



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 01:42 PM BST

PDB ID : 6PAQ
Title : Structure of a bacterial Atm1-family ABC exporter with ATP bound
Authors : Fan, C.; Kaiser, J.T.; Rees, D.C.
Deposited on : 2019-06-11
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

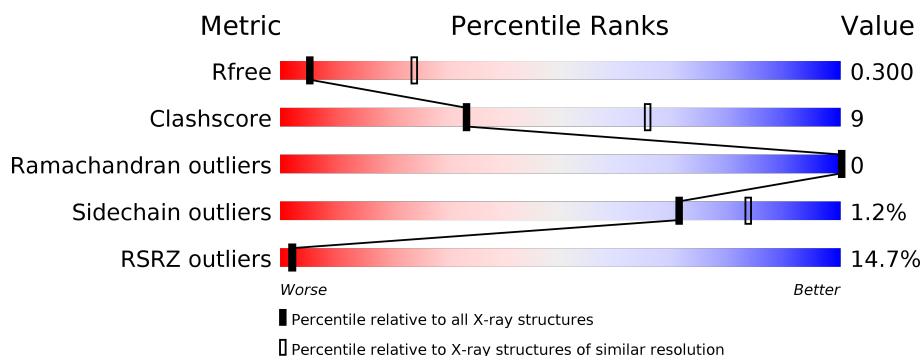
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	614	<div> <div>14%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>8%</div> </div> </div>
1	B	614	<div> <div>13%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8842 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 ATM1-type heavy metal exporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	Se	0	0	0
			4390	2800	781	797	12			
1	B	567	Total	C	N	O	Se	0	0	0
			4390	2800	781	797	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q2G506
A	523	GLN	GLU	engineered mutation	UNP Q2G506
A	609	HIS	-	expression tag	UNP Q2G506
A	610	HIS	-	expression tag	UNP Q2G506
A	611	HIS	-	expression tag	UNP Q2G506
A	612	HIS	-	expression tag	UNP Q2G506
A	613	HIS	-	expression tag	UNP Q2G506
A	614	HIS	-	expression tag	UNP Q2G506
B	1	MSE	-	initiating methionine	UNP Q2G506
B	523	GLN	GLU	engineered mutation	UNP Q2G506
B	609	HIS	-	expression tag	UNP Q2G506
B	610	HIS	-	expression tag	UNP Q2G506
B	611	HIS	-	expression tag	UNP Q2G506
B	612	HIS	-	expression tag	UNP Q2G506
B	613	HIS	-	expression tag	UNP Q2G506
B	614	HIS	-	expression tag	UNP Q2G506

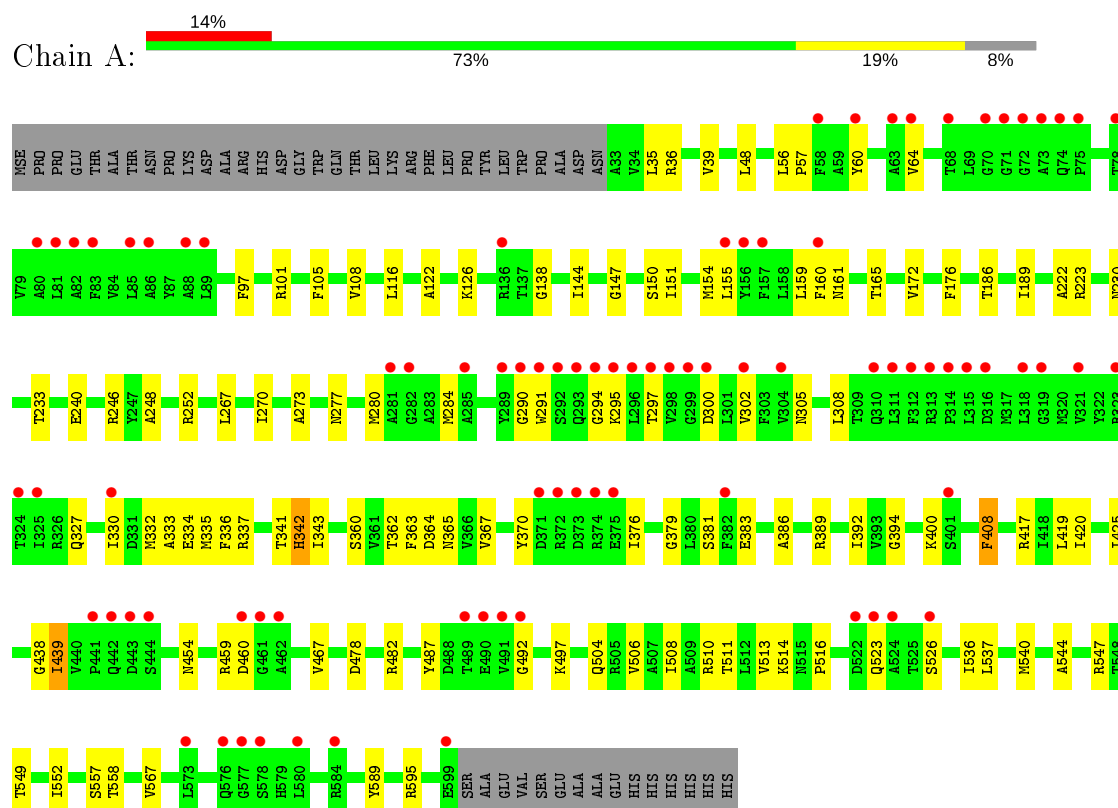
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



