



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:42 am BST

PDB ID : 1ZFN
Title : Structural Analysis of Escherichia coli ThiF
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Deposited on : 2005-04-20
Resolution : 2.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

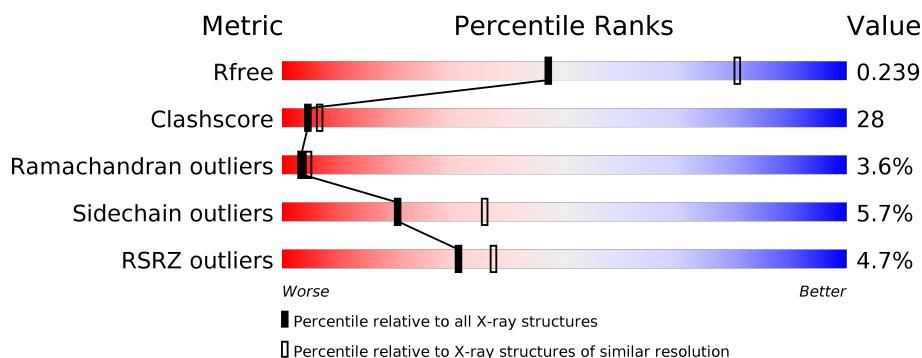
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 ≥ 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	253	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>37%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	253	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>36%</div> <div>• •</div> <div>8%</div> </div> </div>
1	C	253	<div> <div>5%</div> <div> <div></div> <div>49%</div> <div>42%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	253	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>• •</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7315 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 Adenylyltransferase thiF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1841	1144	329	356	12			
1	B	232	Total	C	N	O	S	0	0	0
			1741	1088	308	334	11			
1	C	244	Total	C	N	O	S	0	0	0
			1841	1144	329	356	12			
1	D	235	Total	C	N	O	S	0	0	0
			1764	1101	312	340	11			

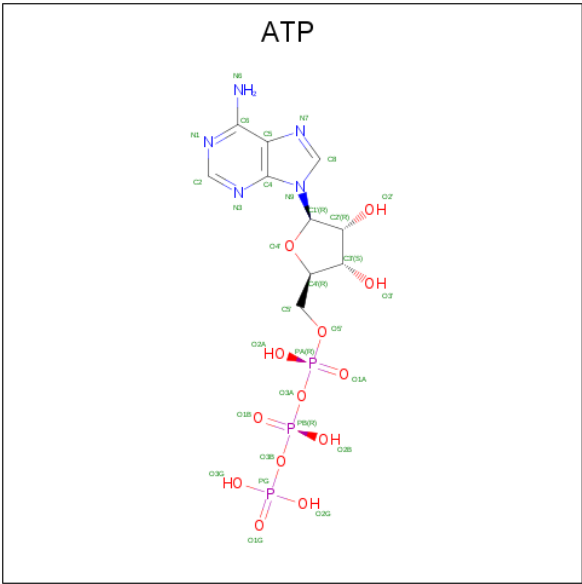
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP P30138
A	0	SER	-	cloning artifact	UNP P30138
B	-1	GLY	-	cloning artifact	UNP P30138
B	0	SER	-	cloning artifact	UNP P30138
C	-1	GLY	-	cloning artifact	UNP P30138
C	0	SER	-	cloning artifact	UNP P30138
D	-1	GLY	-	cloning artifact	UNP P30138
D	0	SER	-	cloning artifact	UNP P30138

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

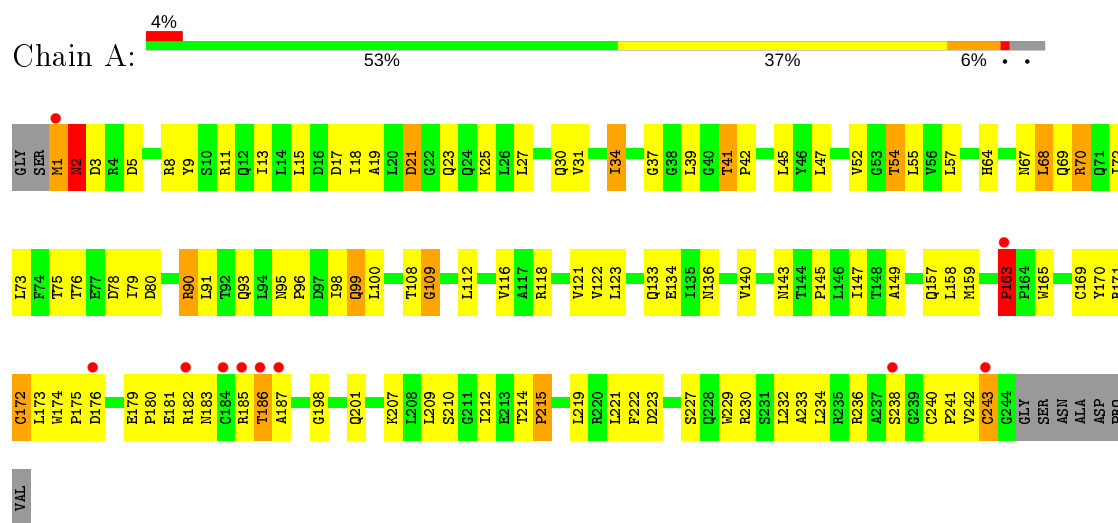
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



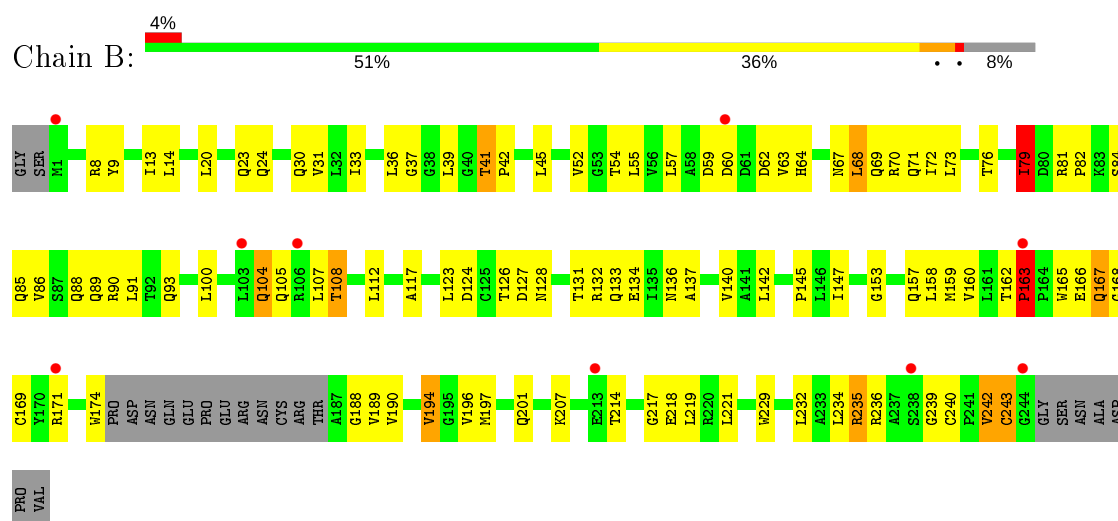
3 Residue-property plots [i](#)

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: Adenylyltransferase thiF

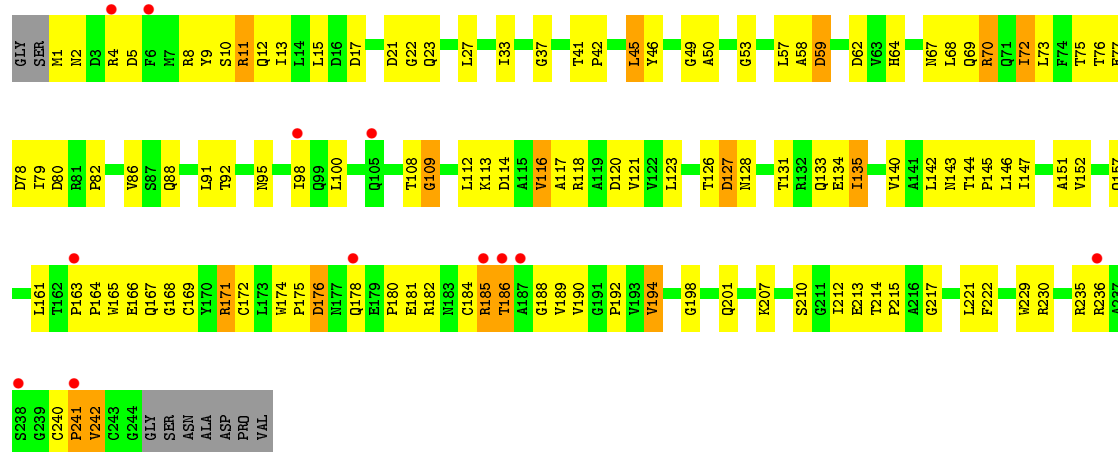


• Molecule 1: Adenylyltransferase thiF

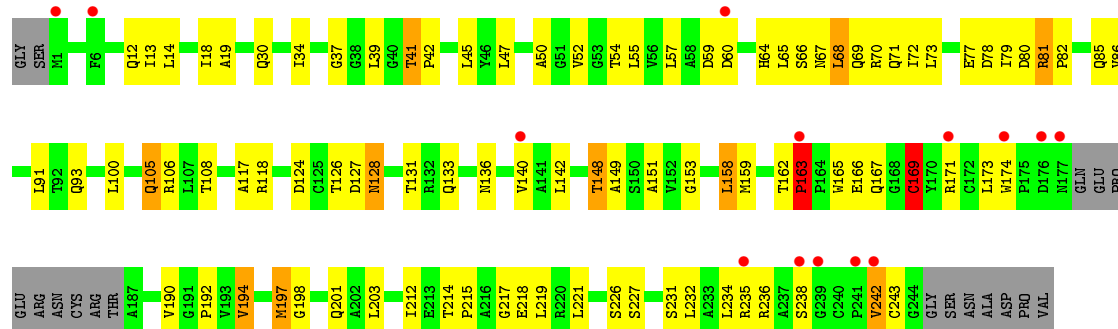


• Molecule 1: Adenylyltransferase thiF





• Molecule 1: Adenylyltransferase thiF



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	360.30 Å 360.30 Å 360.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 44.02 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.75) 99.8 (44.02-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.65 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.268 0.250 , 0.239	Depositor DCC
R_{free} test set	2936 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7315	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.44	2/1865 (0.1%)	0.66	0/2534
1	B	0.40	0/1762	0.67	0/2392
1	C	0.38	1/1865 (0.1%)	0.63	0/2534
1	D	0.41	0/1786	0.70	1/2426 (0.0%)
All	All	0.41	3/7278 (0.0%)	0.66	1/9886 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	5.40	2.08	1.77
1	C	166	GLU	CD-OE1	5.20	1.31	1.25
1	A	243	CYS	CB-SG	-5.01	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	CYS	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1841	0	1859	125	1
1	B	1741	0	1769	105	0
1	C	1841	0	1858	132	0
1	D	1764	0	1786	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	2	0
All	All	7315	0	7320	415	1

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 28.

