Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 09:14 pm GMT

PDB ID	:	6ZHU
Title	:	Yeast Uba1 in complex with Ubc3 and ATP
Authors	:	Misra, M.; Schindelin, H.
Deposited on	:	2020-06-23
Resolution	:	3.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

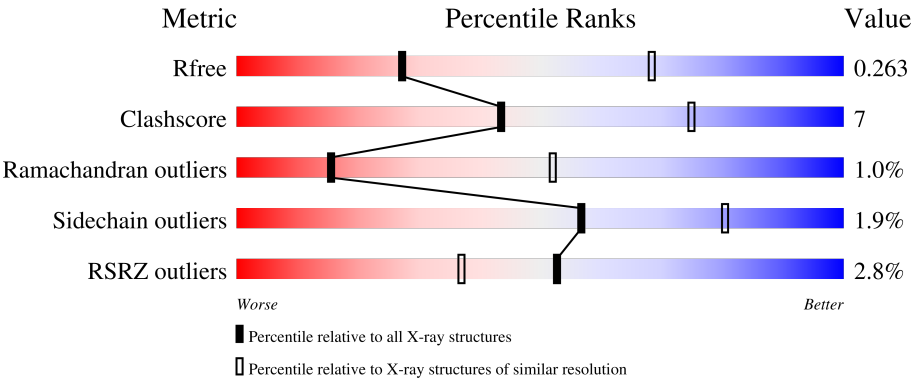
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	295	7% 39% 18% 40%
1	D	295	4% 41% 16% 41%
1	F	295	3% 40% 17% 40%
1	H	295	9% 37% 22% 40%
2	A	1024	% 83% 14%

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Mol	Chain	Length	Quality of chain
2	C	1024	85% 11%
2	E	1024	2% 80% 16%
2	G	1024	3% 83% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 73822 atoms, of which 36603 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

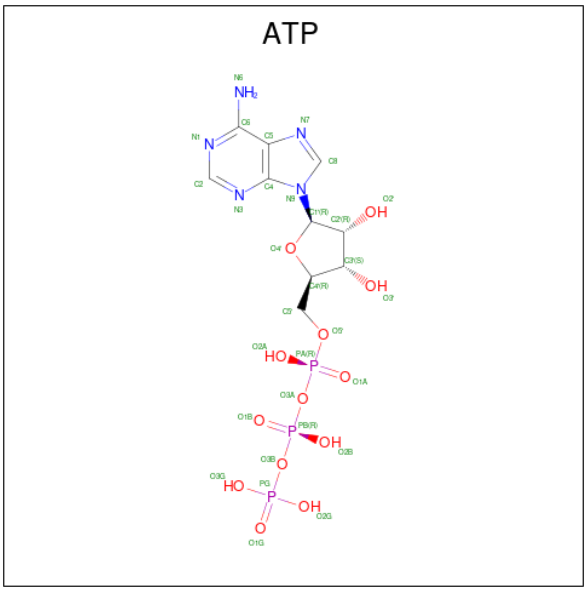
- Molecule 1 is a protein called Ubiquitin-conjugating enzyme E2-34 kDa.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	177	Total	C	H	N	O	S	0	0	0
			2821	910	1390	242	273	6			
1	F	178	Total	C	H	N	O	S	0	0	0
			2841	915	1402	243	274	7			
1	D	173	Total	C	H	N	O	S	0	0	0
			2753	892	1354	234	267	6			
1	H	178	Total	C	H	N	O	S	0	0	0
			2841	915	1402	243	274	7			

- Molecule 2 is a protein called Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	995	Total	C	H	N	O	S	0	0	0
			15611	5005	7760	1297	1526	23			
2	E	993	Total	C	H	N	O	S	0	0	0
			15590	4999	7751	1294	1523	23			
2	C	995	Total	C	H	N	O	S	0	0	0
			15612	5005	7761	1297	1526	23			
2	G	992	Total	C	H	N	O	S	0	0	0
			15572	4996	7739	1294	1520	23			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	E	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	G	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		

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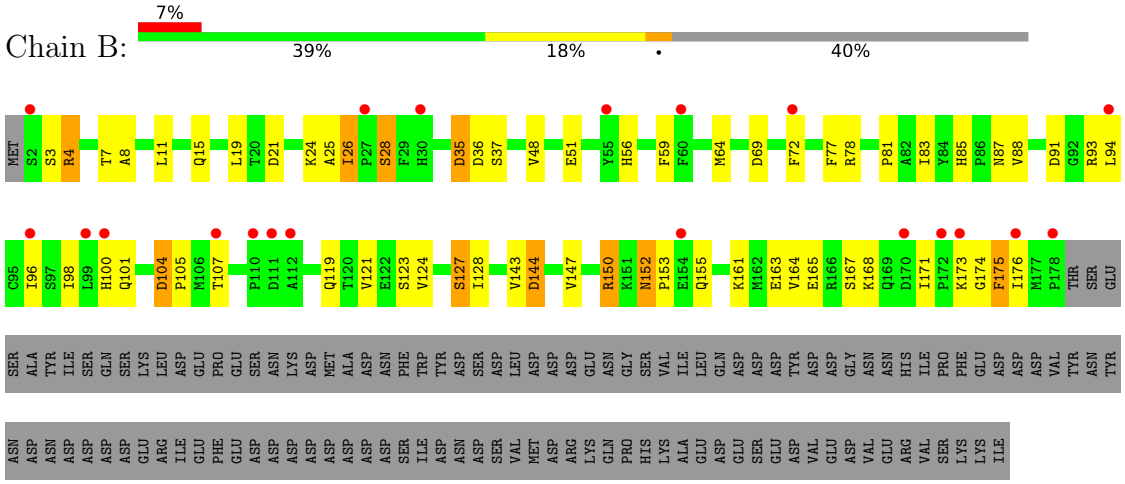
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	2	Total O 2 2	0	0
5	C	2	Total O 2 2	0	0
5	G	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

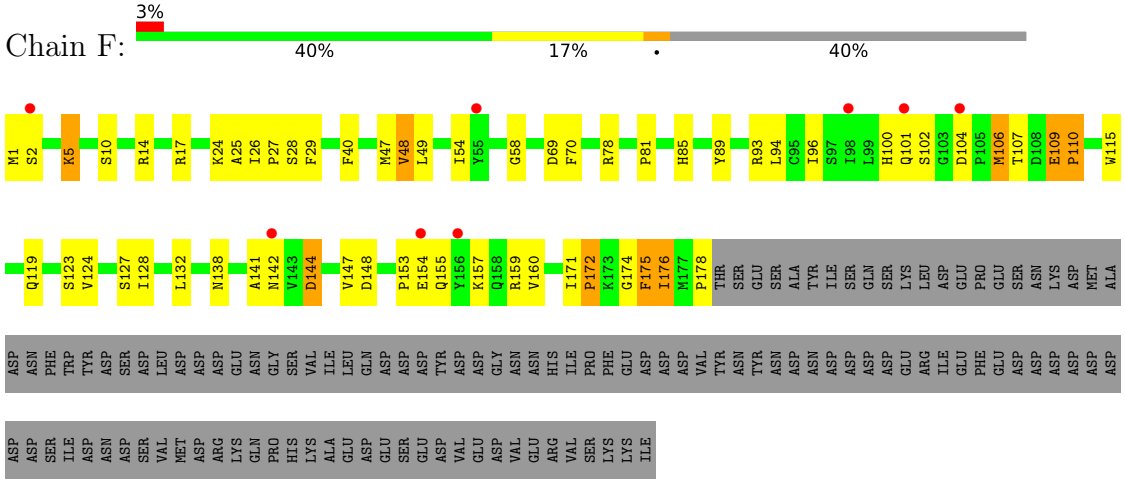
• Molecule 1: Ubiquitin-conjugating enzyme E2-34 kDa

Chain B:



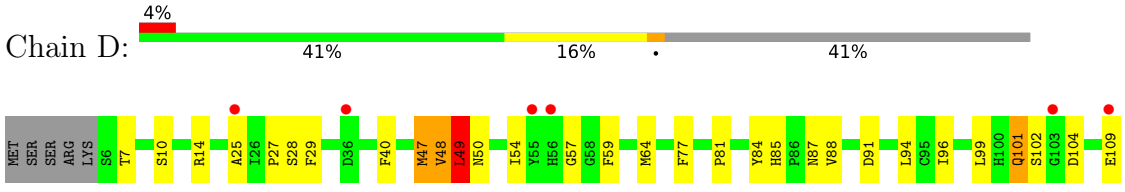
• Molecule 1: Ubiquitin-conjugating enzyme E2-34 kDa

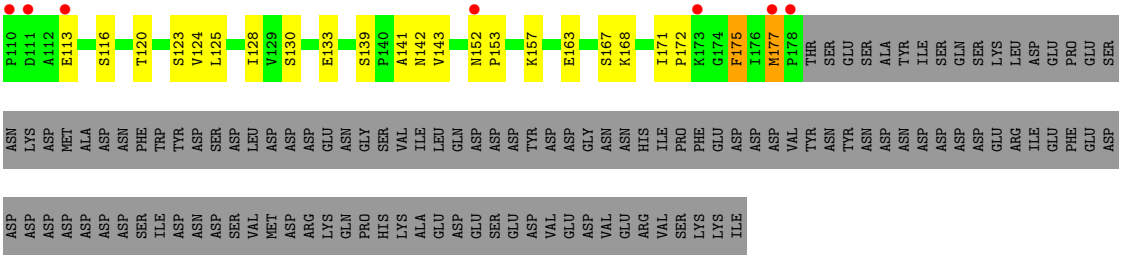
Chain F:



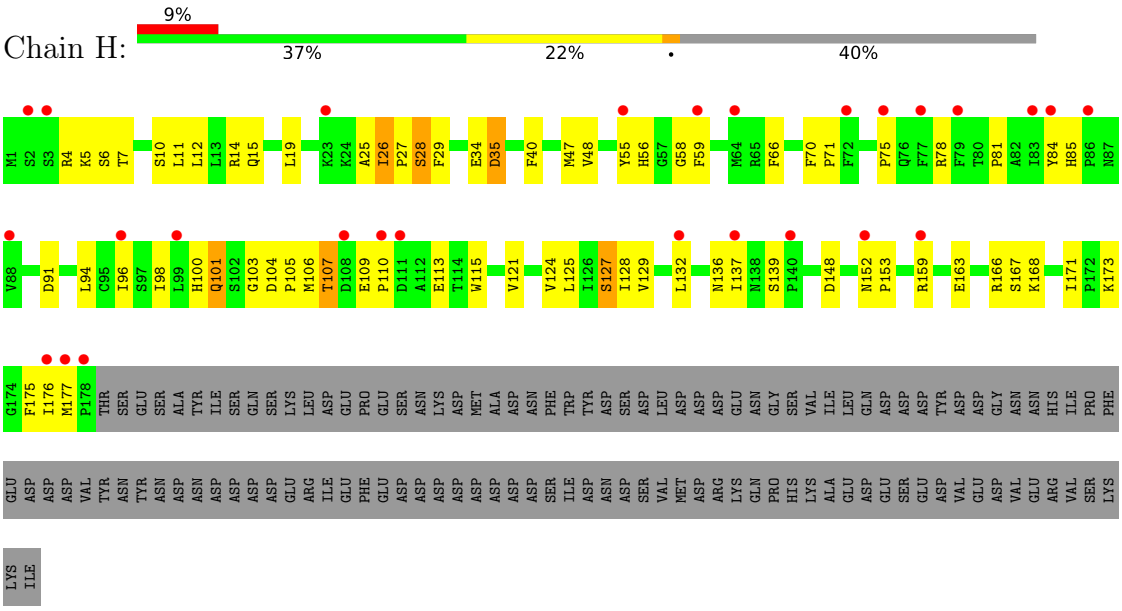
• Molecule 1: Ubiquitin-conjugating enzyme E2-34 kDa

Chain D:

