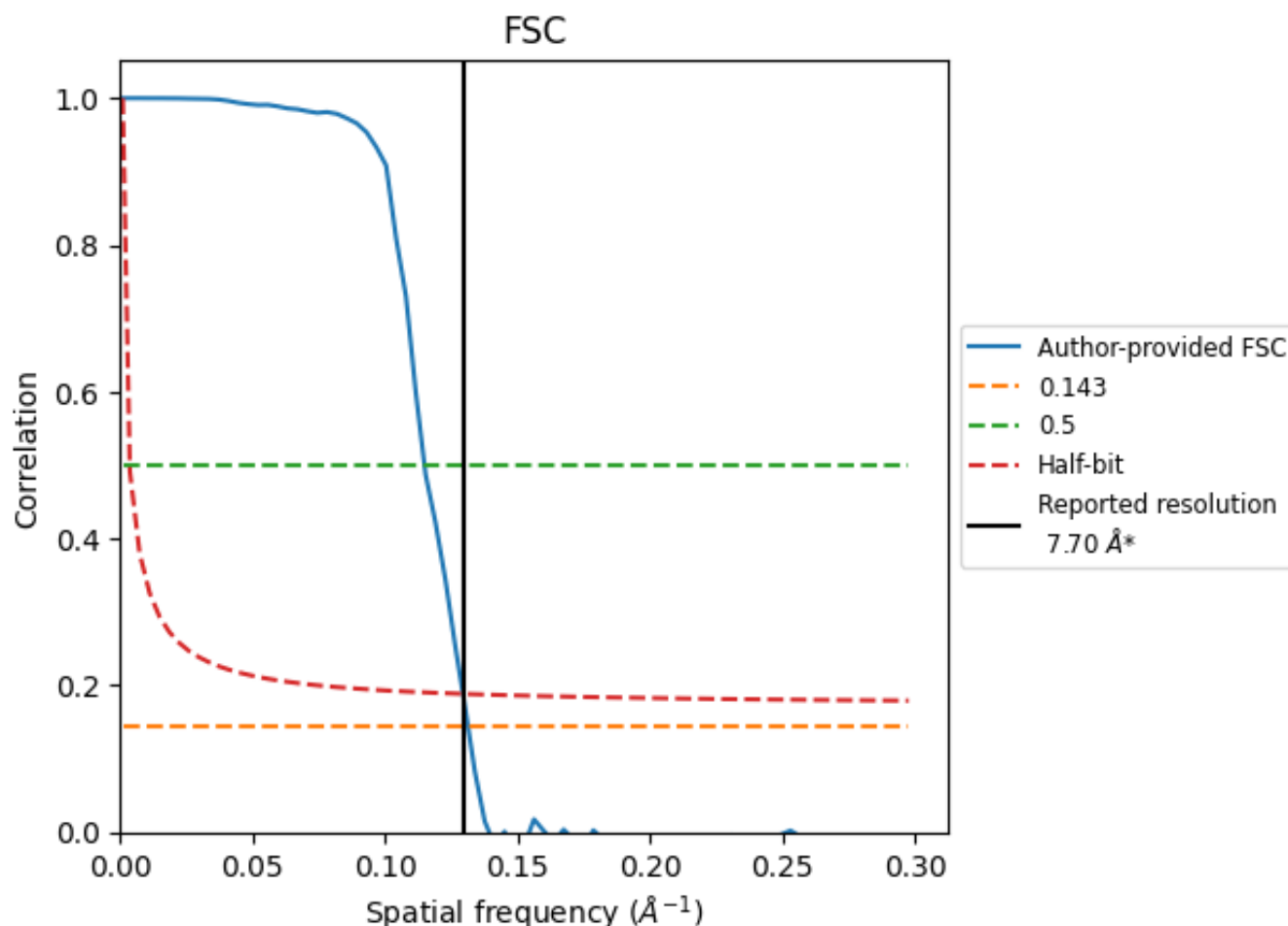
\*Reported resolution corresponds to spatial frequency of 0.130 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.130 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

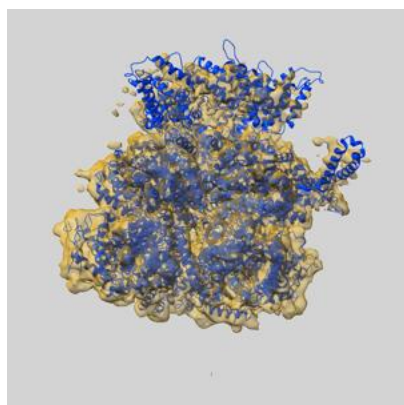
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.70	-	-
Author-provided FSC curve	7.62	8.70	7.73
Unmasked-calculated*	-	-	-

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

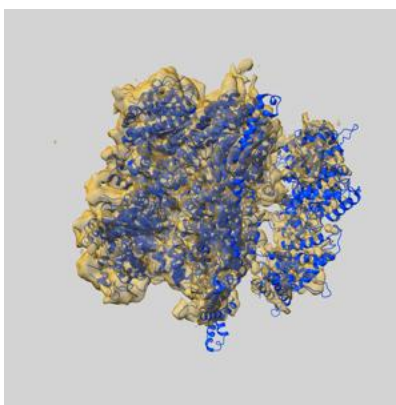
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0375 and PDB model 6N8T. Per-residue inclusion information can be found in section [3](#) on page [6](#).

