



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:20 AM UTC

PDB ID : 7KO2 / pdb_00007ko2
Title : Restraining state of near full-length Hsp70 DnaK
Authors : Wang, W.; Hendrickson, W.A.
Deposited on : 2020-11-06
Resolution : 2.64 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

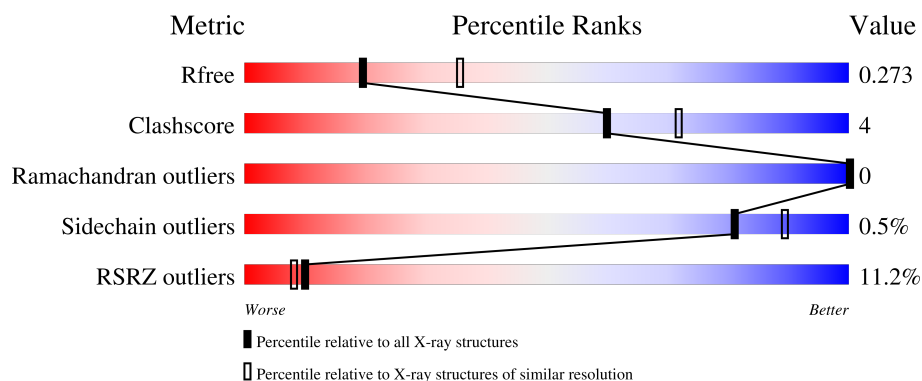
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	609	10% 86% 12%
1	B	609	11% 88% 11%
1	C	609	17% 87% 11%
1	D	609	7% 89% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18470 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4515	2800	785	914	16			
1	B	603	Total	C	N	O	S	0	0	0
			4547	2820	791	921	15			
1	C	595	Total	C	N	O	S	0	0	0
			4487	2788	781	904	14			
1	D	600	Total	C	N	O	S	0	0	0
			4533	2814	789	914	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
A	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
B	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
C	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
C	199	ALA	THR	engineered mutation	UNP A0A6D2W465
C	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
D	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
D	199	ALA	THR	engineered mutation	UNP A0A6D2W465
D	529	CYS	PHE	engineered mutation	UNP A0A6D2W465

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

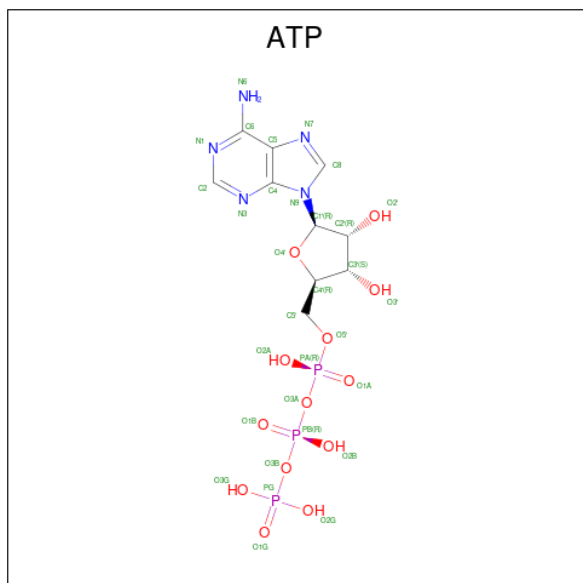
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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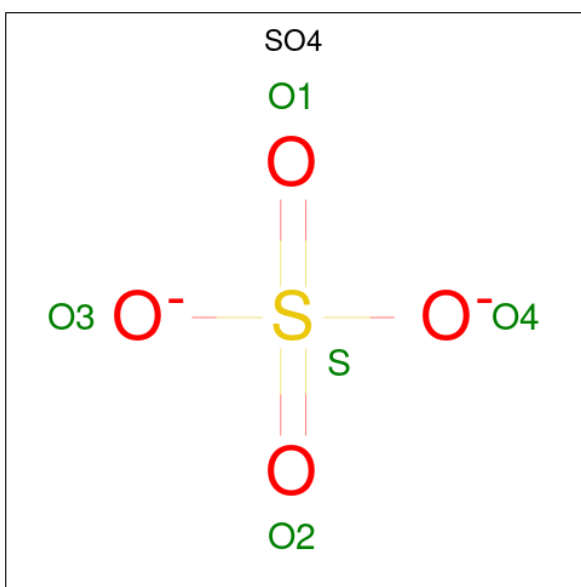
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

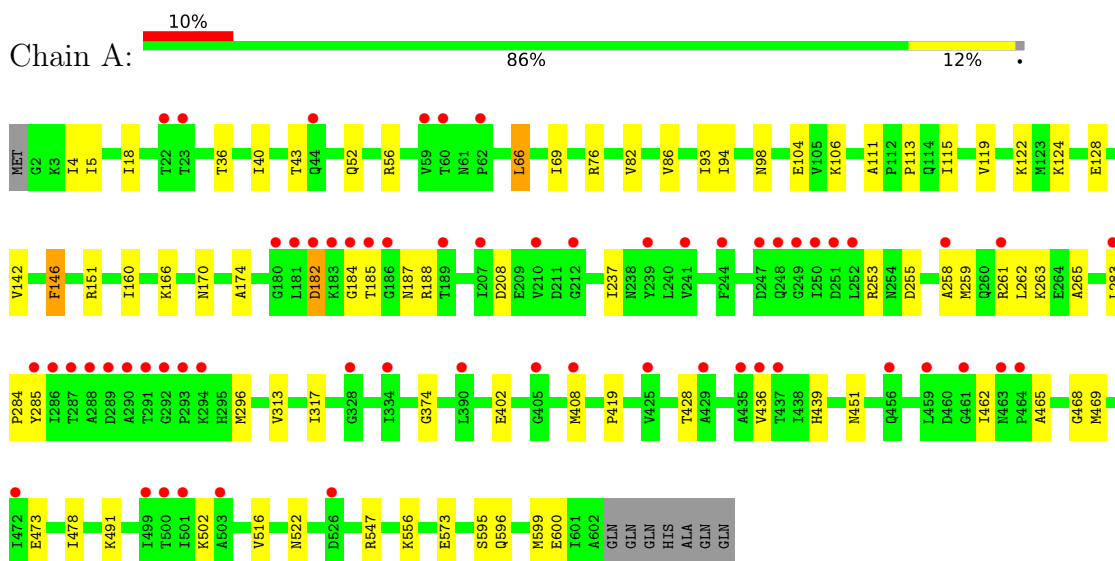
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	63	Total	O	0	0
			63	63		
5	C	70	Total	O	0	0
			70	70		
5	D	52	Total	O	0	0
			52	52		

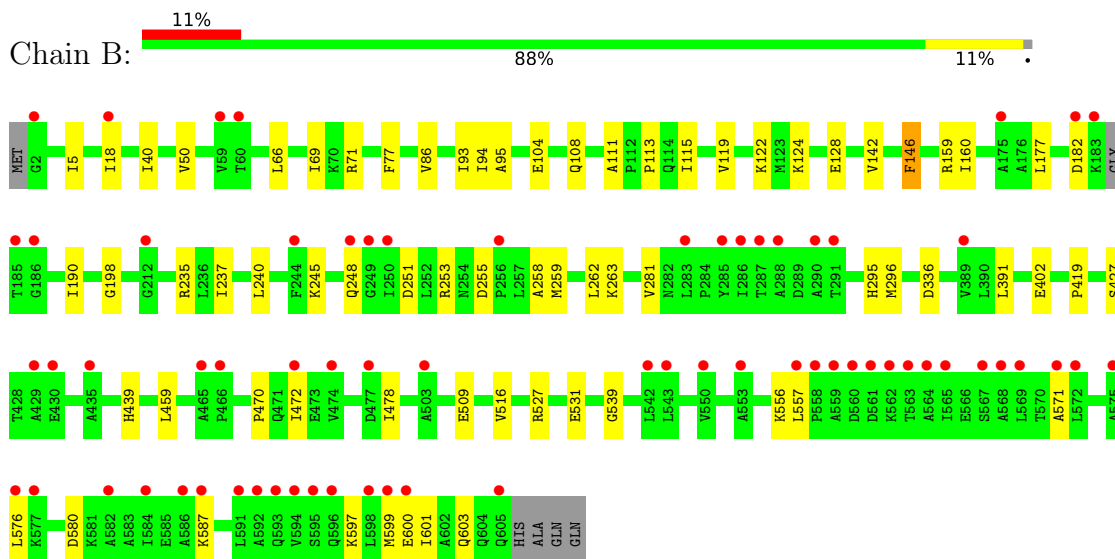
3 Residue-property plots [i](#)

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.

