Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:13 PM EDT

PDB ID	:	1FQ1
Title	:	CRYSTAL STRUCTURE OF KINASE ASSOCIATED PHOSPHATASE (KAP) IN COMPLEX WITH PHOSPHO-CDK2
Authors	:	Song, H.; Hanlon, N.; Brown, N.R.; Noble, M.E.M.; Johnson, L.N.; Barford, D.
Deposited on	:	2000-09-01
Resolution	:	3.00 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

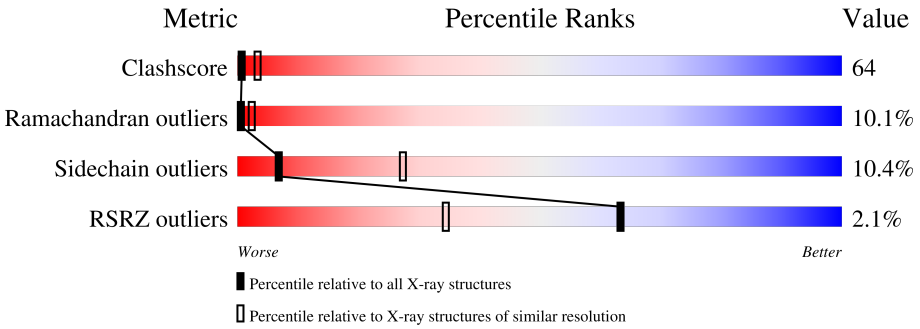
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	A	212	% 35% 39% 11% 14%
2	B	298	3% 18% 65% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3853 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 CYCLIN-DEPENDENT KINASE INHIBITOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1439	902	254	271	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	SER	CYS	ENGINEERED MUTATION	UNP Q16667

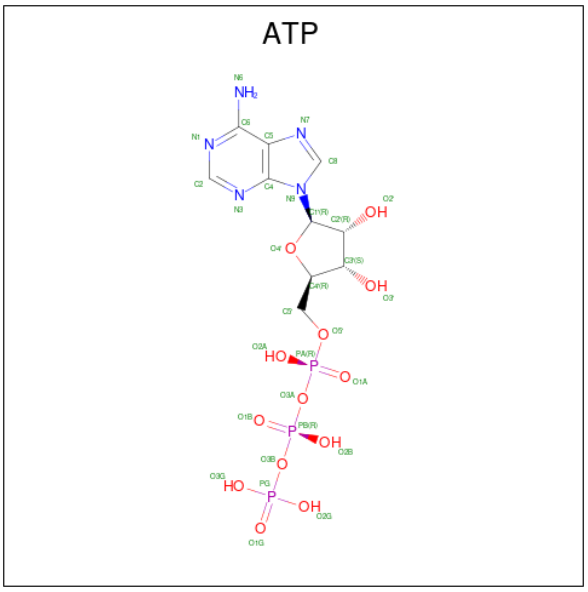
- Molecule 2 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	296	Total	C	N	O	P	S	0	0	0
			2382	1547	403	423	1	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



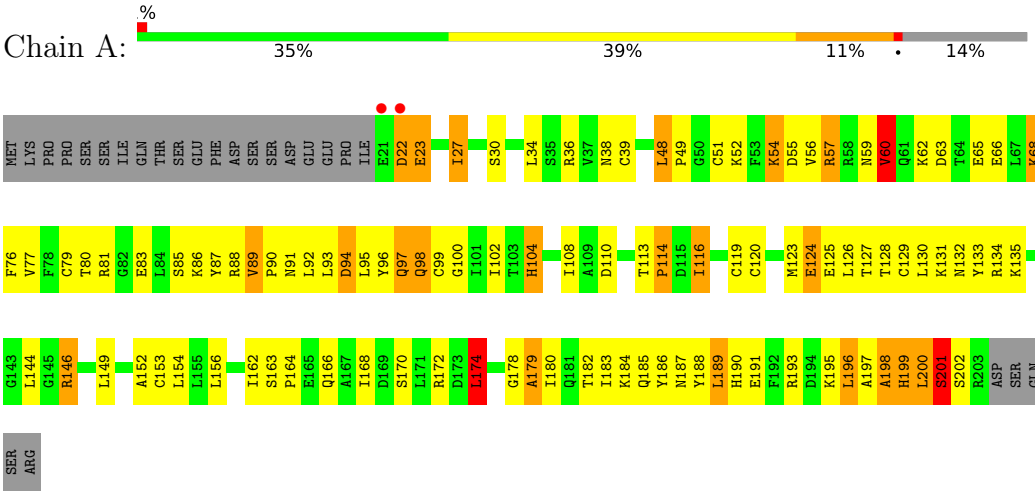
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	31	10	5	13	3	0	0

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.

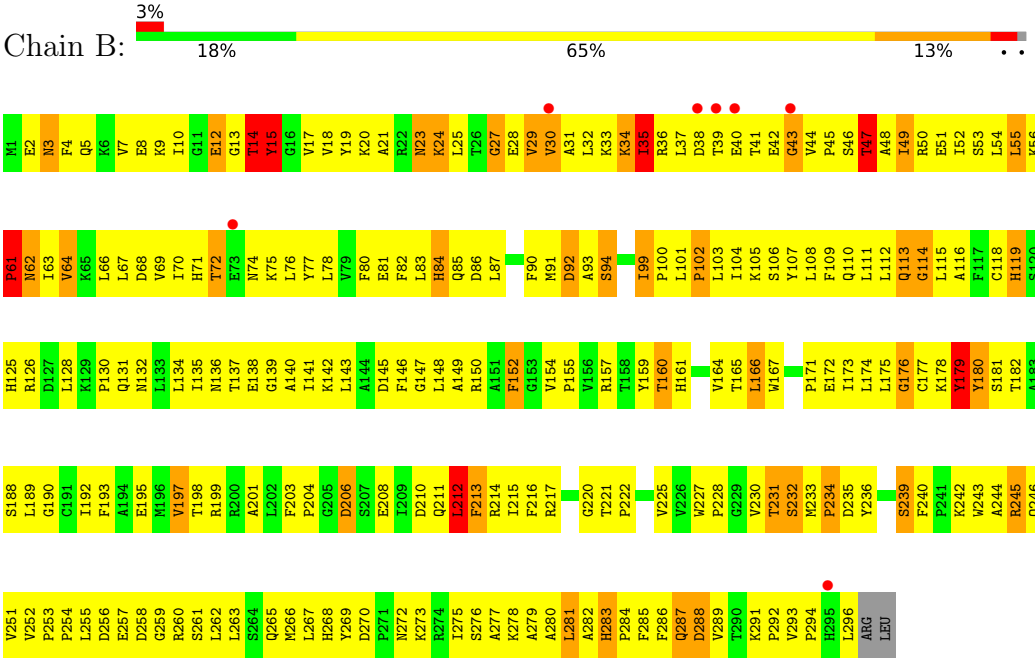
• Molecule 1: CYCLIN-DEPENDENT KINASE INHIBITOR 3

Chain A:



• Molecule 2: CELL DIVISION PROTEIN KINASE 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.45Å 134.45Å 65.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 38.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.00) 99.7 (38.81-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.313 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	87.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3853	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: TPO, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.71	0/1465	0.91	5/1979 (0.3%)
2	B	0.57	2/2432 (0.1%)	0.91	6/3300 (0.2%)
All	All	0.63	2/3897 (0.1%)	0.91	11/5279 (0.2%)

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
2	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	47	THR	C-N	-8.38	1.14	1.34
2	B	35	ILE	C-N	-6.47	1.19	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	35	ILE	O-C-N	-15.35	98.14	122.70
2	B	47	THR	C-N-CA	-11.08	93.99	121.70
2	B	35	ILE	CA-C-N	9.66	138.46	117.20
2	B	166	LEU	CA-CB-CG	5.86	128.77	115.30
2	B	212	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	174	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	23	GLU	N-CA-C	5.67	126.31	111.00
2	B	35	ILE	C-N-CA	5.25	134.84	121.70
1	A	22	ASP	N-CA-C	5.18	124.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	199	HIS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	35	ILE	Mainchain
2	B	47	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1439	0	1436	125	0
2	B	2382	0	2424	378	0
3	B	1	0	0	0	0
4	B	31	0	12	3	0
All	All	3853	0	3872	491	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 64.

