



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:16 AM UTC

PDB ID : 4B9Q / pdb_00004b9q
Title : Open conformation of ATP-bound Hsp70 homolog DnaK
Authors : Kopp, J.; Mayer, M.P.; Sinning, I.
Deposited on : 2012-09-06
Resolution : 2.40 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

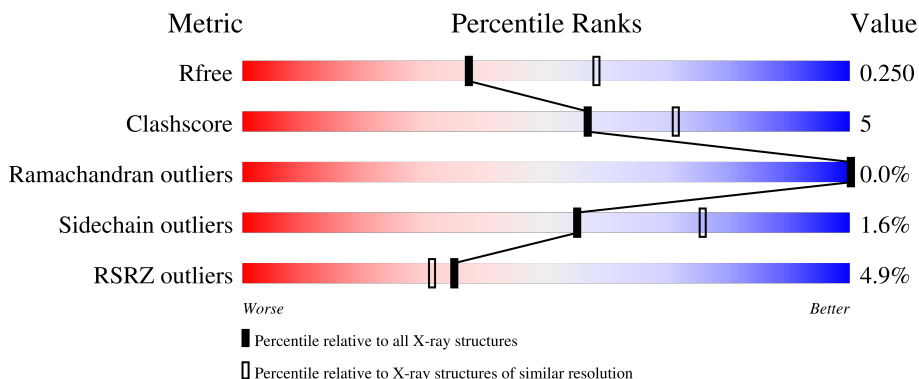
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	605	5% 88% 11% ..
1	B	605	4% 87% 11% .
1	C	605	6% 86% 12% .
1	D	605	3% 87% 11% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18760 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	Se	0	0	0
			4554	2826	792	919	3	14			
1	B	597	Total	C	N	O	S	Se	0	0	0
			4534	2812	789	916	3	14			
1	C	595	Total	C	N	O	S	Se	0	0	0
			4515	2803	785	910	3	14			
1	D	595	Total	C	N	O	S	Se	0	0	0
			4515	2802	784	912	3	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	GLU	engineered mutation	UNP P0A6Y8
A	199	ALA	THR	engineered mutation	UNP P0A6Y8
A	529	CYS	PHE	engineered mutation	UNP P0A6Y8
B	47	CYS	GLU	engineered mutation	UNP P0A6Y8
B	199	ALA	THR	engineered mutation	UNP P0A6Y8
B	529	CYS	PHE	engineered mutation	UNP P0A6Y8
C	47	CYS	GLU	engineered mutation	UNP P0A6Y8
C	199	ALA	THR	engineered mutation	UNP P0A6Y8
C	529	CYS	PHE	engineered mutation	UNP P0A6Y8
D	47	CYS	GLU	engineered mutation	UNP P0A6Y8
D	199	ALA	THR	engineered mutation	UNP P0A6Y8
D	529	CYS	PHE	engineered mutation	UNP P0A6Y8

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



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		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total	O	0	0
			164	164		

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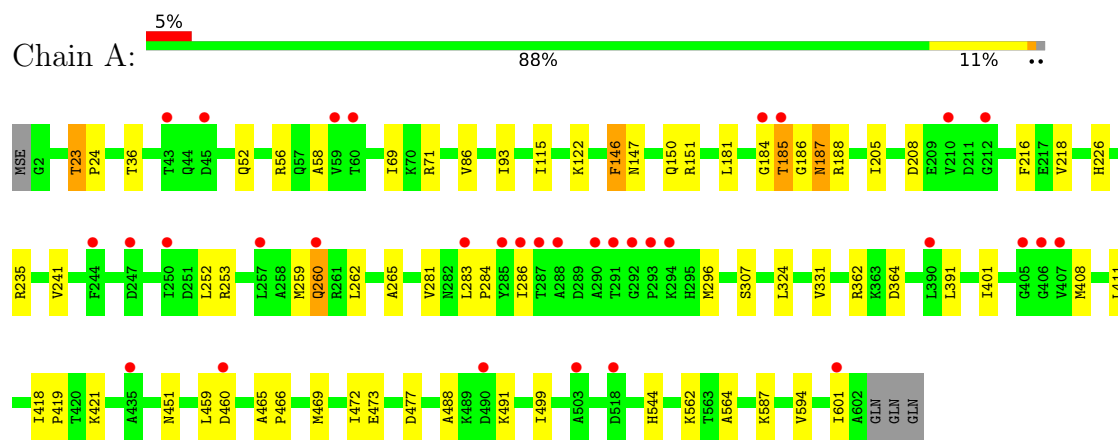
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	145	Total 145	O 145	0	0
4	C	115	Total 115	O 115	0	0
4	D	90	Total 90	O 90	0	0

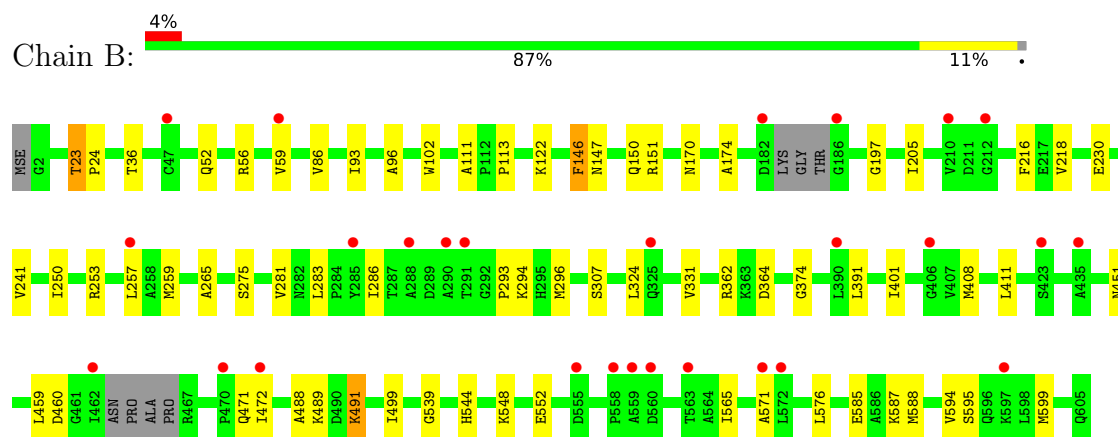
3 Residue-property plots [i](#)

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.