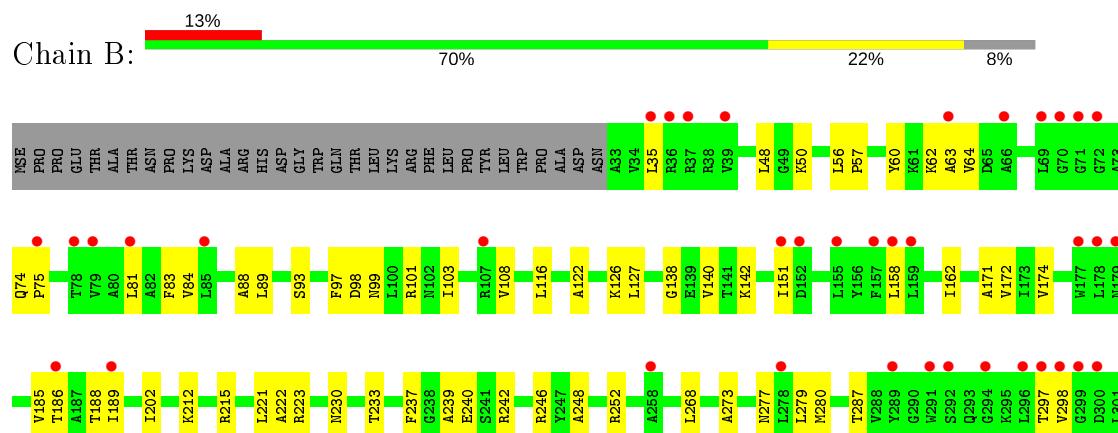
3 Residue-property plots

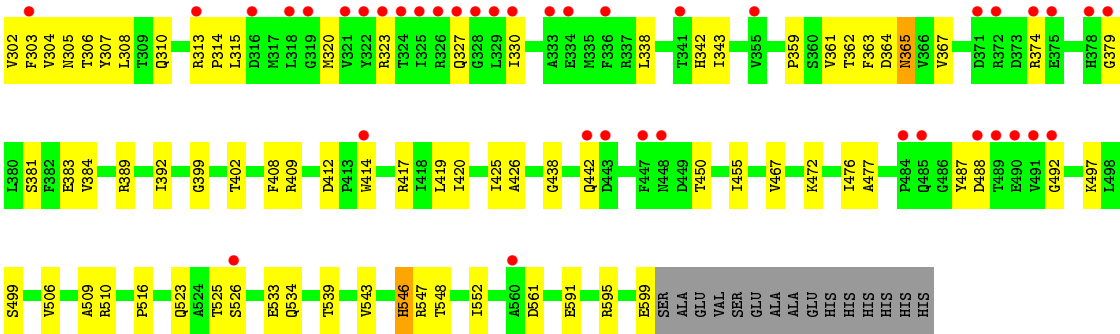
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATM1-type heavy metal exporter



- Molecule 1: ATM1-type heavy metal exporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.35Å 115.35Å 184.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 3.30 38.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.63-3.30) 99.7 (38.63-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, REFMAC	Depositor
R, R_{free}	0.235 , 0.290 0.236 , 0.300	Depositor DCC
R_{free} test set	1438 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8842	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/4454	0.42	0/6027
1	B	0.24	0/4454	0.42	0/6027
All	All	0.24	0/8908	0.42	0/12054

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	4390	0	4486	75	0
1	B	4390	0	4486	84	0
2	A	31	0	12	1	0
2	B	31	0	12	4	0
All	All	8842	0	8996	154	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 9.