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)
2:B:83:LEU:HD11	2:B:136:ASN:HB3	1.23	1.13
2:B:33:LYS:HG2	2:B:34:LYS:H	1.11	1.08
1:A:27:ILE:HD12	1:A:27:ILE:H	1.10	1.07
1:A:27:ILE:H	1:A:27:ILE:CD1	1.70	1.02
2:B:46:SER:O	2:B:48:ALA:N	1.94	1.01
2:B:46:SER:C	2:B:48:ALA:H	1.57	0.98
2:B:164:VAL:HG12	2:B:165:THR:H	1.28	0.97
2:B:31:ALA:HB2	2:B:82:PHE:HA	1.47	0.96
2:B:62:ASN:ND2	2:B:110:GLN:HB3	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:VAL:HG12	2:B:252:VAL:HG23	1.49	0.95
2:B:155:PRO:HA	2:B:179:TYR:HA	1.49	0.94
2:B:85:GLN:HG3	2:B:135:ILE:HD11	1.49	0.93
2:B:197:VAL:HG11	2:B:252:VAL:HG13	1.52	0.92
1:A:172:ARG:NE	1:A:179:ALA:HB3	1.86	0.91
1:A:27:ILE:HD12	1:A:27:ILE:N	1.85	0.91
2:B:171:PRO:O	2:B:175:LEU:HD12	1.72	0.89
1:A:141:TYR:HB3	2:B:160:TPO:HG21	1.53	0.89
1:A:27:ILE:HD13	1:A:66:GLU:HG2	1.54	0.88
2:B:106:SER:O	2:B:110:GLN:HG3	1.74	0.88
2:B:132:ASN:HD22	2:B:145:ASP:HB3	1.38	0.88
2:B:262:LEU:HD21	2:B:266:MET:SD	2.13	0.87
2:B:4:PHE:H	2:B:24:LYS:HE3	1.39	0.87
2:B:132:ASN:ND2	2:B:145:ASP:HB3	1.89	0.86
2:B:33:LYS:HG2	2:B:34:LYS:N	1.90	0.85
2:B:258:ASP:HB3	2:B:285:PHE:HB2	1.57	0.85
1:A:172:ARG:HE	1:A:179:ALA:HB3	1.43	0.84
2:B:197:VAL:HG11	2:B:252:VAL:CG1	2.08	0.83
1:A:183:ILE:HG13	2:B:208:GLU:HB2	1.60	0.83
2:B:136:ASN:HD21	2:B:140:ALA:HB3	1.40	0.83
2:B:124:LEU:HD21	2:B:152:PHE:HA	1.59	0.82
2:B:136:ASN:ND2	2:B:140:ALA:HB3	1.93	0.82
2:B:10:ILE:HD11	2:B:20:LYS:HB2	1.62	0.82
2:B:157:ARG:HD2	2:B:159:TYR:OH	1.80	0.82
2:B:253:PRO:HA	2:B:260:ARG:HH12	1.44	0.82
2:B:4:PHE:N	2:B:24:LYS:HE3	1.95	0.81
2:B:167:TRP:CZ3	2:B:204:PRO:HB3	2.15	0.80
2:B:248:PHE:HE1	2:B:263:LEU:HD23	1.46	0.80
2:B:230:VAL:HG23	2:B:231:THR:H	1.46	0.80
2:B:206:ASP:N	2:B:206:ASP:OD1	2.15	0.80
1:A:123:MET:HE1	1:A:154:LEU:N	1.98	0.79
2:B:138:GLU:O	2:B:293:VAL:HG22	1.83	0.79
1:A:123:MET:HE1	1:A:153:CYS:C	2.03	0.79
2:B:37:LEU:HD13	2:B:45:PRO:HD3	1.64	0.79
2:B:83:LEU:CD1	2:B:136:ASN:HB3	2.08	0.79
1:A:54:LYS:HZ2	2:B:15:TYR:HD1	1.31	0.78
2:B:37:LEU:O	2:B:38:ASP:HB2	1.85	0.77
2:B:34:LYS:HD3	2:B:35:ILE:N	2.00	0.77
2:B:102:PRO:HB2	2:B:292:PRO:HG2	1.65	0.77
2:B:106:SER:HB2	2:B:292:PRO:HD2	1.66	0.76
2:B:62:ASN:HD21	2:B:110:GLN:HB3	1.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:LEU:C	2:B:262:LEU:HD23	2.06	0.76
2:B:33:LYS:CG	2:B:34:LYS:H	1.95	0.76
2:B:230:VAL:O	2:B:232:SER:N	2.19	0.75
2:B:3:ASN:CG	2:B:24:LYS:HB3	2.06	0.75
2:B:109:PHE:HA	2:B:112:LEU:HD12	1.68	0.75
1:A:89:VAL:N	1:A:90:PRO:HD3	2.00	0.75
1:A:116:ILE:HD13	1:A:195:LYS:HB3	1.69	0.74
1:A:116:ILE:HD11	1:A:195:LYS:HE3	1.68	0.73
2:B:145:ASP:C	2:B:147:GLY:H	1.89	0.73
2:B:255:LEU:O	2:B:260:ARG:NH2	2.22	0.73
1:A:30:SER:HB3	1:A:174:LEU:HD22	1.70	0.73
2:B:155:PRO:HA	2:B:179:TYR:CA	2.19	0.73
2:B:246:GLN:HG2	2:B:250:LYS:HD2	1.69	0.73
1:A:123:MET:HE3	1:A:154:LEU:HA	1.71	0.72
2:B:50:ARG:HE	2:B:150:ARG:HE	1.35	0.72
1:A:110:ASP:OD2	2:B:159:TYR:HD1	1.71	0.72
2:B:52:ILE:HG23	2:B:66:LEU:HD21	1.71	0.72
1:A:183:ILE:HG13	2:B:208:GLU:CB	2.20	0.72
2:B:230:VAL:C	2:B:232:SER:H	1.92	0.71
2:B:137:THR:O	2:B:293:VAL:HG13	1.90	0.71
1:A:187:ASN:O	1:A:191:GLU:HG3	1.89	0.71
2:B:230:VAL:HG23	2:B:231:THR:N	2.06	0.71
2:B:128:LEU:HD13	2:B:189:LEU:HD21	1.72	0.70
2:B:253:PRO:CA	2:B:260:ARG:HH12	2.04	0.70
2:B:206:ASP:OD1	2:B:210:ASP:OD2	2.09	0.70
1:A:164:PRO:O	1:A:168:ILE:HG13	1.91	0.70
2:B:116:ALA:HB2	2:B:277:ALA:HB1	1.74	0.70
2:B:195:GLU:CD	2:B:201:ALA:HA	2.13	0.70
2:B:258:ASP:HB3	2:B:285:PHE:CB	2.20	0.69
2:B:67:LEU:HD11	2:B:81:GLU:HA	1.72	0.69
2:B:108:LEU:HG	2:B:112:LEU:HD11	1.75	0.69
1:A:48:LEU:HB3	1:A:51:CYS:HB2	1.75	0.69
2:B:248:PHE:CE1	2:B:263:LEU:HD23	2.28	0.69
1:A:73:GLN:HE21	1:A:135:LYS:H	1.42	0.68
2:B:195:GLU:OE1	2:B:201:ALA:HA	1.94	0.68
2:B:181:SER:O	2:B:184:VAL:HG22	1.94	0.67
2:B:278:LYS:HA	2:B:281:LEU:HD12	1.76	0.67
2:B:112:LEU:HD22	2:B:280:ALA:HB1	1.75	0.67
2:B:138:GLU:HA	2:B:293:VAL:HG13	1.76	0.67
2:B:212:LEU:HD22	2:B:216:PHE:CE1	2.30	0.67
2:B:184:VAL:HG23	2:B:185:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:HD13	1:A:66:GLU:CG	2.23	0.67
2:B:262:LEU:HD23	2:B:263:LEU:N	2.10	0.67
2:B:46:SER:C	2:B:48:ALA:N	2.22	0.67
2:B:165:THR:HG22	2:B:167:TRP:CD1	2.29	0.66
1:A:30:SER:HB3	1:A:174:LEU:CD2	2.25	0.66
2:B:23:ASN:C	2:B:25:LEU:H	1.99	0.66
2:B:48:ALA:O	2:B:52:ILE:HG13	1.94	0.66
2:B:69:VAL:C	2:B:70:ILE:HD12	2.16	0.66
2:B:50:ARG:HH21	2:B:150:ARG:NE	1.93	0.66
1:A:80:THR:OG1	1:A:83:GLU:HG3	1.96	0.65
2:B:220:GLY:HA2	2:B:243:TRP:O	1.97	0.65
2:B:37:LEU:HD22	2:B:45:PRO:HD3	1.78	0.65
1:A:196:LEU:HD22	1:A:196:LEU:O	1.97	0.65
2:B:105:LYS:HE2	2:B:285:PHE:CZ	2.31	0.65
2:B:128:LEU:HD13	2:B:189:LEU:CD2	2.27	0.65
1:A:114:PRO:HG2	1:A:119:CYS:HB2	1.79	0.65
2:B:164:VAL:HG12	2:B:165:THR:N	2.07	0.65
2:B:50:ARG:NE	2:B:150:ARG:HE	1.96	0.64
2:B:84:HIS:CE1	2:B:296:LEU:HD22	2.32	0.64
1:A:86:LYS:O	1:A:86:LYS:HG3	1.98	0.64
2:B:204:PRO:O	2:B:214:ARG:NE	2.31	0.64
2:B:256:ASP:O	2:B:260:ARG:HB2	1.98	0.64
2:B:66:LEU:HG	2:B:66:LEU:O	1.99	0.63
2:B:10:ILE:HD11	2:B:20:LYS:CB	2.28	0.63
2:B:164:VAL:CG1	2:B:165:THR:H	2.09	0.63
2:B:212:LEU:O	2:B:215:ILE:N	2.31	0.63
2:B:228:PRO:HD2	2:B:270:ASP:OD2	1.98	0.63
1:A:200:LEU:HD23	1:A:201:SER:N	2.14	0.63
2:B:33:LYS:HE3	2:B:80:PHE:CE1	2.34	0.63
2:B:125:HIS:O	2:B:126:ARG:HB2	1.98	0.63
2:B:60:HIS:ND1	2:B:61:PRO:HD2	2.13	0.62
2:B:213:PHE:HD1	2:B:213:PHE:H	1.47	0.62
1:A:141:TYR:CD1	1:A:142:GLY:N	2.68	0.62