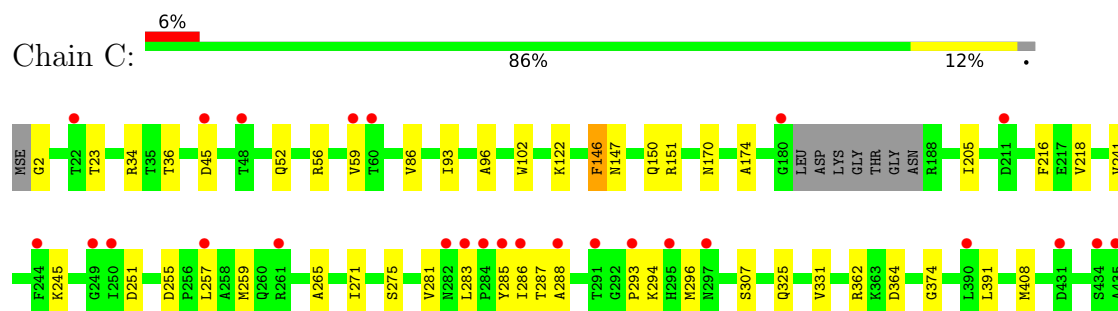
• Molecule 1: CHAPERONE PROTEIN DNAK

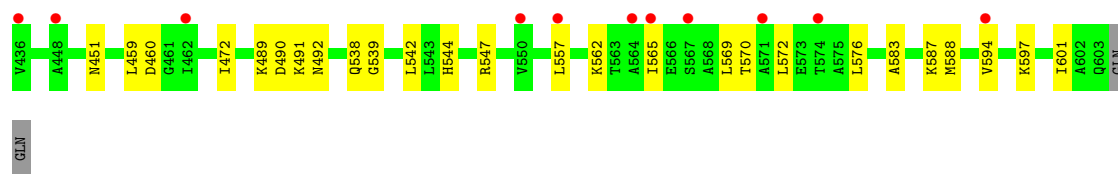


• Molecule 1: CHAPERONE PROTEIN DNAK

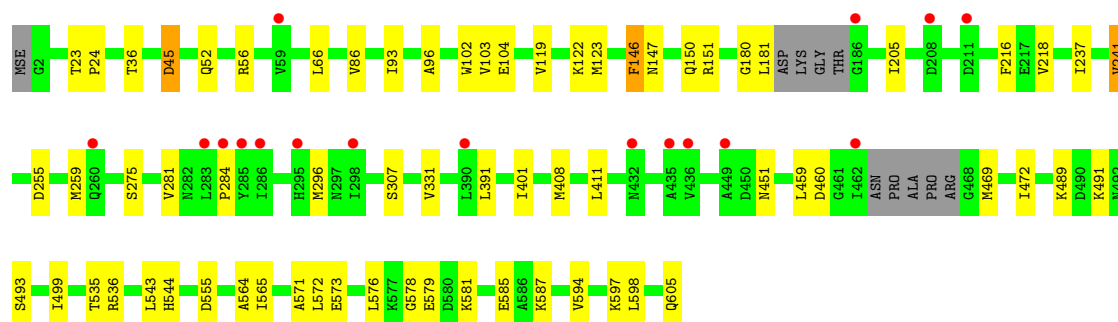
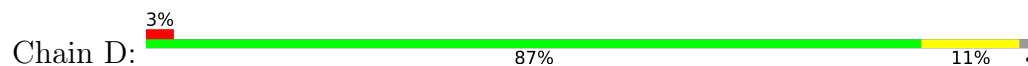


• Molecule 1: CHAPERONE PROTEIN DNAK





• 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	202.33Å 77.47Å 182.96Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	59.72 – 2.40 59.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (59.72-2.40) 99.6 (59.72-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.196 , 0.239 0.208 , 0.250	Depositor DCC
R_{free} test set	5503 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.0	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	0.94	EDS
Total number of atoms	18760	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 24.59 % 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 3.7239e-03.*

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: MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/4591	0.82	0/6182
1	B	0.53	0/4567	0.80	0/6144
1	C	0.54	0/4551	0.83	1/6127 (0.0%)
1	D	0.51	0/4548	0.79	0/6119
All	All	0.54	0/18257	0.81	1/24572 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	TYR	N-CA-C	5.38	118.61	111.30

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	4554	0	4605	52	0
1	B	4534	0	4579	40	0
1	C	4515	0	4565	45	0
1	D	4515	0	4562	39	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	12	1	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	164	0	0	3	0
4	B	145	0	0	2	0
4	C	115	0	0	3	0
4	D	90	0	0	1	0
All	All	18760	0	18359	167	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 5.

