Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 07:53 AM EDT

PDB ID	:	3TPQ
Title	:	Crystal structure of wild-type MAL RPEL domain in complex with five G-actins
Authors	:	Hirano, H.; Matsuura, Y.
Deposited on	:	2011-09-08
Resolution	:	3.45 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 (i) 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 (i)) were used in the production of this report:

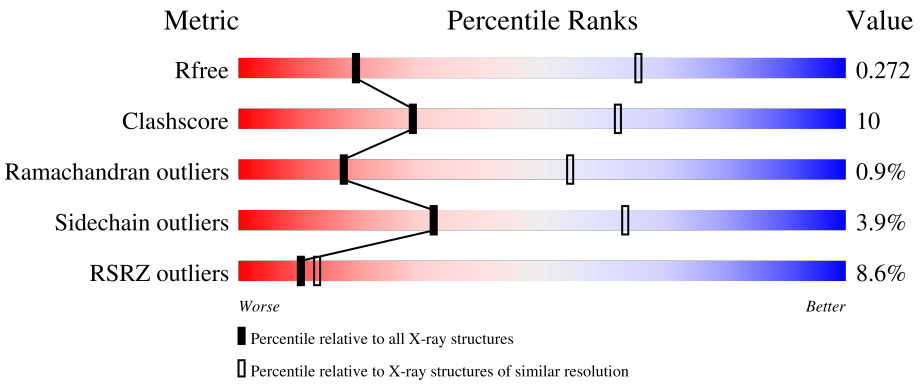
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	375	% 74% 16% • • 8%
1	B	375	3% 75% 18% • 5%
1	C	375	6% 82% 11% • • 5%
1	D	375	5% 81% 13% • 5%
1	E	375	27% 74% 9% • 15%

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Mol	Chain	Length	Quality of chain
2	M	117	29% 51% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14613 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.

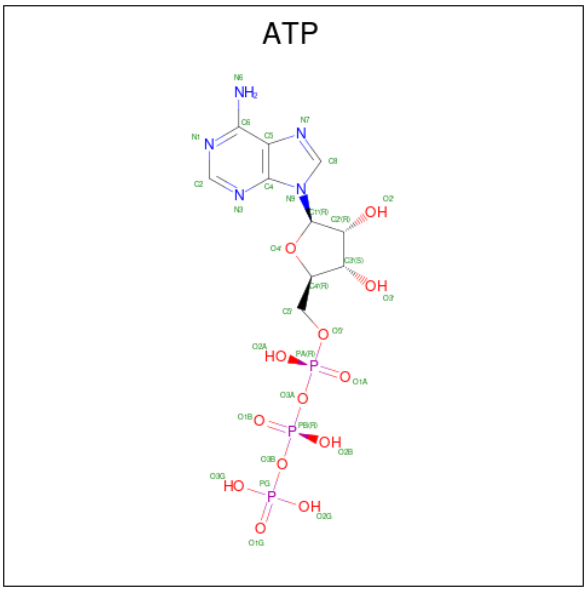
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	2700	1714	448	519	19	0	0	0
1	B	358	2790	1771	464	536	19	0	0	0
1	C	358	2784	1768	461	536	19	0	0	0
1	D	358	2794	1773	464	538	19	0	0	0
1	E	318	2485	1581	412	474	18	0	0	0

- Molecule 2 is a protein called MAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	117	900	556	174	167	3	0	0	0

- Molecule 3 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		
3	A	1	31	10	5	13	3	0	0
3	B	1	31	10	5	13	3	0	0
3	C	1	31	10	5	13	3	0	0
3	D	1	31	10	5	13	3	0	0
3	E	1	31	10	5	13	3	0	0

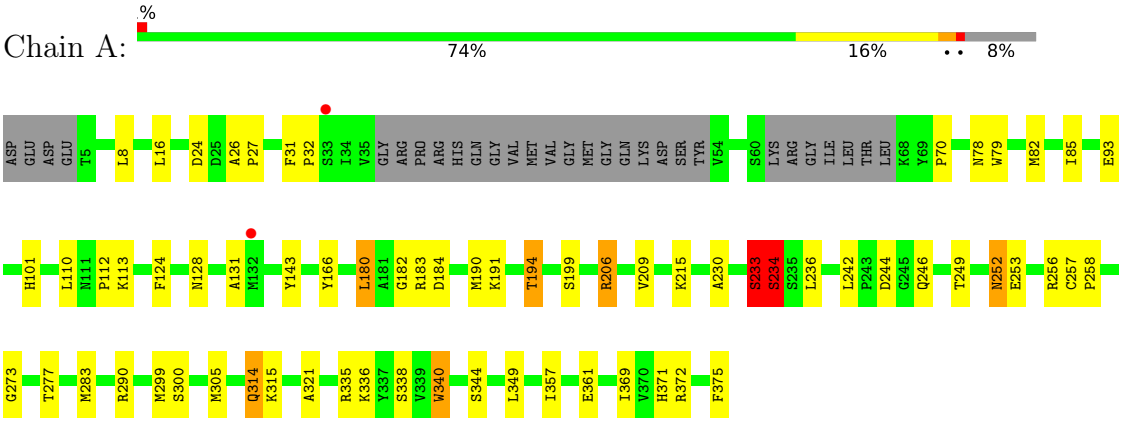
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0

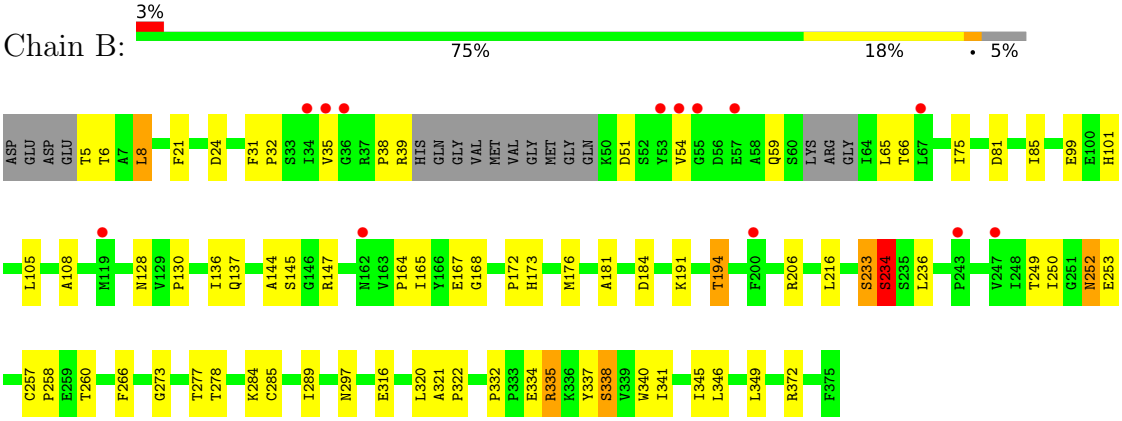
3 Residue-property plots (i)

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.

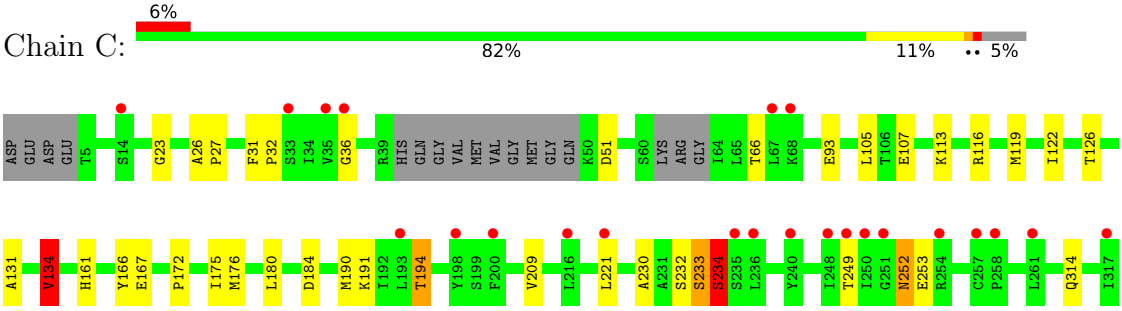
• Molecule 1: Actin, alpha skeletal muscle

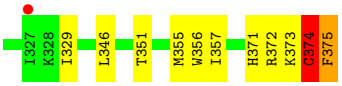


• Molecule 1: Actin, alpha skeletal muscle



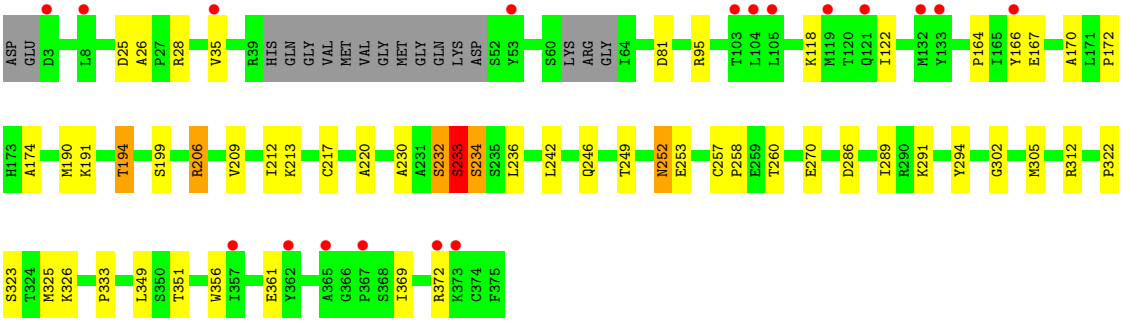
• Molecule 1: Actin, alpha skeletal muscle





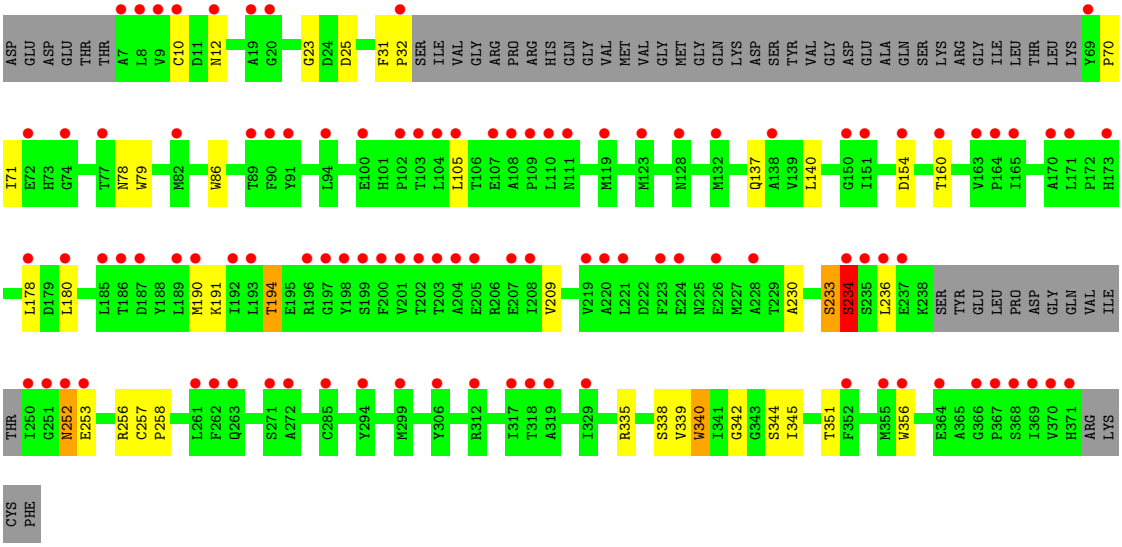
• Molecule 1: Actin, alpha skeletal muscle