1:A:91:ASN:ND2	1:A:95:LEU:HG	2.15	0.62
2:B:37:LEU:HD13	2:B:45:PRO:CD	2.29	0.61
2:B:30:VAL:HG13	2:B:32:LEU:H	1.65	0.61
2:B:116:ALA:HB2	2:B:277:ALA:CB	2.30	0.61
2:B:227:TRP:CE3	2:B:269:TYR:HB3	2.34	0.61
2:B:68:ASP:CG	2:B:69:VAL:H	2.03	0.61
1:A:198:ALA:C	1:A:200:LEU:H	2.03	0.61
1:A:68:LYS:NZ	1:A:99:CYS:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HA	1:A:90:PRO:HG3	1.82	0.61
2:B:157:ARG:NE	2:B:159:TYR:HE2	1.99	0.61
2:B:39:THR:HG22	2:B:40:GLU:N	2.15	0.60
2:B:248:PHE:HA	2:B:251:VAL:HB	1.83	0.60
2:B:280:ALA:O	2:B:282:ALA:N	2.34	0.60
2:B:68:ASP:OD1	2:B:69:VAL:N	2.33	0.60
2:B:280:ALA:C	2:B:282:ALA:H	2.05	0.60
1:A:141:TYR:HB3	2:B:160:TPO:CG2	2.27	0.60
2:B:92:ASP:O	2:B:94:SER:N	2.34	0.60
1:A:200:LEU:O	1:A:202:SER:N	2.35	0.60
2:B:82:PHE:CE2	2:B:84:HIS:N	2.70	0.60
2:B:270:ASP:OD1	2:B:272:ASN:HB3	2.03	0.59
2:B:21:ALA:O	2:B:30:VAL:HB	2.02	0.59
2:B:176:GLY:O	2:B:234:PRO:HD2	2.03	0.59
1:A:91:ASN:O	1:A:94:ASP:N	2.36	0.59
2:B:113:GLN:N	2:B:281:LEU:HD21	2.18	0.59
2:B:253:PRO:HA	2:B:260:ARG:NH1	2.15	0.59
2:B:10:ILE:HD12	2:B:10:ILE:H	1.67	0.59
2:B:188:SER:O	2:B:192:ILE:HG13	2.03	0.58
2:B:296:LEU:HD12	2:B:296:LEU:N	2.18	0.58
1:A:127:THR:HG22	1:A:131:LYS:HD3	1.85	0.58
2:B:101:LEU:N	2:B:102:PRO:HD2	2.19	0.58
1:A:123:MET:CE	1:A:154:LEU:HA	2.33	0.58
2:B:10:ILE:HD11	2:B:20:LYS:CA	2.33	0.58
2:B:32:LEU:O	2:B:32:LEU:HD23	2.04	0.58
2:B:52:ILE:CG2	2:B:66:LEU:HD21	2.34	0.58
2:B:50:ARG:HG2	2:B:54:LEU:HD23	1.85	0.57
2:B:51:GLU:O	2:B:55:LEU:HD23	2.04	0.57
2:B:132:ASN:ND2	2:B:145:ASP:CB	2.65	0.57
2:B:105:LYS:HG3	2:B:285:PHE:CE2	2.39	0.57
2:B:126:ARG:NH2	2:B:150:ARG:HG3	2.18	0.57
2:B:41:THR:HG22	2:B:42:GLU:N	2.20	0.57
2:B:252:VAL:HG12	2:B:252:VAL:O	2.04	0.57
2:B:50:ARG:HH12	2:B:148:LEU:CA	2.16	0.57
1:A:27:ILE:HD13	1:A:66:GLU:CB	2.34	0.57
1:A:52:LYS:NZ	1:A:88:ARG:HB2	2.19	0.57
2:B:108:LEU:O	2:B:111:LEU:HB2	2.05	0.57
1:A:146:ARG:N	2:B:160:TPO:O3P	2.36	0.57
2:B:51:GLU:HG3	2:B:146:PHE:C	2.24	0.57
2:B:136:ASN:CG	2:B:140:ALA:HB3	2.24	0.57
1:A:95:LEU:O	1:A:99:CYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:ASP:HB3	2:B:273:LYS:HB2	1.87	0.56
2:B:268:HIS:HD2	2:B:269:TYR:N	2.03	0.56
2:B:31:ALA:HB2	2:B:82:PHE:CA	2.29	0.56
2:B:81:GLU:OE1	2:B:142:LYS:NZ	2.37	0.56
2:B:99:ILE:HG22	2:B:100:PRO:HD2	1.87	0.56
2:B:17:VAL:HG21	2:B:19:TYR:CZ	2.41	0.56
1:A:27:ILE:HG13	1:A:63:ASP:OD1	2.06	0.56
2:B:109:PHE:HD1	2:B:286:PHE:CD1	2.23	0.56
2:B:3:ASN:OD1	2:B:24:LYS:HB3	2.06	0.56
2:B:48:ALA:O	2:B:51:GLU:N	2.38	0.56
2:B:70:ILE:HD12	2:B:70:ILE:N	2.21	0.56
2:B:82:PHE:CD2	2:B:83:LEU:N	2.74	0.56
2:B:167:TRP:CE3	2:B:204:PRO:HA	2.41	0.56
1:A:180:ILE:HG22	1:A:185:GLN:HE21	1.71	0.55
1:A:94:ASP:HA	1:A:97:GLN:HB2	1.88	0.55
2:B:193:PHE:CD2	2:B:263:LEU:HD13	2.42	0.55
2:B:63:ILE:O	2:B:64:VAL:C	2.44	0.55
2:B:252:VAL:HG12	2:B:255:LEU:HB2	1.87	0.55
2:B:288:ASP:OD2	2:B:288:ASP:N	2.33	0.55
1:A:89:VAL:N	1:A:90:PRO:CD	2.66	0.55
2:B:62:ASN:HD22	2:B:110:GLN:HB3	1.66	0.55
2:B:113:GLN:CA	2:B:281:LEU:HD21	2.37	0.55
2:B:222:PRO:HB3	2:B:269:TYR:CD2	2.41	0.55
1:A:149:LEU:CD1	1:A:189:LEU:HD13	2.37	0.55
1:A:104:HIS:N	1:A:104:HIS:CD2	2.75	0.55
2:B:261:SER:O	2:B:265:GLN:HG3	2.06	0.55
2:B:222:PRO:HB3	2:B:269:TYR:CE2	2.42	0.55
1:A:60:VAL:HG13	1:A:89:VAL:HG12	1.88	0.54
1:A:149:LEU:HD12	1:A:189:LEU:HD13	1.90	0.54
2:B:3:ASN:HA	2:B:24:LYS:CE	2.37	0.54
2:B:231:THR:HA	2:B:236:TYR:CD2	2.43	0.54
2:B:50:ARG:HD3	2:B:149:ALA:O	2.08	0.54
2:B:51:GLU:O	2:B:55:LEU:HB2	2.06	0.54
2:B:230:VAL:C	2:B:232:SER:N	2.59	0.54
1:A:163:SER:O	1:A:166:GLN:N	2.40	0.54
2:B:50:ARG:NH1	2:B:149:ALA:N	2.57	0.53
2:B:87:LEU:HG	2:B:91:MET:HG3	1.90	0.53
2:B:60:HIS:CG	2:B:61:PRO:HD2	2.43	0.53
1:A:186:TYR:CZ	1:A:190:HIS:CE1	2.97	0.53
2:B:12:GLU:O	2:B:12:GLU:HG2	2.07	0.53
2:B:20:LYS:HG2	2:B:21:ALA:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:CG1	2:B:32:LEU:H	2.21	0.53
2:B:100:PRO:C	2:B:102:PRO:HD2	2.29	0.53
2:B:105:LYS:HE2	2:B:285:PHE:CE2	2.43	0.53
2:B:165:THR:O	2:B:166:LEU:HB2	2.08	0.53
2:B:190:GLY:HA3	2:B:267:LEU:CD2	2.39	0.53
2:B:262:LEU:CD2	2:B:263:LEU:N	2.71	0.53
1:A:80:THR:O	1:A:83:GLU:N	2.42	0.53
2:B:62:ASN:OD1	2:B:62:ASN:N	2.42	0.53
2:B:222:PRO:HD3	2:B:269:TYR:CZ	2.44	0.53
1:A:68:LYS:NZ	1:A:100:GLY:HA3	2.24	0.53
1:A:184:LYS:NZ	2:B:235:ASP:OD2	2.40	0.53
2:B:64:VAL:HG23	2:B:143:LEU:O	2.09	0.52
2:B:106:SER:CB	2:B:292:PRO:HD2	2.36	0.52
2:B:23:ASN:O	2:B:25:LEU:N	2.42	0.52
2:B:83:LEU:O	2:B:83:LEU:HG	2.09	0.52
2:B:186:ILE:HG22	2:B:186:ILE:O	2.08	0.52
1:A:91:ASN:O	1:A:92:LEU:C	2.48	0.52
2:B:112:LEU:HD22	2:B:280:ALA:CB	2.38	0.52
2:B:262:LEU:C	2:B:262:LEU:CD2	2.78	0.52
2:B:258:ASP:HB3	2:B:285:PHE:CA	2.40	0.52
2:B:52:ILE:O	2:B:56:LYS:HG2	2.09	0.52
2:B:152:PHE:HD1	2:B:152:PHE:H	1.58	0.52
1:A:88:ARG:C	1:A:90:PRO:HD3	2.30	0.52
2:B:66:LEU:HD13	2:B:80:PHE:CE2	2.45	0.52
2:B:173:ILE:HG12	2:B:180:TYR:CD1	2.45	0.52
2:B:280:ALA:C	2:B:282:ALA:N	2.62	0.52
2:B:124:LEU:CD2	2:B:152:PHE:HA	2.35	0.52
2:B:172:GLU:HG2	2:B:173:ILE:HD12	1.92	0.52
2:B:259:GLY:N	2:B:285:PHE:CD1	2.78	0.52
2:B:119:HIS:CD2	2:B:182:THR:HB	2.46	0.51
2:B:253:PRO:C	2:B:255:LEU:H	2.13	0.51
2:B:289:VAL:O	2:B:289:VAL:HG13	2.10	0.51
2:B:136:ASN:OD1	2:B:140:ALA:HB3	2.10	0.51
2:B:227:TRP:HZ2	2:B:233:MET:HE1	1.75	0.51
1:A:193:ARG:HG3	1:A:193:ARG:HH11	1.74	0.51
2:B:3:ASN:OD1	2:B:3:ASN:O	2.28	0.51
2:B:62:ASN:ND2	2:B:110:GLN:CB	2.67	0.51
2:B:173:ILE:HG12	2:B:180:TYR:HD1	1.75	0.51
