



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:32 am BST

PDB ID : 1UA2  
Title : Crystal Structure of Human CDK7  
Authors : Lolli, G.; Lowe, E.D.; Brown, N.R.; Johnson, L.N.  
Deposited on : 2004-08-11  
Resolution : 3.02 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

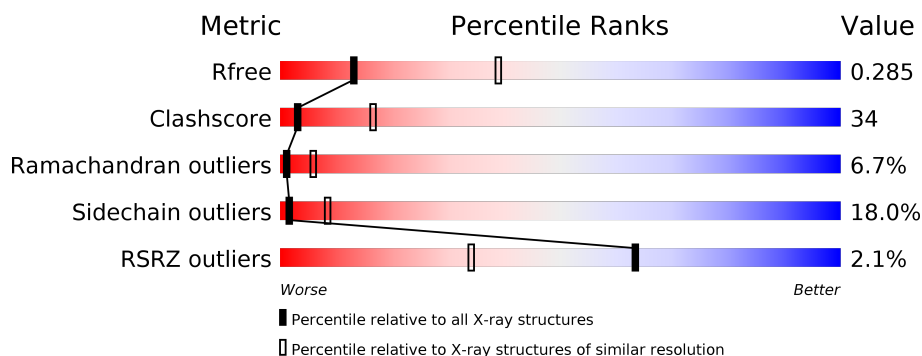
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	346	<div> <div>34%</div> <div>38%</div> <div>9%</div> <div>•</div> <div>17%</div> </div>
1	B	346	<div> <div>%</div> <div>29%</div> <div>37%</div> <div>15%</div> <div>•</div> <div>17%</div> </div>
1	C	346	<div> <div>4%</div> <div>36%</div> <div>36%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>
1	D	346	<div> <div>2%</div> <div>35%</div> <div>35%</div> <div>12%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cell division protein kinase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	B	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	C	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			
1	D	287	Total	C	N	O	P	S	0	0	0
			2291	1480	387	412	1	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	TPO	THR	MODIFIED RESIDUE	UNP P50613
B	170	TPO	THR	MODIFIED RESIDUE	UNP P50613
C	170	TPO	THR	MODIFIED RESIDUE	UNP P50613
D	170	TPO	THR	MODIFIED RESIDUE	UNP P50613

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



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

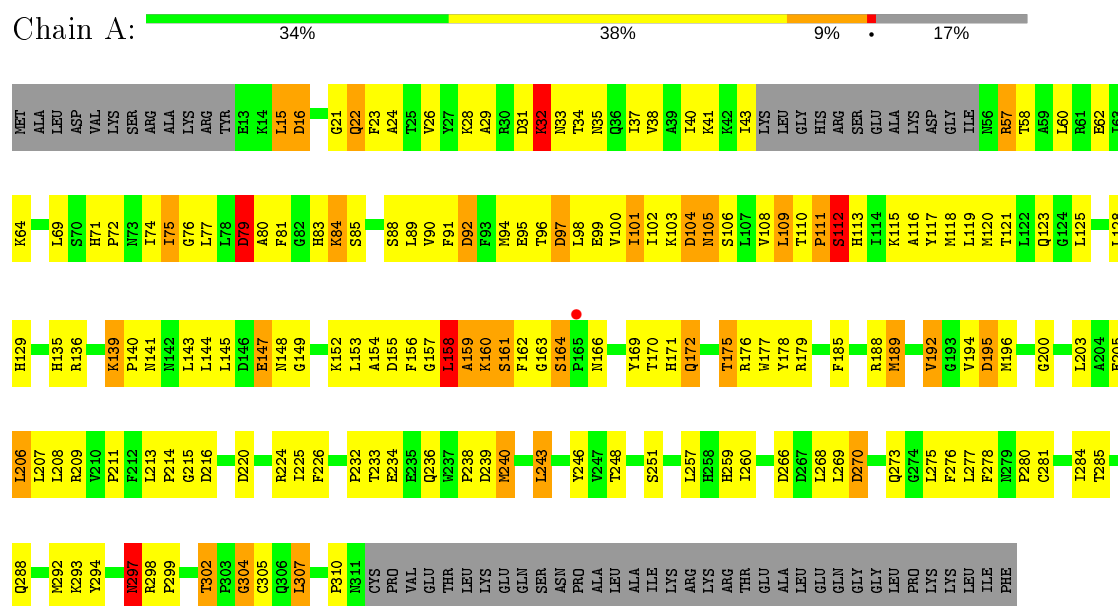
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	13	Total	O	0	0
			13	13		
3	C	12	Total	O	0	0
			12	12		
3	D	7	Total	O	0	0
			7	7		

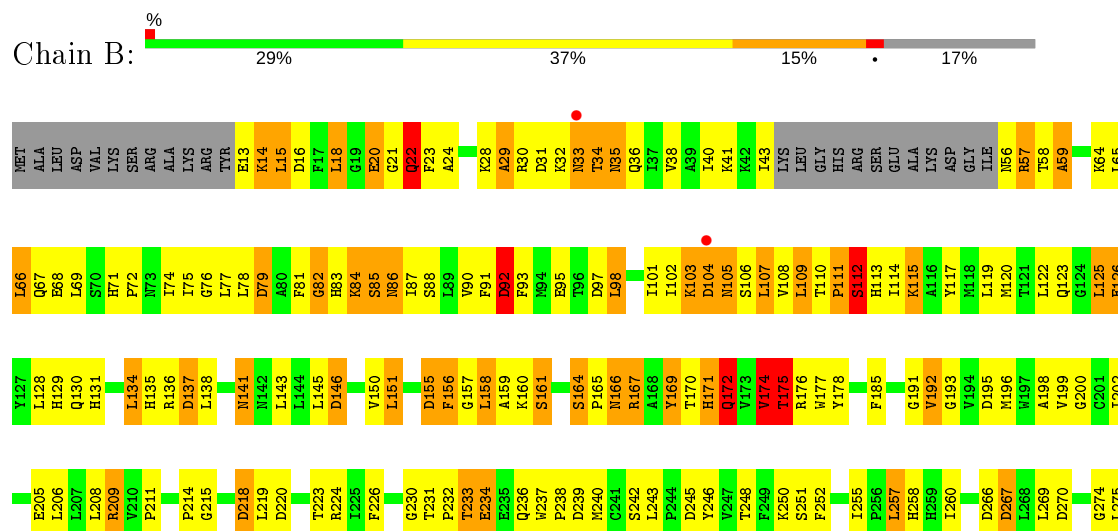
### 3 Residue-property plots

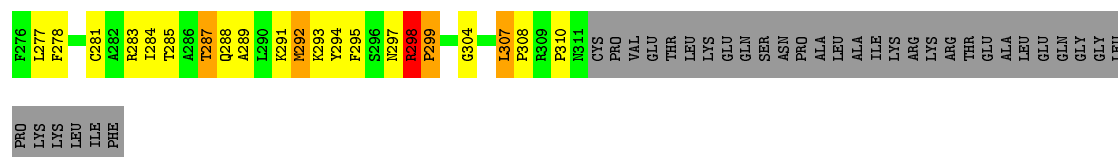
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Cell division protein kinase 7

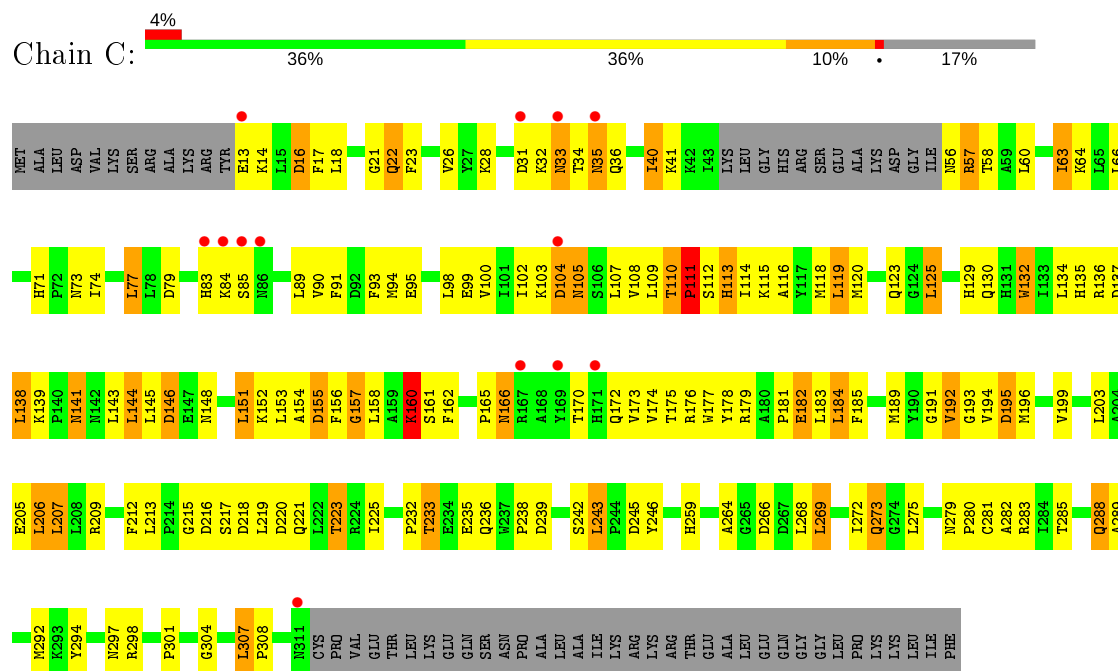


#### • Molecule 1: Cell division protein kinase 7

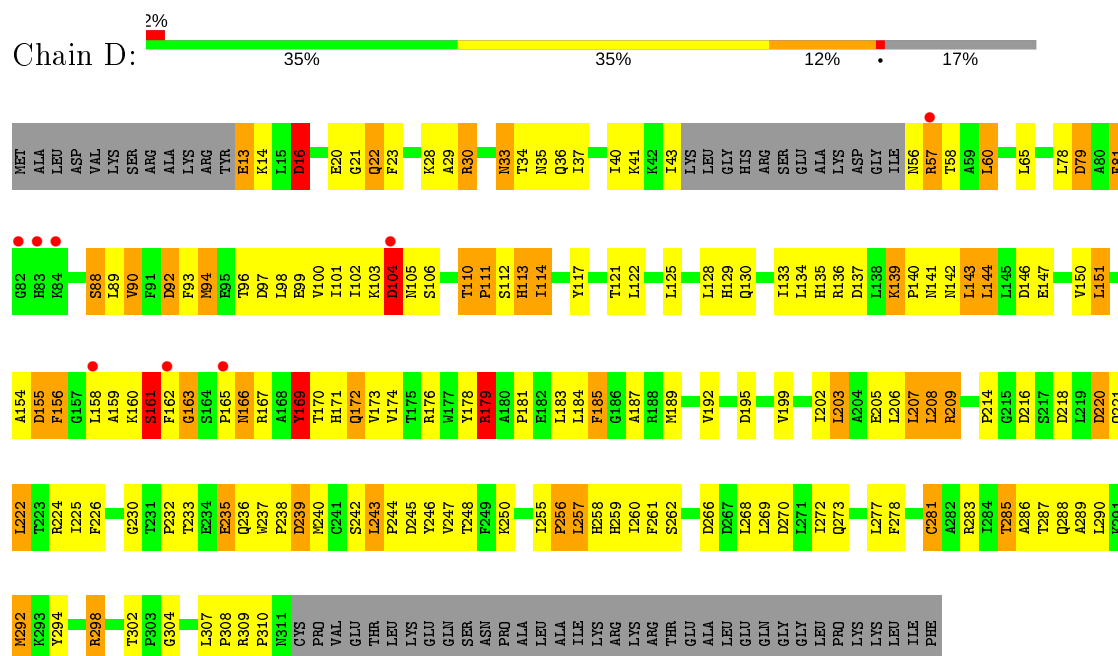




• Molecule 1: Cell division protein kinase 7



• Molecule 1: Cell division protein kinase 7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.50 Å 191.63 Å 75.79 Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	49.45 – 3.02 29.42 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.45-3.02) 91.2 (29.42-2.96)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.95 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.213 , 0.288 0.210 , 0.285	Depositor DCC
$R_{free}$ test set	1767 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 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	0.79	0/2336	1.04	8/3169 (0.3%)
1	B	0.76	0/2336	1.05	16/3169 (0.5%)
1	C	0.76	0/2336	1.00	11/3169 (0.3%)
1	D	0.68	0/2336	0.99	11/3169 (0.3%)
All	All	0.75	0/9344	1.02	46/12676 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	2
All	All	0	9

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	CB-CG-OD2	9.33	126.70	118.30
1	A	92	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	216	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	270	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	195	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	158	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	218	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	97	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	266	ASP	CB-CG-OD2	6.34	124.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	195	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	C	245	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	245	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	218	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	270	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	281	CYS	CA-CB-SG	-6.10	103.02	114.00
1	C	298	ARG	N-CA-C	6.08	127.42	111.00
1	D	220	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	16	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	92	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	104	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	138	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	109	LEU	CB-CG-CD1	-5.93	100.91	111.00
1	B	155	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	79	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	110	THR	OG1-CB-CG2	-5.83	96.59	110.00
1	C	146	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	175	THR	N-CA-C	5.71	126.43	111.00
1	B	104	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	245	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	281	CYS	CA-CB-SG	-5.62	103.89	114.00
1	B	158	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	267	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	298	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	179	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	299	PRO	N-CD-CG	-5.31	95.23	103.20
1	A	220	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	270	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	16	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	92	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	307	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	266	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	266	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	281	CYS	CA-CB-SG	-5.09	104.83	114.00
1	D	155	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	104	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	SER	Peptide
1	A	164	SER	Peptide
1	A	297	ASN	Peptide
1	A	304	GLY	Peptide
1	B	103	LYS	Peptide
1	B	169	TYR	Peptide
1	B	34	THR	Peptide
1	C	111	PRO	Peptide
1	C	297	ASN	Peptide

## 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	2291	0	2300	182	0
1	B	2291	0	2300	169	0
1	C	2291	0	2300	134	0
1	D	2291	0	2300	138	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	0	0
3	A	16	0	0	9	0
3	B	13	0	0	5	0
3	C	12	0	0	1	0
3	D	7	0	0	2	0
All	All	9336	0	9248	625	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 34.

