



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:45 AM UTC

PDB ID : 7KRT / pdb_00007krt
Title : Restraining state of a truncated Hsp70 DnaK
Authors : Wang, W.; Hendrickson, W.A.
Deposited on : 2020-11-20
Resolution : 2.79 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

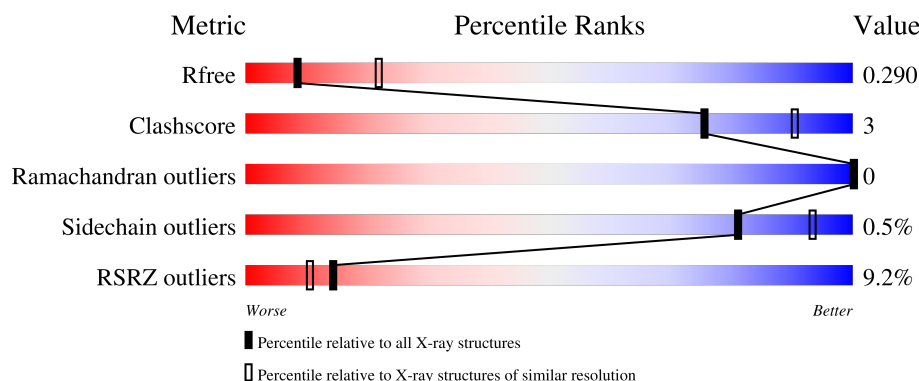
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	600	7% 92% 8%
1	B	600	13% 93% 7%
1	C	600	8% 93% 7%
1	D	600	9% 90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17919 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	599	Total	C	N	O	S	0	0	0
			4457	2764	780	896	17			
1	B	599	Total	C	N	O	S	0	0	0
			4386	2723	769	879	15			
1	C	599	Total	C	N	O	S	0	0	0
			4483	2782	785	900	16			
1	D	599	Total	C	N	O	S	0	0	0
			4426	2743	772	894	17			

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) (labeled as "Ligand of Interest" by depositor).

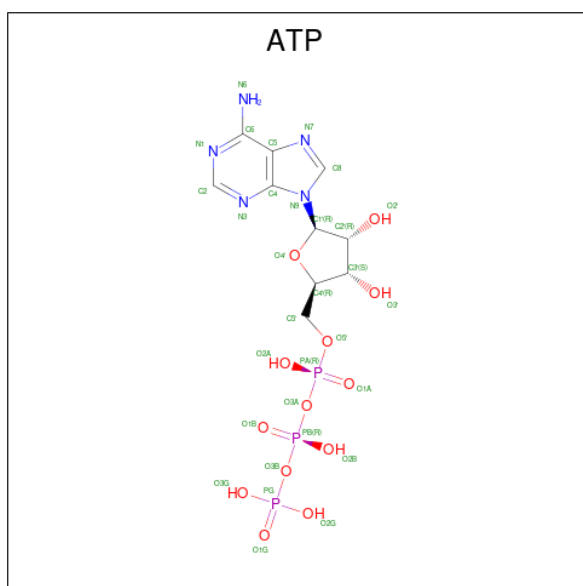
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	9	Total	O	0	0
			9	9		

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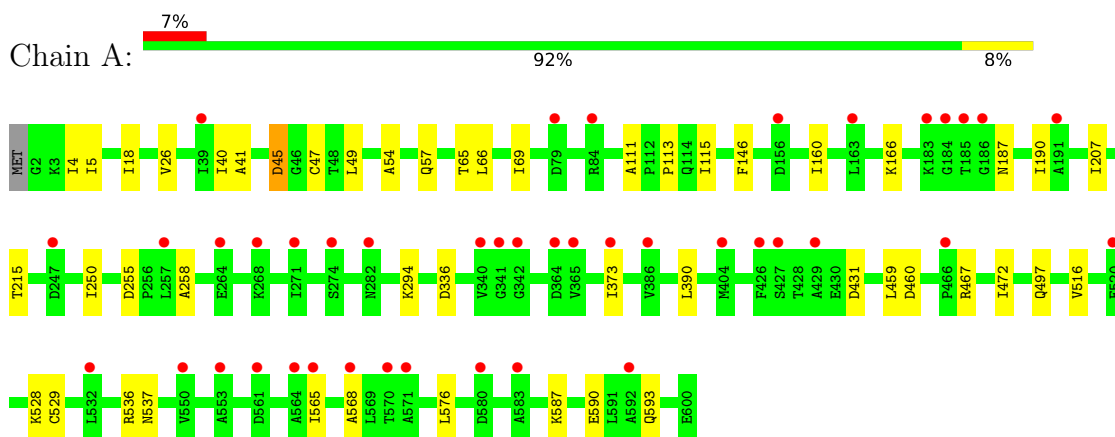
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	10	Total	O	0	0
			10	10		
4	D	8	Total	O	0	0
			8	8		

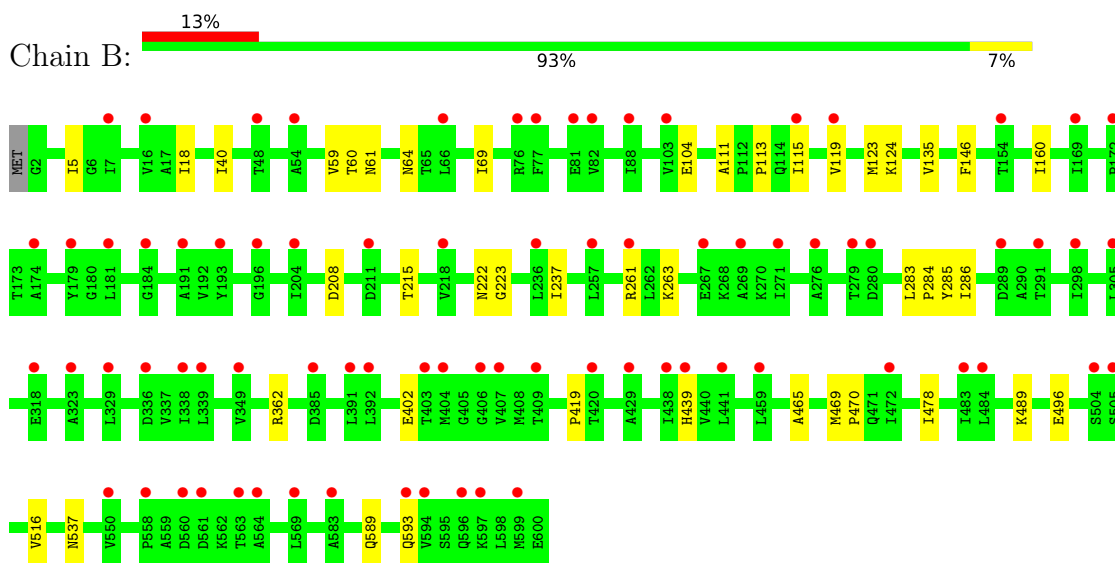
3 Residue-property plots [i](#)

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.