2:B:193:PHE:HD2	2:B:263:LEU:HD13	1.74	0.51
2:B:227:TRP:CG	2:B:230:VAL:HG13	2.46	0.51
1:A:27:ILE:HD11	1:A:63:ASP:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:C	2:B:260:ARG:NH2	2.64	0.51
1:A:152:ALA:CB	1:A:189:LEU:HD21	2.41	0.51
2:B:189:LEU:N	2:B:189:LEU:HD22	2.25	0.51
2:B:68:ASP:CG	2:B:69:VAL:N	2.65	0.50
2:B:87:LEU:O	2:B:91:MET:HG3	2.11	0.50
2:B:157:ARG:CZ	2:B:159:TYR:HE2	2.24	0.50
1:A:76:PHE:CE1	1:A:126:LEU:HD23	2.46	0.50
1:A:80:THR:O	1:A:81:ARG:C	2.48	0.50
2:B:167:TRP:CH2	2:B:204:PRO:HB3	2.46	0.50
2:B:55:LEU:O	2:B:58:LEU:O	2.30	0.50
2:B:103:LEU:HD21	2:B:294:PRO:HB3	1.94	0.50
2:B:113:GLN:O	2:B:114:GLY:C	2.50	0.50
2:B:34:LYS:HD3	2:B:34:LYS:C	2.32	0.50
2:B:61:PRO:O	2:B:142:LYS:HE2	2.12	0.50
2:B:184:VAL:HG23	2:B:185:ASP:N	2.27	0.50
2:B:195:GLU:CG	2:B:201:ALA:HA	2.42	0.50
2:B:113:GLN:O	2:B:115:LEU:N	2.45	0.50
2:B:195:GLU:HG3	2:B:201:ALA:HA	1.93	0.50
2:B:212:LEU:O	2:B:214:ARG:N	2.44	0.50
1:A:52:LYS:HA	1:A:56:VAL:O	2.12	0.50
1:A:141:TYR:HD1	1:A:142:GLY:N	2.09	0.50
2:B:119:HIS:NE2	2:B:182:THR:HB	2.27	0.50
2:B:134:LEU:O	2:B:141:ILE:HG13	2.12	0.50
1:A:178:GLY:O	1:A:179:ALA:O	2.30	0.50
1:A:200:LEU:HD23	1:A:201:SER:H	1.76	0.50
2:B:41:THR:HG23	2:B:42:GLU:OE1	2.12	0.50
2:B:198:THR:O	2:B:199:ARG:HB2	2.12	0.50
2:B:247:ASP:OD2	2:B:249:SER:CB	2.60	0.49
2:B:213:PHE:HD1	2:B:213:PHE:N	2.09	0.49
2:B:124:LEU:HD13	2:B:182:THR:HG22	1.94	0.49
1:A:94:ASP:O	1:A:95:LEU:C	2.50	0.49
2:B:3:ASN:HA	2:B:24:LYS:NZ	2.28	0.49
2:B:213:PHE:N	2:B:213:PHE:CD1	2.78	0.49
2:B:204:PRO:HG2	2:B:214:ARG:CZ	2.43	0.49
2:B:257:GLU:HA	2:B:257:GLU:OE1	2.13	0.49
1:A:87:TYR:CZ	1:A:141:TYR:CD2	3.00	0.49
2:B:29:VAL:O	2:B:30:VAL:HB	2.12	0.49
2:B:48:ALA:O	2:B:49:ILE:C	2.51	0.48
2:B:107:TYR:CD1	2:B:141:ILE:HB	2.49	0.48
2:B:139:GLY:HA2	2:B:294:PRO:HD3	1.95	0.48
2:B:230:VAL:HG23	2:B:231:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:HB1	1:A:189:LEU:HD21	1.96	0.48
2:B:139:GLY:CA	2:B:294:PRO:HD3	2.44	0.48
1:A:102:ILE:HD12	1:A:102:ILE:H	1.78	0.48
1:A:102:ILE:HD13	1:A:134:ARG:HH11	1.79	0.48
2:B:189:LEU:O	2:B:190:GLY:C	2.50	0.48
1:A:91:ASN:ND2	1:A:95:LEU:CG	2.76	0.48
2:B:227:TRP:CZ2	2:B:233:MET:CE	2.97	0.48
1:A:197:ALA:O	1:A:200:LEU:N	2.47	0.48
2:B:60:HIS:CE1	2:B:61:PRO:HD2	2.48	0.48
2:B:66:LEU:HD13	2:B:80:PHE:HE2	1.79	0.47
2:B:107:TYR:O	2:B:111:LEU:HG	2.14	0.47
1:A:108:ILE:HG12	1:A:114:PRO:HB3	1.97	0.47
1:A:162:ILE:HG13	1:A:166:GLN:HE21	1.78	0.47
1:A:180:ILE:CG2	1:A:185:GLN:HB3	2.44	0.47
2:B:23:ASN:N	2:B:27:GLY:HA2	2.29	0.47
2:B:8:GLU:HG2	2:B:9:LYS:N	2.29	0.47
2:B:121:HIS:O	2:B:122:ARG:HB2	2.15	0.47
2:B:247:ASP:OD2	2:B:249:SER:HB3	2.15	0.47
2:B:39:THR:HG22	2:B:40:GLU:H	1.79	0.47
2:B:282:ALA:O	2:B:283:HIS:O	2.32	0.47
2:B:20:LYS:HG3	2:B:82:PHE:CE1	2.50	0.47
1:A:52:LYS:HA	1:A:57:ARG:HA	1.97	0.47
2:B:32:LEU:HD23	2:B:32:LEU:C	2.35	0.47
2:B:197:VAL:CG1	2:B:252:VAL:HG13	2.34	0.47
2:B:222:PRO:HD3	2:B:269:TYR:OH	2.14	0.47
2:B:230:VAL:CG2	2:B:231:THR:H	2.23	0.47
1:A:163:SER:OG	1:A:166:GLN:HG3	2.15	0.47
2:B:82:PHE:HE2	2:B:84:HIS:HA	1.79	0.47
2:B:253:PRO:N	2:B:254:PRO:CD	2.78	0.47
2:B:284:PRO:O	2:B:287:GLN:HB2	2.13	0.47
2:B:111:LEU:O	2:B:112:LEU:C	2.53	0.47
1:A:116:ILE:CD1	1:A:195:LYS:HE3	2.40	0.47
2:B:23:ASN:HB3	2:B:27:GLY:CA	2.44	0.47
2:B:145:ASP:C	2:B:147:GLY:N	2.58	0.47
2:B:13:GLY:O	2:B:14:THR:C	2.54	0.46
2:B:145:ASP:HB2	4:B:381:ATP:O2A	2.15	0.46
2:B:217:ARG:HD2	2:B:243:TRP:CE2	2.50	0.46
2:B:239:SER:O	2:B:240:PHE:C	2.53	0.46
2:B:268:HIS:CD2	2:B:269:TYR:N	2.83	0.46
2:B:259:GLY:N	2:B:285:PHE:HD1	2.13	0.46
2:B:37:LEU:CD1	2:B:45:PRO:HD3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:VAL:N	2:B:253:PRO:HD3	2.30	0.46
2:B:37:LEU:HD12	2:B:41:THR:HG21	1.97	0.46
2:B:104:ILE:O	2:B:107:TYR:HB2	2.16	0.46
2:B:56:LYS:O	2:B:57:GLU:C	2.54	0.46
2:B:60:HIS:HB3	2:B:63:ILE:HD12	1.97	0.46
2:B:180:TYR:N	2:B:180:TYR:CD2	2.83	0.46
2:B:252:VAL:O	2:B:260:ARG:NH1	2.49	0.46
2:B:118:CYS:O	2:B:119:HIS:C	2.53	0.46
1:A:163:SER:O	1:A:166:GLN:HB2	2.16	0.46
2:B:23:ASN:HB3	2:B:27:GLY:N	2.31	0.46
2:B:123:VAL:HG12	2:B:124:LEU:N	2.31	0.46
2:B:230:VAL:CG2	2:B:231:THR:N	2.76	0.46
2:B:3:ASN:HD21	2:B:25:LEU:CD2	2.28	0.46
2:B:138:GLU:C	2:B:293:VAL:HG22	2.36	0.46
2:B:84:HIS:ND1	2:B:296:LEU:HD22	2.31	0.45
2:B:122:ARG:C	2:B:152:PHE:CD1	2.90	0.45
2:B:60:HIS:CD2	2:B:114:GLY:HA2	2.52	0.45
2:B:104:ILE:HG22	2:B:105:LYS:N	2.30	0.45
2:B:122:ARG:HA	2:B:152:PHE:CE1	2.51	0.45
2:B:216:PHE:N	2:B:216:PHE:HD1	2.14	0.45
1:A:92:LEU:HD11	1:A:96:TYR:CZ	2.52	0.45
2:B:44:VAL:HG12	2:B:45:PRO:N	2.31	0.45
2:B:186:ILE:HG21	2:B:275:ILE:O	2.16	0.45
2:B:216:PHE:N	2:B:216:PHE:CD1	2.83	0.45
2:B:50:ARG:HE	2:B:150:ARG:NE	2.11	0.45
2:B:50:ARG:HH12	2:B:147:GLY:C	2.20	0.45
2:B:109:PHE:CA	2:B:112:LEU:HD12	2.44	0.45
2:B:37:LEU:HD12	2:B:41:THR:CG2	2.47	0.45
1:A:120:CYS:O	1:A:124:GLU:HG3	2.17	0.45
2:B:41:THR:CG2	2:B:42:GLU:N	2.79	0.45
2:B:102:PRO:HG2	2:B:103:LEU:H	1.82	0.45
2:B:189:LEU:CD2	2:B:189:LEU:N	2.80	0.45
2:B:50:ARG:NH2	2:B:150:ARG:NE	2.64	0.45
1:A:34:LEU:HB2	1:A:39:CYS:HB3	1.99	0.45
2:B:54:LEU:O	2:B:58:LEU:HB2	2.17	0.45
1:A:73:GLN:NE2	1:A:134:ARG:HA	2.32	0.45
2:B:33:LYS:HE2	4:B:381:ATP:O1A	2.17	0.45
2:B:109:PHE:CD1	2:B:286:PHE:CD1	3.05	0.45
1:A:172:ARG:CD	1:A:179:ALA:HB3	2.46	0.44
2:B:186:ILE:O	2:B:186:ILE:CG2	2.64	0.44
2:B:277:ALA:O	2:B:280:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HA	1:A:69:SER:HB3	1.99	0.44
