



# Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2021 – 07:21 PM EDT

PDB ID : 7KZI  
Title : Intermediate state (QQQ) of near full-length DnaK alternatively fused with a substrate peptide  
Authors : Wang, W.; Hendrickson, W.A.  
Deposited on : 2020-12-10  
Resolution : 2.82 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](mailto: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.

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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 : 2.18  
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) : 2.18

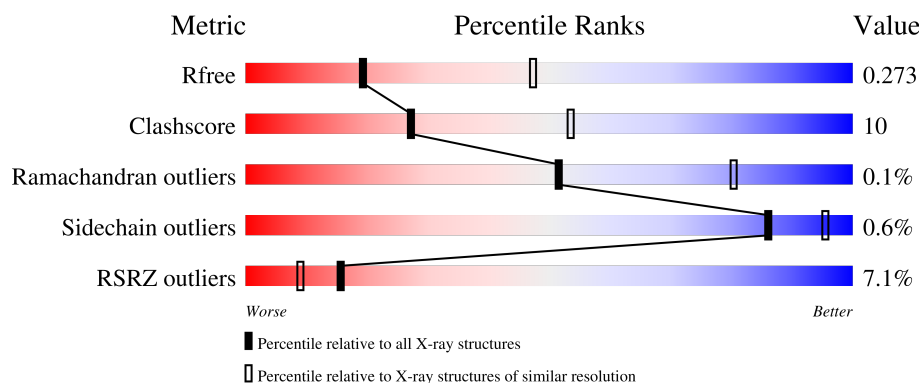
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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  $\geq 3$ , 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	628	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	628	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9233 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.

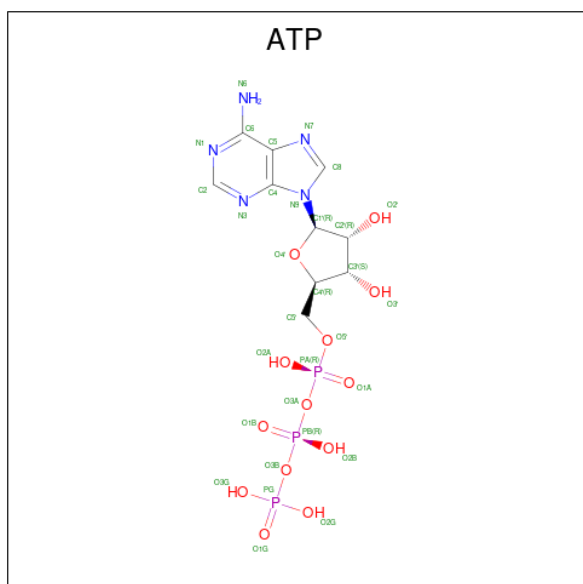
- Molecule 1 is a protein called Chaperone protein DnaK fused with substrate peptide,Chaperone protein DnaK fused with substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4570	2833	801	922	14			
1	B	603	Total	C	N	O	S	0	0	0
			4570	2833	801	922	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0

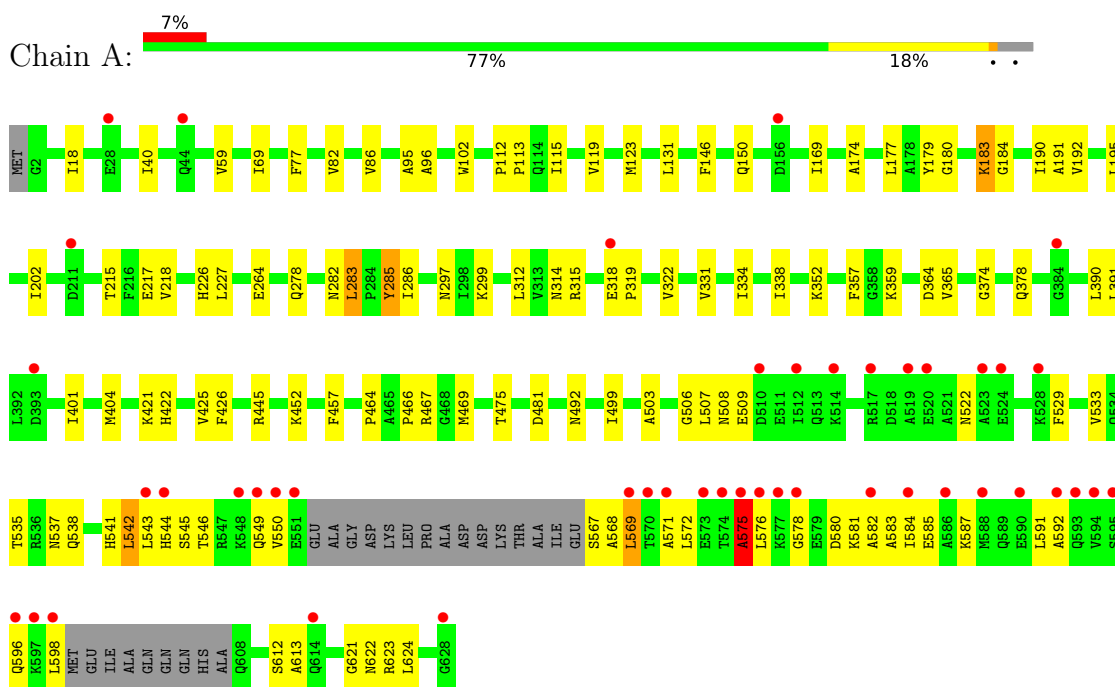
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	B	4	Total 4	O 4	0	0

