Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 10:50 pm GMT

PDB ID	:	6QV0
Title	:	Structure of ATP-bound outward-facing TM287/288 in complex with sybody Sb_TM35
Authors	:	Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.
Deposited on	:	2019-03-01
Resolution	:	3.12 Å(reported)

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

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

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

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

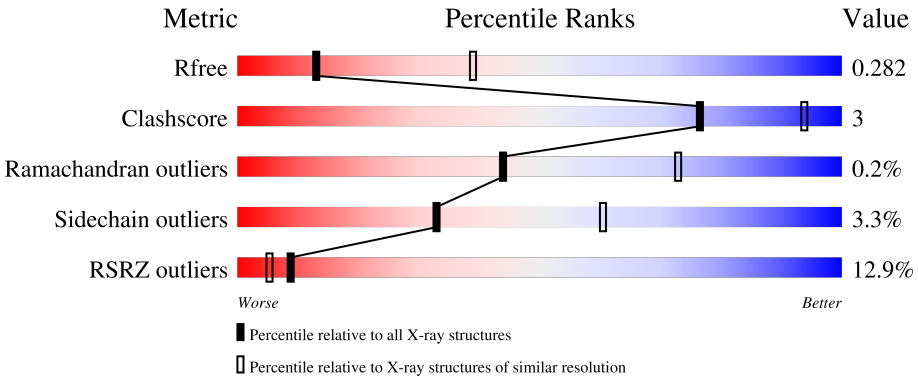
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.12 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}	164625	1668 (3.14-3.10)
Clashscore	180529	1788 (3.14-3.10)
Ramachandran outliers	177936	1696 (3.14-3.10)
Sidechain outliers	177891	1696 (3.14-3.10)
RSRZ outliers	164620	1668 (3.14-3.10)

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	587	11% 85% 11% ·
1	C	587	11% 86% 11% ·
2	B	599	10% 85% 10% · 5%
2	D	599	8% 86% 10% · ·
3	E	128	38% 84% 10% · · ·

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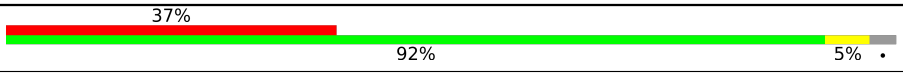
Mol	Chain	Length	Quality of chain
3	F	128	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20086 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 ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			
1	C	569	Total	C	N	O	S	0	0	0
			4470	2882	769	800	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3
A	41	ALA	ASP	engineered mutation	UNP Q9WYC3
C	-9	GLY	-	expression tag	UNP Q9WYC3
C	-8	PRO	-	expression tag	UNP Q9WYC3
C	-7	SER	-	expression tag	UNP Q9WYC3
C	-6	GLY	-	expression tag	UNP Q9WYC3
C	-5	SER	-	expression tag	UNP Q9WYC3
C	-4	GLY	-	expression tag	UNP Q9WYC3
C	-3	GLY	-	expression tag	UNP Q9WYC3
C	-2	GLY	-	expression tag	UNP Q9WYC3
C	-1	GLY	-	expression tag	UNP Q9WYC3
C	0	GLY	-	expression tag	UNP Q9WYC3
C	1	SER	-	expression tag	UNP Q9WYC3
C	41	ALA	ASP	engineered mutation	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			
2	D	574	Total	C	N	O	S	0	0	0
			4573	2957	772	830	14			

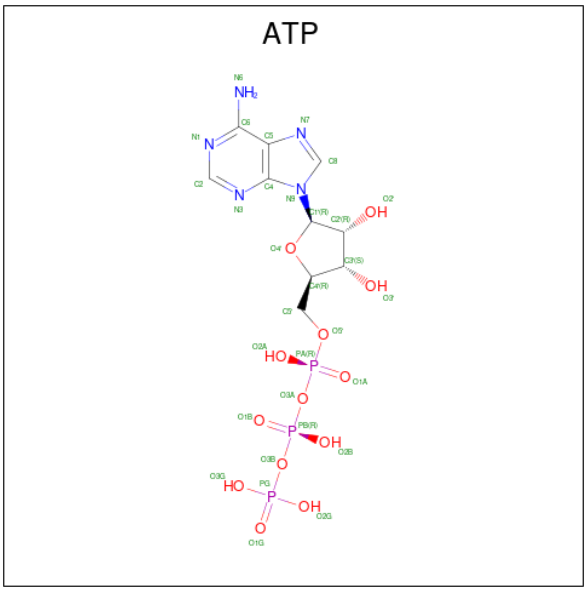
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ALA	ASP	engineered mutation	UNP Q9WYC4
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	65	ALA	ASP	engineered mutation	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Sb_TM35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			955	603	163	186	3			
3	F	124	Total	C	N	O	S	0	0	0
			955	603	163	186	3			

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

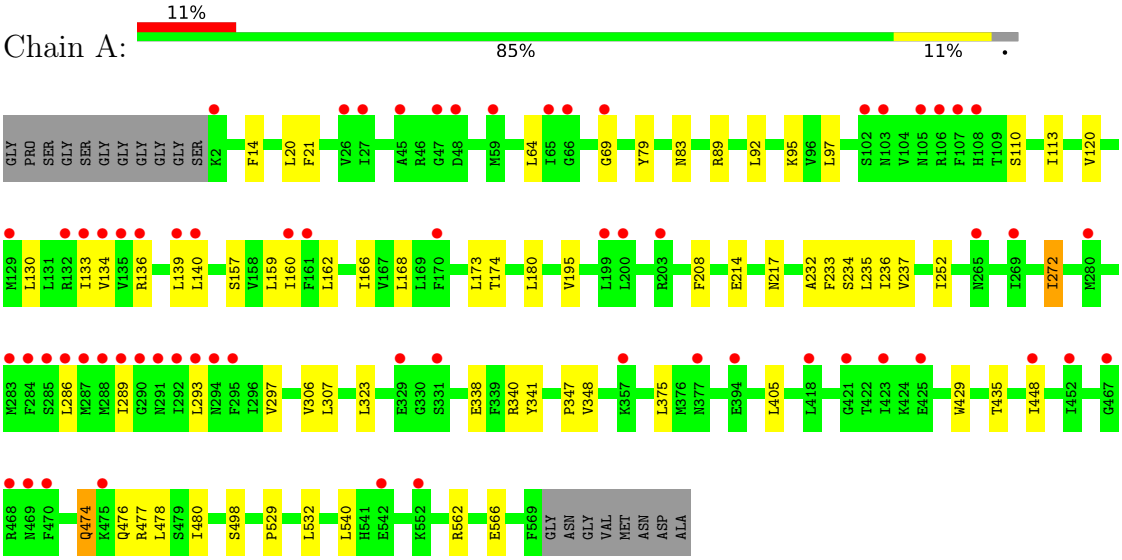
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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.

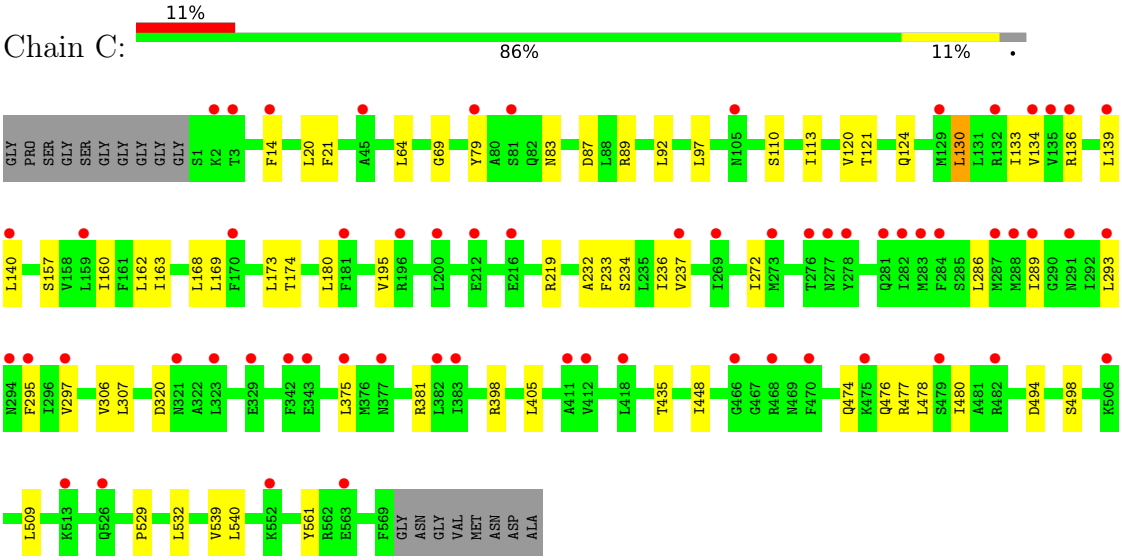
• Molecule 1: ABC transporter, ATP-binding protein