All (154) 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:B:363:PHE:O	1:B:381:SER:HA	1.80	0.81
1:A:363:PHE:O	1:A:381:SER:HA	1.85	0.76
1:A:523:GLN:HG3	1:A:526:SER:HB3	1.71	0.71
1:B:523:GLN:HG3	1:B:526:SER:HB3	1.72	0.70
1:B:63:ALA:HB1	1:B:298:VAL:HG12	1.74	0.68
1:B:116:LEU:HD22	1:B:151:ILE:HG21	1.75	0.67
1:B:362:THR:OG1	1:B:383:GLU:OE2	2.12	0.67
1:A:144:ILE:HA	1:A:335:MSE:HE2	1.77	0.67
1:A:223:ARG:HD3	1:A:246:ARG:HG2	1.76	0.66
1:A:367:VAL:HG22	1:A:379:GLY:H	1.61	0.65
1:A:334:GLU:OE1	1:A:337:ARG:NH1	2.30	0.65
1:B:409:ARG:NH1	1:B:412:ASP:OD1	2.30	0.65
1:A:116:LEU:HD22	1:A:151:ILE:HG21	1.79	0.64
1:B:158:LEU:HA	1:B:162:ILE:HD13	1.79	0.63
1:A:544:ALA:HA	1:A:547:ARG:HB3	1.80	0.63
1:A:417:ARG:HE	1:A:419:LEU:HD21	1.66	0.61
1:A:273:ALA:O	1:A:277:ASN:ND2	2.34	0.60
1:B:273:ALA:O	1:B:277:ASN:ND2	2.33	0.59
2:A:701:ATP:H5'1	1:B:499:SER:HB3	1.86	0.58
1:B:127:LEU:HD22	1:B:342:HIS:HB2	1.86	0.58
1:A:362:THR:OG1	1:A:383:GLU:OE1	2.20	0.57
1:B:138:GLY:HA3	1:B:222:ALA:HA	1.87	0.57
1:B:392:ILE:HB	1:B:552:ILE:HG12	1.87	0.57
1:A:497:LYS:HE3	2:B:701:ATP:HN62	1.70	0.56
1:B:374:ARG:NH2	2:B:701:ATP:O2'	2.38	0.56
1:A:56:LEU:HB3	1:A:57:PRO:HD3	1.87	0.56
1:A:267:LEU:O	1:A:270:ILE:HG13	2.05	0.56
1:B:506:VAL:O	1:B:510:ARG:HG3	2.06	0.56
1:B:57:PRO:HB3	1:B:303:PHE:CE1	2.42	0.55
1:B:467:VAL:HG12	1:B:487:TYR:HE2	1.71	0.55
1:A:280:MSE:HE2	1:A:308:LEU:HB3	1.88	0.55
1:A:389:ARG:HG3	1:A:549:THR:HB	1.87	0.55
1:A:460:ASP:HA	1:B:242:ARG:HH12	1.71	0.54
1:A:147:GLY:HA3	1:A:335:MSE:HE3	1.88	0.54
1:A:337:ARG:O	1:A:341:THR:HG23	2.07	0.54
1:B:417:ARG:HE	1:B:419:LEU:HD21	1.72	0.54
1:B:442:GLN:NE2	2:B:701:ATP:O3G	2.41	0.54
1:A:302:VAL:HA	1:A:305:ASN:ND2	2.22	0.54
1:B:280:MSE:HG2	1:B:308:LEU:HD22	1.90	0.54
1:B:539:THR:O	1:B:543:VAL:HG23	2.07	0.54
1:B:223:ARG:HD3	1:B:246:ARG:HG2	1.89	0.53
1:B:362:THR:HB	1:B:419:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:O	1:B:64:VAL:HG23	2.08	0.53
1:B:546:HIS:O	1:B:546:HIS:CG	2.61	0.53
1:A:122:ALA:O	1:A:126:LYS:HG3	2.09	0.53
1:A:60:TYR:CZ	1:A:302:VAL:HB	2.44	0.53
1:A:35:LEU:HB3	1:A:108:VAL:HG22	1.91	0.52
1:A:506:VAL:O	1:A:510:ARG:HG3	2.08	0.52
1:B:172:VAL:HG22	1:B:307:TYR:CE1	2.43	0.52
1:A:438:GLY:HA3	1:A:516:PRO:HG3	1.92	0.52
1:B:359:PRO:O	1:B:548:THR:OG1	2.21	0.52
1:A:333:ALA:O	1:A:337:ARG:HB2	2.09	0.52
1:B:186:THR:HA	1:B:189:ILE:HG12	1.91	0.52
1:B:367:VAL:HG22	1:B:379:GLY:H	1.75	0.51
1:A:186:THR:HA	1:A:189:ILE:HG12	1.91	0.51
1:B:89:LEU:O	1:B:93:SER:N	2.36	0.51
1:A:492:GLY:HA3	1:A:497:LYS:HG3	1.93	0.51
1:B:420:ILE:HG13	1:B:425:ILE:HD11	1.93	0.51
1:A:536:ILE:HG22	1:A:540:MSE:HE3	1.92	0.50
1:B:472:LYS:HA	1:B:477:ALA:HB2	1.93	0.50
1:A:290:GLY:HA3	1:A:295:LYS:HG3	1.93	0.50
1:A:420:ILE:HG13	1:A:425:ILE:HD11	1.94	0.49
1:B:48:LEU:HB3	1:B:97:PHE:CD2	2.47	0.49
1:B:57:PRO:HG3	1:B:307:TYR:CE2	2.48	0.49
1:B:74:GLN:N	1:B:75:PRO:HD2	2.28	0.49
1:A:101:ARG:HD2	1:A:160:PHE:CD1	2.49	0.48
1:B:525:THR:HB	1:B:533:GLU:HG3	1.94	0.48
1:A:514:LYS:HD2	1:B:237:PHE:HD1	1.78	0.48
1:A:467:VAL:HG12	1:A:487:TYR:HE2	1.77	0.48
1:B:364:ASP:OD2	1:B:417:ARG:NH2	2.47	0.48
1:B:302:VAL:HA	1:B:305:ASN:ND2	2.29	0.47
1:B:365:ASN:H	1:B:381:SER:HG	1.62	0.47
1:B:492:GLY:HA3	1:B:497:LYS:HG3	1.97	0.47
1:B:338:LEU:O	1:B:342:HIS:ND1	2.46	0.47
1:B:361:VAL:HB	1:B:384:VAL:HB	1.97	0.47
1:A:497:LYS:CE	2:B:701:ATP:HN62	2.28	0.46
1:B:142:LYS:HG2	1:B:221:LEU:HD23	1.97	0.46
1:A:138:GLY:HA3	1:A:222:ALA:HA	1.97	0.46
1:B:399:GLY:O	1:B:402:THR:HG22	2.16	0.46
1:A:394:GLY:O	1:A:400:LYS:NZ	2.39	0.46
1:B:172:VAL:HG22	1:B:307:TYR:HE1	1.80	0.46
1:A:161:ASN:O	1:A:165:THR:OG1	2.25	0.46
1:A:36:ARG:O	1:A:39:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:MSE:HA	1:B:323:ARG:NE	2.30	0.46
1:B:62:LYS:NZ	1:B:83:PHE:HA	2.31	0.46
1:B:62:LYS:HZ1	1:B:83:PHE:HA	1.80	0.46
1:A:116:LEU:HD11	1:A:336:PHE:HZ	1.81	0.46
1:A:150:SER:O	1:A:154:MSE:HB2	2.16	0.46
1:A:332:MSE:HB2	1:A:332:MSE:HE3	1.76	0.46
1:B:185:VAL:O	1:B:189:ILE:HG23	2.16	0.46
1:B:313:ARG:HB3	1:B:314:PRO:HD3	1.98	0.46
1:A:364:ASP:OD2	1:A:417:ARG:NH2	2.49	0.45
1:A:459:ARG:H	1:A:513:VAL:HG12	1.81	0.45
1:B:122:ALA:O	1:B:126:LYS:HG3	2.16	0.45
1:B:248:ALA:O	1:B:252:ARG:HG2	2.16	0.45
1:A:408:PHE:CE2	1:A:439:ILE:HG13	2.51	0.45
1:A:557:SER:HB2	1:B:599:GLU:HG3	1.99	0.45