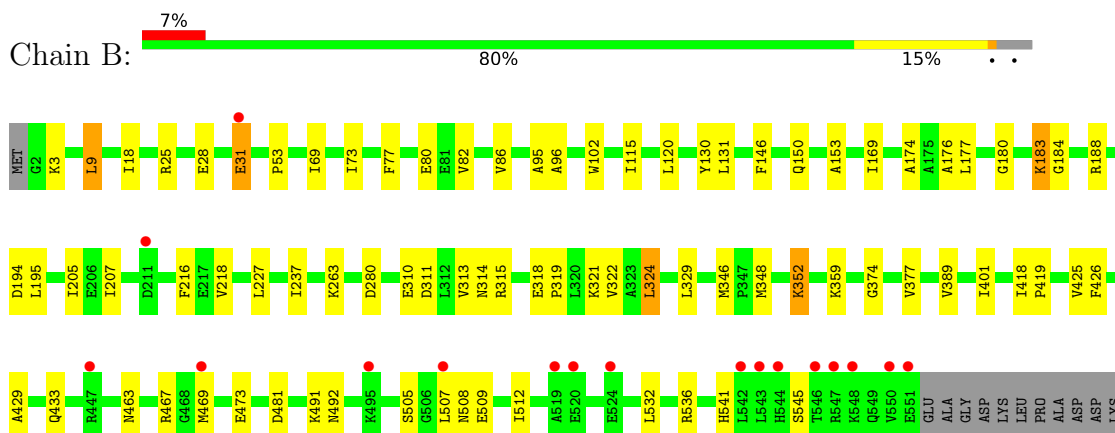
### 3 Residue-property plots

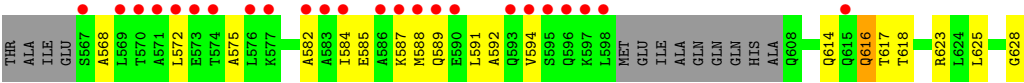
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chaperone protein DnaK fused with substrate peptide,Chaperone protein DnaK fused with substrate peptide



- Molecule 1: Chaperone protein DnaK fused with substrate peptide,Chaperone protein DnaK fused with substrate peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.52Å 121.52Å 457.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 2.82 49.75 – 2.82	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.75-2.82) 77.8 (49.75-2.82)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, $R_{free}$	0.255 , 0.273 0.255 , 0.273	Depositor DCC
$R_{free}$ test set	1926 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, CL, ATP, MG

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	0.57	1/4619 (0.0%)	0.96	10/6237 (0.2%)
1	B	0.61	4/4619 (0.1%)	0.95	14/6237 (0.2%)
All	All	0.59	5/9238 (0.1%)	0.96	24/12474 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	PRO	N-CD	6.83	1.57	1.47
1	B	318	GLU	CB-CG	-5.80	1.41	1.52
1	B	31	GLU	CG-CD	-5.28	1.44	1.51
1	B	183	LYS	CB-CG	-5.20	1.38	1.52
1	B	505	SER	CA-C	5.18	1.66	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	LEU	CA-CB-CG	8.30	134.40	115.30
1	B	227	LEU	CA-CB-CG	7.89	133.46	115.30
1	A	542	LEU	N-CA-C	7.40	130.97	111.00
1	B	507	LEU	CA-CB-CG	7.06	131.54	115.30
1	A	542	LEU	N-CA-CB	-6.41	97.59	110.40
1	B	28	GLU	CA-CB-CG	6.28	127.21	113.40
1	A	575	ALA	N-CA-CB	-6.16	101.48	110.10
1	A	285	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	B	183	LYS	CB-CG-CD	-5.95	96.12	111.60
1	A	283	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	B	329	LEU	CB-CG-CD2	-5.71	101.28	111.00
1	B	9	LEU	CB-CG-CD1	-5.66	101.37	111.00
1	B	9	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	B	31	GLU	CA-CB-CG	-5.47	101.37	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	GLY	N-CA-C	-5.42	99.55	113.10
1	A	184	GLY	N-CA-C	-5.30	99.84	113.10
1	B	280	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	194	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	324	LEU	CA-CB-CG	-5.21	103.33	115.30
1	A	183	LYS	CB-CA-C	-5.18	100.05	110.40
1	A	183	LYS	CB-CG-CD	-5.10	98.34	111.60
1	B	195	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	569	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	352	LYS	CB-CG-CD	-5.01	98.56	111.60