Chain A:



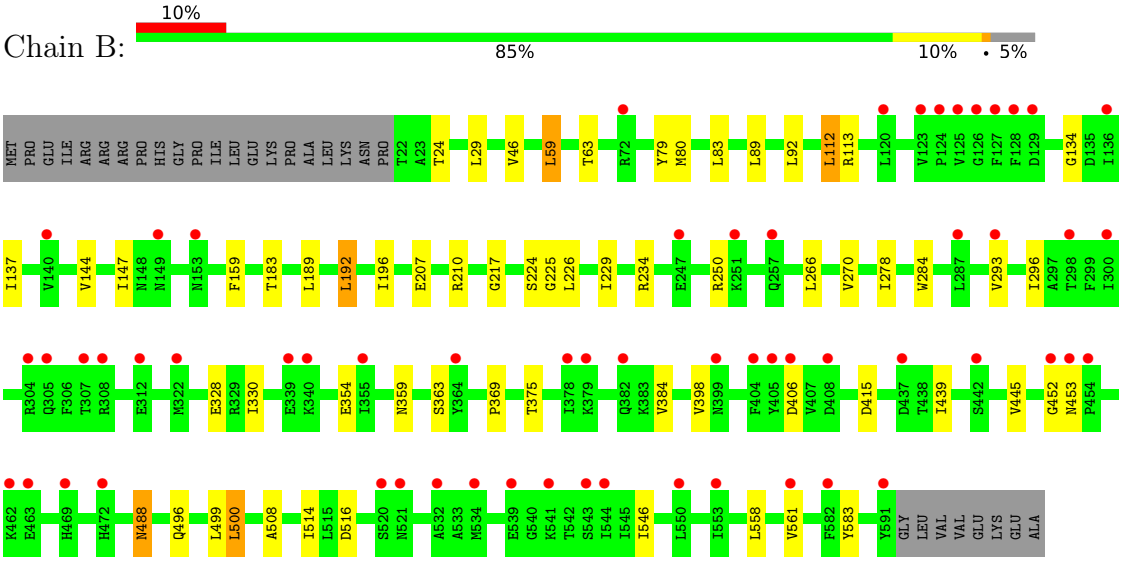
• Molecule 1: ABC transporter, ATP-binding protein

Chain C:



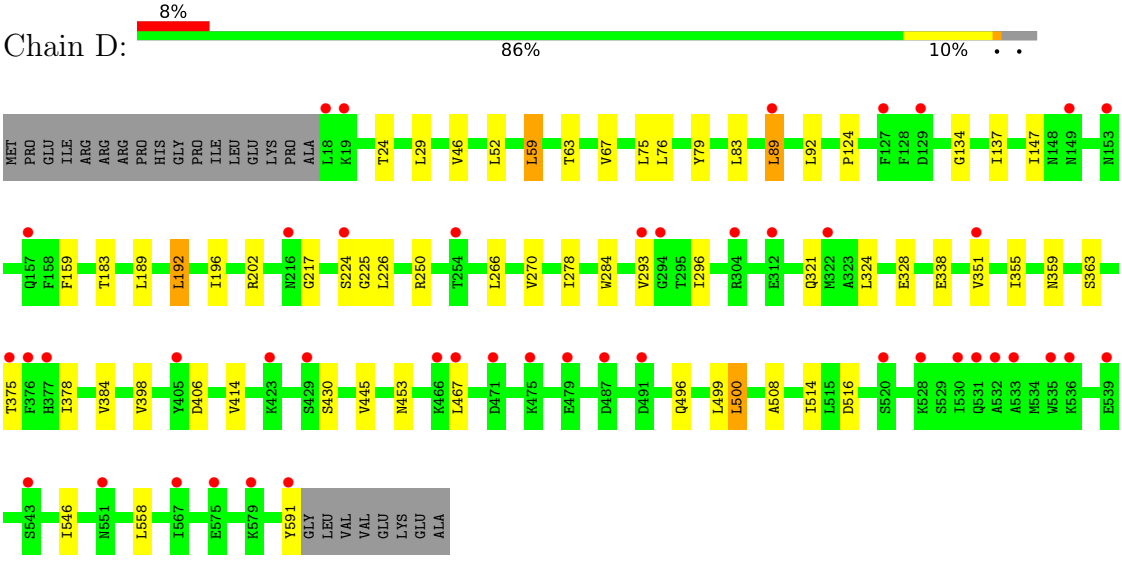
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain B:



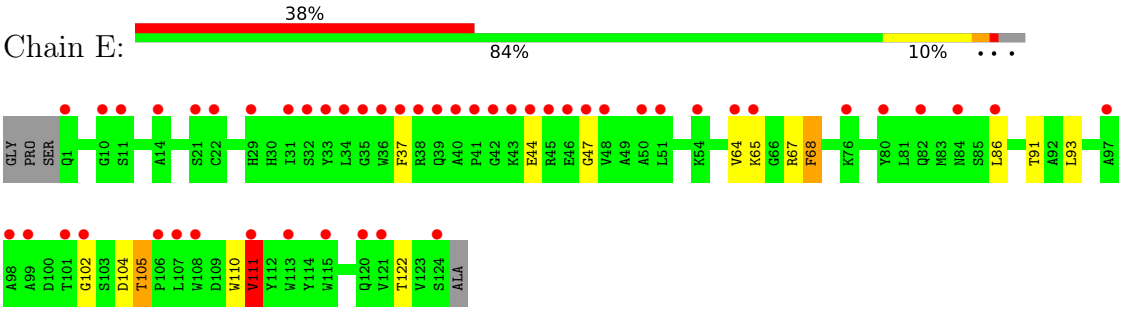
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain D:



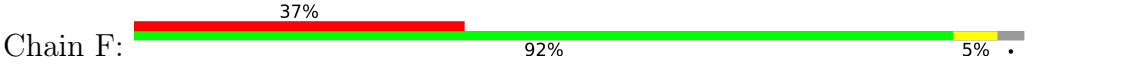
• Molecule 3: Sb_TM35

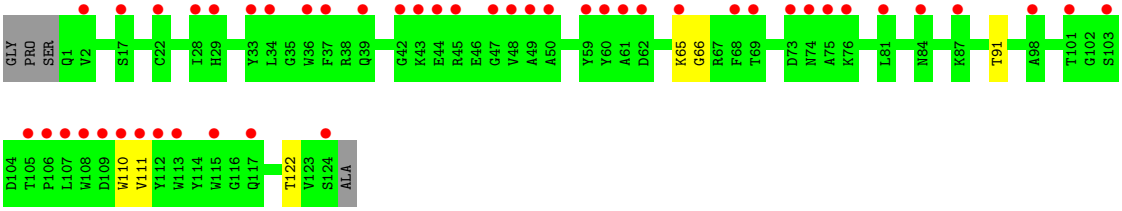
Chain E:



• Molecule 3: Sb_TM35

Chain F:




GLY
PRO
SER
Q1
V2
S17
C22
I28
H29
Y33
L34
G35
W36
F37
R38
Q39
G42
K43
E44
R45
E46
G47
V48
A49
A50
Y59
Y60
A61
D62
K65
G66
R67
F68
T69
D73
N74
A75
K76
L81
N84
K87
T91
A98
T101
G102
S103
D104
T105
P106
L107
W108
D109
W110
V111
Y112
W113
Y114
W115
G116
Q117
T122
V123
S124
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	166.28Å 77.29Å 207.18Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	49.19 – 3.12 49.19 – 3.12	Depositor EDS
% Data completeness (in resolution range)	62.9 (49.19-3.12) 63.1 (49.19-3.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.244 , 0.264 0.261 , 0.282	Depositor DCC
R_{free} test set	2797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	20086	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.41	0/4539	0.58	0/6139
1	C	0.41	0/4545	0.58	0/6147
2	B	0.40	0/4619	0.57	0/6245
2	D	0.41	0/4652	0.58	0/6290
3	E	0.36	0/981	0.53	0/1337
3	F	0.36	0/981	0.51	0/1337
All	All	0.40	0/20317	0.57	0/27495

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

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	4464	0	4666	32	0
1	C	4470	0	4674	24	0
2	B	4541	0	4725	32	0
2	D	4573	0	4762	29	0
3	E	955	0	895	7	0
3	F	955	0	895	3	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	1	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	20086	0	20665	115	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 3.