1:A:240:GLU:OE1	1:A:240:GLU:N	2.49	0.45
1:B:305:ASN:OD1	1:B:306:THR:N	2.49	0.45
1:B:367:VAL:O	1:B:414:TRP:N	2.50	0.45
1:B:50:LYS:HZ3	1:B:171:ALA:HB3	1.82	0.45
1:B:140:VAL:HG23	1:B:338:LEU:HD11	1.99	0.45
1:B:455:ILE:HG23	1:B:509:ALA:HB1	1.99	0.45
1:B:591:GLU:O	1:B:595:ARG:N	2.49	0.45
1:A:297:THR:HG22	1:A:300:ASP:CG	2.37	0.44
1:A:48:LEU:HB3	1:A:97:PHE:CD2	2.51	0.44
1:A:60:TYR:CE2	1:A:302:VAL:HB	2.52	0.44
1:A:105:PHE:HZ	1:A:155:LEU:HD22	1.83	0.44
1:B:212:LYS:HG3	1:B:215:ARG:HH22	1.82	0.44
1:B:476:ILE:O	1:B:476:ILE:HG12	2.18	0.44
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.86	0.44
1:B:35:LEU:HD22	1:B:108:VAL:HG22	1.99	0.44
1:A:230:ASN:HB3	1:A:233:THR:HB	2.00	0.44
1:B:287:THR:HG21	1:B:304:VAL:HG21	1.99	0.43
1:A:360:SER:HB3	1:A:386:ALA:HB2	2.00	0.43
1:B:171:ALA:HA	1:B:174:VAL:HG22	1.99	0.43
1:B:84:VAL:O	1:B:88:ALA:N	2.50	0.43
1:B:438:GLY:HA3	1:B:516:PRO:HG3	2.00	0.43
1:B:450:THR:HB	1:B:488:ASP:HA	2.00	0.43
1:A:417:ARG:NE	1:A:419:LEU:HD21	2.32	0.43
1:B:543:VAL:O	1:B:547:ARG:NH2	2.52	0.43
1:A:478:ASP:HB3	1:A:482:ARG:HH12	1.83	0.42
1:B:188:THR:HG22	1:B:279:LEU:HD11	2.01	0.42
1:A:291:TRP:HB2	1:A:294:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLN:O	1:A:508:ILE:HG13	2.19	0.42
1:A:248:ALA:O	1:A:252:ARG:HG2	2.20	0.42
1:A:370:TYR:H	1:A:376:ILE:HD13	1.84	0.42
1:A:392:ILE:HB	1:A:552:ILE:HG12	2.02	0.42
1:A:567:VAL:HG21	1:A:589:TYR:HB2	2.01	0.42
1:A:454:ASN:O	1:A:510:ARG:HG2	2.20	0.42
1:B:230:ASN:HB3	1:B:233:THR:HB	2.01	0.42
1:B:327:GLN:O	1:B:330:ILE:HG22	2.19	0.42
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.88	0.41
1:B:56:LEU:HD12	1:B:310:GLN:CD	2.41	0.41
1:B:98:ASP:O	1:B:101:ARG:HB3	2.20	0.41
1:A:60:TYR:O	1:A:64:VAL:HG23	2.20	0.41
1:B:409:ARG:NH1	1:B:426:ALA:HA	2.35	0.41
1:B:516:PRO:O	1:B:547:ARG:HD2	2.20	0.41
1:B:417:ARG:NE	1:B:419:LEU:HD21	2.36	0.41
1:A:126:LYS:O	1:A:343:ILE:HD13	2.20	0.41
1:A:172:VAL:HG13	1:A:176:PHE:CD1	2.55	0.41
1:A:537:LEU:HD11	1:A:558:THR:HB	2.01	0.41
1:A:60:TYR:CZ	1:A:64:VAL:HG22	2.56	0.41
1:B:239:ALA:HB2	1:B:242:ARG:HH21	1.85	0.41
1:B:202:ILE:HG21	1:B:268:LEU:HB2	2.02	0.41
1:B:389:ARG:NH1	1:B:561:ASP:O	2.54	0.41
1:A:516:PRO:O	1:A:547:ARG:HD2	2.21	0.40
1:A:330:ILE:HD12	1:A:330:ILE:HA	1.94	0.40
1:B:99:ASN:O	1:B:103:ILE:HG23	2.20	0.40
1:A:342:HIS:ND1	1:A:342:HIS:O	2.54	0.40
1:A:508:ILE:O	1:A:511:THR:HG22	2.22	0.40
1:A:327:GLN:HA	1:A:330:ILE:HG22	2.02	0.40
1:A:595:ARG:HG2	1:B:534:GLN:HG3	2.02	0.40
1:A:284:MSE:SE	1:B:83:PHE:HE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	565/614 (92%)	551 (98%)	14 (2%)	0	100	100
1	B	565/614 (92%)	551 (98%)	14 (2%)	0	100	100
All	All	1130/1228 (92%)	1102 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/478 (94%)	447 (99%)	4 (1%)	78	87
1	B	451/478 (94%)	444 (98%)	7 (2%)	62	79
All	All	902/956 (94%)	891 (99%)	11 (1%)	71	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	HIS
1	A	365	ASN
1	A	408	PHE
1	A	439	ILE
1	B	81	LEU
1	B	240	GLU
1	B	297	THR
1	B	343	ILE
1	B	365	ASN
1	B	408	PHE
1	B	546	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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
2	ATP	A	701	-	26,33,33	0.99	1 (3%)	31,52,52	1.38	4 (12%)
2	ATP	B	701	-	26,33,33	0.95	1 (3%)	31,52,52	1.58	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	701	-	-	3/18/38/38	0/3/3/3
2	ATP	B	701	-	-	8/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ATP	C5-C4	2.59	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ATP	C5-C4	2.37	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C4-C5-N7	-3.54	105.71	109.40
2	B	701	ATP	N3-C2-N1	-3.29	123.54	128.68
2	A	701	ATP	PA-O3A-PB	-2.90	122.87	132.83
2	B	701	ATP	PA-O3A-PB	-2.82	123.15	132.83
2	B	701	ATP	O2A-PA-O1A	2.74	125.77	112.24
2	B	701	ATP	O4'-C4'-C3'	2.73	110.51	105.11
2	A	701	ATP	N3-C2-N1	-2.72	124.43	128.68
2	B	701	ATP	C4-C5-N7	-2.53	106.76	109.40
2	B	701	ATP	C2'-C3'-C4'	-2.28	98.20	102.64
2	A	701	ATP	PB-O3B-PG	-2.22	125.20	132.83
2	B	701	ATP	C3'-C2'-C1'	2.03	104.04	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C4'-C5'-O5'-PA
2	A	701	ATP	PB-O3B-PG-O1G
2	B	701	ATP	PB-O3B-PG-O1G
2	A	701	ATP	PB-O3B-PG-O2G
2	A	701	ATP	PB-O3B-PG-O3G
2	B	701	ATP	PB-O3B-PG-O2G
2	B	701	ATP	PB-O3B-PG-O3G
2	B	701	ATP	C5'-O5'-PA-O3A
2	B	701	ATP	PB-O3A-PA-O1A