All (625) 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:234:GLU:OE2	1:A:238:PRO:HA	1.21	1.34
1:A:43:ILE:CD1	1:A:160:LYS:HE2	1.70	1.21
1:A:32:LYS:NZ	1:A:32:LYS:HB2	1.49	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:CB	1:A:160:LYS:NZ	2.06	1.18
1:A:103:LYS:O	1:A:105:ASN:N	1.75	1.17
1:A:43:ILE:HD11	1:A:160:LYS:CE	1.76	1.15
1:A:24:ALA:HB1	1:A:160:LYS:NZ	1.64	1.09
1:D:255:ILE:HB	1:D:260:ILE:HD11	1.40	1.04
1:B:141:ASN:ND2	1:B:141:ASN:H	1.47	1.04
1:B:141:ASN:HD22	1:B:141:ASN:N	1.51	1.04
1:A:24:ALA:CB	1:A:160:LYS:HZ2	1.68	1.02
1:A:234:GLU:OE2	1:A:238:PRO:CA	2.12	0.98
1:B:174:VAL:O	1:B:175:THR:HG23	1.66	0.94
1:A:32:LYS:HZ2	1:A:32:LYS:HB2	1.22	0.93
1:B:176:ARG:O	1:B:176:ARG:HG3	1.69	0.93
1:A:304:GLY:HA2	1:A:307:LEU:HB2	1.52	0.92
1:D:189:MET:O	1:D:189:MET:HG3	1.69	0.92
1:D:40:ILE:HG13	1:D:90:VAL:HG23	1.52	0.91
1:A:111:PRO:O	1:A:113:HIS:N	2.01	0.91
1:A:41:LYS:HB3	1:A:160:LYS:CE	1.99	0.91
1:A:24:ALA:CB	1:A:160:LYS:HZ3	1.75	0.90
1:A:15:LEU:O	1:A:16:ASP:HB2	1.71	0.90
1:A:41:LYS:HB3	1:A:160:LYS:HE3	1.53	0.90
1:A:40:ILE:HG13	1:A:90:VAL:HG22	1.53	0.89
1:A:41:LYS:HB3	1:A:160:LYS:HZ1	1.34	0.89
1:A:32:LYS:HZ3	1:A:32:LYS:HB2	1.28	0.89
1:C:233:THR:H	1:C:236:GLN:HE21	1.15	0.89
1:C:238:PRO:O	1:C:239:ASP:HB2	1.73	0.88
1:D:257:LEU:HB3	1:D:269:LEU:HD22	1.53	0.88
1:D:94:MET:HE3	1:D:146:ASP:HB3	1.55	0.88
1:A:41:LYS:HB3	1:A:160:LYS:NZ	1.87	0.88
1:A:185:PHE:CD2	1:A:246:TYR:HA	2.07	0.88
1:D:103:LYS:O	1:D:105:ASN:N	2.06	0.88
1:B:164:SER:HB2	1:B:165:PRO:HD3	1.56	0.88
1:C:139:LYS:HE3	1:C:141:ASN:HD21	1.37	0.88
1:A:32:LYS:NZ	1:A:32:LYS:CB	2.37	0.86
1:A:24:ALA:HB2	1:A:160:LYS:NZ	1.88	0.86
1:D:41:LYS:HB2	1:D:160:LYS:HE3	1.57	0.86
1:A:102:ILE:HD11	1:A:206:LEU:HD13	1.58	0.85
1:A:24:ALA:HB1	1:A:160:LYS:HZ3	1.27	0.85
1:A:43:ILE:HD11	1:A:160:LYS:HE2	0.90	0.85
1:B:24:ALA:HB2	1:B:160:LYS:HE2	1.57	0.85
1:C:113:HIS:CD2	1:C:308:PRO:HD3	2.12	0.85
1:D:43:ILE:HG22	1:D:166:ASN:HD22	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASN:HD22	1:D:33:ASN:C	1.81	0.83
1:B:43:ILE:CD1	1:B:160:LYS:HE3	2.08	0.82
1:D:110:THR:HG22	1:D:113:HIS:HB2	1.62	0.82
1:D:238:PRO:O	1:D:239:ASP:HB2	1.78	0.82
1:A:41:LYS:CB	1:A:160:LYS:HZ1	1.92	0.82
1:B:112:SER:N	3:B:383:HOH:O	2.12	0.82
1:A:38:VAL:CG1	1:A:90:VAL:HG13	2.10	0.82
1:B:43:ILE:HG23	1:B:165:PRO:HB3	1.59	0.81
1:B:135:HIS:ND1	1:B:135:HIS:O	2.13	0.81
1:B:125:LEU:HD22	1:B:129:HIS:CE1	2.17	0.80
1:A:136:ARG:HD3	3:A:383:HOH:O	1.82	0.80
1:C:203:LEU:HD21	1:C:268:LEU:HD11	1.61	0.80
1:B:103:LYS:O	1:B:105:ASN:N	2.14	0.80
1:C:102:ILE:HA	1:C:209:ARG:NH1	1.96	0.80
1:C:182:GLU:OE2	1:C:283:ARG:NH1	2.14	0.79
1:D:43:ILE:HG13	1:D:160:LYS:NZ	1.98	0.79
1:A:103:LYS:C	1:A:105:ASN:H	1.85	0.78
1:A:38:VAL:HG11	1:A:90:VAL:HG13	1.65	0.78
1:D:226:PHE:CE2	1:D:232:PRO:HD3	2.20	0.77
1:B:177:TRP:CD1	1:B:214:PRO:HA	2.20	0.76
1:D:111:PRO:HD2	1:D:113:HIS:ND1	2.00	0.75
1:C:120:MET:CE	1:C:151:LEU:H	1.99	0.75
1:C:176:ARG:HG3	1:C:176:ARG:O	1.85	0.75
1:A:157:GLY:O	1:A:159:ALA:N	2.20	0.74
1:A:158:LEU:HA	1:A:163:GLY:H	1.52	0.74
1:A:105:ASN:ND2	1:A:310:PRO:HB3	2.01	0.74
1:B:238:PRO:O	1:B:239:ASP:HB2	1.85	0.74
1:A:158:LEU:C	1:A:160:LYS:H	1.90	0.74
1:C:175:THR:HG21	1:C:178:TYR:HE1	1.50	0.74
1:C:184:LEU:HD21	1:C:221:GLN:HG2	1.70	0.73
1:D:176:ARG:NH1	1:D:218:ASP:OD1	2.21	0.73
1:B:119:LEU:O	1:B:123:GLN:HG3	1.88	0.73
1:B:156:PHE:CE1	1:B:159:ALA:HB2	2.23	0.73
1:B:24:ALA:HB1	1:B:160:LYS:NZ	2.04	0.73
1:B:22:GLN:HB3	1:B:23:PHE:CD1	2.23	0.72
1:B:15:LEU:HB2	1:B:29:ALA:HA	1.71	0.72
1:B:125:LEU:HD13	1:B:196:MET:CE	2.19	0.72
1:D:113:HIS:HD2	1:D:308:PRO:HD3	1.52	0.72
1:A:16:ASP:HB3	1:A:28:LYS:HB3	1.72	0.72
1:D:189:MET:CG	1:D:189:MET:O	2.38	0.72
1:B:22:GLN:HA	1:B:170:TPO:O2P	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:HB3	1:B:231:THR:HG22	1.70	0.72
1:C:103:LYS:O	1:C:105:ASN:N	2.22	0.71
1:C:41:LYS:HE3	1:C:91:PHE:HE1	1.56	0.71
1:A:35:ASN:HB3	3:A:389:HOH:O	1.90	0.70
1:A:125:LEU:HD22	1:A:129:HIS:CE1	2.26	0.70
1:A:175:THR:CG2	1:A:178:TYR:HE1	2.04	0.70
1:B:38:VAL:HG11	1:B:90:VAL:HG13	1.73	0.70
1:D:203:LEU:HD13	1:D:272:ILE:CG1	2.21	0.70
1:C:21:GLY:HA2	1:C:170:TPO:O1P	1.90	0.70
1:A:139:LYS:HE2	1:A:141:ASN:HD21	1.56	0.70
1:B:257:LEU:HD12	1:B:260:ILE:HD12	1.73	0.70
1:D:29:ALA:HB3	1:D:40:ILE:HD13	1.71	0.70
1:A:105:ASN:HD22	1:A:310:PRO:HB3	1.55	0.70
1:B:22:GLN:HB3	1:B:23:PHE:HD1	1.56	0.70
1:D:78:LEU:O	1:D:79:ASP:HB2	1.91	0.69
1:B:174:VAL:C	1:B:175:THR:HG23	2.12	0.69
1:C:102:ILE:HA	1:C:209:ARG:HH11	1.56	0.69
1:B:38:VAL:CG1	1:B:90:VAL:HG13	2.21	0.69
1:A:111:PRO:HD2	1:A:113:HIS:CD2	2.26	0.69
1:C:99:GLU:O	1:C:103:LYS:HB2	1.92	0.69
1:D:57:ARG:HA	1:D:60:LEU:HG	1.74	0.69
1:D:93:PHE:C	1:D:94:MET:HG2	2.13	0.69
1:A:115:LYS:HD3	1:A:294:TYR:CE2	2.28	0.68
1:C:289:ALA:O	1:C:292:MET:HB2	1.92	0.68
1:A:285:THR:OG1	1:A:288:GLN:HG3	1.93	0.68
1:D:89:LEU:HD22	1:D:160:LYS:HG2	1.74	0.68
1:D:111:PRO:HD2	1:D:113:HIS:CE1	2.29	0.68
1:A:15:LEU:O	1:A:16:ASP:CB	2.42	0.68
1:A:140:PRO:HG3	1:A:205:GLU:OE1	1.94	0.68
1:D:23:PHE:HB2	1:D:161:SER:HA	1.75	0.67
1:A:179:ARG:HD3	3:A:393:HOH:O	1.94	0.67
1:C:139:LYS:HE3	1:C:141:ASN:ND2	2.08	0.67
1:A:99:GLU:O	1:A:103:LYS:HB2	1.95	0.67
1:D:102:ILE:HD12	1:D:205:GLU:HB3	1.75	0.67
1:D:122:LEU:HB2	1:D:290:LEU:HD21	1.76	0.67
1:C:111:PRO:HD2	1:C:113:HIS:H	1.60	0.67
1:A:41:LYS:HD3	1:A:160:LYS:HD2	1.77	0.67
1:A:176:ARG:O	1:A:176:ARG:HG3	1.93	0.67
1:A:196:MET:HG2	1:A:284:ILE:O	1.96	0.66
1:B:102:ILE:HD13	1:B:205:GLU:HG2	1.76	0.66
1:D:121:THR:HG23	1:D:143:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:HIS:CE1	1:A:192:VAL:HG12	2.30	0.66
1:D:13:GLU:N	3:D:390:HOH:O	2.27	0.66
1:A:207:LEU:HD21	1:A:268:LEU:HD21	1.77	0.66
1:C:119:LEU:HD12	1:C:301:PRO:HG3	1.78	0.66
1:D:43:ILE:CG1	1:D:160:LYS:HZ3	2.09	0.66
1:B:287:THR:O	1:B:291:LYS:HG3	1.95	0.66
1:D:203:LEU:HD13	1:D:272:ILE:HG12	1.78	0.66
1:B:166:ASN:O	1:B:167:ARG:HG3	1.96	0.66
1:D:43:ILE:HG13	1:D:160:LYS:HZ1	1.60	0.66
1:C:102:ILE:HD11	1:C:206:LEU:HD13	1.78	0.66
1:A:196:MET:HG3	1:A:275:LEU:HD23	1.77	0.66
1:B:307:LEU:HD12	1:B:308:PRO:HD2	1.78	0.66
1:D:94:MET:CE	1:D:146:ASP:HB3	2.24	0.65
1:A:185:PHE:HB3	1:A:243:LEU:HG	1.78	0.65
1:C:219:LEU:O	1:C:223:THR:HG22	1.95	0.65
1:A:185:PHE:CE2	1:A:246:TYR:HA	2.31	0.65
1:B:174:VAL:HG22	1:B:175:THR:H	1.61	0.65
1:B:43:ILE:HD11	1:B:160:LYS:HE3	1.78	0.65
1:D:255:ILE:HB	1:D:260:ILE:CD1	2.23	0.65
1:B:128:LEU:CD2	1:B:135:HIS:HB2	2.27	0.65
1:A:233:THR:HG23	1:A:236:GLN:NE2	2.11	0.65
1:B:232:PRO:HA	1:B:236:GLN:OE1	1.98	0.64
1:C:143:LEU:HB3	1:C:151:LEU:HD11	1.78	0.64
1:D:139:LYS:HB2	1:D:140:PRO:CD	2.27	0.64
1:A:158:LEU:C	1:A:160:LYS:N	2.50	0.64
1:C:233:THR:HG23	1:C:236:GLN:HE21	1.62	0.64
1:A:112:SER:N	3:A:382:HOH:O	2.30	0.64
1:B:105:ASN:ND2	1:B:310:PRO:HB3	2.12	0.64
1:B:43:ILE:HB	1:B:87:ILE:O	1.98	0.64
1:A:34:THR:HA	3:A:388:HOH:O	1.96	0.64
1:B:125:LEU:HD22	1:B:129:HIS:NE2	2.13	0.64
1:B:125:LEU:HD13	1:B:196:MET:HE1	1.80	0.64
1:D:13:GLU:N	1:D:30:ARG:O	2.31	0.64
1:A:136:ARG:NE	3:A:383:HOH:O	2.32	0.63
1:D:185:PHE:HB3	1:D:243:LEU:HG	1.79	0.63
1:C:113:HIS:CD2	1:C:308:PRO:CD	2.82	0.63
1:C:26:VAL:HG22	1:C:41:LYS:HD3	1.80	0.63
1:B:267:ASP:HB2	3:B:384:HOH:O	1.98	0.63
1:C:35:ASN:HD22	1:C:35:ASN:H	1.47	0.62
1:C:185:PHE:CD2	1:C:246:TYR:HA	2.35	0.62
1:D:285:THR:HB	1:D:288:GLN:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:CD	3:A:383:HOH:O	2.42	0.62
1:A:158:LEU:O	1:A:160:LYS:N	2.32	0.62
1:D:113:HIS:CD2	1:D:308:PRO:HD3	2.33	0.62
1:A:113:HIS:ND1	1:A:302:THR:HG21	2.14	0.62
1:A:135:HIS:O	1:A:195:ASP:OD1	2.18	0.62
1:B:43:ILE:HG13	1:B:160:LYS:HE3	1.82	0.62
1:D:258:HIS:HB3	3:D:385:HOH:O	1.99	0.62
1:A:155:ASP:O	1:A:157:GLY:N	2.29	0.62
1:A:21:GLY:O	1:A:23:PHE:N	2.33	0.62
1:A:57:ARG:H	1:A:60:LEU:HD12	1.65	0.62
1:C:13:GLU:N	1:C:31:ASP:HA	2.15	0.61
1:C:264:ALA:HB3	1:C:269:LEU:HD13	1.82	0.61
1:B:43:ILE:HG23	1:B:165:PRO:CB	2.30	0.61
1:C:175:THR:CG2	1:C:178:TYR:HE1	2.12	0.61
1:D:65:LEU:HD11	1:D:133:ILE:HD11	1.82	0.61
1:A:98:LEU:HD22	1:A:143:LEU:HD12	1.82	0.61
1:C:71:HIS:CE1	1:C:73:ASN:HB2	2.35	0.61
1:B:277:LEU:HD12	1:B:283:ARG:HA	1.82	0.61
1:D:117:TYR:CE2	1:D:307:LEU:HD23	2.36	0.61
1:A:43:ILE:HG22	1:A:43:ILE:O	2.01	0.61
1:C:23:PHE:CD1	1:C:161:SER:HB2	2.36	0.61
1:B:111:PRO:C	1:B:113:HIS:H	2.04	0.61
1:C:233:THR:HG23	1:C:236:GLN:NE2	2.14	0.61
1:D:181:PRO:HA	1:D:184:LEU:HD12	1.81	0.61
1:A:102:ILE:HD11	1:A:206:LEU:CD1	2.29	0.60
1:A:75:ILE:HB	1:A:153:LEU:O	2.01	0.60
1:C:41:LYS:NZ	1:C:160:LYS:HD3	2.16	0.60
1:D:170:TPO:O3P	1:D:172:GLN:HB2	2.02	0.60
1:C:189:MET:HG3	1:C:189:MET:O	2.01	0.60
1:D:81:PHE:CE1	1:D:88:SER:HB3	2.35	0.60
1:A:98:LEU:O	1:A:102:ILE:HG12	1.99	0.60
1:A:97:ASP:HA	1:A:144:LEU:HA	1.84	0.60
1:B:105:ASN:HD21	1:B:310:PRO:HB3	1.66	0.60
1:B:43:ILE:CG1	1:B:160:LYS:HE3	2.32	0.60
1:D:43:ILE:CG1	1:D:160:LYS:NZ	2.64	0.60
1:A:115:LYS:HE3	1:A:299:PRO:O	2.01	0.59
1:B:82:GLY:HA3	1:B:87:ILE:HA	1.84	0.59
1:C:135:HIS:CG	1:C:138:LEU:HD13	2.37	0.59
1:C:184:LEU:HD21	1:C:221:GLN:CG	2.32	0.59
1:D:79:ASP:O	1:D:90:VAL:HG12	2.02	0.59
1:A:139:LYS:HE2	1:A:141:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLN:N	1:A:170:TPO:O1P	2.35	0.59
