Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:52 PM EDT

PDB ID	:	4B9Q
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 (i) 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 (i)) were used in the production of this report:

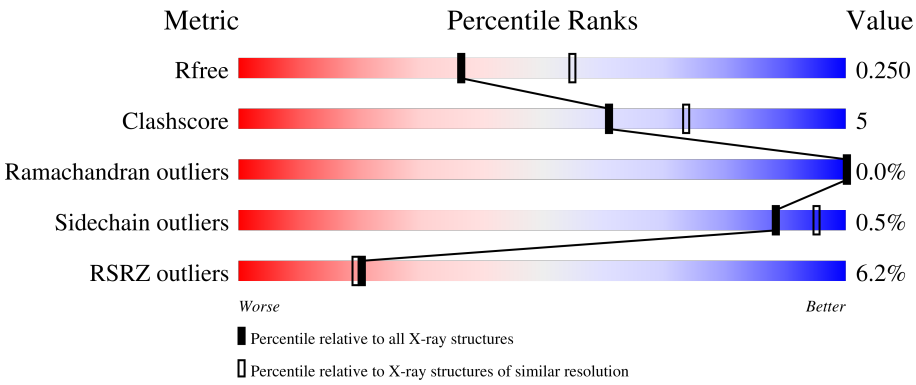
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	6% 89% 10% •
1	B	605	6% 88% 11% •
1	C	605	7% 87% 11% •
1	D	605	5% 88% 10% •

2 Entry composition (i)

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.

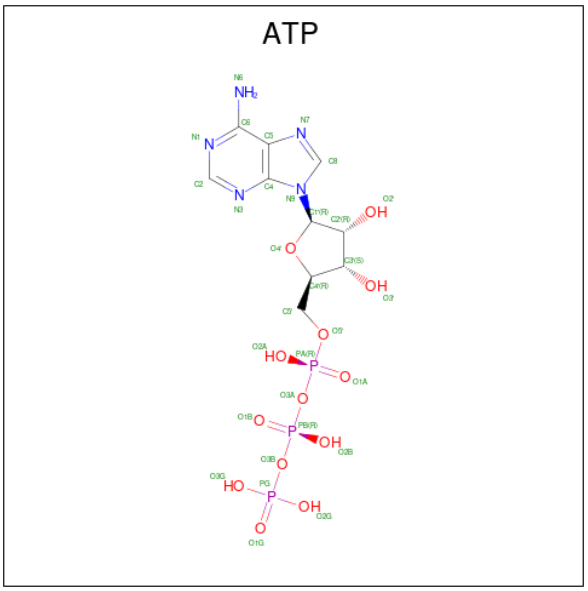
- Molecule 1 is a protein called CHAPERONE PROTEIN DNAK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	601	4554	2826	792	919	3	14	0	0	0
1	B	597	4534	2812	789	916	3	14	0	0	0
1	C	595	4515	2803	785	910	3	14	0	0	0
1	D	595	4515	2802	784	912	3	14	0	0	0

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

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

Continued on next page...

Continued from previous page...

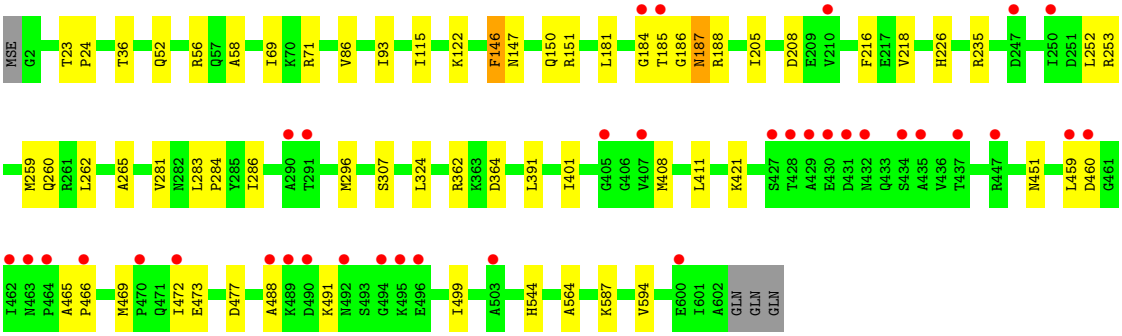
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	145	145	145	0	0
			Total	O		
4	C	115	115	115	0	0
			Total	O		
4	D	90	90	90	0	0

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.

