WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 01:48 pm BST

PDB ID	:	2XSZ
Title	:	The dodecameric human RuvBL1:RuvBL2 complex with truncated domains II
Authors	:	Gorynia, S.; Bandeiras, T.M.; Matias, P.M.; Pinho, F.G.; McVey, C.E.; Vonrhein, C.; Svergun, D.I.; Round, A.; Donner, P.; Carrondo, M.A.
Deposited on	:	2010-10-01
Resolution	:	3.00 Å(reported)

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

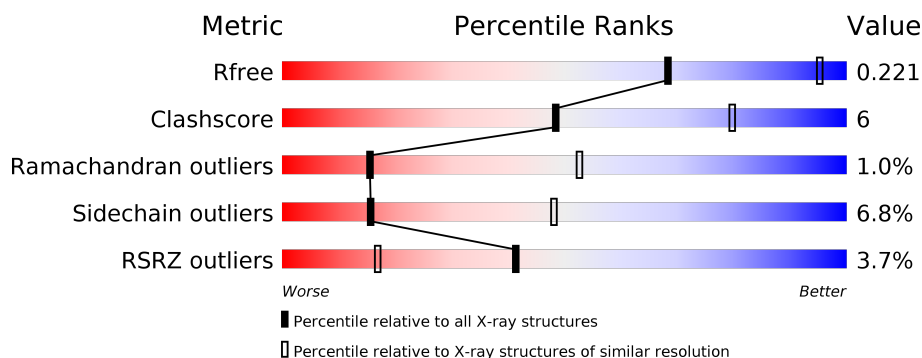|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.221
Clashscore		6
Ramachandran outliers		1.0%
Sidechain outliers		6.8%
RSRZ outliers		3.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
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 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 <=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	367	4% 70% 16% • 13%
1	B	367	5% 70% 16% • 13%
1	C	367	3% 71% 16% • 13%
2	D	378	2% 65% 16% • 18%
2	E	378	2% 62% 20% • 17%
2	F	378	2% 65% 16% • 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14664 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 RUVB-LIKE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	Se	0	0	0
			2430	1530	421	468	4	7			
1	B	319	Total	C	N	O	S	Se	0	0	0
			2435	1531	422	471	4	7			
1	C	320	Total	C	N	O	S	Se	0	0	0
			2425	1525	420	469	4	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9Y265
A	2	VAL	-	expression tag	UNP Q9Y265
A	3	HIS	-	expression tag	UNP Q9Y265
A	4	HIS	-	expression tag	UNP Q9Y265
A	5	HIS	-	expression tag	UNP Q9Y265
A	6	HIS	-	expression tag	UNP Q9Y265
A	7	HIS	-	expression tag	UNP Q9Y265
A	8	HIS	-	expression tag	UNP Q9Y265
A	9	LEU	-	expression tag	UNP Q9Y265
A	10	LEU	-	expression tag	UNP Q9Y265
A	11	VAL	-	expression tag	UNP Q9Y265
A	12	PRO	-	expression tag	UNP Q9Y265
A	13	ARG	-	expression tag	UNP Q9Y265
A	14	GLY	-	expression tag	UNP Q9Y265
A	15	SER	-	expression tag	UNP Q9Y265
B	1	MSE	-	expression tag	UNP Q9Y265
B	2	VAL	-	expression tag	UNP Q9Y265
B	3	HIS	-	expression tag	UNP Q9Y265
B	4	HIS	-	expression tag	UNP Q9Y265
B	5	HIS	-	expression tag	UNP Q9Y265
B	6	HIS	-	expression tag	UNP Q9Y265
B	7	HIS	-	expression tag	UNP Q9Y265
B	8	HIS	-	expression tag	UNP Q9Y265

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	LEU	-	expression tag	UNP Q9Y265
B	10	LEU	-	expression tag	UNP Q9Y265
B	11	VAL	-	expression tag	UNP Q9Y265
B	12	PRO	-	expression tag	UNP Q9Y265
B	13	ARG	-	expression tag	UNP Q9Y265
B	14	GLY	-	expression tag	UNP Q9Y265
B	15	SER	-	expression tag	UNP Q9Y265
C	1	MSE	-	expression tag	UNP Q9Y265
C	2	VAL	-	expression tag	UNP Q9Y265
C	3	HIS	-	expression tag	UNP Q9Y265
C	4	HIS	-	expression tag	UNP Q9Y265
C	5	HIS	-	expression tag	UNP Q9Y265
C	6	HIS	-	expression tag	UNP Q9Y265
C	7	HIS	-	expression tag	UNP Q9Y265
C	8	HIS	-	expression tag	UNP Q9Y265
C	9	LEU	-	expression tag	UNP Q9Y265
C	10	LEU	-	expression tag	UNP Q9Y265
C	11	VAL	-	expression tag	UNP Q9Y265
C	12	PRO	-	expression tag	UNP Q9Y265
C	13	ARG	-	expression tag	UNP Q9Y265
C	14	GLY	-	expression tag	UNP Q9Y265
C	15	SER	-	expression tag	UNP Q9Y265

- Molecule 2 is a protein called RUVB-LIKE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	310	Total 2377	C 1487	N 421	O 457	S 2	Se 10	0	0	0
2	E	315	Total 2426	C 1520	N 428	O 466	S 2	Se 10	0	0	0
2	F	311	Total 2385	C 1493	N 422	O 458	S 2	Se 10	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	expression tag	UNP Q9Y230
D	2	ASP	-	expression tag	UNP Q9Y230
D	3	TYR	-	expression tag	UNP Q9Y230
D	4	LYS	-	expression tag	UNP Q9Y230
D	5	ASP	-	expression tag	UNP Q9Y230
D	6	ASP	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
D	7	ASP	-	expression tag	UNP Q9Y230
D	8	ASP	-	expression tag	UNP Q9Y230
D	9	LYS	-	expression tag	UNP Q9Y230
D	10	GLU	-	expression tag	UNP Q9Y230
D	11	ASN	-	expression tag	UNP Q9Y230
D	12	LEU	-	expression tag	UNP Q9Y230
D	13	TYR	-	expression tag	UNP Q9Y230
D	14	PHE	-	expression tag	UNP Q9Y230
D	15	GLN	-	expression tag	UNP Q9Y230
D	16	GLY	-	expression tag	UNP Q9Y230
E	1	MSE	-	expression tag	UNP Q9Y230
E	2	ASP	-	expression tag	UNP Q9Y230
E	3	TYR	-	expression tag	UNP Q9Y230
E	4	LYS	-	expression tag	UNP Q9Y230
E	5	ASP	-	expression tag	UNP Q9Y230
E	6	ASP	-	expression tag	UNP Q9Y230
E	7	ASP	-	expression tag	UNP Q9Y230
E	8	ASP	-	expression tag	UNP Q9Y230
E	9	LYS	-	expression tag	UNP Q9Y230
E	10	GLU	-	expression tag	UNP Q9Y230
E	11	ASN	-	expression tag	UNP Q9Y230
E	12	LEU	-	expression tag	UNP Q9Y230
E	13	TYR	-	expression tag	UNP Q9Y230
E	14	PHE	-	expression tag	UNP Q9Y230
E	15	GLN	-	expression tag	UNP Q9Y230
E	16	GLY	-	expression tag	UNP Q9Y230
F	1	MSE	-	expression tag	UNP Q9Y230
F	2	ASP	-	expression tag	UNP Q9Y230
F	3	TYR	-	expression tag	UNP Q9Y230
F	4	LYS	-	expression tag	UNP Q9Y230
F	5	ASP	-	expression tag	UNP Q9Y230
F	6	ASP	-	expression tag	UNP Q9Y230
F	7	ASP	-	expression tag	UNP Q9Y230
F	8	ASP	-	expression tag	UNP Q9Y230
F	9	LYS	-	expression tag	UNP Q9Y230
F	10	GLU	-	expression tag	UNP Q9Y230
F	11	ASN	-	expression tag	UNP Q9Y230
F	12	LEU	-	expression tag	UNP Q9Y230
F	13	TYR	-	expression tag	UNP Q9Y230
F	14	PHE	-	expression tag	UNP Q9Y230
F	15	GLN	-	expression tag	UNP Q9Y230
F	16	GLY	-	expression tag	UNP Q9Y230

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

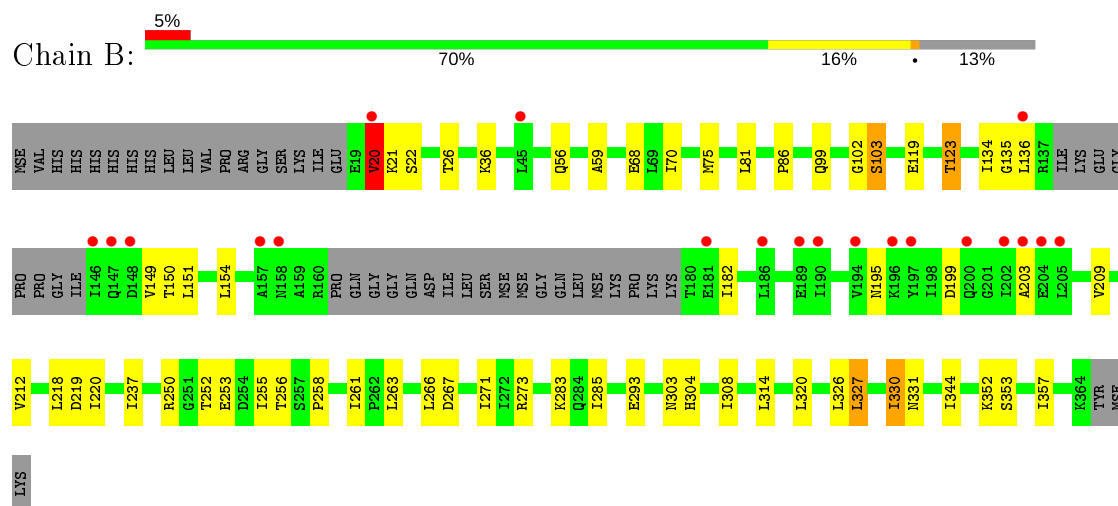| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
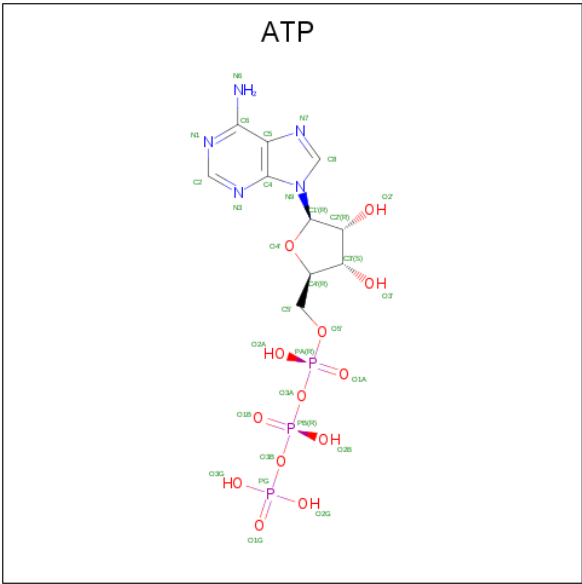
3 Residue-property plots ⓘ