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	4570	0	4618	120	1
1	B	4570	0	4618	89	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	1	0	0	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	9233	0	9260	187	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (187) 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:569:LEU:HD23	1:A:591:LEU:CD2	1.82	1.10
1:A:543:LEU:HD23	1:A:572:LEU:HD22	1.49	0.94
1:A:575:ALA:O	1:A:584:ILE:HG22	1.71	0.91
1:A:467:ARG:NH1	1:A:541:HIS:NE2	2.23	0.86
1:A:331:VAL:O	1:A:334:ILE:HG22	1.76	0.86
1:A:535:THR:HG22	1:A:584:ILE:HD11	1.57	0.86
1:A:467:ARG:CZ	1:A:541:HIS:CD2	2.58	0.86
1:A:543:LEU:CD2	1:A:572:LEU:HD22	2.04	0.86
1:B:572:LEU:HD13	1:B:587:LYS:HB2	1.58	0.84
1:A:467:ARG:NH1	1:A:541:HIS:CD2	2.46	0.83
1:A:535:THR:HG22	1:A:584:ILE:CD1	2.10	0.82
1:B:183:LYS:NZ	1:B:207:ILE:HG21	1.94	0.82
1:A:469:MET:HE1	1:B:314:ASN:C	2.01	0.81
1:B:180:GLY:HA2	1:B:183:LYS:HE3	1.63	0.80
1:A:466:PRO:HG2	1:A:469:MET:HG3	1.63	0.80
1:B:183:LYS:HZ3	1:B:207:ILE:HG21	1.46	0.78
1:B:346:MET:HE2	1:B:348:MET:HB3	1.66	0.77
1:A:508:ASN:OD1	1:A:509:GLU:N	2.17	0.76
1:A:546:THR:HA	1:A:549:GLN:HB2	1.69	0.75
1:A:180:GLY:HA2	1:A:183:LYS:HZ2	1.53	0.73
1:B:218:VAL:HG21	1:B:481:ASP:OD2	1.89	0.72
1:B:310:GLU:HA	1:B:348:MET:HE3	1.71	0.72
1:A:535:THR:CG2	1:A:584:ILE:HD11	2.19	0.71
1:A:190:ILE:C	1:A:334:ILE:HD11	2.10	0.71
1:A:469:MET:CE	1:B:314:ASN:HB3	2.20	0.71
1:B:314:ASN:OD1	1:B:352:LYS:HE2	1.92	0.70
1:B:508:ASN:OD1	1:B:509:GLU:N	2.25	0.69
1:B:508:ASN:O	1:B:512:ILE:N	2.24	0.68
1:A:592:ALA:O	1:A:596:GLN:NE2	2.18	0.68
1:B:180:GLY:HA2	1:B:183:LYS:CE	2.23	0.68
1:A:180:GLY:HA2	1:A:183:LYS:NZ	2.08	0.68
1:A:314:ASN:OD1	1:A:352:LYS:HE2	1.94	0.67
1:A:538:GLN:O	1:A:541:HIS:HB3	1.94	0.67
1:A:575:ALA:O	1:A:584:ILE:CG2	2.42	0.67
1:A:569:LEU:HD23	1:A:591:LEU:HD22	1.72	0.66
1:B:582:ALA:HA	1:B:585:GLU:HB2	1.78	0.66
1:A:569:LEU:HD23	1:A:591:LEU:HD21	1.78	0.65
1:B:237:ILE:HD11	1:B:263:LYS:HA	1.80	0.64
1:A:569:LEU:HD23	1:A:591:LEU:HD23	1.77	0.64
1:B:591:LEU:HA	1:B:594:VAL:HG12	1.80	0.62
1:B:174:ALA:O	1:B:374:GLY:HA3	1.99	0.62
1:A:96:ALA:HB2	1:A:102:TRP:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:O	1:A:576:LEU:HG	2.01	0.61
1:A:572:LEU:O	1:A:572:LEU:HD23	2.00	0.61
1:A:543:LEU:HD23	1:A:572:LEU:CD2	2.27	0.61
1:A:469:MET:HE1	1:B:314:ASN:CB	2.31	0.60
1:A:575:ALA:HB3	1:A:587:LYS:HG3	1.83	0.60
1:B:69:ILE:HG13	1:B:115:ILE:HG21	1.82	0.60
1:A:334:ILE:O	1:A:359:LYS:NZ	2.34	0.60
1:B:77:PHE:CD2	1:B:95:ALA:HB2	2.36	0.60
1:B:541:HIS:O	1:B:545:SER:HB2	2.01	0.60
1:A:218:VAL:HG21	1:A:481:ASP:OD2	2.02	0.59
1:B:401:ILE:HD11	1:B:426:PHE:CE2	2.37	0.59
1:B:18:ILE:HD13	1:B:131:LEU:HD21	1.85	0.58
1:B:218:VAL:HG11	1:B:481:ASP:OD1	2.03	0.58
1:A:466:PRO:HG2	1:A:469:MET:CG	2.33	0.57
1:A:613:ALA:HB1	1:B:352:LYS:HE3	1.85	0.57
1:A:318:GLU:OE1	1:B:463:ASN:HB2	2.05	0.57
1:A:334:ILE:HG21	1:A:357:PHE:CD1	2.39	0.57
1:A:283:LEU:HD13	1:A:286:ILE:HD13	1.86	0.57
1:A:469:MET:HE1	1:B:314:ASN:HB3	1.87	0.57
1:B:584:ILE:HG22	1:B:588:MET:CE	2.35	0.56
1:A:77:PHE:CD2	1:A:95:ALA:HB2	2.41	0.55
1:B:177:LEU:HD23	1:B:377:VAL:HG12	1.89	0.55
1:B:568:ALA:HB3	1:B:591:LEU:HD11	1.88	0.55
1:A:278:GLN:OE1	1:A:299:LYS:HD2	2.07	0.55
1:B:18:ILE:CD1	1:B:131:LEU:HD11	2.37	0.55
1:B:3:LYS:HD2	1:B:131:LEU:HD13	1.90	0.54
1:B:18:ILE:HD11	1:B:131:LEU:HD11	1.89	0.53
1:A:69:ILE:HG13	1:A:115:ILE:HG21	1.91	0.53
1:A:469:MET:HE2	1:B:314:ASN:HB3	1.89	0.52
1:B:532:LEU:HD13	1:B:536:ARG:NH2	2.24	0.52
1:B:575:ALA:O	1:B:584:ILE:HG12	2.08	0.52
1:A:567:SER:HB3	1:A:569:LEU:HG	1.92	0.52
1:B:584:ILE:HG22	1:B:588:MET:HE2	1.92	0.52
1:A:569:LEU:CD2	1:A:591:LEU:CD2	2.74	0.51
1:B:25:ARG:HD3	1:B:130:TYR:OH	2.10	0.51
1:A:218:VAL:HG21	1:A:481:ASP:CG	2.31	0.51
1:B:183:LYS:HZ3	1:B:207:ILE:CG2	2.18	0.51
1:B:433:GLN:NE2	1:B:628:GLY:HA3	2.25	0.51
1:A:452:LYS:HZ3	1:A:506:GLY:N	2.10	0.50
1:A:546:THR:O	1:A:550:VAL:HG23	2.12	0.49
1:A:227:LEU:HD22	1:A:312:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASN:O	1:B:322:VAL:HG11	2.12	0.49
1:A:492:ASN:OD1	1:B:319:PRO:HG3	2.12	0.49
1:A:352:LYS:NZ	1:B:614:GLN:O	2.28	0.49
1:A:612:SER:HB2	1:B:321:LYS:NZ	2.26	0.49
1:B:585:GLU:HA	1:B:588:MET:SD	2.52	0.49
1:A:575:ALA:CB	1:A:587:LYS:HG3	2.43	0.49
1:A:421:LYS:HE3	1:A:475:THR:HG21	1.95	0.48
1:A:314:ASN:HB3	1:B:469:MET:HE1	1.96	0.48