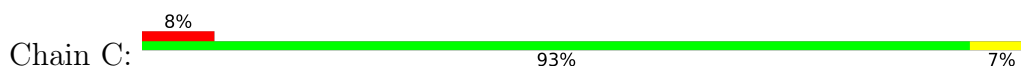
• Molecule 1: Chaperone protein DnaK

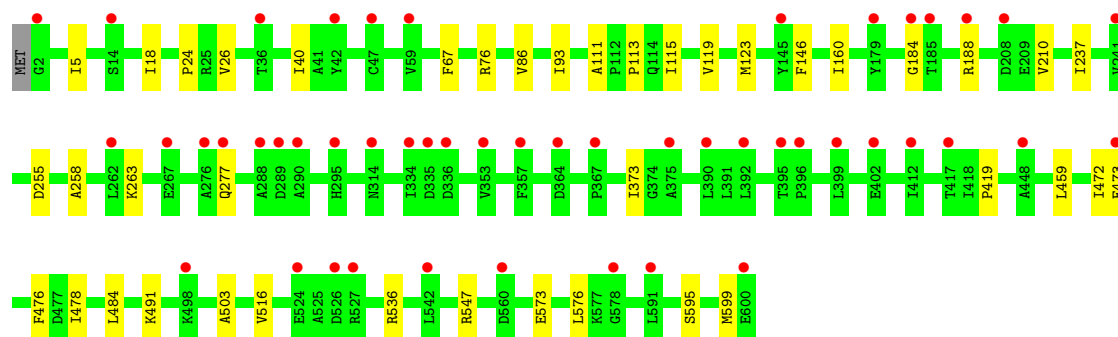


• Molecule 1: Chaperone protein DnaK

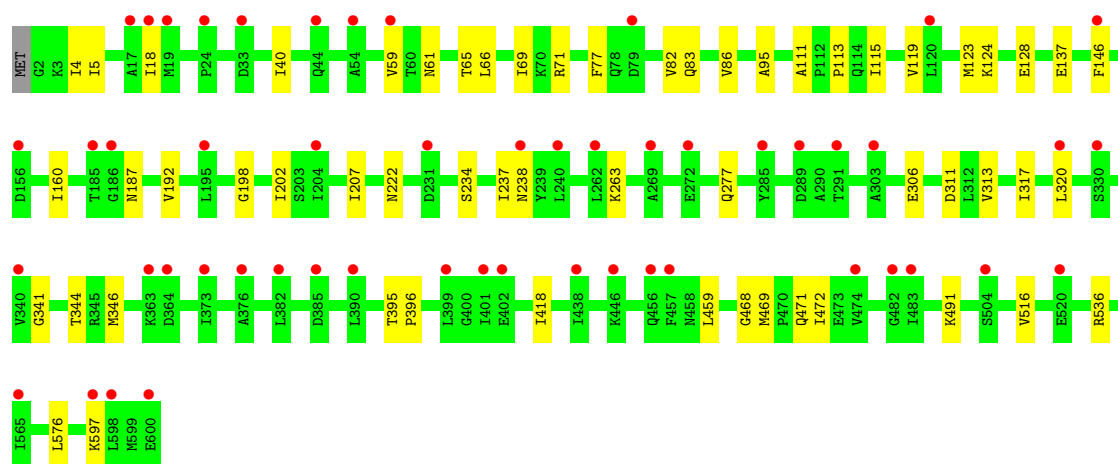
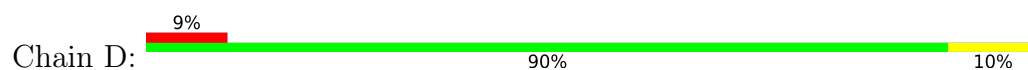


• Molecule 1: Chaperone protein DnaK





● Molecule 1: Chaperone protein DnaK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.47Å 199.53Å 94.23Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	47.02 – 2.79 47.02 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.02-2.79) 90.6 (47.02-2.79)	Depositor EDS
R_{merge}	0.71	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.279 , 0.308 0.285 , 0.290	Depositor DCC
R_{free} test set	3539 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17919	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.20	0/4508	0.39	0/6102
1	B	0.11	0/4435	0.31	0/6014
1	C	0.11	0/4534	0.32	0/6137
1	D	0.18	1/4476 (0.0%)	0.30	0/6067
All	All	0.16	1/17953 (0.0%)	0.33	0/24320

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	396	PRO	N-CD	9.35	1.60	1.47

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	4457	0	4418	27	0
1	B	4386	0	4302	25	0
1	C	4483	0	4482	24	0
1	D	4426	0	4364	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	12	0	0	0	0
4	B	9	0	0	0	0
4	C	10	0	0	0	0
4	D	8	0	0	0	0
All	All	17919	0	17614	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (106) 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:190:ILE:HG22	1:A:336:ASP:HB2	1.74	0.69
1:B:160:ILE:HA	1:B:516:VAL:HG22	1.79	0.65
1:A:565:ILE:HA	1:A:568:ALA:HB3	1.78	0.64
1:B:208:ASP:OD1	1:B:215:THR:OG1	2.15	0.64
1:A:5:ILE:HG22	1:A:18:ILE:HG22	1.78	0.64
1:D:160:ILE:HA	1:D:516:VAL:HG22	1.78	0.64
1:C:210:VAL:O	1:C:210:VAL:HG23	2.00	0.62
1:D:536:ARG:NH1	1:D:576:LEU:O	2.33	0.62
1:B:362:ARG:HH12	1:C:188:ARG:HH22	1.51	0.58
1:A:537:ASN:HD21	1:C:277:GLN:HB3	1.68	0.58
1:A:160:ILE:HA	1:A:516:VAL:HG22	1.85	0.58
1:C:40:ILE:HD13	1:C:115:ILE:HG22	1.86	0.57
1:D:124:LYS:NZ	1:D:128:GLU:OE2	2.38	0.57
1:A:250:ILE:HD12	1:A:294:LYS:HD2	1.87	0.56
1:A:45:ASP:OD1	1:A:45:ASP:N	2.35	0.56
1:C:547:ARG:NH2	1:C:573:GLU:OE2	2.35	0.56
1:C:160:ILE:HA	1:C:516:VAL:HG22	1.88	0.55
1:D:40:ILE:HD13	1:D:115:ILE:HG22	1.89	0.55
1:D:237:ILE:HD11	1:D:263:LYS:HA	1.89	0.54
1:B:284:PRO:HG3	1:D:59:VAL:HG11	1.90	0.54
1:A:40:ILE:HD12	1:A:40:ILE:N	2.23	0.54
1:D:459:LEU:HD13	1:D:472:ILE:HG21	1.90	0.53
1:C:24:PRO:HB2	1:C:373:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ALA:HB1	1:C:113:PRO:HD2	1.91	0.53
1:B:283:LEU:HD13	1:B:286:ILE:HD13	1.90	0.52
1:D:471:GLN:HB3	1:D:491:LYS:HE2	1.91	0.52
1:C:5:ILE:HG22	1:C:18:ILE:HG22	1.92	0.51
1:B:537:ASN:ND2	1:D:277:GLN:OE1	2.44	0.51
1:B:465:ALA:HB1	1:B:469:MET:HE2	1.93	0.51
1:D:469:MET:O	1:D:471:GLN:NE2	2.42	0.51
1:A:111:ALA:HB1	1:A:113:PRO:HD2	1.93	0.50
1:D:306:GLU:HG2	1:D:346:MET:HE2	1.93	0.50
1:A:41:ALA:HB3	1:A:49:LEU:HB2	1.94	0.50
1:A:54:ALA:O	1:A:57:GLN:HG3	2.11	0.50
1:B:419:PRO:HA	1:B:478:ILE:O	2.12	0.50
1:B:111:ALA:HB1	1:B:113:PRO:HD2	1.94	0.50
1:D:311:ASP:N	1:D:311:ASP:OD1	2.40	0.50
1:C:76:ARG:NH2	1:C:503:ALA:O	2.44	0.50
1:A:66:LEU:HB3	1:A:69:ILE:HD11	1.95	0.49
1:C:237:ILE:HD11	1:C:263:LYS:HA	1.95	0.49
1:A:536:ARG:NH1	1:A:576:LEU:O	2.46	0.48
1:B:5:ILE:HG22	1:B:18:ILE:HG22	1.94	0.48
1:D:202:ILE:HD13	1:D:320:LEU:CD2	2.43	0.48
1:B:61:ASN:HD21	1:B:64:ASN:HB2	1.79	0.48
1:C:473:GLU:HB2	1:C:491:LYS:HG3	1.95	0.48
1:D:77:PHE:O	1:D:83:GLN:NE2	2.46	0.48
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.73	0.47
1:C:255:ASP:HB3	1:C:258:ALA:HB3	1.96	0.47
1:A:57:GLN:NE2	1:A:65:THR:OG1	2.37	0.47
1:B:61:ASN:ND2	1:B:64:ASN:HB2	2.29	0.47
1:B:222:ASN:OD1	1:B:223:GLY:N	2.46	0.47
1:C:86:VAL:HG22	1:C:93:ILE:HB	1.95	0.47
1:B:362:ARG:NH1	1:C:188:ARG:HH22	2.13	0.47
1:A:40:ILE:HD13	1:A:115:ILE:HG22	1.98	0.46
1:D:4:ILE:HG12	1:D:137:GLU:HB3	1.98	0.46
1:D:313:VAL:O	1:D:317:ILE:HG12	2.16	0.46
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.96	0.46
1:C:459:LEU:HD13	1:C:472:ILE:HG21	1.97	0.45
1:D:61:ASN:O	1:D:65:THR:OG1	2.28	0.45
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.98	0.45
1:D:71:ARG:HD3	1:D:198:GLY:HA3	1.98	0.45
1:D:187:ASN:HA	1:D:207:ILE:O	2.16	0.45
1:D:192:VAL:O	1:D:202:ILE:HD12	2.16	0.45
1:D:5:ILE:HG22	1:D:18:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASN:HA	1:A:207:ILE:O	2.16	0.45
1:A:460:ASP:O	1:A:497:GLN:NE2	2.51	0.44
1:C:419:PRO:HA	1:C:478:ILE:O	2.16	0.44
1:D:111:ALA:HB1	1:D:113:PRO:HD2	2.00	0.44
1:C:184:GLY:HA3	1:C:188:ARG:CZ	2.48	0.43
1:D:66:LEU:HB3	1:D:69:ILE:HD11	1.99	0.43
1:D:597:LYS:HE2	1:D:597:LYS:HB3	1.84	0.43
1:B:119:VAL:O	1:B:123:MET:HG2	2.19	0.43
1:C:26:VAL:HG23	1:C:373:ILE:HD11	1.99	0.43
1:C:476:PHE:HB3	1:C:484:LEU:HD11	2.00	0.43
1:A:587:LYS:O	1:A:590:GLU:HG3	2.18	0.43
1:C:119:VAL:O	1:C:123:MET:HG2	2.19	0.43
1:D:341:GLY:O	1:D:344:THR:OG1	2.29	0.43
1:D:202:ILE:CD1	1:D:320:LEU:HD22	2.48	0.43
1:A:190:ILE:HA	1:A:336:ASP:O	2.18	0.42
1:A:459:LEU:HD13	1:A:472:ILE:HG21	2.01	0.42
1:B:402:GLU:HB3	1:B:439:HIS:HB3	2.01	0.42
1:A:590:GLU:HA	1:A:593:GLN:HG2	2.01	0.42
1:D:234:SER:O	1:D:238:ASN:ND2	2.48	0.42
1:D:119:VAL:O	1:D:123:MET:HG2	2.20	0.42
1:A:4:ILE:HD13	1:A:166:LYS:HG3	2.02	0.42
1:C:536:ARG:NH1	1:C:576:LEU:O	2.52	0.42
1:B:59:VAL:HG13	1:B:60:THR:HG23	2.01	0.41
1:B:237:ILE:HD11	1:B:263:LYS:HA	2.02	0.41
1:D:202:ILE:HG12	1:D:320:LEU:HD23	2.02	0.41
1:A:431:ASP:H	1:A:467:ARG:HH21	1.68	0.41
1:B:124:LYS:HE2	1:B:135:VAL:O	2.21	0.41
1:A:255:ASP:HB3	1:A:258:ALA:HB3	2.02	0.41
1:B:469:MET:HB3	1:B:470:PRO:HD3	2.03	0.41
1:D:395:THR:HG23	1:D:418:ILE:CG2	2.51	0.41
1:D:468:GLY:O	1:D:471:GLN:NE2	2.48	0.41
1:D:77:PHE:CD2	1:D:95:ALA:HB2	2.56	0.41
1:A:215:THR:HG23	1:A:390:LEU:HD22	2.03	0.40
1:B:261:ARG:NH1	1:B:285:TYR:O	2.45	0.40
1:B:69:ILE:HD12	1:B:69:ILE:H	1.87	0.40
1:B:589:GLN:O	1:B:593:GLN:HG3	2.22	0.40
1:D:202:ILE:HD13	1:D:320:LEU:HD22	2.04	0.40
1:A:26:VAL:HG23	1:A:373:ILE:HD11	2.03	0.40
1:C:67:PHE:CE1	1:C:263:LYS:HE2	2.56	0.40
1:B:489:LYS:HG2	1:B:496:GLU:HA	2.04	0.40
1:C:595:SER:O	1:C:599:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:VAL:O	1:D:86:VAL:HG23	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	597/600 (100%)	591 (99%)	6 (1%)	0	100	100
1	B	597/600 (100%)	589 (99%)	8 (1%)	0	100	100
1	C	597/600 (100%)	593 (99%)	4 (1%)	0	100	100
1	D	597/600 (100%)	592 (99%)	5 (1%)	0	100	100
All	All	2388/2400 (100%)	2365 (99%)	23 (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	464/491 (94%)	460 (99%)	4 (1%)	70	89
1	B	446/491 (91%)	444 (100%)	2 (0%)	84	94
1	C	473/491 (96%)	472 (100%)	1 (0%)	87	96
1	D	459/491 (94%)	457 (100%)	2 (0%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1842/1964 (94%)	1833 (100%)	9 (0%)	81	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	47	CYS
1	A	146	PHE
1	A	529	CYS
1	B	104	GLU
1	B	146	PHE
1	C	146	PHE
1	D	146	PHE
1	D	222	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	52	GLN
1	A	187	ASN
1	A	432	ASN
1	A	534	GLN
1	A	537	ASN
1	A	549	GLN
1	B	52	GLN
1	B	61	ASN
1	B	64	ASN
1	B	83	GLN
1	B	458	ASN
1	B	589	GLN
1	C	44	GLN
1	C	52	GLN
1	C	63	GLN
1	C	248	GLN
1	C	260	GLN
1	C	378	GLN
1	C	415	ASN
1	C	534	GLN
1	C	541	HIS
1	D	147	ASN