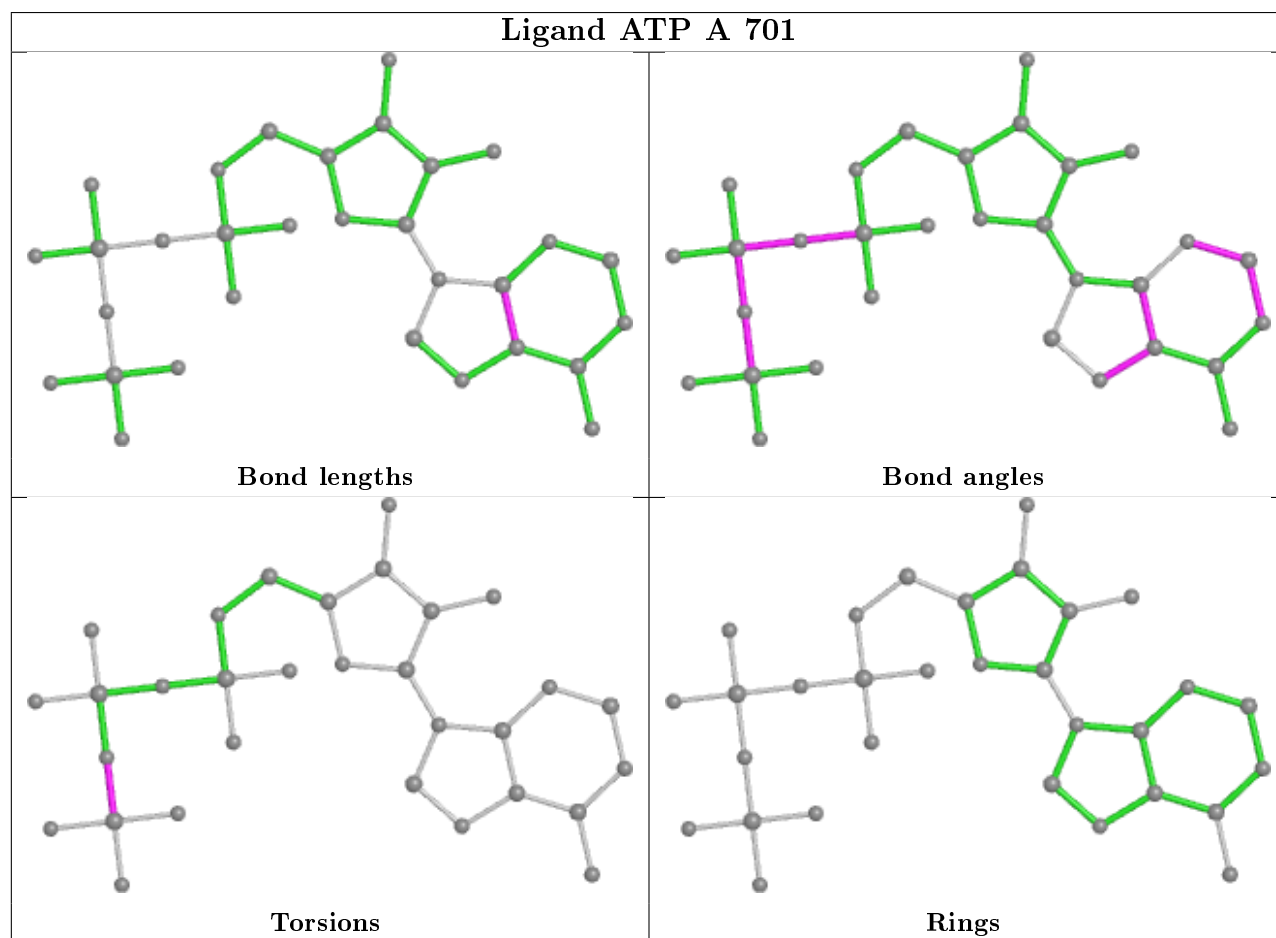
There are no ring outliers.