Chain D:



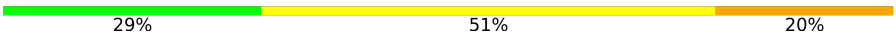
• Molecule 1: Actin, alpha skeletal muscle

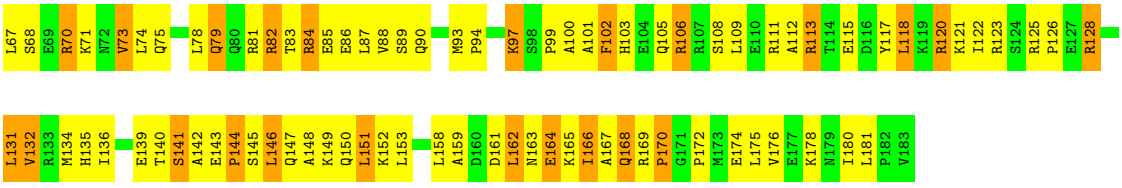
Chain E:



• Molecule 2: MAL

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.74Å 180.74Å 382.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.70 – 3.45 68.70 – 3.45	Depositor EDS
% Data completeness (in resolution range)	84.3 (68.70-3.45) 84.3 (68.70-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.273 0.224 , 0.272	Depositor DCC
R_{free} test set	2080 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	111.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 105.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14613	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CA

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	0.70	2/2758 (0.1%)	0.80	1/3740 (0.0%)
1	B	0.78	0/2850	0.91	5/3865 (0.1%)
1	C	0.71	0/2844	0.84	5/3858 (0.1%)
1	D	0.71	1/2854 (0.0%)	0.84	1/3870 (0.0%)
1	E	0.60	4/2539 (0.2%)	0.71	0/3443
2	M	0.82	1/911 (0.1%)	1.03	3/1231 (0.2%)
All	All	0.71	8/14756 (0.1%)	0.84	15/20007 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	161	ASP	CB-CG	7.93	1.68	1.51
1	A	340	TRP	CD2-CE2	6.34	1.49	1.41
1	E	340	TRP	CD2-CE2	5.36	1.47	1.41
1	A	79	TRP	CD2-CE2	5.35	1.47	1.41
1	E	86	TRP	CD2-CE2	5.30	1.47	1.41
1	E	79	TRP	CD2-CE2	5.28	1.47	1.41
1	D	356	TRP	CD2-CE2	5.10	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	356	TRP	CD2-CE2	5.06	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	119	MET	CG-SD-CE	6.66	110.85	100.20
1	D	206	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	374	CYS	N-CA-C	6.52	128.62	111.00
2	M	162	LEU	CA-CB-CG	6.41	130.05	115.30
2	M	70	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	M	131	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	346	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	C	134	VAL	CB-CA-C	-5.76	100.46	111.40
1	B	335	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	C	346	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	B	147	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	119	MET	CB-CG-SD	-5.29	96.54	112.40
1	B	105	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	299	MET	CG-SD-CE	5.19	108.50	100.20
1	B	8	LEU	CB-CG-CD1	-5.04	102.42	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	SER	Peptide
1	A	234	SER	Peptide
1	B	234	SER	Peptide
1	C	234	SER	Peptide
1	D	233	SER	Peptide
1	D	234	SER	Peptide
1	E	234	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2700	0	2648	54	0
1	B	2790	0	2735	47	0
1	C	2784	0	2724	46	0
1	D	2794	0	2739	40	0
1	E	2485	0	2445	33	0
2	M	900	0	885	108	0
3	A	31	0	12	2	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	14613	0	14236	280	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 10.