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Mol	Chain	Res	Type
1	D	187	ASN
1	D	415	ASN
1	D	432	ASN
1	D	492	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	D	702	2	32,33,33	1.40	3 (9%)	48,52,52	1.22	5 (10%)
3	ATP	B	702	2	32,33,33	1.55	4 (12%)	48,52,52	1.23	6 (12%)
3	ATP	C	702	2	32,33,33	1.44	4 (12%)	48,52,52	1.19	5 (10%)
3	ATP	A	702	2	32,33,33	1.49	4 (12%)	48,52,52	1.21	7 (14%)

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	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
3	ATP	A	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	-4.26	1.54	1.59
3	A	702	ATP	PB-O3A	-4.18	1.55	1.59
3	B	702	ATP	PA-O3A	-4.02	1.55	1.59
3	D	702	ATP	PB-O3A	-4.02	1.55	1.59
3	B	702	ATP	PB-O3B	-3.73	1.55	1.59
3	C	702	ATP	PB-O3B	-3.69	1.55	1.59
3	C	702	ATP	PB-O3A	-3.65	1.55	1.59
3	A	702	ATP	PB-O3B	-3.57	1.55	1.59
3	D	702	ATP	PA-O3A	-3.51	1.55	1.59
3	A	702	ATP	PA-O3A	-3.44	1.55	1.59
3	C	702	ATP	PA-O3A	-3.14	1.56	1.59
3	D	702	ATP	PB-O3B	-2.77	1.56	1.59
3	C	702	ATP	PG-O2G	-2.09	1.47	1.54
3	A	702	ATP	PG-O2G	-2.02	1.47	1.54
3	B	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	3.16	114.20	110.58
3	D	702	ATP	C4-C5-N7	3.13	114.16	110.58
3	C	702	ATP	C4-C5-N7	3.12	114.15	110.58
3	B	702	ATP	C5-C4-N3	-2.95	122.65	126.72
3	B	702	ATP	C4-C5-N7	2.81	113.80	110.58
3	D	702	ATP	C5-C4-N3	-2.72	122.96	126.72
3	C	702	ATP	C5-C4-N3	-2.70	123.00	126.72
3	A	702	ATP	C5-C4-N3	-2.65	123.06	126.72
3	A	702	ATP	O2B-PB-O3A	2.48	113.96	107.27
3	C	702	ATP	O2B-PB-O3A	2.44	113.86	107.27
3	B	702	ATP	O2B-PB-O3A	2.40	113.77	107.27
3	B	702	ATP	N3-C4-N9	2.33	131.14	127.17
3	D	702	ATP	N3-C4-N9	2.28	131.04	127.17
3	C	702	ATP	N3-C4-N9	2.21	130.92	127.17
3	A	702	ATP	N3-C4-N9	2.20	130.91	127.17
3	B	702	ATP	O3G-PG-O3B	2.19	111.96	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	ATP	O2B-PB-O3A	2.14	113.05	107.27
3	B	702	ATP	N6-C6-N1	-2.09	113.72	118.38
3	D	702	ATP	C2-N1-C6	-2.06	115.34	118.73
3	A	702	ATP	O3G-PG-O3B	2.06	111.55	104.64
3	C	702	ATP	O2A-PA-O3A	2.05	112.80	107.27
3	A	702	ATP	O2A-PA-O3A	2.01	112.71	107.27
3	A	702	ATP	C2-N1-C6	-2.01	115.43	118.73