All (415) 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:1:MET:SD	1:A:1:MET:CE	2.08	1.42
1:D:69:GLN:NE2	1:D:70:ARG:HD3	1.65	1.11
1:C:167:GLN:HG3	1:C:217:GLY:HA3	1.45	0.98
1:C:75:THR:HG22	1:C:77:GLU:H	1.31	0.94
1:D:167:GLN:HG3	1:D:217:GLY:HA3	1.50	0.92
1:D:45:LEU:HD21	1:D:73:LEU:HD13	1.50	0.92
1:A:54:THR:HG23	1:A:99:GLN:HB3	1.51	0.91
1:B:236:ARG:HH21	1:C:176:ASP:HB2	1.35	0.91
1:C:186:THR:HG22	1:C:188:GLY:H	1.35	0.90
1:C:117:ALA:HB2	1:C:142:LEU:HD13	1.52	0.89
1:D:158:LEU:HD12	1:D:159:MET:N	1.89	0.87
1:B:69:GLN:OE1	1:B:70:ARG:HD3	1.75	0.86
1:C:69:GLN:HE21	1:C:70:ARG:HE	1.23	0.84
1:B:157:GLN:HG2	1:B:219:LEU:HD11	1.59	0.83
1:C:123:LEU:HD22	1:C:147:ILE:HB	1.60	0.82
1:A:75:THR:HG22	1:A:78:ASP:OD2	1.81	0.81
1:C:69:GLN:NE2	1:C:70:ARG:HE	1.79	0.81
1:C:11:ARG:CG	1:C:11:ARG:HH11	1.94	0.81
1:B:242:VAL:HG23	1:B:243:CYS:H	1.45	0.80
1:C:8:ARG:HH12	1:C:95:ASN:HA	1.47	0.77
1:C:46:TYR:CZ	1:D:72:ILE:HD11	2.19	0.77
1:C:145:PRO:HG3	1:C:163:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:HG3	1:A:54:THR:HB	1.66	0.76
1:D:60:ASP:HB2	1:D:105:GLN:C	2.06	0.76
1:C:11:ARG:HG2	1:C:11:ARG:HH11	1.52	0.75
1:D:69:GLN:HE22	1:D:70:ARG:HD3	1.49	0.75
1:B:81:ARG:HE	1:B:85:GLN:NE2	1.85	0.74
1:D:162:THR:HB	1:D:163:PRO:HD2	1.68	0.74
1:C:23:GLN:HE21	1:C:27:LEU:CD1	2.01	0.73
1:C:64:HIS:H	1:C:67:ASN:ND2	1.85	0.73
1:C:45:LEU:HG	1:D:72:ILE:HG23	1.69	0.73
1:D:57:LEU:HD11	1:D:91:LEU:HD12	1.71	0.73
1:A:45:LEU:HD13	1:A:73:LEU:HD13	1.71	0.73
1:B:169:CYS:SG	1:B:242:VAL:HG21	2.29	0.73
1:A:57:LEU:HD11	1:A:91:LEU:HD12	1.69	0.73
1:A:34:ILE:H	1:A:34:ILE:HD12	1.53	0.73
1:C:11:ARG:N	1:C:11:ARG:HD2	2.03	0.73
1:C:198:GLY:HA2	1:C:201:GLN:HE21	1.55	0.72
1:A:64:HIS:H	1:A:67:ASN:ND2	1.87	0.72
1:B:167:GLN:HG3	1:B:217:GLY:CA	2.19	0.72
1:B:68:LEU:HD11	1:B:76:THR:HA	1.72	0.72
1:A:173:LEU:HA	1:D:235:ARG:HG3	1.72	0.71
1:A:136:ASN:HD21	1:A:169:CYS:HB2	1.52	0.71
1:B:147:ILE:HD12	1:B:160:VAL:HG22	1.72	0.71
1:C:10:SER:OG	1:C:11:ARG:HD2	1.91	0.70
1:B:236:ARG:NH2	1:C:176:ASP:HB2	2.06	0.70
1:A:2:ASN:ND2	1:A:3:ASP:H	1.89	0.70
1:C:131:THR:O	1:C:135:ILE:HD13	1.91	0.70
1:C:75:THR:HG23	1:D:93:GLN:O	1.91	0.70
1:A:136:ASN:ND2	1:A:170:TYR:H	1.90	0.70
1:D:82:PRO:O	1:D:86:VAL:HG23	1.92	0.70
1:A:41:THR:HG22	1:A:42:PRO:HD3	1.72	0.70
1:A:37:GLY:O	1:A:41:THR:HB	1.92	0.70
1:C:186:THR:HG22	1:C:188:GLY:N	2.06	0.70
1:C:186:THR:C	1:C:188:GLY:H	1.95	0.69
1:B:60:ASP:HB2	1:B:105:GLN:C	2.12	0.69
1:D:133:GLN:OE1	1:D:171:ARG:HG2	1.93	0.69
1:B:158:LEU:HD12	1:B:159:MET:H	1.59	0.68
1:D:153:GLY:O	1:D:190:VAL:HG23	1.93	0.68
1:C:157:GLN:HG2	1:C:221:LEU:HD22	1.76	0.67
1:D:117:ALA:HB2	1:D:142:LEU:HD13	1.75	0.67
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.60	0.67
1:B:45:LEU:HD13	1:B:73:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PHE:HB2	1:A:229:TRP:CZ3	2.30	0.67
1:C:45:LEU:HG	1:D:72:ILE:CG2	2.24	0.67
1:A:2:ASN:CG	1:A:3:ASP:H	1.99	0.66
1:B:158:LEU:HD12	1:B:159:MET:N	2.10	0.66
1:B:20:LEU:O	1:B:24:GLN:HG3	1.96	0.66
1:C:17:ASP:O	1:C:212:ILE:HD11	1.96	0.66
1:C:168:GLY:CA	1:C:236:ARG:HB3	2.25	0.66
1:C:8:ARG:NH1	1:C:95:ASN:HA	2.11	0.66
1:B:13:ILE:HD11	1:B:23:GLN:HG2	1.78	0.65
1:A:108:THR:HG22	1:A:109:GLY:H	1.60	0.65
1:D:78:ASP:O	1:D:81:ARG:HG3	1.96	0.65
1:D:197:MET:HE2	1:D:197:MET:N	2.11	0.65
1:A:99:GLN:CA	1:A:99:GLN:HE21	2.10	0.65
1:A:185:ARG:O	1:A:187:ALA:N	2.25	0.65
1:A:207:LYS:HE3	1:A:214:THR:OG1	1.97	0.65
1:B:167:GLN:HG3	1:B:217:GLY:HA2	1.77	0.64
1:D:214:THR:HG23	1:D:215:PRO:HD2	1.80	0.64
1:D:128:ASN:ND2	1:D:131:THR:OG1	2.31	0.64
1:D:41:THR:HG21	1:D:72:ILE:N	2.13	0.64
1:C:140:VAL:HA	1:C:165:TRP:CZ2	2.33	0.64
1:B:219:LEU:HD23	1:B:232:LEU:HD12	1.79	0.63
1:A:45:LEU:CD1	1:A:73:LEU:HD13	2.29	0.63
1:A:136:ASN:HD21	1:A:170:TYR:H	1.46	0.62
1:C:75:THR:CG2	1:D:93:GLN:HB3	2.29	0.62
1:A:64:HIS:H	1:A:67:ASN:HD22	1.46	0.62
1:C:147:ILE:HD12	1:C:147:ILE:N	2.15	0.62
1:A:2:ASN:HB3	1:A:5:ASP:HB2	1.82	0.62
1:A:23:GLN:HE21	1:A:27:LEU:HG	1.65	0.62
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.64	0.62
1:C:182:ARG:O	1:C:185:ARG:HB2	1.99	0.62
1:A:158:LEU:HD12	1:A:159:MET:H	1.64	0.61
1:B:117:ALA:HB2	1:B:142:LEU:HD13	1.81	0.61
1:B:124:ASP:OD2	1:B:132:ARG:HG2	2.01	0.61
1:D:158:LEU:HD12	1:D:158:LEU:C	2.20	0.61
1:D:79:ILE:O	1:D:80:ASP:HB2	2.00	0.61
1:A:230:ARG:HH22	1:D:218:GLU:CD	2.03	0.61
1:B:207:LYS:HE2	1:B:214:THR:OG1	2.01	0.61
1:A:34:ILE:HD11	1:A:122:VAL:CG1	2.30	0.61
1:B:167:GLN:HG3	1:B:217:GLY:HA3	1.82	0.61
1:C:23:GLN:O	1:C:27:LEU:HD13	2.00	0.61
1:A:76:THR:O	1:A:79:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:VAL:HG12	1:C:192:PRO:HD2	1.82	0.60
1:A:145:PRO:HG3	1:A:163:PRO:HD3	1.81	0.60
1:D:64:HIS:H	1:D:67:ASN:ND2	1.99	0.60
1:C:64:HIS:H	1:C:67:ASN:HD22	1.48	0.60
1:A:55:LEU:HB2	1:A:100:LEU:HD23	1.82	0.60
1:D:12:GLN:HE22	1:D:50:ALA:HA	1.66	0.59
1:D:47:LEU:O	1:D:52:VAL:HG23	2.02	0.59
1:B:128:ASN:ND2	1:B:131:THR:OG1	2.34	0.59
1:C:186:THR:C	1:C:188:GLY:N	2.55	0.59
1:B:64:HIS:O	1:B:67:ASN:HB2	2.02	0.59
1:A:45:LEU:HD23	1:B:72:ILE:HB	1.85	0.59
1:C:168:GLY:HA2	1:C:236:ARG:HB3	1.85	0.59
1:D:167:GLN:O	1:D:236:ARG:HB3	2.03	0.59
1:A:182:ARG:HG3	1:A:182:ARG:O	2.03	0.58
1:C:37:GLY:HA3	3:C:346:ATP:H5'2	1.85	0.58
1:B:137:ALA:HB2	1:B:171:ARG:NH2	2.17	0.58
1:A:198:GLY:HA2	1:A:201:GLN:HE21	1.68	0.58
1:C:92:THR:OG1	1:C:100:LEU:HD12	2.03	0.58
1:A:169:CYS:H	1:A:172:CYS:HB2	1.69	0.58
1:B:39:LEU:HD23	1:B:194:VAL:HG12	1.85	0.58
1:A:99:GLN:HA	1:A:99:GLN:HE21	1.67	0.58
1:C:41:THR:HG23	1:C:73:LEU:HB2	1.85	0.58
1:D:39:LEU:O	1:D:42:PRO:HD2	2.03	0.58
1:A:15:LEU:HD12	1:A:18:ILE:HD12	1.86	0.58
1:A:140:VAL:HG13	1:A:165:TRP:NE1	2.19	0.57
1:A:13:ILE:HD11	1:A:23:GLN:HG2	1.86	0.57
1:C:12:GLN:HE22	1:C:50:ALA:HA	1.69	0.57
1:A:207:LYS:NZ	1:A:214:THR:HG21	2.20	0.57
1:B:136:ASN:HD22	1:B:171:ARG:HH11	1.53	0.57
1:C:2:ASN:OD1	1:C:4:ARG:HB3	2.05	0.57
1:B:145:PRO:HG3	1:B:163:PRO:CD	2.35	0.56
1:B:162:THR:HB	1:B:163:PRO:HD2	1.87	0.56
1:A:140:VAL:HA	1:A:165:TRP:CZ2	2.40	0.56