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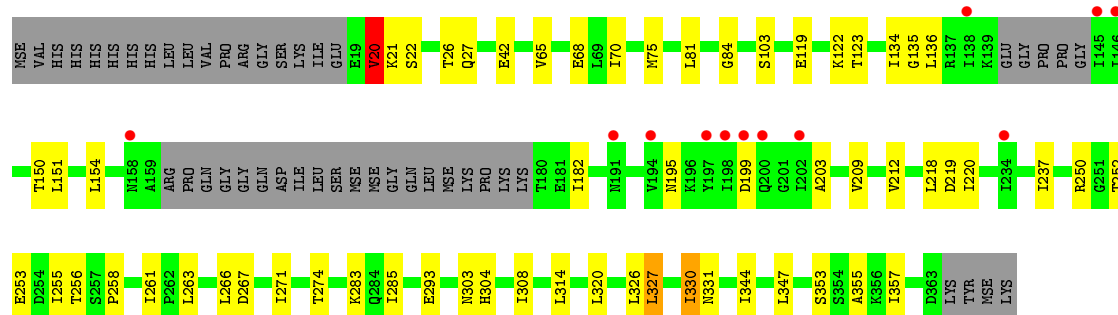
• Molecule 1: RUVB-LIKE 1
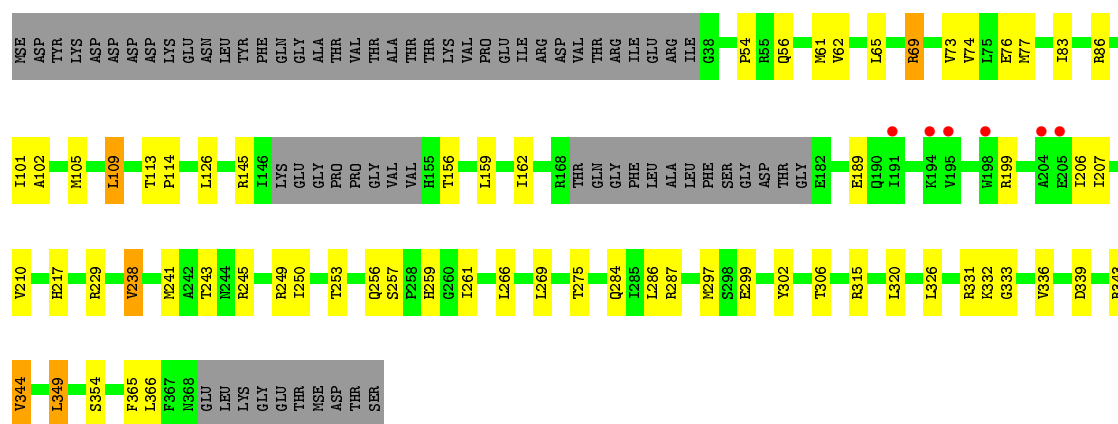

• Molecule 1: RUVB-LIKE 1
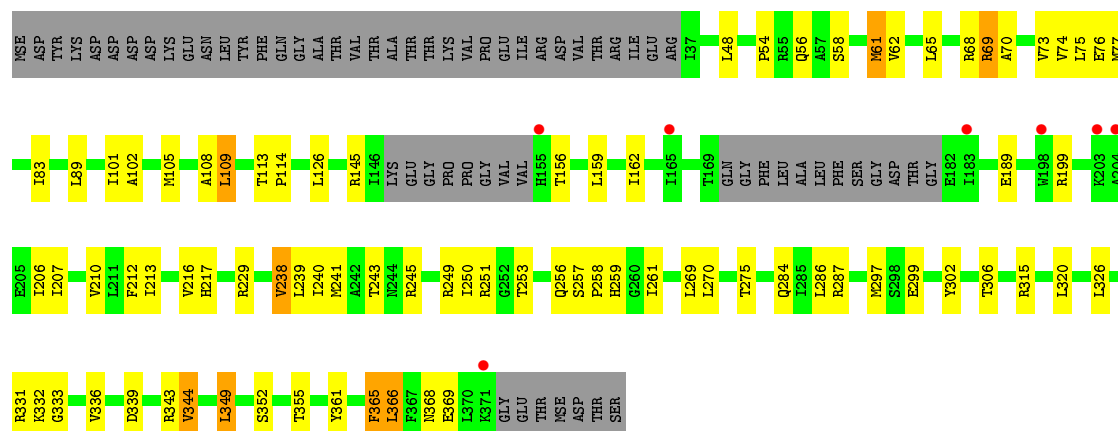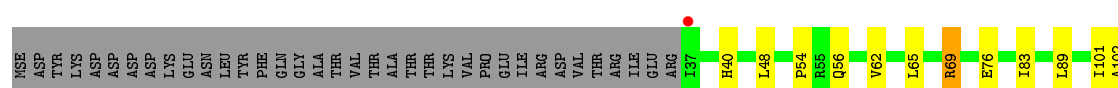

• Molecule 1: RUVB-LIKE 1
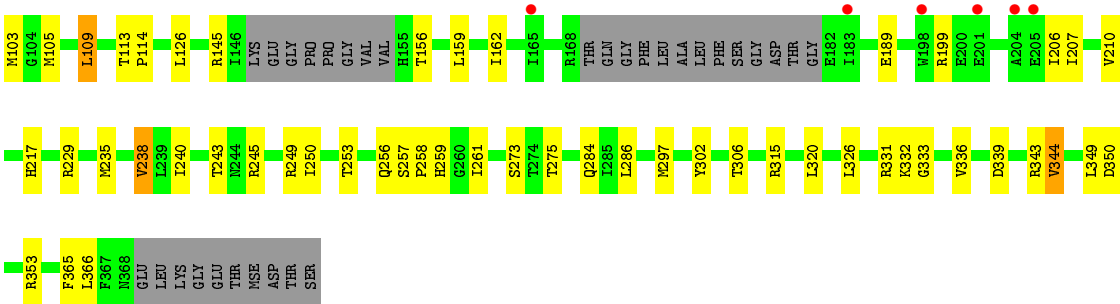
MSE VAL HIS HIS HIS HIS HIS LEU LEU VAL PRO ARG GLY SER LYS ILE GLU E19 V20 K21 S22 T26 Q27 E42 V65 E68 L69 I70 M75 L81 G84 S103 E119 K122 T123 I134 G135 L136 R137 I138 K139 GLU GLY PRO GLY I145 I146

T150 L151 L154 N158 A159 ARG PRO GLN GLY GLN ASP ILE LEU SER MSE MSE GLY GLN LEU MSE PRO LYS LYS T180 E181 I182 N191 V194 N195 K196 Y197 I198 D199 Q200 G201 I202 A203 V209 V212 L218 D219 I220 I234 I237 R250 G251 T252

E253 D254 I255 T256 S257 P258 I261 P262 L263 L266 D267 I271 T274 K283 Q284 I285 E293 N303 H304 I308 L314 L320 L326 L327 I330 N331 I344 L347 S353 S354 A355 K356 I357 D363 LYS TYR MSE LYS

• Molecule 2: RUVB-LIKE 2

Chain D:
2%
65%   16%   18%

MSE ASP TYR LYS ASP ASP ASP LYS GLU ASN LEU TYR PHE GLN GLY ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG ILE G38 P54 R55 Q56 M61 V62 L65 R69 V73 V74 L75 E76 M77 I83 R86

I101 A102 M105 L109 T113 P114 L126 R145 I146 LYS GLY GLY PRO PRO GLY VAL VAL H155 T156 L159 I162 R168 THR GLN GLY PHE LEU ALA LEU PHE SER GLY ASP THR GLY E182 E189 Q190 I191 K194 V195 W198 R199 A204 E205 I206 I207

V210 H217 R229 V238 M241 A242 T243 N244 R245 R249 I250 T253 Q256 S257 P258 H259 G260 I261 L266 L269 T275 Q284 I285 L286 R287 M297 S298 E299 Y302 T306 R315 L320 L326 R331 K332 G333 V336 D339 R343

V344 L349 S354 F365 L366 F367 N368 GLU LEU LYS GLU THR MSE ASP THR SER

• Molecule 2: RUVB-LIKE 2

Chain E:
2%
62%   20%   •   17%

MSE ASP TYR LYS ASP ASP ASP LYS GLU ASN LEU TYR PHE GLN GLY ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG I37 L48 P54 R55 Q56 A57 S58 M61 V62 L65 R68 R69 A70 V73 V74 L75 E76 M77

I83 L89 I101 A102 M105 A108 L109 T113 P114 L126 R145 I146 LYS GLY GLY PRO PRO GLY VAL VAL H155 T156 L159 I162 I165 T169 GLN GLY PHE LEU ALA LEU PHE SER GLY THR GLY E182 I183 E189 W198 R199 K203 A204

E205 I206 I207 V210 I211 F212 I213 V216 H217 R229 V238 L239 I240 M241 A242 T243 N244 R245 R249 I250 R251 G252 T253 Q256 S257 P258 H259 G260 I261 L269 L270 T275 Q284 I285 L286 R287 M297 S298 E299 Y302 T306 R315 L320 L326

R331 K332 G333 V336 D339 R343 V344 F367 L349 S352 T355 Y361 F365 L366 F367 N368 E369 L370 K371 GLY GLU THR MSE ASP THR SER

• Molecule 2: RUVB-LIKE 2

Chain F:
2%
65%   16%   •   18%

MSE ASP TYR LYS ASP ASP ASP LYS GLU ASN LEU TYR PHE GLN GLY ALA THR VAL THR ALA THR THR LYS VAL PRO GLU ILE ARG ASP VAL THR ARG ILE GLU ARG I37 H40 L48 P54 R55 Q56 V62 L65 R69 E76 I83 L89 I101 A102

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	111.82Å 187.93Å 244.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 3.00 46.14 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.14-3.00) 99.5 (46.14-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.0	Depositor
R, R_{free}	0.178 , 0.205 0.196 , 0.221	Depositor DCC
R_{free} test set	2632 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 74.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14664	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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

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	0/2450	0.67	0/3294
1	B	0.44	0/2455	0.65	0/3301
1	C	0.45	0/2445	0.66	0/3289
2	D	0.45	0/2395	0.68	0/3214
2	E	0.45	0/2445	0.67	0/3280
2	F	0.47	0/2403	0.68	0/3225
All	All	0.45	0/14593	0.67	0/19603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2430	0	2514	30	0
1	B	2435	0	2509	31	0
1	C	2425	0	2482	29	0
2	D	2377	0	2392	32	0
2	E	2426	0	2449	40	0
2	F	2385	0	2403	36	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	F	31	0	12	0	0
All	All	14664	0	14821	177	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 6.