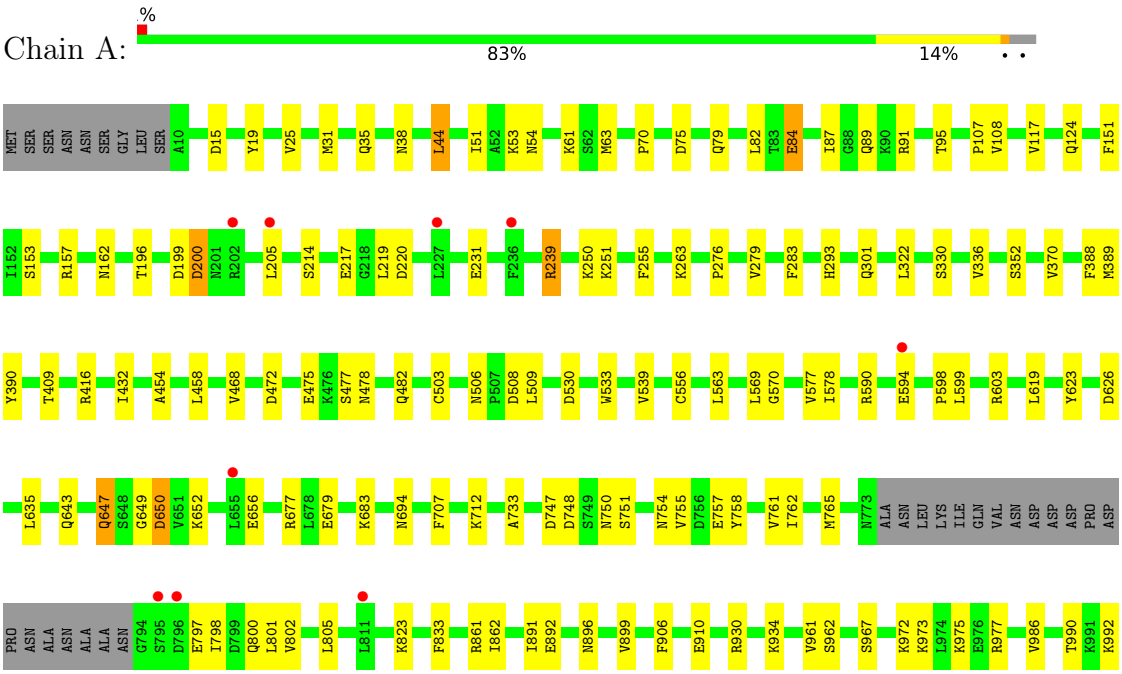




• Molecule 1: Ubiquitin-conjugating enzyme E2-34 kDa

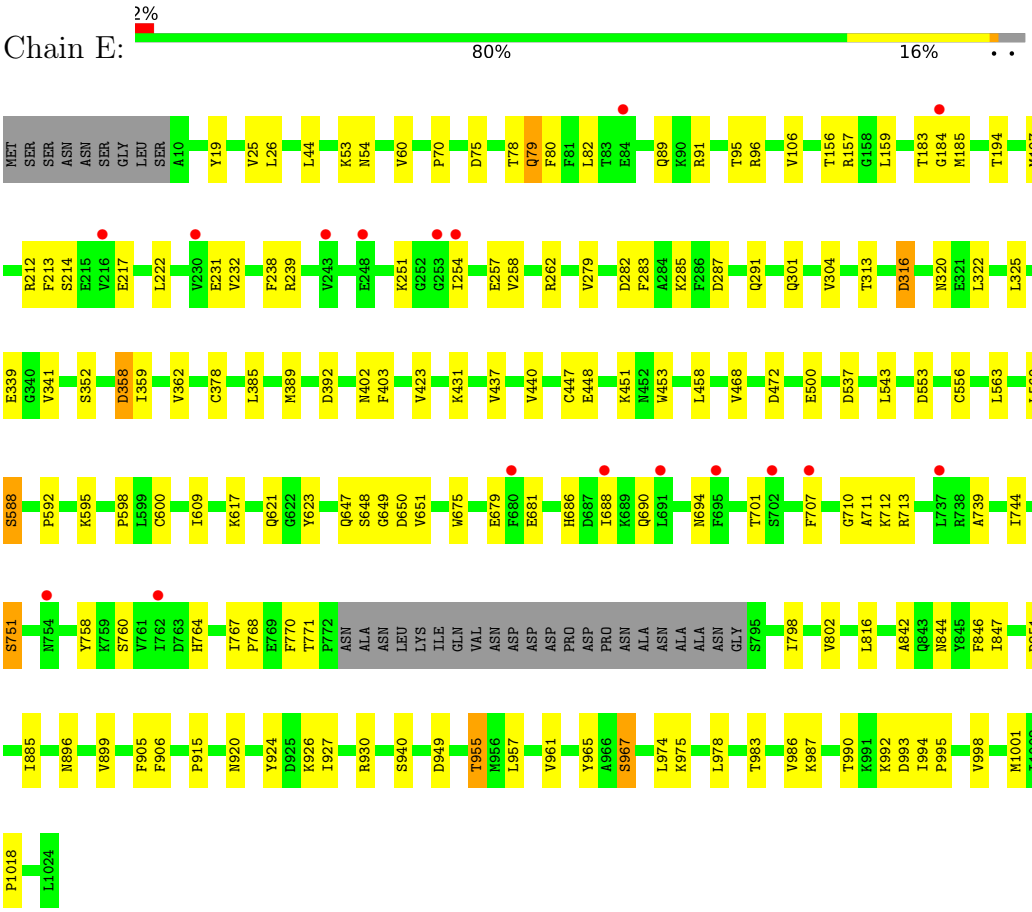


• Molecule 2: Ubiquitin-activating enzyme E1 1



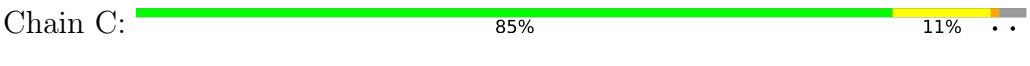
• Molecule 2: Ubiquitin-activating enzyme E1 1

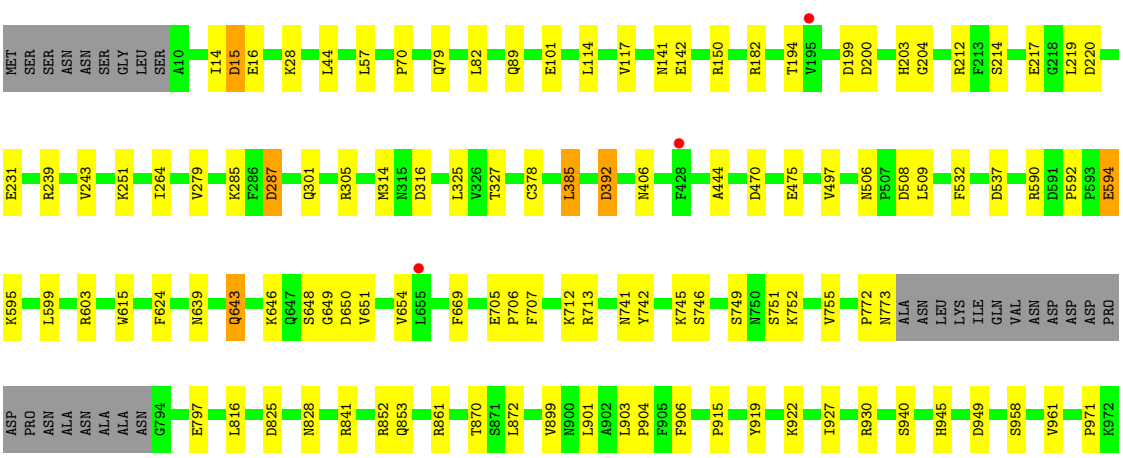
Chain E:

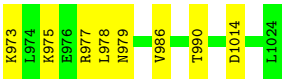


• Molecule 2: Ubiquitin-activating enzyme E1 1

Chain C:

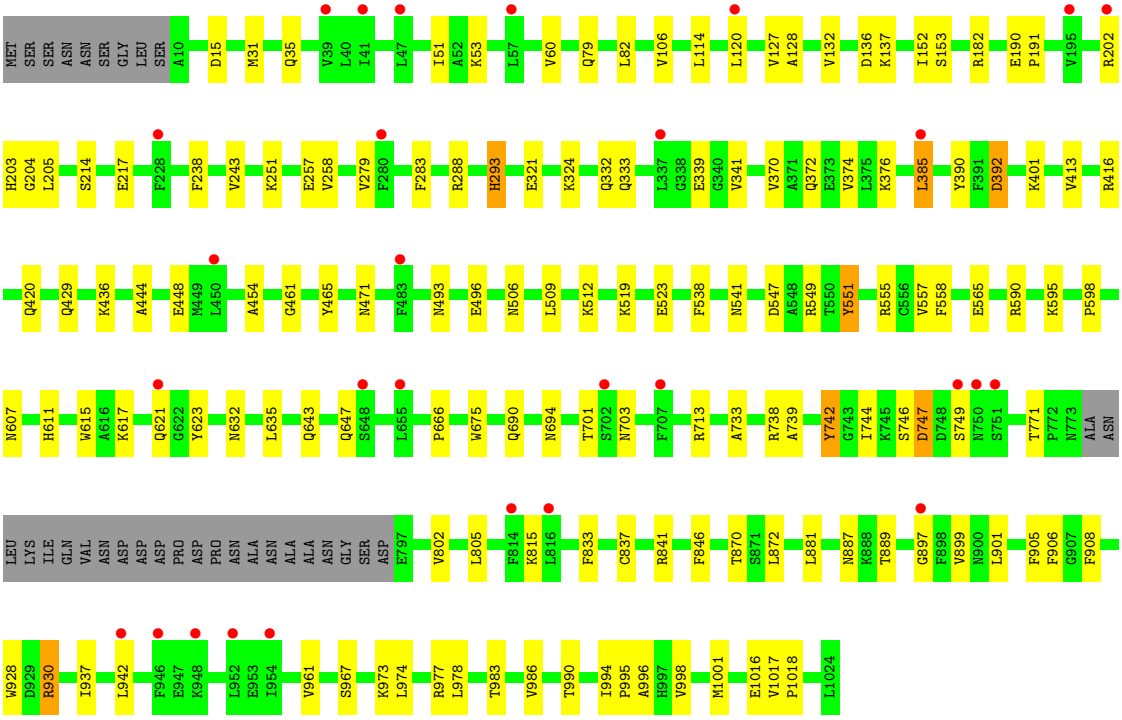






• Molecule 2: Ubiquitin-activating enzyme E1 1

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.64Å 152.41Å 252.57Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	49.81 – 3.18 49.81 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.81-3.18) 97.5 (49.81-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.217 , 0.263 0.217 , 0.263	Depositor DCC
R_{free} test set	4766 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	85.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	73822	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	B	0.59	0/1470	0.75	1/1997 (0.1%)
1	D	0.71	1/1438 (0.1%)	0.80	1/1956 (0.1%)
1	F	0.65	0/1478	0.75	0/2007
1	H	0.58	0/1478	0.68	0/2007
2	A	0.82	9/8014 (0.1%)	0.84	8/10842 (0.1%)
2	C	0.81	6/8014 (0.1%)	0.84	7/10842 (0.1%)
2	E	0.80	6/8002 (0.1%)	0.84	11/10826 (0.1%)
2	G	0.72	4/7996 (0.1%)	0.76	0/10818
All	All	0.77	26/37890 (0.1%)	0.81	28/51295 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	84	GLU	CG-CD	6.86	1.62	1.51
2	E	556	CYS	CB-SG	-6.63	1.71	1.82
2	G	837	CYS	CB-SG	-6.57	1.71	1.82
2	E	378	CYS	CB-SG	-6.44	1.71	1.82
2	E	447	CYS	CB-SG	-6.24	1.71	1.82
2	A	503	CYS	CB-SG	-6.14	1.71	1.82
2	C	532	PHE	CG-CD2	-5.93	1.29	1.38
2	C	979	ASN	C-N	5.73	1.47	1.34
2	A	556	CYS	CB-SG	-5.72	1.72	1.81
2	C	378	CYS	CB-SG	-5.68	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	987	LYS	CD-CE	5.68	1.65	1.51
2	G	551	TYR	CD2-CE2	-5.67	1.30	1.39
2	C	497	VAL	CB-CG2	-5.51	1.41	1.52
2	A	1006	CYS	CB-SG	-5.44	1.73	1.81
2	C	475	GLU	CG-CD	5.34	1.59	1.51
2	A	19	TYR	CG-CD2	-5.29	1.32	1.39
2	A	896	ASN	CB-CG	-5.28	1.39	1.51
2	A	590	ARG	C-N	5.27	1.46	1.34
1	D	109	GLU	C-N	5.23	1.44	1.34
2	E	896	ASN	CB-CG	-5.20	1.39	1.51
2	A	468	VAL	CB-CG1	-5.14	1.42	1.52
2	G	551	TYR	CD1-CE1	-5.08	1.31	1.39
2	G	523	GLU	CG-CD	5.05	1.59	1.51
2	C	101	GLU	CG-CD	5.04	1.59	1.51
2	A	577	VAL	CB-CG1	-5.02	1.42	1.52
2	E	19	TYR	CE1-CZ	-5.02	1.32	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	537	ASP	CB-CG-OD1	7.36	124.93	118.30
2	A	416	ARG	NE-CZ-NH1	-7.15	116.72	120.30
2	E	262	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	C	287	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	D	49	LEU	CA-CB-CG	6.36	129.93	115.30
2	E	358	ASP	CB-CG-OD2	6.33	123.99	118.30
2	C	537	ASP	CB-CG-OD1	6.17	123.85	118.30
2	C	212	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	C	713	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	A	157	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	19	LEU	CB-CG-CD1	5.98	121.17	111.00
2	A	44	LEU	CB-CG-CD1	-5.97	100.85	111.00
2	E	212	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	A	626	ASP	CB-CG-OD1	5.50	123.25	118.30
2	E	949	ASP	CB-CG-OD1	5.48	123.23	118.30
2	A	219	LEU	CB-CG-CD1	5.39	120.16	111.00
2	E	569	LEU	CB-CG-CD2	-5.37	101.87	111.00
2	A	472	ASP	CB-CG-OD1	-5.24	113.59	118.30
2	A	416	ARG	NE-CZ-NH2	5.23	122.92	120.30
2	C	57	LEU	CB-CG-CD1	-5.17	102.21	111.00
2	A	569	LEU	CB-CG-CD2	-5.14	102.26	111.00
2	E	472	ASP	CB-CG-OD2	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	993	ASP	CB-CG-OD1	5.10	122.89	118.30
2	C	150	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	C	1014	ASP	CB-CG-OD1	5.04	122.83	118.30
2	E	282	ASP	CB-CG-OD2	-5.03	113.78	118.30
2	E	282	ASP	CB-CG-OD1	5.03	122.82	118.30
2	E	262	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	100	HIS	Peptide
1	F	172	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1431	1390	1390	40	0
1	D	1399	1354	1354	40	0
1	F	1439	1402	1402	51	0
1	H	1439	1402	1402	46	0
2	A	7851	7760	7759	74	1
2	C	7851	7761	7759	74	0
2	E	7839	7751	7750	95	1
2	G	7833	7739	7747	92	2
3	A	31	11	12	0	0
3	C	31	11	12	2	0
3	E	31	11	12	2	0
3	G	31	11	12	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	3	0	0	0	0
5	C	2	0	0	1	0
5	E	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	2	0	0	3	0
All	All	37219	36603	36611	491	2

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 7.