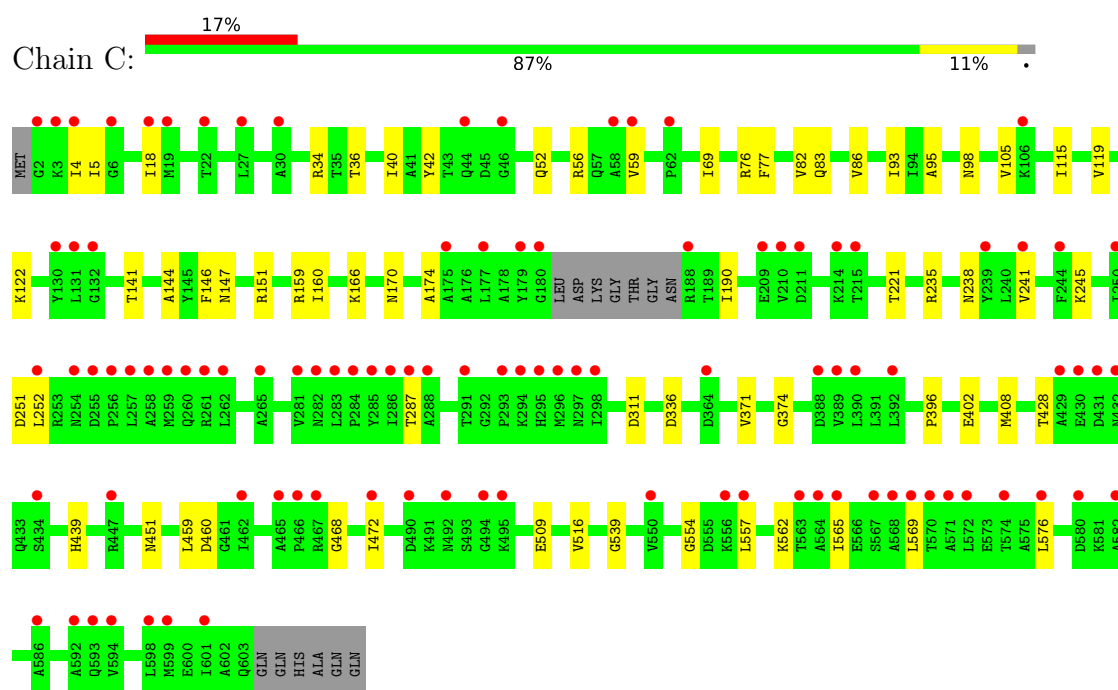
• Molecule 1: Chaperone protein DnaK



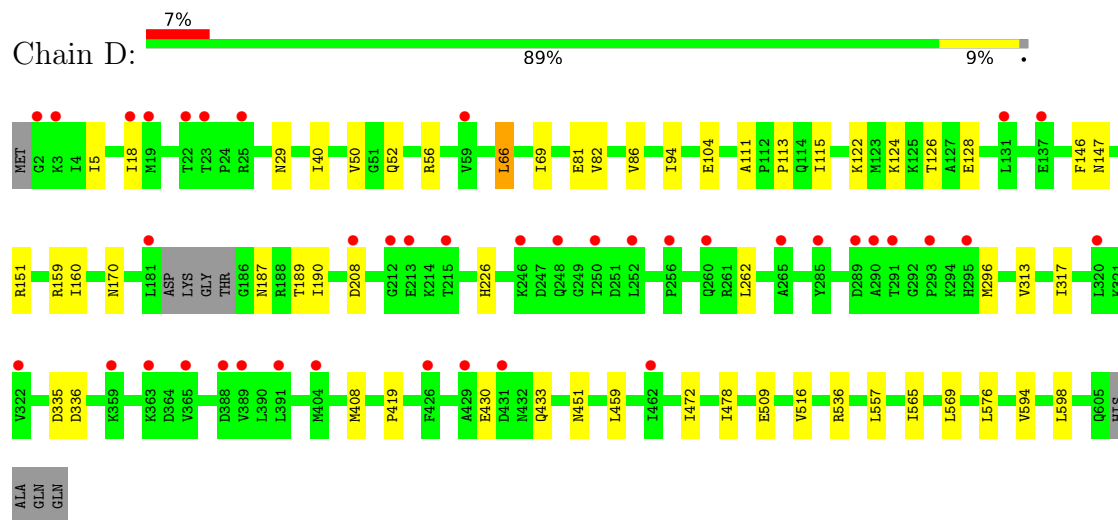
• Molecule 1: Chaperone protein DnaK



• Molecule 1: Chaperone protein DnaK



• Molecule 1: Chaperone protein DnaK



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.43Å 77.49Å 182.74Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	49.54 – 2.64 49.54 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.54-2.64) 90.2 (49.54-2.64)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.241 , 0.287 0.243 , 0.273	Depositor DCC
R_{free} test set	2048 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18470	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1428e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.13	0/4566	0.31	0/6177
1	B	0.13	0/4597	0.32	0/6218
1	C	0.13	0/4537	0.31	0/6136
1	D	0.12	0/4583	0.31	0/6197
All	All	0.12	0/18283	0.31	0/24728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4515	0	4513	45	0
1	B	4547	0	4561	39	0
1	C	4487	0	4516	40	0
1	D	4533	0	4566	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	B	5	0	0	2	0
5	A	70	0	0	2	0
5	B	63	0	0	0	0
5	C	70	0	0	2	0
5	D	52	0	0	1	0
All	All	18470	0	18204	155	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 4.