1:C:53:GLY:O	1:C:98:ILE:HG23	2.05	0.56
1:C:126:THR:O	1:C:128:ASN:N	2.38	0.56
1:C:171:ARG:NH1	1:C:241:PRO:HG2	2.21	0.56
1:B:219:LEU:HG	1:B:221:LEU:HD21	1.87	0.56
1:A:145:PRO:HG3	1:A:163:PRO:CD	2.35	0.56
1:B:30:GLN:HG3	1:B:54:THR:HB	1.88	0.56
1:B:33:ILE:HD12	1:B:123:LEU:HD12	1.87	0.56
1:B:82:PRO:HG2	1:B:85:GLN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLN:CG	1:C:217:GLY:HA3	2.29	0.56
1:C:45:LEU:HD13	1:C:73:LEU:HD13	1.87	0.56
1:B:166:GLU:HB3	1:B:167:GLN:NE2	2.21	0.56
1:B:63:VAL:O	1:B:79:ILE:O	2.22	0.56
1:C:123:LEU:CD2	1:C:147:ILE:HB	2.34	0.56
1:C:151:ALA:HB3	1:C:194:VAL:HG13	1.88	0.56
1:B:41:THR:HG22	1:B:42:PRO:HD3	1.88	0.55
1:C:142:LEU:O	1:C:144:THR:HG23	2.06	0.55
1:C:126:THR:O	1:C:127:ASP:C	2.44	0.55
1:A:2:ASN:ND2	1:A:3:ASP:N	2.55	0.55
1:B:37:GLY:O	1:B:41:THR:HB	2.07	0.55
1:A:93:GLN:O	1:B:76:THR:HG23	2.06	0.55
1:D:69:GLN:HE21	1:D:70:ARG:HD3	1.68	0.55
1:D:41:THR:HG23	1:D:73:LEU:H	1.71	0.55
1:A:240:CYS:HB3	1:A:243:CYS:O	2.07	0.55
1:C:133:GLN:OE1	1:C:133:GLN:HA	2.06	0.55
1:B:9:TYR:O	1:B:13:ILE:HD13	2.07	0.54
1:B:163:PRO:O	1:B:165:TRP:CD1	2.61	0.54
1:B:36:LEU:HG	1:B:59:ASP:HB2	1.89	0.54
1:D:45:LEU:HD21	1:D:73:LEU:CD1	2.29	0.54
1:A:17:ASP:O	1:A:212:ILE:HD11	2.08	0.54
1:C:112:LEU:HD21	1:C:135:ILE:HD12	1.90	0.54
1:B:90:ARG:HA	1:B:93:GLN:HE21	1.71	0.54
1:A:31:VAL:HB	1:A:55:LEU:HD23	1.88	0.54
1:B:55:LEU:HB2	1:B:100:LEU:HD23	1.90	0.54
1:B:168:GLY:N	1:B:236:ARG:HB3	2.21	0.54
1:C:72:ILE:HB	1:D:45:LEU:HD13	1.90	0.54
1:D:219:LEU:HG	1:D:221:LEU:HD21	1.89	0.54
1:C:75:THR:HB	1:C:78:ASP:OD2	2.08	0.54
1:C:75:THR:HG21	1:D:93:GLN:HB3	1.89	0.54
1:A:175:PRO:HG3	1:D:235:ARG:NH2	2.23	0.53
1:B:41:THR:HG22	1:B:42:PRO:CD	2.38	0.53
1:C:140:VAL:HG13	1:C:165:TRP:NE1	2.23	0.53
1:A:230:ARG:NH2	1:D:218:GLU:OE1	2.41	0.53
1:A:173:LEU:CA	1:D:235:ARG:HG3	2.38	0.53
1:A:41:THR:HG22	1:A:42:PRO:CD	2.37	0.53
1:D:136:ASN:O	1:D:140:VAL:HG23	2.08	0.53
1:A:68:LEU:HD13	1:A:76:THR:HG22	1.89	0.53
1:B:41:THR:HG22	1:B:42:PRO:N	2.23	0.53
1:C:11:ARG:NH1	3:D:446:ATP:O2G	2.41	0.53
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PRO:O	1:C:86:VAL:HG23	2.08	0.53
1:A:232:LEU:CD2	1:D:231:SER:HB3	2.39	0.53
1:A:108:THR:HG23	1:A:134:GLU:OE2	2.09	0.52
1:B:136:ASN:HD22	1:B:171:ARG:NH1	2.06	0.52
1:A:240:CYS:O	1:A:242:VAL:N	2.42	0.52
1:A:34:ILE:N	1:A:34:ILE:HD12	2.23	0.52
1:A:45:LEU:CD2	1:B:72:ILE:HB	2.40	0.52
1:D:219:LEU:HB2	1:D:234:LEU:HD21	1.91	0.52
1:B:107:LEU:HB3	1:B:112:LEU:HD13	1.91	0.52
1:C:8:ARG:HG2	1:C:9:TYR:CD2	2.45	0.52
1:C:174:TRP:CH2	1:C:180:PRO:HB3	2.44	0.52
1:C:58:ALA:O	1:C:59:ASP:HB2	2.10	0.52
1:B:60:ASP:HB2	1:B:105:GLN:CA	2.40	0.52
1:C:213:GLU:O	1:C:213:GLU:HG3	2.09	0.51
1:C:69:GLN:NE2	1:C:70:ARG:NE	2.52	0.51
1:D:72:ILE:HD13	1:D:72:ILE:N	2.24	0.51
1:B:153:GLY:O	1:B:190:VAL:HG23	2.10	0.51
1:C:185:ARG:O	1:C:186:THR:C	2.48	0.51
1:D:67:ASN:O	1:D:71:GLN:HG3	2.09	0.51
1:A:68:LEU:HD11	1:A:76:THR:HA	1.92	0.51
1:A:57:LEU:HD11	1:A:91:LEU:CD1	2.38	0.51
1:A:159:MET:HE1	1:A:170:TYR:CD1	2.45	0.51
1:D:169:CYS:SG	1:D:171:ARG:N	2.81	0.51
1:A:219:LEU:HD23	1:A:232:LEU:HD12	1.92	0.51
1:A:240:CYS:C	1:A:242:VAL:H	2.12	0.51
1:A:96:PRO:HD3	1:B:76:THR:HG21	1.93	0.51
1:C:112:LEU:O	1:C:116:VAL:HG23	2.11	0.51
1:D:167:GLN:HG3	1:D:217:GLY:CA	2.32	0.51
1:B:242:VAL:HG23	1:B:243:CYS:N	2.20	0.51
1:C:214:THR:HG23	1:C:215:PRO:HD2	1.92	0.51
1:D:39:LEU:HD23	1:D:194:VAL:HG12	1.93	0.51
1:D:41:THR:CG2	1:D:73:LEU:H	2.23	0.51
1:C:117:ALA:HB2	1:C:142:LEU:CD1	2.35	0.50
1:C:73:LEU:O	1:C:73:LEU:HG	2.12	0.50
1:B:219:LEU:HB2	1:B:234:LEU:HD21	1.94	0.50
1:A:123:LEU:HD22	1:A:147:ILE:HB	1.93	0.50
1:B:8:ARG:HG3	1:B:9:TYR:CD2	2.47	0.50
1:D:34:ILE:HG22	1:D:126:THR:CG2	2.42	0.50
1:A:187:ALA:HB1	1:B:14:LEU:HB3	1.94	0.50
1:B:31:VAL:HG23	1:B:52:VAL:HG11	1.93	0.49
1:A:163:PRO:O	1:A:165:TRP:CD1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:CG	1:A:90:ARG:HH11	2.25	0.49
1:B:84:SER:OG	1:B:104:GLN:HB2	2.13	0.49
1:A:9:TYR:O	1:A:13:ILE:HD13	2.12	0.49
1:C:75:THR:N	1:C:78:ASP:OD2	2.46	0.49
1:C:109:GLY:O	1:C:113:LYS:HG3	2.12	0.49
1:C:145:PRO:HG3	1:C:163:PRO:CD	2.41	0.49
1:C:185:ARG:O	1:C:186:THR:O	2.31	0.49
1:C:46:TYR:CE2	1:D:72:ILE:HD11	2.47	0.49
1:B:39:LEU:O	1:B:42:PRO:HD2	2.13	0.48
1:A:95:ASN:OD1	1:A:98:ILE:HG12	2.13	0.48
1:C:207:LYS:NZ	1:C:214:THR:HG21	2.28	0.48
1:C:210:SER:OG	1:C:212:ILE:HG12	2.13	0.48
1:C:42:PRO:O	1:C:46:TYR:HD1	1.96	0.48
1:C:75:THR:CG2	1:C:76:THR:N	2.76	0.48
1:A:42:PRO:HB3	1:A:72:ILE:HD11	1.96	0.48
1:C:57:LEU:HD11	1:C:91:LEU:HD12	1.94	0.48
1:A:157:GLN:CG	1:A:219:LEU:HD11	2.44	0.48
1:C:11:ARG:CG	1:C:11:ARG:NH1	2.63	0.48
1:A:91:LEU:HB2	1:A:100:LEU:HD13	1.96	0.48
1:A:79:ILE:O	1:A:80:ASP:HB2	2.13	0.47
1:B:82:PRO:O	1:B:86:VAL:HG23	2.13	0.47
1:C:120:ASP:O	1:C:145:PRO:HD2	2.14	0.47
1:A:236:ARG:HH12	1:A:243:CYS:HB3	1.78	0.47
1:C:8:ARG:HE	1:D:65:LEU:HD11	1.79	0.47
1:C:11:ARG:NE	1:D:66:SER:HB2	2.29	0.47
1:A:186:THR:O	1:A:186:THR:HG22	2.14	0.47
1:B:157:GLN:HG3	1:B:221:LEU:HD22	1.96	0.47
1:D:60:ASP:HB2	1:D:105:GLN:CA	2.44	0.47
1:C:11:ARG:H	1:C:11:ARG:HD2	1.78	0.47
1:C:235:ARG:HG3	1:C:235:ARG:O	2.14	0.47
1:C:186:THR:HG21	1:D:14:LEU:C	2.35	0.47
1:C:1:MET:HE3	1:C:5:ASP:HB3	1.96	0.47
1:B:218:GLU:OE1	1:C:230:ARG:NH2	2.48	0.47
1:B:218:GLU:CD	1:C:230:ARG:HH22	2.18	0.47
1:A:181:GLU:C	1:A:183:ASN:H	2.18	0.47
1:B:41:THR:CG2	1:B:72:ILE:HG13	2.45	0.47
1:C:171:ARG:NH2	1:C:175:PRO:HA	2.29	0.47
1:D:214:THR:HG23	1:D:215:PRO:CD	2.45	0.47
1:A:52:VAL:O	1:A:98:ILE:HD12	2.15	0.47
1:B:57:LEU:HD11	1:B:91:LEU:HD12	1.96	0.47
1:A:172:CYS:SG	1:A:236:ARG:HA	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:HG21	1:B:131:THR:HG21	1.97	0.46
1:B:218:GLU:HA	1:B:234:LEU:HG	1.96	0.46
1:C:118:ARG:HG2	1:C:118:ARG:O	2.15	0.46
1:B:133:GLN:O	1:B:171:ARG:NH2	2.48	0.46
1:C:118:ARG:HB2	1:C:118:ARG:NH1	2.30	0.46
1:C:222:PHE:HB2	1:C:229:TRP:CZ3	2.51	0.46
1:D:39:LEU:HD11	1:D:149:ALA:O	2.14	0.46
1:C:240:CYS:C	1:C:242:VAL:H	2.18	0.46
1:B:197:MET:O	1:B:201:GLN:HG3	2.16	0.46