All (491) 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:D:91:ASP:OD2	2:C:603:ARG:NH2	1.83	1.11
3:G:1101:ATP:O2B	5:G:1201:HOH:O	1.77	1.00
1:B:150:ARG:NH2	2:A:694:ASN:O	1.98	0.95
2:E:623:TYR:OH	2:E:679:GLU:OE1	1.83	0.95
2:C:705:GLU:HG2	2:C:706:PRO:HD2	1.57	0.85
1:H:28:SER:OG	1:H:47:MET:O	2.01	0.79
2:E:231:GLU:OE2	2:E:239:ARG:NH1	2.18	0.75
3:C:1101:ATP:O2B	5:C:1201:HOH:O	2.04	0.75
2:C:182:ARG:NH2	2:C:203:HIS:O	2.19	0.75
1:B:119:GLN:OE1	1:B:123:SER:OG	2.01	0.74
1:H:59:PHE:N	1:H:167:SER:OG	2.20	0.74
2:E:690:GLN:OE1	2:E:694:ASN:ND2	2.20	0.73
2:A:643:GLN:O	2:A:647:GLN:HG2	1.91	0.70
2:C:705:GLU:CG	2:C:706:PRO:HD2	2.21	0.69
3:E:1101:ATP:O1B	5:E:1201:HOH:O	2.11	0.69
2:A:79:GLN:HG2	2:A:82:LEU:HG	1.75	0.68
2:A:599:LEU:HD22	2:A:603:ARG:NH1	2.08	0.68
1:H:28:SER:OG	1:H:28:SER:O	2.11	0.68
2:A:70:PRO:HA	2:A:89:GLN:O	1.93	0.68
2:E:760:SER:O	2:E:764:HIS:NE2	2.27	0.68
3:E:1101:ATP:O2G	5:E:1201:HOH:O	2.13	0.67
2:C:594:GLU:OE1	2:C:861:ARG:NH1	2.28	0.67
2:G:746:SER:O	2:G:747:ASP:OD1	2.12	0.67
2:E:986:VAL:O	2:E:990:THR:HG22	1.95	0.66
2:G:872:LEU:HD13	2:G:901:LEU:HD21	1.78	0.66
2:G:182:ARG:NE	2:G:204:GLY:O	2.27	0.66
2:G:973:LYS:O	2:G:977:ARG:HG2	1.96	0.65
2:E:316:ASP:O	2:E:320:ASN:ND2	2.29	0.64
2:E:686:HIS:NE2	2:E:768:PRO:O	2.30	0.64
1:F:144:ASP:N	1:F:144:ASP:OD1	2.30	0.64
2:A:973:LYS:O	2:A:977:ARG:HG2	1.97	0.64
2:E:437:VAL:HG21	2:E:458:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1101:ATP:O1G	5:G:1201:HOH:O	2.14	0.64
1:B:37:SER:O	2:A:962:SER:HA	1.98	0.63
2:E:285:LYS:NZ	2:E:392:ASP:OD1	2.26	0.63
1:D:28:SER:O	1:D:28:SER:OG	2.11	0.63
1:D:101:GLN:H	1:D:101:GLN:HE21	1.45	0.62
2:C:79:GLN:HG2	2:C:82:LEU:HG	1.81	0.62
2:A:899:VAL:HG12	2:A:906:PHE:HD1	1.64	0.62
2:A:619:LEU:HD21	2:A:623:TYR:CZ	2.35	0.62
2:A:899:VAL:HG12	2:A:906:PHE:CD1	2.33	0.62
1:D:94:LEU:HD13	1:D:96:ILE:HD11	1.79	0.62
2:A:652:LYS:NZ	2:A:656:GLU:OE2	2.30	0.62
2:E:437:VAL:HG11	2:E:453:TRP:CH2	2.35	0.61
2:G:461:GLY:O	2:G:512:LYS:NZ	2.34	0.61
1:H:163:GLU:OE2	1:H:166:ARG:NH1	2.33	0.61
1:H:105:PRO:HG2	2:G:202:ARG:HB2	1.83	0.60
2:A:199:ASP:O	2:A:200:ASP:HB2	2.00	0.60
2:C:705:GLU:HG2	2:C:706:PRO:CD	2.30	0.60
2:C:973:LYS:O	2:C:977:ARG:HG2	2.00	0.60
2:G:288:ARG:NH1	2:G:392:ASP:OD2	2.34	0.60
1:B:104:ASP:HB3	1:B:105:PRO:CD	2.32	0.60
2:A:754:ASN:HB3	2:A:757:GLU:OE2	2.01	0.60
2:G:986:VAL:O	2:G:990:THR:HG22	2.02	0.60
2:E:688:ILE:HG13	2:E:844:ASN:ND2	2.16	0.60
1:B:4:ARG:HE	1:B:11:LEU:HD21	1.67	0.59
2:C:594:GLU:OE1	2:C:861:ARG:NH2	2.36	0.59
2:G:152:ILE:HD11	2:G:374:VAL:HG22	1.85	0.59
1:D:141:ALA:O	1:D:143:VAL:N	2.36	0.59
1:F:27:PRO:HB2	1:F:49:LEU:HD22	1.85	0.58
1:F:171:ILE:HG12	1:F:172:PRO:HD2	1.83	0.58
2:C:392:ASP:OD1	2:C:392:ASP:C	2.40	0.58
1:D:64:MET:HG3	1:D:77:PHE:HD2	1.69	0.58
1:F:94:LEU:HD12	1:F:94:LEU:N	2.19	0.58
2:C:961:VAL:HG12	2:C:961:VAL:O	2.02	0.58
1:H:78:ARG:NH2	1:H:91:ASP:O	2.37	0.57
2:A:279:VAL:O	2:A:389:MET:HG3	2.02	0.57
2:A:454:ALA:HA	2:A:509:LEU:HD11	1.86	0.57
1:F:109:GLU:HB2	1:F:110:PRO:HD3	1.87	0.57
2:G:928:TRP:O	2:G:930:ARG:NH1	2.38	0.57
2:C:915:PRO:HD2	2:C:927:ILE:CD1	2.36	0.56
1:F:94:LEU:HD22	1:F:96:ILE:HD11	1.88	0.56
2:C:669:PHE:CE1	2:C:746:SER:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:PHE:CE1	1:D:125:LEU:HB3	2.41	0.56
2:G:416:ARG:HH12	2:G:506:ASN:HA	1.70	0.56
2:G:558:PHE:O	2:G:930:ARG:NH2	2.39	0.55
1:D:141:ALA:C	1:D:143:VAL:H	2.10	0.55
2:E:75:ASP:OD2	2:E:91:ARG:NH1	2.38	0.55
1:D:28:SER:HB2	1:D:49:LEU:HD23	1.88	0.55
1:F:94:LEU:CD2	1:F:96:ILE:HD11	2.36	0.55
2:E:899:VAL:HG12	2:E:906:PHE:CD2	2.42	0.55
2:C:444:ALA:HB1	2:C:870:THR:HG21	1.89	0.55
1:F:124:VAL:O	1:F:128:ILE:HG12	2.07	0.55
1:F:138:ASN:O	2:E:712:LYS:NZ	2.27	0.55
2:A:117:VAL:HG12	2:C:755:VAL:HG11	1.88	0.55
1:H:4:ARG:HB3	2:G:1016:GLU:OE2	2.07	0.54
2:G:152:ILE:HD11	2:G:374:VAL:CG2	2.38	0.54
2:G:666:PRO:HD2	2:G:742:TYR:CD2	2.42	0.54
1:F:47:MET:HA	1:F:58:GLY:O	2.07	0.54
1:H:47:MET:HA	1:H:58:GLY:O	2.07	0.54
2:A:986:VAL:O	2:A:990:THR:HG22	2.07	0.54
2:C:745:LYS:NZ	2:C:749:SER:OG	2.39	0.54
1:B:21:ASP:OD2	1:B:24:LYS:HG3	2.07	0.54
2:E:940:SER:OG	2:E:978:LEU:O	2.23	0.54
1:F:171:ILE:HD11	1:F:178:PRO:HD3	1.88	0.54
2:A:748:ASP:OD2	2:A:758:TYR:OH	2.19	0.54
2:A:961:VAL:O	2:A:961:VAL:HG12	2.07	0.53
2:E:205:LEU:O	2:E:232:VAL:HG11	2.06	0.53
2:G:690:GLN:O	2:G:694:ASN:ND2	2.42	0.53
2:E:183:THR:HG22	2:E:184:GLY:N	2.24	0.53
1:B:161:LYS:O	1:B:165:GLU:HG2	2.08	0.53
2:A:652:LYS:HE3	2:A:797:GLU:OE2	2.07	0.53
2:E:325:LEU:O	2:E:329:LEU:HD13	2.08	0.53
2:G:128:ALA:HB1	2:G:132:VAL:HG11	1.90	0.53
1:B:3:SER:O	1:B:4:ARG:HB2	2.09	0.53
1:H:48:VAL:HG21	1:H:55:TYR:CB	2.39	0.53
1:F:24:LYS:O	1:F:26:ILE:N	2.41	0.53
2:E:257:GLU:HG2	2:E:258:VAL:N	2.24	0.52
2:G:416:ARG:NH1	2:G:506:ASN:HA	2.24	0.52
1:B:124:VAL:O	1:B:128:ILE:HG12	2.09	0.52
2:G:733:ALA:HB1	2:G:833:PHE:HB2	1.92	0.52
1:D:96:ILE:CD1	1:D:128:ILE:HD13	2.39	0.52
2:E:70:PRO:HA	2:E:89:GLN:O	2.09	0.52
2:E:79:GLN:HG2	2:E:82:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:79:GLN:CG	2:G:82:LEU:HB2	2.39	0.52
1:B:7:THR:HG22	1:B:8:ALA:N	2.25	0.52
2:E:53:LYS:HE3	2:E:54:ASN:OD1	2.09	0.52
3:G:1101:ATP:PG	5:G:1201:HOH:O	2.66	0.52
2:C:44:LEU:O	2:C:79:GLN:NE2	2.40	0.52
2:C:751:SER:OG	2:C:752:LYS:N	2.43	0.52
2:G:79:GLN:HG3	2:G:82:LEU:HB2	1.91	0.52
1:F:5:LYS:H	1:F:5:LYS:HD2	1.75	0.52
1:F:54:ILE:HG12	1:F:160:VAL:HG11	1.92	0.52
1:F:24:LYS:O	1:F:26:ILE:HG12	2.09	0.51
2:G:897:GLY:HA2	2:G:908:PHE:HD1	1.75	0.51
2:A:478:ASN:O	2:A:482:GLN:HG3	2.10	0.51
2:E:553:ASP:OD2	2:E:587:SER:OG	2.25	0.51
2:E:713:ARG:NH2	2:E:846:PHE:O	2.34	0.51
2:G:623:TYR:CD2	2:G:675:TRP:HH2	2.28	0.51
1:D:101:GLN:HE21	1:D:101:GLN:N	2.08	0.51
2:A:823:LYS:HD2	2:A:862:ILE:HD11	1.92	0.51
1:F:109:GLU:HB2	1:F:110:PRO:CD	2.41	0.51
2:G:182:ARG:HD3	2:G:205:LEU:HD23	1.91	0.51
2:G:1017:VAL:CG1	2:G:1018:PRO:HD2	2.41	0.51
1:F:109:GLU:OE1	1:F:110:PRO:HD2	2.11	0.50
2:C:872:LEU:HD22	2:C:899:VAL:HG21	1.92	0.50
1:B:98:ILE:HD13	1:B:127:SER:OG	2.10	0.50
1:B:96:ILE:CD1	1:B:128:ILE:HD13	2.41	0.50
1:B:152:ASN:N	1:B:153:PRO:CD	2.75	0.50
1:H:27:PRO:O	1:H:28:SER:HB3	2.11	0.50
2:E:359:ILE:HD11	2:E:423:VAL:HG21	1.93	0.50
2:C:594:GLU:OE1	2:C:861:ARG:CZ	2.59	0.50
2:G:283:PHE:CZ	2:G:905:PHE:HE1	2.29	0.50
1:F:85:HIS:CD2	1:F:132:LEU:HD12	2.46	0.50
1:D:59:PHE:N	1:D:167:SER:OG	2.45	0.50
2:A:205:LEU:HD11	2:A:255:PHE:CE1	2.47	0.50
2:A:986:VAL:HG11	2:A:994:ILE:HD11	1.94	0.50
2:G:643:GLN:O	2:G:647:GLN:HG2	2.12	0.50
1:B:85:HIS:CD2	1:B:87:ASN:H	2.30	0.49
2:C:285:LYS:NZ	2:C:392:ASP:OD1	2.31	0.49
1:B:144:ASP:O	1:B:147:VAL:HG22	2.13	0.49
1:F:78:ARG:NH1	2:E:648:SER:O	2.45	0.49
2:C:182:ARG:CZ	2:C:204:GLY:HA3	2.42	0.49
1:D:171:ILE:HG22	1:D:175:PHE:HB3	1.93	0.49
2:A:231:GLU:OE1	2:A:239:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PHE:O	1:B:167:SER:HB2	2.12	0.49
1:B:88:VAL:O	1:B:143:VAL:HG21	2.12	0.49
1:H:98:ILE:HD13	1:H:127:SER:OG	2.12	0.49
1:B:100:HIS:NE2	2:A:598:PRO:HA	2.28	0.49
1:F:119:GLN:HE21	1:F:123:SER:CB	2.25	0.49
2:E:183:THR:CG2	2:E:184:GLY:N	2.76	0.49
2:E:681:GLU:HG2	2:E:767:ILE:HG23	1.94	0.49
2:E:990:THR:HG23	2:E:992:LYS:HB2	1.95	0.49
1:H:84:TYR:HB3	1:H:163:GLU:HG3	1.93	0.49
1:H:168:LYS:O	1:H:171:ILE:HG23	2.12	0.49
2:A:44:LEU:HD13	2:A:95:THR:HG21	1.95	0.49
2:G:257:GLU:HG2	2:G:258:VAL:N	2.28	0.49
1:F:148:ASP:O	1:F:153:PRO:HD2	2.13	0.49
1:D:25:ALA:C	1:D:27:PRO:HD3	2.33	0.48
1:D:28:SER:O	1:D:29:PHE:CG	2.66	0.48
2:C:141:ASN:O	2:C:142:GLU:C	2.51	0.48
2:E:205:LEU:HD12	2:E:238:PHE:CE2	2.48	0.48
2:E:983:THR:HB	2:E:994:ILE:HD13	1.95	0.48
2:G:937:ILE:HD11	2:G:942:LEU:HD13	1.95	0.48
2:G:1017:VAL:HG13	2:G:1018:PRO:HD2	1.95	0.48
1:D:175:PHE:CD1	1:D:175:PHE:N	2.81	0.48
1:H:12:LEU:HD22	1:H:66:PHE:CE2	2.49	0.48
1:F:171:ILE:CG1	1:F:172:PRO:HD2	2.43	0.48
1:D:94:LEU:HB3	1:D:96:ILE:HG13	1.95	0.48
2:G:541:ASN:ND2	2:G:565:GLU:OE1	2.47	0.48
2:A:707:PHE:CE1	2:A:712:LYS:HE3	2.48	0.48
2:A:733:ALA:HB1	2:A:833:PHE:HB2	1.96	0.48
2:G:690:GLN:OE1	2:G:694:ASN:ND2	2.47	0.48
1:H:104:ASP:HA	2:G:595:LYS:HE2	1.95	0.48
2:A:972:LYS:HD3	2:A:975:LYS:HE3	1.95	0.48
1:F:109:GLU:CB	1:F:110:PRO:CD	2.91	0.48
2:E:915:PRO:HB2	2:E:926:LYS:HB2	1.96	0.48
2:C:231:GLU:OE2	2:C:239:ARG:NH1	2.47	0.48
1:B:153:PRO:HG2	1:B:155:GLN:HG2	1.96	0.47
2:E:851:ASP:OD1	2:E:851:ASP:N	2.41	0.47
2:C:599:LEU:HD13	2:C:603:ARG:NH1	2.29	0.47
2:G:974:LEU:HD11	2:G:978:LEU:HD11	1.96	0.47
1:B:51:GLU:N	1:B:51:GLU:OE1	2.47	0.47
2:E:710:GLY:O	2:E:712:LYS:N	2.47	0.47
2:C:14:ILE:HD12	2:C:28:LYS:HG3	1.95	0.47
2:C:287:ASP:N	2:C:287:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:HB2	1:B:72:PHE:CZ	2.50	0.47
1:D:177:MET:O	1:D:177:MET:SD	2.73	0.47
1:F:155:GLN:HB3	1:F:159:ARG:NH2	2.29	0.47
2:A:599:LEU:HD13	2:A:603:ARG:HH12	1.80	0.47
2:G:31:MET:O	2:G:35:GLN:HG3	2.15	0.47
1:B:48:VAL:HB	1:B:56:HIS:HA	1.97	0.47
1:D:152:ASN:N	1:D:153:PRO:CD	2.78	0.47
2:A:217:GLU:OE1	2:A:251:LYS:HE3	2.15	0.47
2:A:506:ASN:OD1	2:A:508:ASP:HB2	2.15	0.47
2:E:899:VAL:HG12	2:E:906:PHE:HD2	1.79	0.47
2:G:994:ILE:HG21	2:G:1001:MET:CE	2.45	0.47
1:H:124:VAL:O	1:H:128:ILE:HG12	2.15	0.47
2:A:563:LEU:HB3	2:A:578:ILE:HB	1.97	0.47
2:E:287:ASP:O	2:E:291:GLN:HG2	2.14	0.47
2:E:965:TYR:HE1	2:E:974:LEU:CD2	2.27	0.46
1:F:138:ASN:OD1	2:E:701:THR:HG21	2.16	0.46
1:D:96:ILE:HD11	1:D:128:ILE:HD13	1.97	0.46
2:A:475:GLU:CD	2:A:477:SER:HG	2.19	0.46
2:E:798:ILE:O	2:E:802:VAL:HG23	2.15	0.46
2:G:79:GLN:HG2	2:G:82:LEU:HD22	1.97	0.46
1:H:94:LEU:HD13	1:H:96:ILE:HD11	1.96	0.46
1:H:171:ILE:HD12	1:H:175:PHE:CE1	2.51	0.46
1:B:91:ASP:OD2	2:A:603:ARG:NH2	2.49	0.46
1:H:66:PHE:HD1	1:H:75:PRO:HB3	1.80	0.46
2:A:755:VAL:HG11	2:C:117:VAL:HG12	1.96	0.46
2:C:899:VAL:HG12	2:C:906:PHE:HD2	1.80	0.46
1:D:29:PHE:CZ	1:D:125:LEU:HB3	2.49	0.46
1:D:57:GLY:O	1:D:168:LYS:HE3	2.15	0.46
2:A:15:ASP:C	2:A:15:ASP:OD1	2.54	0.46
1:F:1:MET:SD	2:E:592:PRO:HD3	2.56	0.46
1:D:130:SER:HA	1:D:133:GLU:HG2	1.98	0.46
2:E:322:LEU:HD22	2:E:352:SER:HB2	1.98	0.46
2:G:339:GLU:O	2:G:341:VAL:HG23	2.16	0.46
1:B:164:VAL:O	1:B:168:LYS:HG3	2.16	0.46
1:D:40:PHE:HD1	2:C:961:VAL:HG13	1.80	0.46
1:D:171:ILE:HG23	1:D:172:PRO:HD2	1.97	0.46
2:E:468:VAL:O	2:E:468:VAL:HG13	2.15	0.46
2:E:957:LEU:HD11	2:E:1003:LEU:HD13	1.98	0.46
2:C:986:VAL:O	2:C:990:THR:HG22	2.15	0.46
2:G:632:ASN:HD21	2:G:815:LYS:HG2	1.80	0.46
2:A:84:GLU:O	2:A:87:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:506:ASN:OD1	2:C:508:ASP:HB2	2.16	0.46
2:C:599:LEU:HD13	2:C:603:ARG:HH12	1.81	0.46
2:G:79:GLN:HG3	2:G:82:LEU:CB	2.46	0.46
1:B:94:LEU:HD13	1:B:96:ILE:HD11	1.98	0.46
1:F:96:ILE:CD1	1:F:128:ILE:HD13	2.45	0.46
1:F:102:SER:HB2	1:F:115:TRP:O	2.16	0.46
1:D:141:ALA:C	1:D:143:VAL:N	2.69	0.46
2:C:217:GLU:OE1	2:C:251:LYS:HE3	2.15	0.46
2:G:321:GLU:O	2:G:324:LYS:HB3	2.16	0.46
2:G:607:ASN:OD1	2:G:611:HIS:CE1	2.69	0.46
1:H:137:ILE:HD11	2:G:701:THR:HB	1.98	0.45
2:E:301:GLN:OE1	2:E:329:LEU:HD11	2.16	0.45
2:G:15:ASP:OD1	2:G:15:ASP:C	2.53	0.45
2:E:767:ILE:HG22	2:E:767:ILE:O	2.16	0.45
2:G:557:VAL:HA	2:G:928:TRP:CZ3	2.51	0.45
