



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:01 PM UTC

PDB ID : 7KZI / pdb_00007kzi
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

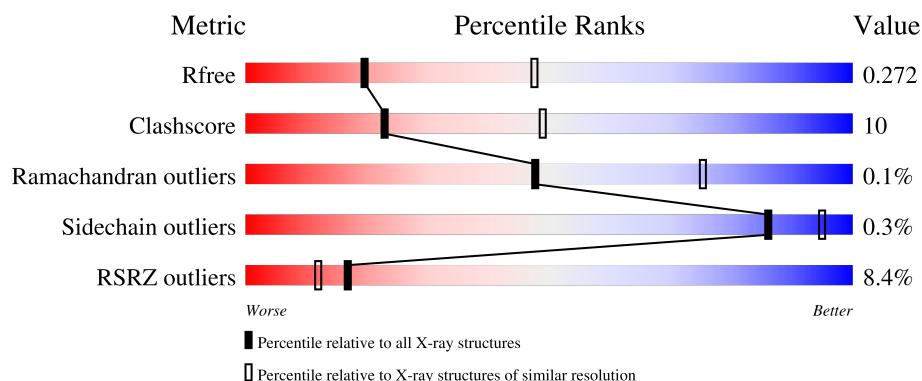
1 Overall quality at a glance

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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 ≥ 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	7% 76% 19% • •
1	B	628	9% 80% 15% • •

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.

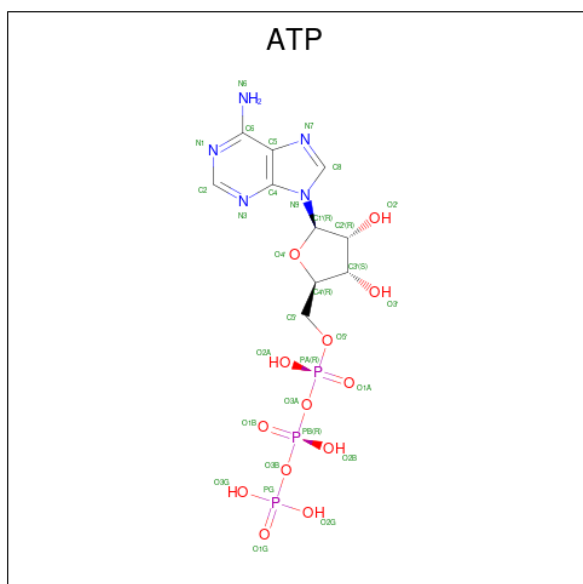
- Molecule 1 is a protein called Chaperone protein DnaK fused with substrate peptide,Chaperone protein DnaK fused with substrate peptide.

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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

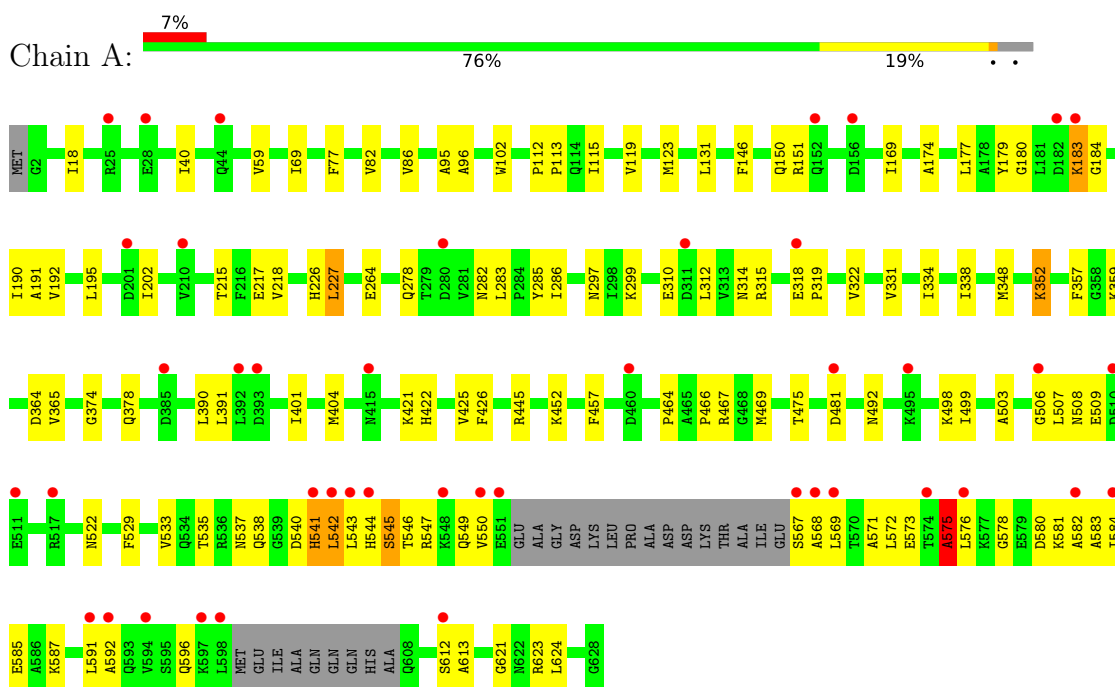
- Molecule 6 is water.