1:A:38:VAL:HG13	1:A:90:VAL:HG13	1.84	0.59
1:C:26:VAL:HG13	1:C:41:LYS:HG2	1.84	0.59
1:D:114:ILE:HG12	1:D:206:LEU:HB3	1.84	0.59
1:A:233:THR:HG23	1:A:236:GLN:HE21	1.68	0.59
1:B:174:VAL:O	1:B:175:THR:CG2	2.47	0.59
1:A:155:ASP:HB2	1:A:159:ALA:HB3	1.85	0.59
1:A:43:ILE:CG1	1:A:160:LYS:HE2	2.31	0.59
1:A:158:LEU:HD23	1:A:162:PHE:HB2	1.85	0.58
1:D:16:ASP:HB2	1:D:28:LYS:HB3	1.85	0.58
1:A:160:LYS:O	1:A:161:SER:C	2.42	0.58
1:D:22:GLN:HB3	1:D:23:PHE:CD1	2.38	0.58
1:B:111:PRO:HD2	1:B:113:HIS:CD2	2.39	0.58
1:A:135:HIS:HE1	1:A:154:ALA:O	1.86	0.58
1:B:108:VAL:O	1:B:209:ARG:NH2	2.37	0.58
1:B:23:PHE:HB2	1:B:161:SER:HA	1.85	0.58
1:C:32:LYS:O	1:C:33:ASN:HB2	2.02	0.58
1:B:134:LEU:HD21	1:B:191:GLY:HA2	1.84	0.58
1:D:207:LEU:HD12	1:D:261:PHE:CD2	2.39	0.58
1:C:259:HIS:HB2	3:C:384:HOH:O	2.03	0.58
1:B:33:ASN:HD22	1:B:34:THR:HG23	1.69	0.57
1:B:161:SER:HB3	2:B:382:ATP:O1G	2.04	0.57
1:D:33:ASN:C	1:D:33:ASN:ND2	2.54	0.57
1:B:298:ARG:HB3	1:B:299:PRO:HD3	1.86	0.57
1:B:220:ASP:O	1:B:223:THR:HG22	2.04	0.57
1:A:240:MET:O	1:A:240:MET:HG3	2.00	0.57
1:C:285:THR:HG23	1:C:288:GLN:NE2	2.20	0.57
1:C:134:LEU:HD21	1:C:191:GLY:HA2	1.85	0.57
1:B:258:HIS:HB3	3:B:387:HOH:O	2.04	0.57
1:C:264:ALA:CB	1:C:269:LEU:HD13	2.35	0.57
1:C:135:HIS:O	1:C:137:ASP:N	2.38	0.57
1:A:143:LEU:HD22	1:A:153:LEU:HD23	1.87	0.56
1:C:116:ALA:O	1:C:120:MET:HG3	2.05	0.56
1:B:28:LYS:O	1:B:29:ALA:HB2	2.04	0.56
1:C:120:MET:HE2	1:C:151:LEU:H	1.70	0.56
1:C:94:MET:HG3	1:C:144:LEU:HB2	1.87	0.56
1:D:22:GLN:HB3	1:D:23:PHE:CE1	2.40	0.56
1:D:237:TRP:CE3	1:D:278:PHE:HB3	2.40	0.56
1:C:158:LEU:HA	1:C:162:PHE:HB2	1.86	0.56
1:D:90:VAL:O	1:D:90:VAL:CG1	2.53	0.56
1:B:71:HIS:HB3	1:B:74:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG11	1:B:90:VAL:CG1	2.35	0.56
1:D:298:ARG:NE	1:D:298:ARG:HA	2.20	0.56
1:D:43:ILE:HG12	1:D:160:LYS:HZ3	1.70	0.56
1:A:285:THR:HG23	1:A:288:GLN:HE21	1.71	0.56
1:C:114:ILE:HD13	1:C:207:LEU:HD13	1.87	0.56
1:D:158:LEU:HA	1:D:163:GLY:H	1.70	0.56
1:D:90:VAL:O	1:D:90:VAL:HG13	2.06	0.56
1:B:13:GLU:O	1:B:15:LEU:N	2.35	0.56
1:C:21:GLY:O	1:C:23:PHE:N	2.39	0.56
1:A:80:ALA:HB2	1:A:89:LEU:HD23	1.88	0.56
1:D:29:ALA:HB3	1:D:40:ILE:CD1	2.36	0.56
1:A:15:LEU:HB2	1:A:29:ALA:HA	1.87	0.56
1:A:32:LYS:HZ3	1:A:32:LYS:CB	2.07	0.56
1:C:60:LEU:O	1:C:64:LYS:HG2	2.06	0.56
1:A:189:MET:HG3	1:A:189:MET:O	2.05	0.55
1:B:92:ASP:OD1	1:B:92:ASP:N	2.36	0.55
1:B:24:ALA:HB2	1:B:160:LYS:CE	2.33	0.55
1:A:205:GLU:O	1:A:209:ARG:N	2.38	0.55
1:A:116:ALA:O	1:A:120:MET:HG3	2.06	0.55
1:B:125:LEU:CD2	1:B:129:HIS:NE2	2.70	0.55
1:A:21:GLY:O	1:A:22:GLN:C	2.44	0.55
1:A:92:ASP:OD1	1:A:92:ASP:N	2.39	0.55
1:C:217:SER:H	1:C:220:ASP:HB3	1.72	0.55
1:A:23:PHE:HB2	1:A:161:SER:HA	1.87	0.55
1:D:220:ASP:O	1:D:224:ARG:HG3	2.07	0.55
1:A:43:ILE:HD11	1:A:160:LYS:HG3	1.89	0.55
1:B:126:GLU:OE1	1:B:287:THR:HB	2.07	0.55
1:B:41:LYS:HB3	1:B:160:LYS:NZ	2.22	0.55
1:C:56:ASN:O	1:C:58:THR:N	2.39	0.55
1:C:213:LEU:HD13	1:C:225:ILE:HG13	1.88	0.54
1:B:24:ALA:HB1	1:B:160:LYS:HZ3	1.70	0.54
1:B:233:THR:HG22	1:B:234:GLU:H	1.72	0.54
1:B:143:LEU:HB3	1:B:151:LEU:HD11	1.90	0.54
1:C:22:GLN:HB3	1:C:23:PHE:CD1	2.43	0.54
1:C:83:HIS:CG	1:C:84:LYS:H	2.25	0.54
1:D:289:ALA:HA	1:D:292:MET:HG3	1.90	0.54
1:A:108:VAL:O	1:A:209:ARG:NH2	2.40	0.54
1:B:146:ASP:CG	1:B:150:VAL:HG22	2.28	0.54
1:C:185:PHE:HB3	1:C:243:LEU:HG	1.88	0.54
1:B:226:PHE:CE2	1:B:232:PRO:HD3	2.43	0.54
1:D:208:LEU:HD13	1:D:261:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LYS:HB2	1:D:160:LYS:CE	2.35	0.54
1:D:136:ARG:HH21	1:D:158:LEU:HD22	1.72	0.54
1:C:63:ILE:HG22	1:C:64:LYS:N	2.24	0.53
1:B:164:SER:CB	1:B:165:PRO:HD3	2.34	0.53
1:B:185:PHE:CD2	1:B:246:TYR:HA	2.43	0.53
1:D:128:LEU:CD1	1:D:135:HIS:HB2	2.38	0.53
1:D:43:ILE:O	1:D:166:ASN:ND2	2.40	0.53
1:D:102:ILE:HG21	1:D:206:LEU:HD12	1.90	0.53
1:C:111:PRO:HD2	1:C:113:HIS:CG	2.43	0.53
1:B:198:ALA:O	1:B:202:ILE:HG13	2.07	0.53
1:C:191:GLY:O	1:C:193:GLY:N	2.41	0.53
1:C:21:GLY:O	1:C:22:GLN:C	2.46	0.53
1:A:32:LYS:HZ2	1:A:32:LYS:CB	2.09	0.53
1:B:31:ASP:O	1:B:33:ASN:N	2.42	0.53
1:C:105:ASN:OD1	1:C:107:LEU:HB3	2.09	0.53
1:C:116:ALA:HA	1:C:301:PRO:HB3	1.91	0.53
1:C:215:GLY:HA2	1:C:220:ASP:OD2	2.09	0.53
1:D:143:LEU:CD2	1:D:151:LEU:HD21	2.39	0.53
1:B:231:THR:HG23	1:B:252:PHE:H	1.74	0.52
1:C:22:GLN:HE21	1:C:174:VAL:HG12	1.74	0.52
1:B:67:GLN:HG2	1:B:77:LEU:HD23	1.92	0.52
1:A:175:THR:CG2	1:A:178:TYR:CE1	2.90	0.52
1:B:81:PHE:O	1:B:82:GLY:O	2.27	0.52
1:C:304:GLY:HA2	1:C:307:LEU:HD22	1.90	0.52
1:A:83:HIS:O	1:A:85:SER:N	2.43	0.52
1:C:23:PHE:HD1	1:C:161:SER:HB2	1.74	0.52
1:C:275:LEU:O	1:C:283:ARG:HD3	2.10	0.52
1:C:175:THR:CG2	1:C:178:TYR:CE1	2.92	0.52
1:B:234:GLU:OE1	1:B:234:GLU:HA	2.09	0.52
1:D:103:LYS:HG2	1:D:104:ASP:H	1.73	0.52
1:B:114:ILE:O	1:B:115:LYS:C	2.48	0.52
1:B:255:ILE:HG22	1:B:260:ILE:HG13	1.92	0.52
1:D:171:HIS:O	1:D:171:HIS:CG	2.63	0.52
1:B:24:ALA:CB	1:B:160:LYS:HE2	2.35	0.51
1:B:237:TRP:CG	1:B:240:MET:HB2	2.45	0.51
1:A:115:LYS:CE	1:A:299:PRO:O	2.58	0.51
1:C:175:THR:HG21	1:C:178:TYR:CE1	2.39	0.51
1:D:155:ASP:OD2	1:D:160:LYS:HB2	2.11	0.51
1:B:105:ASN:OD1	1:B:107:LEU:HB3	2.11	0.51
1:A:117:TYR:HE2	1:A:145:LEU:HD21	1.75	0.51
1:C:179:ARG:HB3	1:C:184:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:THR:OG1	1:D:236:GLN:HG3	2.10	0.51
1:B:24:ALA:CB	1:B:160:LYS:NZ	2.72	0.51
1:B:257:LEU:HB3	1:B:269:LEU:CD2	2.40	0.51
1:A:111:PRO:CD	1:A:111:PRO:O	2.59	0.51
1:A:125:LEU:HD22	1:A:129:HIS:NE2	2.26	0.51
1:C:79:ASP:HB3	1:C:90:VAL:HG12	1.93	0.51
1:D:111:PRO:HD2	1:D:113:HIS:CG	2.45	0.51
1:A:101:ILE:HG23	1:A:108:VAL:HG11	1.93	0.51
2:B:382:ATP:O1B	2:B:382:ATP:O2A	2.29	0.51
1:A:96:THR:CG2	1:A:100:VAL:HG11	2.41	0.51
1:A:41:LYS:HD3	1:A:160:LYS:CD	2.39	0.50
1:C:73:ASN:O	1:C:152:LYS:HA	2.11	0.50
1:B:102:ILE:O	1:B:209:ARG:NH1	2.45	0.50
1:D:155:ASP:HB2	1:D:159:ALA:HB3	1.93	0.50
1:A:58:THR:O	1:A:62:GLU:HG2	2.11	0.50
1:B:83:HIS:O	1:B:85:SER:N	2.45	0.50
1:D:139:LYS:HB2	1:D:140:PRO:HD3	1.92	0.50
1:B:56:ASN:HB2	1:B:59:ALA:HB2	1.92	0.50
1:A:104:ASP:O	1:A:106:SER:N	2.45	0.50
1:A:238:PRO:O	1:A:239:ASP:CB	2.59	0.50
1:B:285:THR:H	1:B:288:GLN:HB2	1.77	0.50
1:C:111:PRO:HD2	1:C:113:HIS:ND1	2.26	0.50
1:A:118:MET:HA	1:A:118:MET:CE	2.42	0.50
1:A:41:LYS:O	1:A:88:SER:HA	2.12	0.49
1:C:182:GLU:HG2	1:C:280:PRO:HG3	1.94	0.49
1:B:129:HIS:CG	1:B:192:VAL:HG12	2.46	0.49
1:B:285:THR:HG22	3:B:388:HOH:O	2.11	0.49
1:C:232:PRO:HA	1:C:236:GLN:NE2	2.26	0.49
1:D:147:GLU:H	1:D:147:GLU:CD	2.15	0.49
1:D:233:THR:C	1:D:235:GLU:N	2.62	0.49
1:B:117:TYR:CE2	1:B:145:LEU:HD11	2.47	0.49
1:D:98:LEU:HD21	1:D:206:LEU:HD11	1.93	0.49
1:C:89:LEU:HB2	1:C:160:LYS:NZ	2.26	0.49
1:C:103:LYS:C	1:C:105:ASN:H	2.16	0.49
1:C:16:ASP:HB2	1:C:28:LYS:HB3	1.94	0.49
1:A:41:LYS:CA	1:A:160:LYS:HZ1	2.26	0.49
1:B:156:PHE:CD1	1:B:159:ALA:HB2	2.48	0.49
1:D:257:LEU:CD2	1:D:273:GLN:HB2	2.42	0.49
1:A:101:ILE:O	1:A:209:ARG:NH1	2.46	0.48
1:A:103:LYS:C	1:A:105:ASN:N	2.51	0.48
1:B:35:ASN:HA	3:B:391:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:CD1	1:C:153:LEU:HD12	2.43	0.48
1:A:115:LYS:HD3	1:A:294:TYR:CZ	2.48	0.48
1:D:185:PHE:CD2	1:D:246:TYR:HA	2.48	0.48
1:D:240:MET:O	1:D:243:LEU:HB2	2.13	0.48
1:D:256:PRO:O	1:D:259:HIS:N	2.46	0.48
1:B:135:HIS:O	1:B:137:ASP:N	2.46	0.48
1:C:90:VAL:O	1:C:90:VAL:HG13	2.12	0.48
1:A:178:TYR:OH	1:A:205:GLU:OE1	2.30	0.48
1:A:16:ASP:CB	1:A:28:LYS:HB3	2.42	0.48
1:B:84:LYS:O	1:B:84:LYS:HG3	2.14	0.48
1:B:174:VAL:HG22	1:B:175:THR:N	2.29	0.48
1:C:178:TYR:OH	1:C:205:GLU:OE2	2.17	0.48
1:A:177:TRP:CD1	1:A:214:PRO:HA	2.48	0.48
1:B:257:LEU:HB3	1:B:269:LEU:HD22	1.94	0.48
1:D:135:HIS:HD2	1:D:137:ASP:H	1.61	0.48
1:B:76:GLY:O	1:B:91:PHE:HA	2.14	0.48
1:B:115:LYS:HE2	1:B:299:PRO:O	2.13	0.48
1:B:267:ASP:O	1:B:294:TYR:HB2	2.14	0.48
1:C:203:LEU:HD21	1:C:268:LEU:CD1	2.40	0.48
1:D:113:HIS:ND1	1:D:302:THR:HG21	2.28	0.48
1:A:226:PHE:CD1	1:A:232:PRO:HD3	2.48	0.48
1:C:95:GLU:H	1:C:146:ASP:HA	1.78	0.48
1:D:285:THR:HG22	1:D:288:GLN:H	1.79	0.48
1:B:13:GLU:C	1:B:15:LEU:H	2.16	0.47
1:B:200:GLY:HA2	1:B:275:LEU:HD13	1.96	0.47
1:D:140:PRO:HD3	1:D:178:TYR:CZ	2.49	0.47
1:A:102:ILE:CD1	1:A:206:LEU:CD1	2.92	0.47
1:A:26:VAL:HG11	2:A:381:ATP:C8	2.49	0.47
1:A:97:ASP:HB3	1:A:144:LEU:HD23	1.96	0.47
1:A:157:GLY:C	1:A:159:ALA:N	2.68	0.47
1:A:71:HIS:CE1	1:A:72:PRO:HG2	2.49	0.47
1:B:157:GLY:C	1:B:159:ALA:H	2.18	0.47
1:B:24:ALA:HB1	1:B:160:LYS:HZ1	1.80	0.47
1:C:108:VAL:O	1:C:209:ARG:NH2	2.47	0.47
1:C:203:LEU:HD12	1:C:203:LEU:O	2.15	0.47
1:C:238:PRO:O	1:C:239:ASP:CB	2.50	0.47
1:C:66:LEU:HD23	1:C:77:LEU:HB2	1.95	0.47
1:D:122:LEU:HD21	1:D:199:VAL:HG11	1.94	0.47
2:B:382:ATP:O2G	2:B:382:ATP:O3A	2.32	0.47
1:B:98:LEU:HA	1:B:98:LEU:HD12	1.78	0.47
1:C:73:ASN:HD21	1:C:120:MET:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:THR:N	1:C:236:GLN:HE21	1.98	0.47
1:B:304:GLY:O	1:B:307:LEU:HB2	2.14	0.47
1:D:142:ASN:HB3	1:D:154:ALA:HB3	1.97	0.47
1:D:43:ILE:HG22	1:D:166:ASN:ND2	2.23	0.47
1:B:143:LEU:HD13	1:B:151:LEU:HD11	1.96	0.47
1:A:158:LEU:O	1:A:163:GLY:HA3	2.15	0.46
1:A:259:HIS:HD2	3:A:397:HOH:O	1.98	0.46
1:A:31:ASP:O	1:A:32:LYS:C	2.54	0.46
1:C:113:HIS:HD2	1:C:308:PRO:CD	2.28	0.46