All (177) 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:68:GLU:HB2	2:D:326:LEU:HD21	1.53	0.88
1:B:68:GLU:HB2	2:E:326:LEU:HD21	1.55	0.85
2:E:243:THR:HG21	2:E:259:HIS:HB3	1.60	0.83
2:D:243:THR:HG21	2:D:259:HIS:HB3	1.62	0.82
2:F:243:THR:HG21	2:F:259:HIS:HB3	1.61	0.81
1:A:283:LYS:HD3	1:A:303:ASN:HA	1.66	0.76
1:C:68:GLU:HB2	2:F:326:LEU:HD21	1.71	0.73
2:F:350:ASP:OD1	2:F:353:ARG:HB2	1.91	0.70
2:E:320:LEU:HD22	2:E:344:VAL:HG13	1.76	0.67
1:B:273:ARG:HB2	2:E:349:LEU:HD11	1.77	0.65
2:E:287:ARG:NH2	2:E:299:GLU:OE1	2.30	0.65
2:E:302:TYR:O	2:E:306:THR:HG23	1.99	0.62
1:A:252:THR:HB	1:A:255:ILE:HD12	1.82	0.62
2:E:210:VAL:HG13	2:E:240:ILE:HD12	1.81	0.62
1:C:252:THR:HB	1:C:255:ILE:HD12	1.82	0.61
2:F:302:TYR:O	2:F:306:THR:HG23	2.01	0.61
1:B:252:THR:HB	1:B:255:ILE:HD12	1.81	0.61
1:C:70:ILE:HG13	1:C:75:MSE:HG3	1.83	0.61
2:D:302:TYR:O	2:D:306:THR:HG23	2.01	0.60
1:B:36:LYS:HA	1:B:99:GLN:HE21	1.66	0.60
1:C:135:GLY:HA2	1:C:150:THR:HA	1.84	0.60
2:F:286:LEU:HD12	2:F:306:THR:HG22	1.83	0.60
2:D:286:LEU:HD12	2:D:306:THR:HG22	1.84	0.60
2:D:145:ARG:HG2	2:D:156:THR:HG22	1.85	0.59
1:A:135:GLY:HA2	1:A:150:THR:HA	1.85	0.59
1:B:135:GLY:HA2	1:B:150:THR:HA	1.84	0.59
2:E:365:PHE:O	2:E:368:ASN:HB2	2.02	0.59
2:E:145:ARG:HG2	2:E:156:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ARG:HG2	2:F:156:THR:HG22	1.85	0.58
2:D:102:ALA:HA	2:D:105:MSE:HE3	1.86	0.57
2:E:73:VAL:HG12	2:E:77:MSE:HE2	1.87	0.57
2:F:210:VAL:HG13	2:F:240:ILE:HD12	1.85	0.57
1:B:70:ILE:HG13	1:B:75:MSE:HG3	1.86	0.56
2:D:74:VAL:HA	2:D:77:MSE:HE3	1.86	0.56
2:D:73:VAL:HG12	2:D:77:MSE:HE2	1.86	0.56
2:E:102:ALA:HA	2:E:105:MSE:HE3	1.87	0.56
2:F:102:ALA:HA	2:F:105:MSE:HE3	1.87	0.56
2:E:259:HIS:HB2	2:E:261:ILE:HD12	1.88	0.56
2:D:56:GLN:HA	2:D:65:LEU:HD21	1.87	0.56
1:A:81:LEU:HD23	1:A:271:ILE:HG12	1.88	0.56
1:A:279:PRO:O	1:A:283:LYS:HG3	2.06	0.55
2:F:56:GLN:HA	2:F:65:LEU:HD21	1.89	0.55
2:E:56:GLN:HA	2:E:65:LEU:HD21	1.89	0.54
2:D:101:ILE:HG22	2:D:105:MSE:HE2	1.88	0.54
2:D:217:HIS:CG	2:D:245:ARG:HD2	2.43	0.54
2:E:286:LEU:HD12	2:E:306:THR:HG22	1.90	0.54
2:E:101:ILE:HG22	2:E:105:MSE:HE2	1.89	0.54
2:F:217:HIS:CG	2:F:245:ARG:HD2	2.42	0.54
2:F:349:LEU:CD2	2:F:353:ARG:NH1	2.72	0.53
2:E:217:HIS:CG	2:E:245:ARG:HD2	2.43	0.53
2:F:259:HIS:HB2	2:F:261:ILE:HD12	1.89	0.53
2:D:259:HIS:HB2	2:D:261:ILE:HD12	1.91	0.53
2:F:101:ILE:HG22	2:F:105:MSE:HE2	1.91	0.53
1:C:81:LEU:HD23	1:C:271:ILE:HG12	1.91	0.52
1:A:355:ALA:HB2	2:F:258:PRO:HB3	1.91	0.52
2:D:266:LEU:HD23	2:D:269:LEU:HD12	1.92	0.52
2:E:89:LEU:HB2	2:E:269:LEU:HD13	1.91	0.52
1:B:327:LEU:HD12	1:B:344:ILE:HG12	1.90	0.52
2:E:213:ILE:HD12	2:E:239:LEU:HD11	1.91	0.52
1:A:327:LEU:HD12	1:A:344:ILE:HG12	1.92	0.52
2:F:349:LEU:HD22	2:F:353:ARG:NH1	2.25	0.52
1:A:70:ILE:HG13	1:A:75:MSE:HG3	1.91	0.51
1:A:258:PRO:HB2	1:A:266:LEU:HD21	1.93	0.51
1:B:134:ILE:HB	1:B:151:LEU:HD12	1.92	0.51
2:E:74:VAL:HG22	2:E:270:LEU:HD13	1.93	0.51
2:F:89:LEU:HD11	2:F:243:THR:HG22	1.92	0.51
1:B:209:VAL:HG22	1:B:237:ILE:HG23	1.92	0.51
1:B:81:LEU:HD23	1:B:271:ILE:HG12	1.93	0.50
1:A:209:VAL:HG22	1:A:237:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ILE:HD11	2:E:257:SER:HB2	1.94	0.50
2:E:297:MSE:HG3	2:E:336:VAL:HB	1.94	0.50
2:D:297:MSE:HG3	2:D:336:VAL:HB	1.93	0.50
1:C:258:PRO:HB2	1:C:266:LEU:HD21	1.94	0.50
1:C:327:LEU:HD12	1:C:344:ILE:HG12	1.92	0.50
2:D:54:PRO:HD3	2:D:69:ARG:HB2	1.94	0.49
1:B:283:LYS:HD3	1:B:303:ASN:HA	1.94	0.49
1:A:134:ILE:HB	1:A:151:LEU:HD12	1.94	0.49
1:C:209:VAL:HG22	1:C:237:ILE:HG23	1.94	0.49
2:E:159:LEU:HA	2:E:162:ILE:HD12	1.95	0.49
2:F:249:ARG:HA	2:F:256:GLN:HA	1.95	0.49
1:A:219:ASP:HA	1:A:250:ARG:HB3	1.95	0.49
1:B:20:VAL:HG12	1:B:21:LYS:H	1.77	0.49
2:F:159:LEU:HA	2:F:162:ILE:HD12	1.95	0.49
1:C:134:ILE:HB	1:C:151:LEU:HD12	1.95	0.48
1:C:219:ASP:HA	1:C:250:ARG:HB3	1.94	0.48
2:E:212:PHE:HA	2:E:240:ILE:O	2.13	0.48
2:F:297:MSE:HG3	2:F:336:VAL:HB	1.93	0.48
2:D:159:LEU:HA	2:D:162:ILE:HD12	1.95	0.48
1:B:330:ILE:HD11	2:D:76:GLU:HG3	1.95	0.48
2:E:109:LEU:HB3	2:E:113:THR:HG21	1.95	0.48
1:B:258:PRO:HB2	1:B:266:LEU:HD21	1.94	0.48
2:D:241:MSE:HE1	2:D:269:LEU:HD21	1.96	0.48
2:E:61:MSE:HE2	2:E:68:ARG:HD2	1.94	0.48
1:B:219:ASP:HA	1:B:250:ARG:HB3	1.95	0.48
1:B:326:LEU:HD23	2:D:76:GLU:HB3	1.96	0.48
1:A:285:ILE:HG21	1:A:314:LEU:HD21	1.96	0.47
2:F:350:ASP:N	2:F:350:ASP:OD1	2.30	0.47
1:A:252:THR:O	1:A:253:GLU:HG2	2.14	0.47
2:F:250:ILE:HD11	2:F:257:SER:HB2	1.94	0.47
2:F:210:VAL:CG1	2:F:240:ILE:HD12	2.45	0.47
2:F:54:PRO:HD3	2:F:69:ARG:HB2	1.96	0.47
1:C:267:ASP:HA	2:F:315:ARG:HD2	1.95	0.47
2:E:249:ARG:HA	2:E:256:GLN:HA	1.96	0.47
1:B:267:ASP:HA	2:E:315:ARG:HD2	1.96	0.47
1:C:65:VAL:HG13	2:F:326:LEU:HD23	1.96	0.47
1:B:353:SER:O	1:B:357:ILE:HG12	2.14	0.47
2:D:250:ILE:HD11	2:D:257:SER:HB2	1.95	0.47
2:D:349:LEU:HD12	2:D:354:SER:HA	1.97	0.47
1:A:320:LEU:HD22	1:A:344:ILE:HG22	1.97	0.46
1:A:353:SER:O	1:A:357:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLY:HA3	1:C:274:THR:OG1	2.15	0.46
2:D:109:LEU:HB3	2:D:113:THR:HG21	1.96	0.46
1:A:123:THR:HG23	2:D:126:LEU:HB3	1.98	0.46
2:D:249:ARG:HA	2:D:256:GLN:HA	1.96	0.46
1:B:252:THR:O	1:B:253:GLU:HG2	2.15	0.46
2:E:216:VAL:HG21	2:E:241:MSE:SE	2.66	0.46
1:C:353:SER:O	1:C:357:ILE:HG12	2.16	0.45
1:C:320:LEU:HD22	1:C:344:ILE:HG22	1.98	0.45
1:B:320:LEU:HD22	1:B:344:ILE:HG22	1.98	0.45
1:C:212:VAL:HG11	1:C:218:LEU:HD11	1.99	0.45
1:C:326:LEU:HD23	2:E:76:GLU:HB3	1.99	0.45
1:A:330:ILE:HG22	1:A:331:ASN:HD22	1.82	0.45
1:C:252:THR:O	1:C:253:GLU:HG2	2.17	0.45
1:C:330:ILE:HG22	1:C:331:ASN:HD22	1.82	0.45
1:C:283:LYS:HD3	1:C:303:ASN:HA	1.98	0.45
2:E:366:LEU:O	2:E:369:GLU:HB2	2.16	0.45
2:E:54:PRO:HD3	2:E:69:ARG:HB2	2.00	0.44
1:C:20:VAL:HG12	1:C:21:LYS:H	1.83	0.44
1:B:330:ILE:HG22	1:B:331:ASN:HD22	1.83	0.44
1:C:122:LYS:HD2	2:F:126:LEU:HD21	2.00	0.43
1:B:123:THR:HG23	2:E:126:LEU:HB3	2.01	0.43
1:A:287:LYS:HB2	1:A:302:LEU:HD21	1.99	0.43
1:A:330:ILE:HD11	2:F:76:GLU:HG3	1.99	0.43
2:F:109:LEU:HB3	2:F:113:THR:HG21	1.99	0.43
1:A:151:LEU:HA	1:A:154:LEU:HD12	1.99	0.43
1:B:136:LEU:HD22	1:B:203:ALA:HB1	2.01	0.43
1:B:261:ILE:HB	1:B:266:LEU:HD13	2.01	0.43
1:C:151:LEU:HA	1:C:154:LEU:HD12	2.01	0.43
2:F:320:LEU:HD22	2:F:344:VAL:HG13	2.00	0.43
1:A:261:ILE:HB	1:A:266:LEU:HD13	2.01	0.43
2:F:114:PRO:HD3	2:F:207:ILE:HD12	2.01	0.43
2:D:114:PRO:HD3	2:D:207:ILE:HD12	2.01	0.43
1:B:151:LEU:HA	1:B:154:LEU:HD12	2.00	0.42
1:B:212:VAL:HG11	1:B:218:LEU:HD11	2.01	0.42
1:B:304:HIS:O	1:B:308:ILE:HG12	2.19	0.42
2:E:114:PRO:HD3	2:E:207:ILE:HD12	2.02	0.42
1:A:136:LEU:HD22	1:A:203:ALA:HB1	2.01	0.42
1:A:65:VAL:HG13	2:D:326:LEU:HD23	2.00	0.42
2:F:349:LEU:HD22	2:F:353:ARG:CZ	2.49	0.42
1:B:285:ILE:HG21	1:B:314:LEU:HD21	2.00	0.42
2:E:210:VAL:HG22	2:E:238:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HA	2:D:315:ARG:HD2	2.02	0.42
2:E:62:VAL:HG21	2:E:284:GLN:HB3	2.02	0.42
1:B:56:GLN:HG3	1:B:59:ALA:HB3	2.02	0.42
1:C:304:HIS:O	1:C:308:ILE:HG12	2.20	0.42
1:B:86:PRO:HD2	2:E:361:TYR:OH	2.20	0.42
2:E:75:LEU:HD21	2:E:108:ALA:HB3	2.02	0.42
1:A:212:VAL:HG11	1:A:218:LEU:HD11	2.01	0.41
2:D:284:GLN:HE22	2:D:287:ARG:HD2	1.85	0.41
1:C:285:ILE:HG21	1:C:314:LEU:HD21	2.02	0.41
1:C:136:LEU:HD22	1:C:203:ALA:HB1	2.02	0.41
1:C:355:ALA:HB2	2:E:258:PRO:HB3	2.01	0.41
2:D:320:LEU:HD22	2:D:344:VAL:HG13	2.02	0.41
2:D:62:VAL:HG21	2:D:284:GLN:HB3	2.03	0.41
1:A:326:LEU:HD23	2:F:76:GLU:HB3	2.02	0.41
1:C:347:LEU:HB3	2:E:70:ALA:HB2	2.03	0.41
2:D:287:ARG:NH2	2:D:299:GLU:OE1	2.54	0.41
2:F:210:VAL:HG22	2:F:238:VAL:HG13	2.02	0.41
2:F:62:VAL:HG21	2:F:284:GLN:HB3	2.02	0.41
1:A:280:GLN:HE21	1:A:284:GLN:HG3	1.86	0.41
1:C:261:ILE:HB	1:C:266:LEU:HD13	2.02	0.41
1:B:20:VAL:HG13	1:B:149:VAL:HG13	2.03	0.40
1:A:304:HIS:O	1:A:308:ILE:HG12	2.21	0.40
2:E:284:GLN:HE22	2:E:287:ARG:HD2	1.87	0.40
2:F:297:MSE:HE2	2:F:302:TYR:HA	2.03	0.40
2:F:40:HIS:HB2	2:F:103:MSE:HE3	2.04	0.40
2:D:210:VAL:HG22	2:D:238:VAL:HG13	2.01	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	312/367 (85%)	296 (95%)	12 (4%)	4 (1%)	12	45
1	B	313/367 (85%)	296 (95%)	12 (4%)	5 (2%)	9	40
1	C	314/367 (86%)	299 (95%)	12 (4%)	3 (1%)	15	53
2	D	304/378 (80%)	295 (97%)	7 (2%)	2 (1%)	22	60
2	E	309/378 (82%)	300 (97%)	7 (2%)	2 (1%)	25	64
2	F	305/378 (81%)	297 (97%)	6 (2%)	2 (1%)	22	60
All	All	1857/2235 (83%)	1783 (96%)	56 (3%)	18 (1%)	15	53