1:B:81:ARG:HE	1:B:85:GLN:HE21	1.59	0.46
1:C:168:GLY:HA3	1:C:236:ARG:HB3	1.98	0.46
1:C:33:ILE:HD12	1:C:33:ILE:N	2.31	0.46
1:B:197:MET:HE1	1:B:229:TRP:CH2	2.51	0.46
1:C:108:THR:HG22	1:C:109:GLY:N	2.31	0.46
1:D:124:ASP:HB3	1:D:148:THR:HA	1.98	0.46
1:C:49:GLY:O	1:D:69:GLN:CB	2.63	0.46
1:B:157:GLN:HG3	1:B:221:LEU:CD2	2.46	0.45
1:C:17:ASP:HB3	1:C:212:ILE:HD12	1.98	0.45
1:A:207:LYS:CE	1:A:214:THR:OG1	2.65	0.45
1:A:207:LYS:HZ1	1:A:214:THR:HG21	1.80	0.45
1:A:157:GLN:HG2	1:A:219:LEU:HD11	1.99	0.45
1:B:68:LEU:CD1	1:B:76:THR:HG22	2.46	0.45
1:D:34:ILE:HG22	1:D:126:THR:HG21	1.99	0.45
1:B:189:VAL:HG11	1:B:194:VAL:HG22	1.98	0.45
1:D:13:ILE:O	1:D:19:ALA:HA	2.17	0.45
1:D:226:SER:O	1:D:227:SER:HB2	2.16	0.45
1:D:30:GLN:HG3	1:D:54:THR:CG2	2.46	0.45
1:A:121:VAL:HG23	1:A:209:LEU:HD21	1.99	0.45
1:A:240:CYS:C	1:A:242:VAL:N	2.69	0.45
1:D:60:ASP:HB2	1:D:106:ARG:N	2.30	0.45
1:A:90:ARG:NH1	1:B:90:ARG:CZ	2.80	0.45
1:C:214:THR:HG22	1:C:215:PRO:O	2.17	0.45
1:B:140:VAL:HA	1:B:165:TRP:CZ2	2.52	0.45
1:D:79:ILE:O	1:D:80:ASP:CB	2.63	0.45
1:C:10:SER:OG	1:C:11:ARG:CD	2.63	0.45
1:B:85:GLN:O	1:B:89:GLN:HG3	2.17	0.44
1:D:173:LEU:HG	1:D:174:TRP:CD1	2.52	0.44
1:A:108:THR:O	1:A:109:GLY:C	2.55	0.44
1:A:68:LEU:CD1	1:A:76:THR:HG22	2.47	0.44
1:B:82:PRO:HG2	1:B:85:GLN:CB	2.47	0.44
1:A:169:CYS:N	1:A:172:CYS:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:O	1:A:25:LYS:HG3	2.17	0.44
1:B:188:GLY:O	1:B:189:VAL:HG22	2.17	0.44
1:C:75:THR:HG22	1:C:77:GLU:N	2.15	0.44
1:D:151:ALA:HB3	1:D:194:VAL:HG13	1.98	0.44
1:B:147:ILE:CD1	1:B:160:VAL:HG13	2.47	0.44
1:C:109:GLY:N	1:C:134:GLU:OE2	2.40	0.44
1:C:68:LEU:HD11	1:C:76:THR:HA	1.98	0.44
1:A:185:ARG:C	1:A:187:ALA:H	2.16	0.44
1:A:17:ASP:HB3	1:A:212:ILE:CD1	2.47	0.44
1:D:59:ASP:OD2	3:D:446:ATP:H1'	2.18	0.44
1:B:123:LEU:CD2	1:B:147:ILE:HB	2.47	0.44
1:B:69:GLN:HG2	1:B:69:GLN:O	2.17	0.44
1:B:90:ARG:HA	1:B:93:GLN:NE2	2.33	0.44
1:B:235:ARG:NH2	1:C:175:PRO:HG3	2.32	0.44
1:D:55:LEU:HB2	1:D:100:LEU:HD23	2.00	0.44
1:B:240:CYS:SG	1:B:242:VAL:HG22	2.56	0.44
1:C:79:ILE:O	1:C:80:ASP:HB2	2.17	0.44
1:B:76:THR:HA	1:B:79:ILE:HD13	1.99	0.44
1:C:121:VAL:CG1	1:C:147:ILE:HD13	2.48	0.44
1:C:21:ASP:OD1	1:C:22:GLY:N	2.51	0.44
1:A:169:CYS:SG	1:A:171:ARG:HB3	2.58	0.43
1:B:219:LEU:HG	1:B:221:LEU:CD2	2.48	0.43
1:C:142:LEU:O	1:C:144:THR:N	2.51	0.43
1:C:147:ILE:N	1:C:147:ILE:CD1	2.80	0.43
1:C:57:LEU:CD1	1:C:91:LEU:HD12	2.48	0.43
1:D:242:VAL:HG22	1:D:243:CYS:N	2.32	0.43
1:D:65:LEU:C	1:D:67:ASN:H	2.22	0.43
1:A:149:ALA:HA	1:A:157:GLN:O	2.18	0.43
1:A:233:ALA:HB3	1:D:232:LEU:CD2	2.48	0.43
1:A:90:ARG:NH1	1:B:90:ARG:NH2	2.66	0.43
1:C:8:ARG:HH11	1:C:95:ASN:ND2	2.16	0.43
1:C:186:THR:HG23	1:D:14:LEU:HB3	1.99	0.43
1:D:65:LEU:HD12	1:D:68:LEU:HD12	1.99	0.43
1:C:172:CYS:SG	1:C:236:ARG:HA	2.58	0.43
1:A:67:ASN:O	1:A:69:GLN:N	2.52	0.43
1:D:45:LEU:CD2	1:D:73:LEU:HD13	2.36	0.43
1:A:180:PRO:C	1:A:182:ARG:H	2.22	0.43
1:A:223:ASP:O	1:A:227:SER:N	2.52	0.43
1:A:17:ASP:HB3	1:A:212:ILE:HD12	2.01	0.43
1:B:171:ARG:HD2	1:B:242:VAL:CG1	2.48	0.43
1:C:75:THR:HG23	1:D:93:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:116:VAL:HG23	2.19	0.42
1:A:8:ARG:HH12	1:A:95:ASN:HA	1.84	0.42
1:A:99:GLN:C	1:A:99:GLN:HE21	2.23	0.42
1:B:62:ASP:HA	1:B:82:PRO:HA	2.01	0.42
1:A:179:GLU:HA	1:A:180:PRO:HD3	1.87	0.42
1:A:54:THR:HG23	1:A:99:GLN:CB	2.36	0.42
1:D:140:VAL:HA	1:D:165:TRP:CZ2	2.55	0.42
1:A:159:MET:SD	1:A:234:LEU:HD11	2.58	0.42
1:D:30:GLN:HE22	1:D:118:ARG:HB3	1.85	0.42
1:D:37:GLY:O	1:D:41:THR:HB	2.19	0.42
1:A:232:LEU:HD23	1:D:231:SER:CB	2.49	0.42
1:B:81:ARG:NH2	1:B:89:GLN:OE1	2.53	0.42
1:C:146:LEU:C	1:C:147:ILE:HD12	2.39	0.42
1:C:180:PRO:O	1:C:182:ARG:N	2.52	0.42
1:A:133:GLN:NE2	1:A:174:TRP:O	2.53	0.42
1:B:196:VAL:HG12	1:B:197:MET:HE2	2.02	0.42
1:C:75:THR:HG23	1:D:93:GLN:C	2.40	0.42
1:C:192:PRO:HB2	1:D:203:LEU:HB2	2.00	0.42
1:A:214:THR:HG23	1:A:215:PRO:HD2	2.02	0.42
1:A:2:ASN:CG	1:A:3:ASP:N	2.71	0.42
1:C:13:ILE:C	1:C:15:LEU:H	2.23	0.42
1:D:198:GLY:O	1:D:201:GLN:HB2	2.20	0.42
1:A:69:GLN:HE21	1:A:70:ARG:HE	1.68	0.42
1:D:72:ILE:HD13	1:D:72:ILE:H	1.84	0.42
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.82	0.42
1:A:99:GLN:NE2	1:A:99:GLN:CA	2.81	0.41
1:B:168:GLY:CA	1:B:236:ARG:HB3	2.50	0.41
1:C:163:PRO:N	1:C:164:PRO:HD2	2.34	0.41
1:B:108:THR:HG23	1:B:134:GLU:OE1	2.20	0.41
1:A:232:LEU:HD23	1:D:231:SER:HB3	2.01	0.41
1:A:31:VAL:HB	1:A:55:LEU:CD2	2.51	0.41
1:C:140:VAL:HG13	1:C:165:TRP:CD1	2.55	0.41
1:C:11:ARG:HD3	1:D:66:SER:HB2	2.02	0.41
1:C:176:ASP:OD2	1:C:178:GLN:HB2	2.20	0.41
1:D:47:LEU:HA	1:D:47:LEU:HD23	1.88	0.41
1:A:157:GLN:HG3	1:A:221:LEU:HD23	2.02	0.41
1:A:210:SER:OG	1:A:212:ILE:HG12	2.21	0.41
1:B:128:ASN:ND2	1:B:131:THR:H	2.19	0.41
1:A:8:ARG:HH21	1:B:68:LEU:HD12	1.85	0.41
1:C:75:THR:HG22	1:C:76:THR:N	2.34	0.41
1:A:182:ARG:O	1:A:186:THR:OG1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:GLN:HG3	1:D:54:THR:HG22	2.01	0.41
1:C:17:ASP:HB3	1:C:212:ILE:CD1	2.51	0.41
1:C:186:THR:O	1:C:188:GLY:N	2.53	0.41
1:A:180:PRO:HA	1:D:166:GLU:OE2	2.20	0.41
1:D:171:ARG:HA	1:D:174:TRP:O	2.20	0.41
1:A:39:LEU:O	1:A:42:PRO:HD2	2.20	0.41
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.91	0.41
1:B:112:LEU:CD2	1:B:134:GLU:HG2	2.51	0.41
1:B:137:ALA:HB2	1:B:171:ARG:CZ	2.51	0.41
1:C:152:VAL:HG13	1:C:152:VAL:O	2.20	0.41
1:B:123:LEU:HD22	1:B:147:ILE:HB	2.03	0.41
1:D:77:GLU:H	1:D:77:GLU:CD	2.24	0.41
1:C:184:CYS:O	1:C:186:THR:N	2.54	0.41
1:D:190:VAL:HG12	1:D:192:PRO:HD2	2.03	0.41
1:A:98:ILE:HG22	1:A:99:GLN:N	2.35	0.40
1:A:140:VAL:HG13	1:A:165:TRP:CD1	2.56	0.40
1:B:13:ILE:HD11	1:B:23:GLN:CG	2.48	0.40
1:B:37:GLY:C	1:B:71:GLN:HG2	2.41	0.40
1:D:18:ILE:CD1	1:D:212:ILE:HD11	2.51	0.40
1:A:98:ILE:CG2	1:A:99:GLN:N	2.85	0.40
1:B:76:THR:O	1:B:79:ILE:HB	2.19	0.40
1:A:2:ASN:HB3	1:A:5:ASP:CB	2.49	0.40
1:C:161:LEU:HB3	1:C:165:TRP:HZ3	1.87	0.40
1:C:169:CYS:O	1:C:172:CYS:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:NH1	1:A:118:ARG:NH1[52_565]	1.65	0.55