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

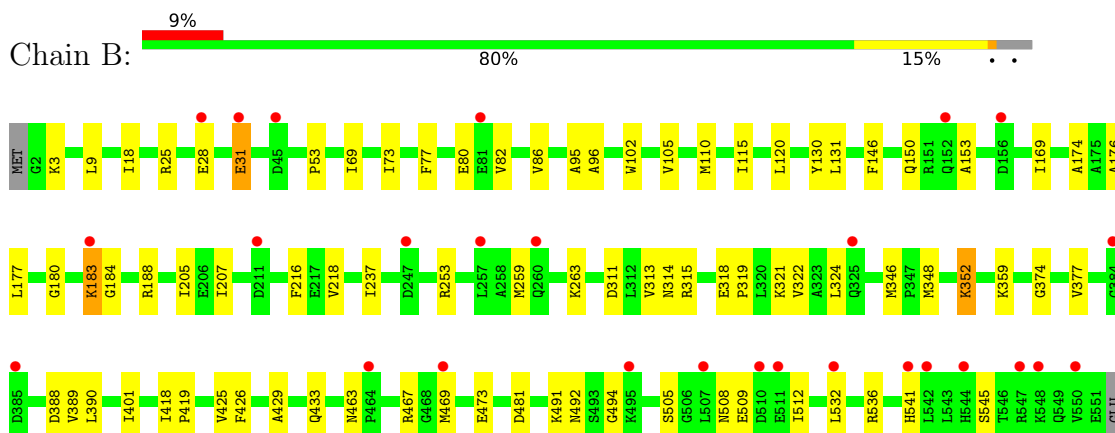
3 Residue-property plots

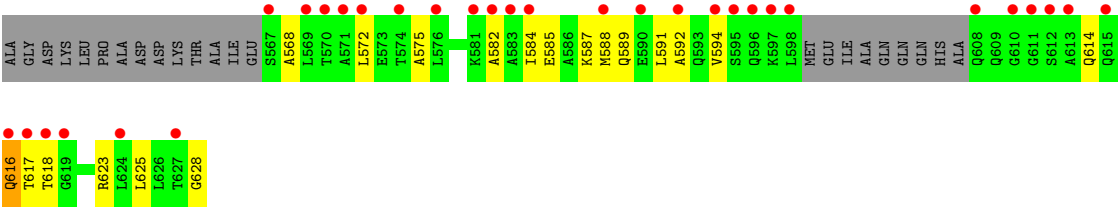
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.255 , 0.273 0.256 , 0.272	Depositor DCC
R_{free} test set	1926 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: SO4, ATP, CL, 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	0.58	2/4619 (0.0%)	1.07	17/6237 (0.3%)
1	B	0.62	1/4619 (0.0%)	1.03	11/6237 (0.2%)
All	All	0.60	3/9238 (0.0%)	1.05	28/12474 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	505	SER	CA-C	9.63	1.66	1.52
1	A	464	PRO	N-CD	6.90	1.57	1.47
1	A	541	HIS	CA-C	5.04	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	LEU	N-CA-C	14.36	130.97	113.16
1	A	573	GLU	N-CA-C	-10.63	98.62	111.69
1	A	542	LEU	N-CA-CB	-8.40	97.59	110.44
1	A	540	ASP	N-CA-C	-7.22	104.35	113.01
1	B	183	LYS	CB-CG-CD	-6.60	96.12	111.30
1	A	547	ARG	N-CA-C	-6.58	104.19	111.36
1	B	28	GLU	CA-CB-CG	6.55	127.21	114.10
1	B	31	GLU	CA-CB-CG	-6.37	101.37	114.10
1	A	575	ALA	N-CA-C	6.16	123.92	110.80
1	B	184	GLY	N-CA-C	-5.75	99.55	113.18
1	A	183	LYS	CB-CG-CD	-5.64	98.34	111.30
1	A	184	GLY	N-CA-C	-5.63	99.84	113.18
1	B	352	LYS	CB-CG-CD	-5.54	98.56	111.30
1	A	545	SER	N-CA-C	5.51	119.11	112.38
1	B	390	LEU	CA-C-N	5.48	129.67	121.72
1	B	390	LEU	C-N-CA	5.48	129.67	121.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	SER	CA-C-O	5.44	125.96	119.10
1	A	544	HIS	N-CA-C	-5.42	105.38	111.28
1	B	388	ASP	N-CA-C	5.40	119.36	112.34
1	A	575	ALA	N-CA-CB	-5.33	101.48	110.49
1	A	507	LEU	CA-CB-CG	5.17	134.40	116.30
1	A	183	LYS	CB-CA-C	-5.12	100.05	109.46
1	A	352	LYS	CB-CG-CD	-5.11	99.54	111.30
1	B	28	GLU	N-CA-CB	5.06	118.43	110.23
1	A	227	LEU	N-CA-CB	5.05	119.53	110.80
1	A	151	ARG	CA-CB-CG	-5.05	104.01	114.10
1	A	183	LYS	CA-CB-CG	5.04	124.17	114.10
1	B	318	GLU	CB-CG-CD	-5.02	104.07	112.60

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	122	1
1	B	4570	0	4618	92	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	193	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 (193) 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:B:584:ILE:HG22	1:B:588:MET:HE3	1.49	0.95
1:A:543:LEU:HD23	1:A:572:LEU:HD22	1.49	0.94
1:B:346:MET:HE2	1:B:348:MET:HB3	1.47	0.93
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:A:469:MET:HE1	1:B:314:ASN:C	2.02	0.85
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:404:MET:HE3	1:A:537:ASN:HB3	1.63	0.80
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:A:190:ILE:C	1:A:334:ILE:HD11	2.10	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:B:218:VAL:HG21	1:B:481:ASP:OD2	1.89	0.72
1:A:535:THR:CG2	1:A:584:ILE:HD11	2.19	0.71
1:A:469:MET:CE	1:B:314:ASN:HB3	2.20	0.71
1:A:469:MET:HE1	1:B:314:ASN:CB	2.21	0.71