All (280) 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:C:372:ARG:O	1:C:373:LYS:HG2	1.23	1.27
2:M:106:ARG:HH11	2:M:106:ARG:HG2	1.18	1.02
1:D:166:TYR:CD1	2:M:175:LEU:HD21	1.96	1.00
2:M:131:LEU:HD12	2:M:136:ILE:HG21	1.44	0.97
1:C:113:LYS:HB3	1:C:371:HIS:HE1	1.29	0.94
1:E:23:GLY:HA2	2:M:142:ALA:HB1	1.50	0.93
1:C:113:LYS:CB	1:C:371:HIS:HE1	1.84	0.90
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.54	0.88
1:D:191:LYS:O	1:D:194:THR:HB	1.72	0.88
1:A:215:LYS:CD	2:M:82:ARG:HH12	1.87	0.87
1:A:112:PRO:HB3	1:E:25:ASP:OD2	1.73	0.87
1:C:113:LYS:HE2	1:C:371:HIS:ND1	1.89	0.87
1:B:191:LYS:O	1:B:194:THR:HB	1.74	0.86
1:C:113:LYS:HB3	1:C:371:HIS:CE1	2.11	0.84
2:M:128:ARG:HH12	2:M:140:THR:HG23	1.42	0.83
1:A:215:LYS:HD3	2:M:82:ARG:HH12	1.43	0.82
2:M:84:ARG:HA	2:M:87:LEU:HD12	1.59	0.82
1:C:113:LYS:HE2	1:C:371:HIS:HD1	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LYS:O	1:C:374:CYS:SG	2.40	0.80
2:M:143:GLU:HG2	2:M:144:PRO:HD2	1.61	0.80
1:C:372:ARG:O	1:C:373:LYS:CG	2.19	0.80
1:B:341:ILE:HG21	2:M:70:ARG:HH22	1.48	0.79
1:E:191:LYS:O	1:E:194:THR:HB	1.83	0.78
1:E:230:ALA:HB1	1:E:236:LEU:HD22	1.65	0.78
1:B:341:ILE:HG21	2:M:70:ARG:NH2	1.98	0.77
1:E:233:SER:OG	1:E:234:SER:N	2.15	0.77
1:B:233:SER:OG	1:B:234:SER:N	2.18	0.76
1:C:373:LYS:O	1:C:374:CYS:CB	2.34	0.73
1:C:113:LYS:HG2	1:C:371:HIS:CE1	2.23	0.72
2:M:106:ARG:HH11	2:M:106:ARG:CG	1.99	0.72
1:B:168:GLY:HA3	2:M:81:ARG:NH1	2.05	0.71
1:A:191:LYS:O	1:A:194:THR:HB	1.91	0.71
1:E:70:PRO:HA	1:E:78:ASN:HB3	1.72	0.71
2:M:143:GLU:HG2	2:M:144:PRO:CD	2.20	0.71
1:C:23:GLY:O	2:M:99:PRO:HA	1.91	0.71
1:E:230:ALA:CB	1:E:236:LEU:HD22	2.21	0.70
1:C:23:GLY:HA2	2:M:97:LYS:O	1.91	0.70
1:B:176:MET:HE2	1:B:284:LYS:HD2	1.73	0.70
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.74	0.70
1:C:372:ARG:C	1:C:373:LYS:HG2	2.11	0.70
1:B:345:ILE:HG23	2:M:71:LYS:HG3	1.73	0.69
2:M:83:THR:HG22	2:M:86:GLU:CD	2.13	0.69
1:A:233:SER:OG	1:A:234:SER:N	2.23	0.69
2:M:168:GLN:O	2:M:168:GLN:HG2	1.93	0.68
1:C:113:LYS:CG	1:C:371:HIS:HE1	2.08	0.67
1:D:351:THR:HB	2:M:166:ILE:HD11	1.77	0.67
1:C:355:MET:SD	1:C:375:PHE:O	2.52	0.67
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.76	0.66
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.76	0.66
1:C:166:TYR:CE1	1:C:167:GLU:HG2	2.31	0.65
2:M:94:PRO:HB2	2:M:103:HIS:NE2	2.11	0.65
1:E:345:ILE:CG2	2:M:153:LEU:HD23	2.27	0.65
1:B:31:PHE:HB2	1:B:32:PRO:HD2	1.78	0.64
2:M:141:SER:CB	2:M:142:ALA:HA	2.28	0.64
1:A:112:PRO:CB	1:E:25:ASP:OD2	2.44	0.64
1:A:143:TYR:HB3	2:M:118:LEU:HD21	1.79	0.64
2:M:151:LEU:C	2:M:151:LEU:HD13	2.19	0.63
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.80	0.63
1:B:8:LEU:HG	1:B:101:HIS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.80	0.62
1:D:230:ALA:HB1	1:D:236:LEU:HD22	1.81	0.62
2:M:88:VAL:HB	2:M:93:MET:HB2	1.81	0.62
1:C:113:LYS:CG	1:C:371:HIS:CE1	2.82	0.61
1:E:230:ALA:HB1	1:E:236:LEU:CD2	2.31	0.61
1:C:167:GLU:OE2	1:C:167:GLU:HA	1.99	0.61
2:M:172:PRO:O	2:M:176:VAL:HG23	2.01	0.61
1:A:215:LYS:CD	2:M:82:ARG:NH1	2.63	0.60
2:M:112:ALA:O	2:M:113:ARG:C	2.38	0.60
1:A:252:ASN:HD22	1:A:253:GLU:N	2.00	0.60
1:D:349:LEU:HD13	2:M:163:ASN:HA	1.84	0.60
1:C:191:LYS:O	1:C:194:THR:HB	2.00	0.60
1:E:25:ASP:HA	2:M:146:LEU:HD21	1.84	0.60
1:A:230:ALA:CB	1:A:236:LEU:HD22	2.32	0.59
2:M:106:ARG:HG2	2:M:106:ARG:NH1	1.98	0.59
1:B:35:VAL:HG21	1:B:81:ASP:HB3	1.85	0.59
1:B:167:GLU:O	2:M:81:ARG:HD3	2.03	0.59
1:B:257:CYS:HB3	1:B:258:PRO:CD	2.33	0.58
1:C:372:ARG:HG2	1:C:373:LYS:N	2.18	0.58
2:M:128:ARG:O	2:M:132:VAL:HG23	2.03	0.58
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.84	0.58
1:E:335:ARG:HA	1:E:338:SER:OG	2.02	0.58
1:A:340:TRP:CZ3	1:A:344:SER:HB2	2.39	0.58
2:M:88:VAL:HG23	2:M:93:MET:O	2.03	0.58
1:D:252:ASN:HD22	1:D:253:GLU:N	2.00	0.58
1:C:131:ALA:HA	1:C:357:ILE:O	2.03	0.58
1:C:122:ILE:O	1:C:126:THR:HB	2.04	0.58
1:A:305:MET:O	2:M:90:GLN:NE2	2.37	0.58
2:M:85:GLU:O	2:M:89:SER:HB2	2.04	0.58
2:M:149:LYS:O	2:M:152:LYS:N	2.36	0.58
2:M:180:ILE:O	2:M:181:LEU:HG	2.04	0.57
1:C:105:LEU:O	1:C:134:VAL:HA	2.05	0.57
1:C:373:LYS:O	1:C:374:CYS:HB2	2.04	0.56
1:C:355:MET:HE2	1:C:375:PHE:CE1	2.40	0.56
1:D:170:ALA:O	1:D:172:PRO:HD3	2.06	0.56
1:D:294:TYR:CD2	1:D:325:MET:HG2	2.40	0.56
2:M:88:VAL:CA	2:M:93:MET:HB2	2.35	0.55
1:D:252:ASN:HD22	1:D:252:ASN:C	2.09	0.55
2:M:117:TYR:HD2	2:M:118:LEU:HD13	1.72	0.55
1:A:113:LYS:CD	2:M:143:GLU:HG3	2.37	0.54
1:B:176:MET:CE	1:B:284:LYS:HD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:131:LEU:HD12	2:M:136:ILE:CG2	2.28	0.54
1:A:252:ASN:HD22	1:A:252:ASN:C	2.11	0.54
1:E:190:MET:HG2	1:E:209:VAL:HG21	1.88	0.54
1:A:230:ALA:CA	1:A:236:LEU:HD22	2.38	0.54
1:B:260:THR:HG23	1:B:266:PHE:HB2	1.89	0.53
2:M:168:GLN:O	2:M:168:GLN:CG	2.56	0.53
2:M:73:VAL:CG2	2:M:74:LEU:N	2.72	0.53
1:C:233:SER:OG	1:C:234:SER:N	2.40	0.53
1:B:252:ASN:HD22	1:B:253:GLU:N	2.06	0.53
1:B:172:PRO:HB3	2:M:100:ALA:HB1	1.91	0.53
1:C:252:ASN:HD22	1:C:253:GLU:N	2.06	0.53
1:A:215:LYS:HD2	2:M:82:ARG:NH1	2.24	0.53
1:B:334:GLU:HG2	1:B:341:ILE:HD12	1.91	0.52
1:E:233:SER:O	1:E:234:SER:HB3	2.09	0.52
1:B:6:THR:O	1:B:6:THR:HG22	2.08	0.52
1:E:345:ILE:HG21	2:M:153:LEU:HD23	1.90	0.52
2:M:86:GLU:O	2:M:89:SER:HB3	2.10	0.52
1:D:351:THR:HG21	2:M:167:ALA:HB2	1.92	0.51
1:B:21:PHE:O	1:B:24:ASP:HB2	2.11	0.51
1:A:300:SER:HA	1:A:335:ARG:HB2	1.93	0.51
1:D:242:LEU:HD12	1:D:246:GLN:HB3	1.92	0.51
1:D:257:CYS:HB3	1:D:258:PRO:CD	2.40	0.51
1:B:349:LEU:HD21	2:M:75:GLN:HB2	1.93	0.51
2:M:83:THR:CG2	2:M:86:GLU:HG3	2.40	0.51
1:C:23:GLY:O	2:M:99:PRO:CA	2.58	0.51
1:A:290:ARG:HH12	1:D:26:ALA:HB3	1.75	0.51
1:B:233:SER:O	1:B:234:SER:CB	2.58	0.51
1:C:166:TYR:CD1	1:C:167:GLU:HG2	2.44	0.51
2:M:164:GLU:CD	2:M:165:LYS:N	2.64	0.51
1:C:113:LYS:HE2	1:C:371:HIS:CE1	2.46	0.50
1:E:233:SER:O	1:E:234:SER:CB	2.58	0.50
2:M:88:VAL:CB	2:M:93:MET:HB2	2.41	0.50
2:M:128:ARG:NH1	2:M:140:THR:HG23	2.20	0.50
1:B:273:GLY:O	1:B:277:THR:HG23	2.12	0.50
2:M:170:PRO:HA	2:M:174:GLU:OE2	2.12	0.50
1:A:31:PHE:CE2	1:A:93:GLU:HG3	2.47	0.50
1:A:16:LEU:HD23	1:A:32:PRO:HA	1.93	0.49
1:B:173:HIS:ND1	2:M:94:PRO:HG3	2.27	0.49
1:A:321:ALA:O	1:D:95:ARG:NH2	2.46	0.49
1:E:190:MET:HG3	1:E:209:VAL:HG11	1.94	0.49
1:C:107:GLU:OE1	1:C:116:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HA	1:A:78:ASN:HB3	1.95	0.49
1:A:283:MET:CE	1:D:28:ARG:HD3	2.43	0.49
1:C:26:ALA:HB1	1:C:27:PRO:HD2	1.95	0.48
1:C:31:PHE:CE2	1:C:93:GLU:HG3	2.48	0.48
1:C:375:PHE:OXT	2:M:113:ARG:NH2	2.46	0.48
1:A:113:LYS:HD2	2:M:143:GLU:HG3	1.95	0.48
1:B:335:ARG:HA	1:B:338:SER:OG	2.12	0.48
1:D:190:MET:SD	1:D:206:ARG:HG3	2.53	0.48
1:B:54:VAL:HG13	1:B:85:ILE:HD13	1.94	0.48