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	242/253 (96%)	208 (86%)	24 (10%)	10 (4%)	3	3
1	B	228/253 (90%)	198 (87%)	23 (10%)	7 (3%)	4	6
1	C	242/253 (96%)	202 (84%)	28 (12%)	12 (5%)	2	2
1	D	231/253 (91%)	203 (88%)	23 (10%)	5 (2%)	6	11
All	All	943/1012 (93%)	811 (86%)	98 (10%)	34 (4%)	3	5

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	68	LEU
1	A	186	THR
1	C	127	ASP
1	C	143	ASN
1	C	181	GLU
1	C	186	THR
1	D	163	PRO
1	A	19	ALA
1	A	109	GLY
1	B	79	ILE
1	B	163	PRO
1	C	176	ASP
1	C	185	ARG
1	D	128	ASN
1	A	143	ASN
1	A	238	SER
1	B	68	LEU
1	B	104	GLN
1	B	239	GLY
1	B	243	CYS
1	C	59	ASP
1	D	68	LEU
1	A	163	PRO
1	C	242	VAL
1	D	127	ASP
1	D	238	SER
1	A	215	PRO
1	A	241	PRO
1	C	116	VAL
1	C	72	ILE

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Mol	Chain	Res	Type
1	C	241	PRO
1	C	109	GLY
1	B	242	VAL

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	199/205 (97%)	187 (94%)	12 (6%)	19	33
1	B	187/205 (91%)	177 (95%)	10 (5%)	22	38
1	C	199/205 (97%)	189 (95%)	10 (5%)	24	42
1	D	190/205 (93%)	178 (94%)	12 (6%)	18	31
All	All	775/820 (94%)	731 (94%)	44 (6%)	20	36

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	11	ARG
1	A	21	ASP
1	A	34	ILE
1	A	41	THR
1	A	54	THR
1	A	70	ARG
1	A	90	ARG
1	A	99	GLN
1	A	163	PRO
1	A	172	CYS
1	A	176	ASP
1	B	41	THR
1	B	79	ILE
1	B	88	GLN
1	B	108	THR
1	B	127	ASP
1	B	163	PRO

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Mol	Chain	Res	Type
1	B	167	GLN
1	B	174	TRP
1	B	194	VAL
1	B	235	ARG
1	C	11	ARG
1	C	45	LEU
1	C	62	ASP
1	C	70	ARG
1	C	88	GLN
1	C	114	ASP
1	C	135	ILE
1	C	171	ARG
1	C	189	VAL
1	C	194	VAL
1	D	41	THR
1	D	81	ARG
1	D	85	GLN
1	D	105	GLN
1	D	108	THR
1	D	148	THR
1	D	158	LEU
1	D	163	PRO
1	D	169	CYS
1	D	194	VAL
1	D	197	MET
1	D	242	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	12	GLN
1	A	67	ASN
1	A	99	GLN
1	A	136	ASN
1	A	143	ASN
1	A	201	GLN
1	B	12	GLN
1	B	23	GLN
1	B	85	GLN
1	B	93	GLN
1	B	104	GLN

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Mol	Chain	Res	Type
1	B	128	ASN
1	B	167	GLN
1	B	201	GLN
1	C	23	GLN
1	C	30	GLN
1	C	67	ASN
1	C	69	GLN
1	C	128	ASN
1	C	157	GLN
1	C	177	ASN
1	C	201	GLN
1	D	12	GLN
1	D	30	GLN
1	D	67	ASN
1	D	69	GLN
1	D	95	ASN
1	D	104	GLN
1	D	105	GLN
1	D	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	A	253	-	26,33,33	1.98	8 (30%)	31,52,52	2.21	11 (35%)
3	ATP	B	253	-	26,33,33	1.92	8 (30%)	31,52,52	2.20	11 (35%)
3	ATP	D	446	-	26,33,33	2.01	8 (30%)	31,52,52	2.16	9 (29%)
3	ATP	C	346	-	26,33,33	1.69	7 (26%)	31,52,52	2.28	12 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	253	-	-	8/18/38/38	0/3/3/3
3	ATP	B	253	-	-	9/18/38/38	0/3/3/3
3	ATP	D	446	-	-	9/18/38/38	0/3/3/3
3	ATP	C	346	-	-	10/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	446	ATP	C2'-C1'	-5.50	1.45	1.53
3	B	253	ATP	C2'-C1'	-4.88	1.46	1.53
3	A	253	ATP	C2'-C1'	-4.52	1.46	1.53
3	A	253	ATP	C2-N3	4.46	1.39	1.32
3	C	346	ATP	C2-N3	4.15	1.38	1.32
3	B	253	ATP	C2-N3	4.15	1.38	1.32
3	D	446	ATP	C2-N3	4.08	1.38	1.32
3	C	346	ATP	C2'-C1'	-3.77	1.48	1.53
3	B	253	ATP	C2-N1	3.36	1.40	1.33
3	A	253	ATP	C2-N1	3.34	1.40	1.33
3	D	446	ATP	C2-N1	3.17	1.39	1.33
3	A	253	ATP	C3'-C4'	3.10	1.60	1.53
3	A	253	ATP	PA-O1A	-3.07	1.40	1.50
3	C	346	ATP	C2-N1	3.04	1.39	1.33
3	D	446	ATP	O4'-C4'	-2.96	1.38	1.45
3	C	346	ATP	C3'-C4'	2.79	1.60	1.53
3	D	446	ATP	PA-O1A	-2.68	1.41	1.50
3	B	253	ATP	O4'-C4'	-2.66	1.39	1.45
3	B	253	ATP	O5'-C5'	-2.56	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	253	ATP	PA-O1A	-2.55	1.41	1.50
3	D	446	ATP	C3'-C4'	2.53	1.59	1.53
3	D	446	ATP	O5'-C5'	-2.48	1.35	1.44
3	A	253	ATP	O4'-C4'	-2.47	1.39	1.45
3	A	253	ATP	PG-O1G	-2.43	1.42	1.50
3	D	446	ATP	PG-O1G	-2.43	1.42	1.50
3	B	253	ATP	C3'-C4'	2.42	1.59	1.53
3	A	253	ATP	O5'-C5'	-2.42	1.35	1.44
3	C	346	ATP	PG-O2G	2.27	1.63	1.54
3	C	346	ATP	PA-O1A	-2.11	1.43	1.50
3	C	346	ATP	O5'-C5'	-2.09	1.36	1.44
3	B	253	ATP	PG-O1G	-2.00	1.44	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	253	ATP	N3-C2-N1	-6.11	119.12	128.68
3	A	253	ATP	N3-C2-N1	-6.11	119.12	128.68
3	D	446	ATP	N3-C2-N1	-6.07	119.19	128.68
3	C	346	ATP	N3-C2-N1	-5.87	119.51	128.68
3	C	346	ATP	O4'-C4'-C5'	4.24	123.34	109.37
3	B	253	ATP	O3'-C3'-C2'	4.24	125.55	111.82
3	D	446	ATP	O3'-C3'-C2'	4.24	125.55	111.82
3	C	346	ATP	O3'-C3'-C2'	4.09	125.04	111.82
3	A	253	ATP	O3'-C3'-C2'	3.91	124.47	111.82
3	C	346	ATP	C5-C6-N6	3.87	126.24	120.35
3	B	253	ATP	O4'-C4'-C5'	3.85	122.05	109.37
3	D	446	ATP	O4'-C4'-C5'	3.85	122.04	109.37
3	A	253	ATP	O4'-C4'-C5'	3.79	121.83	109.37
3	D	446	ATP	C3'-C2'-C1'	3.55	106.32	100.98
3	A	253	ATP	C5-C6-N6	3.38	125.49	120.35
3	B	253	ATP	C5-C6-N6	3.12	125.09	120.35
3	B	253	ATP	O3G-PG-O1G	-3.09	98.59	110.68
3	D	446	ATP	C5-C6-N6	3.07	125.02	120.35
3	C	346	ATP	C3'-C2'-C1'	3.07	105.60	100.98
3	B	253	ATP	O2G-PG-O1G	3.06	122.68	110.68
3	D	446	ATP	O3G-PG-O1G	-3.00	98.94	110.68
3	D	446	ATP	O2G-PG-O1G	2.98	122.37	110.68
3	A	253	ATP	C3'-C2'-C1'	2.97	105.45	100.98
3	A	253	ATP	O3G-PG-O1G	-2.96	99.10	110.68
3	B	253	ATP	C2'-C3'-C4'	-2.90	97.00	102.64
3	C	346	ATP	O3G-PG-O2G	2.80	118.36	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	253	ATP	O3G-PG-O2G	2.72	118.05	107.64
3	A	253	ATP	C2'-C3'-C4'	-2.72	97.36	102.64
3	C	346	ATP	O3G-PG-O1G	-2.71	100.08	110.68
3	A	253	ATP	O2G-PG-O1G	2.70	121.26	110.68
3	C	346	ATP	C2'-C3'-C4'	-2.63	97.54	102.64
3	D	446	ATP	O3G-PG-O2G	2.58	117.51	107.64
3	B	253	ATP	O4'-C1'-C2'	-2.54	103.21	106.93
3	B	253	ATP	O3G-PG-O2G	2.48	117.12	107.64
3	B	253	ATP	C3'-C2'-C1'	2.45	104.66	100.98
3	C	346	ATP	O2G-PG-O1G	2.34	119.84	110.68
3	B	253	ATP	C1'-N9-C4	-2.30	122.61	126.64
3	C	346	ATP	O4'-C1'-C2'	-2.29	103.58	106.93
3	A	253	ATP	O4'-C1'-C2'	-2.23	103.67	106.93
3	D	446	ATP	C2'-C3'-C4'	-2.21	98.34	102.64
3	C	346	ATP	O5'-C5'-C4'	2.15	116.37	108.99
3	C	346	ATP	C1'-N9-C4	-2.11	122.94	126.64
3	A	253	ATP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	253	ATP	PB-O3B-PG-O2G
3	A	253	ATP	C5'-O5'-PA-O3A
3	D	446	ATP	PB-O3B-PG-O2G
3	D	446	ATP	PB-O3A-PA-O5'
3	D	446	ATP	C5'-O5'-PA-O2A
3	D	446	ATP	C5'-O5'-PA-O3A
3	B	253	ATP	PB-O3B-PG-O2G
3	B	253	ATP	PB-O3A-PA-O5'
3	B	253	ATP	C5'-O5'-PA-O1A
3	B	253	ATP	C5'-O5'-PA-O2A
3	B	253	ATP	O4'-C4'-C5'-O5'
3	C	346	ATP	C5'-O5'-PA-O1A
3	C	346	ATP	C5'-O5'-PA-O2A
3	A	253	ATP	O4'-C4'-C5'-O5'
3	A	253	ATP	C3'-C4'-C5'-O5'
3	D	446	ATP	O4'-C4'-C5'-O5'
3	D	446	ATP	C3'-C4'-C5'-O5'
3	B	253	ATP	C3'-C4'-C5'-O5'
3	C	346	ATP	O4'-C4'-C5'-O5'
3	C	346	ATP	C3'-C4'-C5'-O5'