1:D:120:THR:HG23	1:D:123:SER:H	1.80	0.45
1:H:25:ALA:O	1:H:26:ILE:C	2.54	0.45
2:A:599:LEU:HD22	2:A:603:ARG:HH12	1.80	0.45
2:C:745:LYS:HZ1	2:C:749:SER:CB	2.29	0.45
2:G:995:PRO:HD2	2:G:998:VAL:HG21	1.97	0.45
1:D:54:ILE:HG21	1:D:157:LYS:NZ	2.32	0.45
2:A:619:LEU:HD21	2:A:623:TYR:CE2	2.52	0.45
2:E:159:LEU:HA	2:E:362:VAL:HG21	1.98	0.45
1:H:176:ILE:HG23	1:H:177:MET:H	1.80	0.45
2:E:185:MET:HG2	2:E:254:ILE:HG12	1.99	0.45
2:E:563:LEU:HB3	2:E:578:ILE:HB	1.99	0.45
2:C:314:MET:HE2	2:C:406:ASN:HA	1.98	0.45
2:A:53:LYS:HE3	2:A:54:ASN:OD1	2.17	0.45
2:A:293:HIS:HD2	2:A:336:VAL:HG11	1.82	0.45
2:G:132:VAL:HG13	2:G:137:LYS:HG3	1.97	0.45
1:F:27:PRO:HB2	1:F:49:LEU:CD2	2.46	0.45
2:A:61:LYS:O	2:A:107:PRO:HD2	2.16	0.45
2:C:16:GLU:OE1	2:C:853:GLN:HG3	2.16	0.45
2:C:509:LEU:HD12	2:C:509:LEU:N	2.32	0.45
1:B:64:MET:HG3	1:B:77:PHE:HD2	1.81	0.45
1:F:101:GLN:HG3	2:E:598:PRO:HG3	1.99	0.45
2:E:279:VAL:O	2:E:389:MET:HG3	2.17	0.45
2:A:151:PHE:CE1	2:A:153:SER:HB2	2.51	0.45
2:E:994:ILE:HG12	2:E:1001:MET:CE	2.46	0.45
2:C:301:GLN:O	2:C:305:ARG:HG3	2.17	0.45
2:G:132:VAL:CG2	2:G:136:ASP:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:137:LYS:HE2	2:G:153:SER:OG	2.17	0.45
1:B:64:MET:HG3	1:B:77:PHE:CD2	2.52	0.44
1:B:168:LYS:O	1:B:171:ILE:HG12	2.17	0.44
1:D:54:ILE:HG21	1:D:157:LYS:HZ3	1.82	0.44
2:C:279:VAL:HG21	2:C:385:LEU:HG	1.99	0.44
2:C:825:ASP:HB3	2:C:828:ASN:ND2	2.32	0.44
1:F:107:THR:OG1	1:F:110:PRO:O	2.35	0.44
2:A:63:MET:O	2:A:108:VAL:HA	2.18	0.44
2:E:748:ASP:O	2:E:749:SER:C	2.55	0.44
2:C:243:VAL:HG12	2:C:243:VAL:O	2.18	0.44
2:C:940:SER:OG	2:C:978:LEU:O	2.32	0.44
2:G:887:ASN:O	2:G:889:THR:HG23	2.17	0.44
1:F:17:ARG:CZ	2:E:955:THR:HG21	2.47	0.44
1:D:84:TYR:HB3	1:D:163:GLU:HG3	1.99	0.44
2:E:70:PRO:HG2	2:G:996:ALA:HB1	1.98	0.44
2:C:919:TYR:O	2:C:922:LYS:HB2	2.18	0.44
1:F:2:SER:HA	2:E:588:SER:O	2.17	0.44
1:H:5:LYS:C	1:H:7:THR:H	2.20	0.44
2:A:432:ILE:HG23	2:A:458:LEU:HD12	2.00	0.44
2:C:114:LEU:O	2:C:114:LEU:HG	2.18	0.44
1:B:104:ASP:HB3	1:B:105:PRO:HD2	2.00	0.44
1:F:147:VAL:HG11	2:E:694:ASN:OD1	2.17	0.44
1:F:171:ILE:HD11	1:F:178:PRO:CD	2.47	0.44
1:D:99:LEU:HD21	1:D:124:VAL:HG13	1.99	0.44
2:E:690:GLN:O	2:E:694:ASN:ND2	2.47	0.44
2:E:842:ALA:HB1	2:E:847:ILE:O	2.18	0.44
2:G:615:TRP:CD2	2:G:841:ARG:HD2	2.52	0.44
1:H:121:VAL:O	1:H:125:LEU:CD2	2.66	0.44
2:A:79:GLN:CG	2:A:82:LEU:HG	2.45	0.44
2:G:332:GLN:OE1	2:G:333:GLN:NE2	2.45	0.44
1:B:35:ASP:O	1:B:37:SER:N	2.51	0.44
2:E:920:ASN:OD1	2:E:1009:ASP:HB2	2.18	0.44
2:C:592:PRO:HG2	2:C:595:LYS:HE2	1.99	0.44
1:F:154:GLU:HA	1:F:157:LYS:HD2	2.00	0.44
2:E:78:THR:OG1	2:E:358:ASP:OD1	2.24	0.44
2:G:293:HIS:CG	2:G:390:TYR:HH	2.36	0.44
1:H:100:HIS:CE1	2:G:598:PRO:HA	2.53	0.43
2:A:533:TRP:HZ3	2:A:539:VAL:HG21	1.83	0.43
2:G:51:ILE:HD13	2:G:370:VAL:HG11	1.99	0.43
1:D:171:ILE:CG2	1:D:172:PRO:HD2	2.49	0.43
1:H:11:LEU:HD11	1:H:15:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:ILE:CD1	1:H:128:ILE:HD13	2.48	0.43
2:A:761:VAL:O	2:A:765:MET:HG3	2.18	0.43
2:C:470:ASP:OD1	3:C:1101:ATP:O2'	2.33	0.43
2:G:53:LYS:NZ	2:G:448:GLU:OE2	2.51	0.43
1:H:148:ASP:O	1:H:153:PRO:HD2	2.18	0.43
2:C:264:ILE:HG21	2:C:264:ILE:HD13	1.71	0.43
2:G:444:ALA:HB1	2:G:870:THR:HG21	2.01	0.43
2:E:44:LEU:HD13	2:E:95:THR:HG21	1.99	0.43
2:E:60:VAL:O	2:E:106:VAL:HG22	2.18	0.43
2:E:915:PRO:HD2	2:E:927:ILE:CD1	2.48	0.43
2:G:203:HIS:HB2	2:G:205:LEU:HG	2.00	0.43
1:F:28:SER:O	1:F:29:PHE:CG	2.72	0.43
2:A:38:ASN:ND2	2:A:124:GLN:OE1	2.52	0.43
1:B:88:VAL:HG22	1:B:94:LEU:HD21	1.99	0.43
2:C:649:GLY:O	2:C:651:VAL:N	2.49	0.43
2:G:973:LYS:HE3	2:G:977:ARG:HH22	1.82	0.43
1:F:106:MET:SD	1:F:107:THR:N	2.89	0.43
1:D:28:SER:HA	1:D:47:MET:HB2	2.01	0.43
2:A:801:LEU:O	2:A:805:LEU:HG	2.19	0.43
2:C:742:TYR:CE2	2:C:816:LEU:HD21	2.53	0.43
1:B:88:VAL:HG22	1:B:94:LEU:CD2	2.49	0.43
1:H:29:PHE:HZ	1:H:129:VAL:HG23	1.83	0.43
1:H:106:MET:O	1:H:107:THR:C	2.57	0.43
2:A:934:LYS:HZ2	2:A:1023:HIS:CE1	2.36	0.43
2:E:924:TYR:CD2	2:E:1018:PRO:HG3	2.54	0.43
1:H:101:GLN:HB3	1:H:115:TRP:HB3	2.00	0.43
1:H:109:GLU:HB2	1:H:110:PRO:CD	2.49	0.43
2:A:677:ARG:HD3	2:A:762:ILE:HD12	2.01	0.43
2:E:156:THR:O	2:E:157:ARG:HD3	2.19	0.43
2:C:592:PRO:HG2	2:C:595:LYS:CE	2.49	0.43
2:G:203:HIS:CD2	2:G:238:PHE:HD2	2.37	0.43
1:B:15:GLN:OE1	1:B:121:VAL:HG23	2.19	0.43
1:H:121:VAL:O	1:H:125:LEU:HD23	2.18	0.43
2:E:402:ASN:HB2	2:E:403:PHE:CD1	2.54	0.43
2:E:440:VAL:HG12	2:E:543:LEU:HD21	1.99	0.43
2:C:624:PHE:HA	2:C:741:ASN:HD21	1.84	0.42
2:G:675:TRP:CE3	2:G:738:ARG:HD2	2.53	0.42
1:F:155:GLN:HB3	1:F:159:ARG:HH22	1.84	0.42
2:E:80:PHE:CD2	2:E:451:LYS:HD2	2.54	0.42
2:C:199:ASP:O	2:C:200:ASP:C	2.57	0.42
2:C:872:LEU:HD13	2:C:901:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:903:LEU:H	2:C:904:PRO:HA	1.84	0.42
2:C:945:HIS:O	2:C:949:ASP:HB2	2.19	0.42
1:F:47:MET:O	1:F:48:VAL:HB	2.20	0.42
2:E:750:ASN:O	2:E:751:SER:HB2	2.18	0.42
2:E:995:PRO:HD2	2:E:998:VAL:HG21	2.01	0.42
2:G:607:ASN:OD1	2:G:611:HIS:HE1	2.01	0.42
2:G:994:ILE:HD13	2:G:1001:MET:CE	2.50	0.42
1:D:124:VAL:O	1:D:128:ILE:HG12	2.19	0.42
2:A:599:LEU:HD13	2:A:603:ARG:NH1	2.35	0.42
2:E:283:PHE:CZ	2:E:905:PHE:HE1	2.37	0.42
2:E:623:TYR:CD2	2:E:675:TRP:CH2	3.08	0.42
2:G:454:ALA:HA	2:G:509:LEU:HD11	2.01	0.42
1:B:3:SER:O	1:B:4:ARG:CB	2.68	0.42
1:H:19:LEU:CD2	1:H:26:ILE:CD1	2.97	0.42
2:A:25:VAL:HG22	2:A:570:GLY:HA2	2.02	0.42
2:A:623:TYR:OH	2:A:679:GLU:OE1	2.27	0.42
2:E:301:GLN:O	2:E:304:VAL:HG12	2.19	0.42
2:E:431:LYS:HE3	2:E:885:ILE:O	2.20	0.42
1:H:98:ILE:HG22	1:H:113:GLU:HA	2.01	0.42
2:A:75:ASP:OD2	2:A:91:ARG:NH1	2.52	0.42
2:G:802:VAL:HA	2:G:805:LEU:HD12	2.02	0.42
1:F:10:SER:O	1:F:14:ARG:HG3	2.20	0.42
1:H:70:PHE:CE2	1:H:71:PRO:HB3	2.54	0.42
2:E:392:ASP:OD1	2:E:392:ASP:C	2.58	0.42
2:C:646:LYS:O	2:C:648:SER:N	2.44	0.42
2:G:549:ARG:NE	2:G:565:GLU:OE2	2.52	0.42
2:G:551:TYR:O	2:G:555:ARG:HG2	2.20	0.42
2:G:742:TYR:N	2:G:742:TYR:CD1	2.87	0.42
1:H:84:TYR:CD2	1:H:159:ARG:HG2	2.54	0.42
2:C:182:ARG:CZ	2:C:203:HIS:O	2.68	0.42
2:G:127:VAL:HG22	2:G:152:ILE:CG1	2.50	0.42
2:G:538:PHE:CZ	2:G:881:LEU:CD1	3.02	0.42
1:B:7:THR:HG22	1:B:8:ALA:H	1.85	0.42
1:D:85:HIS:CD2	1:D:87:ASN:H	2.38	0.42
2:E:983:THR:CB	2:E:994:ILE:HD13	2.50	0.42
2:C:961:VAL:O	2:C:961:VAL:CG1	2.67	0.42
1:H:152:ASN:N	1:H:153:PRO:CD	2.83	0.42
2:C:615:TRP:CD2	2:C:841:ARG:HD2	2.55	0.42
1:H:34:GLU:HG3	1:H:35:ASP:N	2.35	0.41
2:A:276:PRO:HD2	2:A:336:VAL:HG22	2.01	0.41
2:A:283:PHE:CE1	2:E:975:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:639:ASN:O	2:C:643:GLN:OE1	2.37	0.41
2:C:915:PRO:HD2	2:C:927:ILE:HD11	2.02	0.41
1:B:174:GLY:O	1:B:175:PHE:C	2.58	0.41
1:F:89:TYR:CZ	1:F:141:ALA:HB1	2.56	0.41
1:F:172:PRO:O	1:F:174:GLY:N	2.53	0.41
1:D:48:VAL:O	1:D:48:VAL:HG12	2.20	0.41
2:E:44:LEU:O	2:E:79:GLN:NE2	2.47	0.41
2:E:213:PHE:HB2	2:E:222:LEU:HD23	2.02	0.41
2:E:217:GLU:OE1	2:E:251:LYS:HE3	2.20	0.41
2:C:872:LEU:HD21	2:C:899:VAL:HG11	2.02	0.41
2:G:413:VAL:O	2:G:413:VAL:HG23	2.20	0.41
2:G:471:ASN:ND2	2:G:519:LYS:HB2	2.34	0.41
2:G:617:LYS:HE2	2:G:621:GLN:NE2	2.35	0.41
1:D:28:SER:HB2	1:D:49:LEU:CD2	2.50	0.41
2:A:990:THR:HG23	2:A:992:LYS:HB2	2.02	0.41
2:C:15:ASP:C	2:C:15:ASP:OD1	2.58	0.41
1:F:109:GLU:CG	1:F:110:PRO:HD2	2.50	0.41
2:A:594:GLU:OE2	2:A:861:ARG:NH1	2.44	0.41
2:A:649:GLY:O	2:A:650:ASP:C	2.58	0.41
2:G:436:LYS:HB3	2:G:465:TYR:CZ	2.55	0.41
1:F:89:TYR:CE1	1:F:141:ALA:HB1	2.56	0.41
1:F:93:ARG:C	1:F:94:LEU:HD12	2.40	0.41
2:C:305:ARG:CZ	2:C:325:LEU:HD21	2.51	0.41
2:C:650:ASP:O	2:C:654:VAL:HG23	2.20	0.41
2:G:420:GLN:HB3	2:G:429:GLN:NE2	2.36	0.41
1:H:4:ARG:O	1:H:5:LYS:HB2	2.20	0.41
1:H:10:SER:O	1:H:14:ARG:HG3	2.20	0.41
2:A:961:VAL:O	2:A:961:VAL:CG1	2.69	0.41
2:C:70:PRO:HA	2:C:89:GLN:O	2.20	0.41
1:H:85:HIS:CD2	1:H:132:LEU:HD12	2.56	0.41
1:H:136:ASN:ND2	1:H:139:SER:OG	2.53	0.41
2:A:31:MET:O	2:A:35:GLN:HG3	2.20	0.41
2:A:892:GLU:HG2	2:A:910:GLU:OE1	2.20	0.41
2:C:752:LYS:HD3	2:C:752:LYS:HA	1.89	0.41
2:G:279:VAL:HG21	2:G:385:LEU:CD1	2.51	0.41
1:B:26:ILE:O	1:B:28:SER:N	2.53	0.41
2:A:51:ILE:HD13	2:A:370:VAL:HG11	2.02	0.41
2:A:530:ASP:OD2	2:A:999:SER:HB3	2.21	0.41
2:A:748:ASP:HA	2:A:751:SER:O	2.20	0.41
2:E:617:LYS:HE2	2:E:621:GLN:NE2	2.35	0.41
2:C:615:TRP:CE3	2:C:841:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:707:PHE:CE1	2:C:712:LYS:HE3	2.56	0.41
2:C:899:VAL:HG12	2:C:906:PHE:CD2	2.56	0.41
1:F:102:SER:HB3	2:E:595:LYS:HE3	2.03	0.41
2:A:798:ILE:O	2:A:802:VAL:HG23	2.21	0.41
2:E:331:VAL:O	2:E:331:VAL:HG12	2.20	0.41
2:E:448:GLU:HG3	2:E:870:THR:HG22	2.03	0.41
2:E:739:ALA:HB1	2:E:744:ILE:O	2.21	0.41
2:G:60:VAL:O	2:G:106:VAL:HG22	2.21	0.41
2:G:190:GLU:HB3	2:G:191:PRO:CD	2.51	0.41
2:G:376:LYS:NZ	2:G:901:LEU:O	2.46	0.41
2:G:538:PHE:CZ	2:G:881:LEU:HD11	2.55	0.41
1:B:78:ARG:HD3	1:B:93:ARG:NH2	2.36	0.41
1:F:40:PHE:HD1	2:E:961:VAL:HG13	1.86	0.41
1:F:69:ASP:O	1:F:70:PHE:C	2.59	0.41
1:D:7:THR:O	1:D:7:THR:HG22	2.20	0.41
1:H:137:ILE:CD1	2:G:701:THR:HB	2.50	0.41
2:E:25:VAL:HG12	2:E:26:LEU:HD23	2.03	0.41
2:G:114:LEU:HD11	2:G:120:LEU:HD21	2.03	0.41
2:G:739:ALA:HB1	2:G:744:ILE:O	2.21	0.41
1:B:83:ILE:HA	1:B:163:GLU:OE2	2.22	0.40
1:F:175:PHE:O	1:F:176:ILE:O	2.38	0.40
1:H:48:VAL:CG1	1:H:56:HIS:HA	2.51	0.40
2:E:748:ASP:OD2	2:E:758:TYR:OH	2.39	0.40
2:E:983:THR:HA	2:E:994:ILE:CD1	2.51	0.40
2:G:372:GLN:HG3	2:G:376:LYS:HE3	2.04	0.40
2:G:983:THR:HG22	2:G:994:ILE:CD1	2.50	0.40
1:B:85:HIS:HB3	1:B:88:VAL:CG2	2.51	0.40
1:H:40:PHE:HD1	2:G:961:VAL:HG13	1.87	0.40
2:E:750:ASN:OD1	2:E:750:ASN:N	2.54	0.40
2:G:448:GLU:HG3	2:G:870:THR:HG22	2.02	0.40
1:F:28:SER:O	1:F:28:SER:OG	2.33	0.40
1:D:10:SER:HB2	1:D:14:ARG:NH2	2.37	0.40
2:A:162:ASN:HB3	2:A:390:TYR:CD1	2.56	0.40
2:A:619:LEU:HD11	2:A:683:LYS:HE3	2.03	0.40
2:E:707:PHE:O	2:E:712:LYS:HD2	2.22	0.40
2:E:961:VAL:O	2:E:961:VAL:HG12	2.21	0.40
2:C:971:PRO:O	2:C:975:LYS:HG2	2.22	0.40
2:G:713:ARG:NH2	2:G:846:PHE:O	2.50	0.40
2:A:322:LEU:HD22	2:A:352:SER:HB2	2.04	0.40
2:E:339:GLU:O	2:E:341:VAL:HG23	2.22	0.40
2:E:649:GLY:O	2:E:651:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:219:LEU:O	2:C:220:ASP:C	2.58	0.40
2:G:493:ASN:ND2	2:G:496:GLU:OE1	2.46	0.40
1:D:88:VAL:HG22	1:D:94:LEU:CD2	2.51	0.40
2:A:891:ILE:HD13	2:A:891:ILE:HG21	1.91	0.40
2:E:955:THR:O	2:E:967:SER:N	2.53	0.40
2:C:772:PRO:O	2:C:773:ASN:C	2.59	0.40
2:G:217:GLU:HB2	2:G:251:LYS:O	2.21	0.40
2:G:899:VAL:HG12	2:G:906:PHE:CD2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:800:GLN:HE22	2:G:401:LYS:O[2_445]	1.49	0.11
2:E:96:ARG:HH21	2:G:703:ASN:OD1[2_455]	1.52	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	175/295 (59%)	153 (87%)	10 (6%)	12 (7%)	1 7
1	D	171/295 (58%)	153 (90%)	14 (8%)	4 (2%)	6 32
1	F	176/295 (60%)	149 (85%)	19 (11%)	8 (4%)	2 16
1	H	176/295 (60%)	156 (89%)	11 (6%)	9 (5%)	2 14
2	A	991/1024 (97%)	943 (95%)	44 (4%)	4 (0%)	34 69
2	C	991/1024 (97%)	940 (95%)	49 (5%)	2 (0%)	47 78
2	E	989/1024 (97%)	937 (95%)	47 (5%)	5 (0%)	29 66
2	G	988/1024 (96%)	935 (95%)	51 (5%)	2 (0%)	47 78
All	All	4657/5276 (88%)	4366 (94%)	245 (5%)	46 (1%)	15 52