1:B:314:ASN:OD1	1:B:352:LYS:HE2	1.92	0.70
1:A:469:MET:HE1	1:B:314:ASN:HB3	1.74	0.69
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:B:253:ARG:HA	1:B:259:MET:HE2	1.78	0.66
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:B:183:LYS:HZ1	1:B:207:ILE:HG21	1.62	0.64
1:B:183:LYS:HZ3	1:B:207:ILE:HG21	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:346:MET:HE1	1:B:348:MET:HE2	1.84	0.58
1:B:18:ILE:HD13	1:B:131:LEU:HD21	1.85	0.58
1:A:314:ASN:HB3	1:B:469:MET:HE2	1.84	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:218:VAL:HG21	1:A:481:ASP:CG	2.31	0.56
1:A:77:PHE:CD2	1:A:95:ALA:HB2	2.41	0.55
1:A:179:TYR:CD2	1:A:183:LYS:NZ	2.72	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:B:568:ALA:C	1:B:591:LEU:HD21	2.34	0.52
1:B:532:LEU:HD13	1:B:536:ARG:NH2	2.24	0.52
1:A:180:GLY:HA2	1:A:183:LYS:HZ3	1.74	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: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:452:LYS:HZ3	1:A:506:GLY:N	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLN:NE2	1:B:628:GLY:HA3	2.25	0.51
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
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: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: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:O	1:B:169:ILE:HG13	2.14	0.47
1:A:112:PRO:HB2	1:A:113:PRO:HD3	1.96	0.47
1:A:180:GLY:CA	1:A:183:LYS:HZ3	2.27	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:A:282:ASN:ND2	1:A:297:ASN:OD1	2.38	0.47
1:B:584:ILE:HG22	1:B:588:MET:CE	2.35	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:180:GLY:HA2	1:A:183:LYS:HZ2	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:HA	1:A:348:MET:HE1	1.99	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
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:227:LEU:HD21	1:A:315:ARG:NH2	2.32	0.44
1:B:346:MET:CE	1:B:348:MET:HE2	2.47	0.44
1:A:82:VAL:O	1:A:86:VAL:HG23	2.18	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:A:498:LYS:NZ	1:B:494:GLY:O	2.47	0.44
1:B:253:ARG:HG2	1:B:259:MET:HE2	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:B:587:LYS:HZ3	1:B:587:LYS:HB3	1.83	0.43
1:A:469:MET:CE	1:B:314:ASN:C	2.83	0.43
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:B:105:VAL:HB	1:B:110:MET:HE2	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: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:314:ASN:HB3	1:B:469:MET:CE	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:425:VAL:HG12	1:B:623:ARG:HD3	2.02	0.41
1:B:469:MET:HE3	1:B:469:MET:HB2	1.80	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:110:MET:HE3	1:B:110:MET:HB2	1.97	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: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: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