All (155) 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:C:557:LEU:HB3	1:C:562:LYS:HZ2	1.56	0.71
1:D:160:ILE:HA	1:D:516:VAL:HG22	1.72	0.71
1:D:187:ASN:H	1:D:208:ASP:HA	1.57	0.69
1:D:151:ARG:NH2	1:D:170:ASN:OD1	2.27	0.67
1:B:160:ILE:HA	1:B:516:VAL:HG22	1.75	0.67
1:B:539:GLY:HA3	1:B:576:LEU:HD21	1.77	0.66
1:B:557:LEU:HA	1:B:601:ILE:HD11	1.79	0.64
1:A:547:ARG:NH2	1:A:573:GLU:OE1	2.29	0.63
1:A:36:THR:HG21	1:A:122:LYS:HD3	1.82	0.61
1:B:190:ILE:HG22	1:B:336:ASP:HB2	1.83	0.61
1:B:5:ILE:HG22	1:B:18:ILE:HG22	1.82	0.61
1:D:190:ILE:HG22	1:D:336:ASP:HB2	1.82	0.61
1:C:159:ARG:NH2	1:C:509:GLU:OE2	2.31	0.60
1:A:151:ARG:NH2	1:A:170:ASN:OD1	2.31	0.60
1:B:235:ARG:NH1	4:B:703:SO4:S	2.75	0.59
1:C:428:THR:OG1	1:C:468:GLY:N	2.34	0.59
1:C:40:ILE:HD13	1:C:115:ILE:HG22	1.85	0.58
1:C:40:ILE:HD11	1:C:119:VAL:HG23	1.86	0.58
1:A:94:ILE:HD13	1:A:104:GLU:HB2	1.86	0.57
1:D:29:ASN:HA	1:D:126:THR:HG21	1.87	0.56
1:D:159:ARG:NH2	1:D:509:GLU:OE2	2.31	0.56
1:C:235:ARG:NH2	1:C:311:ASP:OD2	2.39	0.55
1:B:50:VAL:HB	1:B:122:LYS:HD2	1.89	0.55
1:A:187:ASN:HA	1:A:208:ASP:HA	1.89	0.55
1:B:177:LEU:HD21	1:B:391:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HB	1:D:122:LYS:HD2	1.87	0.55
1:C:160:ILE:HA	1:C:516:VAL:HG22	1.88	0.55
1:C:190:ILE:HG22	1:C:336:ASP:HB2	1.89	0.55
1:A:473:GLU:HB2	1:A:491:LYS:HG2	1.88	0.54
1:D:430:GLU:N	1:D:433:GLN:OE1	2.40	0.54
1:C:539:GLY:HA3	1:C:576:LEU:HD21	1.90	0.53
1:D:5:ILE:HG22	1:D:18:ILE:HG22	1.91	0.53
1:B:124:LYS:NZ	1:B:128:GLU:OE2	2.42	0.53
1:B:177:LEU:HD11	1:B:391:LEU:HD21	1.90	0.53
1:C:77:PHE:O	1:C:83:GLN:NE2	2.36	0.53
1:A:5:ILE:HG22	1:A:18:ILE:HG22	1.91	0.52
1:C:36:THR:HG21	1:C:122:LYS:HD3	1.91	0.52
1:A:43:THR:O	1:A:106:LYS:NZ	2.41	0.52
1:A:66:LEU:HB3	1:A:69:ILE:HD11	1.91	0.52
1:A:184:GLY:HA3	1:A:188:ARG:HE	1.74	0.52
1:B:159:ARG:NH2	1:B:509:GLU:OE2	2.32	0.52
1:D:29:ASN:HA	1:D:126:THR:CG2	2.40	0.52
1:D:124:LYS:NZ	1:D:128:GLU:OE2	2.43	0.52
1:C:5:ILE:HG22	1:C:18:ILE:HG22	1.91	0.51
1:B:245:LYS:HE2	1:B:251:ASP:HB2	1.91	0.51
1:C:151:ARG:NH2	1:C:170:ASN:OD1	2.35	0.51
1:D:536:ARG:HG3	1:D:576:LEU:HD22	1.93	0.51
1:B:580:ASP:OD1	1:B:580:ASP:N	2.44	0.51
1:C:557:LEU:HB3	1:C:562:LYS:NZ	2.25	0.50
1:B:571:ALA:HB1	1:B:587:LYS:HD2	1.93	0.50
1:A:436:VAL:HG22	1:A:462:ILE:HD11	1.93	0.50
1:B:599:MET:O	1:B:603:GLN:HG2	2.11	0.50
1:B:419:PRO:HA	1:B:478:ILE:O	2.11	0.50
1:B:255:ASP:HB3	1:B:258:ALA:HB3	1.94	0.50
1:D:66:LEU:HB3	1:D:69:ILE:HD11	1.93	0.50
1:A:124:LYS:NZ	1:A:128:GLU:OE2	2.45	0.48
1:C:4:ILE:HD13	1:C:166:LYS:HG3	1.94	0.48
1:C:252:LEU:HD21	1:C:287:THR:HG21	1.95	0.48
1:B:235:ARG:NH1	4:B:703:SO4:O1	2.44	0.48
1:B:262:LEU:HD13	1:B:296:MET:HE1	1.96	0.48
1:A:160:ILE:HA	1:A:516:VAL:HG22	1.94	0.48
1:D:565:ILE:HD13	1:D:598:LEU:HD22	1.94	0.48
1:B:402:GLU:HB3	1:B:439:HIS:HB3	1.96	0.48
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.96	0.48
1:D:262:LEU:HD13	1:D:296:MET:HE1	1.96	0.47
1:A:419:PRO:HA	1:A:478:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:NH1	1:C:98:ASN:O	2.47	0.47
1:B:248:GLN:NE2	1:B:295:HIS:O	2.48	0.47
1:B:556:LYS:HD3	1:B:601:ILE:HG23	1.96	0.47
1:A:40:ILE:HD11	1:A:119:VAL:HG23	1.97	0.47
1:B:40:ILE:HD11	1:B:119:VAL:HG23	1.97	0.47
1:C:221:THR:O	5:C:801:HOH:O	2.20	0.46
1:D:111:ALA:HB1	1:D:113:PRO:HD2	1.97	0.46
1:A:255:ASP:HB3	1:A:258:ALA:HB3	1.97	0.46
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.97	0.46
1:C:86:VAL:HG22	1:C:93:ILE:HB	1.98	0.46
1:A:40:ILE:HD13	1:A:115:ILE:HG22	1.97	0.46
1:B:94:ILE:HD13	1:B:104:GLU:HB2	1.98	0.46
1:A:522:ASN:HB3	5:A:808:HOH:O	2.16	0.46
1:B:253:ARG:HA	1:B:259:MET:SD	2.55	0.46
1:A:142:VAL:HB	1:A:146:PHE:CD2	2.51	0.46
1:D:313:VAL:O	1:D:317:ILE:HG12	2.16	0.46
1:A:86:VAL:HG22	1:A:93:ILE:HB	1.98	0.46
1:A:76:ARG:NH1	1:A:98:ASN:O	2.41	0.46
1:C:174:ALA:O	1:C:374:GLY:HA3	2.16	0.46
1:C:554:GLY:O	1:C:562:LYS:NZ	2.38	0.46
1:A:170:ASN:ND2	5:A:825:HOH:O	2.49	0.45
1:B:66:LEU:HB3	1:B:69:ILE:HD11	1.98	0.45
1:C:460:ASP:OD1	1:C:460:ASP:N	2.47	0.45
1:C:408:MET:HG3	1:C:451:ASN:ND2	2.31	0.45
1:D:56:ARG:NH1	5:D:807:HOH:O	2.41	0.45
1:A:265:ALA:HB2	1:A:283:LEU:HD11	1.97	0.45
1:A:402:GLU:HB3	1:A:439:HIS:HB3	1.99	0.45
1:D:147:ASN:O	1:D:151:ARG:HG3	2.17	0.45
1:A:253:ARG:HA	1:A:259:MET:SD	2.57	0.45
1:B:69:ILE:HG13	1:B:115:ILE:HG21	2.00	0.44
1:B:86:VAL:HG22	1:B:93:ILE:HB	1.97	0.44
1:D:557:LEU:HD21	1:D:565:ILE:HD12	1.98	0.44
1:A:111:ALA:HB1	1:A:113:PRO:HD2	1.99	0.44
1:B:597:LYS:O	1:B:600:GLU:HB3	2.17	0.44
1:A:408:MET:HG3	1:A:451:ASN:ND2	2.33	0.44
1:A:596:GLN:O	1:A:600:GLU:HG3	2.17	0.44
1:A:4:ILE:HD13	1:A:166:LYS:HG3	1.99	0.44
1:A:408:MET:HG3	1:A:451:ASN:HD22	1.82	0.44
1:C:565:ILE:O	1:C:569:LEU:HG	2.18	0.44
1:D:94:ILE:HD13	1:D:104:GLU:HB2	1.98	0.44
1:D:459:LEU:HD13	1:D:472:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HD13	1:B:281:VAL:HG11	2.00	0.43
1:C:147:ASN:O	1:C:151:ARG:HG3	2.18	0.43
1:A:556:LYS:HA	1:A:556:LYS:HD3	1.78	0.43
1:D:81:GLU:HB3	1:D:226:HIS:CE1	2.52	0.43
1:A:261:ARG:NH1	1:A:285:TYR:O	2.52	0.43
1:A:595:SER:O	1:A:599:MET:HG2	2.18	0.43
1:A:174:ALA:O	1:A:374:GLY:HA3	2.19	0.43
1:B:142:VAL:HB	1:B:146:PHE:CD2	2.54	0.43
1:B:527:ARG:HH11	1:B:531:GLU:CD	2.26	0.43
1:D:82:VAL:O	1:D:86:VAL:HG23	2.19	0.43
1:A:182:ASP:N	1:A:182:ASP:OD1	2.51	0.43
1:B:427:SER:OG	1:B:470:PRO:O	2.36	0.42
1:C:238:ASN:HA	1:C:241:VAL:HG22	2.01	0.42
1:C:245:LYS:HE2	1:C:251:ASP:HB2	2.00	0.42
1:A:52:GLN:O	1:A:56:ARG:HG3	2.19	0.42
1:C:144:ALA:O	1:C:396:PRO:HG3	2.19	0.42
1:C:34:ARG:NH1	5:C:820:HOH:O	2.52	0.42
1:D:189:THR:O	1:D:335:ASP:N	2.52	0.42
1:A:502:LYS:HD2	1:A:502:LYS:HA	1.83	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.20	0.42
1:A:262:LEU:HD13	1:A:296:MET:HE1	2.02	0.42
1:B:111:ALA:HB1	1:B:113:PRO:HD2	2.02	0.42
1:C:402:GLU:HB3	1:C:439:HIS:HB3	2.01	0.42
1:D:40:ILE:HD13	1:D:115:ILE:HG22	2.01	0.42
1:D:419:PRO:HA	1:D:478:ILE:O	2.20	0.42
1:A:313:VAL:O	1:A:317:ILE:HG12	2.20	0.41
1:A:428:THR:OG1	1:A:468:GLY:N	2.53	0.41
1:C:141:THR:HG21	1:C:371:VAL:HG12	2.02	0.41
1:A:237:ILE:HD11	1:A:263:LYS:HA	2.01	0.41
1:B:77:PHE:CD2	1:B:95:ALA:HB2	2.55	0.41
1:C:408:MET:HG3	1:C:451:ASN:HD22	1.85	0.41
1:D:52:GLN:O	1:D:56:ARG:HG3	2.21	0.41
1:C:235:ARG:HH21	1:C:311:ASP:CG	2.27	0.41
1:A:184:GLY:HA2	1:A:185:THR:CB	2.50	0.41
1:D:208:ASP:OD1	1:D:208:ASP:N	2.53	0.41
1:B:459:LEU:HD13	1:B:472:ILE:HG21	2.02	0.41
1:C:52:GLN:O	1:C:56:ARG:HG3	2.21	0.41
1:B:237:ILE:HD11	1:B:263:LYS:HA	2.02	0.41
1:C:42:TYR:CD1	1:C:105:VAL:HG11	2.55	0.41
1:C:69:ILE:HG13	1:C:115:ILE:HG21	2.03	0.41
1:B:71:ARG:HD2	1:B:198:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PHE:CD2	1:C:95:ALA:HB2	2.57	0.40
1:C:82:VAL:O	1:C:86:VAL:HG23	2.22	0.40
1:C:459:LEU:HD13	1:C:472:ILE:HG21	2.03	0.40
1:D:408:MET:HG3	1:D:451:ASN:HD22	1.86	0.40
1:A:284:PRO:HG2	1:C:59:VAL:HG21	2.03	0.40
1:A:465:ALA:HB1	1:A:469:MET:HG3	2.04	0.40
1:D:565:ILE:O	1:D:569:LEU:HG	2.21	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	599/609 (98%)	592 (99%)	7 (1%)	0	100	100
1	B	599/609 (98%)	594 (99%)	5 (1%)	0	100	100
1	C	591/609 (97%)	584 (99%)	7 (1%)	0	100	100
1	D	596/609 (98%)	591 (99%)	5 (1%)	0	100	100
All	All	2385/2436 (98%)	2361 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	479/498 (96%)	476 (99%)	3 (1%)	78	87
1	B	486/498 (98%)	483 (99%)	3 (1%)	78	87
1	C	479/498 (96%)	478 (100%)	1 (0%)	87	94
1	D	486/498 (98%)	483 (99%)	3 (1%)	78	87
All	All	1930/1992 (97%)	1920 (100%)	10 (0%)	81	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	146	PHE
1	A	182	ASP
1	B	108	GLN
1	B	146	PHE
1	B	182	ASP
1	C	146	PHE
1	D	66	LEU
1	D	146	PHE
1	D	594	VAL