1:C:31:PHE:HB2	1:C:32:PRO:HD2	1.95	0.48
1:E:12:ASN:HB3	1:E:71:ILE:CD1	2.43	0.48
1:A:314:GLN:O	1:A:315:LYS:C	2.52	0.48
2:M:101:ALA:O	2:M:102:PHE:CB	2.62	0.48
1:C:161:HIS:HA	1:C:176:MET:O	2.14	0.47
1:A:180:LEU:HA	1:A:184:ASP:OD1	2.14	0.47
1:A:8:LEU:HG	1:A:101:HIS:HB3	1.97	0.47
1:C:180:LEU:HA	1:C:184:ASP:OD1	2.14	0.47
1:D:213:LYS:O	1:D:217:CYS:HB2	2.15	0.47
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.95	0.47
1:A:257:CYS:HB3	1:A:258:PRO:CD	2.44	0.47
1:B:285:CYS:HB3	1:B:289:ILE:HD11	1.97	0.47
1:E:31:PHE:HB2	1:E:32:PRO:HD2	1.95	0.47
1:E:252:ASN:ND2	1:E:256:ARG:HH11	2.13	0.47
1:A:82:MET:O	1:A:85:ILE:HB	2.14	0.47
1:B:24:ASP:HB2	1:B:340:TRP:HH2	1.79	0.47
1:E:178:LEU:HD21	1:E:180:LEU:HD23	1.97	0.47
2:M:143:GLU:CG	2:M:144:PRO:HD2	2.40	0.47
1:A:273:GLY:O	1:A:277:THR:HG23	2.15	0.47
1:C:172:PRO:HA	1:C:175:ILE:HD12	1.96	0.47
1:B:75:ILE:HD13	1:B:108:ALA:HB3	1.98	0.46
1:C:375:PHE:CD2	1:C:375:PHE:N	2.78	0.46
1:D:258:PRO:C	1:D:260:THR:N	2.67	0.46
1:E:252:ASN:HD22	1:E:253:GLU:N	2.13	0.46
1:B:252:ASN:HD22	1:B:252:ASN:C	2.19	0.46
1:D:361:GLU:HB3	1:D:369:ILE:CD1	2.45	0.46
1:E:154:ASP:O	1:E:160:THR:HA	2.16	0.46
1:E:252:ASN:HD21	1:E:256:ARG:HH11	1.63	0.46
1:D:167:GLU:O	2:M:169:ARG:NE	2.38	0.46
1:D:209:VAL:HA	1:D:212:ILE:HD12	1.98	0.46
2:M:83:THR:HG23	2:M:86:GLU:H	1.81	0.46
2:M:111:ARG:O	2:M:112:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:180:ILE:O	2:M:181:LEU:CB	2.64	0.46
1:B:144:ALA:HB1	2:M:70:ARG:HH12	1.80	0.46
1:C:131:ALA:HB1	1:C:356:TRP:HB3	1.97	0.46
1:D:234:SER:HA	1:D:236:LEU:H	1.81	0.46
1:D:233:SER:O	1:D:234:SER:HB2	2.16	0.46
1:D:291:LYS:HE2	1:D:326:LYS:HG3	1.98	0.46
2:M:120:ARG:O	2:M:122:ILE:N	2.49	0.46
1:B:164:PRO:C	1:B:165:ILE:HG13	2.36	0.45
2:M:94:PRO:HB2	2:M:103:HIS:CE1	2.50	0.45
1:A:26:ALA:HB1	1:A:27:PRO:CD	2.35	0.45
1:A:183:ARG:HG2	1:A:206:ARG:HH12	1.82	0.45
1:A:335:ARG:HA	1:A:338:SER:OG	2.17	0.45
1:B:337:TYR:O	1:B:341:ILE:HG13	2.16	0.45
1:A:131:ALA:HA	1:A:357:ILE:O	2.17	0.45
1:D:232:SER:OG	1:D:233:SER:N	2.48	0.45
1:E:23:GLY:CA	2:M:142:ALA:HB1	2.34	0.45
1:D:351:THR:HG21	2:M:167:ALA:CA	2.47	0.45
1:D:333:PRO:HB2	2:M:135:HIS:HB2	1.98	0.45
2:M:83:THR:CG2	2:M:86:GLU:CG	2.95	0.45
2:M:174:GLU:O	2:M:178:LYS:HB2	2.18	0.44
1:B:316:GLU:O	1:B:320:LEU:HG	2.18	0.44
2:M:83:THR:O	2:M:86:GLU:HB2	2.18	0.44
2:M:151:LEU:C	2:M:151:LEU:CD1	2.86	0.44
1:B:39:ARG:HA	1:B:66:THR:HG23	2.00	0.44
1:B:233:SER:O	1:B:234:SER:HB3	2.17	0.44
1:D:230:ALA:HB1	1:D:236:LEU:CD2	2.47	0.44
1:C:314:GLN:OE1	1:C:329:ILE:HG12	2.17	0.44
2:M:122:ILE:HG22	2:M:123:ARG:N	2.32	0.44
2:M:151:LEU:HD13	2:M:151:LEU:O	2.18	0.44
1:A:244:ASP:OD2	1:A:246:GLN:HG2	2.18	0.44
1:C:36:GLY:HA2	1:C:66:THR:O	2.18	0.44
1:D:220:ALA:O	1:D:312:ARG:HD3	2.18	0.44
2:M:158:LEU:HD23	2:M:159:ALA:N	2.33	0.44
1:D:286:ASP:O	1:D:289:ILE:HG12	2.18	0.43
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.78	0.43
1:B:99:GLU:O	1:B:130:PRO:HD3	2.18	0.43
1:B:181:ALA:O	1:B:184:ASP:HB2	2.18	0.43
1:A:24:ASP:HB2	1:A:340:TRP:HH2	1.82	0.43
1:B:216:LEU:HD13	1:B:250:ILE:HG21	2.00	0.43
1:A:110:LEU:HD22	2:M:145:SER:HA	2.01	0.43
1:A:215:LYS:HD3	2:M:82:ARG:NH1	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HG2	1:A:371:HIS:CE1	2.54	0.43
1:B:278:THR:HG21	1:B:297:ASN:HD21	1.84	0.43
1:C:230:ALA:C	1:C:232:SER:H	2.22	0.43
1:D:118:LYS:HE2	1:D:122:ILE:HD11	2.01	0.43
1:E:137:GLN:HA	1:E:339:VAL:HG13	2.01	0.43
1:E:345:ILE:HG22	2:M:153:LEU:HD23	2.00	0.43
2:M:134:MET:O	2:M:135:HIS:HB3	2.18	0.43
2:M:73:VAL:HG22	2:M:74:LEU:N	2.34	0.43
1:E:10:CYS:HB3	1:E:105:LEU:HD23	2.00	0.43
1:E:257:CYS:HB3	1:E:258:PRO:CD	2.49	0.42
1:A:166:TYR:CD1	2:M:131:LEU:HD11	2.54	0.42
1:A:233:SER:O	1:A:234:SER:CB	2.66	0.42
1:B:341:ILE:CG2	2:M:70:ARG:NH2	2.75	0.42
1:E:345:ILE:HG23	2:M:150:GLN:HG3	2.01	0.42
1:A:375:PHE:CE2	2:M:125:ARG:NH1	2.87	0.42
1:D:302:GLY:O	1:D:305:MET:HG2	2.20	0.42
1:E:140:LEU:O	1:E:342:GLY:HA3	2.19	0.42
2:M:139:GLU:HA	2:M:140:THR:HA	1.82	0.42
2:M:143:GLU:O	2:M:144:PRO:C	2.58	0.42
1:B:332:PRO:O	1:B:335:ARG:HG2	2.19	0.42
2:M:75:GLN:O	2:M:79:GLN:HG2	2.19	0.42
1:D:291:LYS:HA	1:D:325:MET:SD	2.60	0.42
1:D:166:TYR:CE1	2:M:175:LEU:HD21	2.48	0.42
1:A:252:ASN:ND2	1:A:256:ARG:HD3	2.35	0.41
1:D:35:VAL:HG21	1:D:81:ASP:HB3	2.02	0.41
1:D:118:LYS:HD2	1:D:118:LYS:HA	1.89	0.41
2:M:120:ARG:C	2:M:122:ILE:H	2.24	0.41
2:M:141:SER:OG	2:M:142:ALA:HA	2.20	0.41
2:M:82:ARG:HD3	2:M:87:LEU:HD21	2.02	0.41
1:A:182:GLY:HA3	3:A:1377:ATP:O3'	2.20	0.41
1:C:372:ARG:NH1	1:C:373:LYS:HE2	2.35	0.41
1:B:99:GLU:HG3	1:B:128:ASN:HB2	2.02	0.41
1:C:372:ARG:CG	1:C:373:LYS:N	2.82	0.41
1:D:190:MET:HG3	1:D:209:VAL:HG11	2.03	0.41
1:B:38:PRO:HA	1:B:65:LEU:HD23	2.02	0.41
1:B:321:ALA:HB1	1:B:322:PRO:HD2	2.02	0.41
2:M:83:THR:O	2:M:86:GLU:N	2.52	0.41
2:M:164:GLU:HA	2:M:167:ALA:HB3	2.02	0.41
1:A:314:GLN:HE21	1:A:314:GLN:HB2	1.67	0.41
1:B:136:ILE:O	1:B:137:GLN:C	2.59	0.41
2:M:78:LEU:HD23	2:M:78:LEU:HA	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:THR:CB	2:M:166:ILE:HD11	2.47	0.41
2:M:117:TYR:CZ	2:M:121:LYS:HG3	2.56	0.41
1:A:242:LEU:HD12	1:A:246:GLN:HG3	2.03	0.41
1:A:336:LYS:HE3	3:A:1377:ATP:C8	2.56	0.41
1:A:361:GLU:HB3	1:A:369:ILE:CD1	2.51	0.41
2:M:118:LEU:HD12	2:M:118:LEU:HA	1.88	0.41
1:A:349:LEU:HD11	2:M:118:LEU:HB3	2.02	0.40
2:M:131:LEU:HB3	2:M:136:ILE:HB	2.03	0.40
1:D:164:PRO:HG2	1:D:174:ALA:HB3	2.04	0.40
2:M:112:ALA:O	2:M:115:GLU:N	2.55	0.40
2:M:125:ARG:HA	2:M:126:PRO:HD3	1.81	0.40
2:M:180:ILE:HG22	2:M:181:LEU:HD23	2.02	0.40
1:A:124:PHE:O	1:A:128:ASN:HA	2.21	0.40
1:E:340:TRP:CZ3	1:E:344:SER:HB2	2.56	0.40
2:M:120:ARG:C	2:M:122:ILE:N	2.74	0.40
2:M:147:GLN:O	2:M:148:ALA:C	2.59	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	340/375 (91%)	325 (96%)	13 (4%)	2 (1%)	25 62
1	B	352/375 (94%)	339 (96%)	11 (3%)	2 (1%)	25 62
1	C	352/375 (94%)	334 (95%)	14 (4%)	4 (1%)	14 50
1	D	352/375 (94%)	337 (96%)	13 (4%)	2 (1%)	25 62
1	E	312/375 (83%)	301 (96%)	9 (3%)	2 (1%)	25 62
2	M	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	3 26
All	All	1823/1992 (92%)	1728 (95%)	79 (4%)	16 (1%)	17 54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	SER
1	B	233	SER
1	B	234	SER
1	C	374	CYS
1	E	234	SER
2	M	144	PRO
1	A	233	SER
1	C	134	VAL
1	E	233	SER
1	D	233	SER
1	C	233	SER
2	M	97	LYS
1	C	234	SER
2	M	102	PHE
1	D	322	PRO
2	M	170	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	291/318 (92%)	283 (97%)	8 (3%)	44	73
1	B	300/318 (94%)	289 (96%)	11 (4%)	34	64
1	C	299/318 (94%)	291 (97%)	8 (3%)	44	73
1	D	301/318 (95%)	292 (97%)	9 (3%)	41	70
1	E	267/318 (84%)	264 (99%)	3 (1%)	73	88
2	M	90/106 (85%)	68 (76%)	22 (24%)	0	3
All	All	1548/1696 (91%)	1487 (96%)	61 (4%)	32	64