All (115) 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)
3:E:102:GLY:H	3:E:111:VAL:HG11	1.51	0.73
2:B:46:VAL:HG11	2:B:159:PHE:HB3	1.72	0.71
2:D:46:VAL:HG11	2:D:159:PHE:HB3	1.72	0.71
2:D:284:TRP:HH2	3:F:110:TRP:HA	1.65	0.62
1:A:562:ARG:O	1:A:566:GLU:HG2	2.03	0.59
1:C:130:LEU:O	1:C:134:VAL:HB	2.04	0.57
1:A:83:ASN:HD21	2:B:250:ARG:HH21	1.53	0.56
3:F:91:THR:HG23	3:F:122:THR:HA	1.87	0.56
3:E:91:THR:HG23	3:E:122:THR:HA	1.88	0.56
2:B:359:ASN:H	2:B:375:THR:HB	1.71	0.54
2:B:439:ILE:HG23	2:B:488:ASN:HD21	1.72	0.54
2:D:359:ASN:H	2:D:375:THR:HB	1.72	0.54
1:A:133:ILE:HG22	1:A:136:ARG:HD3	1.89	0.53
2:B:112:LEU:HD23	2:B:330:ILE:HG21	1.90	0.53
2:B:384:VAL:HG22	2:B:558:LEU:HB3	1.91	0.53
2:D:384:VAL:HG22	2:D:558:LEU:HB3	1.91	0.53
3:E:37:PHE:HD1	3:E:47:GLY:HA2	1.74	0.53
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.90	0.52
1:C:21:PHE:HD2	1:C:69:GLY:HA2	1.74	0.52
1:A:234:SER:HA	1:A:237:VAL:HG22	1.91	0.52
2:B:284:TRP:HE1	3:E:110:TRP:HB3	1.74	0.51
1:A:21:PHE:HD1	1:A:69:GLY:HA2	1.76	0.51
1:C:133:ILE:HG22	1:C:136:ARG:HD3	1.93	0.51
2:D:445:VAL:HG13	2:D:500:LEU:HD21	1.93	0.51
1:A:341:TYR:HD1	1:A:348:VAL:HG21	1.76	0.50
1:C:234:SER:HA	1:C:237:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:ASP:HA	2:D:546:ILE:HB	1.95	0.49
1:A:180:LEU:HB3	1:A:232:ALA:HB2	1.93	0.49
1:A:474:GLN:HE22	4:B:600:ATP:H3'	1.78	0.49
1:C:160:ILE:HA	1:C:163:ILE:HD12	1.94	0.49
2:B:59:LEU:HB3	2:B:83:LEU:HD13	1.95	0.49
1:C:180:LEU:HB3	1:C:232:ALA:HB2	1.93	0.49
2:D:59:LEU:HB3	2:D:83:LEU:HD13	1.95	0.49
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.94	0.49
2:D:355:ILE:HG13	2:D:378:ILE:HB	1.94	0.49
1:A:476:GLN:HE22	1:A:498:SER:H	1.61	0.48
2:B:516:ASP:HA	2:B:546:ILE:HB	1.95	0.48
1:C:83:ASN:HD21	2:D:250:ARG:HH21	1.61	0.48
1:A:340:ARG:HG3	1:A:347:PRO:HA	1.95	0.48
1:A:477:ARG:HA	1:A:480:ILE:HD12	1.95	0.48
1:C:477:ARG:HA	1:C:480:ILE:HD12	1.95	0.48
2:B:113:ARG:HG3	2:B:144:VAL:HG11	1.96	0.47
1:C:195:VAL:HG13	2:D:137:ILE:HG12	1.94	0.47
1:A:97:LEU:HA	2:B:226:LEU:HD11	1.96	0.47
1:A:162:LEU:O	1:A:166:ILE:HG12	2.15	0.47
1:A:195:VAL:HG13	2:B:137:ILE:HG12	1.96	0.47
1:C:97:LEU:HA	2:D:226:LEU:HD11	1.95	0.47
1:C:539:VAL:HG21	1:C:561:TYR:HD2	1.80	0.47
1:A:208:PHE:HB3	2:B:452:GLY:HA2	1.98	0.46
2:B:398:VAL:HG13	2:B:514:ILE:HD13	1.96	0.46
2:D:398:VAL:HG13	2:D:514:ILE:HD13	1.97	0.46
1:C:529:PRO:HA	1:C:532:LEU:HD12	1.98	0.46
2:D:202:ARG:HB2	2:D:321:GLN:HE21	1.81	0.46
1:C:157:SER:HA	1:C:160:ILE:HD12	1.98	0.45
1:A:529:PRO:HA	1:A:532:LEU:HD12	1.98	0.45
2:B:63:THR:HG22	2:B:79:TYR:HB3	1.99	0.45
3:E:105:THR:HG21	3:E:111:VAL:HG22	1.99	0.44
1:A:92:LEU:HD11	1:A:306:VAL:HG13	1.98	0.44
1:C:110:SER:HA	1:C:113:ILE:HD12	1.99	0.44
2:D:496:GLN:HA	2:D:499:LEU:HD12	2.00	0.44
2:B:207:GLU:HA	2:B:210:ARG:HG2	2.00	0.44
1:A:286:LEU:HA	1:A:289:ILE:HD12	1.99	0.43
2:B:445:VAL:HG13	2:B:500:LEU:HD21	1.99	0.43
1:A:130:LEU:O	1:A:134:VAL:HB	2.18	0.43
2:B:144:VAL:O	2:B:147:ILE:HG13	2.18	0.43
1:A:341:TYR:CD1	1:A:348:VAL:HG21	2.53	0.43
1:A:429:TRP:HH2	2:B:229:ILE:HG12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:O	2:B:196:ILE:HG12	2.18	0.43
1:C:286:LEU:HA	1:C:289:ILE:HD12	1.99	0.43
2:D:183:THR:HG23	2:D:278:ILE:HG21	2.01	0.43
1:A:375:LEU:HD22	1:A:540:LEU:HD11	2.00	0.43
2:B:24:THR:HG21	2:B:328:GLU:HG2	2.00	0.43
2:B:496:GLN:HA	2:B:499:LEU:HD12	2.00	0.43
2:D:63:THR:HG22	2:D:79:TYR:HB3	2.00	0.43
1:A:110:SER:HA	1:A:113:ILE:HD12	2.00	0.43
1:A:429:TRP:CE3	2:B:234:ARG:HG3	2.54	0.43
2:D:355:ILE:HG22	2:D:414:VAL:HG22	2.00	0.43
1:A:89:ARG:HG3	1:A:120:VAL:HG11	2.01	0.42
1:A:252:ILE:HG23	2:B:80:MET:HG2	2.01	0.42
1:C:476:GLN:HE22	1:C:498:SER:H	1.66	0.42
2:D:192:LEU:O	2:D:196:ILE:HG12	2.19	0.42
2:D:67:VAL:HG11	2:D:76:LEU:HB2	2.00	0.42
1:C:89:ARG:HG3	1:C:120:VAL:HG11	2.01	0.42
2:B:183:THR:HG23	2:B:278:ILE:HG21	2.01	0.42
1:C:92:LEU:HD11	1:C:306:VAL:HG13	2.00	0.42
2:B:134:GLY:HA3	2:B:217:GLY:HA2	2.02	0.42
3:E:64:VAL:HG13	3:E:68:PHE:H	1.84	0.42
2:D:189:LEU:HD23	2:D:270:VAL:HG13	2.02	0.42
2:D:24:THR:HG21	2:D:328:GLU:HG2	2.00	0.42
1:A:214:GLU:HA	1:A:217:ASN:HB2	2.02	0.41
1:A:272:ILE:H	1:A:272:ILE:HG13	1.62	0.41
2:B:189:LEU:HD23	2:B:270:VAL:HG13	2.02	0.41
2:B:354:GLU:HB3	2:B:415:ASP:HA	2.02	0.41
1:C:381:ARG:HH11	1:C:398:ARG:HD2	1.85	0.41
1:C:448:ILE:HG12	1:C:478:LEU:HG	2.02	0.41
3:E:67:ARG:HH21	3:E:86:LEU:HA	1.85	0.41
2:D:134:GLY:HA3	2:D:217:GLY:HA2	2.02	0.41
2:D:293:VAL:HA	2:D:296:ILE:HD12	2.03	0.41
2:B:293:VAL:HA	2:B:296:ILE:HD12	2.03	0.41
1:A:157:SER:HA	1:A:160:ILE:HD12	2.03	0.41
1:A:448:ILE:HG12	1:A:478:LEU:HG	2.02	0.41
2:B:453:ASN:HB2	2:B:508:ALA:HA	2.03	0.41
1:C:174:THR:HA	1:C:297:VAL:HG11	2.02	0.41
2:D:52:LEU:HD11	2:D:89:LEU:HD23	2.03	0.41
2:D:351:VAL:HG11	2:D:430:SER:HB3	2.03	0.41
1:C:121:THR:HA	1:C:124:GLN:HG2	2.02	0.40
2:D:124:PRO:HD3	2:D:338:GLU:HA	2.03	0.40
2:D:202:ARG:HH22	2:D:324:LEU:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:ILE:HG12	2:D:384:VAL:HG21	2.02	0.40
2:B:363:SER:HB2	2:B:369:PRO:HA	2.03	0.40
2:B:561:VAL:HG21	2:B:583:TYR:HB2	2.04	0.40
1:C:375:LEU:HD22	1:C:540:LEU:HD11	2.02	0.40
2:D:453:ASN:HB2	2:D:508:ALA:HA	2.02	0.40
3:F:65:LYS:HB3	3:F:66:GLY:H	1.74	0.40
1:A:174:THR:HA	1:A:297:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	566/587 (96%)	549 (97%)	17 (3%)	0	100 100
1	C	567/587 (97%)	548 (97%)	19 (3%)	0	100 100
2	B	568/599 (95%)	551 (97%)	16 (3%)	1 (0%)	44 73
2	D	572/599 (96%)	558 (98%)	13 (2%)	1 (0%)	44 73
3	E	122/128 (95%)	108 (88%)	10 (8%)	4 (3%)	3 16
3	F	122/128 (95%)	117 (96%)	5 (4%)	0	100 100
All	All	2517/2628 (96%)	2431 (97%)	80 (3%)	6 (0%)	44 73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	111	VAL
3	E	44	GLU
3	E	65	LYS
3	E	104	ASP
2	B	225	GLY
2	D	225	GLY