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	415	ASN
1	B	415	ASN
1	B	456	GLN
1	B	471	GLN
1	C	415	ASN
1	C	538	GLN
1	C	596	GLN
1	D	108	GLN
1	D	456	GLN
1	D	492	ASN
1	D	538	GLN
1	D	593	GLN

5.3.3 RNA ⓘ

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, 4 are monoatomic - leaving 5 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	SO4	B	703	-	4,4,4	0.22	0	6,6,6	0.12	0
3	ATP	C	702	2	32,33,33	1.42	4 (12%)	48,52,52	1.19	5 (10%)
3	ATP	D	702	2	32,33,33	1.40	3 (9%)	48,52,52	1.22	5 (10%)
3	ATP	A	702	2	32,33,33	1.48	4 (12%)	48,52,52	1.21	7 (14%)
3	ATP	B	702	2	32,33,33	1.55	4 (12%)	48,52,52	1.23	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	702	2	-	0/22/38/38	0/3/3/3
3	ATP	D	702	2	-	0/22/38/38	0/3/3/3
3	ATP	B	702	2	-	0/22/38/38	0/3/3/3
3	ATP	C	702	2	-	0/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ATP	PB-O3A	-4.33	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ATP	PB-O3A	-4.09	1.55	1.59
3	D	702	ATP	PB-O3A	-4.00	1.55	1.59
3	B	702	ATP	PA-O3A	-3.93	1.55	1.59
3	B	702	ATP	PB-O3B	-3.67	1.55	1.59
3	C	702	ATP	PB-O3B	-3.63	1.55	1.59
3	C	702	ATP	PB-O3A	-3.60	1.55	1.59
3	A	702	ATP	PB-O3B	-3.51	1.55	1.59
3	D	702	ATP	PA-O3A	-3.47	1.55	1.59
3	A	702	ATP	PA-O3A	-3.40	1.55	1.59
3	C	702	ATP	PA-O3A	-3.08	1.56	1.59
3	D	702	ATP	PB-O3B	-2.76	1.56	1.59
3	C	702	ATP	PG-O2G	-2.07	1.47	1.54
3	B	702	ATP	PG-O2G	-2.03	1.47	1.54
3	A	702	ATP	PG-O2G	-2.01	1.47	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ATP	C4-C5-N7	3.22	114.26	110.58
3	D	702	ATP	C4-C5-N7	3.19	114.23	110.58
3	C	702	ATP	C4-C5-N7	3.05	114.07	110.58
3	B	702	ATP	C5-C4-N3	-2.91	122.71	126.72
3	B	702	ATP	C4-C5-N7	2.84	113.83	110.58
3	C	702	ATP	C5-C4-N3	-2.72	122.96	126.72
3	D	702	ATP	C5-C4-N3	-2.68	123.03	126.72
3	A	702	ATP	C5-C4-N3	-2.60	123.14	126.72
3	A	702	ATP	O2B-PB-O3A	2.47	113.95	107.27
3	C	702	ATP	O2B-PB-O3A	2.44	113.88	107.27
3	B	702	ATP	O2B-PB-O3A	2.43	113.84	107.27
3	B	702	ATP	N3-C4-N9	2.28	131.04	127.17
3	D	702	ATP	N3-C4-N9	2.24	130.98	127.17
3	A	702	ATP	N3-C4-N9	2.20	130.91	127.17
3	B	702	ATP	O3G-PG-O3B	2.19	111.99	104.64
3	C	702	ATP	N3-C4-N9	2.18	130.87	127.17
3	D	702	ATP	O2B-PB-O3A	2.14	113.05	107.27
3	B	702	ATP	N6-C6-N1	-2.08	113.74	118.38
3	A	702	ATP	O3G-PG-O3B	2.07	111.56	104.64
3	C	702	ATP	O2A-PA-O3A	2.05	112.81	107.27
3	A	702	ATP	C2-N1-C6	-2.04	115.39	118.73
3	D	702	ATP	C2-N1-C6	-2.03	115.40	118.73
3	A	702	ATP	O2A-PA-O3A	2.01	112.72	107.27

There are no chirality outliers.