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	597/628 (95%)	577 (97%)	19 (3%)	1 (0%)	43	71
1	B	597/628 (95%)	582 (98%)	15 (2%)	0	100	100
All	All	1194/1256 (95%)	1159 (97%)	34 (3%)	1 (0%)	48	75

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%)	492 (100%)	0	100	100
1	B	492/511 (96%)	489 (99%)	3 (1%)	78	92
All	All	984/1022 (96%)	981 (100%)	3 (0%)	86	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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 (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	226	HIS
1	A	422	HIS
1	A	432	ASN
1	A	522	ASN
1	A	537	ASN
1	A	549	GLN
1	A	608	GLN
1	A	614	GLN
1	B	254	ASN
1	B	433	GLN
1	B	616	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	SO4	B	701	-	4,4,4	0.29	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	703	-	4,4,4	0.34	0	6,6,6	0.29	0
2	ATP	B	702	4	32,33,33	1.46	4 (12%)	48,52,52	1.37	9 (18%)
3	SO4	A	702	-	4,4,4	0.33	0	6,6,6	0.44	0
3	SO4	A	703	-	4,4,4	0.35	0	6,6,6	0.26	0
2	ATP	A	701	4	32,33,33	1.36	2 (6%)	48,52,52	1.39	8 (16%)

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	B	702	4	-	2/22/38/38	0/3/3/3
2	ATP	A	701	4	-	0/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	ATP	PB-O3A	-3.99	1.55	1.59
2	A	701	ATP	PB-O3A	-3.87	1.55	1.59
2	B	702	ATP	PA-O3A	-3.83	1.55	1.59
2	A	701	ATP	PA-O3A	-3.45	1.55	1.59
2	B	702	ATP	C8-N9	2.18	1.41	1.37
2	B	702	ATP	C5-C4	-2.10	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C4-C5-N7	3.42	114.49	110.58
2	B	702	ATP	C4-C5-N7	3.37	114.44	110.58
2	A	701	ATP	C2-N1-C6	-2.96	113.87	118.73
2	B	702	ATP	C2-N1-C6	-2.91	113.95	118.73
2	A	701	ATP	C5-C4-N3	-2.83	122.81	126.72
2	B	702	ATP	O2A-PA-O3A	2.75	114.71	107.27
2	A	701	ATP	N3-C4-N9	2.64	131.66	127.17
2	B	702	ATP	C5-C4-N3	-2.58	123.16	126.72
2	A	701	ATP	C3'-C2'-C1'	2.54	106.27	101.46
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'	2.27	107.00	102.61
2	B	702	ATP	N3-C4-N9	2.25	131.00	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	ATP	C3'-C2'-C1'	2.24	105.71	101.46
2	B	702	ATP	C5-C6-N1	2.24	123.19	117.51
2	A	701	ATP	C5-C6-N1	2.22	123.15	117.51
2	A	701	ATP	C6-C5-N7	-2.00	128.23	132.09

There are no chirality outliers.