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	194	THR
1	A	199	SER
1	A	206	ARG
1	A	249	THR
1	A	252	ASN
1	A	314	GLN
1	A	372	ARG
1	B	5	THR
1	B	51	ASP
1	B	59	GLN
1	B	145	SER
1	B	194	THR
1	B	206	ARG
1	B	236	LEU
1	B	249	THR
1	B	252	ASN
1	B	338	SER
1	B	372	ARG
1	C	51	ASP
1	C	194	THR
1	C	221	LEU
1	C	249	THR
1	C	252	ASN
1	C	351	THR
1	C	374	CYS
1	C	375	PHE
1	D	25	ASP
1	D	194	THR
1	D	199	SER
1	D	232	SER
1	D	249	THR
1	D	252	ASN
1	D	270	GLU
1	D	323	SER
1	D	372	ARG
1	E	194	THR
1	E	252	ASN
1	E	351	THR
2	M	67	LEU
2	M	68	SER
2	M	73	VAL
2	M	79	GLN

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Mol	Chain	Res	Type
2	M	82	ARG
2	M	84	ARG
2	M	105	GLN
2	M	106	ARG
2	M	108	SER
2	M	109	LEU
2	M	113	ARG
2	M	118	LEU
2	M	120	ARG
2	M	128	ARG
2	M	132	VAL
2	M	141	SER
2	M	146	LEU
2	M	151	LEU
2	M	162	LEU
2	M	164	GLU
2	M	166	ILE
2	M	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	252	ASN
1	A	280	ASN
1	A	314	GLN
1	B	252	ASN
1	B	280	ASN
1	C	161	HIS
1	C	252	ASN
1	C	280	ASN
1	C	371	HIS
1	D	246	GLN
1	D	252	ASN
1	D	280	ASN
1	E	162	ASN
1	E	173	HIS
1	E	252	ASN
1	E	280	ASN
2	M	72	ASN
2	M	79	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	1377	4	26,33,33	1.08	2 (7%)	31,52,52	1.66	6 (19%)
3	ATP	B	1377	4	26,33,33	1.03	2 (7%)	31,52,52	1.55	7 (22%)
3	ATP	C	1377	4	26,33,33	1.15	2 (7%)	31,52,52	1.42	7 (22%)
3	ATP	E	1377	4	26,33,33	0.95	1 (3%)	31,52,52	1.42	6 (19%)
3	ATP	D	1377	4	26,33,33	1.25	2 (7%)	31,52,52	1.72	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
3	ATP	A	1377	4	-	2/18/38/38	0/3/3/3
3	ATP	B	1377	4	-	1/18/38/38	0/3/3/3
3	ATP	C	1377	4	-	1/18/38/38	0/3/3/3
3	ATP	E	1377	4	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	1377	4	-	2/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1377	ATP	C2-N3	3.35	1.37	1.32
3	C	1377	ATP	C5-C4	3.02	1.48	1.40
3	E	1377	ATP	C5-C4	2.81	1.48	1.40
3	D	1377	ATP	C4-N3	-2.75	1.31	1.35
3	A	1377	ATP	C5-C4	2.59	1.47	1.40
3	B	1377	ATP	C5-C4	2.56	1.47	1.40
3	C	1377	ATP	C2-N3	2.21	1.35	1.32
3	A	1377	ATP	C2'-C1'	-2.14	1.50	1.53
3	B	1377	ATP	C2-N3	2.12	1.35	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1377	ATP	C4-C5-N7	-5.75	103.40	109.40
3	A	1377	ATP	N3-C2-N1	-3.91	122.57	128.68
3	A	1377	ATP	PA-O3A-PB	-3.84	119.65	132.83
3	B	1377	ATP	C4-C5-N7	-3.83	105.41	109.40
3	D	1377	ATP	PA-O3A-PB	-3.67	120.24	132.83
3	A	1377	ATP	C1'-N9-C4	-3.61	120.31	126.64
3	B	1377	ATP	O2B-PB-O1B	3.39	129.01	112.24
3	D	1377	ATP	O4'-C1'-C2'	-3.28	102.13	106.93
3	C	1377	ATP	C4-C5-N7	-3.24	106.02	109.40
3	E	1377	ATP	C4-C5-N7	-3.15	106.11	109.40
3	A	1377	ATP	N6-C6-N1	3.12	125.04	118.57
3	E	1377	ATP	PA-O3A-PB	-3.01	122.50	132.83
3	B	1377	ATP	O2G-PG-O3B	-2.93	94.80	104.64
3	C	1377	ATP	PA-O3A-PB	-2.86	123.03	132.83
3	B	1377	ATP	PA-O3A-PB	-2.81	123.20	132.83
3	C	1377	ATP	N3-C2-N1	-2.77	124.35	128.68
3	A	1377	ATP	C2-N1-C6	2.48	122.99	118.75
3	E	1377	ATP	O2A-PA-O1A	2.36	123.91	112.24
3	D	1377	ATP	O2G-PG-O3B	-2.30	96.92	104.64
3	B	1377	ATP	O2G-PG-O1G	2.25	119.48	110.68
3	C	1377	ATP	C1'-N9-C4	-2.18	122.80	126.64
3	C	1377	ATP	O3G-PG-O2G	2.12	115.75	107.64
3	E	1377	ATP	O2G-PG-O3B	-2.10	97.60	104.64
3	B	1377	ATP	C5-C6-N6	2.10	123.54	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1377	ATP	C2-N1-C6	-2.09	115.17	118.75
3	B	1377	ATP	PB-O3B-PG	-2.08	125.69	132.83
3	E	1377	ATP	O2B-PB-O1B	2.05	122.39	112.24
3	C	1377	ATP	PB-O3B-PG	-2.04	125.81	132.83
3	C	1377	ATP	O3G-PG-O3B	-2.02	97.86	104.64
3	E	1377	ATP	N3-C2-N1	-2.01	125.54	128.68
3	A	1377	ATP	C5-C6-N6	-2.00	117.31	120.35
3	D	1377	ATP	O3G-PG-O2G	2.00	115.29	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1377	ATP	PG-O3B-PB-O1B
3	B	1377	ATP	PG-O3B-PB-O1B
3	D	1377	ATP	PG-O3B-PB-O1B
3	E	1377	ATP	PG-O3B-PB-O1B
3	C	1377	ATP	PB-O3B-PG-O2G
3	E	1377	ATP	PG-O3B-PB-O2B
3	A	1377	ATP	C5'-O5'-PA-O1A
3	D	1377	ATP	C5'-O5'-PA-O1A