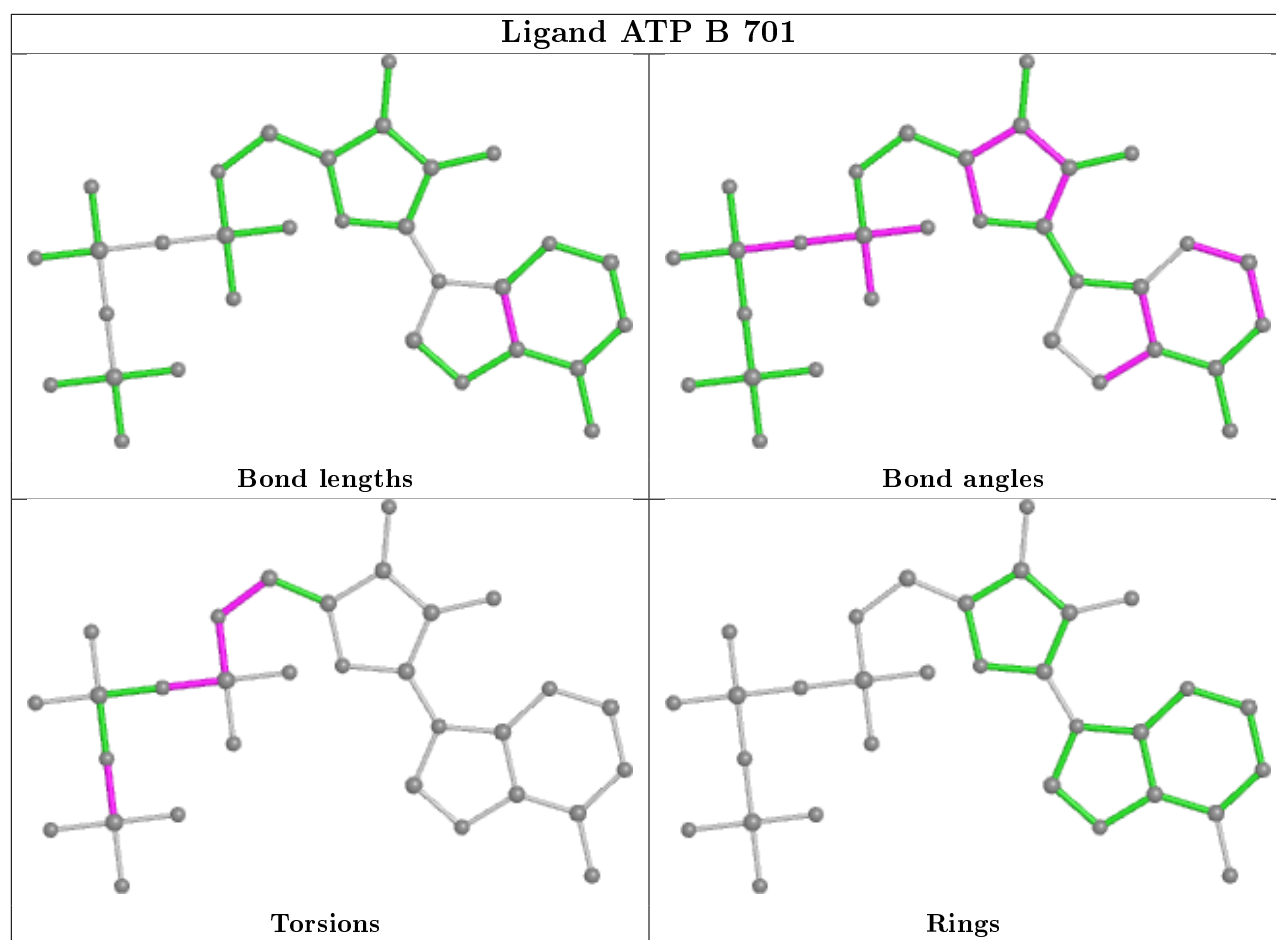
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ATP	1	0
2	B	701	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/614 (90%)	0.73	85 (15%) 2 2	53, 111, 218, 242	32 (5%)
1	B	555/614 (90%)	0.46	78 (14%) 2 2	55, 115, 229, 253	40 (7%)
All	All	1110/1228 (90%)	0.59	163 (14%) 2 2	53, 113, 225, 253	72 (6%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	34.6
1	B	71	GLY	20.4
1	B	70	GLY	18.8
1	A	82	ALA	14.6
1	A	85	LEU	14.1
1	A	78	THR	13.9
1	A	314	PRO	11.7
1	A	297	THR	11.2
1	B	325	ILE	10.3
1	A	599	GLU	10.0
1	A	294	GLY	9.1
1	B	324	THR	8.9
1	A	70	GLY	8.5
1	A	291	TRP	8.4
1	A	81	LEU	8.3
1	A	72	GLY	8.1
1	A	89	LEU	8.0
1	A	290	GLY	8.0
1	A	319	GLY	7.7
1	A	295	LYS	7.4
1	A	315	LEU	7.3
1	B	329	LEU	7.2
1	A	299	GLY	7.2
1	B	330	ILE	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	7.1
1	A	312	PHE	7.0
1	A	74	GLN	6.7
1	B	321	VAL	6.4
1	A	325	ILE	6.4
1	B	299	GLY	6.3
1	B	333	ALA	6.2
1	A	292	SER	6.1
1	A	318	LEU	6.0
1	B	297	THR	5.9
1	A	321	VAL	5.6
1	B	300	ASP	5.5
1	A	293	GLN	5.5
1	B	328	GLY	5.4
1	A	460	ASP	5.4
1	B	319	GLY	5.4
1	A	374	ARG	5.2
1	A	324	THR	5.2
1	B	81	LEU	5.1
1	A	442	GLN	5.0
1	A	73	ALA	4.9
1	A	373	ASP	4.8
1	A	298	VAL	4.8
1	B	178	LEU	4.8
1	A	316	ASP	4.8
1	B	322	TYR	4.8
1	A	282	GLY	4.8
1	A	371	ASP	4.7
1	B	158	LEU	4.7
1	B	318	LEU	4.7
1	A	83	PHE	4.7
1	B	155	LEU	4.6
1	A	489	THR	4.5
1	A	523	GLN	4.4
1	A	444	SER	4.2
1	B	375	GLU	4.2
1	A	576	GLN	4.1
1	A	60	TYR	4.1
1	A	155	LEU	4.1
1	A	441	PRO	4.1
1	B	323	ARG	4.1
1	B	75	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	488	ASP	3.9
1	A	580	LEU	3.9
1	B	316	ASP	3.8
1	A	68	THR	3.8
1	B	327	GLN	3.8
1	B	414	TRP	3.8
1	A	86	ALA	3.7
1	A	63	ALA	3.7
1	B	159	LEU	3.6
1	A	522	ASP	3.6
1	A	524	ALA	3.5
1	A	64	VAL	3.4
1	B	303	PHE	3.4
1	B	334	GLU	3.4
1	A	58	PHE	3.4
1	B	298	VAL	3.4
1	A	526	SER	3.4
1	B	326	ARG	3.4
1	A	300	ASP	3.3
1	A	372	ARG	3.2
1	B	37	ARG	3.2
1	B	289	TYR	3.2
1	B	179	ASN	3.1
1	B	39	VAL	3.1
1	B	443	ASP	3.1
1	B	448	ASN	3.1
1	B	485	GLN	3.1
1	B	442	GLN	3.0
1	B	78	THR	3.0
1	B	151	ILE	3.0
1	A	75	PRO	3.0
1	B	355	VAL	3.0
1	B	296	LEU	3.0
1	B	35	LEU	3.0
1	B	378	HIS	2.9
1	B	490	GLU	2.9
1	A	462	ALA	2.9
1	A	461	GLY	2.8
1	B	63	ALA	2.8
1	A	584	ARG	2.8
1	B	36	ARG	2.8
1	A	375	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	289	TYR	2.8
1	A	492	GLY	2.8
1	B	292	SER	2.8
1	B	66	ALA	2.8
1	B	371	ASP	2.7
1	A	313	ARG	2.7
1	A	156	TYR	2.7
1	A	323	ARG	2.6
1	A	490	GLU	2.6
1	B	186	THR	2.6
1	B	72	GLY	2.5
1	B	258	ALA	2.5
1	B	489	THR	2.5
1	A	88	ALA	2.5
1	B	152	ASP	2.4
1	A	281	ALA	2.4
1	A	443	ASP	2.4
1	A	401	SER	2.4
1	A	160	PHE	2.4
1	B	107	ARG	2.3
1	A	578	SER	2.3
1	A	157	PHE	2.3
1	B	313	ARG	2.3
1	B	484	PRO	2.3
1	B	291	TRP	2.3
1	A	310	GLN	2.3
1	A	136	ARG	2.3
1	A	296	LEU	2.3
1	A	577	GLY	2.3
1	B	379	GLY	2.3
1	B	189	ILE	2.3
1	B	85	LEU	2.2
1	B	79	VAL	2.2
1	B	526	SER	2.2
1	A	304	VAL	2.2
1	A	573	LEU	2.2
1	B	157	PHE	2.2
1	A	491	VAL	2.2
1	B	69	LEU	2.2
1	B	336	PHE	2.2
1	B	491	VAL	2.1
1	B	278	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	372	ARG	2.1
1	A	330	ILE	2.1
1	B	492	GLY	2.1
1	B	447	PHE	2.1
1	B	294	GLY	2.1
1	B	341	THR	2.1
1	A	302	VAL	2.1
1	A	382	PHE	2.0
1	B	177	TRP	2.0
1	B	560	ALA	2.0
1	B	374	ARG	2.0
1	A	80	ALA	2.0
1	A	285	ALA	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](#)