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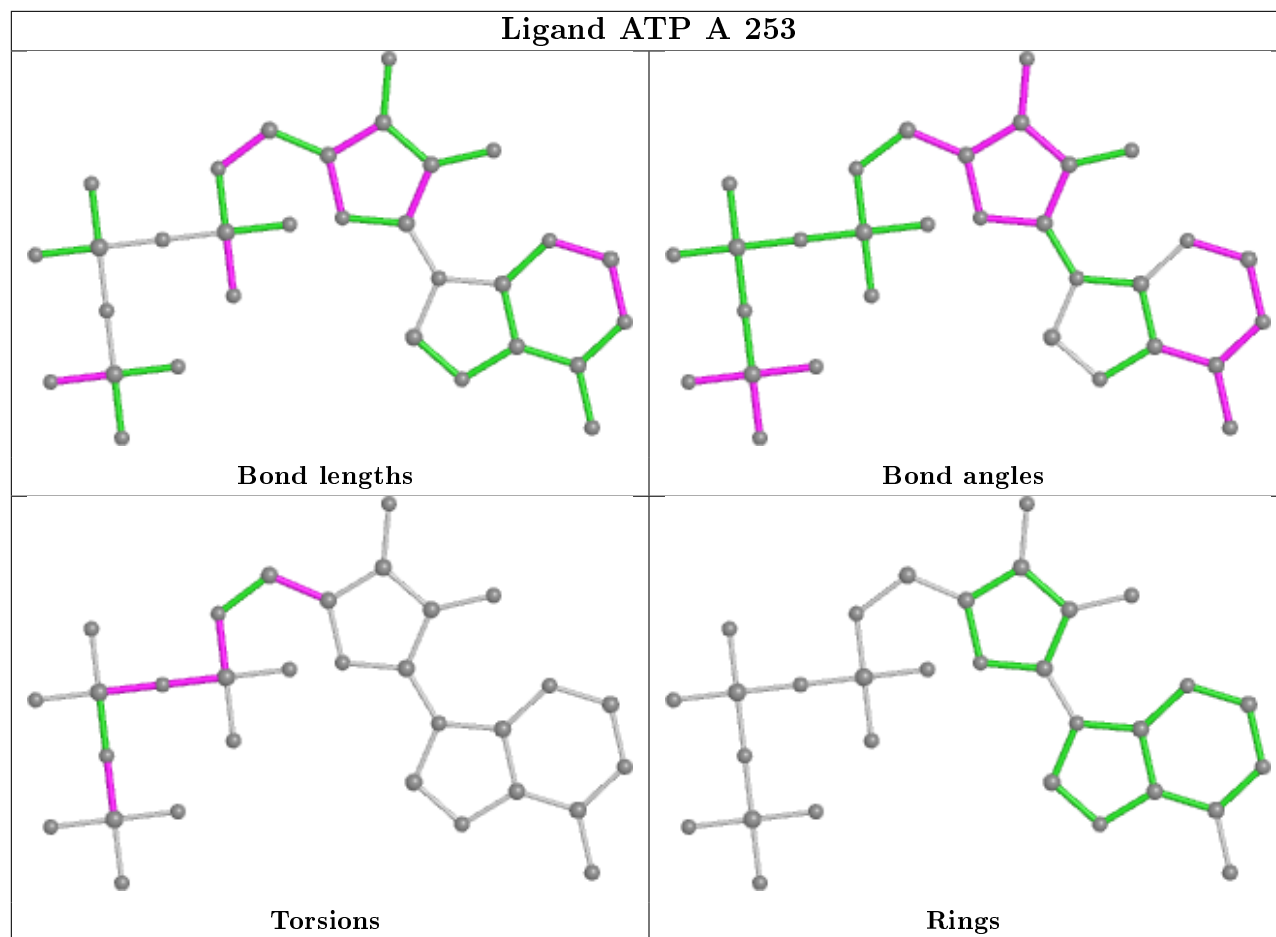
Mol	Chain	Res	Type	Atoms
3	A	253	ATP	PB-O3A-PA-O5'
3	C	346	ATP	PB-O3A-PA-O5'
3	D	446	ATP	PB-O3B-PG-O1G
3	B	253	ATP	PB-O3B-PG-O1G
3	C	346	ATP	PB-O3B-PG-O1G
3	A	253	ATP	PA-O3A-PB-O1B
3	D	446	ATP	PA-O3A-PB-O1B
3	B	253	ATP	PA-O3A-PB-O1B
3	C	346	ATP	PA-O3A-PB-O1B
3	A	253	ATP	C5'-O5'-PA-O2A
3	A	253	ATP	PB-O3B-PG-O1G
3	C	346	ATP	PB-O3B-PG-O2G
3	B	253	ATP	C5'-O5'-PA-O3A
3	C	346	ATP	C5'-O5'-PA-O3A
3	D	446	ATP	PA-O3A-PB-O2B
3	C	346	ATP	PA-O3A-PB-O2B

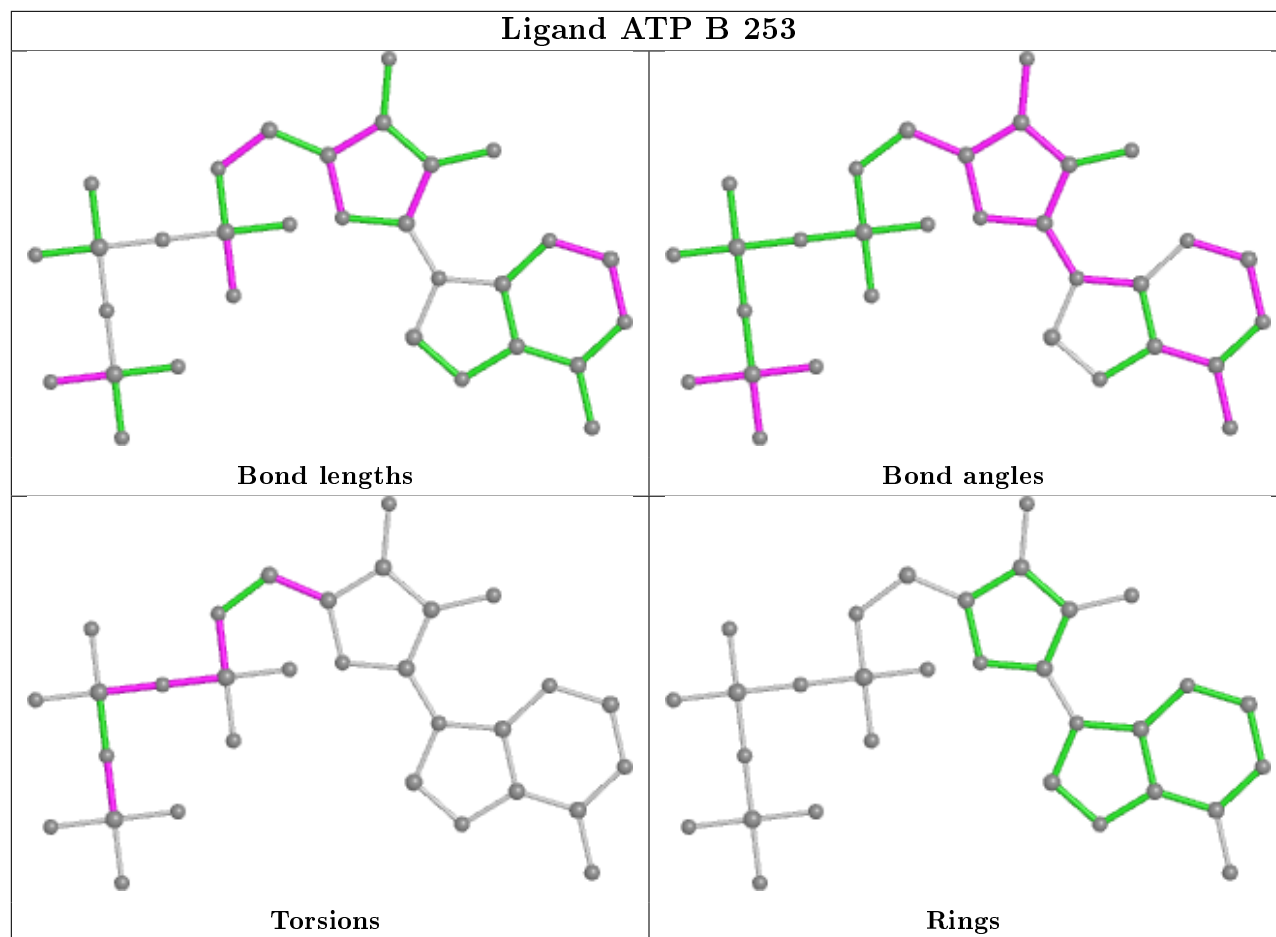
There are no ring outliers.