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ARG
1	B	28	SER
1	B	36	ASP
1	F	109	GLU
1	F	142	ASN
1	F	176	ILE
1	H	107	THR
1	H	173	LYS
2	E	711	ALA
2	G	747	ASP
1	B	104	ASP
1	B	107	THR
1	B	175	PHE
1	F	48	VAL
1	F	110	PRO
1	H	35	ASP
1	H	103	GLY
2	A	650	ASP
2	E	751	SER
1	B	25	ALA
1	B	81	PRO
1	F	25	ALA
2	A	200	ASP
2	A	647	GLN
2	E	197	MET
2	E	650	ASP
2	C	594	GLU
1	B	35	ASP
1	B	176	ILE
1	F	81	PRO
1	D	50	ASN
1	D	142	ASN
1	H	28	SER
1	H	101	GLN
2	A	220	ASP
2	G	749	SER
1	F	104	ASP
1	H	6	SER
2	E	647	GLN
2	C	15	ASP
1	B	173	LYS
1	H	26	ILE

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Mol	Chain	Res	Type
1	H	81	PRO
1	D	48	VAL
1	D	81	PRO
1	B	152	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	163/276 (59%)	158 (97%)	5 (3%)	40	71
1	D	159/276 (58%)	149 (94%)	10 (6%)	18	50
1	F	164/276 (59%)	159 (97%)	5 (3%)	41	72
1	H	164/276 (59%)	163 (99%)	1 (1%)	86	94
2	A	876/900 (97%)	862 (98%)	14 (2%)	62	83
2	C	876/900 (97%)	864 (99%)	12 (1%)	67	85
2	E	875/900 (97%)	857 (98%)	18 (2%)	53	79
2	G	874/900 (97%)	862 (99%)	12 (1%)	67	85
All	All	4151/4704 (88%)	4074 (98%)	77 (2%)	57	80