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	494/503 (98%)	475 (96%)	19 (4%)	28	57
1	C	495/503 (98%)	472 (95%)	23 (5%)	23	51
2	B	506/531 (95%)	495 (98%)	11 (2%)	47	69
2	D	510/531 (96%)	496 (97%)	14 (3%)	40	65
3	E	97/99 (98%)	93 (96%)	4 (4%)	26	55
3	F	97/99 (98%)	96 (99%)	1 (1%)	73	85
All	All	2199/2266 (97%)	2127 (97%)	72 (3%)	33	60

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	20	LEU
1	A	64	LEU
1	A	79	TYR
1	A	95	LYS
1	A	139	LEU
1	A	140	LEU
1	A	159	LEU
1	A	168	LEU
1	A	173	LEU
1	A	235	LEU
1	A	272	ILE
1	A	293	LEU
1	A	307	LEU
1	A	323	LEU
1	A	338	GLU
1	A	405	LEU
1	A	435	THR
1	A	474	GLN
2	B	29	LEU
2	B	59	LEU
2	B	89	LEU

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Mol	Chain	Res	Type
2	B	92	LEU
2	B	112	LEU
2	B	192	LEU
2	B	224	SER
2	B	266	LEU
2	B	406	ASP
2	B	488	ASN
2	B	500	LEU
1	C	14	PHE
1	C	20	LEU
1	C	64	LEU
1	C	79	TYR
1	C	87	ASP
1	C	130	LEU
1	C	139	LEU
1	C	140	LEU
1	C	162	LEU
1	C	168	LEU
1	C	169	LEU
1	C	173	LEU
1	C	219	ARG
1	C	272	ILE
1	C	293	LEU
1	C	295	PHE
1	C	307	LEU
1	C	320	ASP
1	C	405	LEU
1	C	435	THR
1	C	474	GLN
1	C	494	ASP
1	C	509	LEU
2	D	29	LEU
2	D	59	LEU
2	D	75	LEU
2	D	89	LEU
2	D	92	LEU
2	D	147	ILE
2	D	192	LEU
2	D	224	SER
2	D	266	LEU
2	D	363	SER
2	D	406	ASP

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Mol	Chain	Res	Type
2	D	467	LEU
2	D	500	LEU
2	D	591	TYR
3	E	68	PHE
3	E	93	LEU
3	E	105	THR
3	E	111	VAL
3	F	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	215	ASN
1	A	474	GLN
2	B	133	HIS
2	B	268	ASN
2	B	305	GLN
2	B	453	ASN
1	C	83	ASN
2	D	133	HIS
2	D	195	GLN
2	D	257	GLN
2	D	268	ASN
2	D	321	GLN
2	D	453	ASN
2	D	494	GLN
3	E	27	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	ATP	C	600	5	26,33,33	0.56	0	31,52,52	0.67	1 (3%)
4	ATP	D	600	5	26,33,33	0.57	0	31,52,52	0.74	1 (3%)
4	ATP	B	600	5	26,33,33	0.57	0	31,52,52	0.72	1 (3%)
4	ATP	A	600	5	26,33,33	0.60	0	31,52,52	0.68	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	600	5	-	6/18/38/38	0/3/3/3
4	ATP	D	600	5	-	5/18/38/38	0/3/3/3
4	ATP	B	600	5	-	3/18/38/38	0/3/3/3
4	ATP	A	600	5	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	600	ATP	C5-C6-N6	2.30	123.85	120.35
4	B	600	ATP	C5-C6-N6	2.27	123.80	120.35
4	A	600	ATP	C5-C6-N6	2.22	123.73	120.35
4	C	600	ATP	C5-C6-N6	2.22	123.72	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ATP	C5'-O5'-PA-O2A
4	A	600	ATP	C5'-O5'-PA-O3A
4	C	600	ATP	PB-O3B-PG-O2G
4	A	600	ATP	O4'-C4'-C5'-O5'
4	A	600	ATP	C3'-C4'-C5'-O5'
4	C	600	ATP	PB-O3B-PG-O3G
4	B	600	ATP	C5'-O5'-PA-O3A
4	D	600	ATP	C5'-O5'-PA-O3A
4	B	600	ATP	PG-O3B-PB-O1B
4	B	600	ATP	PA-O3A-PB-O1B
4	C	600	ATP	PG-O3B-PB-O2B
4	D	600	ATP	PG-O3B-PB-O2B
4	A	600	ATP	C5'-O5'-PA-O1A
4	A	600	ATP	PG-O3B-PB-O2B
4	D	600	ATP	PA-O3A-PB-O2B
4	A	600	ATP	PA-O3A-PB-O2B
4	D	600	ATP	C3'-C4'-C5'-O5'
4	C	600	ATP	PA-O3A-PB-O1B
4	C	600	ATP	PA-O3A-PB-O2B
4	D	600	ATP	PA-O3A-PB-O1B
4	C	600	ATP	PB-O3B-PG-O1G

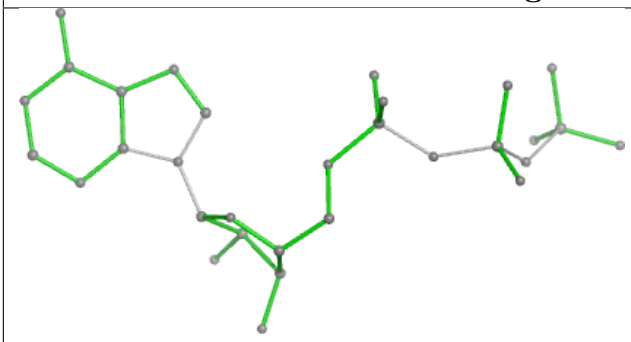
There are no ring outliers.