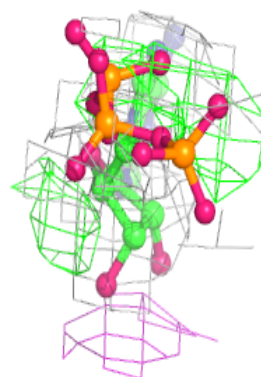
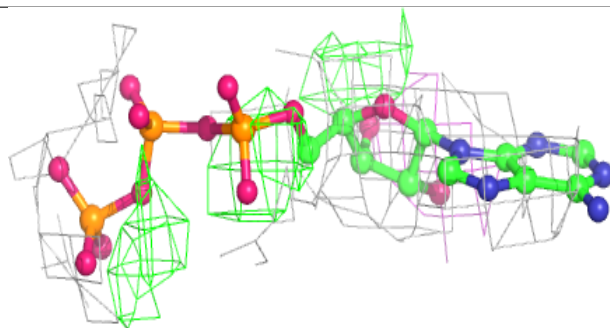
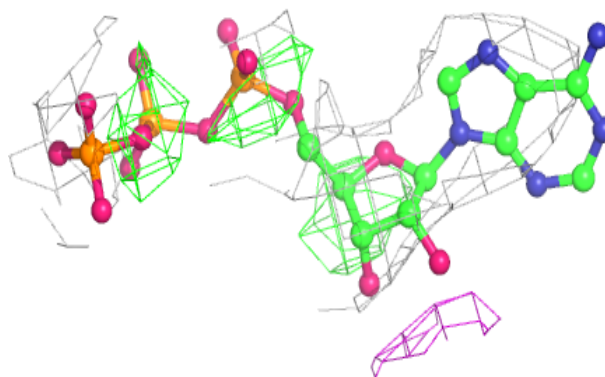
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	A	701	31/31	0.83	0.48	108,151,198,242	0
2	ATP	B	701	31/31	0.85	0.43	102,164,210,240	0