All (167) 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:184:GLY:HA2	1:A:185:THR:CB	1.43	1.38
1:A:184:GLY:CA	1:A:185:THR:HB	1.44	1.30
1:A:184:GLY:HA3	1:A:188:ARG:HE	1.50	0.74
1:A:186:GLY:O	1:A:187:ASN:C	2.29	0.74
1:D:571:ALA:HB1	1:D:587:LYS:HE2	1.69	0.72
1:B:585:GLU:HA	1:B:588:MSE:HE2	1.70	0.72
4:A:2096:HOH:O	1:C:56:ARG:NH2	2.24	0.69
1:A:473:GLU:HB2	1:A:491:LYS:HG2	1.75	0.67
1:C:557:LEU:HD23	1:C:562:LYS:HG3	1.77	0.66
1:C:147:ASN:O	1:C:151:ARG:HG3	1.97	0.65
1:D:147:ASN:O	1:D:151:ARG:HG3	1.95	0.65
1:A:147:ASN:O	1:A:151:ARG:HG3	1.97	0.65
1:A:187:ASN:HA	1:A:208:ASP:HA	1.78	0.64
1:B:147:ASN:O	1:B:151:ARG:HG3	1.98	0.64
1:D:543:LEU:HD11	1:D:573:GLU:HG3	1.81	0.62
1:A:544:HIS:CG	1:C:307:SER:HB2	2.34	0.62
1:C:245:LYS:HE2	1:C:251:ASP:HB2	1.82	0.62
1:A:307:SER:HB2	1:C:544:HIS:CG	2.36	0.61
1:A:185:THR:HG22	1:A:185:THR:O	2.01	0.60
1:B:544:HIS:CG	1:D:307:SER:HB2	2.37	0.59
1:A:185:THR:O	1:A:185:THR:CG2	2.51	0.58
1:B:59:VAL:HG21	1:D:284:PRO:HG2	1.85	0.57
1:A:186:GLY:O	1:A:188:ARG:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD12	1:A:296:MSE:CE	2.36	0.56
1:B:36:THR:HG21	1:B:122:LYS:HD3	1.90	0.53
1:D:459:LEU:HD13	1:D:472:ILE:HG21	1.90	0.53
1:A:86:VAL:HG22	1:A:93:ILE:HB	1.90	0.53
1:B:205:ILE:HG12	1:B:218:VAL:HG22	1.89	0.53
1:C:538:GLN:HB3	1:C:588:MSE:HE1	1.90	0.53
1:A:459:LEU:HD13	1:A:472:ILE:HG21	1.90	0.53
1:C:408:MSE:HG3	1:C:451:ASN:ND2	2.24	0.53
1:A:283:LEU:HD12	1:A:296:MSE:HE1	1.91	0.53
1:B:307:SER:HB2	1:D:544:HIS:CG	2.43	0.53
1:B:408:MSE:HG3	1:B:451:ASN:ND2	2.24	0.52
1:A:36:THR:HG21	1:A:122:LYS:HD3	1.91	0.52
1:B:86:VAL:HG22	1:B:93:ILE:HB	1.91	0.52
1:A:408:MSE:HG3	1:A:451:ASN:ND2	2.25	0.52
1:C:491:LYS:HG3	1:D:469:MSE:SE	2.60	0.51
1:D:408:MSE:HG3	1:D:451:ASN:ND2	2.25	0.51
1:C:36:THR:HG21	1:C:122:LYS:HD3	1.93	0.51
1:A:205:ILE:HG12	1:A:218:VAL:HG22	1.93	0.51
1:D:52:GLN:O	1:D:56:ARG:HG3	2.10	0.51
1:A:262:LEU:HD13	1:A:296:MSE:HE1	1.93	0.50
1:C:539:GLY:HA3	1:C:576:LEU:HD21	1.92	0.50
1:B:459:LEU:HD13	1:B:472:ILE:HG21	1.92	0.50
1:B:253:ARG:HA	1:B:259:MSE:SE	2.61	0.50
1:C:459:LEU:HD13	1:C:472:ILE:HG21	1.93	0.50
1:B:539:GLY:HA3	1:B:576:LEU:HD21	1.93	0.50
1:B:281:VAL:HG12	1:B:296:MSE:HE3	1.95	0.49
1:A:252:LEU:HD21	1:A:286:ILE:HG12	1.94	0.49
1:A:184:GLY:CA	1:A:185:THR:CB	2.30	0.49
1:A:186:GLY:C	1:A:188:ARG:N	2.70	0.49
1:A:488:ALA:HB2	1:A:499:ILE:HD11	1.94	0.49
1:C:565:ILE:HD13	1:C:594:VAL:HG12	1.95	0.49
1:C:86:VAL:HG22	1:C:93:ILE:HB	1.95	0.48
1:A:52:GLN:O	1:A:56:ARG:HG3	2.13	0.48
1:A:253:ARG:HA	1:A:259:MSE:SE	2.63	0.48
1:D:36:THR:HG21	1:D:122:LYS:HD3	1.93	0.48
1:C:52:GLN:O	1:C:56:ARG:HG3	2.14	0.48
1:C:542:LEU:HD23	1:C:588:MSE:HG2	1.96	0.47
1:C:205:ILE:HG12	1:C:218:VAL:HG22	1.95	0.47
1:C:547:ARG:HE	1:C:569:LEU:HD13	1.79	0.47
1:D:216:PHE:HB2	1:D:391:LEU:HD12	1.96	0.47
1:B:565:ILE:HG12	1:B:594:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASP:OD1	1:A:460:ASP:N	2.44	0.47
1:B:460:ASP:OD1	1:B:460:ASP:N	2.43	0.47
1:D:104:GLU:O	4:D:2019:HOH:O	2.21	0.46
1:C:583:ALA:O	1:C:587:LYS:HG2	2.15	0.46
1:D:86:VAL:HG22	1:D:93:ILE:HB	1.98	0.46
1:C:216:PHE:HB2	1:C:391:LEU:HD12	1.98	0.45
1:D:281:VAL:HG12	1:D:296:MSE:HE3	1.97	0.45
1:B:216:PHE:HB2	1:B:391:LEU:HD12	1.99	0.45
1:A:265:ALA:HB2	1:A:283:LEU:HD11	1.98	0.45
1:C:408:MSE:HG3	1:C:451:ASN:HD22	1.82	0.45
1:B:489:LYS:HE3	1:B:489:LYS:HB2	1.82	0.44
1:B:548:LYS:HG3	1:B:552:GLU:OE2	2.17	0.44
1:C:2:GLY:N	4:C:2001:HOH:O	2.51	0.44
1:D:146:PHE:CD2	1:D:150:GLN:HB3	2.52	0.44
1:B:151:ARG:NH2	1:B:170:ASN:OD1	2.36	0.44
1:B:293:PRO:O	1:B:294:LYS:HD3	2.17	0.44
1:D:565:ILE:HD13	1:D:598:LEU:HD22	1.99	0.44
1:A:69:ILE:HG13	1:A:115:ILE:HG21	2.00	0.44
1:A:71:ARG:NH2	1:A:226:HIS:CE1	2.86	0.44
1:C:490:ASP:OD1	1:C:492:ASN:N	2.49	0.44
1:C:491:LYS:CG	1:D:469:MSE:SE	3.16	0.44
1:A:58:ALA:O	1:A:260:GLN:NE2	2.36	0.44
1:C:151:ARG:NH2	1:C:170:ASN:OD1	2.34	0.44
1:A:235:ARG:NH1	4:A:2090:HOH:O	2.51	0.44
1:C:460:ASP:OD1	1:C:460:ASP:N	2.44	0.44
1:A:184:GLY:HA2	1:A:185:THR:HB	0.56	0.43
1:B:96:ALA:HB2	1:B:102:TRP:CD1	2.53	0.43
1:B:571:ALA:O	1:B:587:LYS:HG3	2.18	0.43
1:B:265:ALA:HB2	1:B:283:LEU:HD11	2.00	0.43
1:A:284:PRO:HG2	1:C:59:VAL:HG21	1.99	0.43
1:B:23:THR:HA	1:B:24:PRO:HD3	1.77	0.43
1:C:265:ALA:HB2	1:C:283:LEU:HD11	2.00	0.43
1:C:281:VAL:HG12	1:C:296:MSE:HE3	2.00	0.43
1:D:205:ILE:HG12	1:D:218:VAL:HG22	1.99	0.43
1:D:408:MSE:HG3	1:D:451:ASN:HD22	1.83	0.43
1:C:34:ARG:NH1	4:C:2013:HOH:O	2.43	0.43
1:D:66:LEU:HD21	1:D:103:VAL:HG21	2.00	0.43
1:D:119:VAL:O	1:D:123:MSE:HG2	2.18	0.43
1:A:216:PHE:HB2	1:A:391:LEU:HD12	1.99	0.43
1:A:401:ILE:HG23	1:A:411:LEU:HD11	2.00	0.43
1:A:408:MSE:HG3	1:A:451:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ALA:HB2	1:B:499:ILE:HD11	2.01	0.43
1:B:52:GLN:O	1:B:56:ARG:HG3	2.18	0.43
1:D:564:ALA:HB1	1:D:594:VAL:HG11	2.00	0.43
1:A:307:SER:HB2	1:C:544:HIS:ND1	2.34	0.42
1:D:401:ILE:HG23	1:D:411:LEU:HD11	2.00	0.42
1:A:421:LYS:HG2	1:A:477:ASP:OD1	2.19	0.42
1:B:471:GLN:O	1:B:491:LYS:HB2	2.19	0.42
1:C:286:ILE:CD1	1:C:296:MSE:HE2	2.50	0.42
1:D:23:THR:HA	1:D:24:PRO:HD3	1.78	0.42
1:B:408:MSE:HG3	1:B:451:ASN:HD22	1.84	0.42
1:C:597:LYS:O	1:C:601:ILE:HG13	2.20	0.42
1:C:146:PHE:CD2	1:C:150:GLN:HB3	2.54	0.42
1:B:362:ARG:NH2	1:B:364:ASP:OD2	2.53	0.42
1:C:96:ALA:HB2	1:C:102:TRP:CD1	2.55	0.42
1:D:535:THR:OG1	1:D:581:LYS:HE3	2.19	0.42
1:A:281:VAL:HG12	1:A:296:MSE:HE3	2.01	0.42
1:D:45:ASP:OD2	1:D:579:GLU:HG3	2.19	0.42
1:D:572:LEU:O	1:D:576:LEU:HG	2.20	0.42
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.88	0.42
1:D:237:ILE:O	1:D:241:VAL:HG13	2.19	0.42
1:D:489:LYS:HE3	1:D:489:LYS:HB2	1.80	0.42
1:D:96:ALA:HB2	1:D:102:TRP:CD1	2.55	0.42
1:D:255:ASP:O	1:D:259:MSE:HG2	2.19	0.42
1:C:489:LYS:HB2	1:C:489:LYS:HE3	1.78	0.42
1:D:460:ASP:OD1	1:D:460:ASP:N	2.42	0.42
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.85	0.41
1:A:362:ARG:NH2	1:A:364:ASP:OD2	2.53	0.41
1:C:287:THR:OG1	1:C:288:ALA:N	2.53	0.41
1:D:581:LYS:HE2	1:D:585:GLU:OE2	2.19	0.41
1:B:52:GLN:HB3	4:B:2026:HOH:O	2.21	0.41
1:D:536:ARG:NH2	1:D:578:GLY:O	2.51	0.41
1:A:459:LEU:HD23	1:A:499:ILE:HG12	2.00	0.41
1:C:257:LEU:HD12	1:C:257:LEU:HA	1.83	0.41
1:D:587:LYS:HD2	1:D:587:LYS:HA	1.91	0.41
1:A:564:ALA:HB1	1:A:594:VAL:HG21	2.03	0.41
1:A:466:PRO:HG2	1:A:469:MSE:HG2	2.02	0.41
1:C:255:ASP:O	1:C:259:MSE:HG2	2.20	0.41
1:A:146:PHE:CD2	1:A:150:GLN:HB3	2.54	0.41
1:D:459:LEU:HD23	1:D:499:ILE:HG12	2.02	0.41
1:A:587:LYS:NZ	4:A:2161:HOH:O	2.53	0.41
1:A:465:ALA:HB1	1:A:469:MSE:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:SER:O	1:B:599:MSE:HG2	2.20	0.41
1:A:418:ILE:HA	1:A:419:PRO:C	2.46	0.41
1:B:146:PHE:CD2	1:B:150:GLN:HB3	2.56	0.41
1:B:174:ALA:O	1:B:374:GLY:HA3	2.21	0.41
1:B:250:ILE:HD12	1:B:294:LYS:HG3	2.03	0.41
1:A:23:THR:HA	1:A:24:PRO:HD3	1.78	0.40
1:B:111:ALA:HB1	1:B:113:PRO:HD2	2.03	0.40
1:C:325:GLN:OE1	4:C:2092:HOH:O	2.22	0.40
1:D:180:GLY:C	1:D:181:LEU:HD12	2.46	0.40
1:C:362:ARG:NH2	1:C:364:ASP:OD2	2.54	0.40
1:D:597:LYS:HA	1:D:597:LYS:HD3	1.83	0.40
1:B:56:ARG:HD3	4:B:2026:HOH:O	2.20	0.40
1:B:324:LEU:HA	1:B:324:LEU:HD23	1.85	0.40
1:C:572:LEU:HD13	1:C:587:LYS:HB2	2.02	0.40
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.87	0.40
1:B:197:GLY:O	1:B:230:GLU:HG2	2.22	0.40
1:B:401:ILE:HG23	1:B:411:LEU:HD11	2.03	0.40
1:B:565:ILE:HD11	1:B:595:SER:HA	2.02	0.40
1:C:174:ALA:O	1:C:374:GLY:HA3	2.22	0.40
1:C:271:ILE:HG12	2:C:700:ATP:C5	2.56	0.40
1:C:293:PRO:O	1:C:294:LYS:HD2	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	599/605 (99%)	584 (98%)	14 (2%)	1 (0%)	43	58
1	B	591/605 (98%)	583 (99%)	8 (1%)	0	100	100
1	C	591/605 (98%)	583 (99%)	8 (1%)	0	100	100
1	D	589/605 (97%)	581 (99%)	8 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2370/2420 (98%)	2331 (98%)	38 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASN