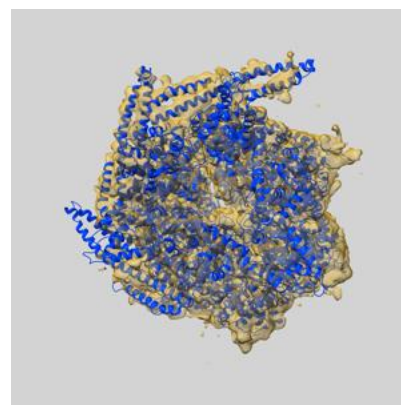
### 9.1 Map-model overlay [i](#)



X



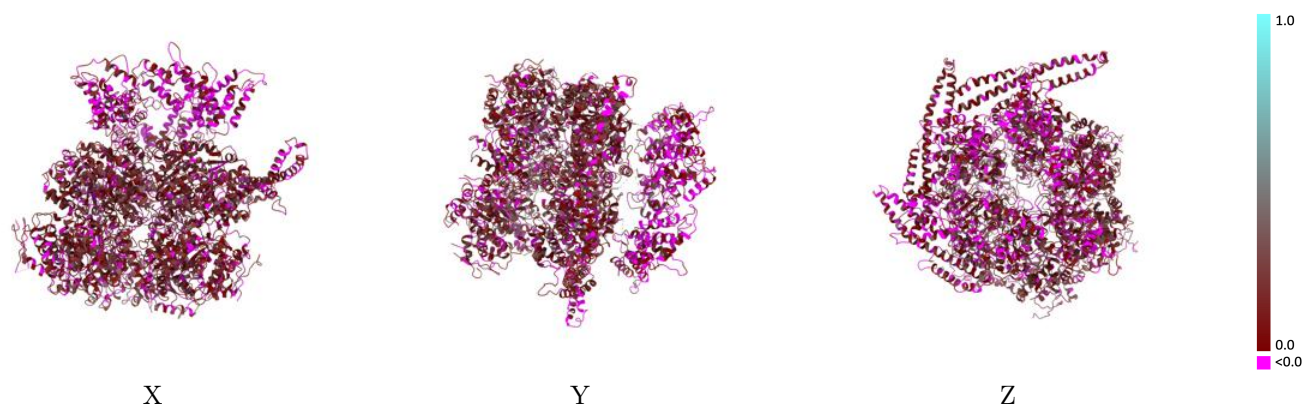
Y



Z

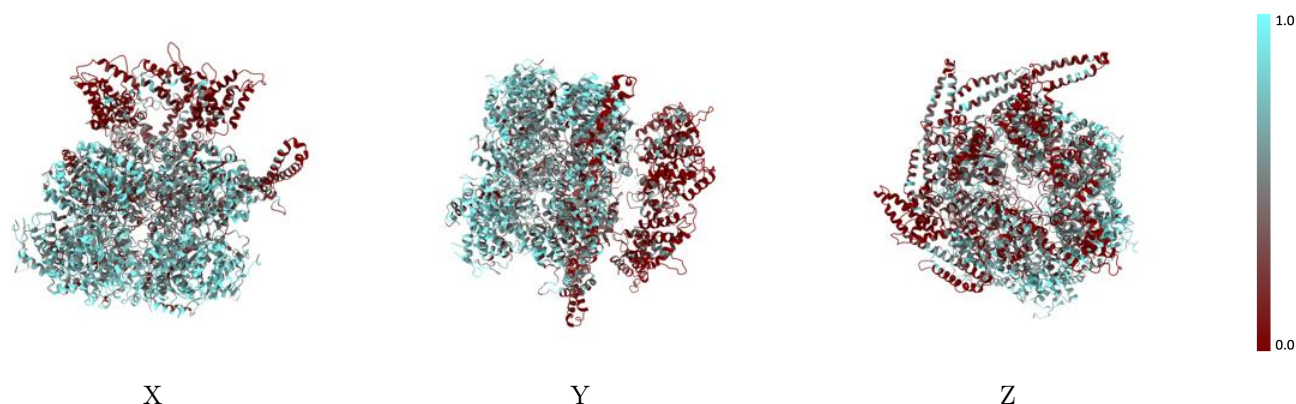
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