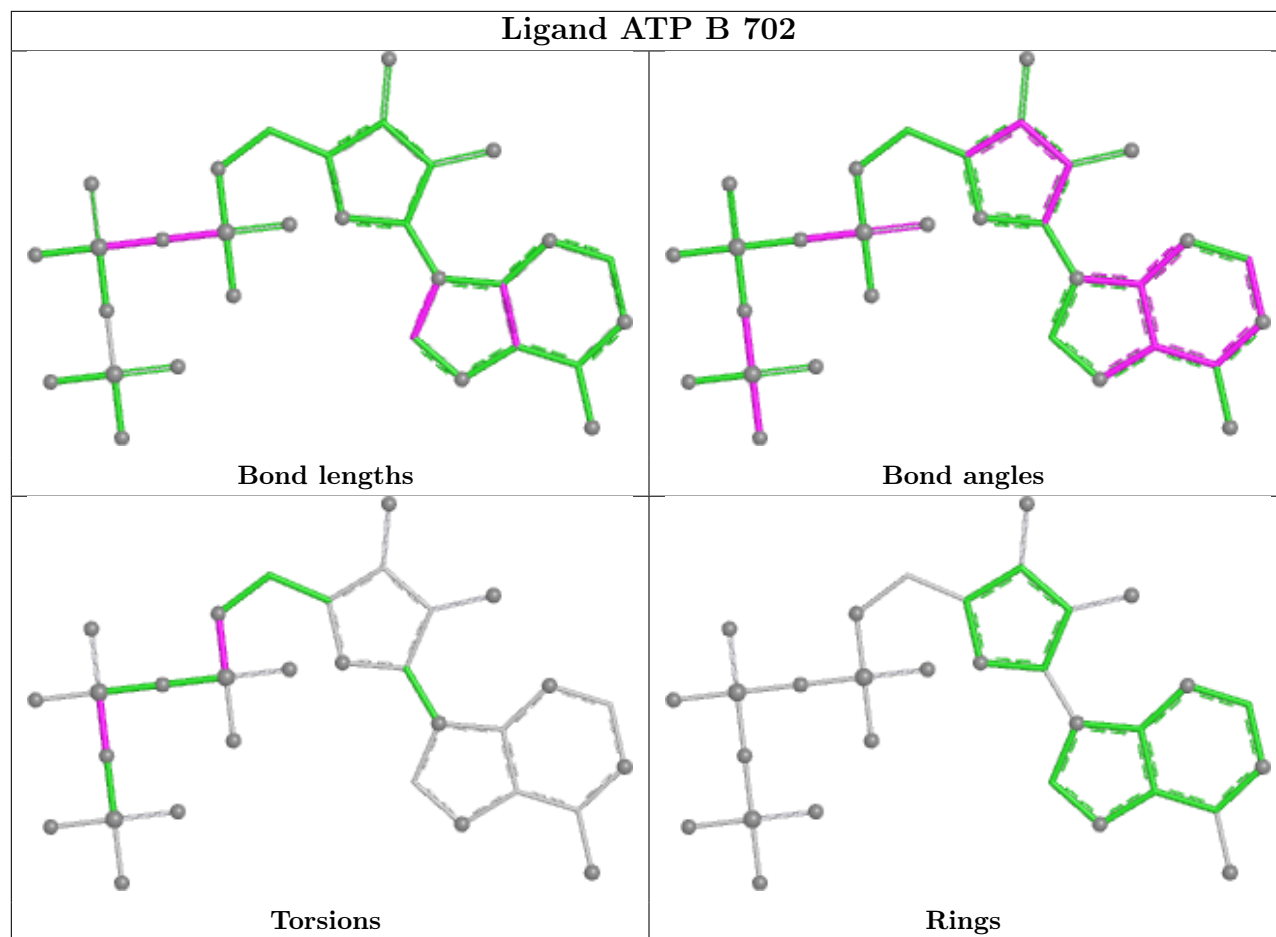
All (2) torsion outliers are listed below:

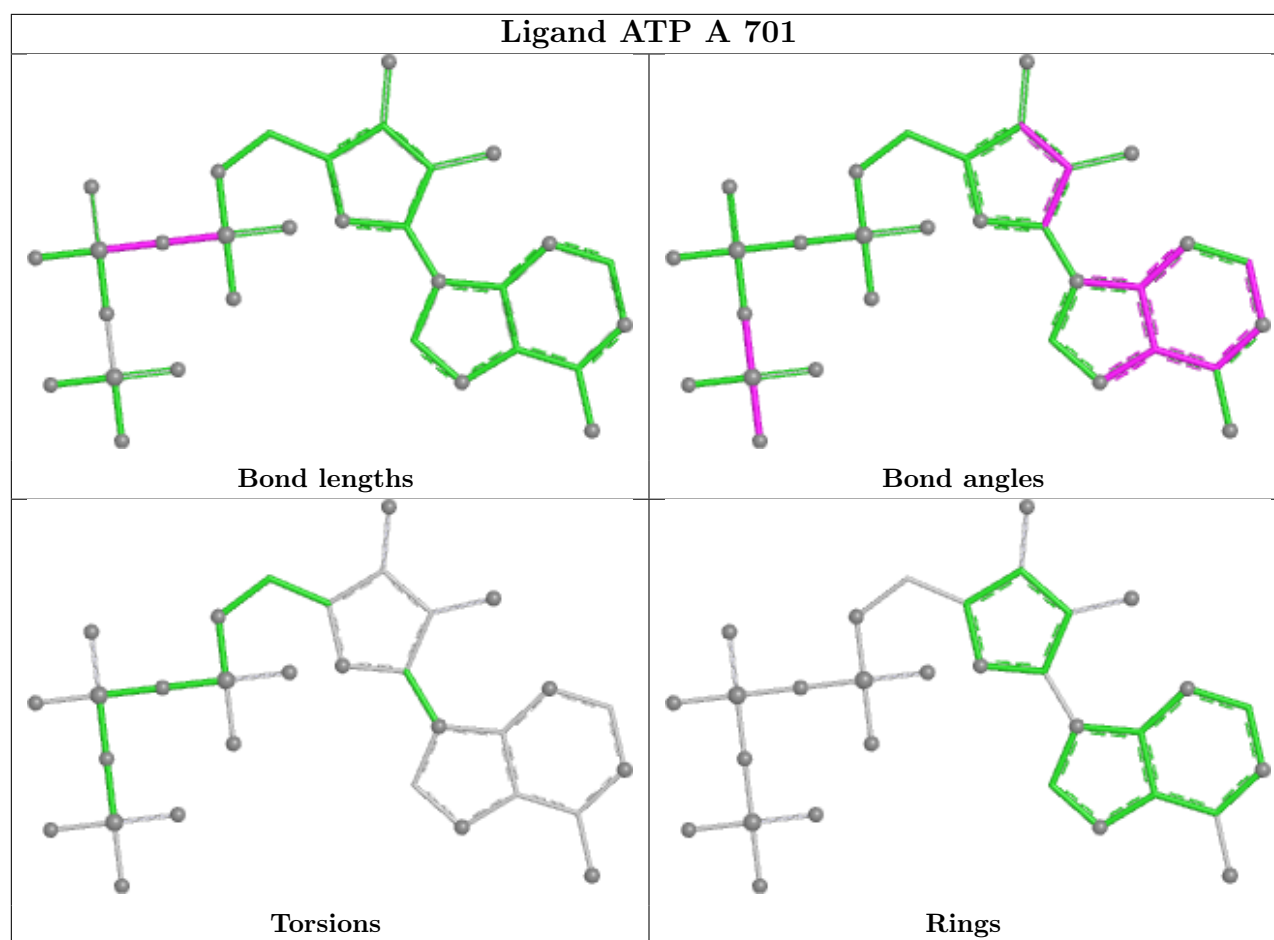
Mol	Chain	Res	Type	Atoms
2	B	702	ATP	C5'-O5'-PA-O1A
2	B	702	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	603/628 (96%)	0.50	43 (7%) 22 16	37, 65, 140, 191	0
1	B	603/628 (96%)	0.49	58 (9%) 13 10	33, 55, 154, 221	0
All	All	1206/1256 (96%)	0.49	101 (8%) 17 12	33, 61, 147, 221	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	MET	6.0
1	B	31	GLU	5.8
1	A	156	ASP	5.8
1	B	569	LEU	5.4
1	B	576	LEU	5.4
1	B	598	LEU	5.0
1	A	544	HIS	4.8
1	B	544	HIS	4.5
1	A	598	LEU	4.5
1	B	616	GLN	4.1
1	A	569	LEU	4.0
1	A	318	GLU	3.9
1	A	592	ALA	3.9
1	B	183	LYS	3.8
1	A	576	LEU	3.7
1	A	28	GLU	3.6
1	B	550	VAL	3.5
1	A	541	HIS	3.4
1	B	570	THR	3.4
1	A	542	LEU	3.3
1	B	627	THR	3.3
1	B	548	LYS	3.3
1	A	543	LEU	3.2
1	B	592	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	567	SER	3.1
1	B	211	ASP	3.1
1	B	152	GLN	3.1
1	A	550	VAL	3.0
1	B	584	ILE	3.0
1	B	542	LEU	3.0
1	B	582	ALA	3.0
1	A	481	ASP	3.0
1	B	595	SER	3.0
1	B	596	GLN	2.9
1	B	572	LEU	2.9
1	B	567	SER	2.8
1	A	392	LEU	2.8
1	B	260	GLN	2.8
1	B	617	THR	2.8
1	B	611	GLY	2.8
1	B	495	LYS	2.8
1	B	612	SER	2.8
1	B	615	GLN	2.7
1	B	583	ALA	2.7
1	A	597	LYS	2.7
1	B	619	GLY	2.7
1	B	571	ALA	2.7
1	A	201	ASP	2.7
1	B	156	ASP	2.7
1	A	510	ASP	2.6
1	A	460	ASP	2.6
1	B	81	GLU	2.6
1	A	511	GLU	2.5
1	B	618	THR	2.5
1	A	548	LYS	2.5
1	B	610	GLY	2.5
1	B	28	GLU	2.5
1	A	393	ASP	2.4
1	B	541	HIS	2.4
1	B	510	ASP	2.4
1	B	384	GLY	2.4
1	A	280	ASP	2.4
1	B	581	LYS	2.3
1	B	325	GLN	2.3
1	A	574	THR	2.3
1	B	574	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	464	PRO	2.3
1	A	210	VAL	2.3
1	A	311	ASP	2.3
1	B	613	ALA	2.3
1	A	152	GLN	2.3
1	A	612	SER	2.3
1	B	507	LEU	2.3
1	A	415	ASN	2.3
1	A	582	ALA	2.3
1	B	597	LYS	2.3
1	B	547	ARG	2.3
1	A	506	GLY	2.3
1	A	385	ASP	2.2
1	B	45	ASP	2.2
1	B	532	LEU	2.2
1	B	624	LEU	2.2
1	A	25	ARG	2.2
1	A	495	LYS	2.2
1	A	568	ALA	2.2
1	A	517	ARG	2.2
1	A	584	ILE	2.2
1	B	608	GLN	2.2
1	B	511	GLU	2.2
1	A	182	ASP	2.1
1	B	257	LEU	2.1
1	A	183	LYS	2.1
1	B	594	VAL	2.1
1	A	551	GLU	2.1
1	B	590	GLU	2.1
1	A	44	GLN	2.0
1	B	385	ASP	2.0
1	A	591	LEU	2.0
1	B	247	ASP	2.0
1	B	588	MET	2.0
1	A	594	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