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	491/480 (102%)	483 (98%)	8 (2%)	55	76
1	B	489/480 (102%)	481 (98%)	8 (2%)	55	76
1	C	487/480 (102%)	480 (99%)	7 (1%)	59	79
1	D	487/480 (102%)	478 (98%)	9 (2%)	51	73
All	All	1954/1920 (102%)	1922 (98%)	32 (2%)	55	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	146	PHE
1	A	185	THR
1	A	241	VAL
1	A	260	GLN
1	A	331	VAL
1	A	562	LYS
1	A	601	ILE
1	B	23	THR
1	B	146	PHE
1	B	241	VAL
1	B	257	LEU
1	B	275	SER
1	B	286	ILE

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Mol	Chain	Res	Type
1	B	331	VAL
1	B	491	LYS
1	C	23	THR
1	C	45	ASP
1	C	146	PHE
1	C	241	VAL
1	C	275	SER
1	C	331	VAL
1	C	570	THR
1	D	45	ASP
1	D	146	PHE
1	D	241	VAL
1	D	275	SER
1	D	331	VAL
1	D	491	LYS
1	D	493	SER
1	D	555	ASP
1	D	605	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	544	HIS
1	A	589	GLN
1	B	226	HIS
1	B	422	HIS
1	B	492	ASN
1	C	13	ASN
1	C	248	GLN
1	C	422	HIS
1	D	187	ASN
1	D	248	GLN
1	D	260	GLN
1	D	422	HIS
1	D	497	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 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$
2	ATP	A	700	3	32,33,33	1.54	6 (18%)	48,52,52	1.82	10 (20%)
2	ATP	C	700	3	32,33,33	1.46	5 (15%)	48,52,52	1.92	16 (33%)
2	ATP	D	700	3	32,33,33	1.45	7 (21%)	48,52,52	1.80	9 (18%)
2	ATP	B	700	3	32,33,33	1.52	7 (21%)	48,52,52	1.68	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	700	3	-	1/22/38/38	0/3/3/3
2	ATP	C	700	3	-	1/22/38/38	0/3/3/3
2	ATP	D	700	3	-	3/22/38/38	0/3/3/3
2	ATP	B	700	3	-	1/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	ATP	C5-C4	5.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ATP	C5-C4	4.75	1.47	1.39
2	C	700	ATP	C5-C4	4.53	1.47	1.39
2	D	700	ATP	C5-C4	4.51	1.47	1.39
2	A	700	ATP	C5-C6	3.03	1.49	1.41
2	A	700	ATP	PB-O3B	3.02	1.62	1.59
2	B	700	ATP	PB-O3B	3.01	1.62	1.59
2	B	700	ATP	C5-C6	2.81	1.48	1.41
2	C	700	ATP	C5-C6	2.77	1.48	1.41
2	D	700	ATP	C5-C6	2.62	1.48	1.41
2	A	700	ATP	PB-O3A	2.56	1.62	1.59
2	C	700	ATP	PB-O3A	2.49	1.62	1.59
2	D	700	ATP	PB-O3A	2.47	1.62	1.59
2	C	700	ATP	C8-N7	2.44	1.36	1.31
2	D	700	ATP	PA-O3A	2.36	1.62	1.59
2	D	700	ATP	C8-N7	2.33	1.36	1.31
2	A	700	ATP	C8-N7	2.27	1.36	1.31
2	D	700	ATP	PB-O3B	2.24	1.61	1.59
2	B	700	ATP	C4-N9	-2.24	1.33	1.37
2	B	700	ATP	C8-N7	2.19	1.35	1.31
2	B	700	ATP	C5-N7	-2.18	1.35	1.39
2	A	700	ATP	PA-O3A	2.12	1.61	1.59
2	C	700	ATP	C4-N9	-2.10	1.33	1.37
2	B	700	ATP	PB-O3A	2.01	1.61	1.59
2	D	700	ATP	C5-N7	-2.01	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ATP	C5-C4-N3	-5.82	118.71	126.72
2	D	700	ATP	C5-C4-N3	-5.79	118.74	126.72
2	C	700	ATP	C5-C4-N3	-4.89	119.98	126.72
2	D	700	ATP	N3-C4-N9	4.74	135.22	127.17
2	A	700	ATP	N3-C4-N9	4.66	135.09	127.17
2	B	700	ATP	C5-C4-N3	-4.60	120.38	126.72
2	C	700	ATP	N3-C4-N9	4.20	134.30	127.17
2	A	700	ATP	C4-C5-N7	-4.05	105.95	110.58
2	C	700	ATP	C4-N9-C8	3.94	109.88	105.74
2	D	700	ATP	C2-N3-C4	3.87	121.28	111.83
2	B	700	ATP	N3-C4-N9	3.82	133.66	127.17
2	B	700	ATP	C4-C5-N7	-3.68	106.38	110.58
2	D	700	ATP	N3-C2-N1	-3.63	123.09	128.58
2	A	700	ATP	C2-N3-C4	3.58	120.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	ATP	N3-C2-N1	-3.54	123.22	128.58
2	C	700	ATP	C2-N3-C4	3.47	120.31	111.83
2	C	700	ATP	C4-C5-N7	-3.45	106.64	110.58
2	D	700	ATP	C4-C5-N7	-3.39	106.70	110.58
2	B	700	ATP	C4-N9-C8	3.36	109.26	105.74
2	A	700	ATP	C4-N9-C8	3.36	109.26	105.74
2	D	700	ATP	C4-N9-C8	3.20	109.10	105.74
2	A	700	ATP	C5-N7-C8	2.95	108.08	103.45
2	B	700	ATP	C2-N3-C4	2.94	119.00	111.83
2	A	700	ATP	N3-C2-N1	-2.83	124.30	128.58
2	B	700	ATP	N3-C2-N1	-2.76	124.40	128.58
2	C	700	ATP	C6-C5-N7	2.70	137.29	132.09
2	C	700	ATP	N9-C8-N7	-2.68	110.13	113.94
2	B	700	ATP	C5-N7-C8	2.66	107.64	103.45
2	C	700	ATP	C5-N7-C8	2.66	107.63	103.45
2	B	700	ATP	C2-N1-C6	2.60	123.00	118.73
2	D	700	ATP	C5-N7-C8	2.55	107.46	103.45
2	A	700	ATP	C6-C5-N7	2.53	136.97	132.09
2	C	700	ATP	O3'-C3'-C4'	-2.43	104.11	111.08
2	A	700	ATP	N9-C8-N7	-2.42	110.50	113.94
2	C	700	ATP	O2B-PB-O1B	2.36	123.41	112.44
2	B	700	ATP	C6-C5-N7	2.31	136.55	132.09
2	D	700	ATP	C6-C5-N7	2.31	136.54	132.09
2	A	700	ATP	O3G-PG-O2G	2.30	116.42	107.80
2	D	700	ATP	N9-C8-N7	-2.28	110.70	113.94
2	C	700	ATP	O3G-PG-O2G	2.25	116.25	107.80
2	B	700	ATP	N9-C8-N7	-2.23	110.77	113.94
2	B	700	ATP	O2B-PB-O1B	2.18	122.60	112.44
2	C	700	ATP	O4'-C1'-N9	2.12	112.16	108.09
2	C	700	ATP	O3A-PA-O1A	-2.11	104.37	110.70
2	C	700	ATP	C4-N9-C1'	-2.08	121.76	126.63
2	C	700	ATP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	700	ATP	PG-O3B-PB-O1B
2	D	700	ATP	PB-O3B-PG-O3G
2	C	700	ATP	PG-O3B-PB-O1B
2	A	700	ATP	PG-O3B-PB-O2B
2	B	700	ATP	PG-O3B-PB-O1B