2:B:23:ASN:C	2:B:25:LEU:N	2.67	0.44
2:B:67:LEU:HD12	2:B:80:PHE:O	2.17	0.44
2:B:227:TRP:CZ2	2:B:233:MET:HE1	2.51	0.44
2:B:291:LYS:O	2:B:292:PRO:C	2.56	0.44
2:B:43:GLY:O	2:B:44:VAL:HB	2.18	0.44
2:B:109:PHE:HA	2:B:112:LEU:CD1	2.44	0.44
2:B:190:GLY:O	2:B:193:PHE:HB3	2.17	0.44
2:B:190:GLY:HA3	2:B:267:LEU:HD23	2.00	0.44
1:A:52:LYS:HA	1:A:57:ARG:HG3	1.99	0.44
1:A:180:ILE:N	1:A:180:ILE:HD13	2.33	0.44
2:B:50:ARG:HH21	2:B:150:ARG:CD	2.30	0.44
2:B:66:LEU:O	2:B:66:LEU:CG	2.63	0.44
2:B:177:CYS:SG	2:B:177:CYS:O	2.75	0.44
2:B:197:VAL:HG12	2:B:198:THR:N	2.32	0.44
2:B:221:THR:CB	2:B:242:LYS:HA	2.48	0.44
2:B:262:LEU:HD23	2:B:266:MET:HB2	1.98	0.44
1:A:197:ALA:O	1:A:200:LEU:HB3	2.18	0.44
1:A:197:ALA:C	1:A:199:HIS:N	2.71	0.44
2:B:82:PHE:HE2	2:B:84:HIS:H	1.58	0.44
1:A:51:CYS:O	1:A:57:ARG:HA	2.17	0.44
2:B:24:LYS:O	2:B:24:LYS:HG2	2.18	0.44
2:B:62:ASN:ND2	2:B:110:GLN:O	2.50	0.44
2:B:105:LYS:HG3	2:B:285:PHE:HE2	1.82	0.44
2:B:71:HIS:O	2:B:72:THR:C	2.56	0.43
2:B:253:PRO:C	2:B:255:LEU:N	2.70	0.43
2:B:136:ASN:HD21	2:B:140:ALA:CB	2.19	0.43
2:B:253:PRO:O	2:B:255:LEU:N	2.50	0.43
2:B:275:ILE:HD11	2:B:279:ALA:C	2.38	0.43
2:B:275:ILE:HG13	2:B:279:ALA:HB3	2.00	0.43
1:A:59:ASN:HB3	1:A:62:LYS:HB2	2.01	0.43
1:A:77:VAL:HG12	1:A:79:CYS:H	1.84	0.43
2:B:139:GLY:N	2:B:294:PRO:HD2	2.33	0.43
2:B:167:TRP:CZ3	2:B:204:PRO:CB	2.97	0.43
2:B:212:LEU:O	2:B:213:PHE:C	2.57	0.43
2:B:214:ARG:NH1	2:B:214:ARG:HG2	2.33	0.43
2:B:39:THR:CG2	2:B:40:GLU:N	2.79	0.43
2:B:74:ASN:C	2:B:75:LYS:HG3	2.38	0.43
2:B:90:PHE:O	2:B:91:MET:C	2.55	0.43
1:A:198:ALA:C	1:A:200:LEU:N	2.70	0.43
2:B:5:GLN:O	2:B:21:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:C	2:B:152:PHE:CE1	2.92	0.43
2:B:101:LEU:N	2:B:102:PRO:CD	2.82	0.43
1:A:196:LEU:HD22	1:A:196:LEU:C	2.38	0.43
1:A:141:TYR:CE1	2:B:161:HIS:HB3	2.54	0.42
1:A:172:ARG:CD	1:A:179:ALA:CB	2.96	0.42
2:B:5:GLN:O	2:B:7:VAL:HG23	2.19	0.42
2:B:109:PHE:CE1	2:B:286:PHE:HB3	2.54	0.42
1:A:98:GLN:HE21	1:A:98:GLN:HB3	1.55	0.42
1:A:52:LYS:HZ3	1:A:52:LYS:HB2	1.85	0.42
1:A:182:THR:HA	2:B:208:GLU:CD	2.40	0.42
2:B:173:ILE:HD11	2:B:180:TYR:HB3	2.01	0.42
1:A:54:LYS:HZ2	2:B:15:TYR:CB	2.32	0.42
1:A:73:GLN:HG3	1:A:135:LYS:H	1.85	0.42
1:A:48:LEU:HD23	1:A:139:HIS:CE1	2.55	0.42
2:B:29:VAL:O	2:B:30:VAL:CB	2.68	0.42
2:B:76:LEU:HD12	2:B:77:TYR:N	2.35	0.42
2:B:157:ARG:NE	2:B:159:TYR:CE2	2.84	0.42
1:A:172:ARG:NE	1:A:179:ALA:CB	2.71	0.42
2:B:275:ILE:HG13	2:B:276:SER:N	2.35	0.42
2:B:109:PHE:CG	2:B:289:VAL:HG21	2.55	0.42
2:B:244:ALA:O	2:B:245:ARG:C	2.58	0.42
1:A:52:LYS:HZ3	1:A:88:ARG:HB2	1.85	0.42
2:B:108:LEU:HA	2:B:111:LEU:HD12	2.01	0.42
2:B:174:LEU:HD11	2:B:211:GLN:CG	2.50	0.42
2:B:189:LEU:HD13	2:B:189:LEU:HA	1.88	0.42
1:A:83:GLU:OE2	1:A:146:ARG:NH2	2.53	0.41
1:A:91:ASN:HD22	1:A:95:LEU:HG	1.84	0.41
2:B:36:ARG:HE	2:B:75:LYS:HE3	1.84	0.41
2:B:86:ASP:HA	2:B:134:LEU:HA	2.02	0.41
2:B:32:LEU:HD21	2:B:77:TYR:CD1	2.54	0.41
1:A:126:LEU:O	1:A:130:LEU:HG	2.20	0.41
2:B:203:PHE:CB	2:B:211:GLN:HE22	2.33	0.41
2:B:247:ASP:OD2	2:B:249:SER:HB2	2.20	0.41
2:B:256:ASP:OD1	2:B:257:GLU:N	2.53	0.41
1:A:116:ILE:H	1:A:116:ILE:HG13	1.49	0.41
1:A:124:GLU:O	1:A:125:GLU:C	2.57	0.41
2:B:112:LEU:HD11	2:B:286:PHE:CZ	2.55	0.41
1:A:182:THR:OG1	1:A:185:GLN:CG	2.68	0.41
2:B:70:ILE:N	2:B:70:ILE:CD1	2.83	0.41
2:B:247:ASP:O	2:B:249:SER:N	2.53	0.41
1:A:27:ILE:CG1	1:A:63:ASP:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG22	1:A:129:CYS:N	2.36	0.41
2:B:18:VAL:HG11	4:B:381:ATP:C8	2.55	0.41
2:B:53:SER:O	2:B:56:LYS:N	2.52	0.41
2:B:103:LEU:CD2	2:B:294:PRO:HB3	2.50	0.41
2:B:165:THR:O	2:B:167:TRP:HD1	2.03	0.41
2:B:174:LEU:HD11	2:B:211:GLN:HG3	2.03	0.41
1:A:49:PRO:HG2	1:A:96:TYR:OH	2.21	0.41
1:A:89:VAL:HB	1:A:92:LEU:HB2	2.02	0.41
2:B:50:ARG:HH12	2:B:148:LEU:N	2.17	0.41
2:B:69:VAL:HG22	2:B:78:LEU:HD22	2.03	0.41
2:B:262:LEU:O	2:B:266:MET:N	2.52	0.41
2:B:167:TRP:CD1	2:B:167:TRP:N	2.88	0.41
1:A:48:LEU:HD11	1:A:89:VAL:HG21	2.03	0.40
2:B:4:PHE:N	2:B:24:LYS:HB2	2.36	0.40
1:A:114:PRO:CG	1:A:119:CYS:HB2	2.50	0.40
1:A:197:ALA:C	1:A:199:HIS:H	2.22	0.40
2:B:135:ILE:HD12	2:B:135:ILE:C	2.42	0.40
2:B:252:VAL:C	2:B:260:ARG:HH12	2.24	0.40
1:A:113:THR:HB	1:A:188:TYR:CD1	2.56	0.40
1:A:132:ASN:O	1:A:134:ARG:HG2	2.21	0.40
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.92	0.40
1:A:201:SER:O	1:A:202:SER:C	2.60	0.40
2:B:167:TRP:CD2	2:B:204:PRO:HA	2.56	0.40
2:B:186:ILE:HD13	2:B:186:ILE:HA	1.95	0.40
1:A:110:ASP:OD2	2:B:159:TYR:CD1	2.62	0.40
1:A:186:TYR:CE1	1:A:190:HIS:HE1	2.40	0.40
2:B:72:THR:HB	2:B:74:ASN:ND2	2.36	0.40
2:B:278:LYS:C	2:B:280:ALA:N	2.74	0.40
2:B:32:LEU:HD21	2:B:77:TYR:HD1	1.87	0.40
2:B:178:LYS:O	2:B:179:TYR:O	2.40	0.40
2:B:190:GLY:HA3	2:B:267:LEU:HD21	2.04	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	181/212 (85%)	151 (83%)	20 (11%)	10 (6%)	2 10
2	B	293/298 (98%)	183 (62%)	72 (25%)	38 (13%)	0 1
All	All	474/510 (93%)	334 (70%)	92 (19%)	48 (10%)	0 2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	23	GLU
1	A	179	ALA
1	A	201	SER
2	B	2	GLU
2	B	3	ASN
2	B	14	THR
2	B	30	VAL
2	B	47	THR
2	B	93	ALA
2	B	94	SER
2	B	152	PHE
2	B	179	TYR
2	B	212	LEU
2	B	231	THR
2	B	247	ASP
2	B	283	HIS
2	B	287	GLN
1	A	54	LYS
1	A	60	VAL
1	A	133	TYR
1	A	144	LEU
2	B	24	LYS
2	B	28	GLU
2	B	29	VAL
2	B	43	GLY
2	B	113	GLN
2	B	176	GLY
2	B	197	VAL
2	B	213	PHE
2	B	234	PRO
2	B	248	PHE
2	B	281	LEU