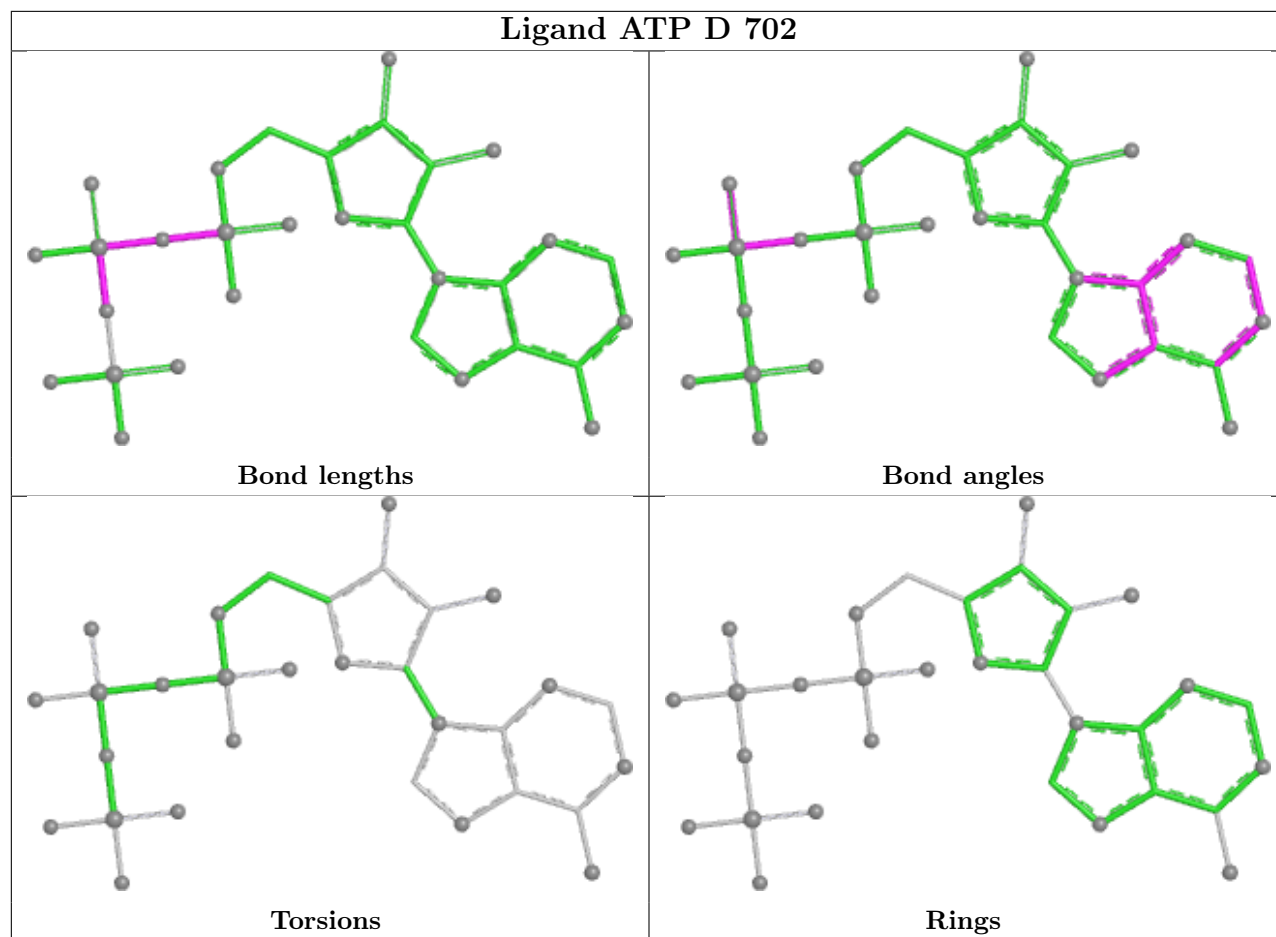
There are no chirality outliers.

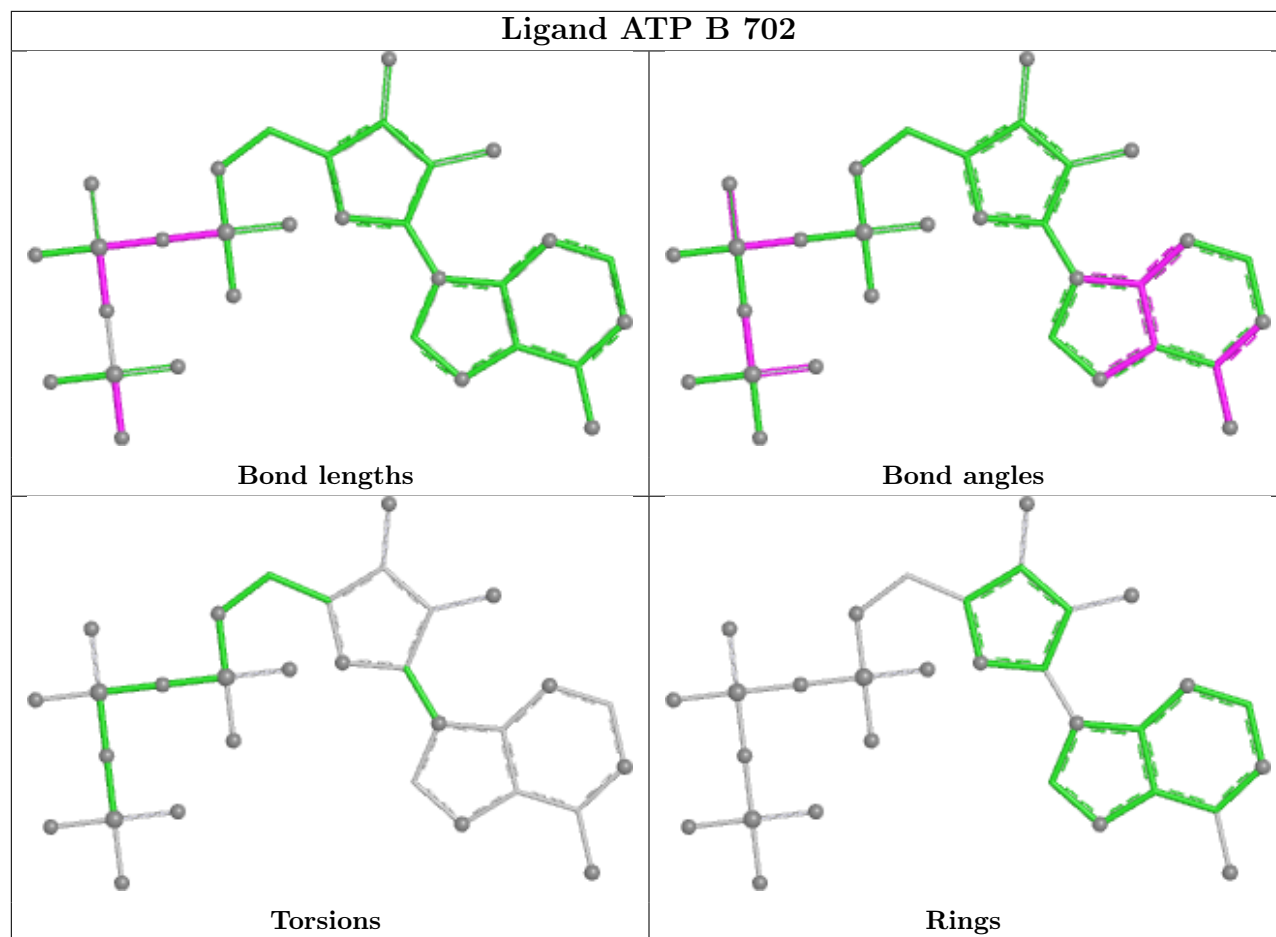
There are no torsion outliers.

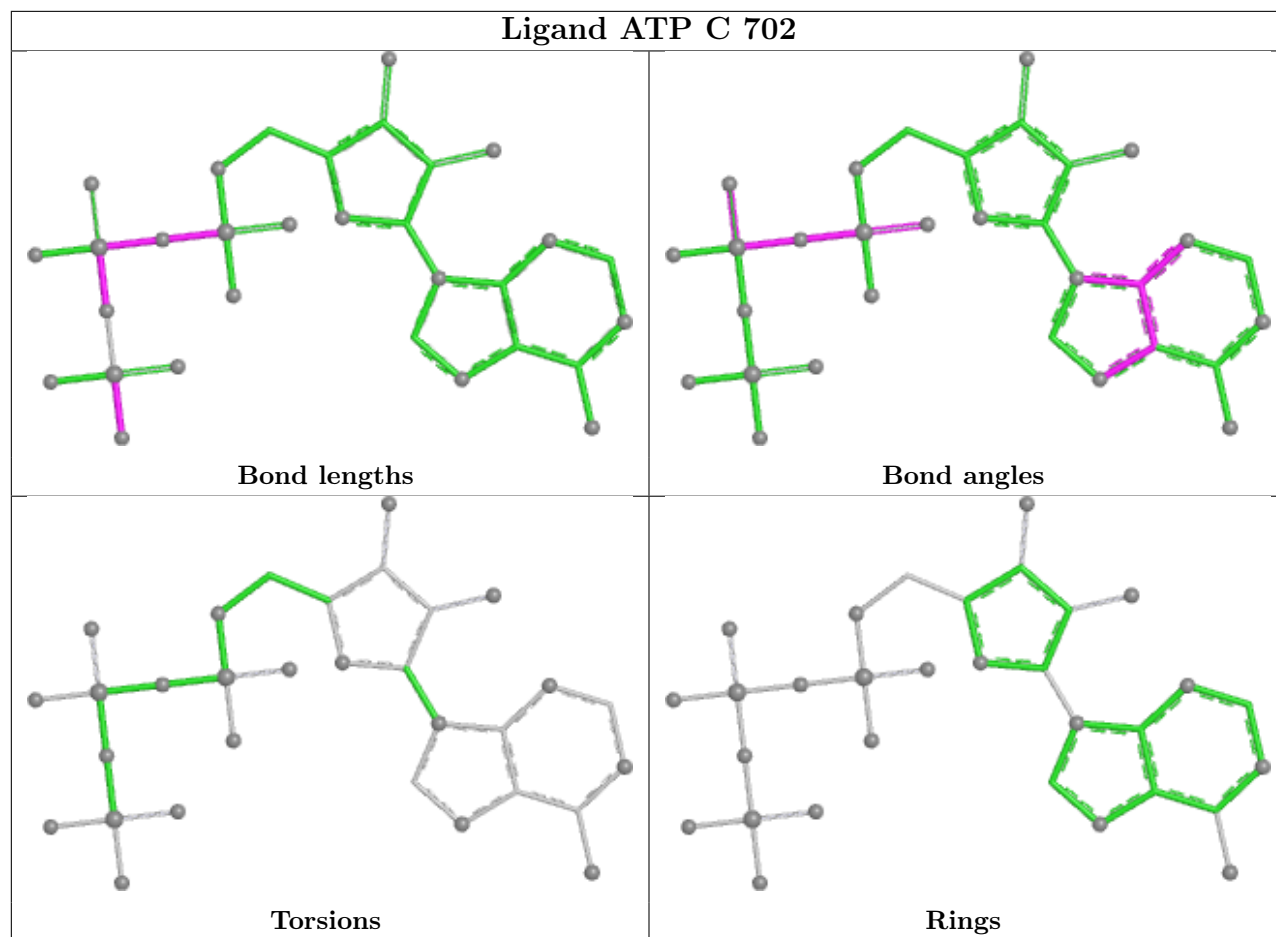
There are no ring outliers.