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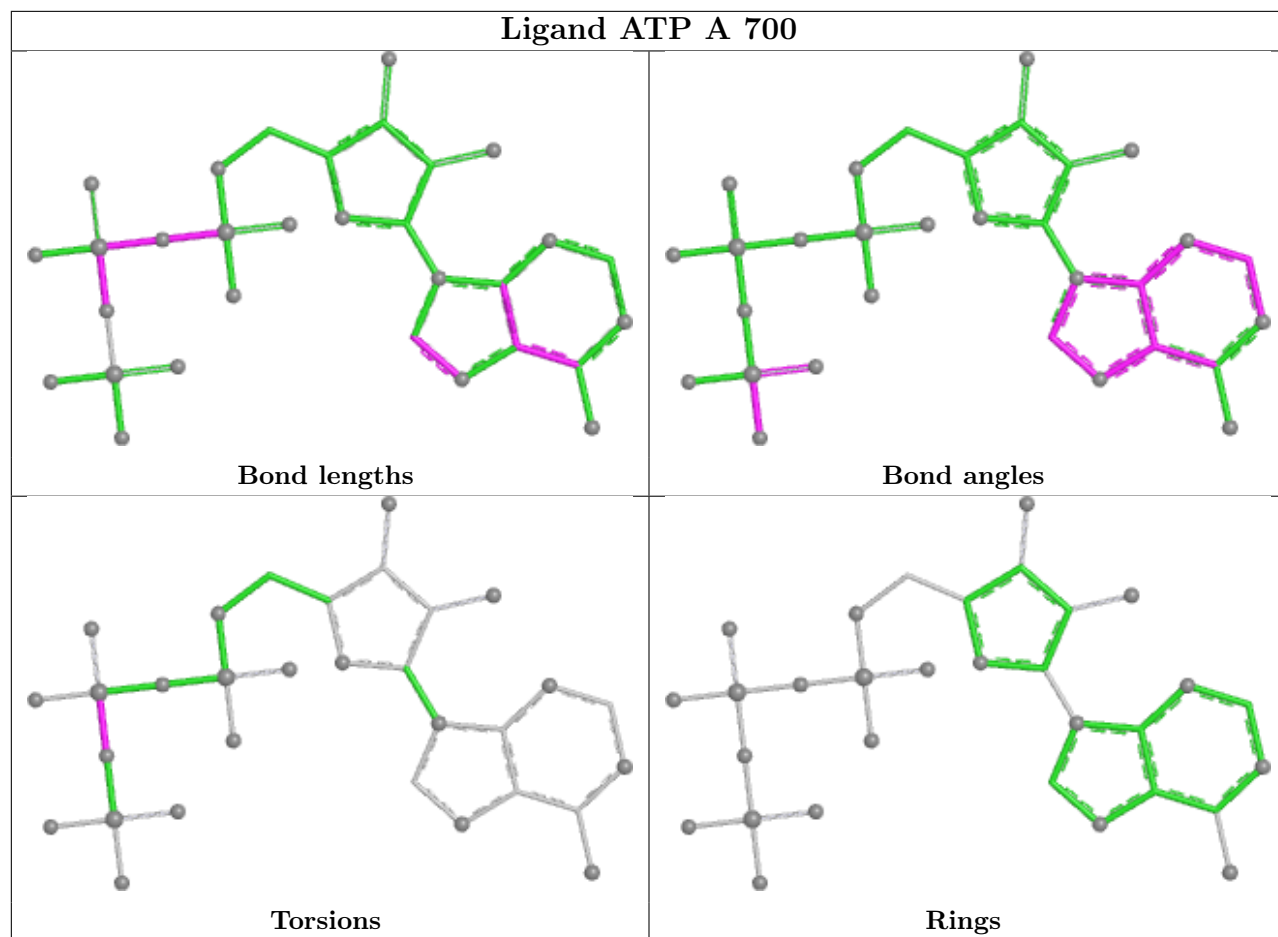
Mol	Chain	Res	Type	Atoms
2	D	700	ATP	PG-O3B-PB-O2B