1:D:214:PRO:HD2	1:D:224:ARG:HH11	1.81	0.46
1:B:237:TRP:HB3	1:B:240:MET:HB2	1.98	0.46
1:A:102:ILE:CD1	1:A:206:LEU:HD13	2.40	0.46
1:B:20:GLU:HG3	1:B:169:TYR:O	2.15	0.46
1:B:64:LYS:HA	1:B:64:LYS:HD3	1.63	0.46
1:C:77:LEU:HD22	1:C:91:PHE:HE2	1.80	0.46
1:D:285:THR:HB	1:D:288:GLN:CG	2.46	0.46
1:D:184:LEU:HD13	1:D:222:LEU:HD13	1.98	0.46
1:D:268:LEU:HB2	1:D:294:TYR:CE1	2.50	0.46
1:A:139:LYS:CE	1:A:141:ASN:HD21	2.27	0.46
1:C:102:ILE:HG23	1:C:209:ARG:HA	1.98	0.46
1:C:118:MET:CE	1:C:118:MET:HA	2.46	0.46
1:C:272:ILE:O	1:C:273:GLN:C	2.54	0.46
1:A:143:LEU:HD22	1:A:153:LEU:CD2	2.46	0.46
1:A:160:LYS:HB3	1:A:161:SER:H	1.49	0.46
1:B:232:PRO:HG3	1:B:278:PHE:CD1	2.51	0.46
1:C:125:LEU:HD11	1:C:195:ASP:HB3	1.97	0.46
1:B:24:ALA:CB	1:B:160:LYS:CE	2.94	0.46
1:B:43:ILE:CG2	1:B:43:ILE:O	2.64	0.46
1:A:200:GLY:HA2	1:A:275:LEU:HD13	1.98	0.46
1:B:171:HIS:O	1:B:172:GLN:HB2	2.16	0.46
1:C:71:HIS:ND1	1:C:73:ASN:HB2	2.31	0.46
1:B:199:VAL:O	1:B:200:GLY:C	2.53	0.45
1:D:65:LEU:HD11	1:D:133:ILE:CD1	2.46	0.45
1:A:21:GLY:C	1:A:170:TPO:O1P	2.54	0.45
1:B:38:VAL:HG13	1:B:90:VAL:HG13	1.98	0.45
1:C:135:HIS:C	1:C:137:ASP:H	2.20	0.45
1:D:23:PHE:HD1	1:D:161:SER:HB3	1.81	0.45
1:B:233:THR:HB	1:B:236:GLN:H	1.82	0.45
1:A:213:LEU:HD13	1:A:225:ILE:HG12	1.98	0.45
1:A:24:ALA:HB2	1:A:160:LYS:HZ3	1.58	0.45
1:C:57:ARG:H	1:C:60:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ARG:HH21	1:D:183:LEU:HD13	1.82	0.45
1:A:96:THR:HG21	1:A:100:VAL:HG11	1.99	0.45
1:B:79:ASP:H	1:B:90:VAL:HB	1.82	0.45
1:A:109:LEU:O	1:A:109:LEU:HG	2.17	0.45
1:B:231:THR:HG21	1:B:250:LYS:O	2.17	0.45
1:B:56:ASN:O	1:B:58:THR:N	2.49	0.45
1:A:185:PHE:CB	1:A:243:LEU:HG	2.45	0.44
1:A:24:ALA:HB3	2:A:381:ATP:O3G	2.17	0.44
1:D:176:ARG:HG3	1:D:176:ARG:O	2.16	0.44
1:D:34:THR:HG22	1:D:36:GLN:H	1.81	0.44
1:D:96:THR:HG21	1:D:100:VAL:HG21	1.99	0.44
1:A:118:MET:O	1:A:119:LEU:C	2.55	0.44
1:C:132:TRP:N	1:C:132:TRP:CD1	2.85	0.44
1:B:230:GLY:HA2	1:B:252:PHE:O	2.18	0.44
1:C:155:ASP:O	1:C:157:GLY:N	2.50	0.44
1:C:182:GLU:HG3	1:C:182:GLU:H	1.18	0.44
1:C:74:ILE:HD13	1:C:153:LEU:HD12	2.00	0.44
1:C:40:ILE:HG13	1:C:90:VAL:HG23	1.99	0.44
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.76	0.44
1:C:18:LEU:HD11	1:C:93:PHE:HE1	1.82	0.44
1:A:270:ASP:O	1:A:273:GLN:HB3	2.17	0.44
1:B:103:LYS:C	1:B:105:ASN:H	2.21	0.44
1:B:21:GLY:O	1:B:22:GLN:C	2.56	0.44
1:B:77:LEU:HA	1:B:77:LEU:HD12	1.85	0.44
1:C:233:THR:H	1:C:236:GLN:NE2	1.98	0.44
1:B:14:LYS:O	1:B:15:LEU:C	2.55	0.44
1:B:214:PRO:O	1:B:224:ARG:HD2	2.17	0.44
1:B:298:ARG:CB	1:B:299:PRO:HD3	2.47	0.44
1:C:158:LEU:C	1:C:160:LYS:H	2.21	0.44
1:C:279:ASN:HB3	1:C:282:ALA:HB3	1.99	0.44
1:D:185:PHE:CE2	1:D:246:TYR:HA	2.52	0.44
1:C:144:LEU:HD11	1:C:154:ALA:HB2	2.00	0.44
1:C:264:ALA:HB3	1:C:269:LEU:CD1	2.48	0.44
1:D:121:THR:CG2	1:D:143:LEU:HD21	2.45	0.44
1:D:187:ALA:HB2	1:D:243:LEU:HD11	2.00	0.44
1:A:38:VAL:HG11	1:A:90:VAL:CG1	2.43	0.44
1:D:97:ASP:OD1	1:D:99:GLU:N	2.51	0.44
1:B:232:PRO:HG3	1:B:278:PHE:CG	2.53	0.44
1:B:74:ILE:HG22	1:B:75:ILE:O	2.18	0.44
1:D:169:TYR:N	1:D:169:TYR:CD2	2.86	0.44
1:A:38:VAL:HG12	1:A:40:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:HD22	1:D:129:HIS:CE1	2.53	0.43
1:A:178:TYR:CD1	1:A:178:TYR:N	2.86	0.43
1:D:114:ILE:HA	1:D:206:LEU:HD23	2.00	0.43
1:A:276:PHE:O	1:A:277:LEU:C	2.56	0.43
1:A:304:GLY:HA2	1:A:307:LEU:HD22	2.01	0.43
1:D:202:ILE:O	1:D:205:GLU:N	2.48	0.43
1:B:109:LEU:HD12	1:B:110:THR:H	1.83	0.43
1:B:141:ASN:HD22	1:B:141:ASN:H	0.66	0.43
1:C:89:LEU:HD12	1:C:160:LYS:HE3	1.99	0.43
1:D:125:LEU:HD22	1:D:129:HIS:NE2	2.33	0.43
1:D:285:THR:HG22	1:D:287:THR:N	2.33	0.43
1:A:157:GLY:O	1:A:158:LEU:C	2.57	0.43
1:C:183:LEU:HD11	1:C:194:VAL:HG22	1.99	0.43
1:D:97:ASP:HB3	1:D:144:LEU:HD12	2.01	0.43
1:A:285:THR:HG23	1:A:288:GLN:NE2	2.33	0.43
1:A:302:THR:OG1	1:A:307:LEU:HD13	2.19	0.43
1:D:226:PHE:O	1:D:230:GLY:N	2.52	0.43
1:A:293:LYS:O	1:A:294:TYR:C	2.56	0.43
1:B:43:ILE:HG23	1:B:165:PRO:CG	2.49	0.43
1:B:86:ASN:N	1:B:86:ASN:ND2	2.67	0.43
1:C:120:MET:HE2	1:C:151:LEU:N	2.33	0.43
1:C:98:LEU:HD21	1:C:206:LEU:HD21	2.01	0.43
1:C:41:LYS:HE3	1:C:91:PHE:CE1	2.45	0.43
1:A:120:MET:O	1:A:121:THR:C	2.57	0.43
1:A:293:LYS:HB3	1:A:297:ASN:ND2	2.34	0.43
1:B:158:LEU:C	1:B:160:LYS:N	2.72	0.43
1:B:176:ARG:NH1	1:B:218:ASP:OD1	2.52	0.43
1:C:125:LEU:HA	1:C:125:LEU:HD23	1.76	0.43
1:D:56:ASN:ND2	1:D:163:GLY:O	2.52	0.43
1:A:41:LYS:HD2	1:A:91:PHE:CE1	2.54	0.43
1:C:181:PRO:HA	1:C:184:LEU:HB2	2.01	0.43
1:C:83:HIS:CG	1:C:84:LYS:N	2.87	0.43
1:D:233:THR:C	1:D:235:GLU:H	2.21	0.43
1:D:243:LEU:HD12	1:D:244:PRO:HD2	2.01	0.43
1:B:289:ALA:O	1:B:292:MET:HB2	2.18	0.43
1:A:278:PHE:O	1:A:280:PRO:HD3	2.18	0.42
1:B:109:LEU:HA	1:B:209:ARG:HH21	1.84	0.42
1:B:211:PRO:HB2	1:B:214:PRO:HG3	2.01	0.42
1:C:212:PHE:O	1:C:213:LEU:HD23	2.19	0.42
1:C:99:GLU:O	1:C:103:LYS:CB	2.66	0.42
1:D:257:LEU:HD21	1:D:273:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TRP:HB2	1:B:178:TYR:CE1	2.54	0.42
1:B:18:LEU:HD11	1:B:93:PHE:HE1	1.84	0.42
1:B:28:LYS:O	1:B:29:ALA:CB	2.67	0.42
1:C:196:MET:O	1:C:199:VAL:HB	2.19	0.42
1:D:214:PRO:HD2	1:D:224:ARG:NH1	2.33	0.42
1:D:21:GLY:O	1:D:22:GLN:C	2.57	0.42
1:B:146:ASP:C	1:B:146:ASP:OD1	2.58	0.42
1:B:193:GLY:O	1:B:283:ARG:NH1	2.49	0.42
1:D:222:LEU:HA	1:D:222:LEU:HD12	1.91	0.42
1:C:279:ASN:HB3	1:C:282:ALA:CB	2.48	0.42
1:D:158:LEU:HB3	1:D:162:PHE:HB2	2.02	0.42
1:D:202:ILE:O	1:D:203:LEU:C	2.56	0.42
1:A:43:ILE:HD11	1:A:160:LYS:CG	2.49	0.42
1:B:274:GLY:O	1:B:284:ILE:HG22	2.20	0.42
1:B:83:HIS:C	1:B:85:SER:H	2.22	0.42
1:C:175:THR:HG23	1:C:177:TRP:CD2	2.54	0.42
1:D:170:TPO:O1P	1:D:170:TPO:HG21	2.19	0.42
1:B:102:ILE:HG21	1:B:205:GLU:HG2	2.01	0.42
1:C:41:LYS:NZ	2:C:383:ATP:O2G	2.53	0.42
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.85	0.42
1:A:196:MET:HG3	1:A:275:LEU:CD2	2.48	0.42
1:B:155:ASP:C	1:B:157:GLY:H	2.23	0.42
1:B:110:THR:HG22	1:B:209:ARG:NE	2.35	0.42
1:C:125:LEU:HD22	1:C:129:HIS:NE2	2.35	0.42
1:A:129:HIS:ND1	1:A:192:VAL:HG12	2.35	0.42
1:A:41:LYS:HD2	1:A:91:PHE:HE1	1.85	0.42
1:B:41:LYS:C	1:B:160:LYS:HZ2	2.23	0.42
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.55	0.42
1:A:149:GLY:HA3	1:A:304:GLY:O	2.19	0.41
1:A:192:VAL:O	1:A:194:VAL:N	2.53	0.41
1:B:111:PRO:C	1:B:113:HIS:N	2.71	0.41
1:B:122:LEU:O	1:B:126:GLU:HB3	2.20	0.41
1:D:23:PHE:HD1	1:D:161:SER:CB	2.33	0.41
1:D:160:LYS:HB3	1:D:161:SER:H	1.47	0.41
1:A:94:MET:HE2	1:A:152:LYS:HB2	2.02	0.41
1:A:37:ILE:HD12	1:A:37:ILE:N	2.34	0.41
1:B:267:ASP:OD2	1:B:297:ASN:ND2	2.53	0.41
1:C:63:ILE:CG2	1:C:64:LYS:N	2.83	0.41
1:D:170:TPO:O2P	1:D:172:GLN:O	2.38	0.41
1:D:285:THR:CG2	1:D:286:ALA:N	2.83	0.41
1:A:74:ILE:HD11	1:A:128:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:HIS:CE1	1:A:154:ALA:O	2.70	0.41
1:B:195:ASP:O	1:B:199:VAL:HG23	2.21	0.41
1:B:66:LEU:HD12	1:B:159:ALA:HB1	2.02	0.41
1:B:293:LYS:O	1:B:295:PHE:N	2.53	0.41
1:C:89:LEU:HB2	1:C:160:LYS:HZ2	1.85	0.41
1:D:221:GLN:O	1:D:225:ILE:HD12	2.20	0.41
1:D:258:HIS:O	1:D:262:SER:HA	2.21	0.41
1:A:102:ILE:O	1:A:209:ARG:NH1	2.53	0.41
1:A:118:MET:HG3	1:A:203:LEU:HD13	2.02	0.41
1:A:119:LEU:HD11	1:A:123:GLN:NE2	2.35	0.41
1:A:75:ILE:HG12	1:A:144:LEU:HD12	2.02	0.41
1:B:237:TRP:CE3	1:B:240:MET:HG3	2.55	0.41
1:A:104:ASP:O	1:A:106:SER:OG	2.36	0.41
1:A:205:GLU:HG2	1:A:211:PRO:HA	2.03	0.41
1:C:41:LYS:HZ1	1:C:160:LYS:HD3	1.86	0.41
1:B:177:TRP:HD1	1:B:215:GLY:H	1.59	0.41
1:C:119:LEU:HD22	1:C:123:GLN:NE2	2.36	0.41
1:A:84:LYS:HG3	3:A:396:HOH:O	2.20	0.41
1:A:76:GLY:O	1:A:91:PHE:HA	2.20	0.41
1:B:174:VAL:C	1:B:175:THR:CG2	2.83	0.41
1:D:135:HIS:HA	1:D:156:PHE:HB3	2.03	0.41
1:A:77:LEU:HD13	1:A:91:PHE:CE2	2.56	0.41
1:B:43:ILE:HD11	1:B:160:LYS:CE	2.47	0.41
1:C:110:THR:HA	1:C:111:PRO:HD3	1.84	0.41
1:B:111:PRO:O	1:B:113:HIS:N	2.53	0.41
1:B:177:TRP:CD1	1:B:215:GLY:N	2.83	0.41
1:A:215:GLY:HA2	1:A:224:ARG:HD2	2.03	0.41
1:B:130:GLN:HE21	1:B:131:HIS:CE1	2.39	0.41
1:C:102:ILE:HD13	1:C:205:GLU:HB3	2.03	0.41
1:D:111:PRO:CD	1:D:113:HIS:CE1	3.03	0.41
1:D:40:ILE:CG1	1:D:90:VAL:HG23	2.35	0.41
1:A:257:LEU:HD23	1:A:260:ILE:HD12	2.03	0.40
1:B:103:LYS:C	1:B:105:ASN:N	2.74	0.40
1:D:143:LEU:CD1	1:D:202:ILE:HD13	2.51	0.40
1:D:257:LEU:HB3	1:D:269:LEU:CD2	2.37	0.40
1:D:277:LEU:HD12	1:D:283:ARG:HA	2.03	0.40
1:D:60:LEU:H	1:D:60:LEU:HD23	1.86	0.40
1:D:78:LEU:O	1:D:79:ASP:CB	2.64	0.40
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.84	0.40
1:D:207:LEU:O	1:D:209:ARG:N	2.55	0.40
1:D:309:ARG:HA	1:D:310:PRO:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:H	1:A:90:VAL:HB	1.85	0.40
1:A:81:PHE:CE1	1:A:88:SER:HB2	2.57	0.40
1:C:114:ILE:O	1:C:115:LYS:C	2.59	0.40
1:A:60:LEU:O	1:A:64:LYS:HG2	2.21	0.40
1:B:156:PHE:HE1	1:B:159:ALA:HB2	1.80	0.40
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.86	0.40
1:B:40:ILE:HG13	1:B:90:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/346 (82%)	242 (86%)	22 (8%)	18 (6%)	1	7
1	B	282/346 (82%)	231 (82%)	26 (9%)	25 (9%)	1	3
1	C	282/346 (82%)	237 (84%)	30 (11%)	15 (5%)	2	11
1	D	282/346 (82%)	227 (80%)	37 (13%)	18 (6%)	1	7
All	All	1128/1384 (82%)	937 (83%)	115 (10%)	76 (7%)	1	6