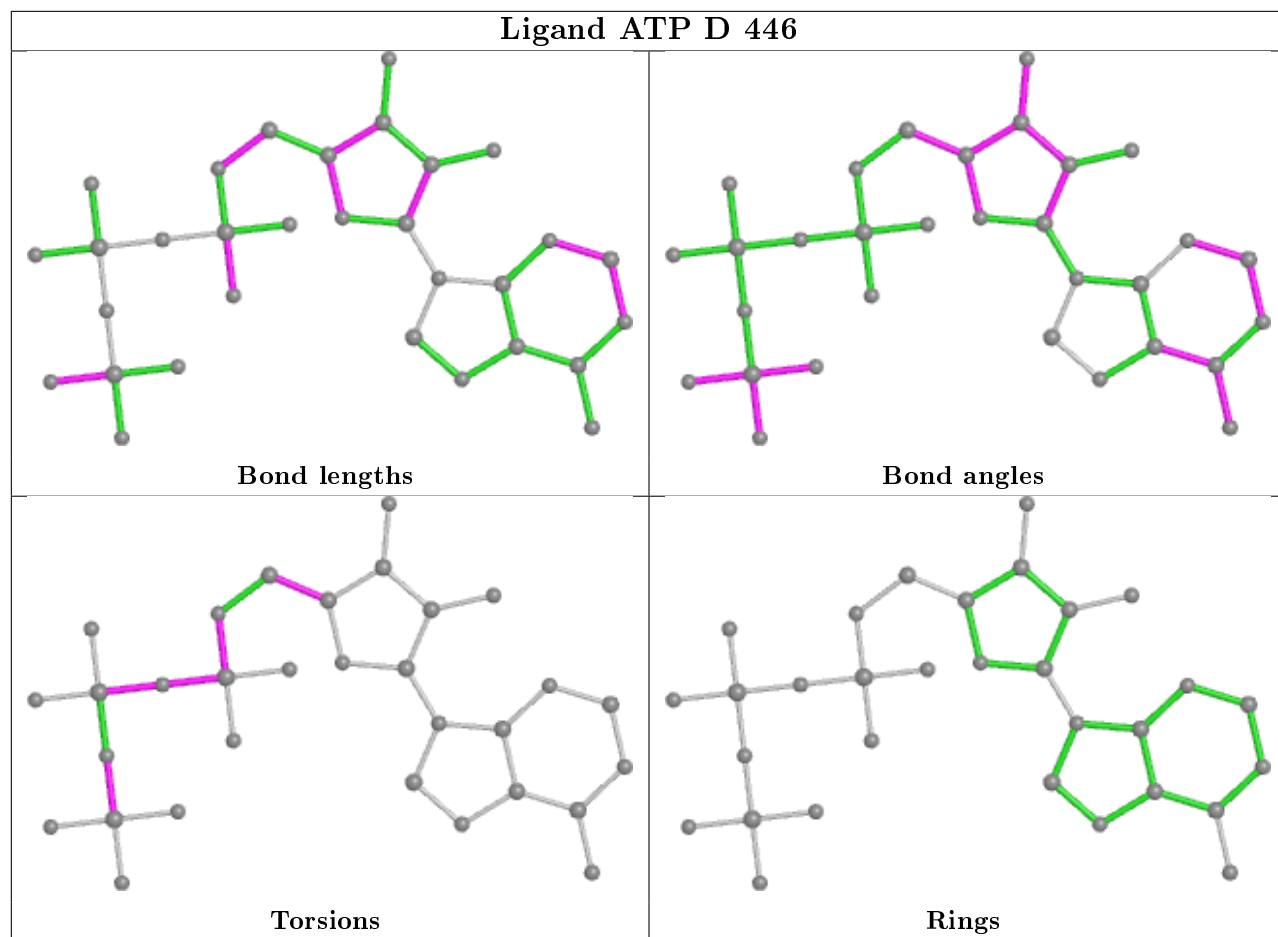
2 monomers are involved in 3 short contacts:

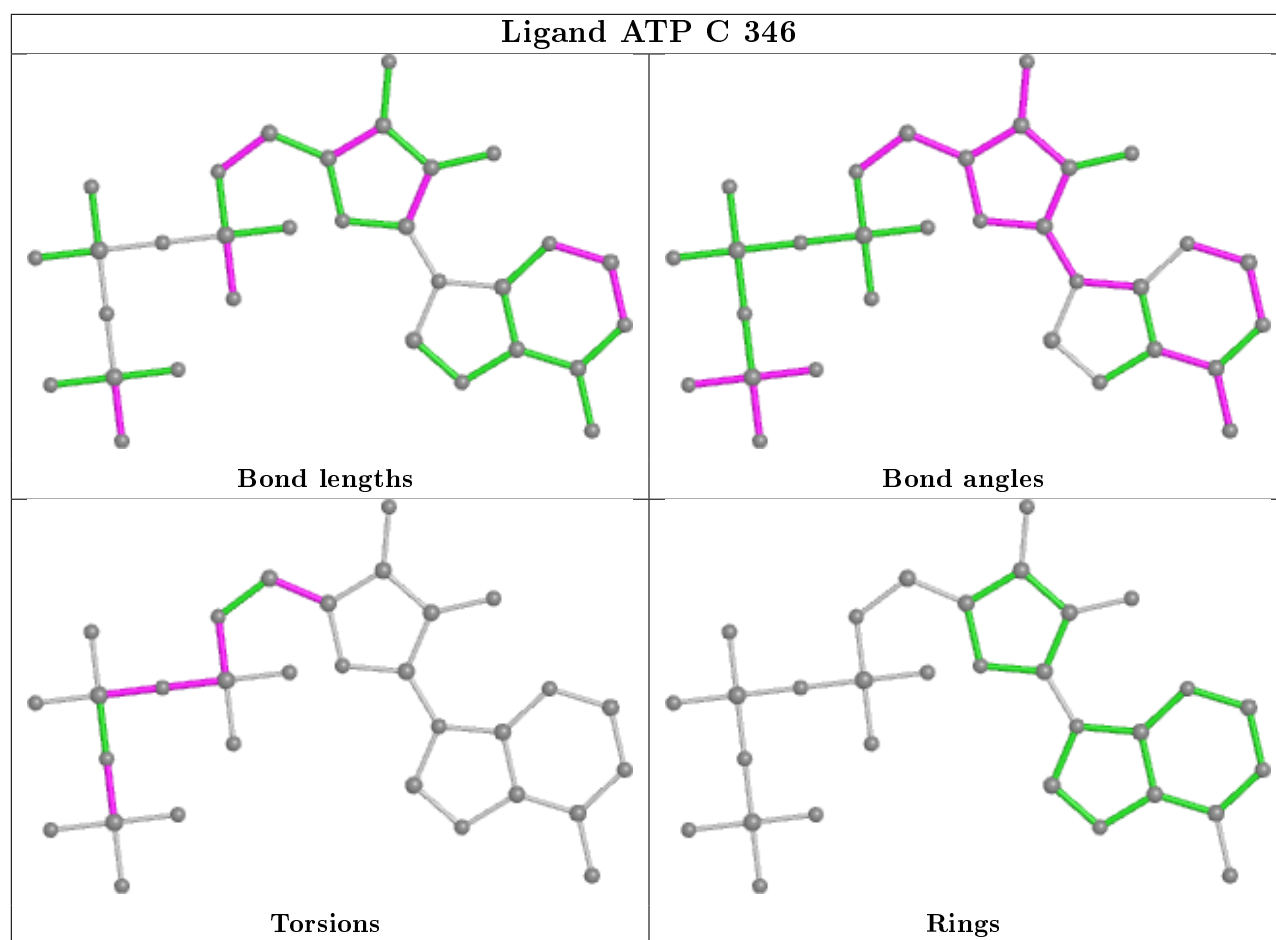
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	446	ATP	2	0
3	C	346	ATP	1	0