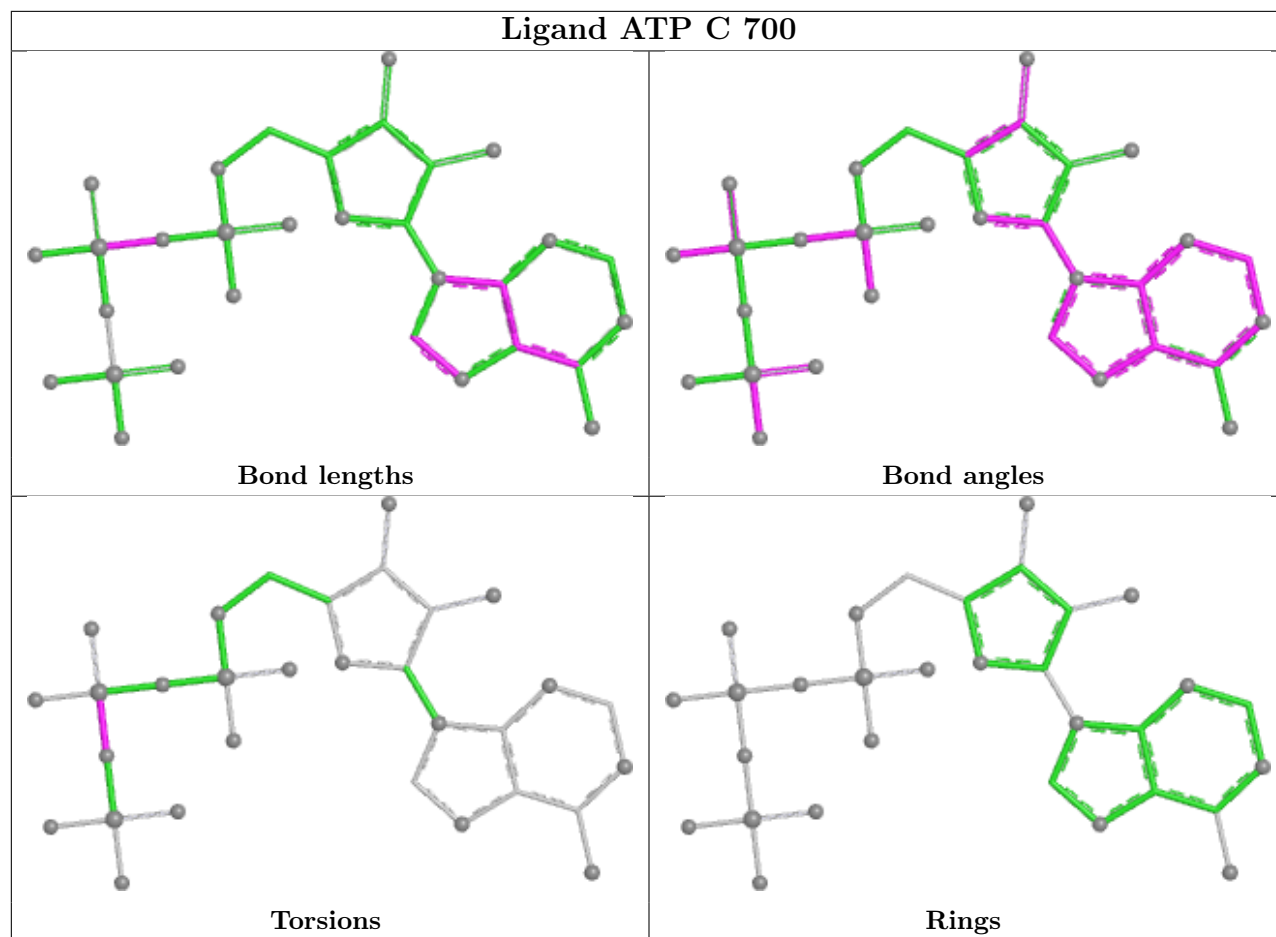
There are no ring outliers.

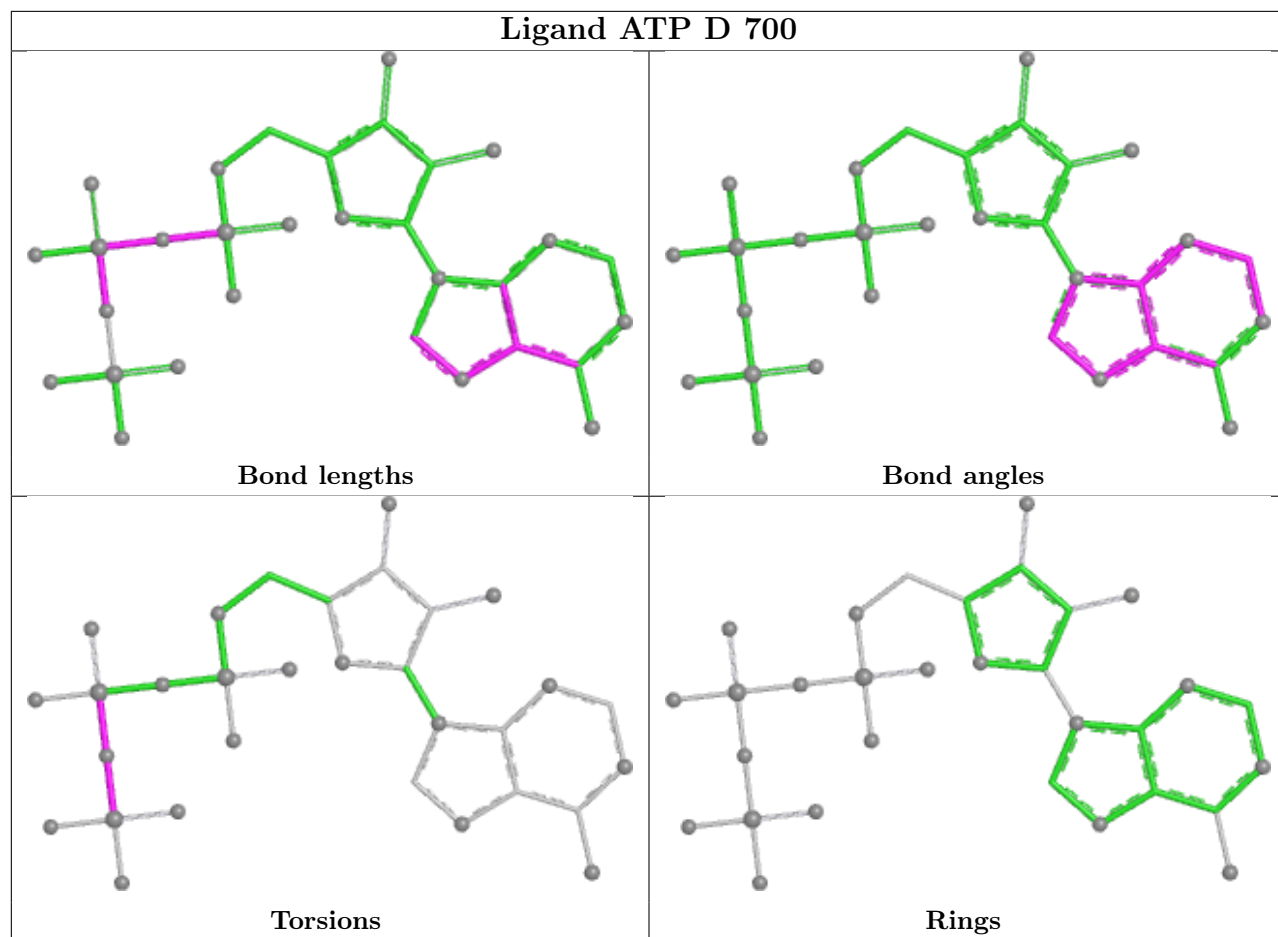
1 monomer is involved in 1 short contact:

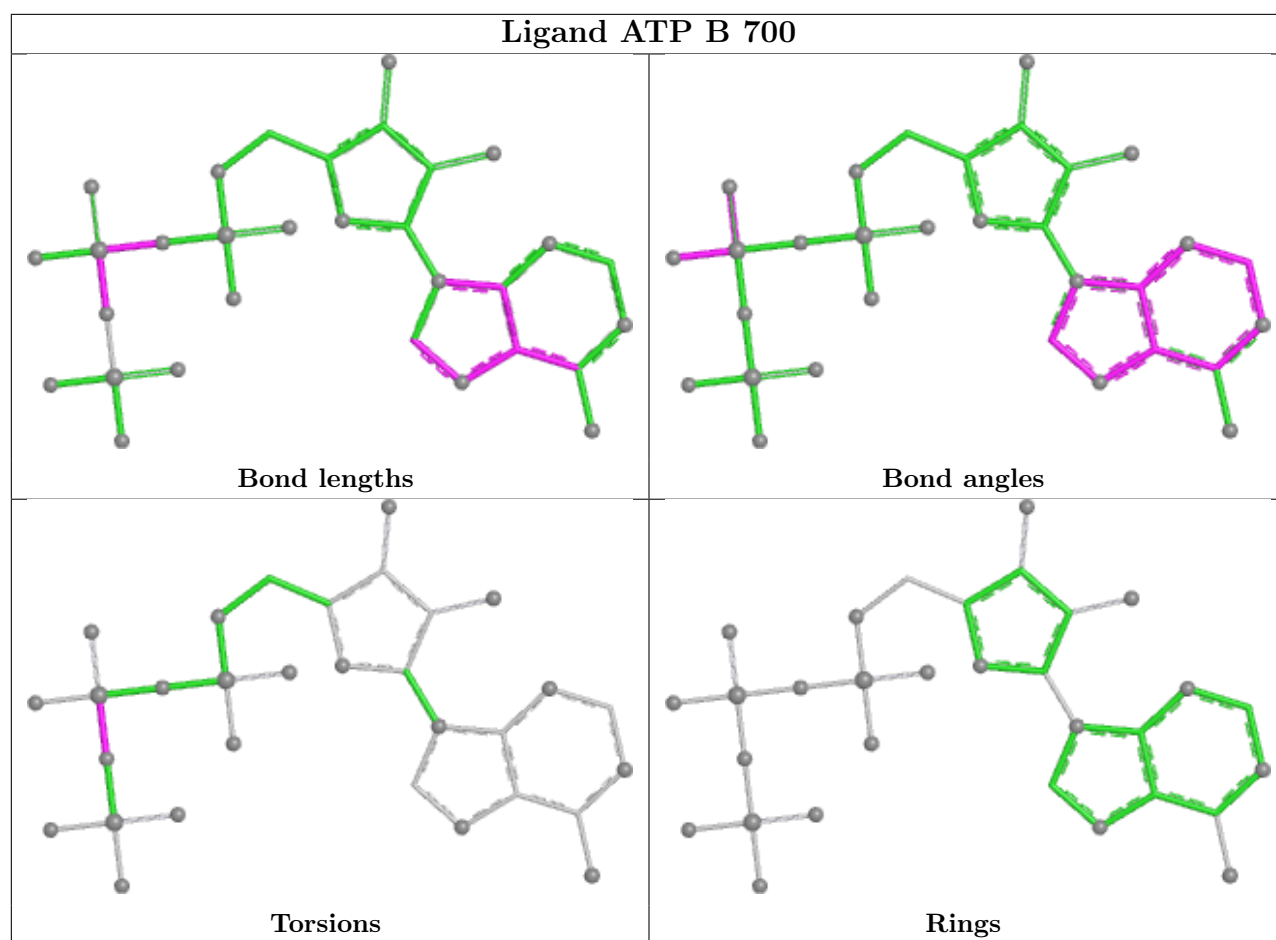
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	ATP	1	0

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	587/605 (97%)	0.27	33 (5%)	30	26	29, 60, 123, 196	0
1	B	583/605 (96%)	0.31	27 (4%)	37	33	31, 64, 130, 172	0
1	C	581/605 (96%)	0.34	37 (6%)	25	22	32, 66, 134, 168	0
1	D	581/605 (96%)	0.28	17 (2%)	53	50	34, 65, 115, 155	0
All	All	2332/2420 (96%)	0.30	114 (4%)	35	31	29, 64, 127, 196	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	286	ILE	4.9
1	A	405	GLY	4.8
1	A	257	LEU	4.5
1	C	59	VAL	4.3
1	C	284	PRO	4.2
1	D	286	ILE	4.1
1	C	295	HIS	4.0
1	C	550	VAL	4.0
1	D	462	ILE	3.8
1	C	257	LEU	3.8
1	C	594	VAL	3.6
1	B	212	GLY	3.6
1	A	260	GLN	3.5
1	C	285	TYR	3.5
1	A	43	THR	3.4
1	A	283	LEU	3.4
1	B	210	VAL	3.4
1	B	291	THR	3.4
1	A	247	ASP	3.4
1	A	185	THR	3.4
1	B	290	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	490	ASP	3.3
1	D	285	TYR	3.3
1	B	285	TYR	3.2
1	B	559	ALA	3.2
1	C	283	LEU	3.2
1	D	295	HIS	3.2
1	A	59	VAL	3.2
1	A	250	ILE	3.1
1	A	184	GLY	3.1
1	C	249	GLY	3.1
1	D	436	VAL	3.0
1	A	291	THR	3.0
1	C	282	ASN	2.9
1	B	257	LEU	2.9
1	A	212	GLY	2.9
1	B	186	GLY	2.9
1	A	503	ALA	2.8
1	C	288	ALA	2.8
1	A	292	GLY	2.8
1	D	186	GLY	2.8
1	A	286	ILE	2.8
1	B	59	VAL	2.8
1	C	60	THR	2.8
1	A	285	TYR	2.7
1	A	287	THR	2.7
1	C	434	SER	2.6
1	D	208	ASP	2.6
1	C	567	SER	2.6
1	C	571	ALA	2.6
1	C	261	ARG	2.6
1	D	449	ALA	2.6
1	D	283	LEU	2.6
1	B	563	THR	2.6
1	C	211	ASP	2.5
1	B	288	ALA	2.5
1	B	571	ALA	2.5
1	C	45	ASP	2.5
1	D	59	VAL	2.5
1	A	288	ALA	2.5
1	A	290	ALA	2.5
1	A	45	ASP	2.4
1	B	555	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	432	ASN	2.4
1	C	291	THR	2.4
1	B	462	ILE	2.4
1	C	250	ILE	2.4
1	A	294	LYS	2.4
1	B	47	CYS	2.4
1	C	435	ALA	2.4
1	C	48	THR	2.4
1	D	284	PRO	2.3
1	C	180	GLY	2.3
1	A	390	LEU	2.3
1	C	557	LEU	2.3
1	A	210	VAL	2.3
1	A	407	VAL	2.3
1	B	560	ASP	2.3
1	B	558	PRO	2.3
1	D	260	GLN	2.3
1	B	390	LEU	2.3
1	B	472	ILE	2.3
1	B	470	PRO	2.2
1	C	436	VAL	2.2
1	B	406	GLY	2.2
1	C	390	LEU	2.2
1	D	298	ILE	2.2
1	A	518	ASP	2.2
1	B	435	ALA	2.2
1	C	448	ALA	2.2
1	A	293	PRO	2.2
1	A	435	ALA	2.1
1	A	460	ASP	2.1
1	B	572	LEU	2.1
1	C	574	THR	2.1
1	B	423	SER	2.1
1	B	597	LYS	2.1
1	A	244	PHE	2.1
1	C	462	ILE	2.1
1	C	565	ILE	2.1
1	B	182	ASP	2.1
1	C	297	ASN	2.1
1	B	325	GLN	2.0
1	D	435	ALA	2.0
1	A	60	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	2.0
1	C	564	ALA	2.0
1	D	390	LEU	2.0
1	A	406	GLY	2.0
1	A	601	ILE	2.0
1	C	22	THR	2.0
1	C	293	PRO	2.0
1	C	431	ASP	2.0
1	D	211	ASP	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 [i](#)