1 monomer is involved in 1 short contact:

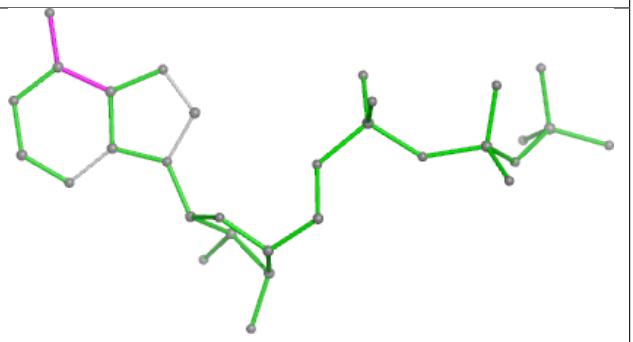
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	ATP	1	0

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 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.

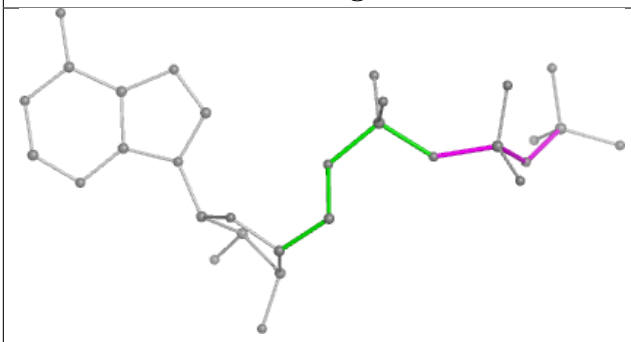
Ligand ATP C 600



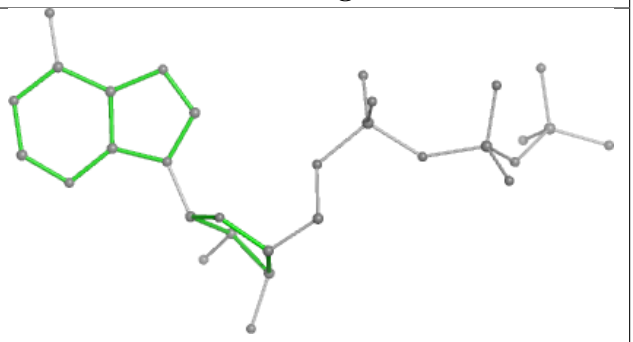
Bond lengths



Bond angles

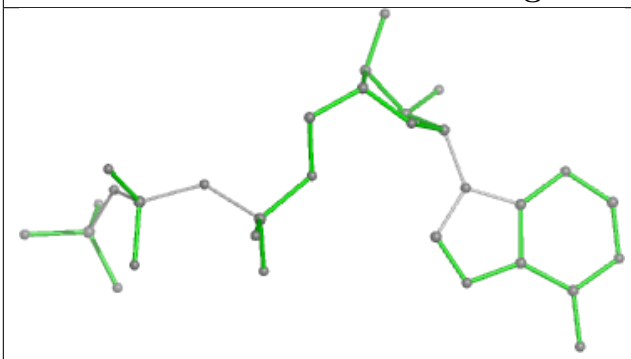


Torsions

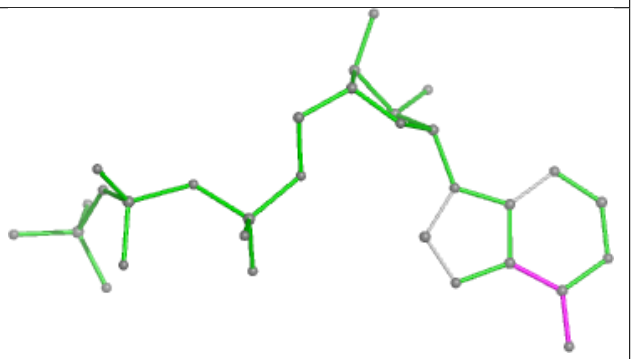


Rings

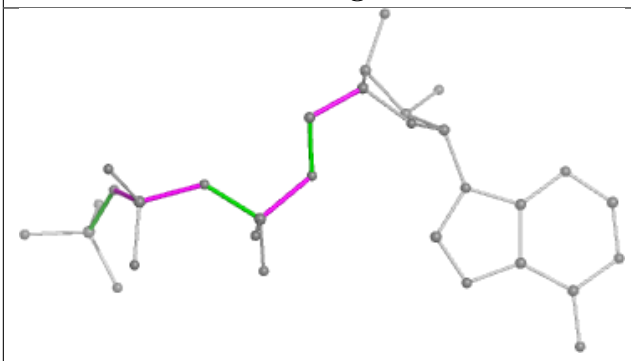
Ligand ATP D 600



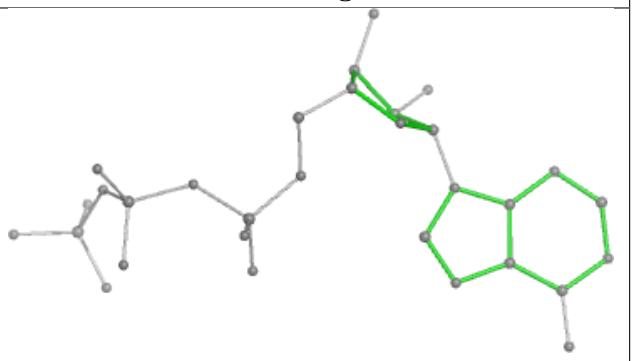
Bond lengths



Bond angles

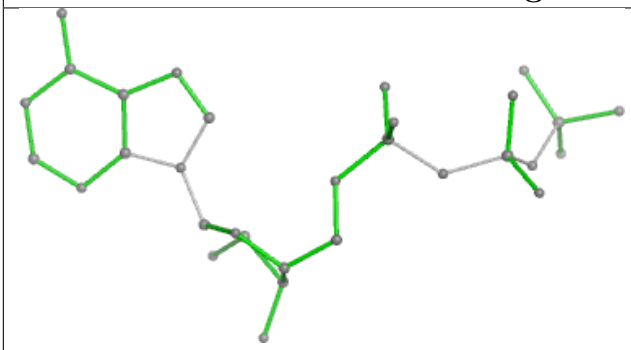


Torsions

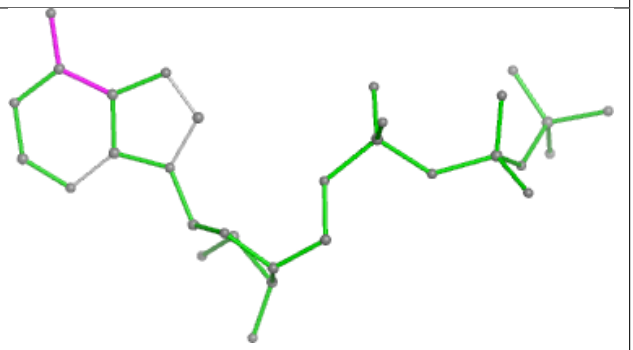


Rings

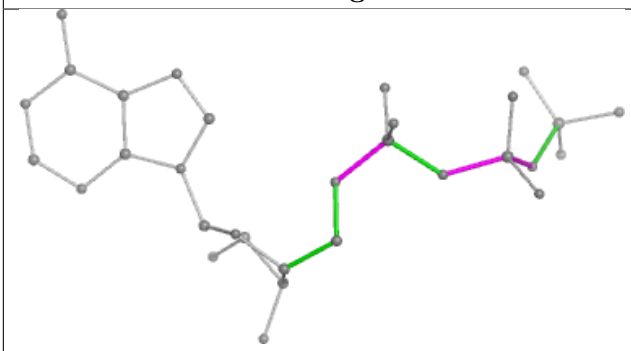
Ligand ATP B 600



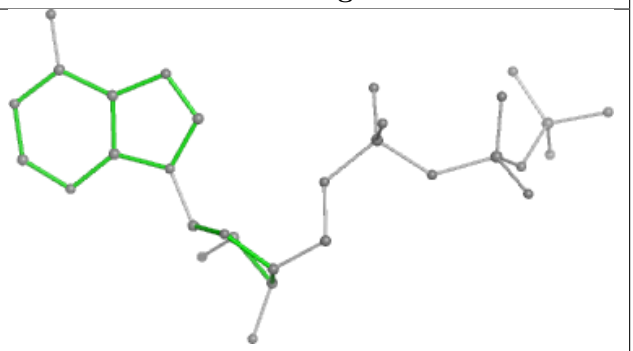
Bond lengths



Bond angles

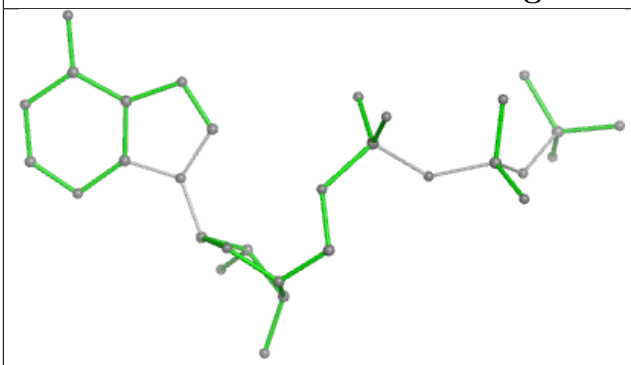


Torsions

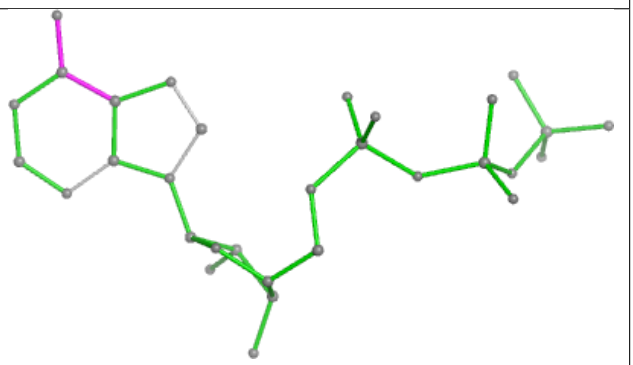


Rings

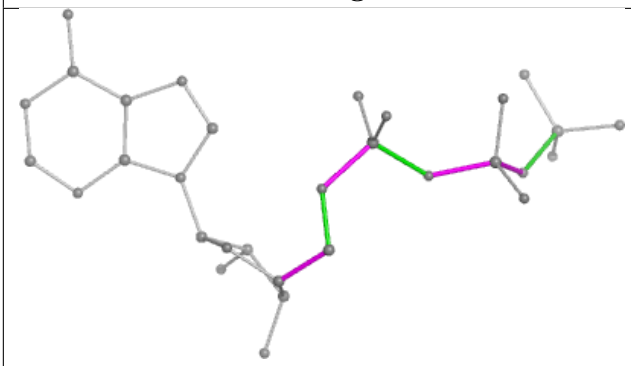
Ligand ATP A 600



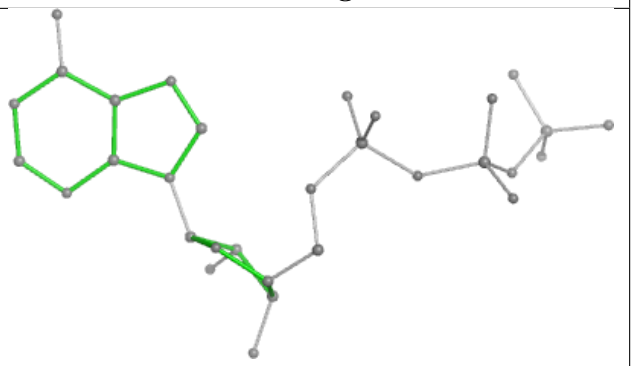
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	568/587 (96%)	0.70	64 (11%)	11	7	26, 54, 102, 126	0
1	C	569/587 (96%)	0.79	62 (10%)	12	7	33, 69, 113, 132	0
2	B	570/599 (95%)	0.71	60 (10%)	13	8	26, 63, 100, 129	0
2	D	574/599 (95%)	0.68	45 (7%)	20	12	32, 64, 91, 119	0
3	E	124/128 (96%)	2.05	49 (39%)	1	0	101, 131, 168, 180	0
3	F	124/128 (96%)	1.83	47 (37%)	1	0	89, 118, 147, 159	0
All	All	2529/2628 (96%)	0.84	327 (12%)	9	5	26, 66, 126, 180	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	TYR	7.2
3	E	42	GLY	7.2
1	A	105	ASN	6.8
3	E	33	TYR	6.4
3	E	11	SER	6.4
3	E	47	GLY	6.1
1	A	200	LEU	6.1
2	D	153	ASN	6.0
3	E	43	LYS	6.0
1	A	283	MET	6.0
3	F	111	VAL	6.0
1	A	293	LEU	5.8
1	C	200	LEU	5.8
1	A	292	ILE	5.8
2	B	339	GLU	5.6
1	A	475	LYS	5.6
1	A	470	PHE	5.6
1	C	294	ASN	5.5
1	A	288	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	5.3
1	A	329	GLU	5.3
1	C	105	ASN	5.2
3	F	75	ALA	5.2
3	E	37	PHE	5.1
3	E	65	LYS	5.1
1	C	343	GLU	5.1
2	B	305	GLN	5.1
3	E	113	TRP	5.0
1	C	291	ASN	4.9
1	C	377	ASN	4.9
1	C	79	TYR	4.9
3	E	44	GLU	4.8
3	E	107	LEU	4.8
2	B	127	PHE	4.7
2	D	535	TRP	4.6
3	F	50	ALA	4.6
3	F	110	TRP	4.5
2	D	18	LEU	4.5
2	B	304	ARG	4.5
3	E	45	ARG	4.4
1	A	394	GLU	4.4
3	F	109	ASP	4.4
1	A	468	ARG	4.4
3	E	40	ALA	4.3
3	E	115	TRP	4.3
1	C	468	ARG	4.2
2	B	129	ASP	4.2
1	A	357	LYS	4.2
1	A	291	ASN	4.2