1:A:191:ALA:N	1:A:334:ILE:HD11	2.27	0.48
1:B:146:PHE:CD2	1:B:150:GLN:HB3	2.48	0.48
1:A:467:ARG:NH1	1:A:541:HIS:CE1	2.82	0.48
1:A:537:ASN:O	1:A:541:HIS:HB2	2.13	0.48
1:B:568:ALA:C	1:B:591:LEU:HD21	2.34	0.48
1:B:9:LEU:HD22	1:B:120:LEU:HD21	1.95	0.47
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.70	0.47
1:A:426:PHE:HE1	1:A:624:LEU:HD12	1.77	0.47
1:B:169:ILE:HG13	1:B:169:ILE:O	2.14	0.47
1:A:112:PRO:HB2	1:A:113:PRO:HD3	1.96	0.47
1:B:313:VAL:HG12	1:B:352:LYS:HG2	1.96	0.47
1:A:174:ALA:O	1:A:374:GLY:HA3	2.14	0.47
1:B:587:LYS:HZ3	1:B:587:LYS:HB3	1.80	0.47
1:A:282:ASN:ND2	1:A:297:ASN:OD1	2.38	0.47
1:A:319:PRO:HG3	1:B:492:ASN:OD1	2.15	0.47
1:A:177:LEU:HD11	1:A:391:LEU:HD11	1.97	0.46
1:A:535:THR:HG22	1:A:584:ILE:HD12	1.92	0.46
1:B:216:PHE:HE2	1:B:389:VAL:HG13	1.80	0.46
1:A:18:ILE:HD13	1:A:131:LEU:HD21	1.97	0.46
1:A:580:ASP:HB3	1:A:583:ALA:CB	2.46	0.46
1:A:425:VAL:HG12	1:A:623:ARG:HD3	1.98	0.46
1:A:621:GLY:N	1:B:311:ASP:OD2	2.49	0.46
1:A:217:GLU:OE2	1:A:503:ALA:HB1	2.16	0.46
1:A:215:THR:HG22	1:A:390:LEU:HD23	1.98	0.46
1:A:226:HIS:HD2	1:B:491:LYS:NZ	2.14	0.46
1:A:334:ILE:HG21	1:A:357:PHE:HD1	1.77	0.46
1:A:571:ALA:O	1:A:587:LYS:HE3	2.15	0.46
1:B:205:ILE:HG12	1:B:218:VAL:HG22	1.97	0.45
1:A:180:GLY:HA2	1:A:183:LYS:HG3	1.98	0.45
1:B:176:ALA:O	1:B:180:GLY:N	2.43	0.45
1:A:192:VAL:O	1:A:202:ILE:HD12	2.16	0.45
1:B:589:GLN:HA	1:B:592:ALA:HB3	1.99	0.45
1:A:578:GLY:O	1:A:580:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HB2	1:A:102:TRP:CG	2.52	0.44
1:A:582:ALA:HA	1:A:585:GLU:HB2	1.98	0.44
1:A:179:TYR:CD2	1:A:183:LYS:NZ	2.72	0.44
1:A:227:LEU:HD21	1:A:315:ARG:NH2	2.32	0.44
1:A:82:VAL:O	1:A:86:VAL:HG23	2.18	0.44
1:A:314:ASN:HB3	1:B:469:MET:CE	2.47	0.44
1:A:543:LEU:CD2	1:A:572:LEU:CD2	2.88	0.44
1:A:623:ARG:HH12	1:B:315:ARG:NH2	2.16	0.44
1:A:422:HIS:HA	1:B:80:GLU:OE2	2.17	0.44
1:A:445:ARG:NH2	1:A:522:ASN:HD22	2.15	0.44
1:B:584:ILE:HG22	1:B:588:MET:HE3	2.00	0.44
1:A:571:ALA:HB1	1:A:587:LYS:NZ	2.33	0.44
1:B:433:GLN:HE22	1:B:628:GLY:CA	2.30	0.44
1:A:580:ASP:HB3	1:A:583:ALA:HB3	1.99	0.43
1:A:576:LEU:HA	1:A:584:ILE:HG22	1.99	0.43
1:B:9:LEU:HA	1:B:9:LEU:HD12	1.77	0.43
1:B:575:ALA:O	1:B:584:ILE:CG1	2.66	0.43
1:A:542:LEU:HA	1:A:545:SER:HB3	2.00	0.43
1:A:180:GLY:CA	1:A:183:LYS:NZ	2.81	0.43
1:A:529:PHE:CZ	1:A:533:VAL:HG21	2.54	0.43
1:A:572:LEU:HD23	1:A:576:LEU:HG	1.99	0.43
1:B:180:GLY:HA2	1:B:183:LYS:NZ	2.34	0.43
1:B:82:VAL:O	1:B:86:VAL:HG23	2.18	0.43
1:A:180:GLY:HA2	1:A:183:LYS:CG	2.48	0.43
1:A:378:GLN:OE1	1:A:391:LEU:HD12	2.19	0.43
1:B:346:MET:CE	1:B:348:MET:HB3	2.42	0.42
1:A:457:PHE:CE2	1:A:499:ILE:HG12	2.54	0.42
1:A:169:ILE:O	1:A:169:ILE:HG13	2.19	0.42
1:B:584:ILE:O	1:B:588:MET:HG3	2.19	0.42
1:A:69:ILE:HG13	1:A:115:ILE:CG2	2.48	0.42
1:A:338:ILE:HD12	1:A:365:VAL:HG21	1.99	0.42
1:B:96:ALA:HB2	1:B:102:TRP:CD2	2.55	0.42
1:A:568:ALA:HB1	1:A:571:ALA:HB3	2.01	0.42
1:A:572:LEU:HD12	1:A:587:LYS:O	2.19	0.42
1:B:429:ALA:HA	1:B:625:LEU:HD13	2.02	0.42
1:B:433:GLN:HE22	1:B:628:GLY:HA3	1.84	0.42
1:A:59:VAL:HG13	1:A:264:GLU:OE2	2.20	0.42
1:A:146:PHE:CD2	1:A:150:GLN:HB3	2.54	0.42
1:B:73:ILE:HG12	1:B:153:ALA:CB	2.50	0.42
1:B:473:GLU:OE1	1:B:491:LYS:HD3	2.20	0.42
1:A:469:MET:CE	1:B:314:ASN:CB	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:VAL:HG12	1:B:623:ARG:HD3	2.02	0.41
1:B:188:ARG:NH2	5:B:705:CL:CL	2.90	0.41
1:A:584:ILE:HG13	1:A:585:GLU:N	2.35	0.41
1:A:315:ARG:HA	1:B:469:MET:HG3	2.02	0.41
1:A:322:VAL:HG11	1:B:492:ASN:O	2.21	0.41
1:B:532:LEU:O	1:B:536:ARG:HB2	2.20	0.41
1:A:40:ILE:HD12	1:A:40:ILE:N	2.36	0.41
1:A:467:ARG:HD3	1:A:541:HIS:CD2	2.56	0.41
1:A:364:ASP:OD1	1:A:364:ASP:N	2.54	0.41
1:A:401:ILE:HD11	1:A:426:PHE:CE2	2.55	0.41
1:A:576:LEU:HA	1:A:584:ILE:CG2	2.51	0.41
1:B:467:ARG:NH1	1:B:541:HIS:CD2	2.88	0.41
1:B:591:LEU:CA	1:B:594:VAL:HG12	2.49	0.41
1:A:404:MET:CE	1:A:537:ASN:HB3	2.50	0.40
1:B:31:GLU:OE2	1:B:53:PRO:HD3	2.19	0.40
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.86	0.40
1:B:359:LYS:HB3	1:B:359:LYS:HE2	1.96	0.40
1:B:616:GLN:H	1:B:616:GLN:HG3	1.41	0.40
1:A:469:MET:HE1	1:B:315:ARG:N	2.35	0.40
1:B:418:ILE:HG23	1:B:419:PRO:HA	2.04	0.40
1:A:119:VAL:O	1:A:123:MET:HG2	2.20	0.40
1:A:581:LYS:HE2	1:A:585:GLU:OE1	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:OH	1:A:285:TYR:OH[9_554]	1.81	0.39