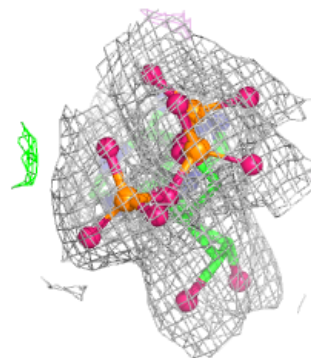
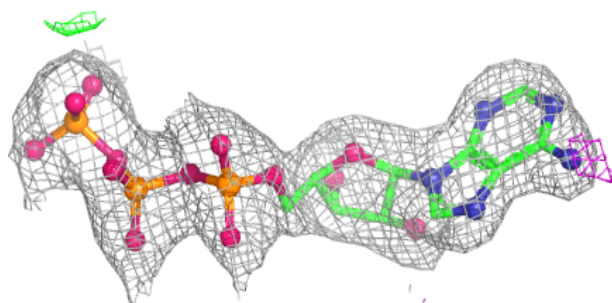
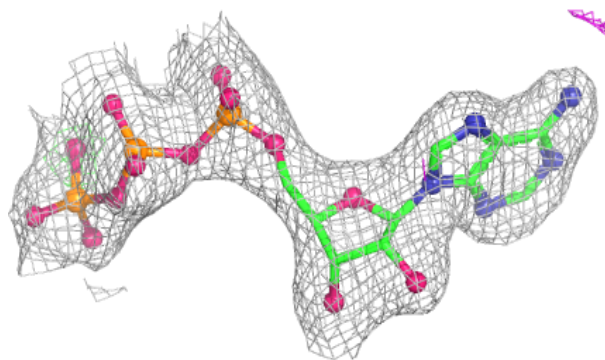
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	C	700	31/31	0.98	0.06	22,42,65,75	0
2	ATP	D	700	31/31	0.98	0.06	30,55,72,73	0
2	ATP	A	700	31/31	0.99	0.04	21,37,48,53	0
2	ATP	B	700	31/31	0.99	0.05	22,39,55,61	0
3	MG	A	701	1/1	0.99	0.05	35,35,35,35	0
3	MG	B	701	1/1	0.99	0.02	33,33,33,33	0
3	MG	C	701	1/1	0.99	0.03	33,33,33,33	0
3	MG	D	701	1/1	0.99	0.04	43,43,43,43	0

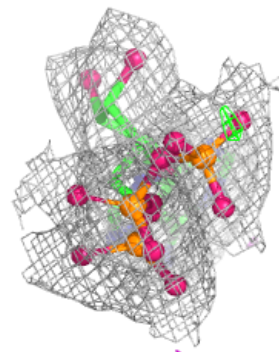
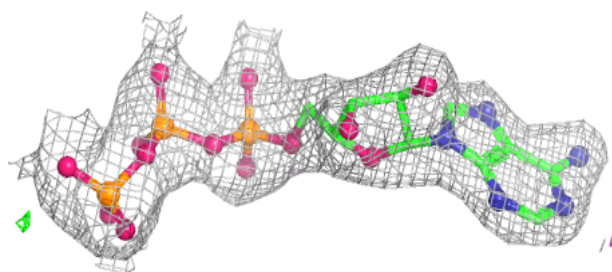
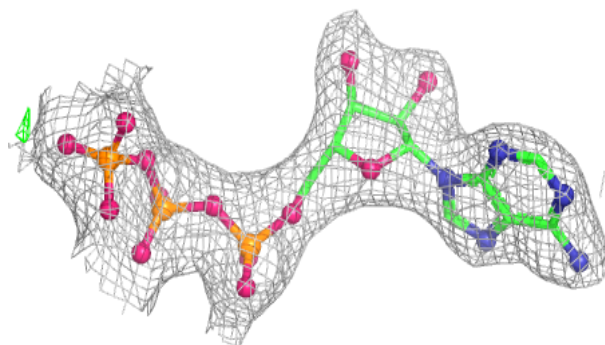
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 700:

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

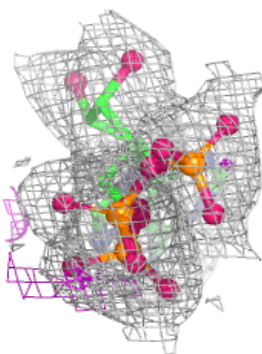
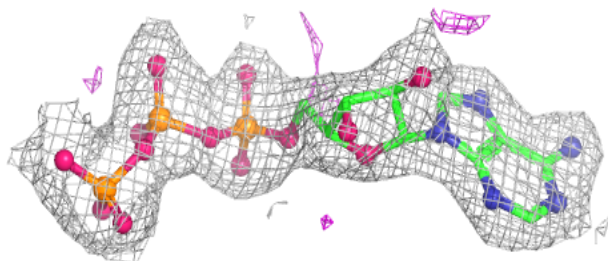
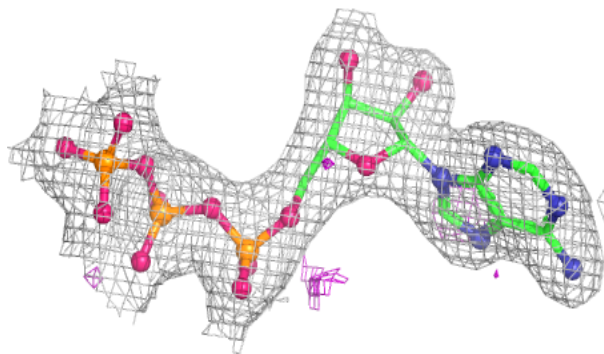
**Electron density around ATP D 700:**

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

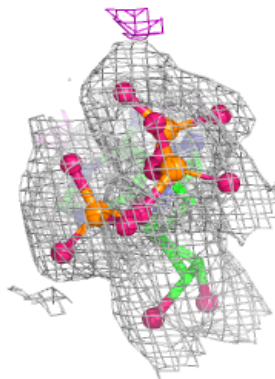
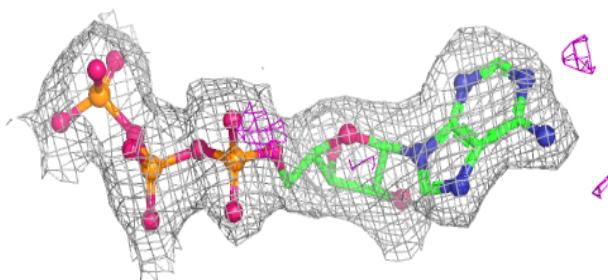
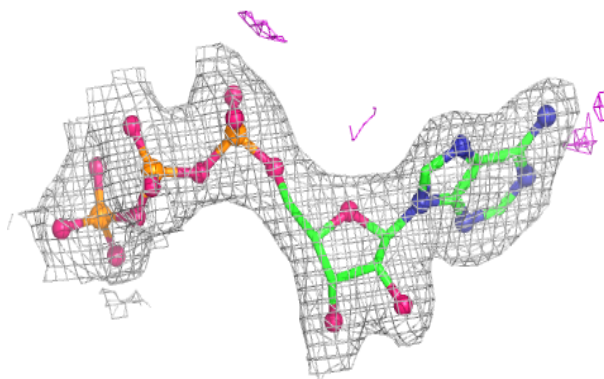


Electron density around ATP A 700:

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

**Electron density around ATP B 700:**

$2mF_o-DF_c$ (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.