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	104	LYS
1	B	20	VAL
1	C	20	VAL
2	D	332	LYS
2	E	332	LYS
2	F	332	LYS
1	B	103	SER
2	F	333	GLY
1	A	22	SER
1	B	22	SER
1	B	102	GLY
1	C	22	SER
2	D	333	GLY
2	E	333	GLY
1	A	182	ILE
1	C	182	ILE
1	B	182	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/299 (89%)	252 (94%)	15 (6%)	21	56
1	B	267/299 (89%)	253 (95%)	14 (5%)	23	59
1	C	263/299 (88%)	248 (94%)	15 (6%)	20	56
2	D	250/305 (82%)	231 (92%)	19 (8%)	13	43
2	E	257/305 (84%)	234 (91%)	23 (9%)	9	35
2	F	251/305 (82%)	232 (92%)	19 (8%)	13	43
All	All	1555/1812 (86%)	1450 (93%)	105 (7%)	16	48

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	26	THR
1	A	42	GLU
1	A	103	SER
1	A	119	GLU
1	A	123	THR
1	A	195	ASN
1	A	199	ASP
1	A	220	ILE
1	A	243	ASN
1	A	256	THR
1	A	263	LEU
1	A	293	GLU
1	A	327	LEU
1	A	330	ILE
1	B	20	VAL
1	B	26	THR
1	B	103	SER
1	B	119	GLU
1	B	123	THR
1	B	195	ASN
1	B	199	ASP
1	B	220	ILE
1	B	256	THR
1	B	263	LEU
1	B	293	GLU
1	B	327	LEU

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Mol	Chain	Res	Type
1	B	330	ILE
1	B	352	LYS
1	C	20	VAL
1	C	26	THR
1	C	27	GLN
1	C	42	GLU
1	C	103	SER
1	C	119	GLU
1	C	123	THR
1	C	195	ASN
1	C	199	ASP
1	C	220	ILE
1	C	256	THR
1	C	263	LEU
1	C	293	GLU
1	C	327	LEU
1	C	330	ILE
2	D	61	MSE
2	D	69	ARG
2	D	83	ILE
2	D	86	ARG
2	D	109	LEU
2	D	189	GLU
2	D	199	ARG
2	D	206	ILE
2	D	229	ARG
2	D	238	VAL
2	D	253	THR
2	D	275	THR
2	D	331	ARG
2	D	339	ASP
2	D	343	ARG
2	D	344	VAL
2	D	349	LEU
2	D	365	PHE
2	D	366	LEU
2	E	48	LEU
2	E	58	SER
2	E	61	MSE
2	E	69	ARG
2	E	83	ILE
2	E	109	LEU

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Mol	Chain	Res	Type
2	E	189	GLU
2	E	199	ARG
2	E	206	ILE
2	E	229	ARG
2	E	238	VAL
2	E	251	ARG
2	E	253	THR
2	E	275	THR
2	E	331	ARG
2	E	339	ASP
2	E	343	ARG
2	E	344	VAL
2	E	349	LEU
2	E	352	SER
2	E	355	THR
2	E	365	PHE
2	E	366	LEU
2	F	48	LEU
2	F	69	ARG
2	F	83	ILE
2	F	109	LEU
2	F	189	GLU
2	F	199	ARG
2	F	206	ILE
2	F	229	ARG
2	F	235	MSE
2	F	238	VAL
2	F	253	THR
2	F	273	SER
2	F	275	THR
2	F	331	ARG
2	F	339	ASP
2	F	343	ARG
2	F	344	VAL
2	F	365	PHE
2	F	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	280	GLN

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Mol	Chain	Res	Type
1	A	284	GLN
1	A	331	ASN
1	B	48	GLN
1	B	99	GLN
1	B	284	GLN
1	B	331	ASN
1	C	48	GLN
1	C	58	ASN
1	C	284	GLN
1	C	331	ASN
2	D	217	HIS
2	D	284	GLN
2	D	337	GLN
2	D	362	GLN
2	E	217	HIS
2	E	284	GLN
2	E	362	GLN
2	F	217	HIS
2	F	284	GLN
2	F	337	GLN
2	F	362	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ATP	B	501	-	26,33,33	1.58	6 (23%)	31,52,52	1.00	2 (6%)
3	ATP	D	501	-	26,33,33	1.38	5 (19%)	31,52,52	0.89	2 (6%)
3	ATP	F	501	-	26,33,33	1.33	6 (23%)	31,52,52	0.94	2 (6%)
3	ATP	C	501	-	26,33,33	1.49	4 (15%)	31,52,52	1.03	2 (6%)
3	ATP	E	501	-	26,33,33	1.46	5 (19%)	31,52,52	0.85	2 (6%)
3	ATP	A	501	-	26,33,33	1.67	5 (19%)	31,52,52	0.95	2 (6%)