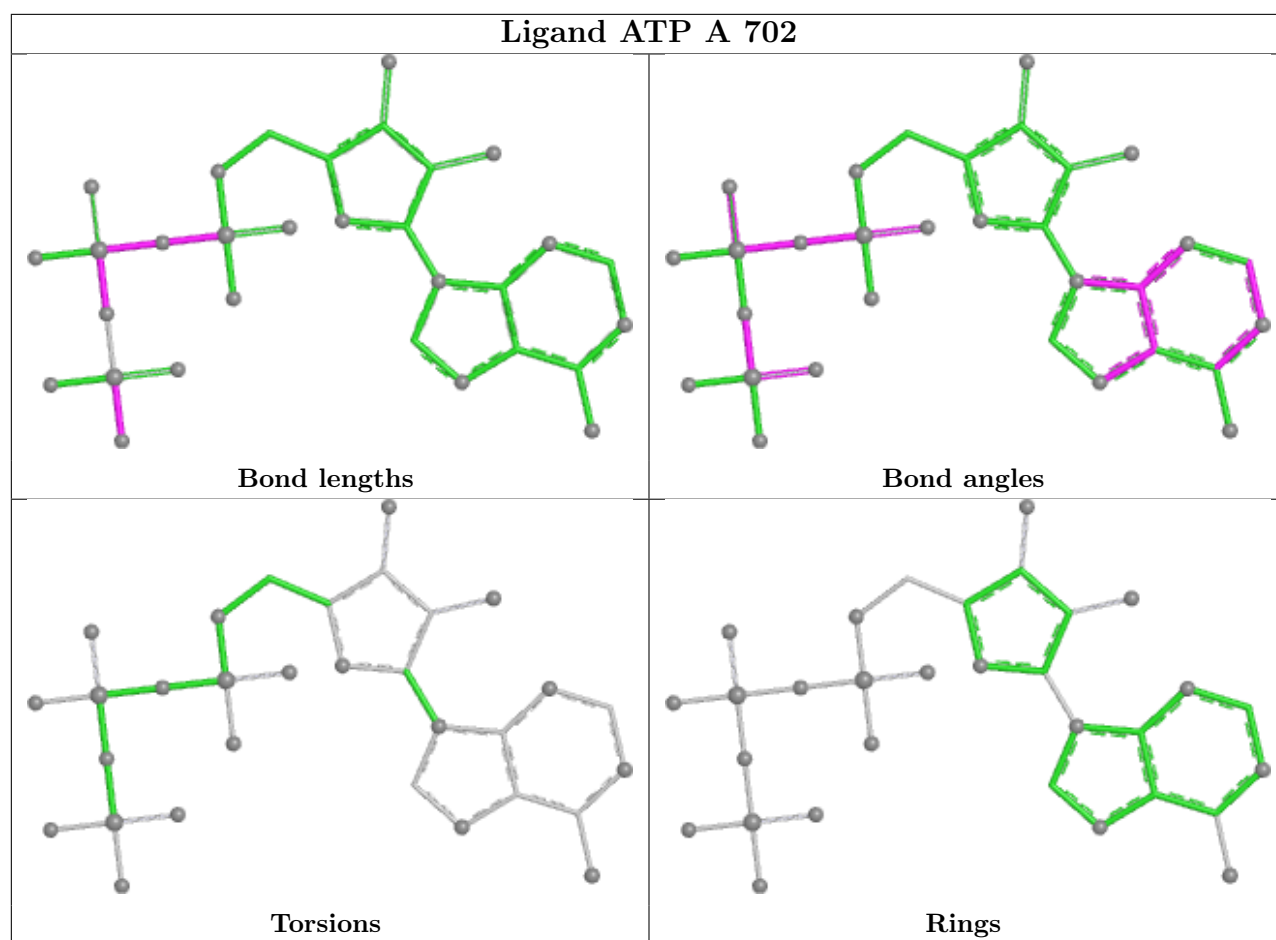
No monomer is involved in short contacts.

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	599/600 (99%)	0.69	42 (7%) 22 16	22, 50, 102, 137	0
1	B	599/600 (99%)	1.02	78 (13%) 7 6	40, 73, 110, 136	0
1	C	599/600 (99%)	0.74	49 (8%) 17 13	23, 51, 86, 112	0
1	D	599/600 (99%)	0.84	52 (8%) 16 11	24, 62, 90, 113	0
All	All	2396/2400 (99%)	0.82	221 (9%) 14 10	22, 59, 100, 137	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	GLY	6.8
1	A	184	GLY	5.9
1	B	280	ASP	5.3
1	B	82	VAL	5.2
1	D	482	GLY	5.1
1	D	340	VAL	4.5
1	B	391	LEU	4.3
1	C	527	ARG	4.3
1	D	17	ALA	4.3
1	A	365	VAL	4.3
1	A	364	ASP	4.3
1	D	457	PHE	4.2
1	B	66	LEU	4.1
1	D	600	GLU	4.1
1	A	79	ASP	4.0
1	A	185	THR	3.9
1	A	568	ALA	3.9
1	B	560	ASP	3.9
1	B	583	ALA	3.8
1	D	19	MET	3.8
1	B	154	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	18	ILE	3.7
1	D	373	ILE	3.7
1	D	438	ILE	3.7
1	A	404	MET	3.7
1	B	204	ILE	3.7
1	D	24	PRO	3.7
1	B	564	ALA	3.6
1	B	484	LEU	3.6
1	B	184	GLY	3.5
1	B	392	LEU	3.5
1	B	336	ASP	3.5
1	B	404	MET	3.5
1	A	565	ILE	3.5
1	A	191	ALA	3.5
1	B	77	PHE	3.5
1	B	48	THR	3.4
1	C	336	ASP	3.4
1	B	407	VAL	3.3
1	C	367	PRO	3.3
1	B	439	HIS	3.3
1	B	406	GLY	3.3
1	D	376	ALA	3.3
1	C	276	ALA	3.2
1	C	591	LEU	3.2
1	C	600	GLU	3.2
1	B	119	VAL	3.2
1	D	120	LEU	3.2
1	D	399	LEU	3.2
1	D	320	LEU	3.1
1	B	276	ALA	3.1
1	D	146	PHE	3.1
1	D	504	SER	3.1
1	D	262	LEU	3.0
1	A	156	ASP	3.0
1	C	277	GLN	3.0
1	D	597	LYS	3.0
1	C	364	ASP	3.0
1	B	289	ASP	3.0
1	A	341	GLY	3.0
1	C	2	GLY	3.0
1	C	185	THR	2.9
1	C	59	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	195	LEU	2.9
1	B	236	LEU	2.9
1	C	526	ASP	2.9
1	B	103	VAL	2.9
1	A	183	LYS	2.9
1	B	339	LEU	2.9
1	C	399	LEU	2.9
1	B	329	LEU	2.9
1	C	560	ASP	2.8
1	B	181	LEU	2.8
1	D	240	LEU	2.8
1	D	598	LEU	2.8
1	B	349	VAL	2.8
1	C	267	GLU	2.8
1	A	271	ILE	2.8
1	B	267	GLU	2.8
1	D	382	LEU	2.7
1	D	289	ASP	2.7
1	D	483	ILE	2.7
1	A	163	LEU	2.7
1	A	257	LEU	2.7
1	A	532	LEU	2.7
1	A	186	GLY	2.7
1	A	429	ALA	2.7
1	B	174	ALA	2.7
1	C	47	CYS	2.6
1	A	466	PRO	2.6
1	B	558	PRO	2.6
1	B	596	GLN	2.6
1	C	498	LYS	2.6
1	C	578	GLY	2.6
1	B	403	THR	2.6
1	D	401	ILE	2.6
1	C	390	LEU	2.6
1	B	88	ILE	2.6
1	C	295	HIS	2.6
1	A	553	ALA	2.6
1	C	375	ALA	2.6
1	A	580	ASP	2.5
1	A	264	GLU	2.5
1	D	59	VAL	2.5
1	A	592	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	271	ILE	2.5
1	B	81	GLU	2.5
1	A	571	ALA	2.5
1	B	269	ALA	2.5
1	B	429	ALA	2.5
1	B	385	ASP	2.5
1	C	542	LEU	2.5
1	B	76	ARG	2.5
1	B	169	ILE	2.5
1	B	561	ASP	2.5
1	A	583	ALA	2.5
1	A	268	LYS	2.4
1	D	291	THR	2.4
1	B	599	MET	2.4
1	D	446	LYS	2.4
1	B	594	VAL	2.4
1	D	285	TYR	2.4
1	A	564	ALA	2.4
1	A	39	ILE	2.4
1	C	36	THR	2.4
1	C	448	ALA	2.4
1	B	409	THR	2.4
1	A	340	VAL	2.4
1	B	323	ALA	2.4
1	C	392	LEU	2.3
1	B	7	ILE	2.3
1	A	84	ARG	2.3
1	B	191	ALA	2.3
1	B	298	ILE	2.3
1	B	483	ILE	2.3
1	B	420	THR	2.3
1	B	505	SER	2.3
1	D	231	ASP	2.3
1	B	218	VAL	2.3
1	B	438	ILE	2.3
1	C	412	ILE	2.3
1	A	570	THR	2.3
1	B	179	TYR	2.3
1	C	179	TYR	2.3
1	D	402	GLU	2.3
1	D	456	GLN	2.3
1	A	426	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	2.3
1	A	373	ILE	2.3
1	D	54	ALA	2.3
1	C	188	ARG	2.3
1	D	330	SER	2.3
1	B	305	LEU	2.3
1	C	353	VAL	2.3
1	A	520	GLU	2.2
1	B	318	GLU	2.2
1	C	524	GLU	2.2
1	D	272	GLU	2.2
1	D	520	GLU	2.2
1	D	79	ASP	2.2
1	D	186	GLY	2.2
1	B	16	VAL	2.2
1	B	597	LYS	2.2
1	C	357	PHE	2.2
1	C	184	GLY	2.2
1	C	289	ASP	2.2
1	D	33	ASP	2.2
1	D	364	ASP	2.2
1	D	385	ASP	2.2
1	B	172	PRO	2.2
1	A	247	ASP	2.2
1	B	211	ASP	2.2
1	B	472	ILE	2.2
1	D	204	ILE	2.2
1	D	565	ILE	2.2
1	B	54	ALA	2.2
1	C	473	GLU	2.2
1	B	279	THR	2.2
1	C	395	THR	2.2
1	B	257	LEU	2.2
1	B	441	LEU	2.2
1	B	563	THR	2.1
1	B	593	GLN	2.1
1	B	459	LEU	2.1
1	C	262	LEU	2.1
1	B	550	VAL	2.1
1	C	208	ASP	2.1
1	C	335	ASP	2.1
1	B	291	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	363	LYS	2.1
1	D	44	GLN	2.1
1	B	569	LEU	2.1
1	C	145	TYR	2.1
1	D	156	ASP	2.1
1	A	427	SER	2.1
1	C	290	ALA	2.1
1	C	402	GLU	2.1
1	A	550	VAL	2.1
1	A	561	ASP	2.1
1	C	14	SER	2.1
1	D	303	ALA	2.1
1	C	314	ASN	2.1
1	B	196	GLY	2.1
1	B	115	ILE	2.1
1	B	193	TYR	2.1
1	D	474	VAL	2.1
1	A	274	SER	2.0
1	B	504	SER	2.0
1	D	185	THR	2.0
1	C	396	PRO	2.0
1	D	238	ASN	2.0
1	B	338	ILE	2.0
1	C	334	ILE	2.0
1	A	386	VAL	2.0
1	C	42	TYR	2.0
1	B	261	ARG	2.0
1	C	288	ALA	2.0
1	D	269	ALA	2.0
1	C	417	THR	2.0
1	A	282	ASN	2.0
1	C	241	VAL	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](#)