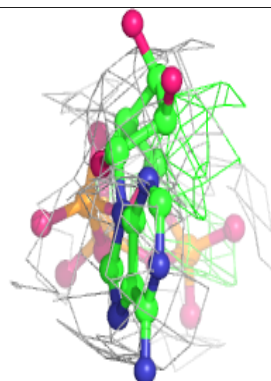
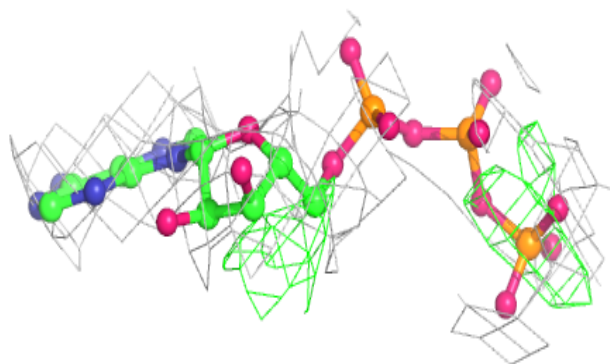
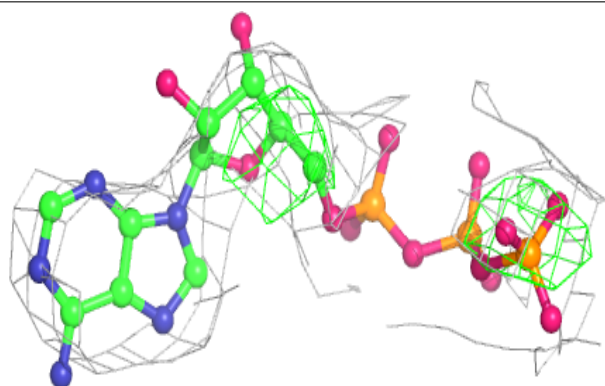
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 701:

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

**Electron density around ATP B 701:**

$2mF_o-DF_c$ (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.