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	ILE
1	B	101	GLN
1	B	127	SER
1	B	144	ASP
1	B	150	ARG
1	F	5	LYS
1	F	106	MET
1	F	127	SER
1	F	144	ASP
1	F	175	PHE
1	D	47	MET

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Mol	Chain	Res	Type
1	D	49	LEU
1	D	101	GLN
1	D	102	SER
1	D	104	ASP
1	D	113	GLU
1	D	116	SER
1	D	139	SER
1	D	175	PHE
1	D	177	MET
1	H	127	SER
2	A	196	THR
2	A	214	SER
2	A	239	ARG
2	A	250	LYS
2	A	263	LYS
2	A	301	GLN
2	A	330	SER
2	A	388	PHE
2	A	409	THR
2	A	635	LEU
2	A	747	ASP
2	A	750	ASN
2	A	930	ARG
2	A	967	SER
2	E	79	GLN
2	E	194	THR
2	E	214	SER
2	E	313	THR
2	E	316	ASP
2	E	385	LEU
2	E	500	GLU
2	E	588	SER
2	E	600	CYS
2	E	609	ILE
2	E	750	ASN
2	E	770	PHE
2	E	771	THR
2	E	816	LEU
2	E	853	GLN
2	E	930	ARG
2	E	955	THR
2	E	967	SER

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Mol	Chain	Res	Type
2	C	194	THR
2	C	214	SER
2	C	316	ASP
2	C	327	THR
2	C	385	LEU
2	C	392	ASP
2	C	590	ARG
2	C	643	GLN
2	C	797	GLU
2	C	852	ARG
2	C	930	ARG
2	C	958	SER
2	G	214	SER
2	G	243	VAL
2	G	293	HIS
2	G	385	LEU
2	G	392	ASP
2	G	547	ASP
2	G	590	ARG
2	G	635	LEU
2	G	742	TYR
2	G	771	THR
2	G	930	ARG
2	G	967	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	HIS
1	D	101	GLN
2	G	611	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	C	1101	4	26,33,33	0.83	0	31,52,52	1.63	5 (16%)
3	ATP	E	1101	4	26,33,33	0.79	0	31,52,52	1.71	6 (19%)
3	ATP	G	1101	4	26,33,33	0.91	1 (3%)	31,52,52	1.83	9 (29%)
3	ATP	A	1101	4	26,33,33	1.07	1 (3%)	31,52,52	1.43	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	1101	4	-	7/18/38/38	0/3/3/3
3	ATP	E	1101	4	-	5/18/38/38	0/3/3/3
3	ATP	G	1101	4	-	7/18/38/38	0/3/3/3
3	ATP	A	1101	4	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ATP	C2-N3	3.13	1.37	1.32
3	G	1101	ATP	O4'-C4'	-2.13	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1101	ATP	C4-C5-N7	-4.99	104.19	109.40
3	G	1101	ATP	N3-C2-N1	-4.19	122.13	128.68
3	E	1101	ATP	N3-C2-N1	-4.14	122.21	128.68
3	G	1101	ATP	C4-C5-N7	-3.74	105.50	109.40
3	E	1101	ATP	C4-C5-N7	-3.39	105.87	109.40
3	E	1101	ATP	O3'-C3'-C4'	-3.34	101.39	111.05
3	C	1101	ATP	N3-C2-N1	-3.34	123.45	128.68
3	A	1101	ATP	N3-C2-N1	-3.31	123.51	128.68
3	A	1101	ATP	C4-C5-N7	-3.23	106.03	109.40
3	G	1101	ATP	O2G-PG-O3B	-3.15	94.06	104.64
3	C	1101	ATP	O2A-PA-O1A	2.76	125.90	112.24
3	G	1101	ATP	O3G-PG-O3B	2.75	113.85	104.64
3	G	1101	ATP	O2B-PB-O1B	2.68	125.48	112.24
3	E	1101	ATP	O2'-C2'-C3'	2.62	120.29	111.82
3	G	1101	ATP	O3G-PG-O2G	2.61	117.62	107.64
3	C	1101	ATP	PA-O3A-PB	-2.61	123.89	132.83
3	E	1101	ATP	PB-O3B-PG	-2.54	124.12	132.83
3	E	1101	ATP	C2'-C3'-C4'	2.51	107.51	102.64
3	A	1101	ATP	C1'-N9-C4	-2.47	122.31	126.64
3	G	1101	ATP	O5'-PA-O1A	-2.32	100.01	109.07
3	C	1101	ATP	O3G-PG-O1G	2.18	119.23	110.68
3	G	1101	ATP	PA-O3A-PB	-2.09	125.66	132.83
3	A	1101	ATP	O2G-PG-O3B	-2.08	97.67	104.64
3	G	1101	ATP	O3B-PG-O1G	-2.04	99.85	111.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	ATP	C5'-O5'-PA-O2A
3	E	1101	ATP	C5'-O5'-PA-O1A
3	C	1101	ATP	C5'-O5'-PA-O2A
3	G	1101	ATP	C5'-O5'-PA-O2A
3	A	1101	ATP	PB-O3A-PA-O1A
3	G	1101	ATP	PB-O3A-PA-O1A
3	A	1101	ATP	C5'-O5'-PA-O3A
3	E	1101	ATP	C5'-O5'-PA-O3A
3	C	1101	ATP	C5'-O5'-PA-O3A
3	G	1101	ATP	C5'-O5'-PA-O3A
3	C	1101	ATP	PB-O3A-PA-O1A
3	C	1101	ATP	PB-O3A-PA-O2A
3	A	1101	ATP	C5'-O5'-PA-O1A
3	E	1101	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	1101	ATP	C5'-O5'-PA-O1A
3	G	1101	ATP	C5'-O5'-PA-O1A
3	A	1101	ATP	PB-O3A-PA-O2A
3	G	1101	ATP	PB-O3A-PA-O2A
3	A	1101	ATP	O4'-C4'-C5'-O5'
3	C	1101	ATP	O4'-C4'-C5'-O5'
3	E	1101	ATP	PB-O3A-PA-O1A
3	G	1101	ATP	O4'-C4'-C5'-O5'
3	C	1101	ATP	PA-O3A-PB-O2B
3	G	1101	ATP	PG-O3B-PB-O1B
3	E	1101	ATP	O4'-C4'-C5'-O5'

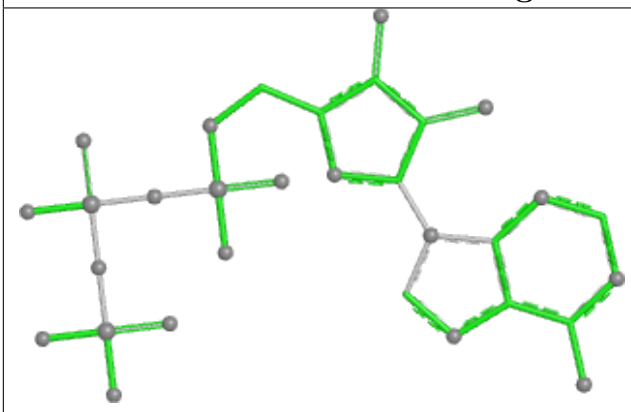
There are no ring outliers.