3	E	124	SER	4.1
2	D	591	TYR	4.1
2	B	399	ASN	4.1
1	A	542	GLU	4.0
1	C	212	GLU	4.0
2	B	308	ARG	4.0
3	F	68	PHE	4.0
3	E	46	GLU	4.0
3	E	14	ALA	4.0
1	C	329	GLU	4.0
3	F	108	TRP	3.9
2	B	442	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	F	107	LEU	3.8
2	B	405	TYR	3.8
1	A	102	SER	3.8
2	B	406	ASP	3.7
1	C	287	MET	3.7
2	D	157	GLN	3.7
1	C	479	SER	3.7
2	B	463	GLU	3.6
2	D	528	LYS	3.6
2	B	553	ILE	3.6
1	C	2	LYS	3.6
1	A	467	GLY	3.6
3	F	87	LYS	3.6
2	B	582	PHE	3.5
2	D	475	LYS	3.5
3	F	17	SER	3.5
2	B	307	THR	3.5
2	B	251	LYS	3.5
1	A	331	SER	3.5
1	A	377	ASN	3.5
3	F	59	TYR	3.5
1	A	47	GLY	3.5
1	C	81	SER	3.4
1	A	45	ALA	3.4
1	C	283	MET	3.4
2	D	532	ALA	3.4
2	D	536	LYS	3.4
1	C	295	PHE	3.4
2	B	312	GLU	3.4
2	B	469	HIS	3.4
3	F	48	VAL	3.4
2	B	126	GLY	3.4
3	F	124	SER	3.4
1	C	411	ALA	3.4
2	D	312	GLU	3.4
1	C	293	LEU	3.4
1	A	136	ARG	3.4
3	F	39	GLN	3.3
1	C	136	ARG	3.3
2	B	300	ILE	3.3
1	C	139	LEU	3.3
3	E	41	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
3	F	76	LYS	3.3
2	B	520	SER	3.3
3	E	76	LYS	3.2
3	F	74	ASN	3.2
3	F	112	TYR	3.2
3	E	36	TRP	3.2
3	F	34	LEU	3.2
1	C	552	LYS	3.2
1	A	469	ASN	3.2
1	A	161	PHE	3.2
1	A	289	ILE	3.2
2	D	129	ASP	3.2
1	A	129	MET	3.2
2	B	120	LEU	3.2
3	E	34	LEU	3.2
1	A	132	ARG	3.1
2	D	575	GLU	3.1
1	A	134	VAL	3.1
1	C	289	ILE	3.1
1	A	66	GLY	3.1
1	A	290	GLY	3.1
2	D	567	ILE	3.1
3	E	106	PRO	3.1
1	C	470	PHE	3.1
2	D	375	THR	3.1
3	F	105	THR	3.1
3	E	39	GLN	3.1
3	E	80	TYR	3.1
2	D	294	GLY	3.0
2	D	531	GLN	3.0
2	B	404	PHE	3.0
1	A	280	MET	3.0
1	A	135	VAL	3.0
2	B	153	ASN	3.0
1	A	160	ILE	3.0
1	C	269	ILE	3.0
2	B	322	MET	3.0
2	D	351	VAL	3.0
3	F	49	ALA	3.0
2	B	247	GLU	3.0
1	C	382	LEU	3.0
3	E	111	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	408	ASP	3.0
1	A	294	ASN	3.0
3	E	22	CYS	2.9
2	B	379	LYS	2.9
3	E	38	ARG	2.9
2	B	561	VAL	2.9
3	E	64	VAL	2.9
1	A	140	LEU	2.9
2	B	123	VAL	2.9
1	A	448	ILE	2.9
1	C	132	ARG	2.9
1	C	412	VAL	2.9
2	D	149	ASN	2.9
3	E	50	ALA	2.8
3	E	101	THR	2.8
3	F	69	THR	2.8
2	B	298	THR	2.8
2	B	437	ASP	2.8
1	A	2	LYS	2.8
2	B	534	MET	2.8
1	C	45	ALA	2.7
1	C	418	LEU	2.7
2	D	530	ILE	2.7
2	D	224	SER	2.7
1	A	423	ILE	2.7
3	F	106	PRO	2.7
3	F	61	ALA	2.7
3	F	36	TRP	2.7
1	C	135	VAL	2.7
1	A	106	ARG	2.7
2	B	355	ILE	2.7
2	D	127	PHE	2.7
3	F	47	GLY	2.7
2	B	382	GLN	2.7
1	C	277	ASN	2.7
1	C	284	PHE	2.7
1	C	342	PHE	2.7
1	C	375	LEU	2.7
1	C	129	MET	2.7
2	B	140	VAL	2.7
1	A	452	ILE	2.6
3	F	84	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	322	MET	2.6