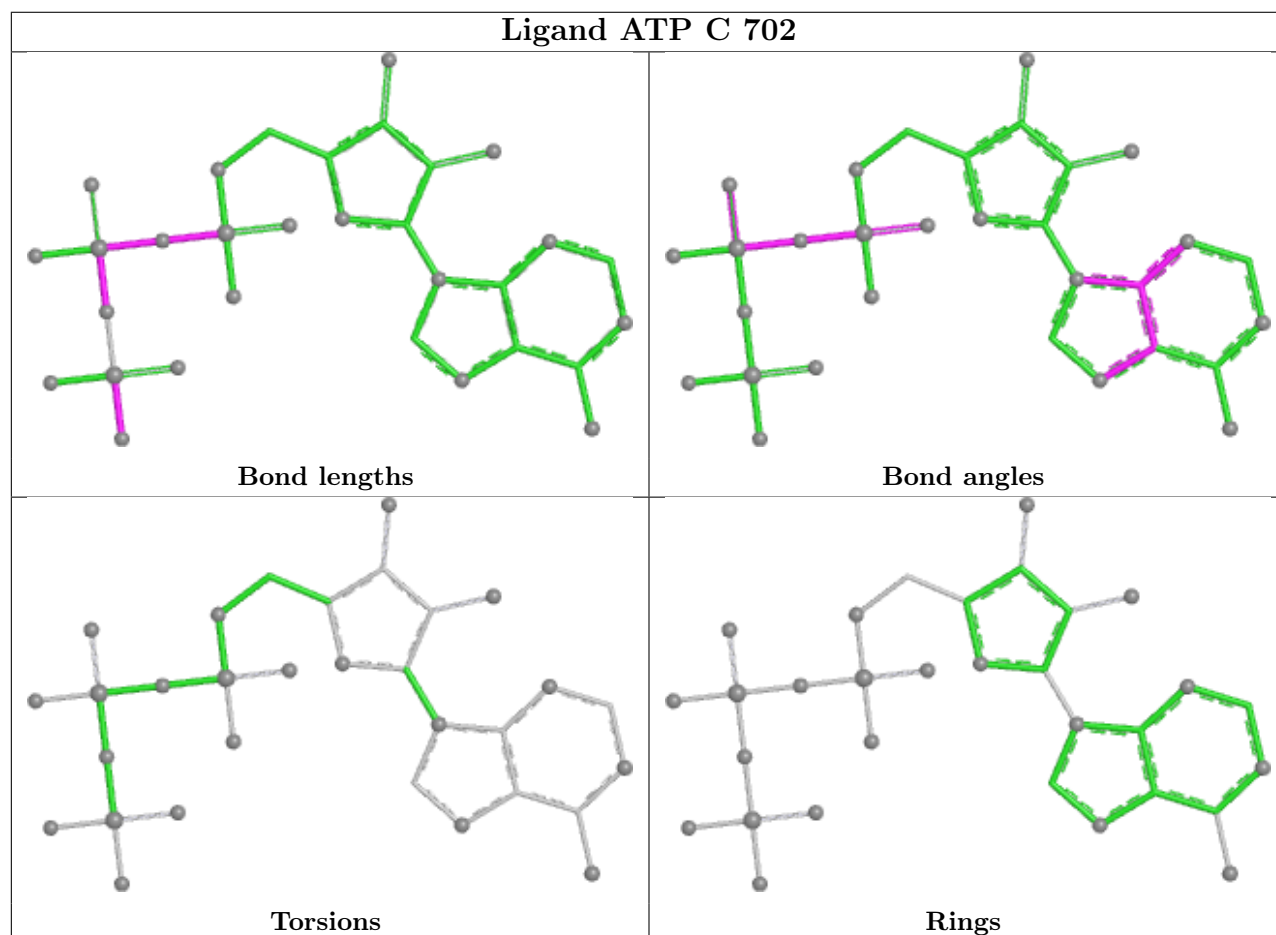
There are no torsion outliers.

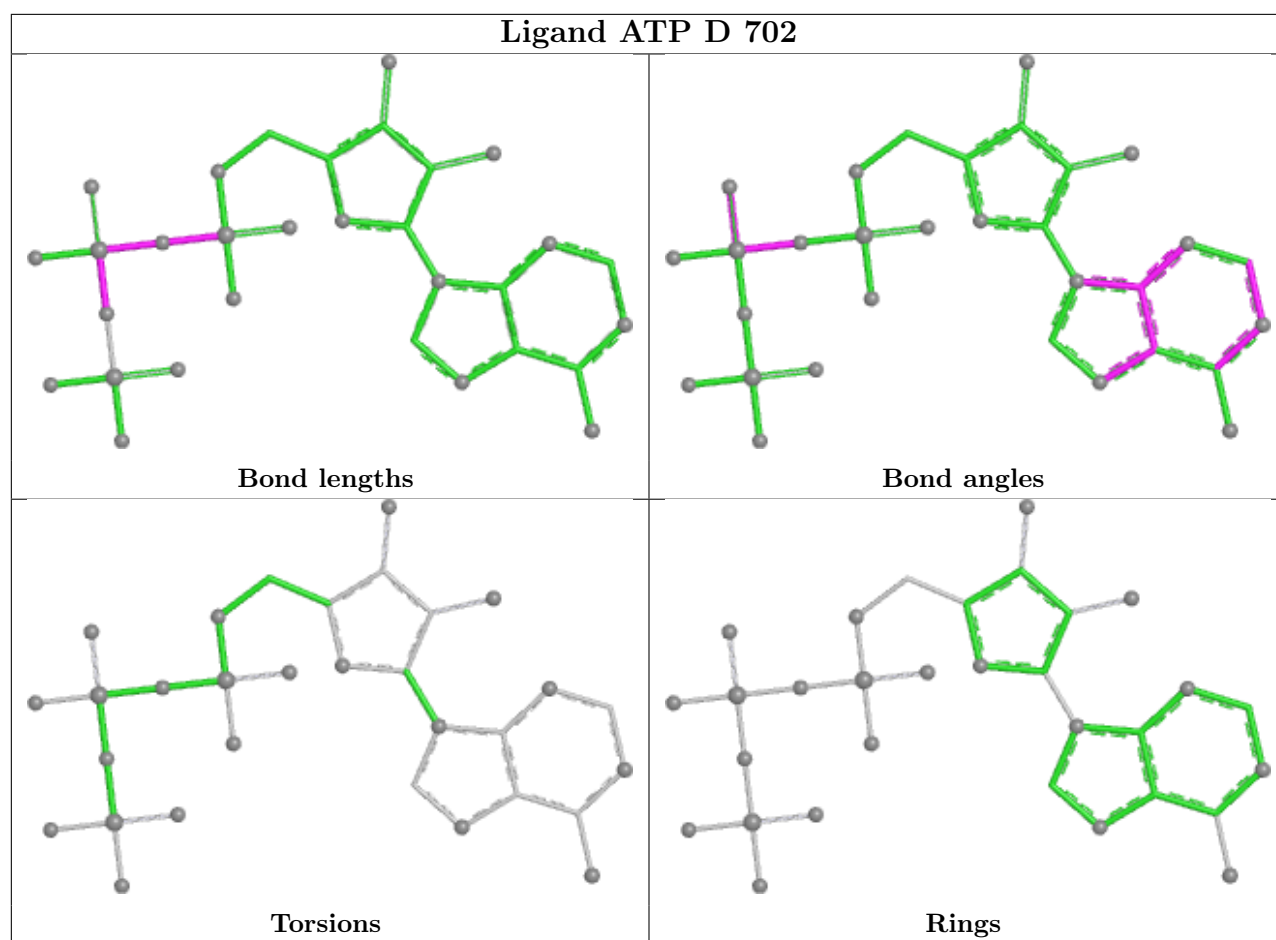
There are no ring outliers.