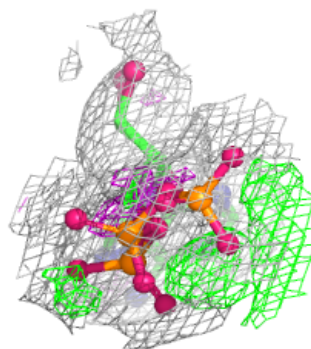
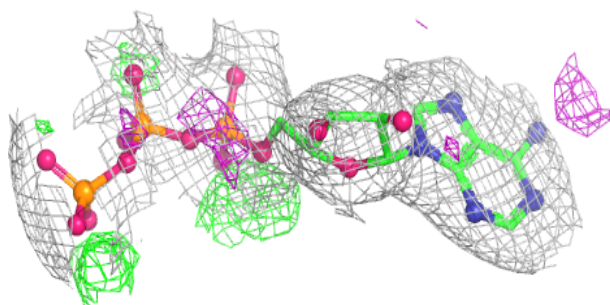
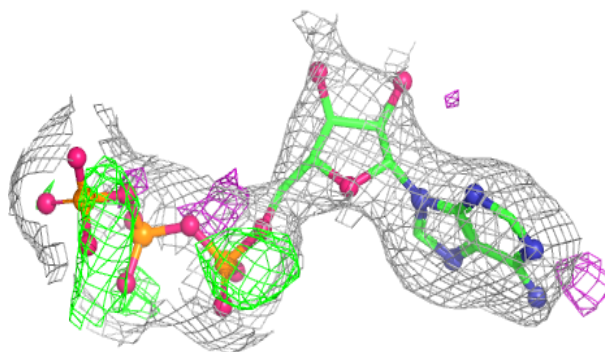
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	702	5/5	0.69	0.13	92,100,104,106	0
3	SO4	B	701	5/5	0.80	0.19	84,91,105,105	0
3	SO4	B	703	5/5	0.81	0.14	75,76,88,95	0
3	SO4	A	703	5/5	0.84	0.14	77,77,85,93	0
2	ATP	A	701	31/31	0.90	0.11	42,50,60,64	0
5	CL	B	705	1/1	0.90	0.28	64,64,64,64	0
2	ATP	B	702	31/31	0.92	0.10	27,39,56,78	0
4	MG	A	704	1/1	0.94	0.08	60,60,60,60	0
4	MG	B	704	1/1	0.98	0.05	43,43,43,43	0