3 monomers are involved in 7 short contacts:

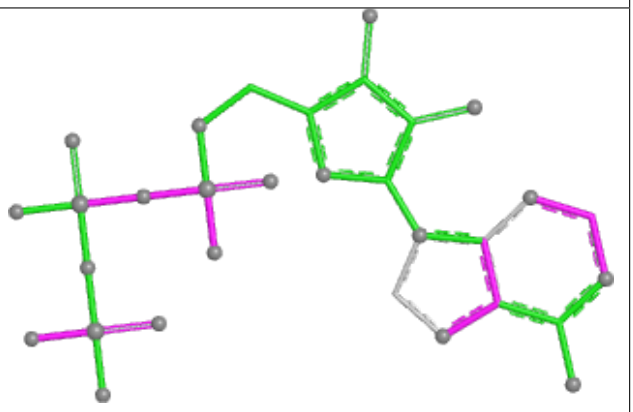
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	ATP	2	0
3	E	1101	ATP	2	0
3	G	1101	ATP	3	0

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

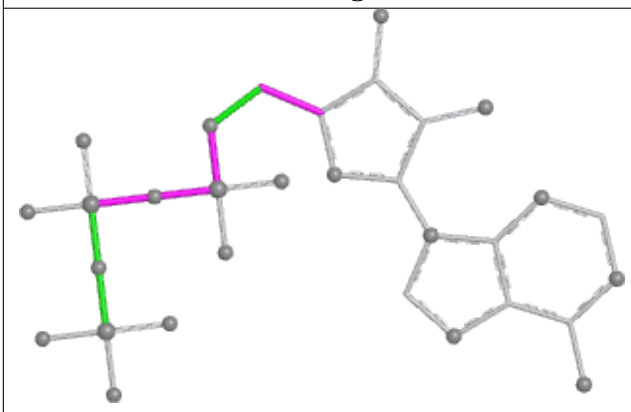
Ligand ATP C 1101



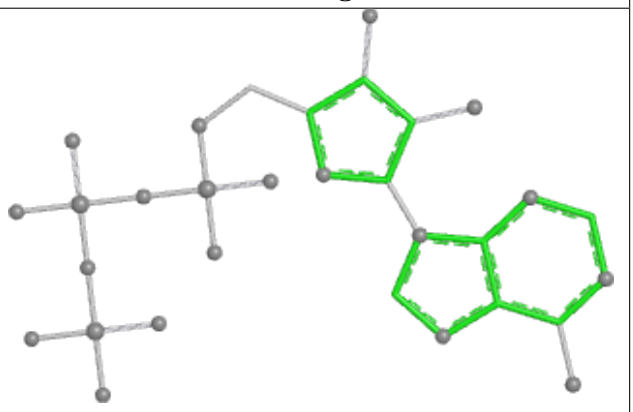
Bond lengths



Bond angles

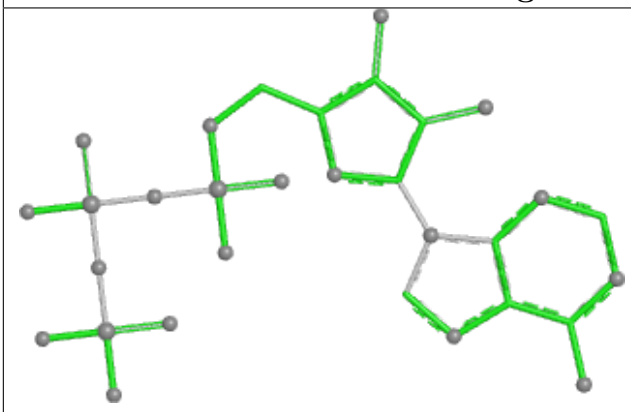


Torsions

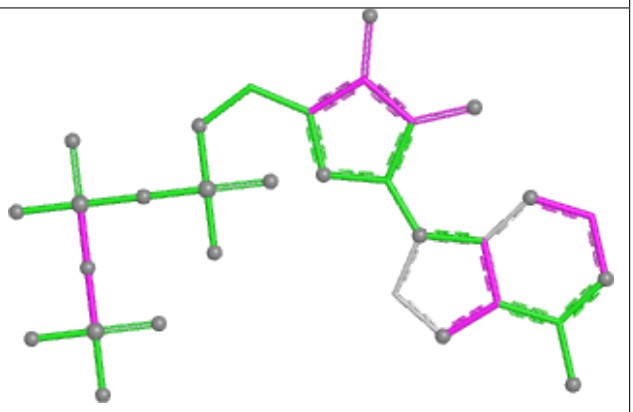


Rings

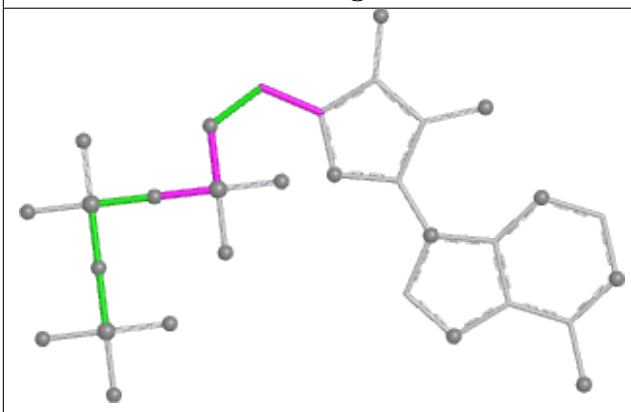
Ligand ATP E 1101



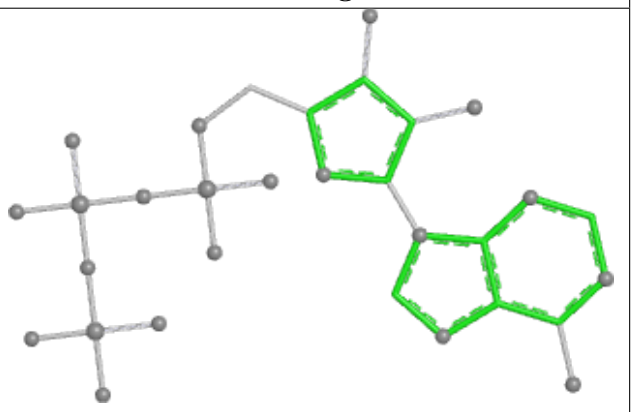
Bond lengths



Bond angles

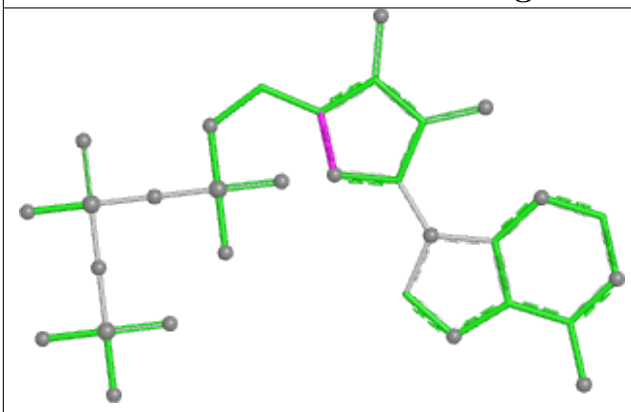


Torsions

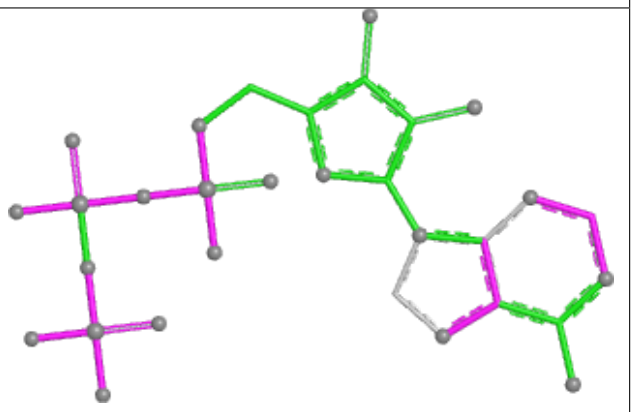


Rings

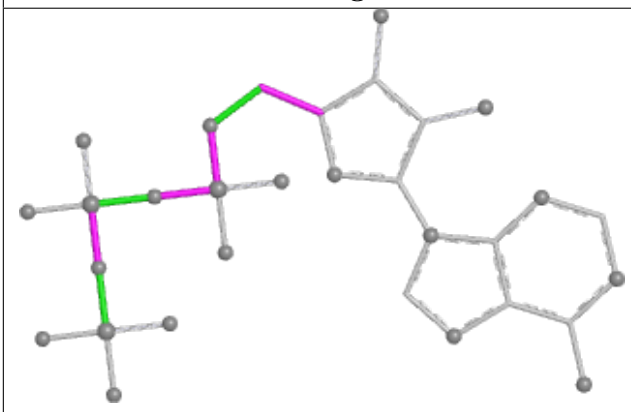
Ligand ATP G 1101



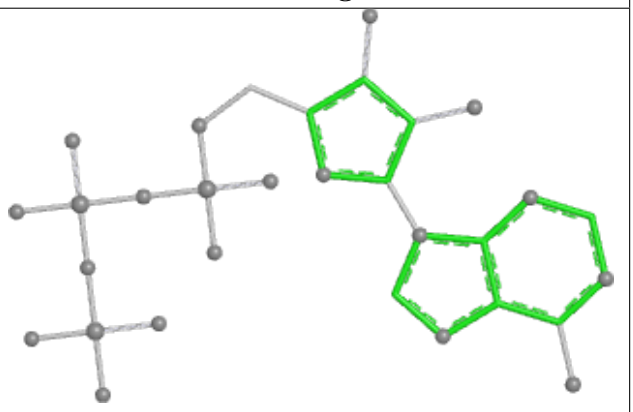
Bond lengths



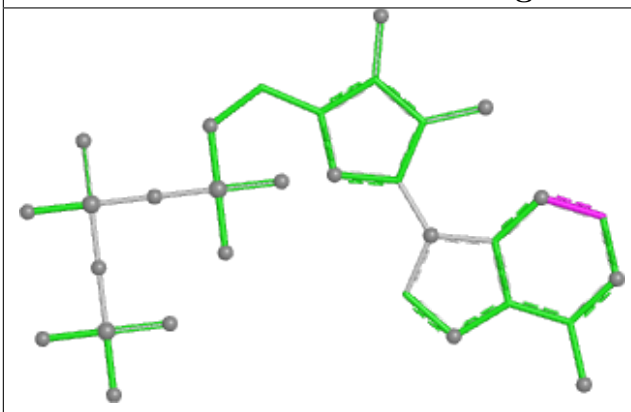
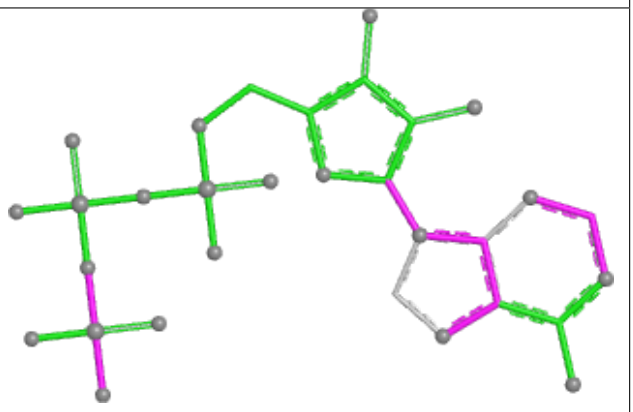
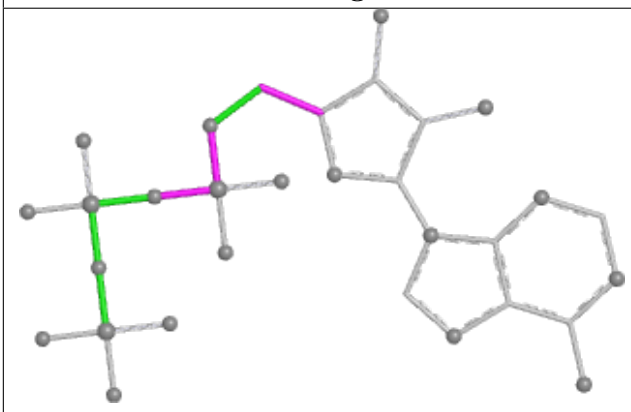
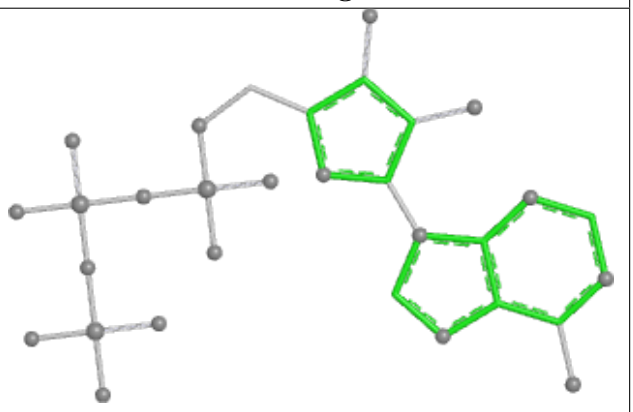
Bond angles