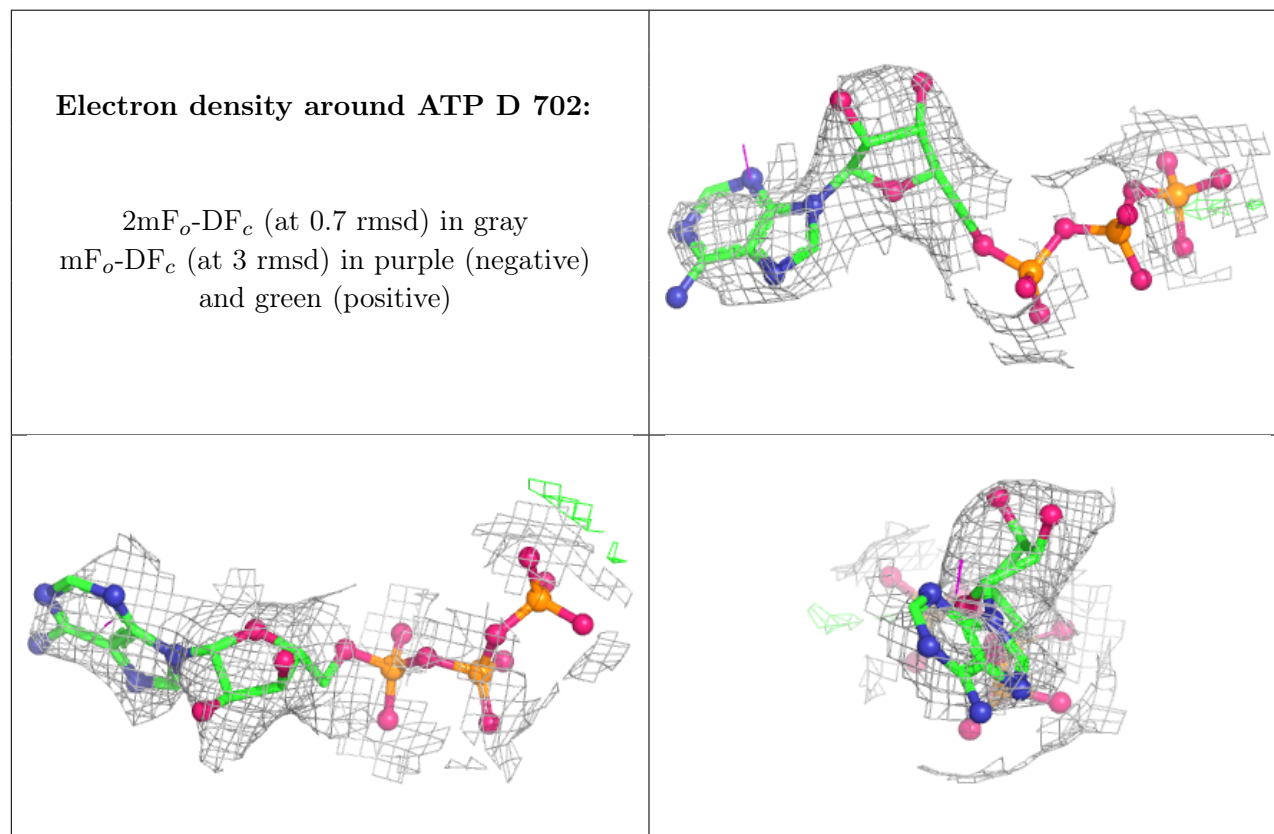
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

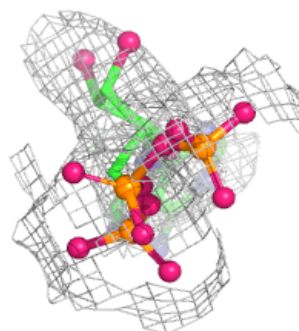
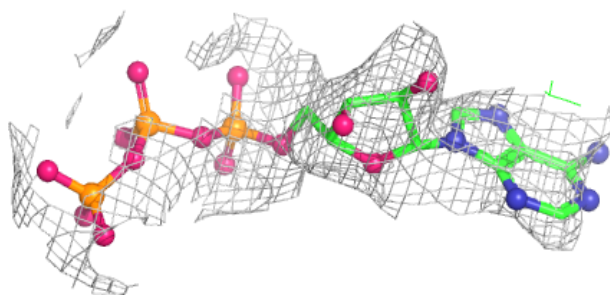
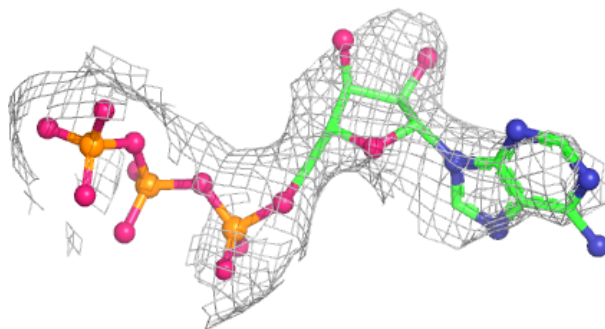
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	D	702	31/31	0.91	0.10	43,59,80,83	0
3	ATP	B	702	31/31	0.93	0.10	38,64,84,88	0
3	ATP	C	702	31/31	0.94	0.08	23,38,48,58	0
3	ATP	A	702	31/31	0.95	0.08	25,33,53,63	0
2	MG	A	701	1/1	0.96	0.06	36,36,36,36	0
2	MG	C	701	1/1	0.98	0.08	41,41,41,41	0
2	MG	B	701	1/1	0.99	0.03	65,65,65,65	0
2	MG	D	701	1/1	0.99	0.03	50,50,50,50	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.