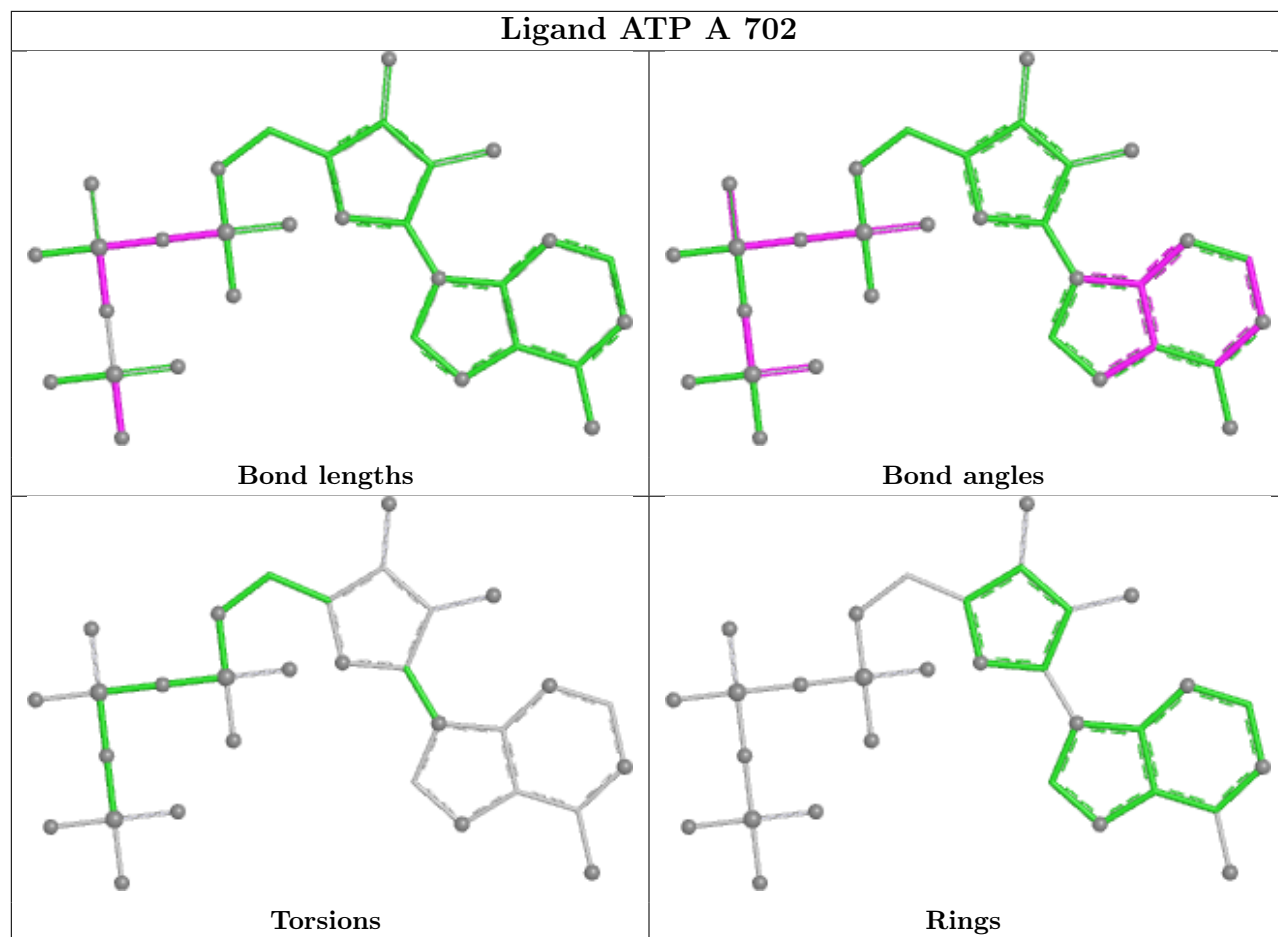
1 monomer is involved in 2 short contacts:

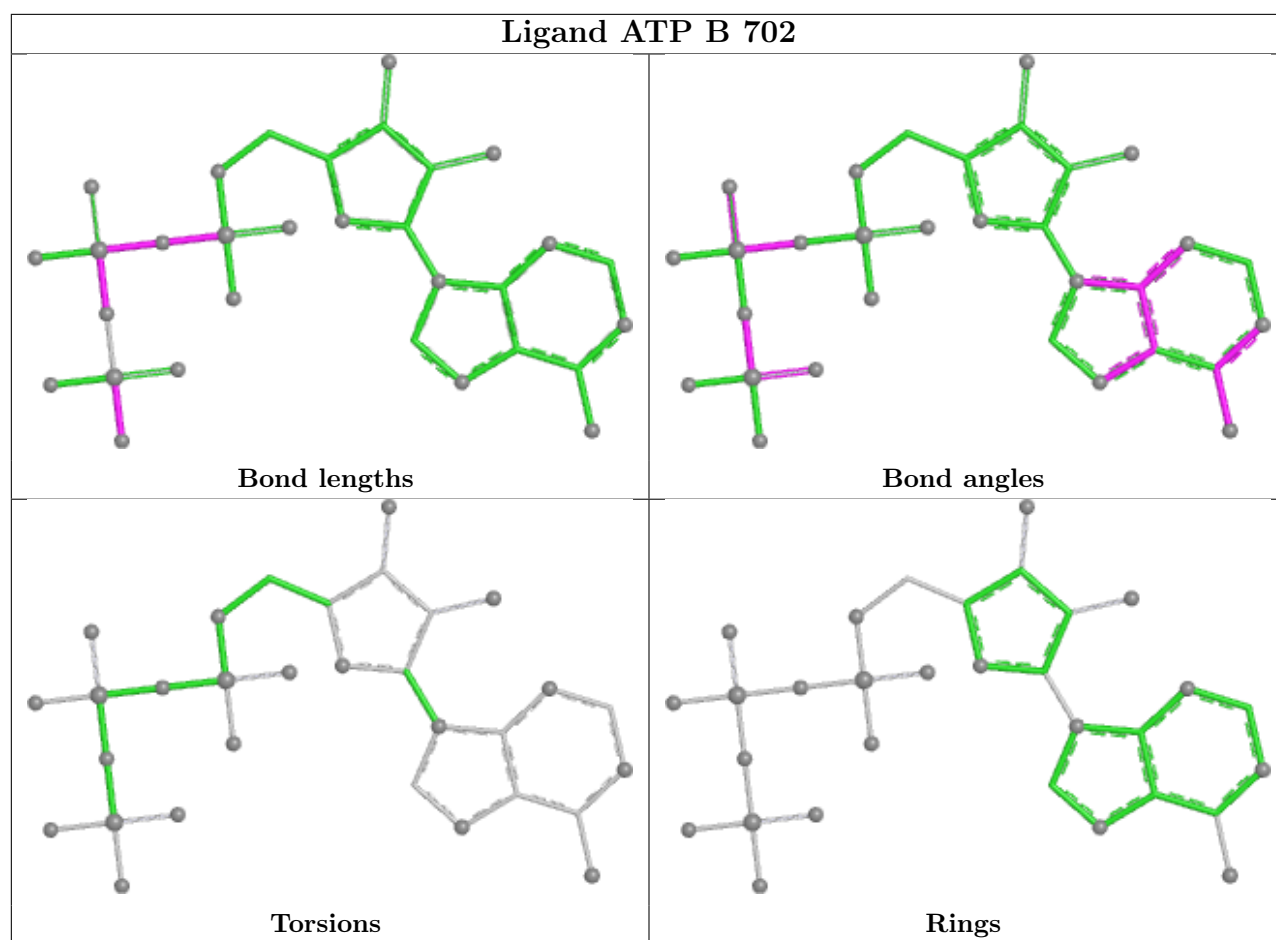
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	SO4	2	0