1	A	26	VAL	2.6
3	F	22	CYS	2.6
3	E	97	ALA	2.6
2	D	376	PHE	2.6
2	D	533	ALA	2.6
2	D	304	ARG	2.6
2	B	125	VAL	2.6
3	E	31	ILE	2.6
2	B	452	GLY	2.6
1	C	288	MET	2.6
1	A	203	ARG	2.6
3	F	103	SER	2.6
1	C	278	TYR	2.5
3	F	45	ARG	2.5
2	B	454	PRO	2.5
2	B	462	LYS	2.5
2	B	287	LEU	2.5
3	F	42	GLY	2.5
1	A	287	MET	2.5
2	B	257	GLN	2.5
3	F	98	ALA	2.5
3	F	29	HIS	2.5
2	D	543	SER	2.5
3	E	99	ALA	2.5
3	E	121	VAL	2.5
3	F	2	VAL	2.5
2	B	378	ILE	2.5
1	C	14	PHE	2.5
2	B	543	SER	2.5
3	E	1	GLN	2.5
3	E	102	GLY	2.5
1	A	425	GLU	2.5
3	E	10	GLY	2.4
3	F	117	GLN	2.4
1	C	323	LEU	2.4
1	A	107	PHE	2.4
1	A	295	PHE	2.4
1	C	513	LYS	2.4
2	D	466	LYS	2.4
3	E	82	GLN	2.4
2	D	520	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	33	TYR	2.4
1	A	265	ASN	2.4
1	A	269	ILE	2.4
1	A	552	LYS	2.4
1	C	506	LYS	2.4
1	C	482	ARG	2.4
2	D	405	TYR	2.4
2	B	544	ILE	2.4
1	A	284	PHE	2.4
2	D	539	GLU	2.4
1	C	273	MET	2.4
3	F	101	THR	2.4
2	D	487	ASP	2.3
3	E	84	ASN	2.3
2	D	293	VAL	2.3
2	D	429	SER	2.3
2	D	491	ASP	2.3
3	E	48	VAL	2.3
3	F	115	TRP	2.3
1	C	383	ILE	2.3
2	B	149	ASN	2.3
2	D	579	LYS	2.3
3	F	113	TRP	2.3
1	C	181	PHE	2.3
1	C	466	GLY	2.3
1	C	170	PHE	2.3
2	B	539	GLU	2.3
1	A	103	ASN	2.2
1	C	475	LYS	2.2
1	A	139	LEU	2.2
1	C	563	GLU	2.2
3	E	21	SER	2.2
1	C	3	THR	2.2
1	C	140	LEU	2.2
2	B	453	ASN	2.2
2	B	521	ASN	2.2
3	F	43	LYS	2.2
3	E	98	ALA	2.2
2	B	541	LYS	2.2
2	D	551	ASN	2.2
1	C	237	VAL	2.2
1	C	297	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	467	LEU	2.2
1	A	69	GLY	2.2
1	A	170	PHE	2.2
1	A	418	LEU	2.2
1	A	27	ILE	2.1
1	C	196	ARG	2.1
1	A	286	LEU	2.1
1	C	134	VAL	2.1
2	B	550	LEU	2.1
2	D	89	LEU	2.1
3	E	32	SER	2.1
3	F	81	LEU	2.1
2	B	532	ALA	2.1
2	D	471	ASP	2.1
1	C	216	GLU	2.1
1	C	159	LEU	2.1
2	D	216	ASN	2.1
3	E	35	GLY	2.1
2	B	72	ARG	2.1
1	A	108	HIS	2.1
2	D	377	HIS	2.1
1	A	59	MET	2.1
3	E	51	LEU	2.1
2	B	293	VAL	2.1
2	D	254	THR	2.1
3	F	28	ILE	2.1
1	C	321	ASN	2.1
1	C	526	GLN	2.1
2	B	340	LYS	2.1
3	F	65	LYS	2.1
3	E	29	HIS	2.1
3	F	44	GLU	2.1
2	B	136	ILE	2.1
2	D	423	LYS	2.1
2	B	591	TYR	2.1
1	C	281	GLN	2.1
2	B	128	PHE	2.1
3	F	37	PHE	2.1
3	F	62	ASP	2.1
3	F	73	ASP	2.1
1	A	199	LEU	2.1
2	B	124	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	108	TRP	2.0
1	C	282	ILE	2.0
2	D	19	LYS	2.0
1	C	276	THR	2.0
2	B	364	TYR	2.0
1	A	65	ILE	2.0
1	A	133	ILE	2.0
3	E	120	GLN	2.0
1	A	285	SER	2.0
3	E	86	LEU	2.0
2	B	472	HIS	2.0
3	E	54	LYS	2.0
2	D	479	GLU	2.0
1	A	421	GLY	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)