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	22	GLN
1	A	84	LYS
1	A	104	ASP
1	A	112	SER
1	A	156	PHE
1	A	158	LEU
1	A	161	SER

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Mol	Chain	Res	Type
1	B	15	LEU
1	B	32	LYS
1	B	33	ASN
1	B	35	ASN
1	B	57	ARG
1	B	82	GLY
1	B	84	LYS
1	B	95	GLU
1	B	104	ASP
1	B	111	PRO
1	B	164	SER
1	B	166	ASN
1	B	174	VAL
1	B	175	THR
1	C	22	GLN
1	C	57	ARG
1	C	104	ASP
1	C	112	SER
1	C	156	PHE
1	C	160	LYS
1	C	166	ASN
1	C	192	VAL
1	D	79	ASP
1	D	104	ASP
1	D	161	SER
1	D	166	ASN
1	D	208	LEU
1	D	257	LEU
1	D	298	ARG
1	A	105	ASN
1	A	160	LYS
1	B	14	LYS
1	B	22	GLN
1	B	36	GLN
1	B	59	ALA
1	B	161	SER
1	B	192	VAL
1	C	33	ASN
1	C	157	GLY
1	C	165	PRO
1	D	114	ILE
1	D	156	PHE

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Mol	Chain	Res	Type
1	D	163	GLY
1	D	165	PRO
1	D	169	TYR
1	D	304	GLY
1	A	111	PRO
1	A	159	ALA
1	A	172	GLN
1	B	29	ALA
1	B	172	GLN
1	B	298	ARG
1	C	14	LYS
1	C	111	PRO
1	C	136	ARG
1	D	22	GLN
1	D	111	PRO
1	A	57	ARG
1	A	147	GLU
1	B	112	SER
1	B	233	THR
1	D	207	LEU
1	A	32	LYS
1	A	297	ASN
1	C	294	TYR
1	D	256	PRO
1	A	175	THR
1	D	101	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/298 (84%)	213 (86%)	36 (14%)	3	14
1	B	249/298 (84%)	200 (80%)	49 (20%)	1	7
1	C	249/298 (84%)	207 (83%)	42 (17%)	2	10
1	D	249/298 (84%)	197 (79%)	52 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	996/1192 (84%)	817 (82%)	179 (18%)	<b>1</b> <b>8</b>