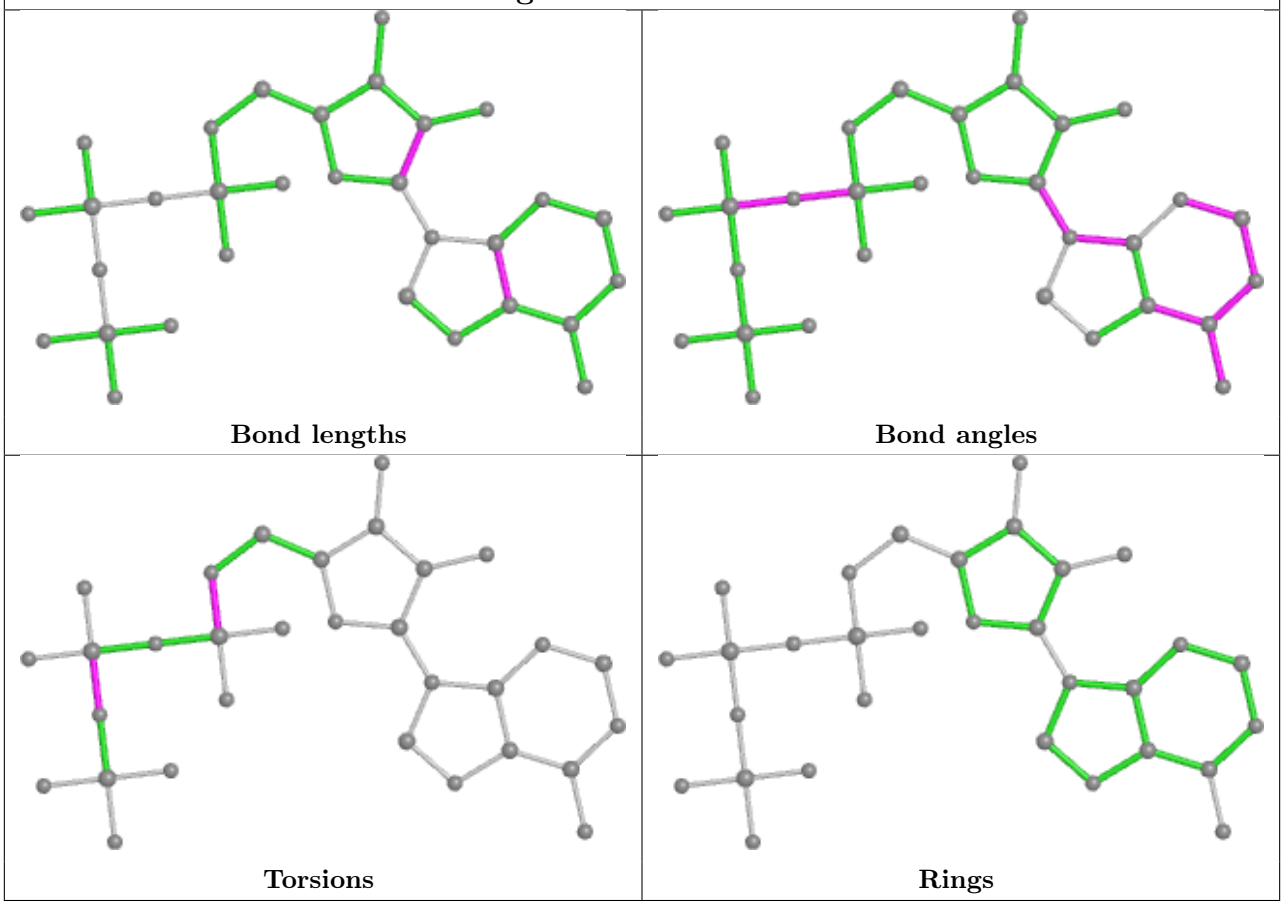
There are no ring outliers.

1 monomer is involved in 2 short contacts:

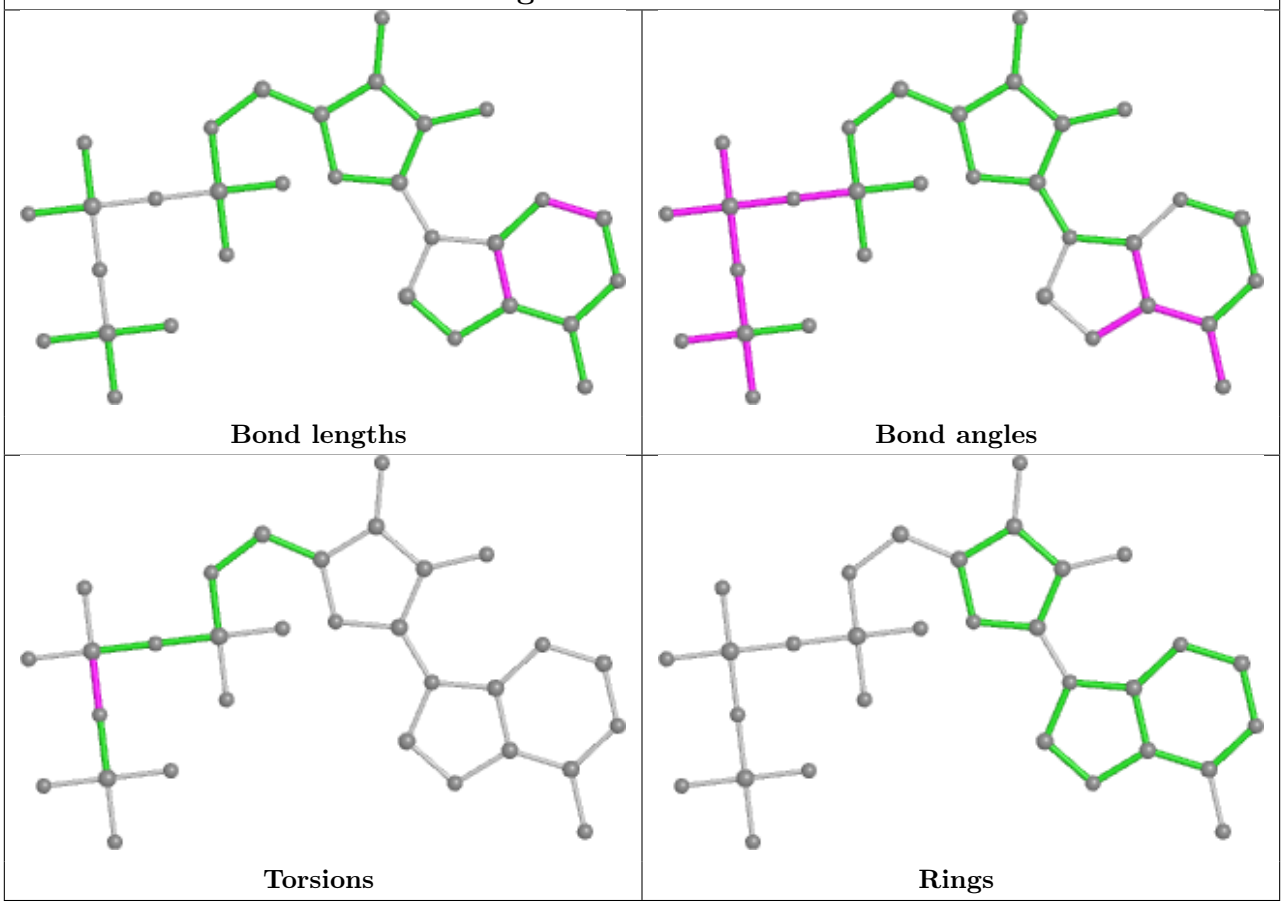
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1377	ATP	2	0

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.