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, 95th 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	244/253 (96%)	0.13	10 (4%) 37 44	33, 63, 100, 141	0
1	B	232/253 (91%)	0.18	9 (3%) 39 46	35, 58, 88, 105	0
1	C	244/253 (96%)	0.23	12 (4%) 29 36	32, 70, 106, 136	0
1	D	235/253 (92%)	0.22	14 (5%) 21 26	32, 56, 92, 141	0
All	All	955/1012 (94%)	0.19	45 (4%) 31 37	32, 61, 100, 141	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ARG	5.5
1	A	185	ARG	4.2
1	D	177	ASN	4.1
1	C	186	THR	4.0
1	A	186	THR	3.9
1	A	184	CYS	3.9
1	D	238	SER	3.7
1	A	1	MET	3.6
1	B	238	SER	3.5
1	D	239	GLY	3.5
1	D	163	PRO	3.5
1	D	242	VAL	3.4
1	D	171	ARG	3.3
1	A	187	ALA	3.3
1	A	238	SER	3.3
1	D	241	PRO	3.2
1	C	4	ARG	3.1
1	C	187	ALA	3.1
1	A	163	PRO	2.9
1	C	105	GLN	2.9
1	C	185	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	178	GLN	2.8
1	B	1	MET	2.8
1	D	140	VAL	2.8
1	D	6	PHE	2.7
1	D	174	TRP	2.6
1	D	235	ARG	2.5
1	B	60	ASP	2.4
1	A	176	ASP	2.4
1	B	244	GLY	2.3
1	D	60	ASP	2.3
1	A	243	CYS	2.3
1	A	182	ARG	2.3
1	D	1	MET	2.2
1	C	6	PHE	2.2
1	D	176	ASP	2.2
1	B	103	LEU	2.1
1	C	238	SER	2.1
1	C	163	PRO	2.1
1	B	106	ARG	2.1
1	B	213	GLU	2.1
1	C	98	ILE	2.0
1	B	163	PRO	2.0
1	C	241	PRO	2.0
1	C	236	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

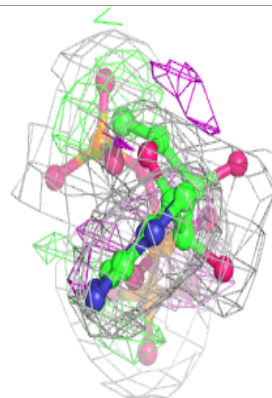
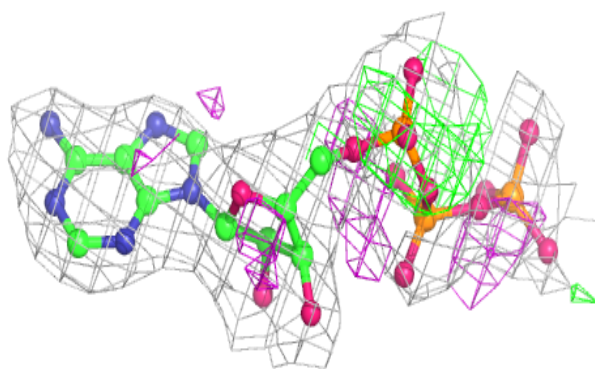
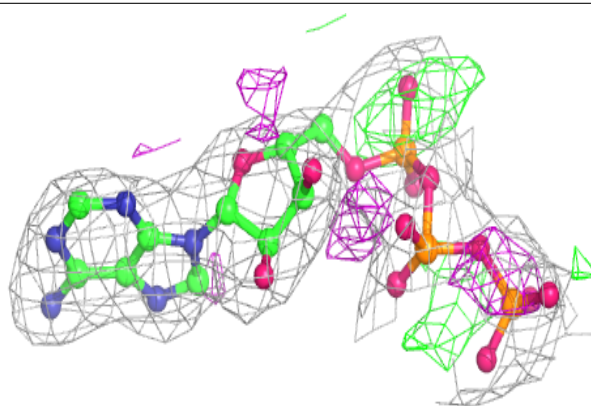
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	C	346	31/31	0.86	0.18	54,60,92,94	0
3	ATP	B	253	31/31	0.93	0.16	46,49,69,70	0
3	ATP	D	446	31/31	0.94	0.16	40,44,59,61	0
3	ATP	A	253	31/31	0.95	0.17	47,54,63,63	0
2	ZN	B	252	1/1	0.96	0.10	69,69,69,69	0
2	ZN	C	345	1/1	0.97	0.09	67,67,67,67	0
2	ZN	D	445	1/1	0.98	0.07	73,73,73,73	0
2	ZN	A	252	1/1	0.99	0.08	64,64,64,64	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.

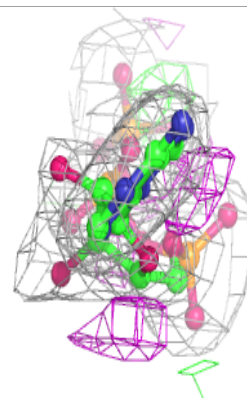
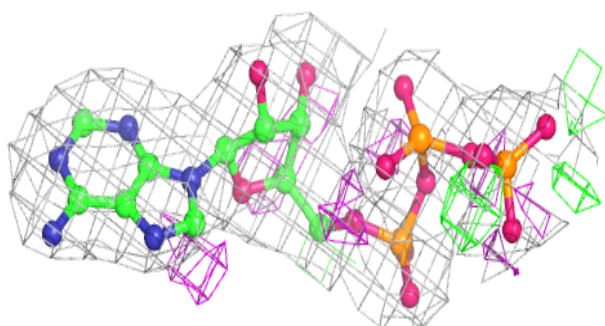
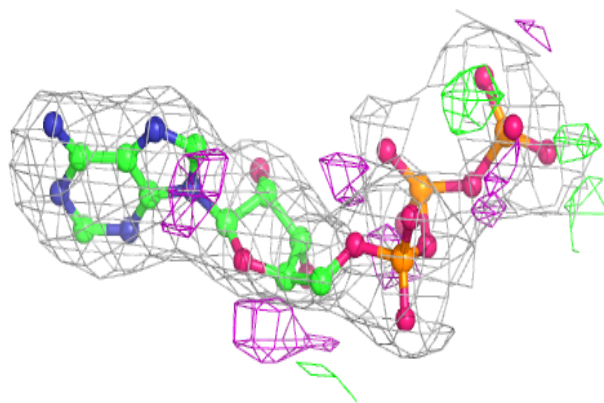
Electron density around ATP C 346:

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

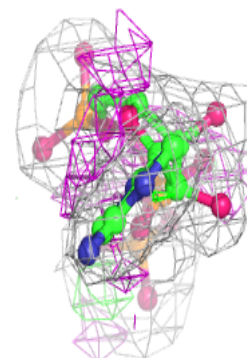
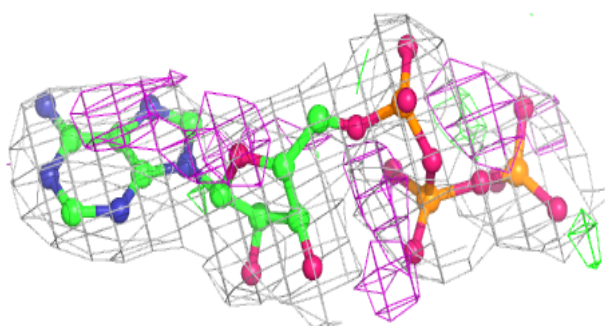
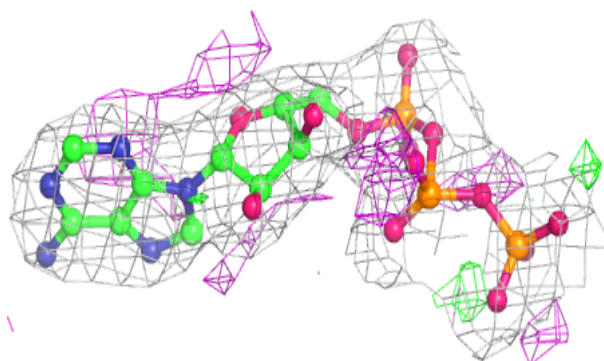


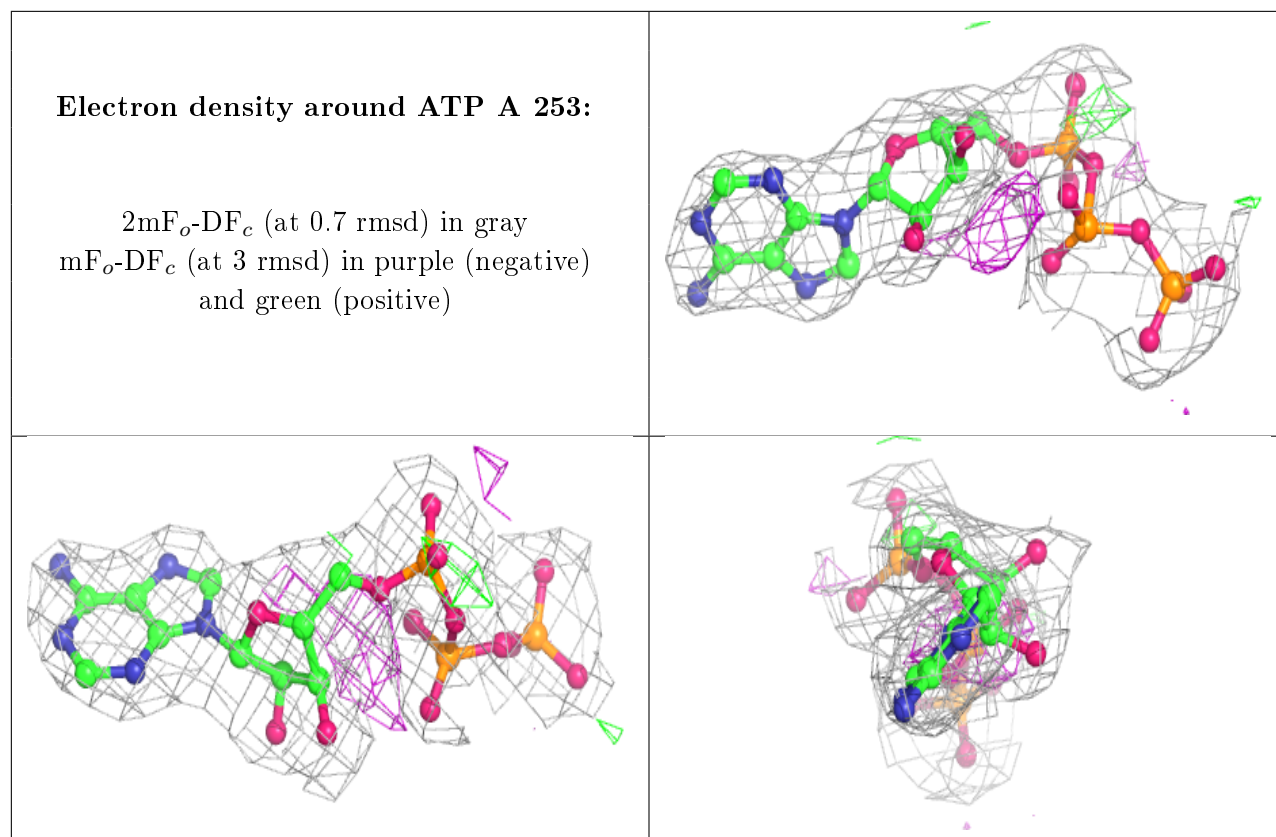
Electron density around ATP B 253:

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

**Electron density around ATP D 446:**

$2mF_o-DF_c$ (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.