## 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	597/628 (95%)	577 (97%)	19 (3%)	1 (0%)	47	76
1	B	597/628 (95%)	582 (98%)	15 (2%)	0	100	100
All	All	1194/1256 (95%)	1159 (97%)	34 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	ALA

### 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	492/511 (96%)	489 (99%)	3 (1%)	86	95
1	B	492/511 (96%)	489 (99%)	3 (1%)	86	95
All	All	984/1022 (96%)	978 (99%)	6 (1%)	86	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	HIS
1	A	598	LEU
1	A	622	ASN
1	B	616	GLN
1	B	617	THR
1	B	618	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	B	433	GLN
1	B	616	GLN



### 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 ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
2	ATP	B	702	4	26,33,33	1.21	2 (7%)	31,52,52	1.63	7 (22%)
2	ATP	A	701	4	26,33,33	1.12	1 (3%)	31,52,52	1.69	6 (19%)
3	SO4	B	703	-	4,4,4	0.23	0	6,6,6	0.33	0
3	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.52	0
3	SO4	A	703	-	4,4,4	0.24	0	6,6,6	0.29	0
3	SO4	B	701	-	4,4,4	0.18	0	6,6,6	0.17	0

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	4	-	0/18/38/38	0/3/3/3
2	ATP	B	702	4	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	ATP	O4'-C1'	2.81	1.45	1.41
2	A	701	ATP	O4'-C1'	2.46	1.44	1.41
2	B	702	ATP	C5-C4	-2.11	1.35	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C4-C5-N7	4.89	114.49	109.40
2	B	702	ATP	C4-C5-N7	4.84	114.44	109.40
2	A	701	ATP	C3'-C2'-C1'	3.51	106.27	100.98
2	B	702	ATP	PA-O3A-PB	-3.44	121.03	132.83
2	B	702	ATP	C3'-C2'-C1'	3.14	105.71	100.98
2	A	701	ATP	PB-O3B-PG	-3.10	122.20	132.83
2	A	701	ATP	C2-N1-C6	-2.86	113.87	118.75
2	B	702	ATP	C2-N1-C6	-2.81	113.95	118.75
2	A	701	ATP	PA-O3A-PB	-2.80	123.21	132.83
2	B	702	ATP	PB-O3B-PG	-2.47	124.33	132.83
2	B	702	ATP	O2G-PG-O3B	2.46	112.89	104.64
2	A	701	ATP	O2G-PG-O3B	2.39	112.65	104.64
2	B	702	ATP	C2'-C3'-C4'	2.24	107.00	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