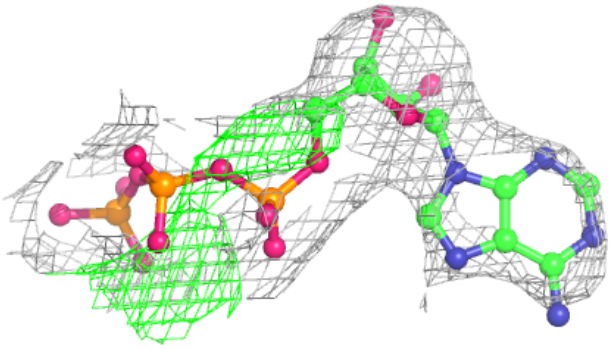
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

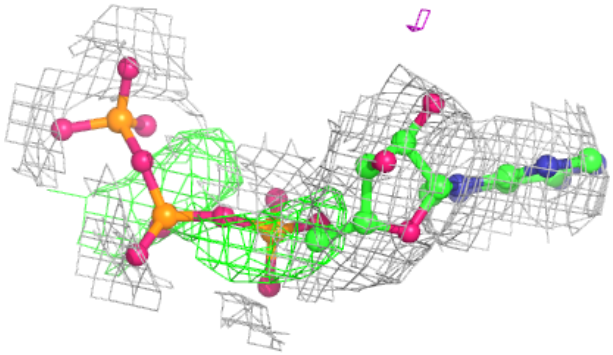
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	D	600	31/31	0.93	0.14	43,49,55,55	0
5	MG	A	601	1/1	0.93	0.20	13,13,13,13	0
4	ATP	B	600	31/31	0.94	0.12	47,52,58,58	0
4	ATP	C	600	31/31	0.95	0.10	65,67,70,70	0
4	ATP	A	600	31/31	0.96	0.09	32,36,38,39	0
5	MG	B	601	1/1	0.97	0.15	34,34,34,34	0
5	MG	C	601	1/1	0.97	0.17	43,43,43,43	0
5	MG	D	601	1/1	0.98	0.17	20,20,20,20	0

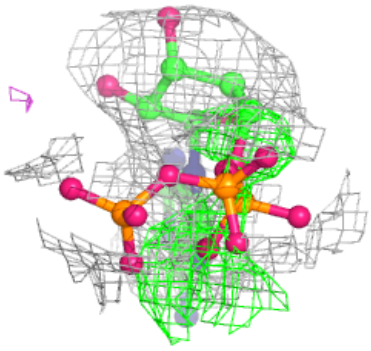
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 600:

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

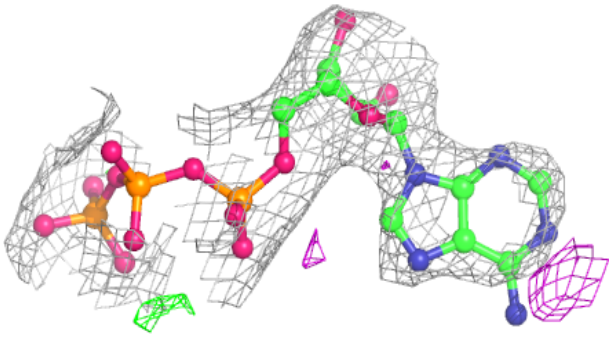


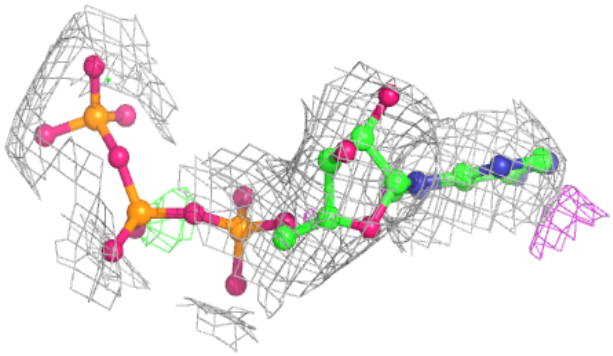


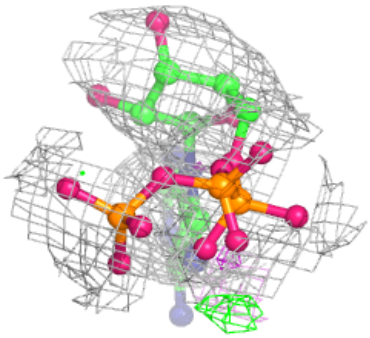


Electron density around ATP B 600:

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

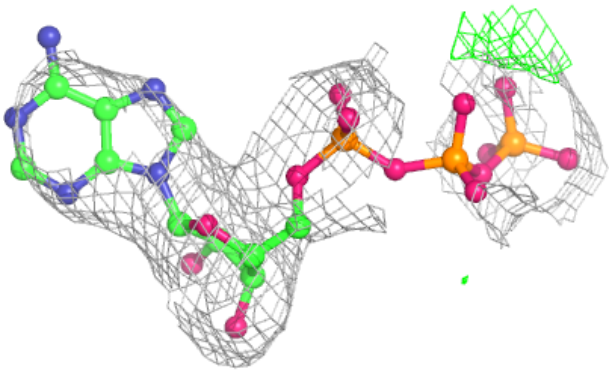


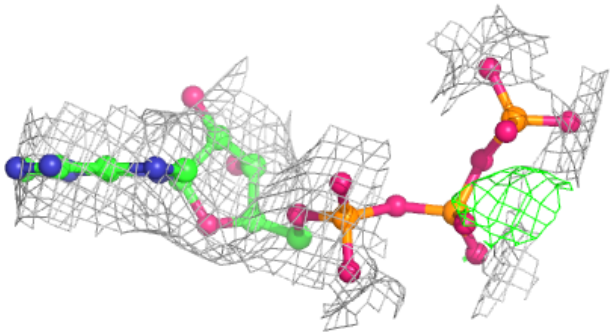


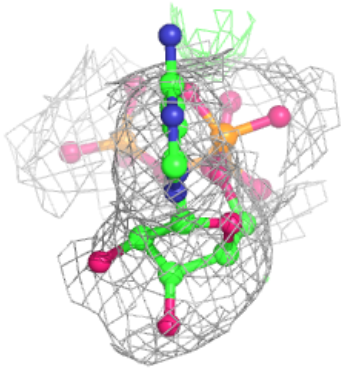


Electron density around ATP C 600:

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

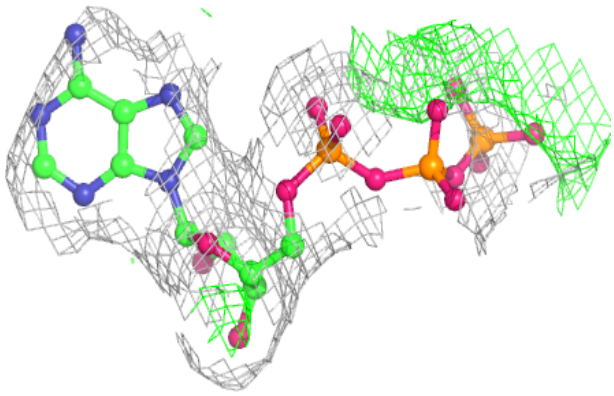


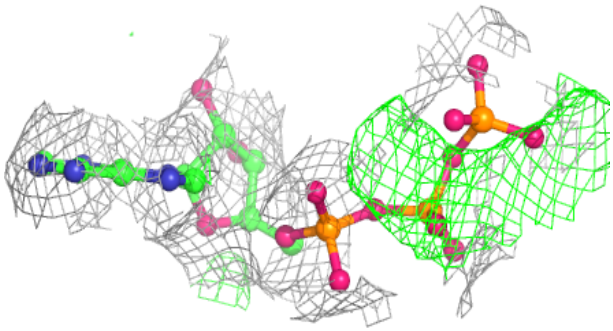


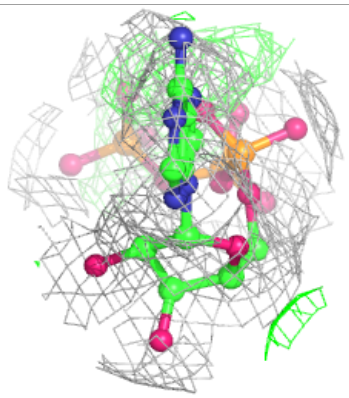


Electron density around ATP A 600:

$2mF_o$-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

There are no such residues in this entry.