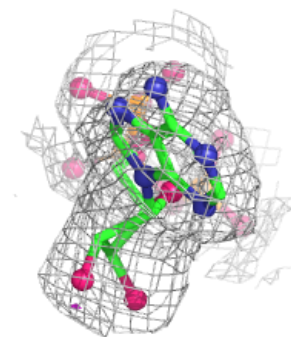
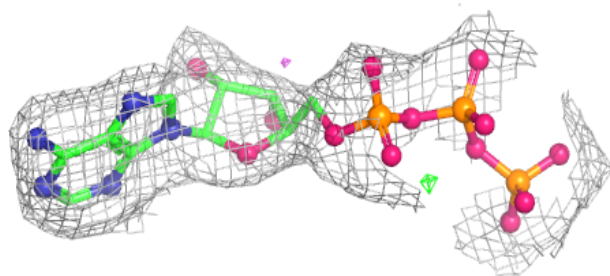
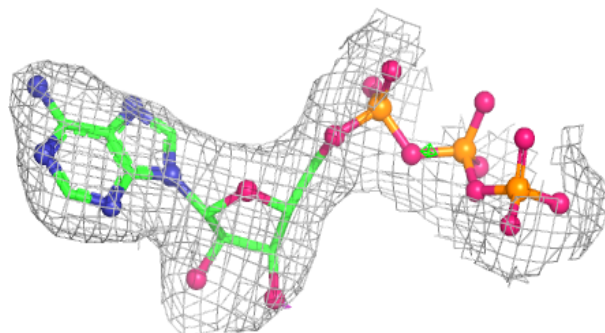


Electron density around ATP B 702:

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

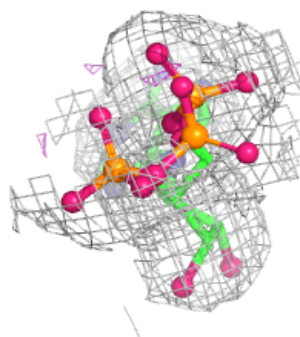
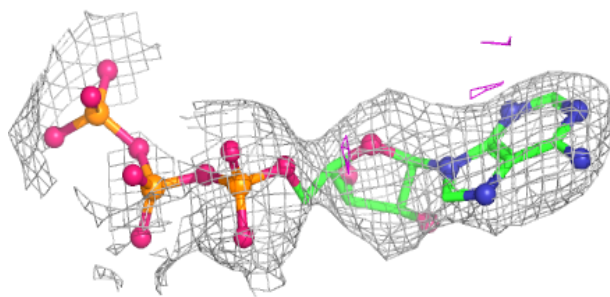
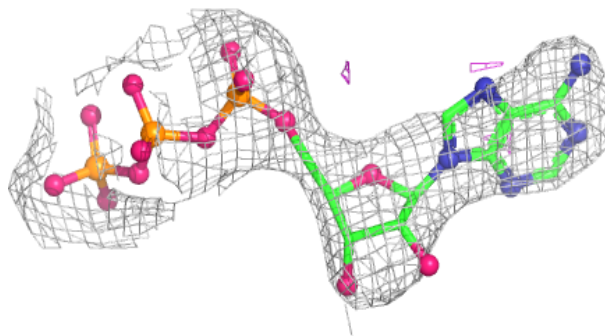
**Electron density around ATP C 702:**

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



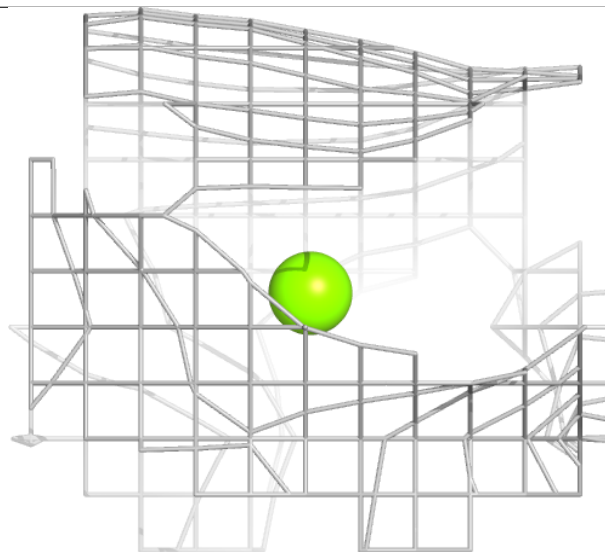
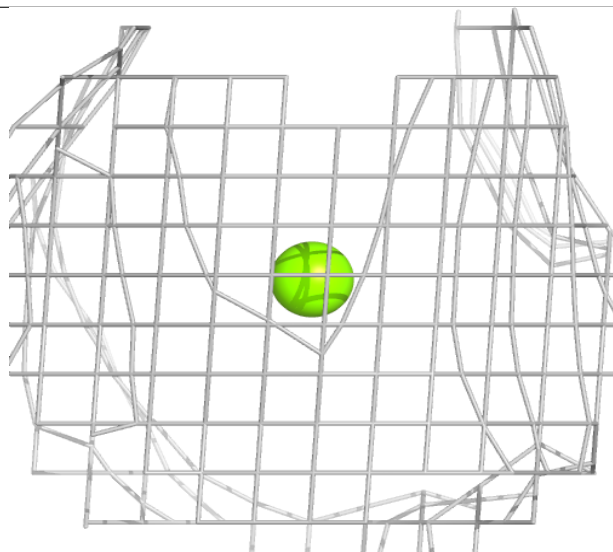
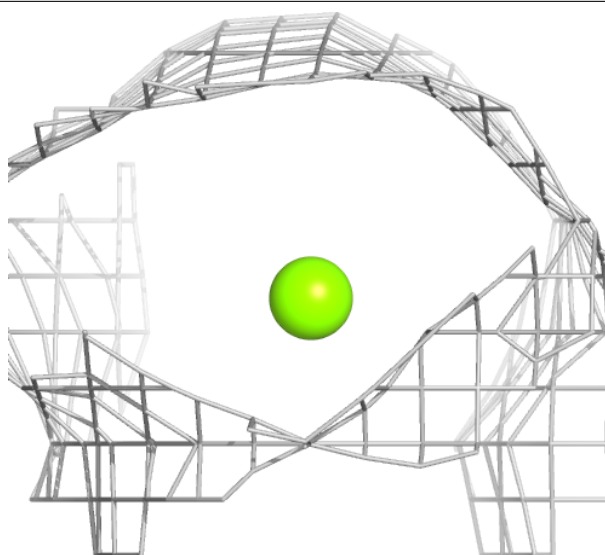
Electron density around ATP A 702:

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



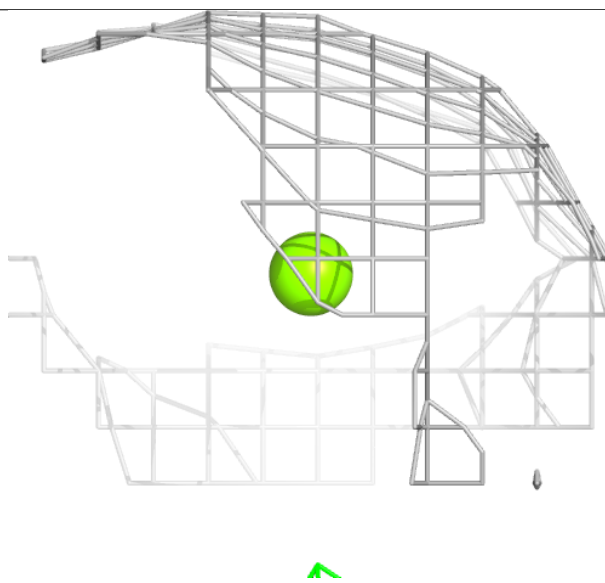
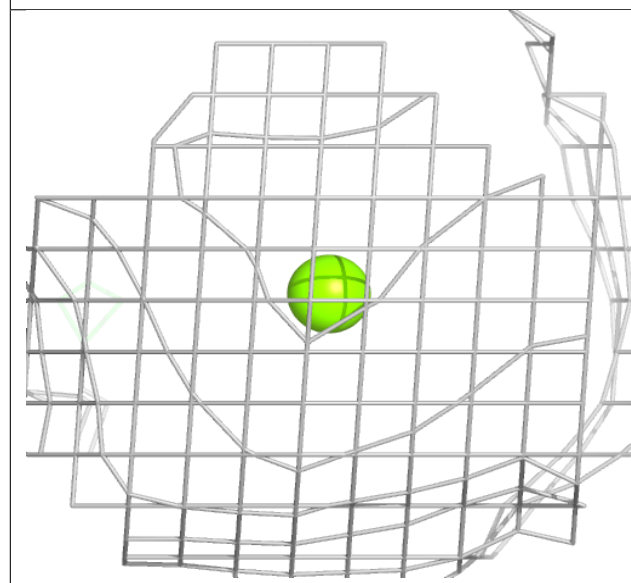
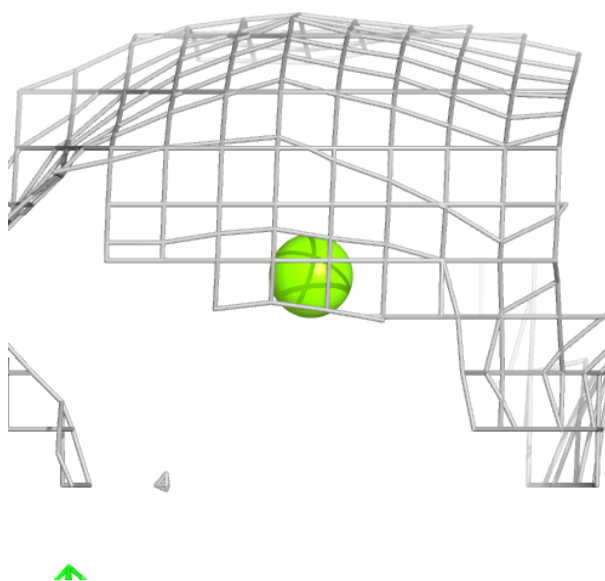
Electron density around MG A 701:

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



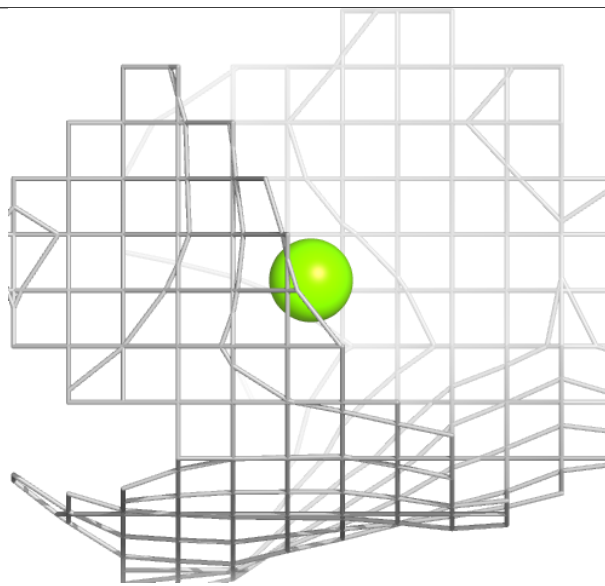
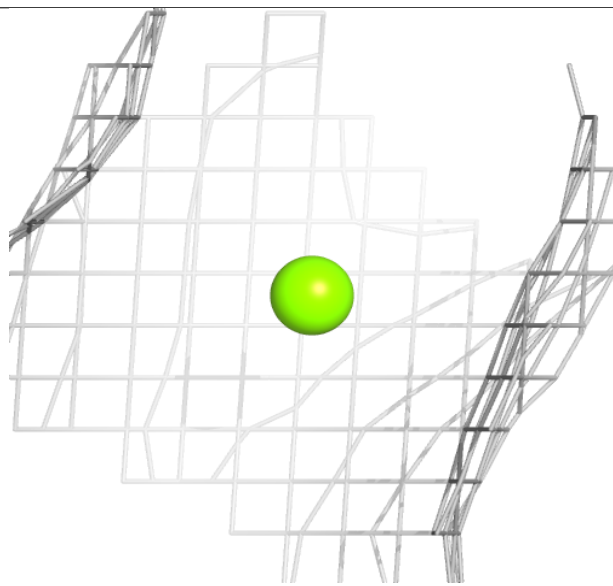
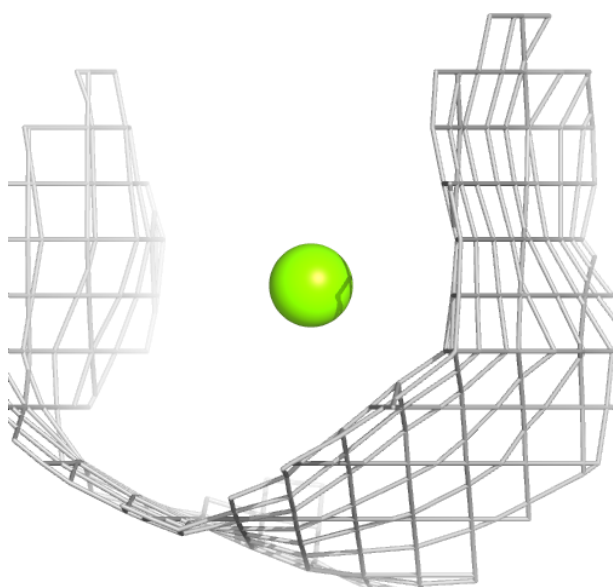
Electron density around MG C 701:

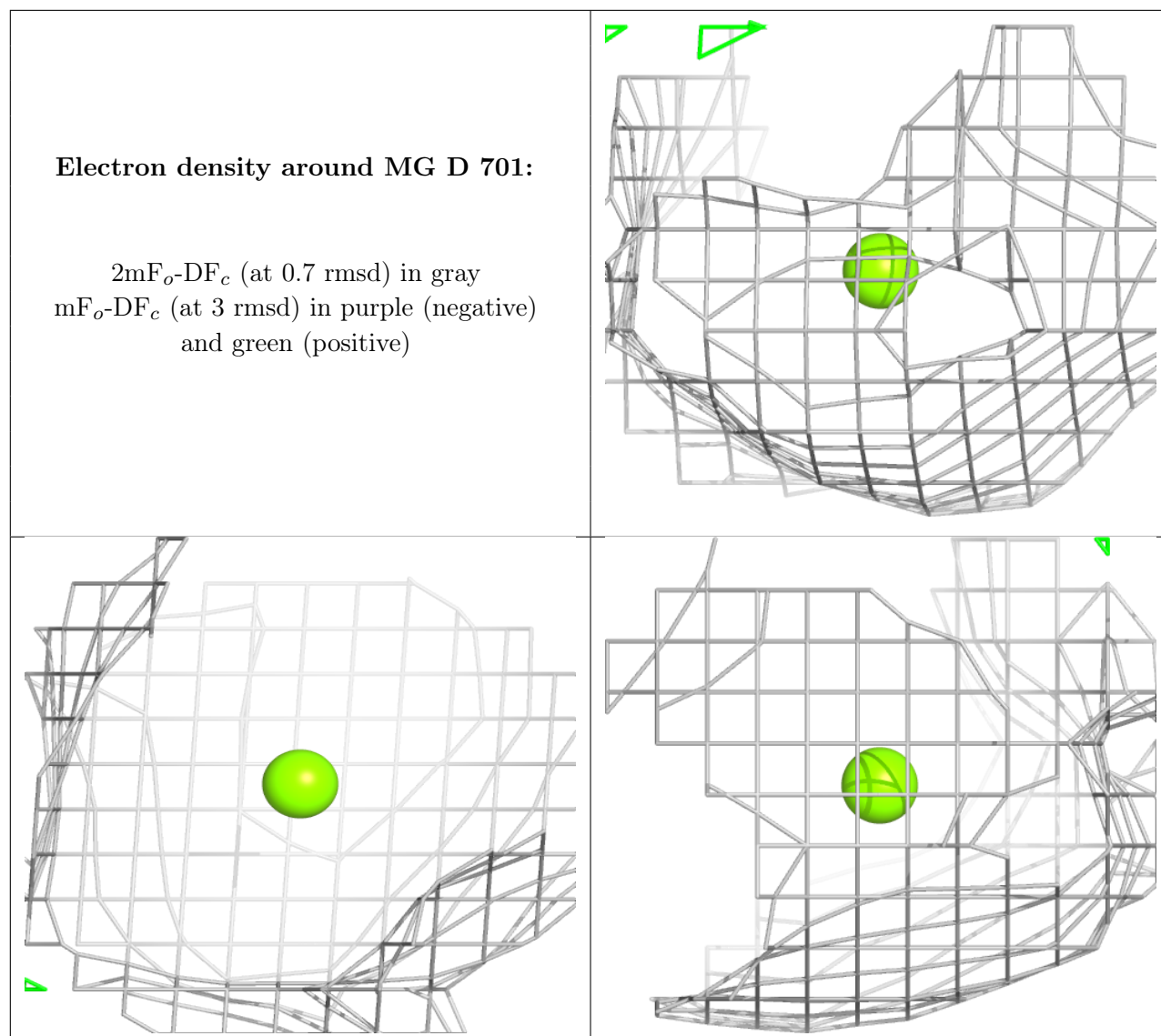
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 701:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.