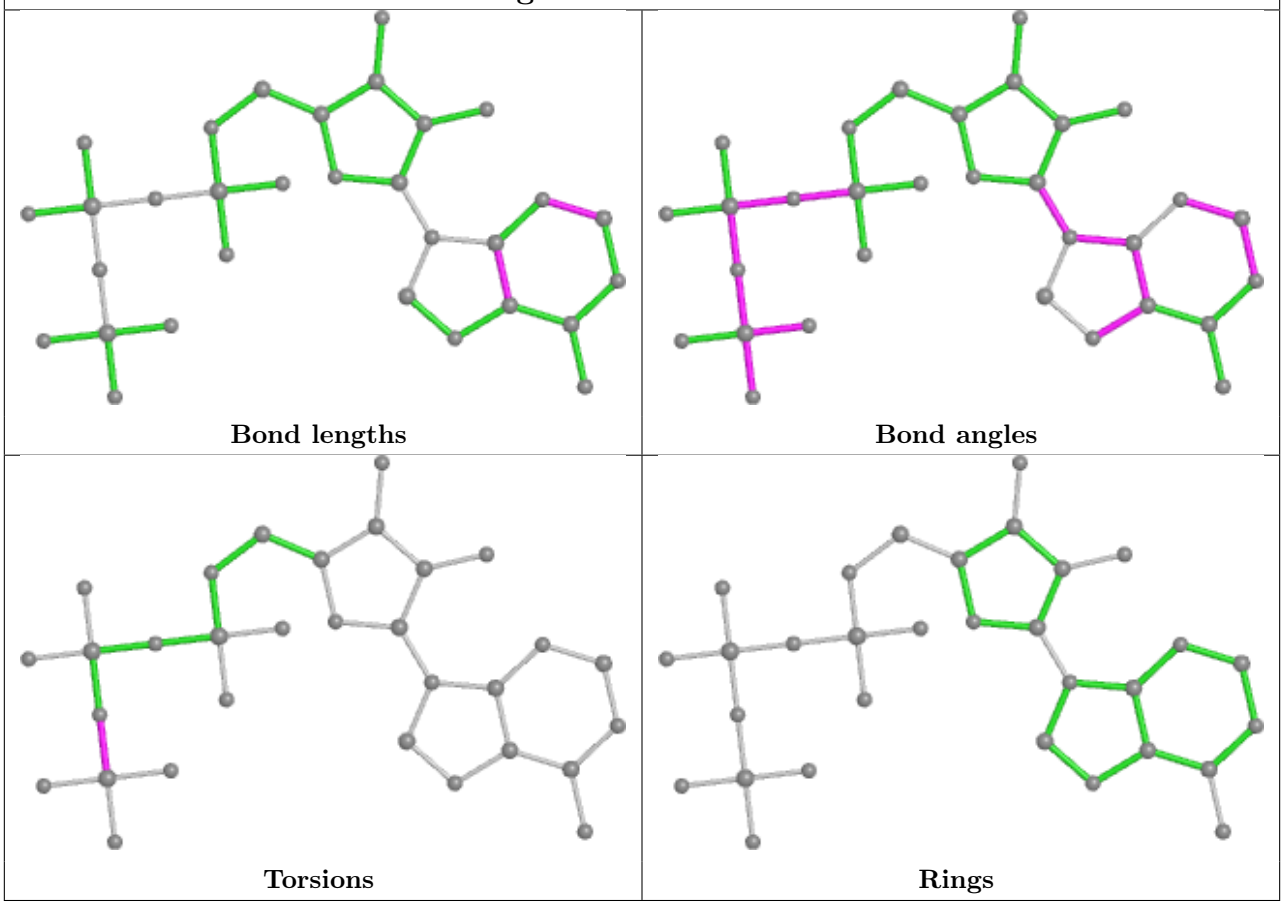
Ligand ATP A 1377



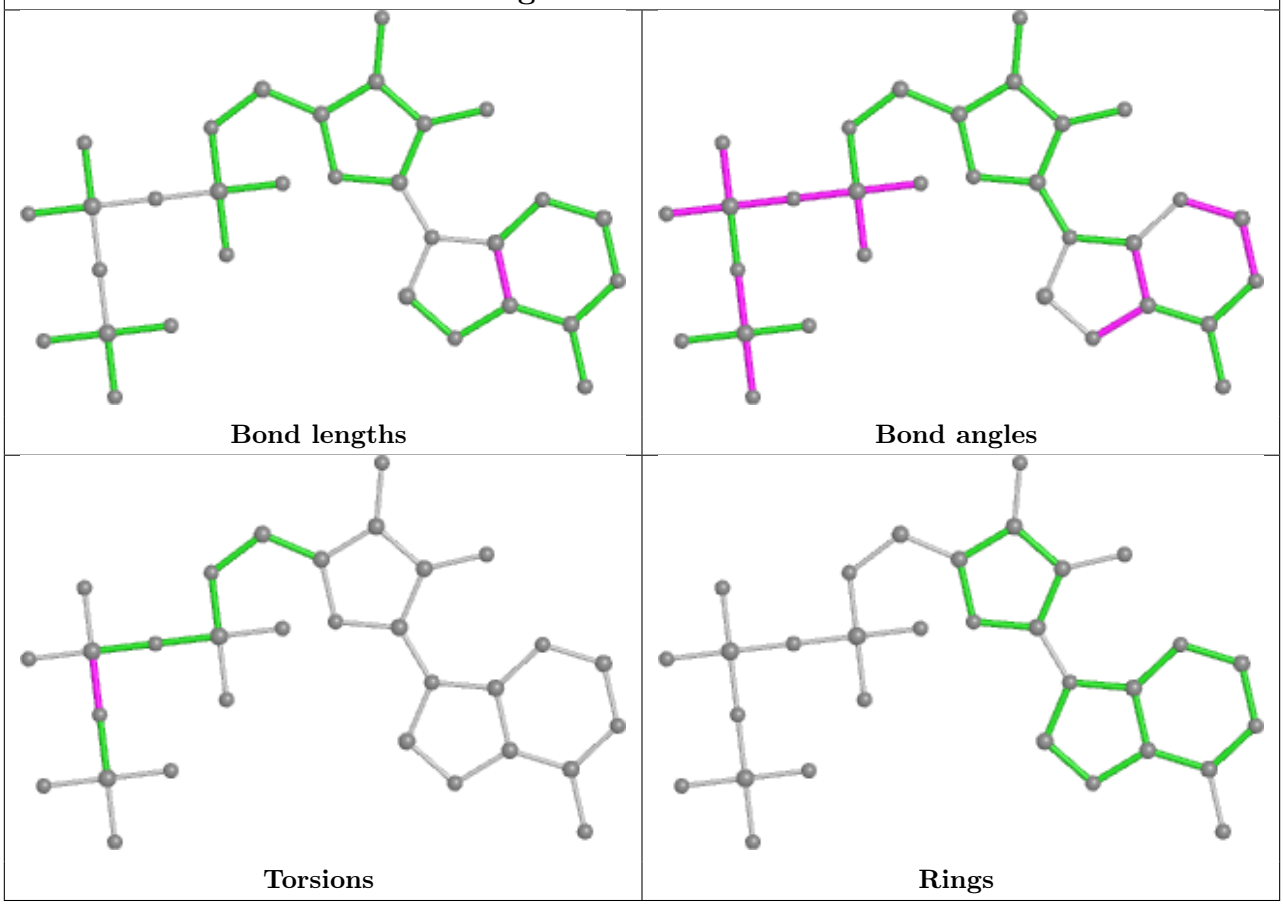
Ligand ATP B 1377



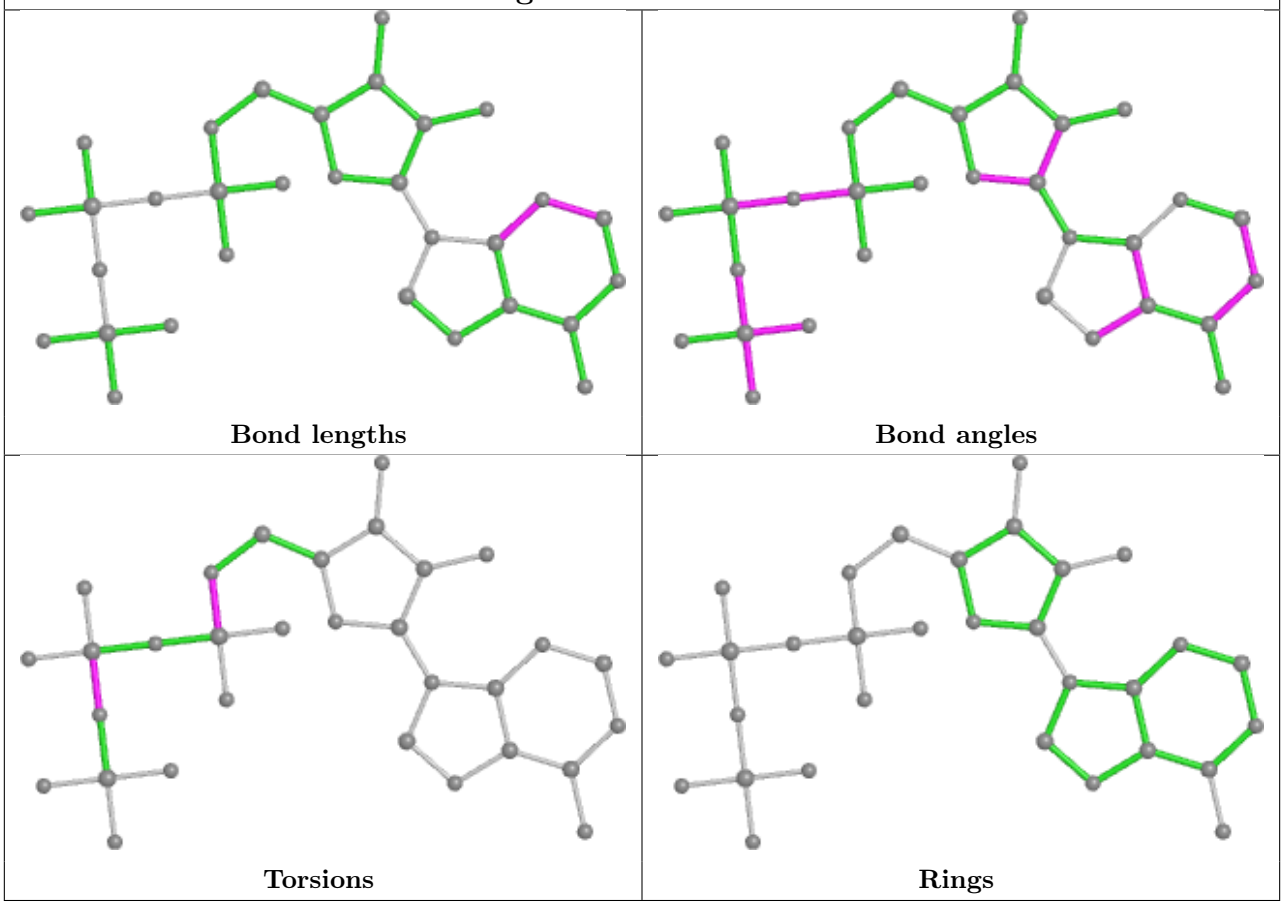
Ligand ATP C 1377



Ligand ATP E 1377



Ligand ATP D 1377



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	346/375 (92%)	0.17	2 (0%) 89 87	77, 140, 187, 211	0
1	B	358/375 (95%)	0.43	13 (3%) 42 41	74, 128, 196, 331	0
1	C	358/375 (95%)	0.44	24 (6%) 17 19	69, 142, 219, 272	0
1	D	358/375 (95%)	0.40	18 (5%) 28 28	67, 136, 200, 297	0
1	E	318/375 (84%)	1.47	102 (32%) 0 0	152, 227, 269, 303	0
2	M	117/117 (100%)	-0.03	0 100 100	81, 128, 196, 205	0
All	All	1855/1992 (93%)	0.53	159 (8%) 10 13	67, 144, 243, 331	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	250	ILE	8.3
1	E	236	LEU	7.3
1	E	200	PHE	6.8
1	E	201	VAL	5.8
1	B	36	GLY	5.7
1	E	170	ALA	5.6
1	E	7	ALA	5.6
1	C	251	GLY	5.4
1	E	261	LEU	5.2
1	E	74	GLY	4.9
1	E	352	PHE	4.8
1	E	150	GLY	4.8
1	E	171	LEU	4.7
1	C	200	PHE	4.7
1	E	369	ILE	4.6
1	E	10	CYS	4.6
1	E	94	LEU	4.6
1	C	236	LEU	4.6
1	E	204	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	317	ILE	4.5
1	E	164	PRO	4.5
1	E	252	ASN	4.4
1	E	154	ASP	4.3
1	E	356	TRP	4.2
1	E	234	SER	4.2
1	E	228	ALA	4.1
1	D	53	TYR	4.1
1	E	250	ILE	4.1
1	E	219	VAL	4.1
1	B	53	TYR	4.0
1	E	262	PHE	4.0
1	D	372	ARG	4.0
1	E	199	SER	4.0
1	B	34	ILE	4.0
1	D	119	MET	4.0
1	E	221	LEU	3.9
1	E	207	GLU	3.9
1	D	133	TYR	3.9
1	E	104	LEU	3.9
1	E	9	VAL	3.8
1	D	3	ASP	3.8
1	E	366	GLY	3.7
1	E	102	PRO	3.7
1	C	36	GLY	3.7
1	E	220	ALA	3.7
1	D	105	LEU	3.7
1	E	89	THR	3.7
1	E	8	LEU	3.6
1	C	216	LEU	3.6
1	D	357	ILE	3.6
1	C	35	VAL	3.6
1	E	189	LEU	3.5
1	E	368	SER	3.5
1	E	103	THR	3.4
1	B	67	LEU	3.4
1	E	110	LEU	3.4
1	C	198	TYR	3.3
1	E	370	VAL	3.3
1	E	82	MET	3.3
1	E	187	ASP	3.3
1	E	251	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	221	LEU	3.3
1	E	132	MET	3.2
1	B	54	VAL	3.2
1	E	163	VAL	3.2
1	E	285	CYS	3.2
1	C	254	ARG	3.1
1	C	193	LEU	3.1
1	E	237	GLU	3.1
1	E	185	LEU	3.1
1	E	294	TYR	3.0
1	E	193	LEU	3.0
1	E	364	GLU	3.0
1	C	248	ILE	3.0
1	E	272	ALA	2.9
1	C	327	ILE	2.9
1	E	91	TYR	2.9
1	B	35	VAL	2.9
1	E	138	ALA	2.9
1	E	371	HIS	2.9
1	D	132	MET	2.9
1	D	103	THR	2.9
1	E	90	PHE	2.8
1	E	318	THR	2.8
1	E	178	LEU	2.8
1	E	235	SER	2.8
1	E	111	ASN	2.8
1	E	151	ILE	2.8
1	E	202	THR	2.8
1	E	123	MET	2.7
1	C	68	LYS	2.7
1	E	108	ALA	2.7
1	E	299	MET	2.7
1	E	271	SER	2.7
1	E	306	TYR	2.7
1	B	200	PHE	2.7
1	E	109	PRO	2.7
1	E	196	ARG	2.6
1	A	33	SER	2.6
1	E	165	ILE	2.6
1	E	19	ALA	2.6
1	A	132	MET	2.6
1	C	240	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	VAL	2.6
1	D	104	LEU	2.5
1	D	373	LYS	2.5
1	D	35	VAL	2.5
1	E	205	GLU	2.5
1	B	55	GLY	2.5
1	E	367	PRO	2.5
1	C	235	SER	2.5
1	C	249	THR	2.4
1	E	105	LEU	2.4
1	E	100	GLU	2.4
1	E	253	GLU	2.4
1	E	197	GLY	2.4
1	E	119	MET	2.4
1	E	20	GLY	2.4
1	D	121	GLN	2.4
1	E	32	PRO	2.3
1	D	365	ALA	2.3
1	E	180	LEU	2.3
1	E	208	ILE	2.3
1	E	312	ARG	2.3
1	E	173	HIS	2.3
1	E	69	TYR	2.3
1	C	258	PRO	2.3
1	C	317	ILE	2.3
1	B	119	MET	2.3
1	B	162	ASN	2.3
1	E	203	THR	2.2
1	D	166	TYR	2.2
1	D	362	TYR	2.2
1	E	12	ASN	2.2
1	D	8	LEU	2.2
1	E	198	TYR	2.2
1	E	263	GLN	2.2
1	C	261	LEU	2.2
1	E	72	GLU	2.2
1	E	355	MET	2.2
1	C	67	LEU	2.2
1	E	223	PHE	2.1
1	C	257	CYS	2.1
1	E	224	GLU	2.1
1	E	192	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	319	ALA	2.1
1	E	107	GLU	2.1
1	E	128	ASN	2.1
1	E	160	THR	2.1
1	D	367	PRO	2.1
1	C	14	SER	2.1
1	C	33	SER	2.1
1	E	186	THR	2.1
1	B	57	GLU	2.0
1	B	243	PRO	2.0
1	E	190	MET	2.0
1	E	77	THR	2.0
1	E	226	GLU	2.0
1	E	329	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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(Å^2)	Q<0.9
3	ATP	E	1377	31/31	0.90	0.12	148,187,237,261	0
4	CA	D	1378	1/1	0.94	0.22	104,104,104,104	0
3	ATP	A	1377	31/31	0.95	0.21	81,103,143,154	0
4	CA	A	1378	1/1	0.95	0.30	108,108,108,108	0
3	ATP	C	1377	31/31	0.95	0.17	98,128,150,163	0
4	CA	E	1378	1/1	0.95	0.16	245,245,245,245	0
3	ATP	B	1377	31/31	0.97	0.21	74,101,120,128	0
4	CA	C	1378	1/1	0.98	0.28	104,104,104,104	0
3	ATP	D	1377	31/31	0.98	0.21	54,79,123,137	0

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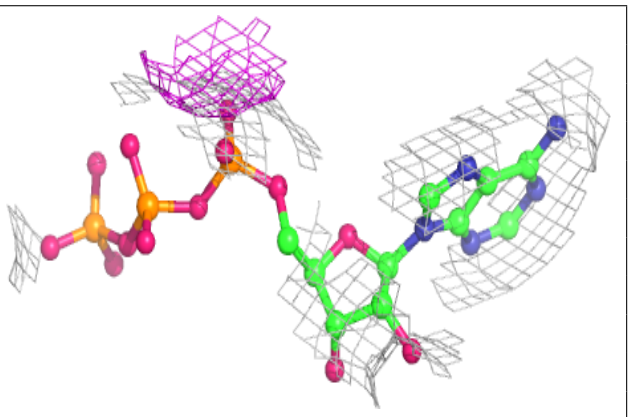
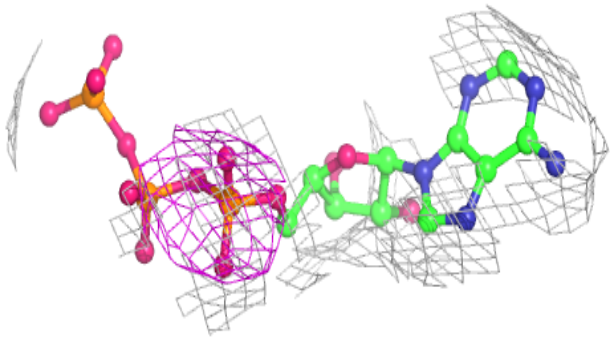
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	1378	1/1	0.98	0.30	81,81,81,81	0

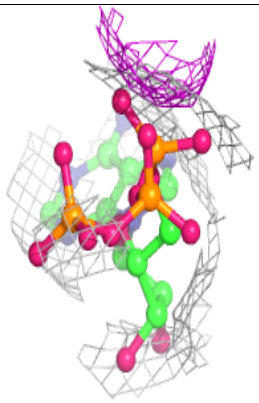
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 1377:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