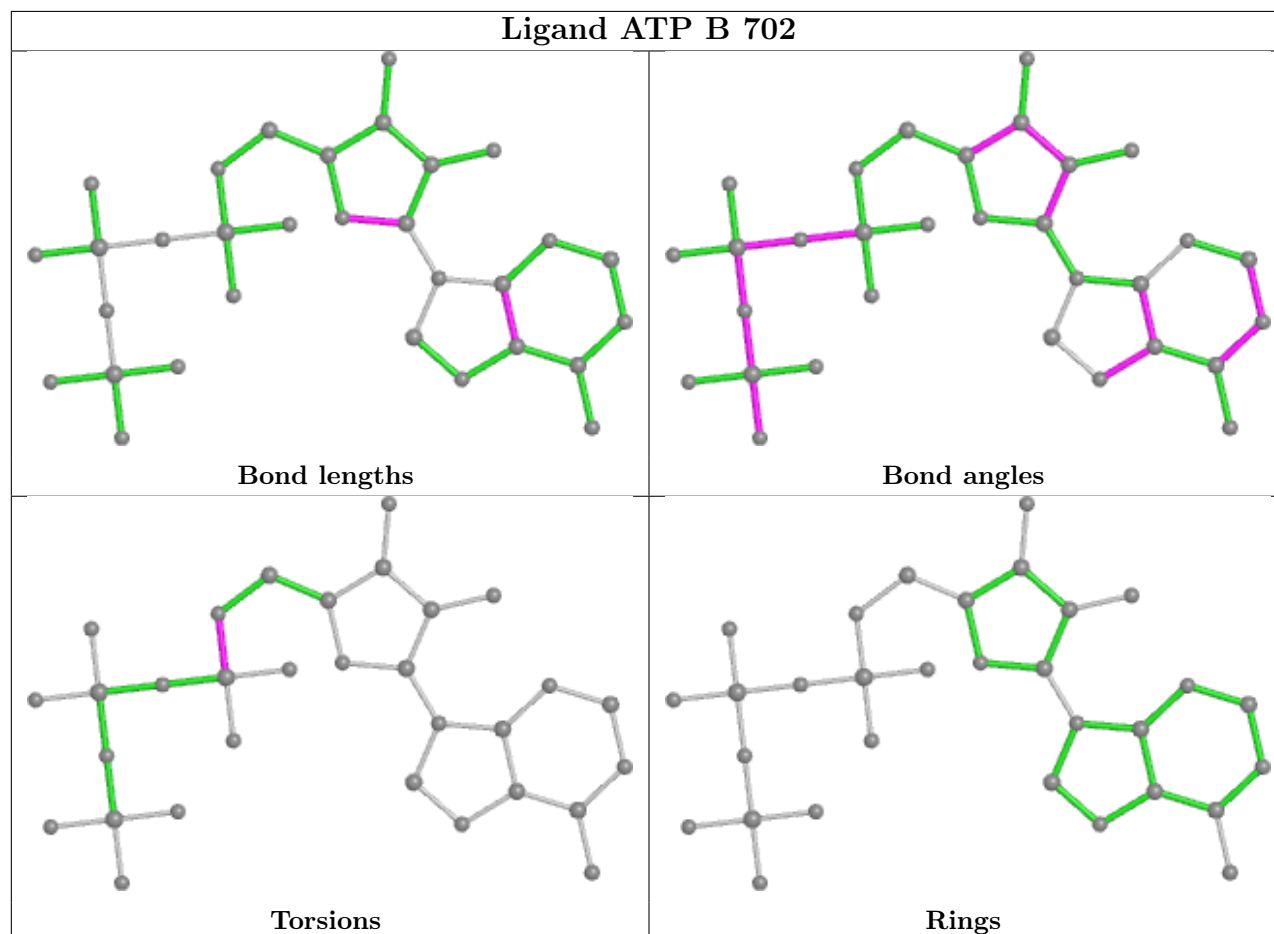
Mol	Chain	Res	Type	Atoms
2	B	702	ATP	C5'-O5'-PA-O3A
2	B	702	ATP	C5'-O5'-PA-O1A
2	B	702	ATP	C5'-O5'-PA-O2A

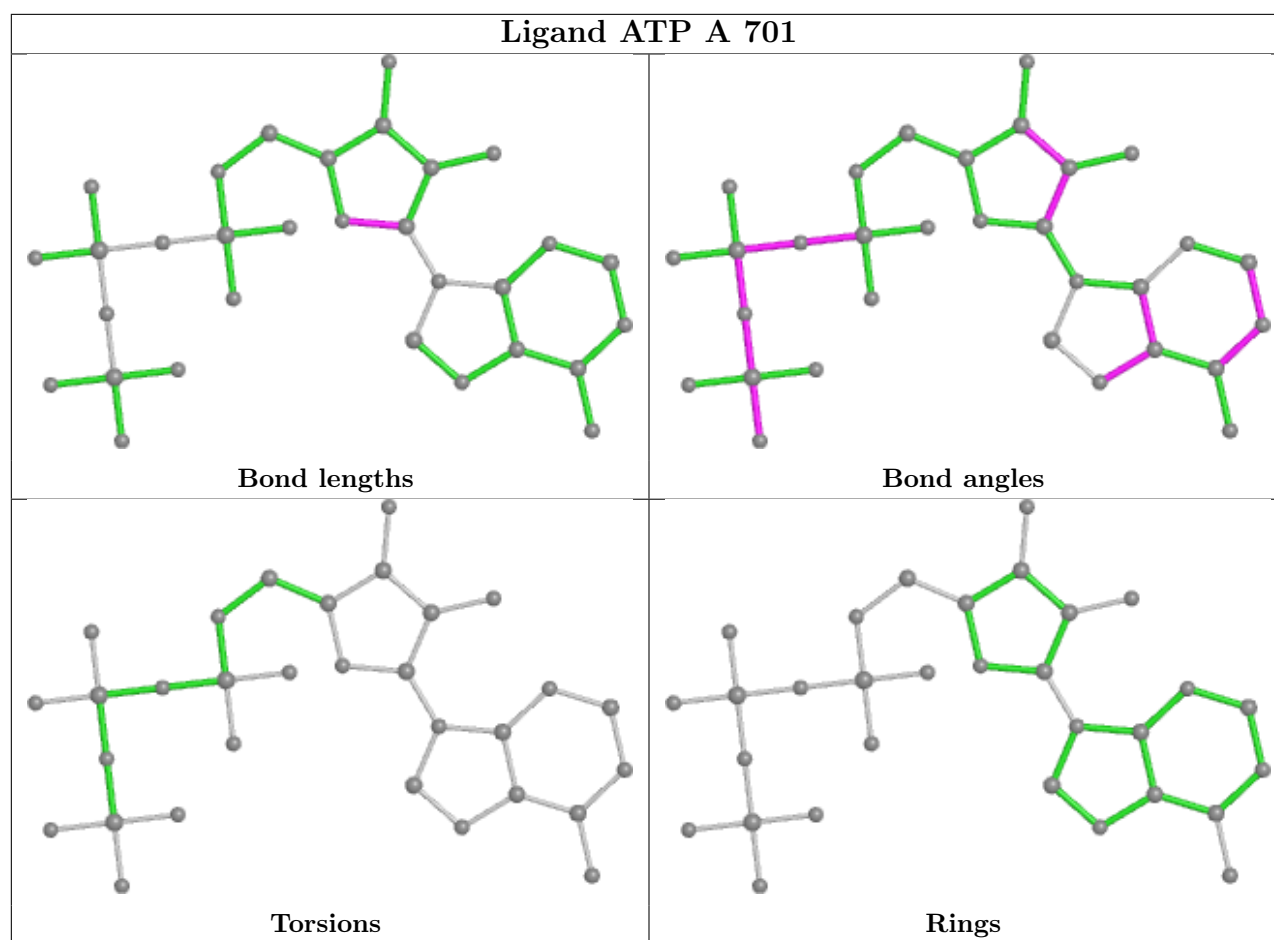
There are no ring outliers.