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	64	VAL
2	B	84	HIS
2	B	114	GLY
2	B	245	ARG
2	B	92	ASP
1	A	124	GLU
1	A	198	ALA
2	B	15	TYR
2	B	72	THR
2	B	102	PRO
2	B	49	ILE
2	B	225	VAL
2	B	27	GLY
2	B	61	PRO

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	A	162/191 (85%)	137 (85%)	25 (15%)	2 13
2	B	260/262 (99%)	241 (93%)	19 (7%)	14 44
All	All	422/453 (93%)	378 (90%)	44 (10%)	7 27

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	38	ASN
1	A	48	LEU
1	A	55	ASP
1	A	57	ARG
1	A	60	VAL
1	A	65	GLU
1	A	68	LYS

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Mol	Chain	Res	Type
1	A	69	SER
1	A	89	VAL
1	A	93	LEU
1	A	94	ASP
1	A	97	GLN
1	A	98	GLN
1	A	104	HIS
1	A	114	PRO
1	A	116	ILE
1	A	146	ARG
1	A	156	LEU
1	A	170	SER
1	A	174	LEU
1	A	189	LEU
1	A	196	LEU
1	A	200	LEU
1	A	201	SER
2	B	14	THR
2	B	15	TYR
2	B	23	ASN
2	B	34	LYS
2	B	55	LEU
2	B	61	PRO
2	B	62	ASN
2	B	99	ILE
2	B	119	HIS
2	B	130	PRO
2	B	131	GLN
2	B	154	VAL
2	B	179	TYR
2	B	180	TYR
2	B	206	ASP
2	B	232	SER
2	B	239	SER
2	B	247	ASP
2	B	288	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	73	GLN