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	32	LYS
1	A	33	ASN
1	A	75	ILE
1	A	79	ASP
1	A	95	GLU
1	A	97	ASP
1	A	101	ILE
1	A	109	LEU
1	A	110	THR
1	A	112	SER
1	A	139	LYS
1	A	147	GLU
1	A	148	ASN
1	A	164	SER
1	A	166	ASN
1	A	169	TYR
1	A	171	HIS
1	A	172	GLN
1	A	188	ARG
1	A	189	MET
1	A	192	VAL
1	A	206	LEU
1	A	208	LEU
1	A	240	MET
1	A	243	LEU
1	A	248	THR
1	A	251	SER
1	A	266	ASP
1	A	269	LEU
1	A	281	CYS
1	A	292	MET
1	A	298	ARG
1	A	302	THR
1	A	305	CYS
1	A	307	LEU
1	B	18	LEU

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Mol	Chain	Res	Type
1	B	20	GLU
1	B	22	GLN
1	B	30	ARG
1	B	57	ARG
1	B	65	LEU
1	B	66	LEU
1	B	68	GLU
1	B	69	LEU
1	B	78	LEU
1	B	79	ASP
1	B	85	SER
1	B	86	ASN
1	B	88	SER
1	B	92	ASP
1	B	98	LEU
1	B	101	ILE
1	B	105	ASN
1	B	106	SER
1	B	107	LEU
1	B	109	LEU
1	B	112	SER
1	B	115	LYS
1	B	120	MET
1	B	125	LEU
1	B	126	GLU
1	B	134	LEU
1	B	136	ARG
1	B	137	ASP
1	B	141	ASN
1	B	146	ASP
1	B	151	LEU
1	B	156	PHE
1	B	167	ARG
1	B	171	HIS
1	B	172	GLN
1	B	174	VAL
1	B	208	LEU
1	B	209	ARG
1	B	219	LEU
1	B	234	GLU
1	B	242	SER
1	B	243	LEU

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Mol	Chain	Res	Type
1	B	248	THR
1	B	251	SER
1	B	257	LEU
1	B	287	THR
1	B	292	MET
1	B	298	ARG
1	C	16	ASP
1	C	17	PHE
1	C	34	THR
1	C	35	ASN
1	C	36	GLN
1	C	40	ILE
1	C	63	ILE
1	C	77	LEU
1	C	85	SER
1	C	100	VAL
1	C	105	ASN
1	C	113	HIS
1	C	119	LEU
1	C	125	LEU
1	C	130	GLN
1	C	132	TRP
1	C	138	LEU
1	C	141	ASN
1	C	144	LEU
1	C	145	LEU
1	C	148	ASN
1	C	151	LEU
1	C	155	ASP
1	C	160	LYS
1	C	166	ASN
1	C	172	GLN
1	C	173	VAL
1	C	182	GLU
1	C	184	LEU
1	C	192	VAL
1	C	206	LEU
1	C	207	LEU
1	C	216	ASP
1	C	223	THR
1	C	233	THR
1	C	235	GLU

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Mol	Chain	Res	Type
1	C	242	SER
1	C	243	LEU
1	C	269	LEU
1	C	273	GLN
1	C	288	GLN
1	C	307	LEU
1	D	13	GLU
1	D	14	LYS
1	D	16	ASP
1	D	20	GLU
1	D	30	ARG
1	D	33	ASN
1	D	35	ASN
1	D	37	ILE
1	D	57	ARG
1	D	58	THR
1	D	60	LEU
1	D	81	PHE
1	D	88	SER
1	D	90	VAL
1	D	92	ASP
1	D	94	MET
1	D	104	ASP
1	D	106	SER
1	D	110	THR
1	D	112	SER
1	D	113	HIS
1	D	130	GLN
1	D	134	LEU
1	D	139	LYS
1	D	141	ASN
1	D	143	LEU
1	D	144	LEU
1	D	150	VAL
1	D	151	LEU
1	D	161	SER
1	D	167	ARG
1	D	169	TYR
1	D	172	GLN
1	D	173	VAL
1	D	174	VAL
1	D	179	ARG

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Mol	Chain	Res	Type
1	D	185	PHE
1	D	192	VAL
1	D	203	LEU
1	D	209	ARG
1	D	216	ASP
1	D	222	LEU
1	D	235	GLU
1	D	239	ASP
1	D	242	SER
1	D	243	LEU
1	D	247	VAL
1	D	248	THR
1	D	250	LYS
1	D	281	CYS
1	D	285	THR
1	D	292	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	135	HIS
1	A	166	ASN
1	A	172	GLN
1	A	236	GLN
1	A	288	GLN
1	B	33	ASN
1	B	56	ASN
1	B	73	ASN
1	B	86	ASN
1	B	131	HIS
1	B	141	ASN
1	B	142	ASN
1	C	22	GLN
1	C	35	ASN
1	C	73	ASN
1	C	86	ASN
1	C	141	ASN
1	C	236	GLN
1	C	288	GLN
1	D	33	ASN
1	D	56	ASN

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Mol	Chain	Res	Type
1	D	135	HIS
1	D	166	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	170	1	8,10,11	3.23	4 (50%)	10,14,16	1.36	0
1	TPO	B	170	1	8,10,11	3.30	4 (50%)	10,14,16	0.88	0
1	TPO	C	170	1	8,10,11	3.25	4 (50%)	10,14,16	0.78	0
1	TPO	D	170	1	8,10,11	3.40	4 (50%)	10,14,16	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	170	1	-	4/9/11/13	-
1	TPO	B	170	1	-	2/9/11/13	-
1	TPO	C	170	1	-	5/9/11/13	-
1	TPO	D	170	1	-	6/9/11/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	TPO	P-O1P	6.71	1.72	1.50
1	B	170	TPO	P-O1P	6.66	1.72	1.50
1	C	170	TPO	P-O1P	6.43	1.71	1.50
1	A	170	TPO	P-O1P	6.24	1.70	1.50
1	D	170	TPO	P-O2P	4.41	1.71	1.54
1	B	170	TPO	P-O3P	4.39	1.71	1.54
1	D	170	TPO	P-O3P	4.35	1.71	1.54
1	C	170	TPO	P-O2P	4.31	1.71	1.54
1	C	170	TPO	P-O3P	4.31	1.71	1.54
1	A	170	TPO	P-O3P	4.23	1.71	1.54
1	A	170	TPO	P-O2P	4.10	1.70	1.54
1	B	170	TPO	P-O2P	3.86	1.69	1.54
1	A	170	TPO	P-OG1	2.61	1.64	1.59
1	D	170	TPO	P-OG1	2.45	1.63	1.59
1	B	170	TPO	P-OG1	2.29	1.63	1.59
1	C	170	TPO	P-OG1	2.05	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	170	TPO	N-CA-CB-CG2
1	A	170	TPO	N-CA-CB-OG1
1	A	170	TPO	C-CA-CB-CG2
1	A	170	TPO	O-C-CA-CB
1	B	170	TPO	N-CA-CB-OG1
1	C	170	TPO	N-CA-CB-CG2
1	C	170	TPO	N-CA-CB-OG1
1	C	170	TPO	C-CA-CB-CG2
1	C	170	TPO	O-C-CA-CB
1	D	170	TPO	N-CA-CB-CG2
1	D	170	TPO	N-CA-CB-OG1
1	D	170	TPO	C-CA-CB-CG2
1	D	170	TPO	CG2-CB-OG1-P
1	B	170	TPO	CB-OG1-P-O1P
1	C	170	TPO	CB-OG1-P-O1P
1	D	170	TPO	CB-OG1-P-O3P
1	D	170	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	170	TPO	2	0
1	B	170	TPO	1	0
1	C	170	TPO	1	0
1	D	170	TPO	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	A	381	-	26,33,33	0.98	2 (7%)	31,52,52	1.44	5 (16%)
2	ATP	B	382	-	26,33,33	1.02	2 (7%)	31,52,52	1.74	7 (22%)
2	ATP	D	384	-	26,33,33	0.91	1 (3%)	31,52,52	1.64	8 (25%)
2	ATP	C	383	-	26,33,33	1.03	2 (7%)	31,52,52	1.63	6 (19%)

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	A	381	-	-	6/18/38/38	0/3/3/3
2	ATP	B	382	-	-	5/18/38/38	0/3/3/3
2	ATP	D	384	-	-	3/18/38/38	0/3/3/3
2	ATP	C	383	-	-	4/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	383	ATP	C5-C4	2.56	1.47	1.40
2	D	384	ATP	C5-C4	2.39	1.47	1.40
2	A	381	ATP	C5-C4	2.38	1.47	1.40
2	B	382	ATP	O4'-C1'	2.33	1.44	1.41
2	C	383	ATP	O4'-C1'	2.19	1.44	1.41
2	B	382	ATP	C5-C4	2.19	1.46	1.40
2	A	381	ATP	C2-N3	2.15	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	381	ATP	PA-O3A-PB	-4.17	118.52	132.83
2	B	382	ATP	PB-O3B-PG	-4.14	118.62	132.83
2	B	382	ATP	C4-C5-N7	-3.84	105.39	109.40
2	C	383	ATP	C3'-C2'-C1'	3.84	106.76	100.98
2	D	384	ATP	N3-C2-N1	-3.84	122.67	128.68
2	D	384	ATP	PB-O3B-PG	-3.73	120.04	132.83
2	B	382	ATP	PA-O3A-PB	-3.62	120.41	132.83
2	C	383	ATP	PA-O3A-PB	-3.50	120.82	132.83
2	A	381	ATP	C4-C5-N7	-3.10	106.17	109.40
2	C	383	ATP	N3-C2-N1	-2.99	124.01	128.68
2	C	383	ATP	PB-O3B-PG	-2.87	122.97	132.83
2	B	382	ATP	C2'-C3'-C4'	2.87	108.21	102.64
2	A	381	ATP	N3-C2-N1	-2.66	124.52	128.68
2	B	382	ATP	C3'-C2'-C1'	2.63	104.94	100.98
2	C	383	ATP	C4-C5-N7	-2.58	106.71	109.40
2	D	384	ATP	PA-O3A-PB	-2.55	124.08	132.83
2	D	384	ATP	C4-C5-N7	-2.52	106.77	109.40
2	B	382	ATP	N3-C2-N1	-2.50	124.76	128.68
2	C	383	ATP	O3B-PG-O1G	-2.36	98.12	111.19
2	A	381	ATP	O2G-PG-O1G	2.20	119.29	110.68
2	D	384	ATP	C2'-C3'-C4'	2.20	106.91	102.64
2	A	381	ATP	O2B-PB-O1B	2.13	122.78	112.24
2	B	382	ATP	O3G-PG-O2G	2.12	115.73	107.64
2	D	384	ATP	C2-N1-C6	2.05	122.26	118.75
2	D	384	ATP	O2B-PB-O1B	2.04	122.33	112.24
2	D	384	ATP	O3G-PG-O2G	2.00	115.29	107.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	381	ATP	PB-O3B-PG-O2G