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	B	501	-	-	3/18/38/38	0/3/3/3
3	ATP	D	501	-	-	4/18/38/38	0/3/3/3
3	ATP	F	501	-	-	4/18/38/38	0/3/3/3
3	ATP	C	501	-	-	3/18/38/38	0/3/3/3
3	ATP	E	501	-	-	4/18/38/38	0/3/3/3
3	ATP	A	501	-	-	3/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ATP	O4'-C1'	5.21	1.48	1.41
3	C	501	ATP	O4'-C1'	4.45	1.47	1.41
3	B	501	ATP	O4'-C1'	4.22	1.47	1.41
3	D	501	ATP	O4'-C1'	4.07	1.46	1.41
3	B	501	ATP	C2-N3	3.84	1.38	1.32
3	A	501	ATP	C2-N3	3.78	1.38	1.32
3	E	501	ATP	O4'-C1'	3.59	1.46	1.41
3	E	501	ATP	C2-N3	3.54	1.37	1.32
3	D	501	ATP	C2-N3	3.26	1.37	1.32
3	C	501	ATP	C2-N3	3.00	1.36	1.32
3	A	501	ATP	C8-N7	-2.71	1.29	1.34
3	A	501	ATP	PG-O1G	2.67	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	ATP	PG-O1G	2.63	1.59	1.50
3	E	501	ATP	C8-N7	-2.61	1.30	1.34
3	B	501	ATP	PG-O1G	2.58	1.58	1.50
3	B	501	ATP	C8-N7	-2.56	1.30	1.34
3	F	501	ATP	O4'-C1'	2.49	1.44	1.41
3	F	501	ATP	C2-N1	2.47	1.38	1.33
3	F	501	ATP	PG-O1G	2.42	1.58	1.50
3	D	501	ATP	C2-N1	2.40	1.38	1.33
3	F	501	ATP	C8-N7	-2.38	1.30	1.34
3	E	501	ATP	PG-O1G	2.36	1.58	1.50
3	F	501	ATP	C2-N3	2.31	1.35	1.32
3	F	501	ATP	C4-N3	2.29	1.38	1.35
3	E	501	ATP	C2-N1	2.28	1.38	1.33
3	B	501	ATP	C2-N1	2.27	1.38	1.33
3	D	501	ATP	PG-O1G	2.11	1.57	1.50
3	C	501	ATP	C8-N7	-2.09	1.31	1.34
3	A	501	ATP	PA-O1A	2.08	1.58	1.50
3	D	501	ATP	C8-N7	-2.06	1.31	1.34
3	B	501	ATP	PA-O1A	2.02	1.58	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	ATP	O2G-PG-O3B	3.33	115.81	104.64
3	A	501	ATP	O2G-PG-O3B	3.10	115.02	104.64
3	F	501	ATP	C5-C6-N6	3.02	124.94	120.35
3	B	501	ATP	O2G-PG-O3B	3.01	114.73	104.64
3	D	501	ATP	C5-C6-N6	2.81	124.63	120.35
3	E	501	ATP	C5-C6-N6	2.69	124.44	120.35
3	D	501	ATP	O2G-PG-O3B	2.54	113.16	104.64
3	C	501	ATP	C5-C6-N6	2.52	124.19	120.35
3	B	501	ATP	C5-C6-N6	2.50	124.14	120.35
3	F	501	ATP	O2G-PG-O3B	2.46	112.87	104.64
3	A	501	ATP	C5-C6-N6	2.36	123.94	120.35
3	E	501	ATP	O2G-PG-O3B	2.17	111.91	104.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	ATP	C5'-O5'-PA-O1A
3	D	501	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	F	501	ATP	PB-O3B-PG-O3G
3	C	501	ATP	C5'-O5'-PA-O1A
3	E	501	ATP	PB-O3B-PG-O3G
3	A	501	ATP	C5'-O5'-PA-O1A
3	D	501	ATP	PA-O3A-PB-O1B
3	F	501	ATP	PA-O3A-PB-O1B
3	E	501	ATP	PA-O3A-PB-O1B
3	B	501	ATP	C5'-O5'-PA-O3A
3	C	501	ATP	C5'-O5'-PA-O3A
3	A	501	ATP	C5'-O5'-PA-O3A
3	B	501	ATP	C5'-O5'-PA-O2A
3	C	501	ATP	C5'-O5'-PA-O2A
3	A	501	ATP	C5'-O5'-PA-O2A
3	D	501	ATP	PA-O3A-PB-O2B
3	E	501	ATP	PA-O3A-PB-O2B
3	D	501	ATP	PB-O3B-PG-O1G
3	F	501	ATP	PB-O3B-PG-O1G
3	E	501	ATP	PB-O3B-PG-O1G
3	F	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 501