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Mol	Chain	Res	Type
1	A	98	GLN
1	A	132	ASN
1	A	166	GLN
1	A	185	GLN
1	A	187	ASN
1	A	190	HIS
2	B	3	ASN
2	B	59	ASN
2	B	132	ASN
2	B	246	GLN
2	B	265	GLN
2	B	268	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	B	160	2	8,10,11	1.82	2 (25%)	10,14,16	0.98	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
2	TPO	B	160	2	-	7/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	160	TPO	P-O3P	-3.25	1.42	1.54
2	B	160	TPO	P-OG1	-3.12	1.53	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	160	TPO	N-CA-CB-CG2
2	B	160	TPO	N-CA-CB-OG1
2	B	160	TPO	C-CA-CB-CG2
2	B	160	TPO	CG2-CB-OG1-P
2	B	160	TPO	CB-OG1-P-O2P
2	B	160	TPO	CA-CB-OG1-P
2	B	160	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	160	TPO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	ATP	B	381	3	26,33,33	1.33	4 (15%)	31,52,52	1.12	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
4	ATP	B	381	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	381	ATP	C4-N3	2.99	1.39	1.35
4	B	381	ATP	C8-N7	-2.66	1.30	1.34
4	B	381	ATP	C2-N3	2.06	1.35	1.32
4	B	381	ATP	C2'-C1'	2.05	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	381	ATP	C4-C5-N7	2.58	112.09	109.40
4	B	381	ATP	O4'-C1'-C2'	-2.24	103.66	106.93
4	B	381	ATP	O3G-PG-O2G	2.20	116.04	107.64
4	B	381	ATP	C3'-C2'-C1'	2.10	104.14	100.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