Torsions



Rings

Ligand ATP A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	177/295 (60%)	0.41	20 (11%) 5 3	80, 130, 186, 201	0
1	D	173/295 (58%)	0.35	13 (7%) 14 7	60, 100, 166, 204	0
1	F	178/295 (60%)	0.34	8 (4%) 33 20	69, 130, 196, 230	0
1	H	178/295 (60%)	0.66	27 (15%) 2 1	99, 138, 177, 207	0
2	A	995/1024 (97%)	-0.10	9 (0%) 84 75	37, 69, 135, 190	0
2	C	995/1024 (97%)	-0.14	3 (0%) 94 92	39, 73, 115, 178	0
2	E	993/1024 (96%)	-0.02	20 (2%) 65 50	45, 75, 160, 208	0
2	G	992/1024 (96%)	0.06	29 (2%) 51 35	63, 98, 147, 185	0
All	All	4681/5276 (88%)	0.02	129 (2%) 53 37	37, 85, 155, 230	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	PRO	7.2
2	G	750	ASN	6.9
1	D	109	GLU	6.5
1	H	111	ASP	5.9
1	F	154	GLU	5.7
2	G	952	LEU	5.3
1	D	25	ALA	5.1
2	G	648	SER	5.0
1	H	152	ASN	5.0
1	H	75	PRO	4.7
1	B	178	PRO	4.6
1	H	59	PHE	4.5
1	F	55	TYR	4.5
1	H	77	PHE	4.4
1	F	156	TYR	4.4
1	B	2	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	154	GLU	4.2
1	H	99	LEU	4.1
1	H	23	LYS	4.1
2	G	57	LEU	4.1
2	E	747	ASP	4.0
2	G	749	SER	4.0
1	B	72	PHE	3.9
2	A	796	ASP	3.9
2	A	594	GLU	3.8
1	H	79	PHE	3.7
1	H	3	SER	3.7
1	D	173	LYS	3.6
2	G	385	LEU	3.6
2	E	254	ILE	3.5
1	D	177	MET	3.5
1	H	177	MET	3.5
1	D	55	TYR	3.5
2	E	205	LEU	3.4
1	H	83	ILE	3.4
1	D	110	PRO	3.3
1	B	111	ASP	3.3
2	G	202	ARG	3.3
1	B	172	PRO	3.3
1	B	110	PRO	3.1
1	D	103	GLY	3.1
2	G	621	GLN	3.1
2	G	751	SER	3.1
1	D	111	ASP	3.1
2	E	202	ARG	3.1
2	G	948	LYS	2.9
1	B	170	ASP	2.9
2	E	707	PHE	2.9
2	G	946	PHE	2.9
2	G	337	LEU	2.9
2	A	202	ARG	2.9
2	G	954	ILE	2.8
1	F	101	GLN	2.8
2	E	216	VAL	2.8
1	H	55	TYR	2.8
2	G	39	VAL	2.7
2	E	762	ILE	2.7
1	B	60	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	110	PRO	2.7
2	E	253	GLY	2.7
2	G	483	PHE	2.6
1	H	72	PHE	2.6
2	E	702	SER	2.6
1	H	176	ILE	2.6
2	E	695	PHE	2.6
1	F	142	ASN	2.6
2	G	942	LEU	2.6
2	G	707	PHE	2.6
1	F	98	ILE	2.6
1	B	107	THR	2.6
1	H	108	ASP	2.5
1	H	84	TYR	2.5
1	D	56	HIS	2.5
1	H	96	ILE	2.5
2	A	811	LEU	2.5
1	H	64	MET	2.5
1	B	94	LEU	2.5
2	A	227	LEU	2.5
2	E	184	GLY	2.5
1	H	86	PRO	2.5
1	H	178	PRO	2.4
1	F	104	ASP	2.4
2	A	655	LEU	2.4
1	B	96	ILE	2.4
2	G	450	LEU	2.4
2	G	195	VAL	2.4
2	E	84	GLU	2.4
1	B	99	LEU	2.4
2	E	737	LEU	2.4
1	B	30	HIS	2.4
2	G	280	PHE	2.3
1	D	36	ASP	2.3
2	A	236	PHE	2.3
2	A	795	SER	2.3
1	B	100	HIS	2.3
2	G	655	LEU	2.3
1	B	112	ALA	2.3
1	H	132	LEU	2.2
2	E	248	GLU	2.2
1	H	140	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	228	PHE	2.2
2	C	428	PHE	2.2
2	C	195	VAL	2.2
2	A	205	LEU	2.2
2	G	47	LEU	2.2
1	F	2	SER	2.2
2	G	120	LEU	2.2
2	E	754	ASN	2.2
1	B	27	PRO	2.1
2	E	680	PHE	2.1
2	G	897	GLY	2.1
1	B	173	LYS	2.1
1	D	113	GLU	2.1
2	G	814	PHE	2.1
2	C	655	LEU	2.1
2	G	816	LEU	2.1
1	D	152	ASN	2.1
1	B	55	TYR	2.1
2	G	702	SER	2.1
1	H	2	SER	2.1
2	E	230	VAL	2.1
2	E	243	VAL	2.1
1	H	137	ILE	2.0
1	H	88	VAL	2.0
2	E	688	ILE	2.0
1	H	159	ARG	2.0
2	E	691	LEU	2.0
2	G	41	ILE	2.0
1	B	176	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

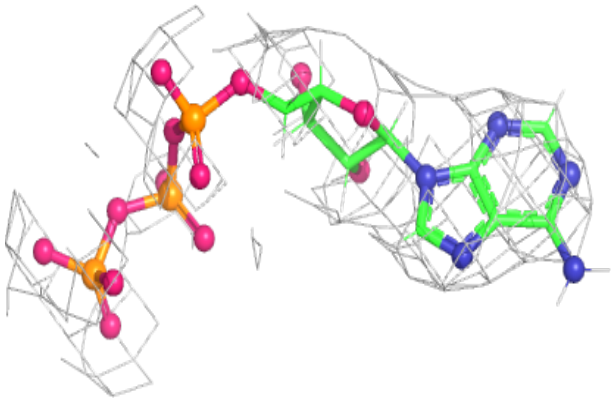
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

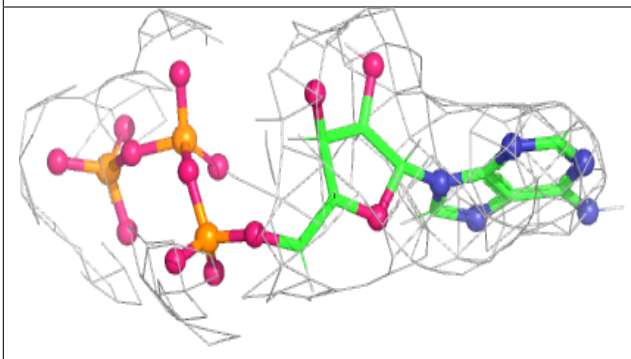
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1102	1/1	0.88	0.15	72,72,72,72	0
3	ATP	G	1101	31/31	0.95	0.19	63,67,81,88	0
3	ATP	C	1101	31/31	0.97	0.22	40,55,69,82	0
3	ATP	A	1101	31/31	0.97	0.18	40,58,71,71	0
3	ATP	E	1101	31/31	0.97	0.19	43,56,67,72	0
4	MG	C	1102	1/1	0.97	0.15	68,68,68,68	0
4	MG	E	1102	1/1	0.98	0.13	67,67,67,67	0
4	MG	G	1102	1/1	0.99	0.19	62,62,62,62	0

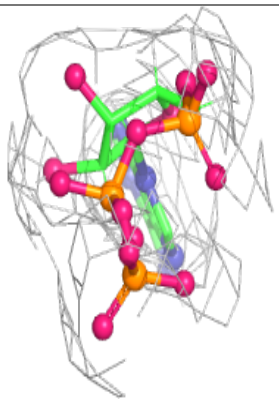
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP G 1101:

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

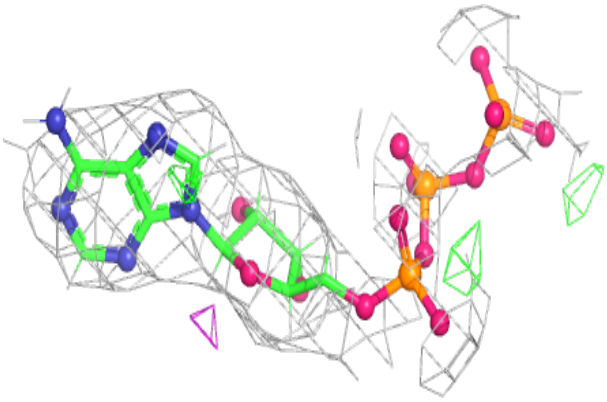


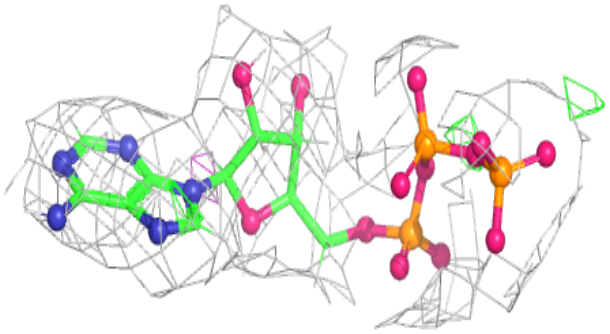


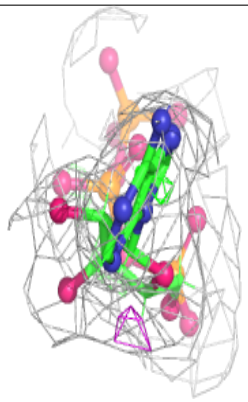


Electron density around ATP C 1101:

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

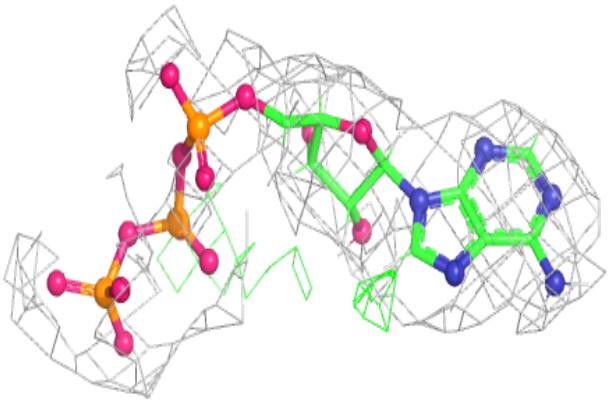


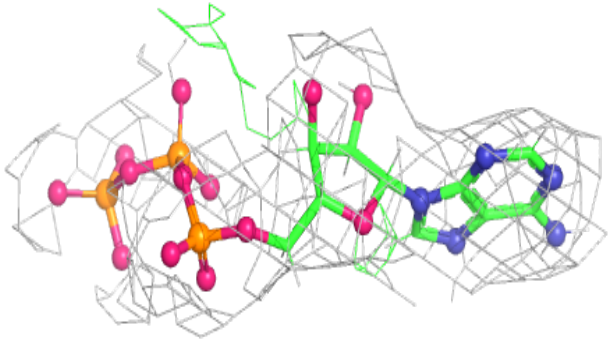


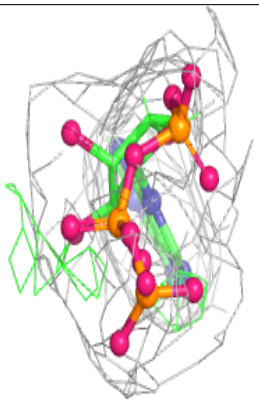


Electron density around ATP A 1101:

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

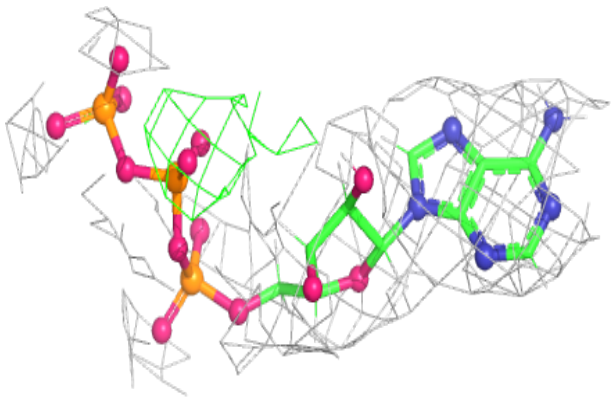


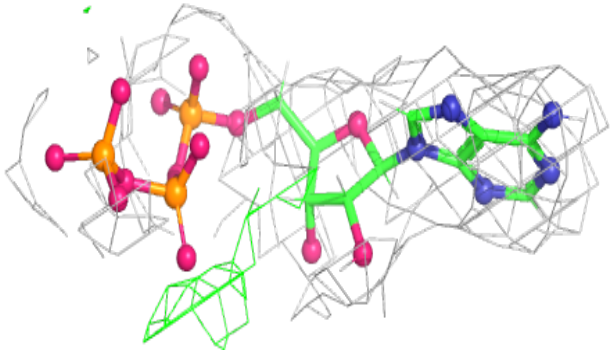


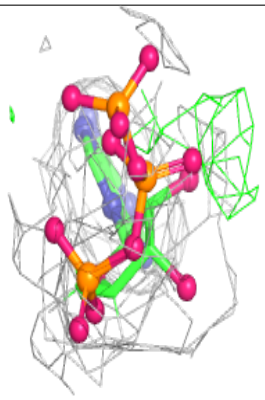


Electron density around ATP E 1101:

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







6.5 Other polymers

There are no such residues in this entry.