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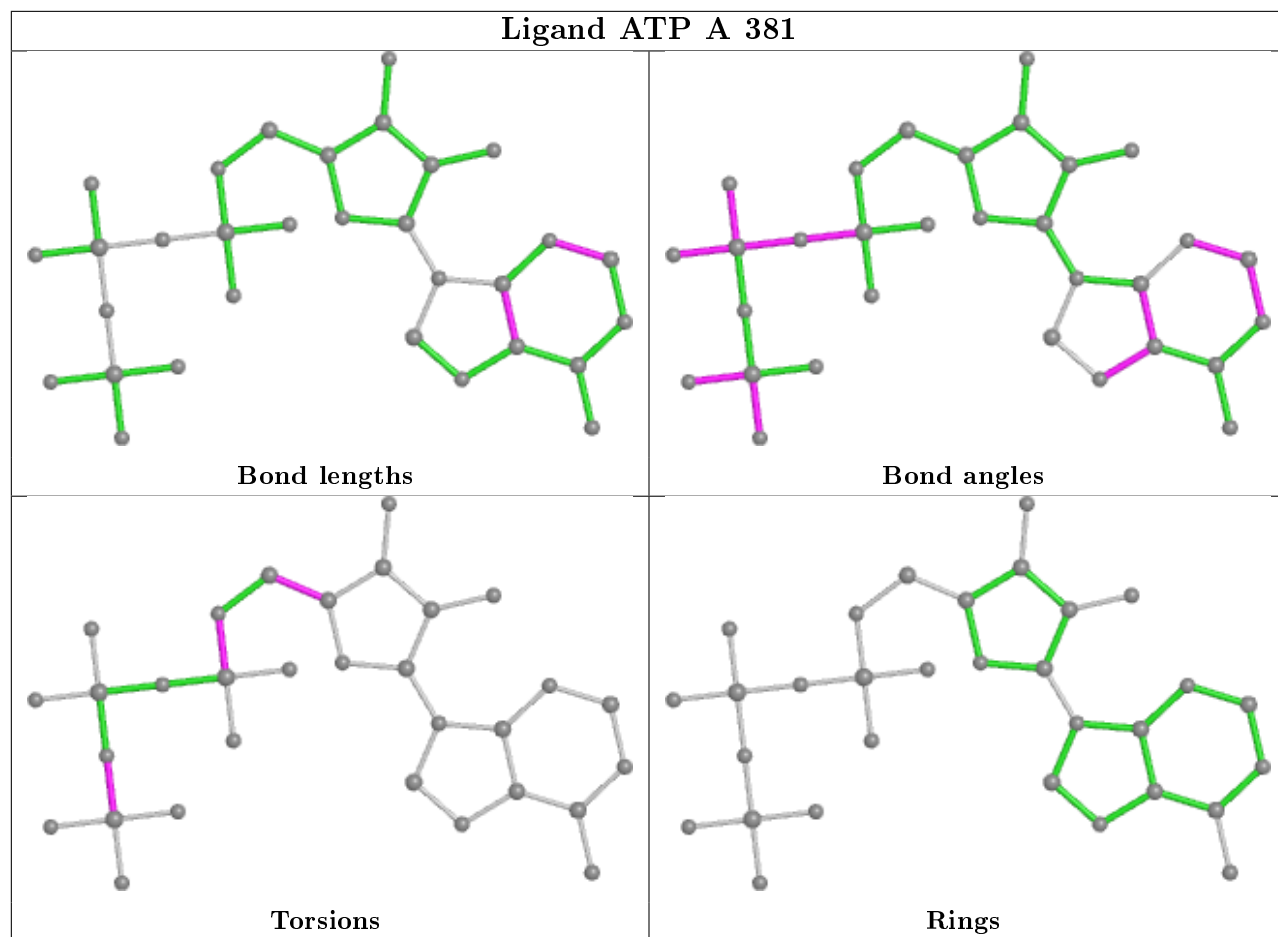
Mol	Chain	Res	Type	Atoms
2	A	381	ATP	PB-O3B-PG-O3G
2	D	384	ATP	O4'-C4'-C5'-O5'
2	C	383	ATP	O4'-C4'-C5'-O5'
2	C	383	ATP	C3'-C4'-C5'-O5'
2	D	384	ATP	C3'-C4'-C5'-O5'
2	A	381	ATP	O4'-C4'-C5'-O5'
2	A	381	ATP	C3'-C4'-C5'-O5'
2	B	382	ATP	PB-O3A-PA-O2A
2	C	383	ATP	PA-O3A-PB-O1B
2	D	384	ATP	C4'-C5'-O5'-PA
2	B	382	ATP	PG-O3B-PB-O3A
2	B	382	ATP	PA-O3A-PB-O2B
2	B	382	ATP	PG-O3B-PB-O1B
2	B	382	ATP	PA-O3A-PB-O1B
2	C	383	ATP	PA-O3A-PB-O2B
2	A	381	ATP	C5'-O5'-PA-O1A
2	A	381	ATP	PB-O3B-PG-O1G

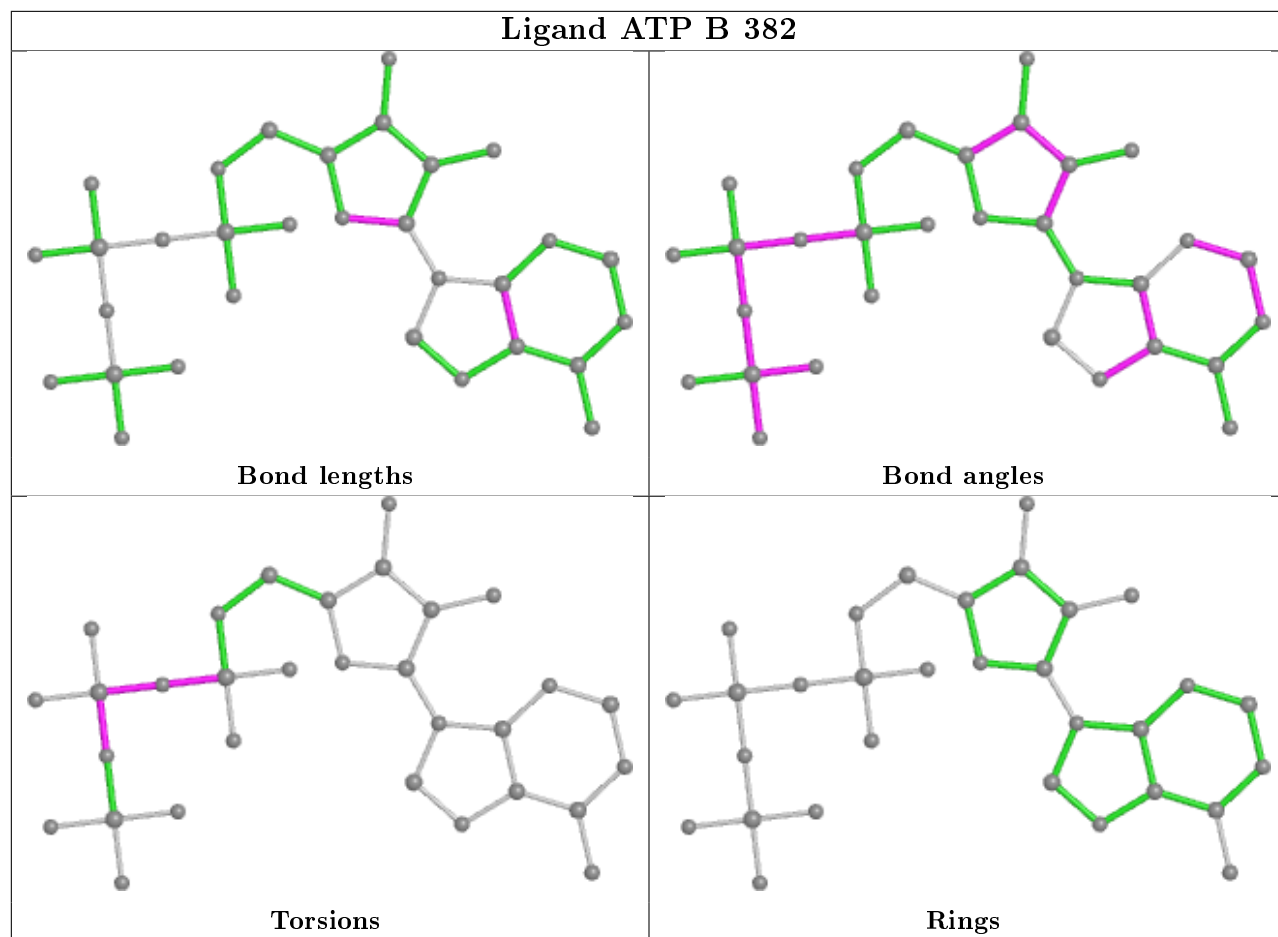
There are no ring outliers.

3 monomers are involved in 6 short contacts:

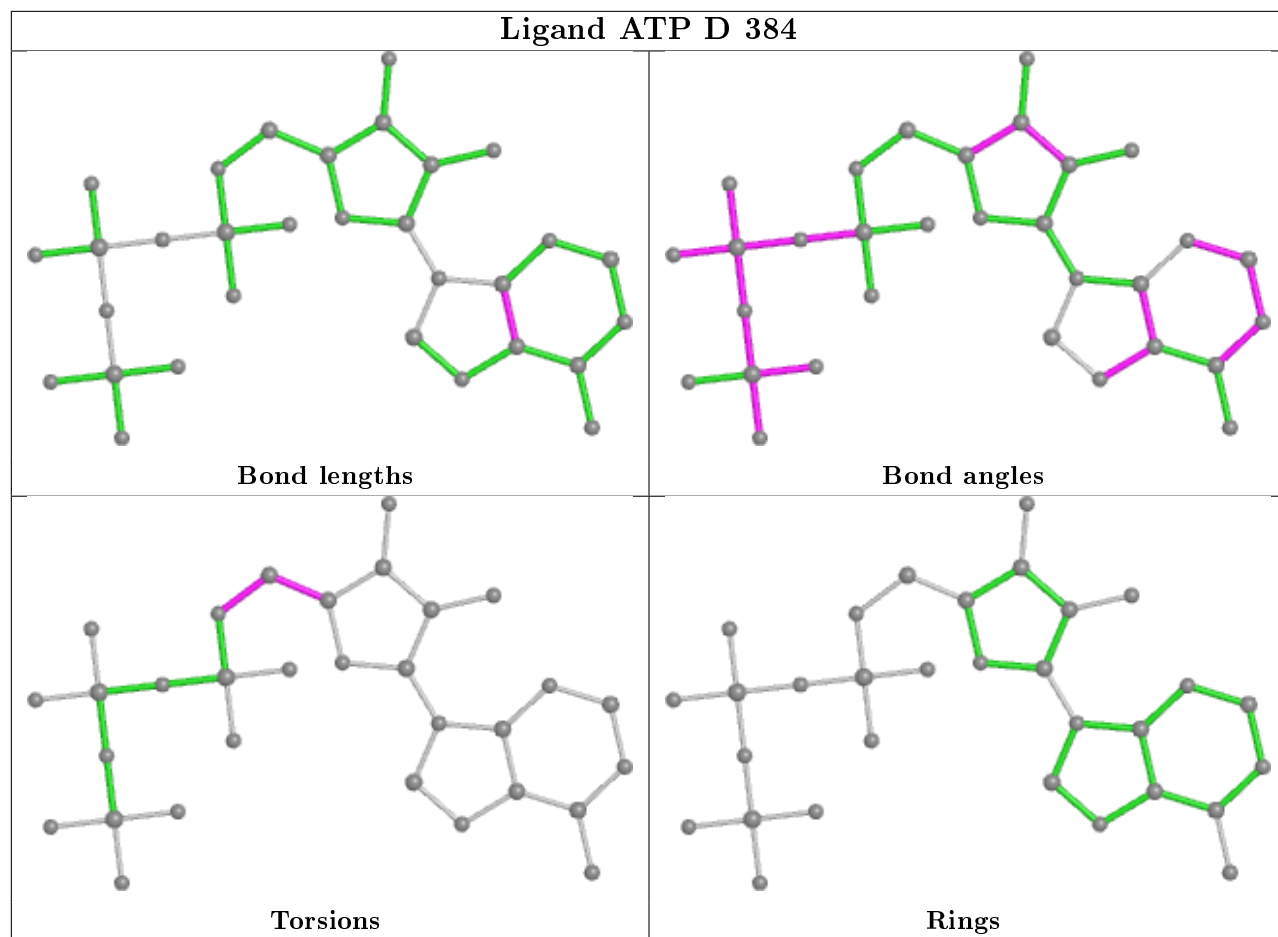
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	381	ATP	2	0
2	B	382	ATP	3	0
2	C	383	ATP	1	0