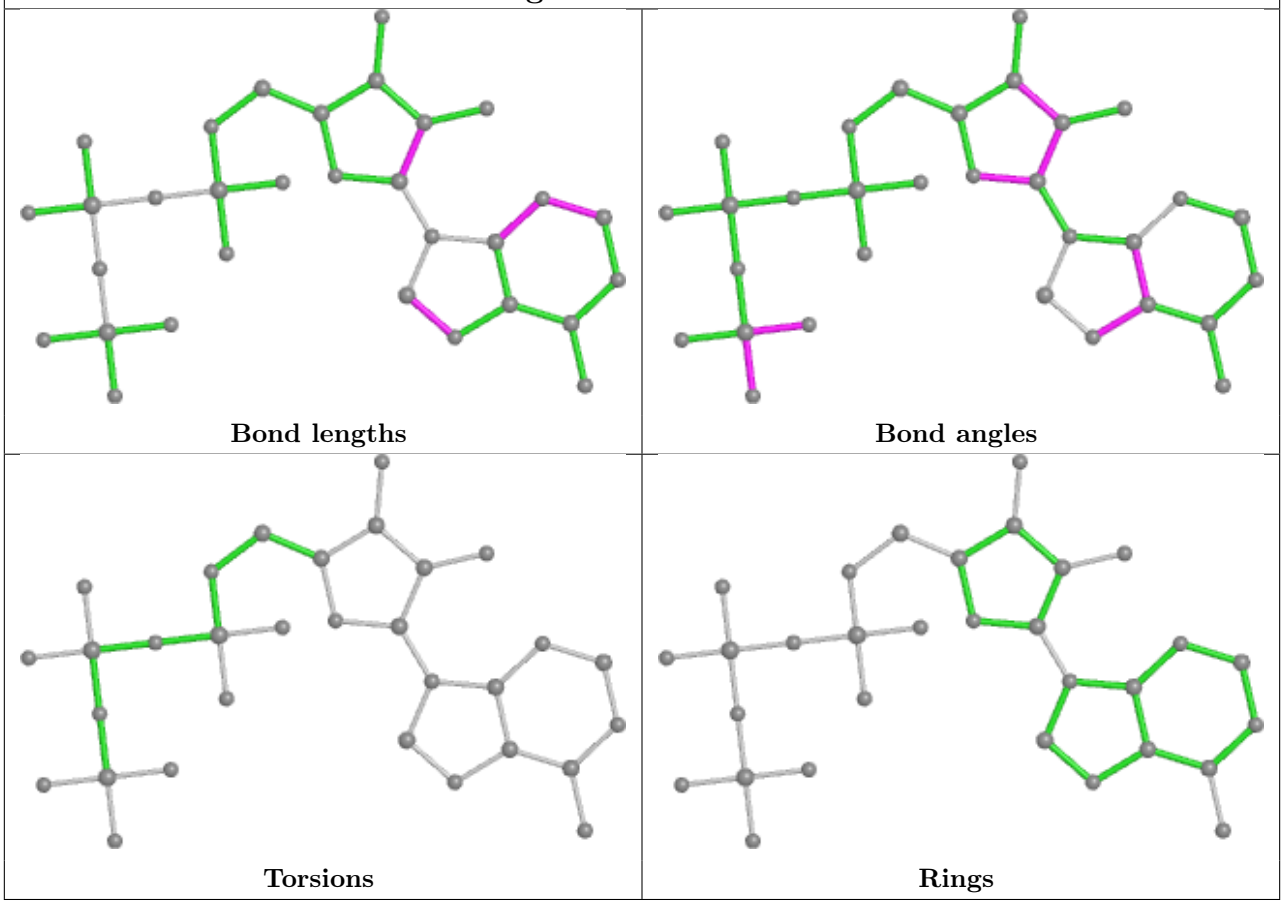
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	381	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 B 381



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	35:ILE	C	36:ARG	N	1.19
1	B	47:THR	C	48:ALA	N	1.14

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	A	183/212 (86%)	-0.46	2 (1%) 80 56	45, 66, 100, 113	0
2	B	295/298 (98%)	-0.11	8 (2%) 54 26	61, 96, 135, 143	0
All	All	478/510 (93%)	-0.25	10 (2%) 63 34	45, 86, 131, 143	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	38	ASP	4.2
2	B	43	GLY	4.2
2	B	39	THR	4.0
1	A	22	ASP	3.2
2	B	30	VAL	2.9
2	B	40	GLU	2.8
1	A	21	GLU	2.3
2	B	295	HIS	2.3
2	B	250	LYS	2.3
2	B	73	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	TPO	B	160	11/12	0.97	0.20	69,75,88,88	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

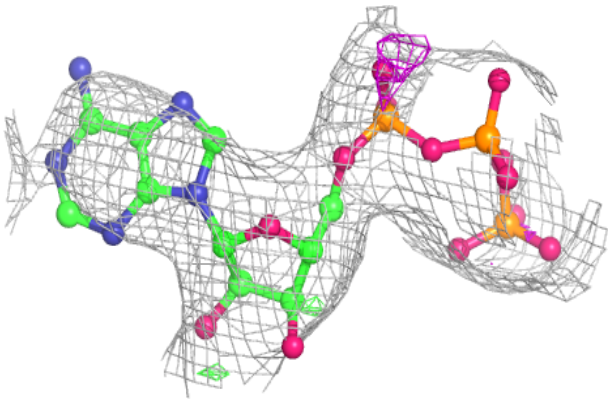
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

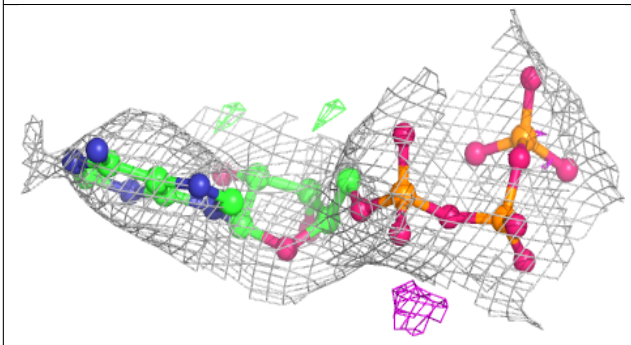
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	B	381	31/31	0.92	0.20	113,121,131,132	0
3	MG	B	383	1/1	0.97	0.16	65,65,65,65	0

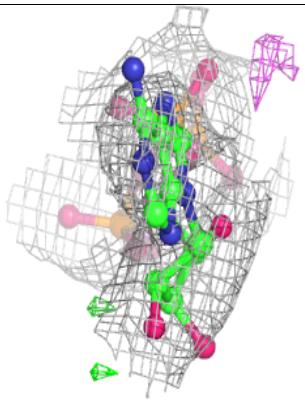
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 381:

$2mF_o$-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.