Bond lengths

Bond angles

Torsions

Rings
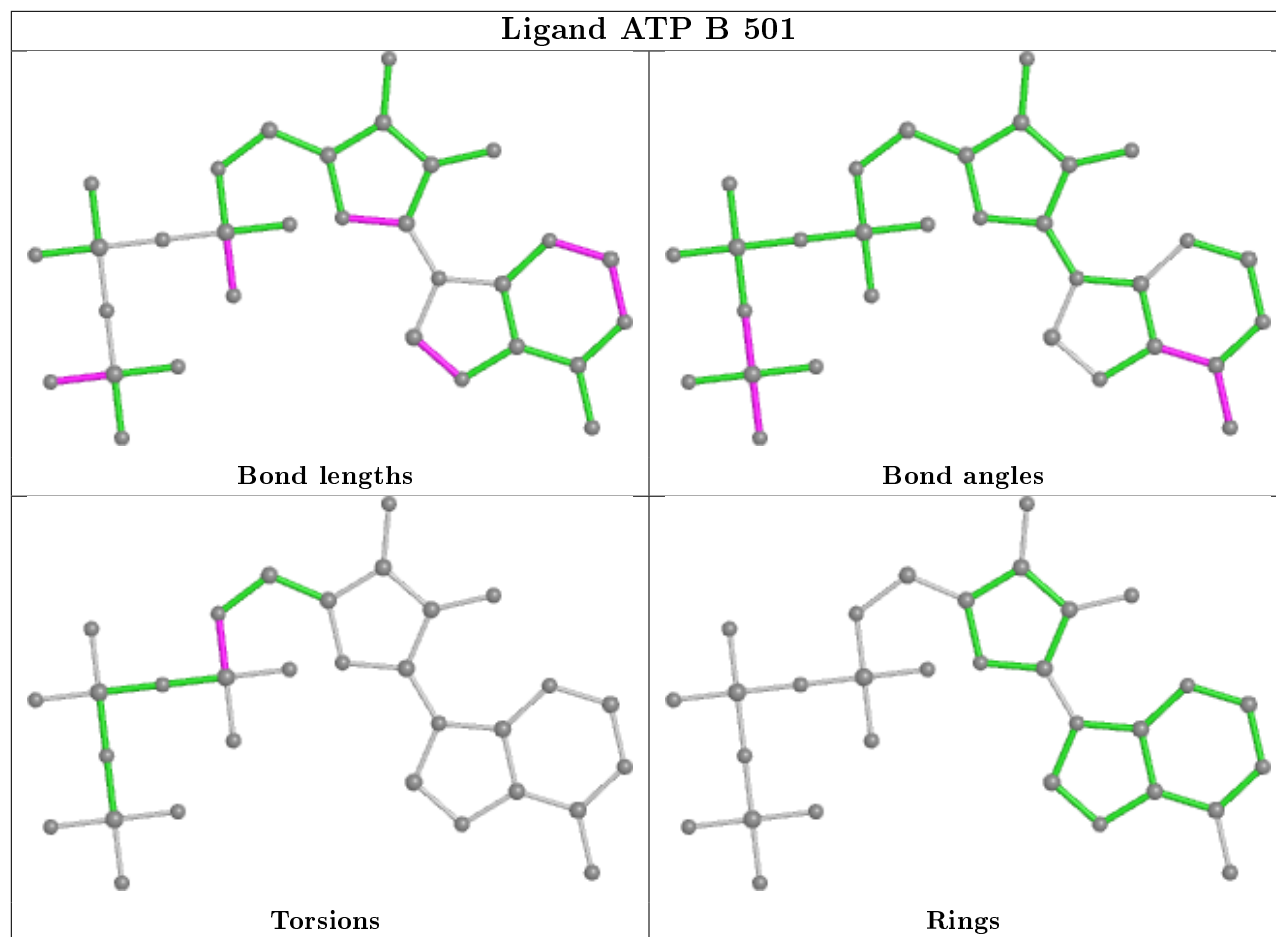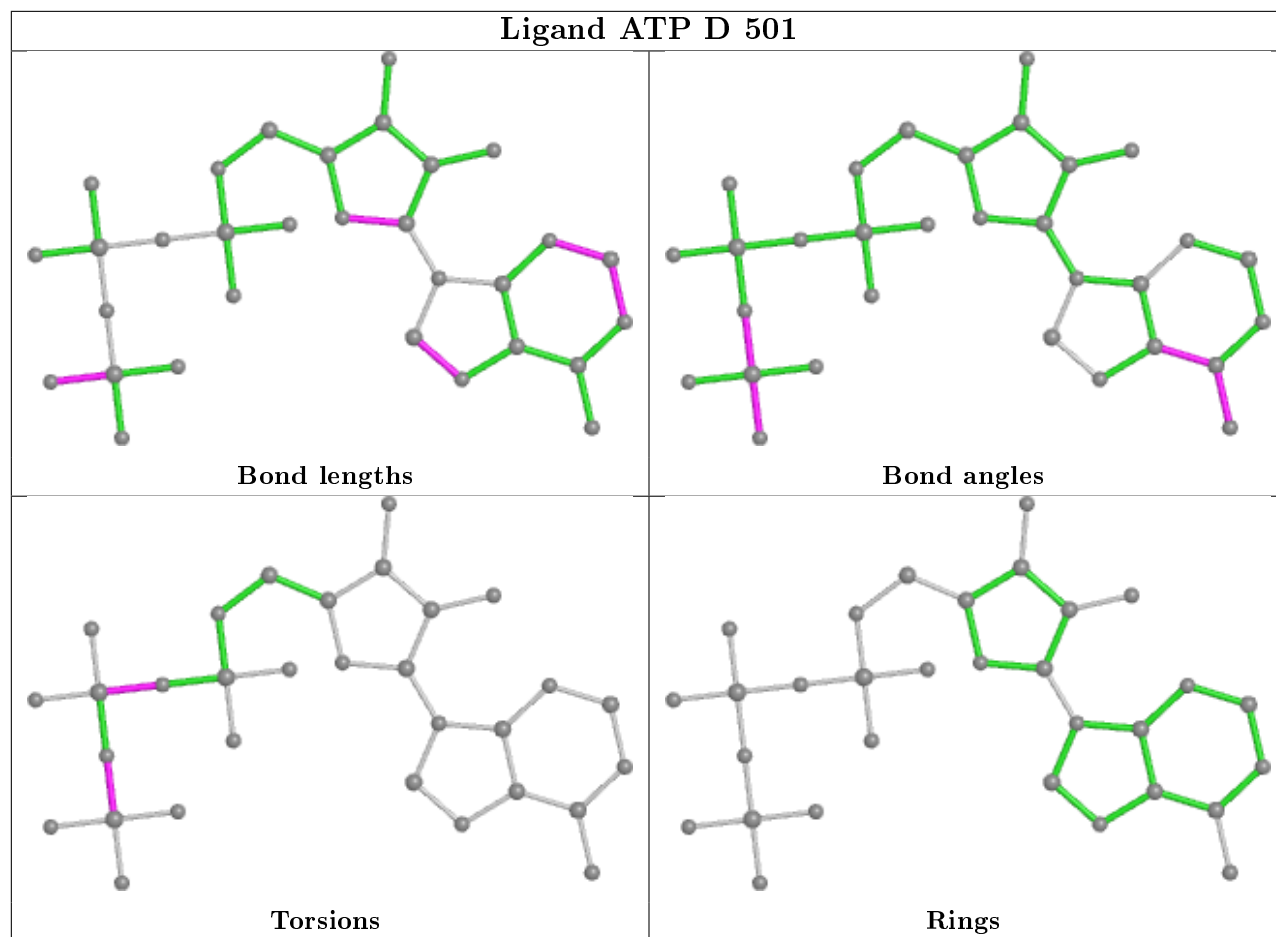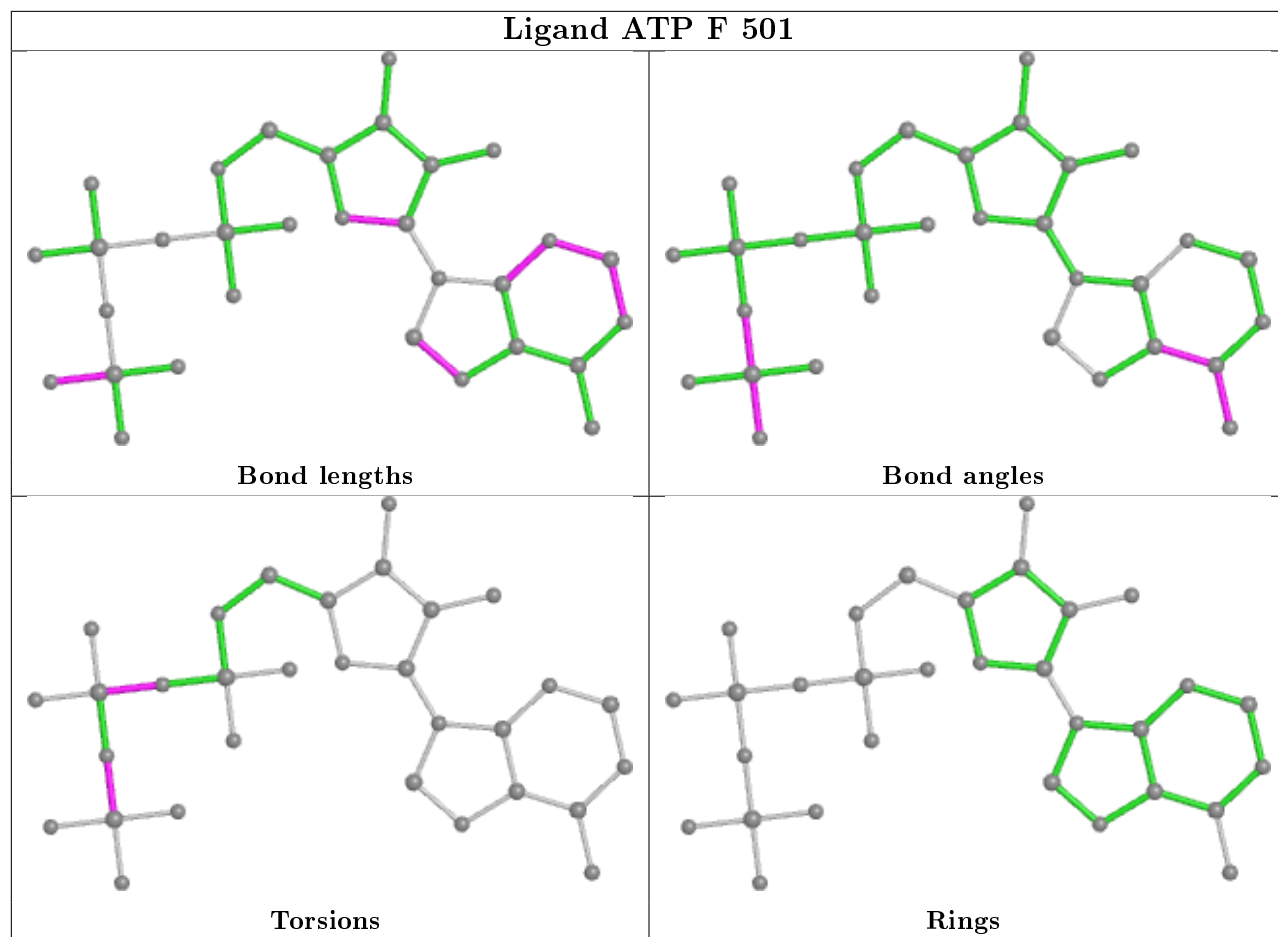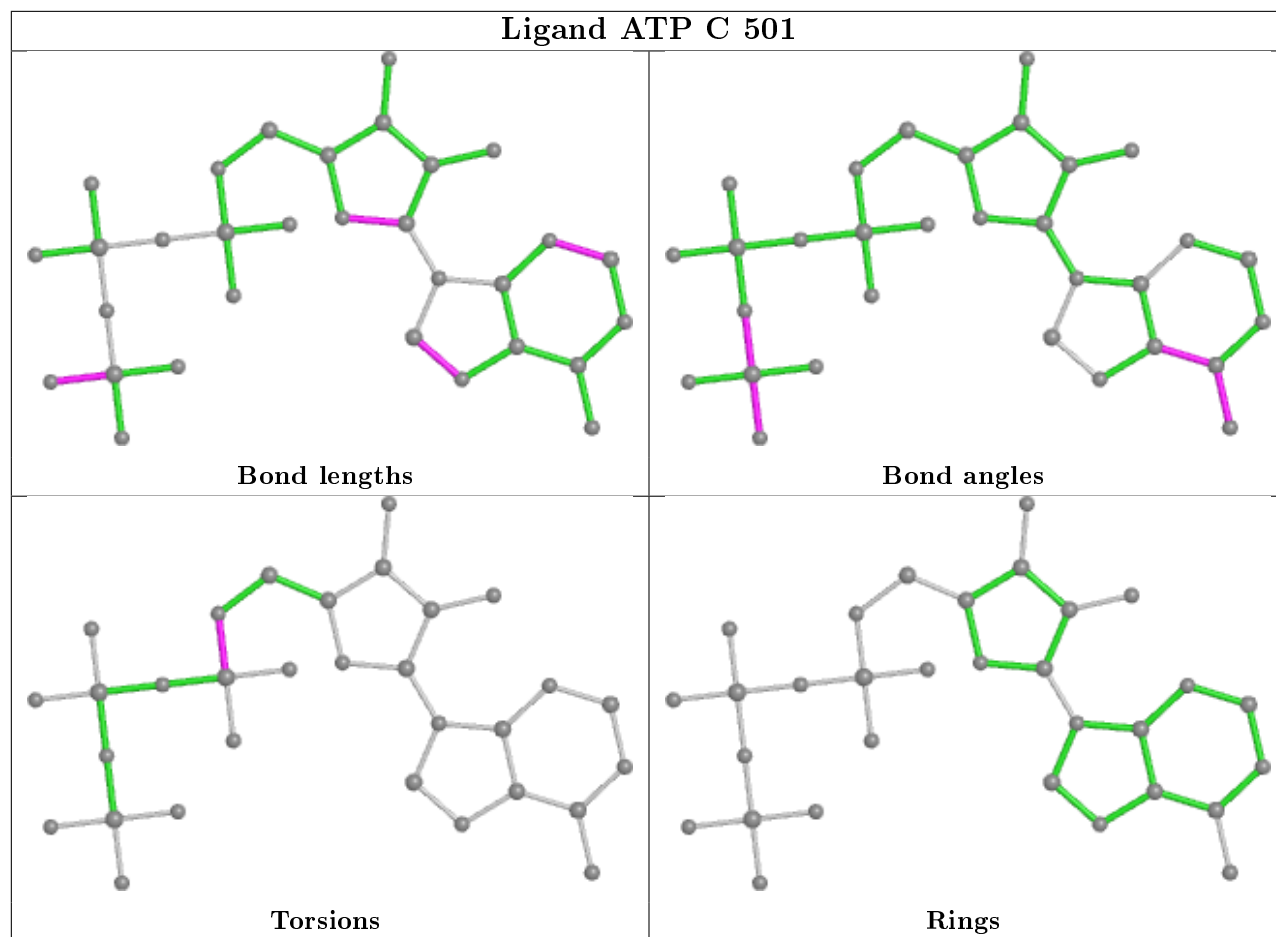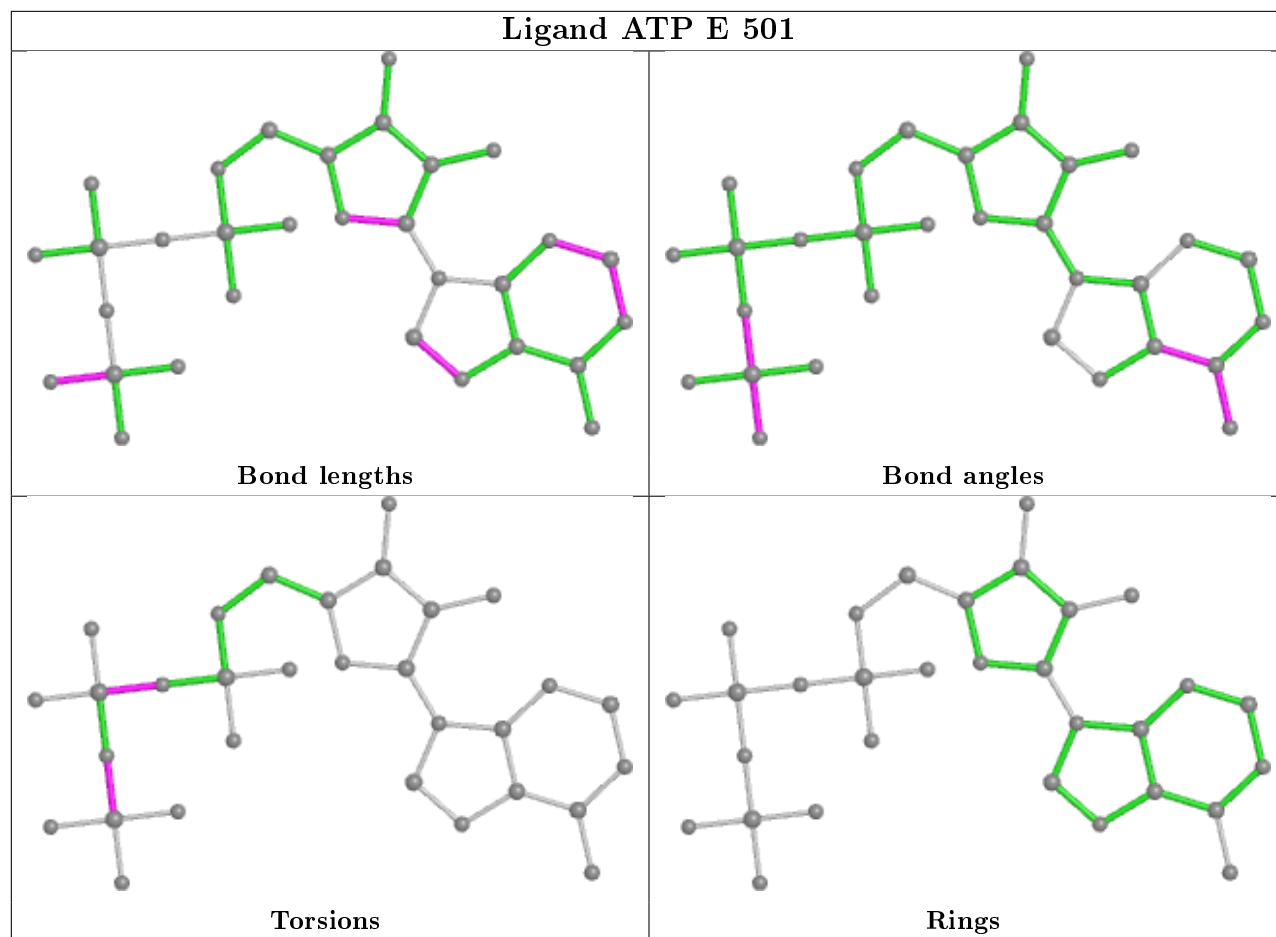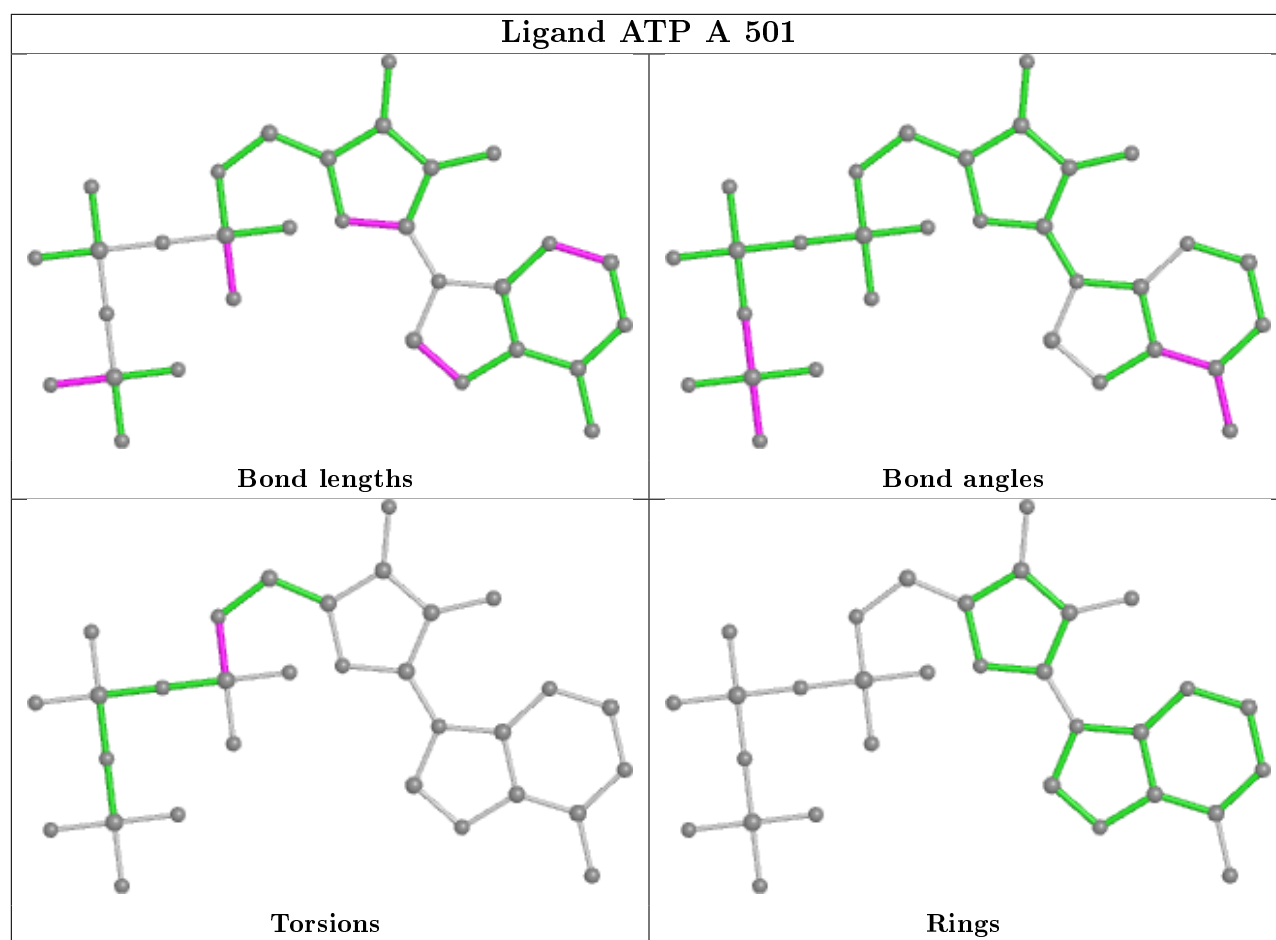
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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(Å²)	Q<0.9
1	A	311/367 (84%)	0.03	16 (5%)	28	10	69, 97, 173, 214	1 (0%)
1	B	312/367 (85%)	0.16	20 (6%)	19	6	74, 113, 169, 211	1 (0%)
1	C	313/367 (85%)	0.06	12 (3%)	40	16	71, 104, 170, 205	1 (0%)
2	D	300/378 (79%)	-0.02	6 (2%)	65	36	74, 106, 168, 202	0
2	E	305/378 (80%)	-0.08	7 (2%)	60	31	79, 108, 167, 196	0
2	F	301/378 (79%)	0.01	7 (2%)	60	31	66, 97, 160, 188	0
All	All	1842/2235 (82%)	0.03	68 (3%)	41	17	66, 105, 169, 214	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	ILE	4.7
1	B	189	GLU	4.7
1	A	194	VAL	4.2
1	B	147	GLN	4.2
1	A	202	ILE	4.1
1	C	202	ILE	4.0
1	C	191	ASN	3.8
1	A	192	LYS	3.8
2	F	165	ILE	3.7
1	B	148	ASP	3.7
1	A	200	GLN	3.6
2	F	205	GLU	3.6
1	B	202	ILE	3.6
1	B	194	VAL	3.5
2	D	198	TRP	3.5
1	B	146	ILE	3.4
1	C	145	ILE	3.4
1	A	203	ALA	3.3
1	B	197	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	197	TYR	3.2
1	B	136	LEU	3.2