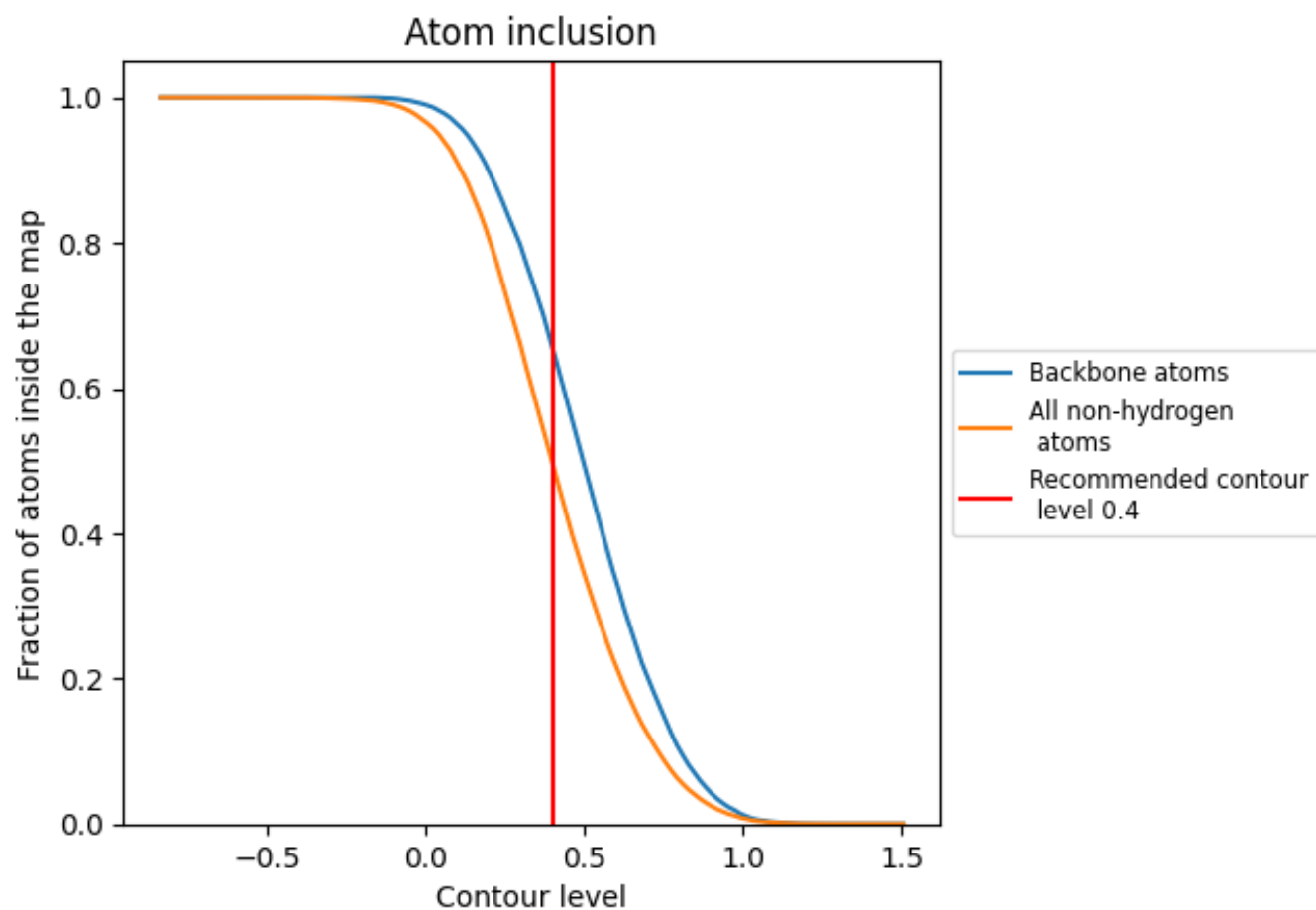
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 49% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.4942	<div><div></div></div> 0.1020
A	<div><div></div></div> 0.4840	<div><div></div></div> 0.0960
B	<div><div></div></div> 0.4896	<div><div></div></div> 0.1020
C	<div><div></div></div> 0.5138	<div><div></div></div> 0.1090
D	<div><div></div></div> 0.5358	<div><div></div></div> 0.1080
E	<div><div></div></div> 0.5071	<div><div></div></div> 0.1070
F	<div><div></div></div> 0.4462	<div><div></div></div> 0.0930

1.0

0.0

<0.0