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	601/609 (98%)	0.74	60 (9%) 12 10	32, 65, 131, 159	0
1	B	603/609 (99%)	0.76	67 (11%) 10 8	32, 66, 129, 170	0
1	C	595/609 (97%)	1.01	101 (16%) 4 3	35, 74, 130, 163	0
1	D	600/609 (98%)	0.73	41 (6%) 23 19	38, 70, 115, 136	0
All	All	2399/2436 (98%)	0.81	269 (11%) 10 8	32, 69, 127, 170	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	SER	6.6
1	A	291	THR	6.5
1	C	285	TYR	6.3
1	A	250	ILE	5.7
1	C	296	MET	5.2
1	A	288	ALA	4.9
1	B	560	ASP	4.9
1	C	563	THR	4.8
1	C	258	ALA	4.8
1	C	295	HIS	4.8
1	C	286	ILE	4.7
1	B	568	ALA	4.7
1	C	283	LEU	4.6
1	C	284	PRO	4.5
1	B	563	THR	4.5
1	C	261	ARG	4.4
1	A	456	GLN	4.3
1	A	252	LEU	4.3
1	B	565	ILE	4.3
1	D	285	TYR	4.3
1	B	569	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	59	VAL	4.2
1	B	572	LEU	4.1
1	B	286	ILE	4.1
1	A	247	ASP	4.0
1	A	286	ILE	4.0
1	D	250	ILE	4.0
1	A	181	LEU	4.0
1	A	186	GLY	3.9
1	C	257	LEU	3.9
1	A	185	THR	3.9
1	C	288	ALA	3.9
1	C	565	ILE	3.9
1	B	564	ALA	3.8
1	C	59	VAL	3.8
1	A	293	PRO	3.8
1	B	288	ALA	3.8
1	C	389	VAL	3.7
1	B	591	LEU	3.7
1	B	593	GLN	3.7
1	A	287	THR	3.7
1	A	258	ALA	3.7
1	A	461	GLY	3.7
1	B	559	ALA	3.6
1	C	287	THR	3.6
1	C	569	LEU	3.6
1	C	293	PRO	3.5
1	D	2	GLY	3.5
1	A	23	THR	3.4
1	B	185	THR	3.4
1	C	58	ALA	3.4
1	C	30	ALA	3.3
1	B	389	VAL	3.3
1	D	215	THR	3.3
1	A	210	VAL	3.3
1	D	295	HIS	3.3
1	C	282	ASN	3.3
1	C	390	LEU	3.3
1	B	285	TYR	3.3
1	C	2	GLY	3.2
1	C	180	GLY	3.2
1	C	466	PRO	3.2
1	C	574	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	260	GLN	3.2
1	A	241	VAL	3.2
1	C	465	ALA	3.1
1	C	244	PHE	3.1
1	C	256	PRO	3.1
1	A	292	GLY	3.1
1	A	249	GLY	3.1
1	C	298	ILE	3.1
1	A	285	TYR	3.0
1	C	599	MET	3.0
1	B	594	VAL	3.0
1	B	605	GLN	3.0
1	B	553	ALA	3.0
1	C	594	VAL	3.0
1	A	390	LEU	2.9
1	B	59	VAL	2.9
1	D	426	PHE	2.9
1	D	320	LEU	2.9
1	C	22	THR	2.9
1	B	503	ALA	2.9
1	C	564	ALA	2.9
1	C	568	ALA	2.9
1	B	466	PRO	2.9
1	A	437	THR	2.9
1	A	290	ALA	2.9
1	A	212	GLY	2.8
1	D	252	LEU	2.8
1	C	467	ARG	2.8
1	A	22	THR	2.8
1	A	503	ALA	2.8
1	C	259	MET	2.8
1	D	246	LYS	2.8
1	A	405	GLY	2.8
1	C	598	LEU	2.8
1	A	436	VAL	2.8
1	B	550	VAL	2.8
1	C	571	ALA	2.8
1	C	250	ILE	2.8
1	A	463	ASN	2.8
1	D	181	LEU	2.8
1	A	244	PHE	2.8
1	B	600	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	281	VAL	2.8
1	D	208	ASP	2.7
1	A	294	LYS	2.7
1	B	562	LYS	2.7
1	C	106	LYS	2.7
1	B	186	GLY	2.7
1	B	567	SER	2.7
1	A	60	THR	2.7
1	B	429	ALA	2.7
1	C	550	VAL	2.7
1	C	570	THR	2.7
1	D	365	VAL	2.7
1	B	557	LEU	2.7
1	B	212	GLY	2.7
1	A	429	ALA	2.7
1	C	429	ALA	2.7
1	C	582	ALA	2.7
1	D	59	VAL	2.7
1	D	3	LYS	2.7
1	B	248	GLN	2.7
1	C	294	LYS	2.7
1	C	495	LYS	2.7
1	A	62	PRO	2.7
1	C	388	ASP	2.7
1	B	291	THR	2.6
1	D	431	ASP	2.6
1	D	293	PRO	2.6
1	B	598	LEU	2.6
1	C	252	LEU	2.6
1	C	576	LEU	2.6
1	A	261	ARG	2.6
1	A	425	VAL	2.6
1	B	571	ALA	2.6
1	C	567	SER	2.6
1	C	593	GLN	2.6
1	D	291	THR	2.6
1	D	137	GLU	2.6
1	B	558	PRO	2.6
1	C	130	TYR	2.5
1	B	249	GLY	2.5
1	C	19	MET	2.5
1	D	363	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	287	THR	2.5
1	C	297	ASN	2.5
1	B	2	GLY	2.5
1	B	465	ALA	2.5
1	D	22	THR	2.5
1	B	576	LEU	2.5
1	C	255	ASP	2.5
1	B	575	ALA	2.5
1	D	290	ALA	2.5
1	C	214	LYS	2.4
1	A	184	GLY	2.4
1	A	328	GLY	2.4
1	B	256	PRO	2.4
1	C	291	THR	2.4
1	D	25	ARG	2.4
1	A	334	ILE	2.4
1	C	557	LEU	2.4
1	B	183	LYS	2.4
1	C	3	LYS	2.4
1	D	429	ALA	2.4
1	D	19	MET	2.4
1	A	464	PRO	2.4
1	A	472	ILE	2.3
1	A	501	ILE	2.3
1	A	408	MET	2.3
1	C	211	ASP	2.3
1	C	580	ASP	2.3
1	C	262	LEU	2.3
1	C	431	ASP	2.3
1	C	44	GLN	2.3
1	C	46	GLY	2.3
1	B	60	THR	2.3
1	C	254	ASN	2.3
1	A	182	ASP	2.3
1	B	561	ASP	2.3
1	D	289	ASP	2.3
1	B	596	GLN	2.3
1	B	474	VAL	2.3
1	B	244	PHE	2.3
1	C	592	ALA	2.3
1	B	577	LYS	2.3
1	A	289	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	526	ASP	2.3
1	C	447	ARG	2.3
1	D	391	LEU	2.3
1	B	435	ALA	2.2
1	C	556	LYS	2.2
1	C	209	GLU	2.2
1	C	434	SER	2.2
1	D	248	GLN	2.2
1	D	389	VAL	2.2
1	B	18	ILE	2.2
1	B	592	ALA	2.2
1	C	265	ALA	2.2
1	D	359	LYS	2.2
1	D	404	MET	2.2
1	D	256	PRO	2.2
1	A	180	GLY	2.2
1	C	6	GLY	2.2
1	C	364	ASP	2.2
1	D	212	GLY	2.2
1	C	179	TYR	2.2
1	C	432	ASN	2.2
1	A	459	LEU	2.2
1	B	587	LYS	2.2
1	C	27	LEU	2.2
1	C	131	LEU	2.2
1	C	132	GLY	2.2
1	A	207	ILE	2.2
1	C	18	ILE	2.2
1	A	435	ALA	2.2
1	B	283	LEU	2.2
1	D	131	LEU	2.2
1	A	499	ILE	2.2
1	B	472	ILE	2.2
1	A	500	THR	2.1
1	A	183	LYS	2.1
1	C	241	VAL	2.1
1	C	490	ASP	2.1
1	D	322	VAL	2.1
1	B	582	ALA	2.1
1	B	586	ALA	2.1
1	C	430	GLU	2.1
1	A	239	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	543	LEU	2.1
1	B	175	ALA	2.1
1	B	290	ALA	2.1
1	C	188	ARG	2.1
1	A	189	THR	2.1
1	D	23	THR	2.1
1	C	177	LEU	2.1
1	B	250	ILE	2.1
1	B	182	ASP	2.1
1	B	477	ASP	2.1
1	D	260	GLN	2.1
1	A	283	LEU	2.1
1	C	392	LEU	2.1
1	C	572	LEU	2.1
1	C	239	TYR	2.1
1	D	18	ILE	2.1
1	A	251	ASP	2.0
1	B	430	GLU	2.0
1	C	586	ALA	2.0
1	D	265	ALA	2.0
1	C	215	THR	2.0
1	B	542	LEU	2.0
1	B	584	ILE	2.0
1	C	601	ILE	2.0
1	D	213	GLU	2.0
1	C	175	ALA	2.0
1	D	388	ASP	2.0
1	B	599	MET	2.0
1	C	62	PRO	2.0
1	A	44	GLN	2.0
1	A	248	GLN	2.0
1	C	4	ILE	2.0
1	C	462	ILE	2.0
1	C	472	ILE	2.0
1	C	492	ASN	2.0
1	C	494	GLY	2.0
1	D	462	ILE	2.0
1	C	210	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](#)