1	B	186	LEU	3.2
1	C	194	VAL	3.1
1	B	190	ILE	3.1
1	A	138	ILE	3.0
2	F	37	ILE	3.0
1	A	199	ASP	3.0
1	B	158	ASN	3.0
2	E	371	LYS	3.0
2	E	155	HIS	3.0
1	A	189	GLU	2.9
1	B	203	ALA	2.8
2	E	198	TRP	2.8
1	C	234	ILE	2.8
1	A	195	ASN	2.8
2	F	183	ILE	2.8
2	F	198	TRP	2.7
1	C	199	ASP	2.6
1	B	204	GLU	2.6
1	C	198	ILE	2.6
2	D	191	ILE	2.6
2	E	165	ILE	2.6
2	D	205	GLU	2.5
1	A	360	ASP	2.5
1	B	205	LEU	2.4
2	E	203	LYS	2.4
1	C	158	ASN	2.4
1	B	157	ALA	2.4
1	A	196	LYS	2.4
2	D	194	LYS	2.4
2	E	183	ILE	2.4
1	B	200	GLN	2.3
1	A	187	ARG	2.3
1	A	205	LEU	2.3
2	D	195	VAL	2.2
1	B	45	LEU	2.2
2	F	201	GLU	2.2
1	C	138	ILE	2.2
1	C	200	GLN	2.1
2	E	204	ALA	2.1
1	A	158	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	196	LYS	2.1
1	B	20	VAL	2.1
1	A	301	ALA	2.1
2	D	204	ALA	2.0
1	B	181	GLU	2.0
2	F	204	ALA	2.0
1	A	197	TYR	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(Å^2)	Q<0.9
3	ATP	B	501	31/31	0.85	0.28	93,97,133,134	0
3	ATP	D	501	31/31	0.91	0.20	90,96,120,121	0
3	ATP	E	501	31/31	0.92	0.21	87,92,124,126	0
3	ATP	C	501	31/31	0.93	0.23	83,88,134,134	0
3	ATP	F	501	31/31	0.93	0.20	77,84,117,119	0
3	ATP	A	501	31/31	0.93	0.20	77,81,123,124	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.