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	603/628 (96%)	0.46	45 (7%) 14 8	37, 65, 140, 191	0
1	B	603/628 (96%)	0.44	41 (6%) 17 10	33, 55, 154, 221	0
All	All	1206/1256 (96%)	0.45	86 (7%) 16 9	33, 61, 147, 221	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	THR	9.8
1	B	574	THR	7.7
1	A	510	ASP	6.4
1	B	590	GLU	6.2
1	B	569	LEU	6.2
1	B	550	VAL	6.1
1	B	593	GLN	5.9
1	A	576	LEU	5.8
1	A	595	SER	5.7
1	B	573	GLU	5.3
1	B	595	SER	5.3
1	B	576	LEU	5.3
1	A	570	THR	5.0
1	B	588	MET	4.8
1	A	569	LEU	4.6
1	B	598	LEU	4.5
1	B	544	HIS	4.3
1	A	548	LYS	4.2
1	A	598	LEU	4.2
1	B	586	ALA	4.1
1	B	583	ALA	4.0
1	A	590	GLU	3.8
1	A	523	ALA	3.8
1	B	546	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	211	ASP	3.7
1	A	551	GLU	3.7
1	A	544	HIS	3.7
1	A	550	VAL	3.6
1	A	593	GLN	3.6
1	B	596	GLN	3.6
1	B	571	ALA	3.4
1	A	575	ALA	3.3
1	B	584	ILE	3.3
1	A	596	GLN	3.3
1	A	584	ILE	3.3
1	B	548	LYS	3.2
1	A	597	LYS	3.2
1	B	211	ASP	3.2
1	A	577	LYS	3.1
1	A	594	VAL	3.1
1	B	597	LYS	3.0
1	B	542	LEU	3.0
1	B	582	ALA	2.9
1	A	571	ALA	2.9
1	B	567	SER	2.8
1	B	524	GLU	2.8
1	A	28	GLU	2.8
1	B	547	ARG	2.8
1	B	551	GLU	2.7
1	B	495	LYS	2.7
1	B	469	MET	2.6
1	B	31	GLU	2.6
1	A	514	LYS	2.6
1	B	615	GLN	2.6
1	A	543	LEU	2.6
1	A	156	ASP	2.6
1	A	628	GLY	2.6
1	B	577	LYS	2.6
1	A	586	ALA	2.6
1	A	592	ALA	2.6
1	B	543	LEU	2.5
1	B	507	LEU	2.5
1	A	574	THR	2.4
1	A	573	GLU	2.4
1	A	44	GLN	2.4
1	B	589	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	614	GLN	2.3
1	A	512	ILE	2.3
1	A	578	GLY	2.3
1	A	524	GLU	2.3
1	A	517	ARG	2.3
1	A	549	GLN	2.3
1	B	587	LYS	2.3
1	A	519	ALA	2.3
1	A	520	GLU	2.2
1	A	588	MET	2.2
1	B	594	VAL	2.2
1	B	447	ARG	2.2
1	A	582	ALA	2.2
1	B	572	LEU	2.1
1	A	528	LYS	2.1
1	A	393	ASP	2.1
1	B	519	ALA	2.1
1	A	384	GLY	2.1
1	B	520	GLU	2.1
1	A	318	GLU	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<sup>th</sup> 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.