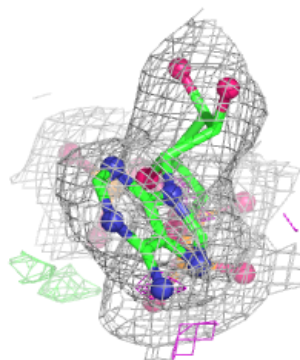
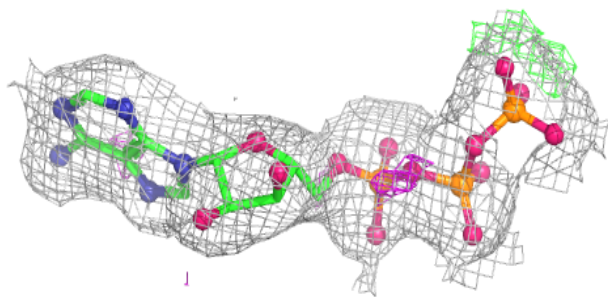
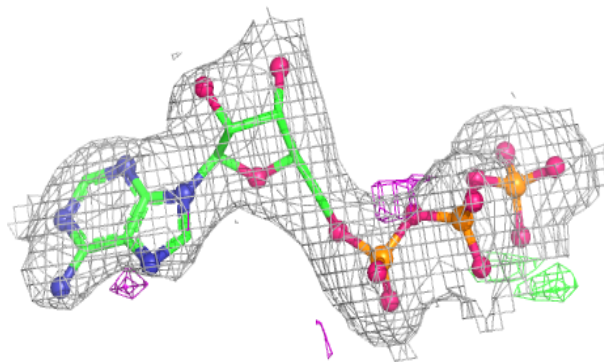
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	703	5/5	0.86	0.18	76,84,112,114	0
3	ATP	A	702	31/31	0.95	0.09	30,49,65,70	0
2	MG	A	701	1/1	0.95	0.07	56,56,56,56	0
3	ATP	C	702	31/31	0.96	0.09	34,48,64,69	0
3	ATP	D	702	31/31	0.96	0.08	26,53,68,76	0
3	ATP	B	702	31/31	0.96	0.08	27,42,54,74	0
2	MG	B	701	1/1	0.98	0.05	35,35,35,35	0
2	MG	D	701	1/1	0.99	0.04	65,65,65,65	0
2	MG	C	701	1/1	0.99	0.04	47,47,47,47	0

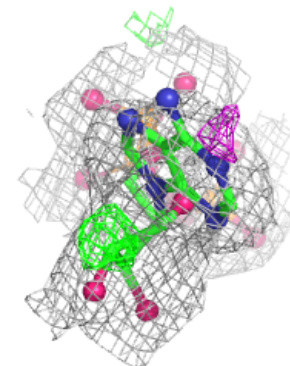
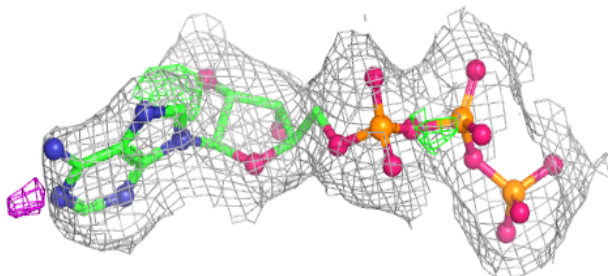
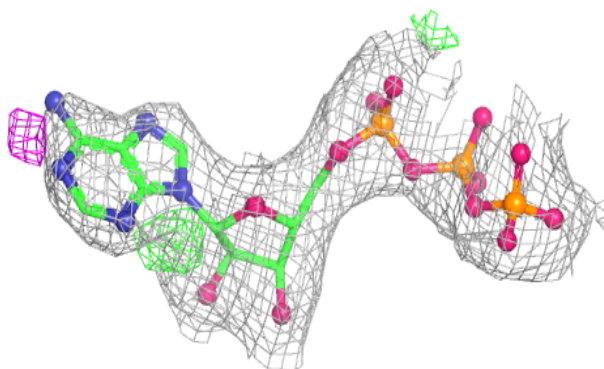
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 702:

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

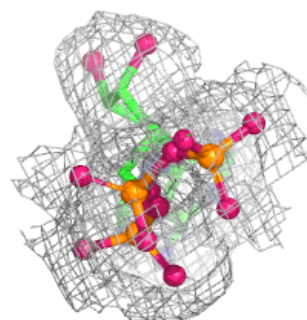
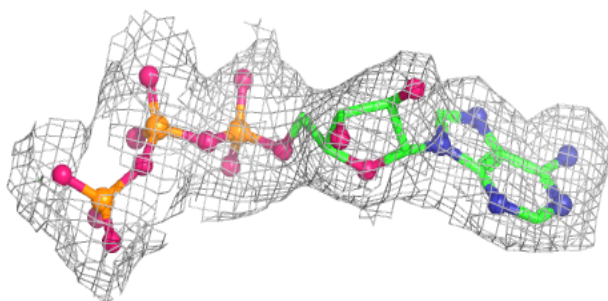
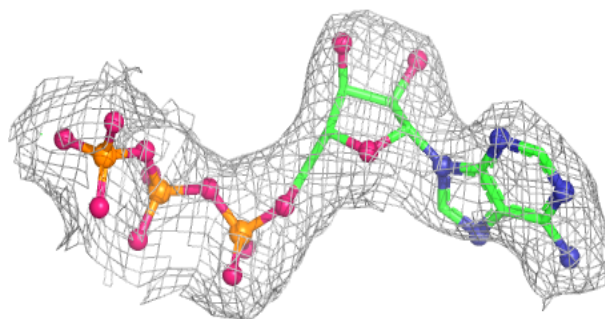
**Electron density around ATP C 702:**

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

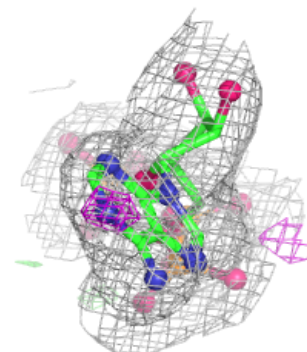
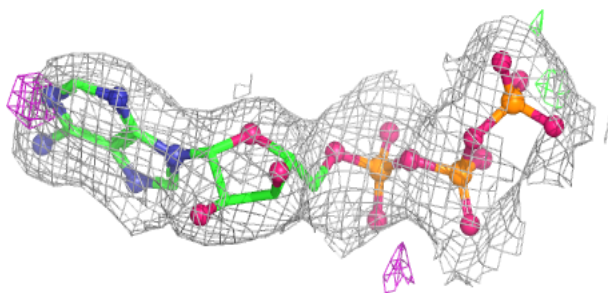
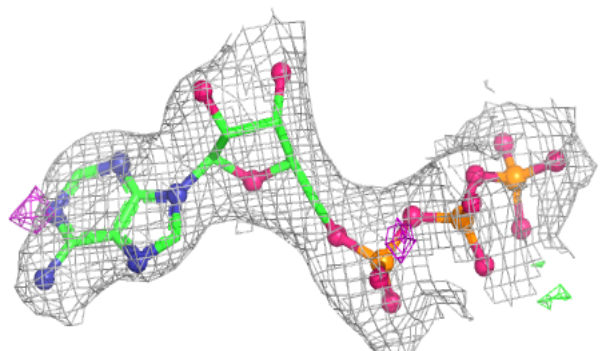


Electron density around ATP D 702:

$2mF_o-DF_c$ (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.