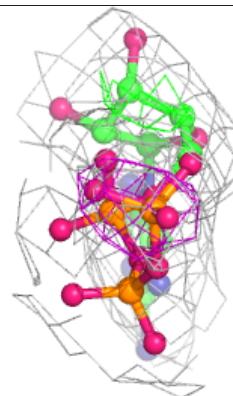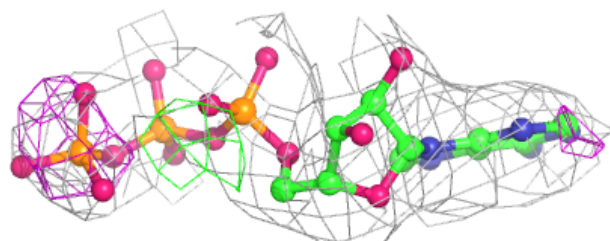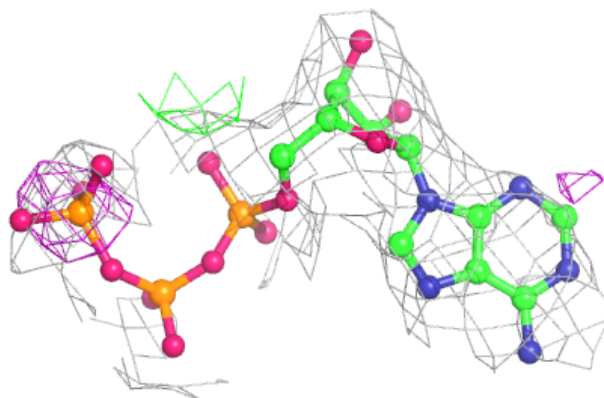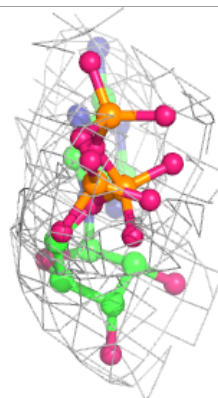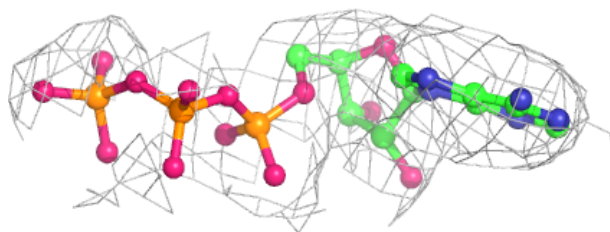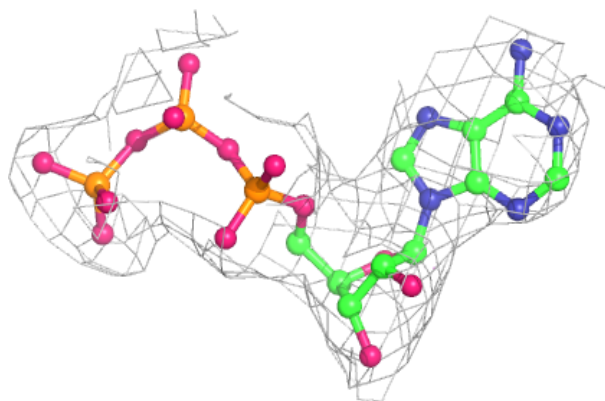
Electron density around ATP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
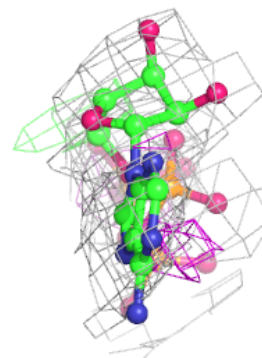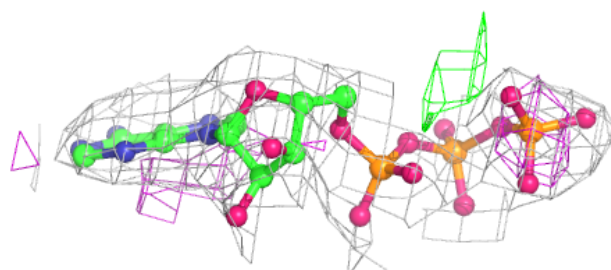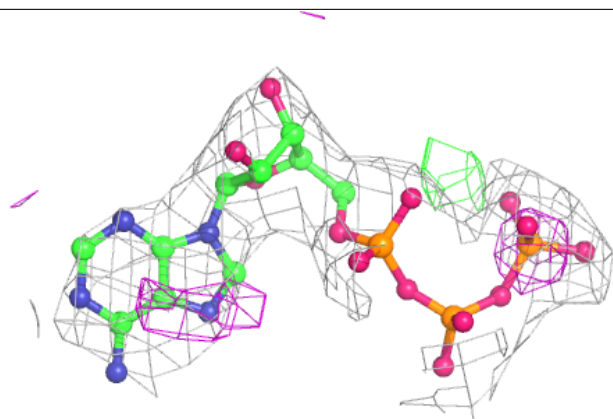
Electron density around ATP D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
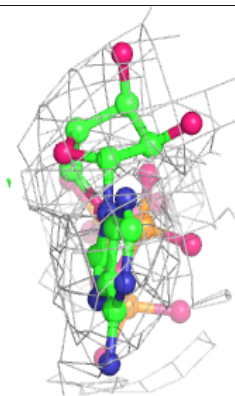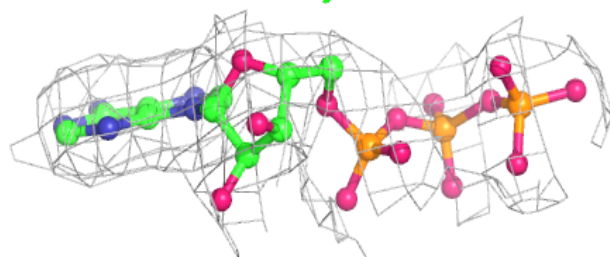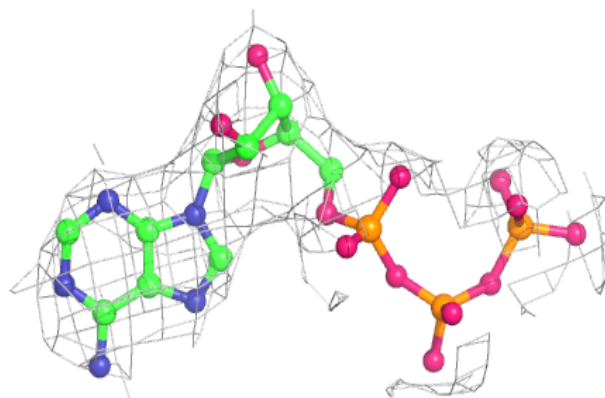and green (positive)
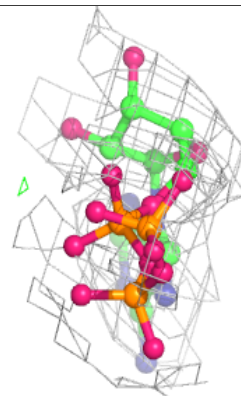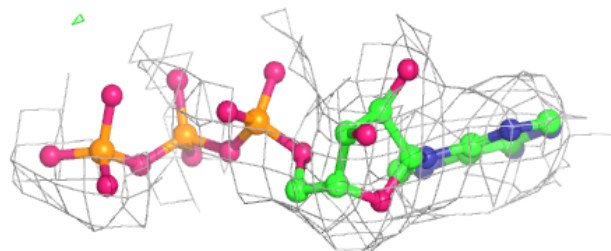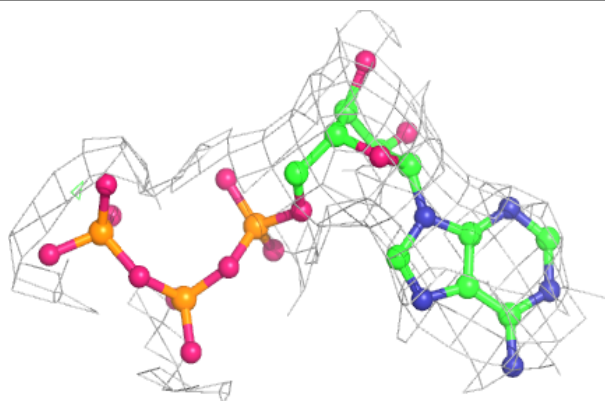
Electron density around ATP E 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
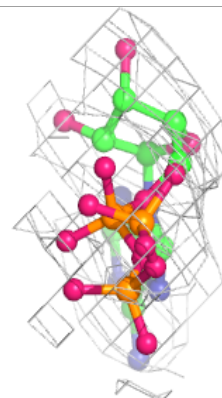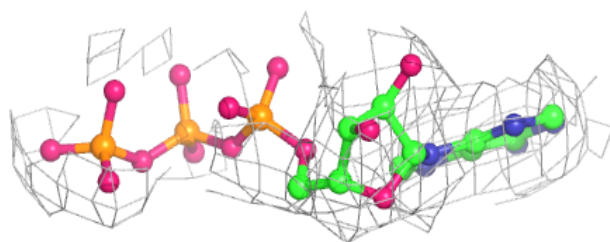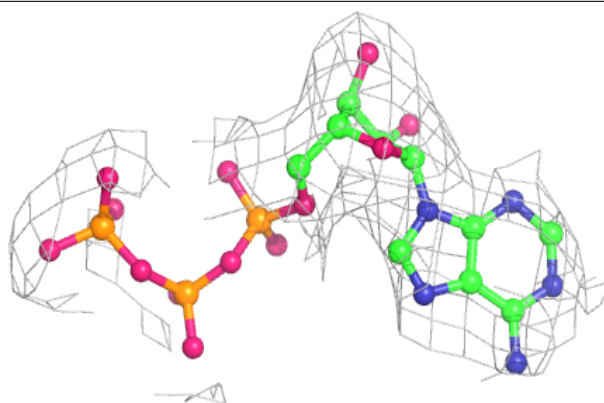
Electron density around ATP C 501:

$2mF_o$-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 F 501:

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

Electron density around ATP A 501:

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

6.5 Other polymers (i)

There are no such residues in this entry.