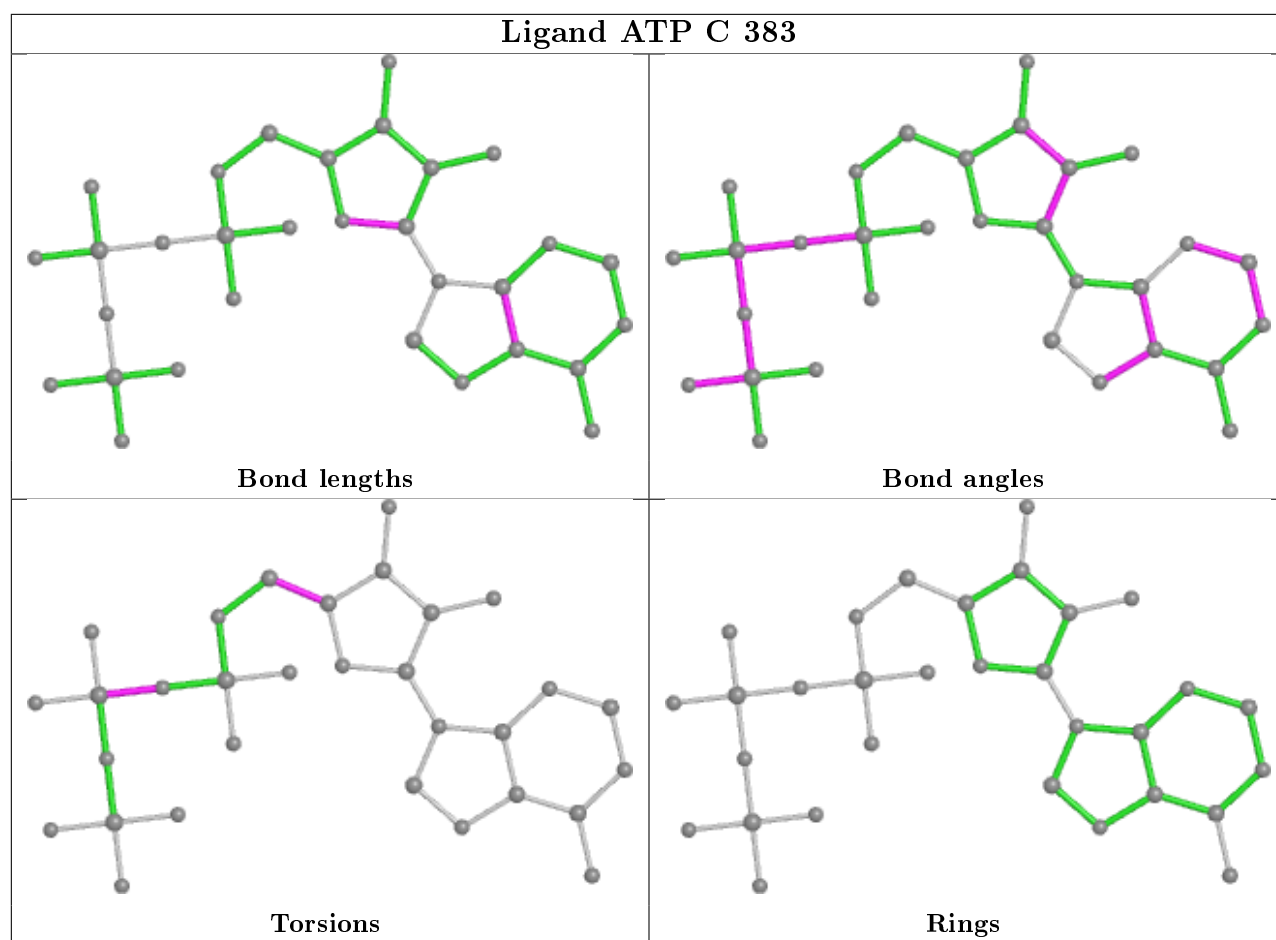
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	286/346 (82%)	-0.39	1 (0%) 94 83	18, 36, 68, 79	0
1	B	286/346 (82%)	-0.35	2 (0%) 87 68	16, 40, 74, 82	0
1	C	286/346 (82%)	-0.17	13 (4%) 33 12	20, 37, 78, 86	0
1	D	286/346 (82%)	-0.22	8 (2%) 53 24	23, 46, 79, 87	0
All	All	1144/1384 (82%)	-0.28	24 (2%) 63 34	16, 40, 74, 87	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	4.1
1	C	33	ASN	3.3
1	A	165	PRO	3.2
1	C	171	HIS	3.2
1	C	84	LYS	2.9
1	D	84	LYS	2.9
1	D	83	HIS	2.8
1	C	83	HIS	2.8
1	C	311	ASN	2.8
1	D	165	PRO	2.7
1	D	158	LEU	2.6
1	C	85	SER	2.5
1	C	104	ASP	2.5
1	C	86	ASN	2.4
1	D	82	GLY	2.3
1	C	169	TYR	2.3
1	D	57	ARG	2.3
1	C	35	ASN	2.2
1	C	13	GLU	2.1
1	D	104	ASP	2.1
1	C	167	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASP	2.1
1	B	33	ASN	2.0
1	D	162	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	D	170	11/12	0.73	0.36	74,76,84,84	0
1	TPO	C	170	11/12	0.82	0.38	76,78,83,84	0
1	TPO	B	170	11/12	0.83	0.26	71,72,77,77	0
1	TPO	A	170	11/12	0.87	0.26	64,65,66,68	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

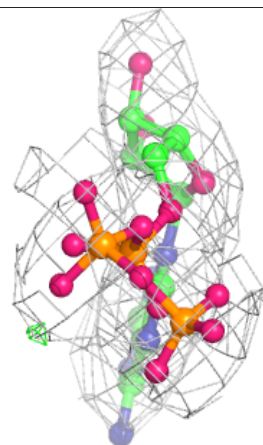
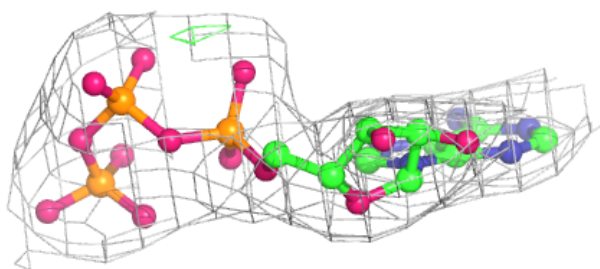
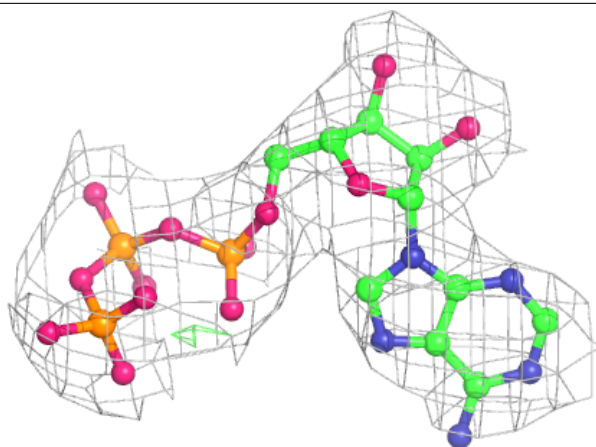
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ATP	C	383	31/31	0.94	0.15	54,59,66,66	0
2	ATP	D	384	31/31	0.95	0.21	59,65,70,70	0
2	ATP	A	381	31/31	0.96	0.12	32,35,46,47	0
2	ATP	B	382	31/31	0.96	0.17	50,57,67,68	0

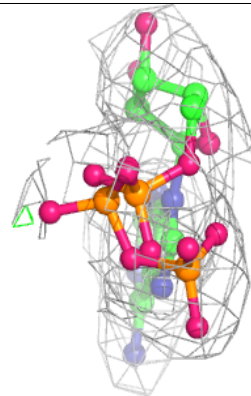
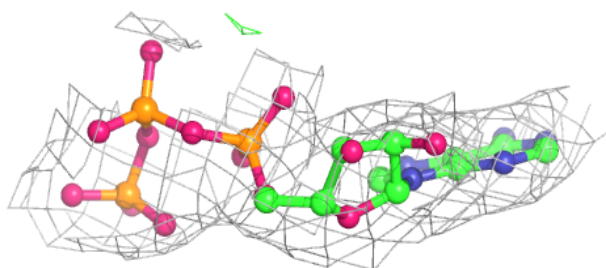
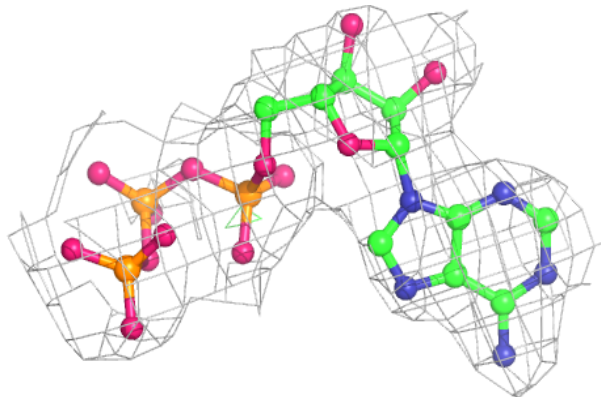
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP C 383:**

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

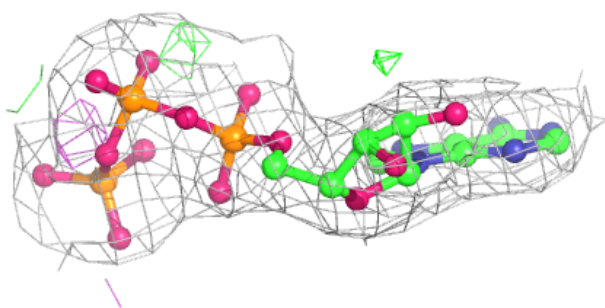
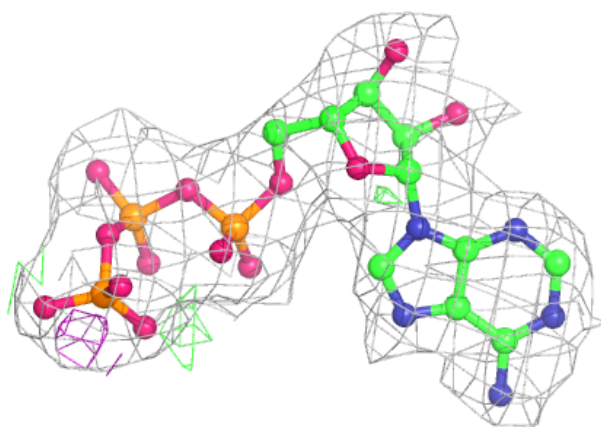
**Electron density around ATP D 384:**

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

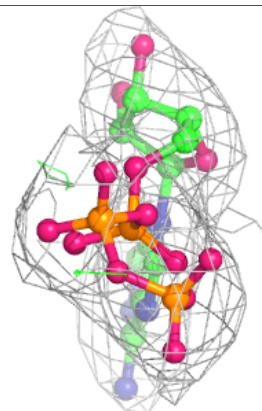
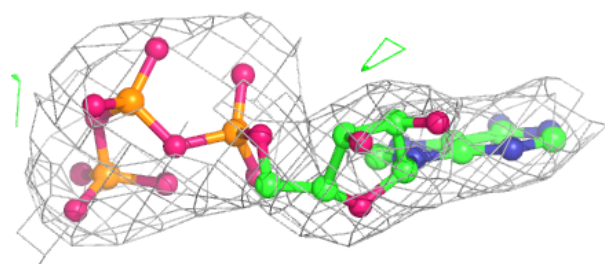
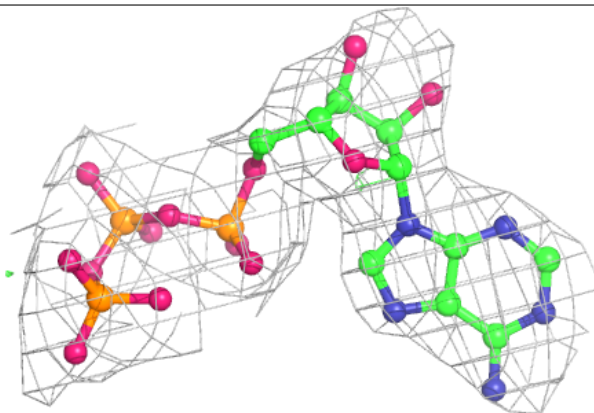


**Electron density around ATP A 381:**

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

**Electron density around ATP B 382:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.