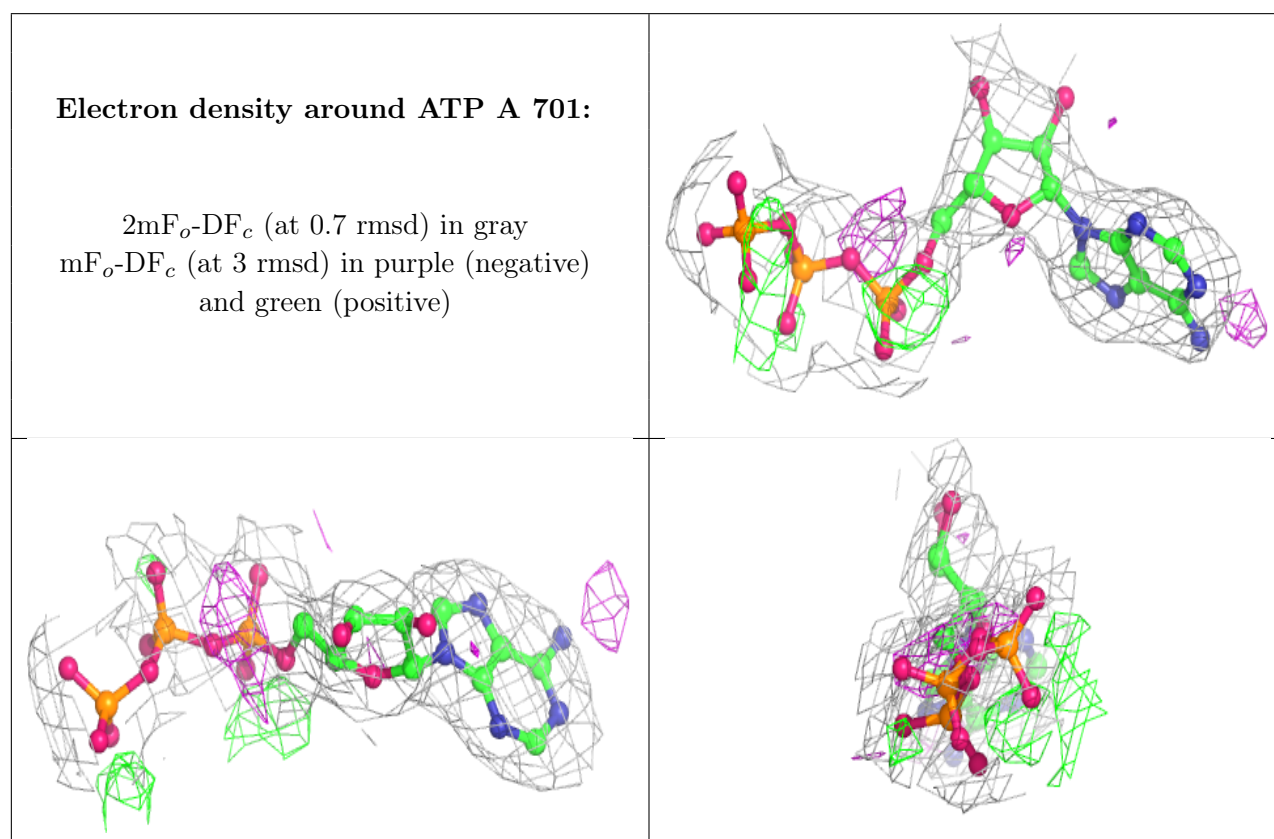
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	704	1/1	0.75	0.17	60,60,60,60	0
3	SO4	A	702	5/5	0.84	0.16	92,100,104,106	0
3	SO4	B	701	5/5	0.92	0.17	84,91,105,105	0

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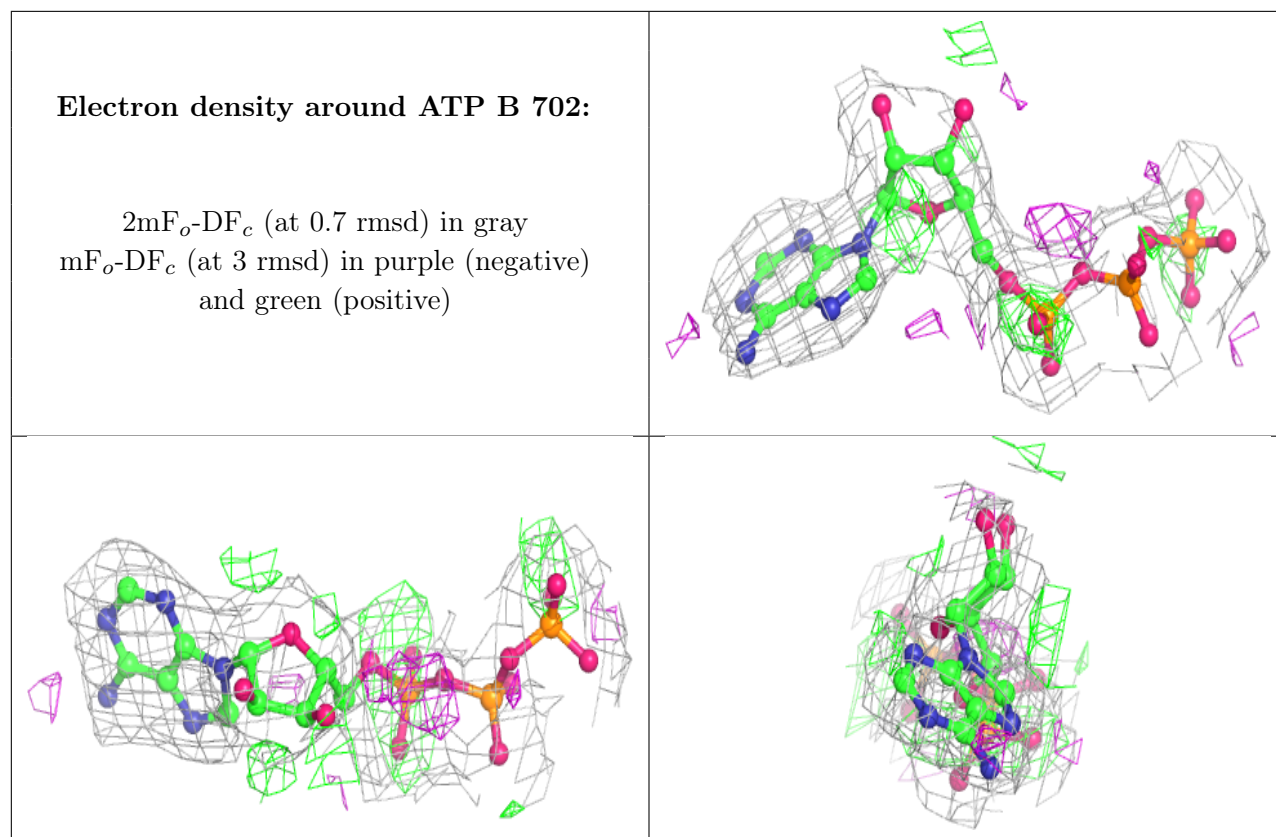
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	703	5/5	0.92	0.13	75,76,88,95	0
2	ATP	A	701	31/31	0.92	0.24	42,50,60,64	0
3	SO4	A	703	5/5	0.93	0.15	77,77,85,93	0
2	ATP	B	702	31/31	0.93	0.25	27,39,56,78	0
4	MG	B	704	1/1	0.95	0.12	43,43,43,43	0
5	CL	B	705	1/1	0.98	0.37	64,64,64,64	0

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.