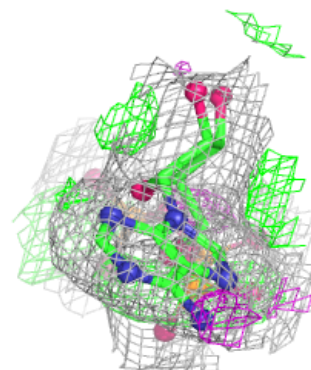
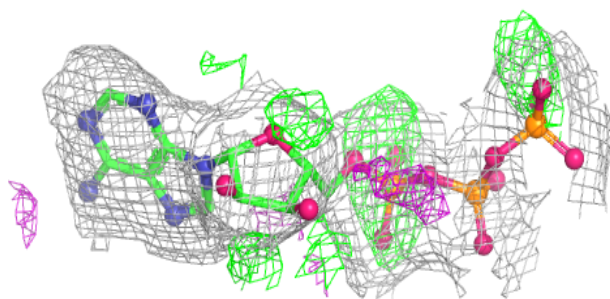
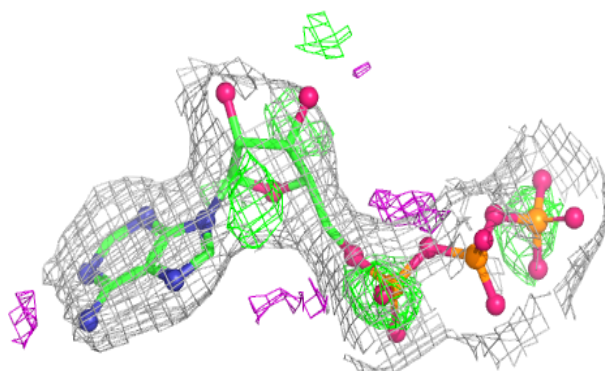
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 702:**

$2mF_o-DF_c$ (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.