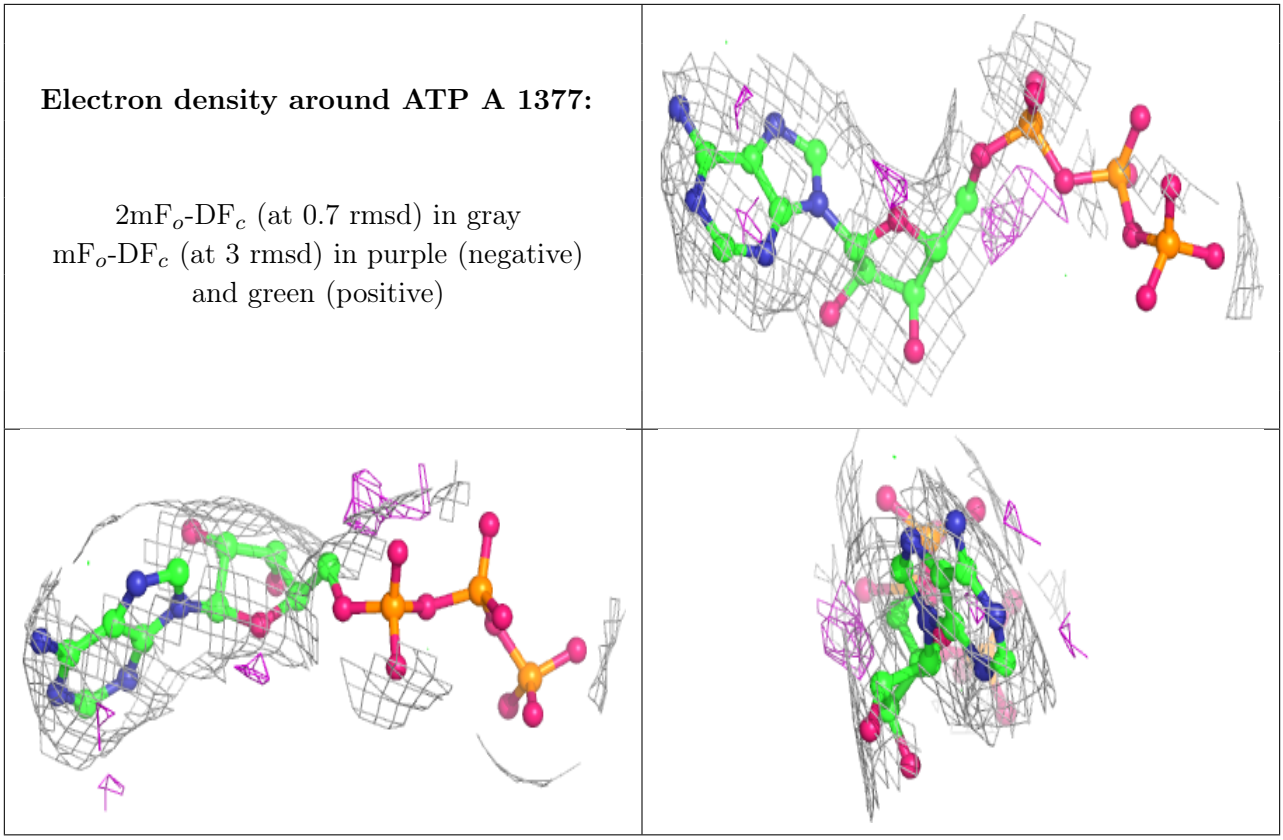






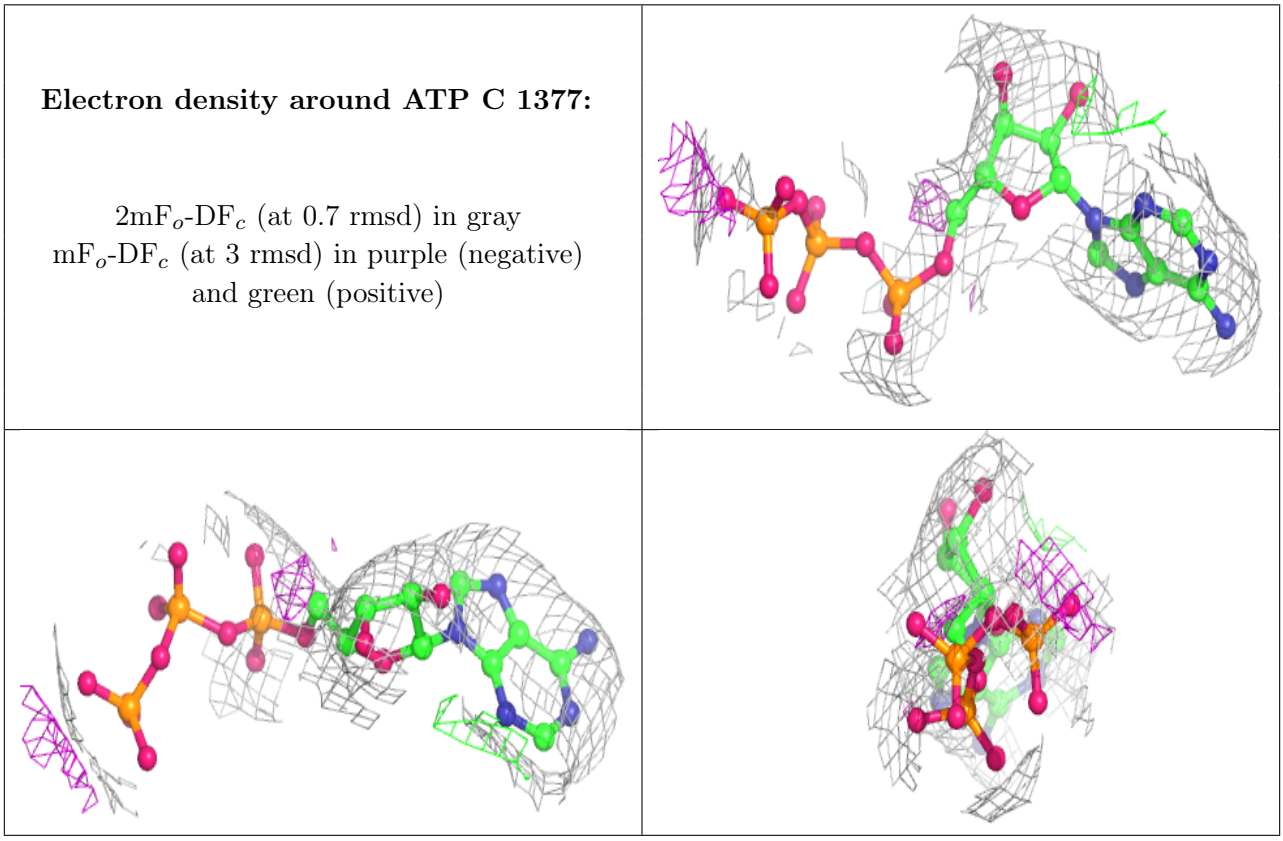
Electron density around ATP A 1377:

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



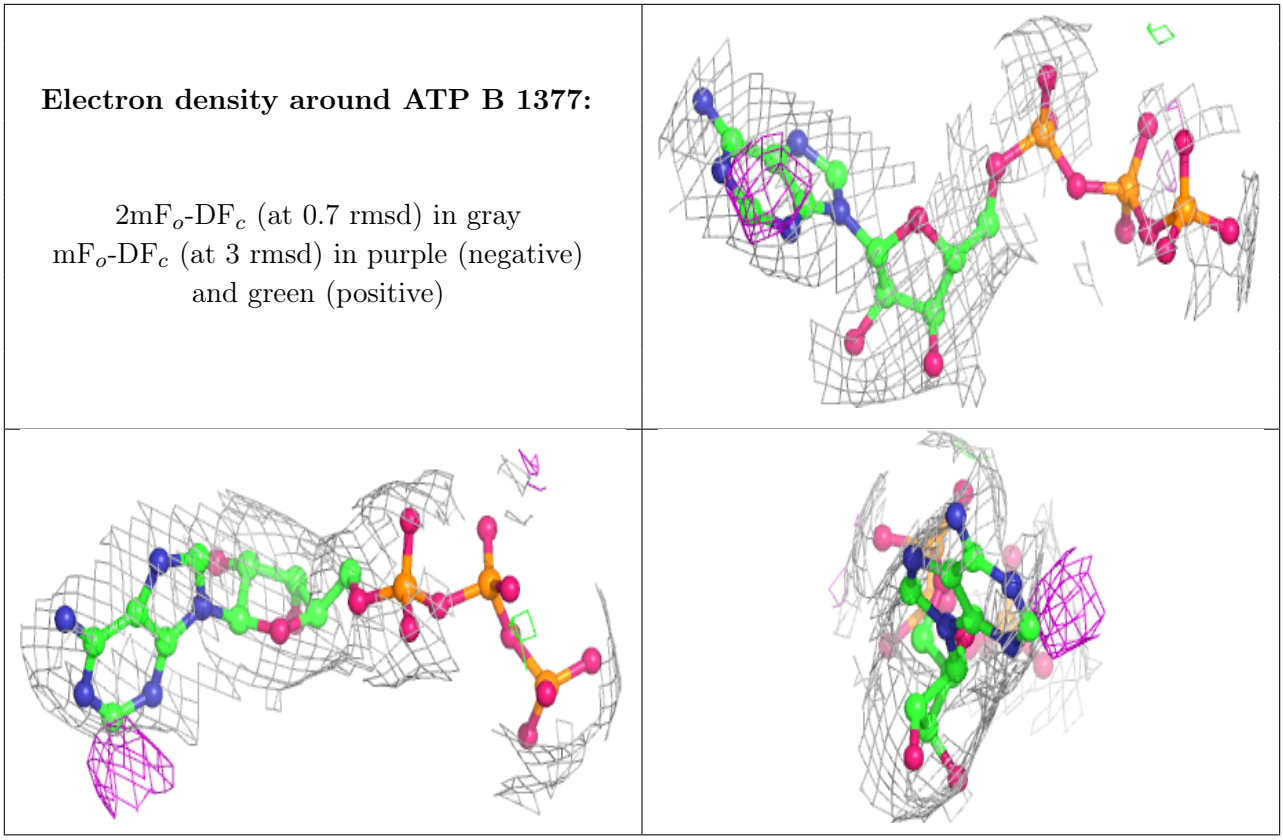
Electron density around ATP C 1377:

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



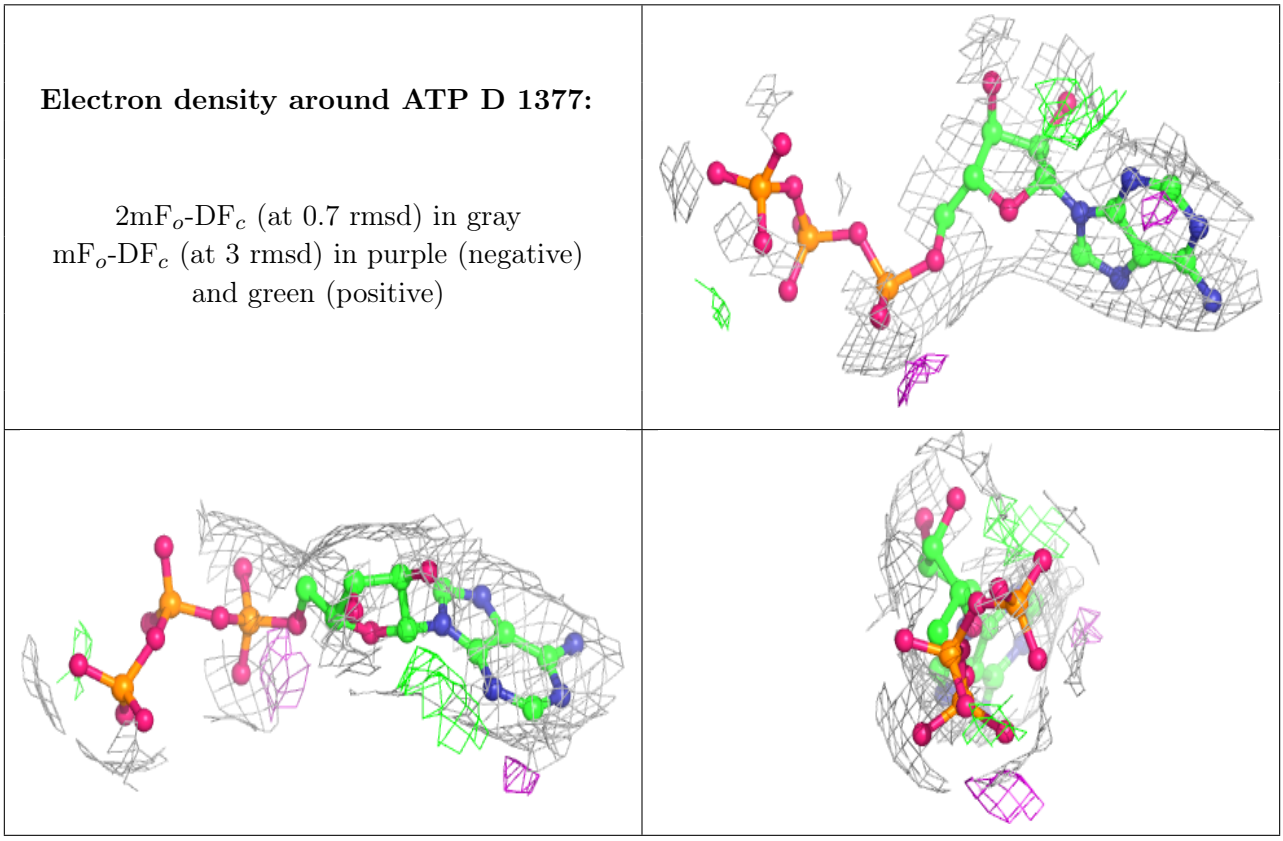
Electron density around ATP B 1377:

$2mF_o$-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 1377:

$2mF_o$-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.