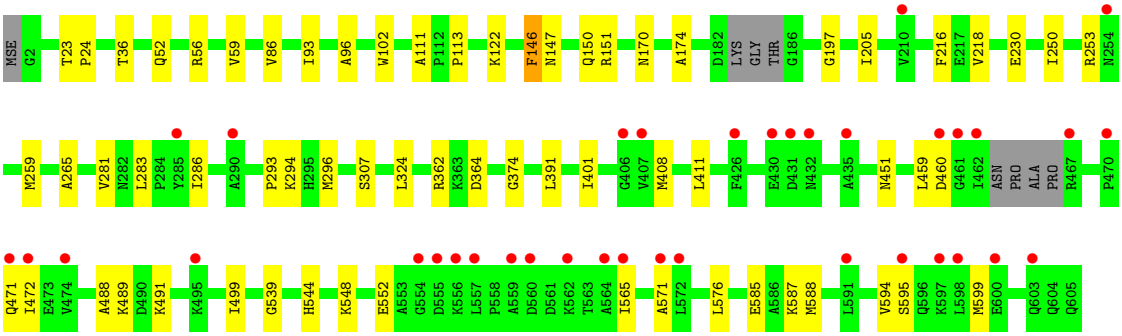
- Molecule 1: CHAPERONE PROTEIN DNAK

Chain A:



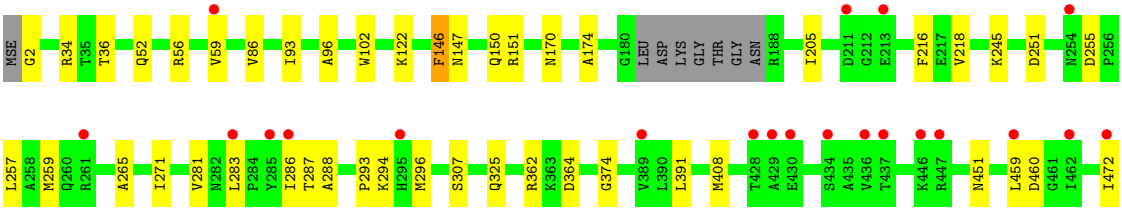
- Molecule 1: CHAPERONE PROTEIN DNAK

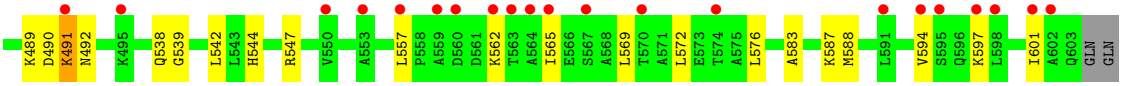
Chain B:



- Molecule 1: CHAPERONE PROTEIN DNAK

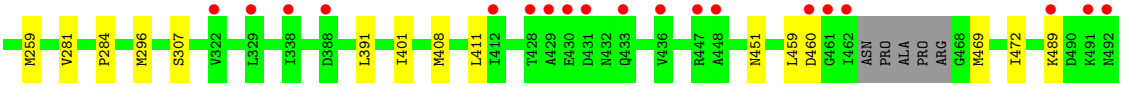
Chain C:

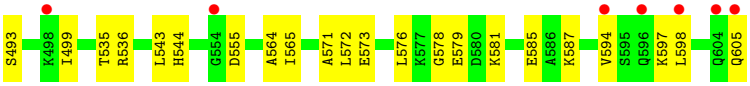




• Molecule 1: CHAPERONE PROTEIN DNAK

Chain D:





4 Data and refinement statistics (i)

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 65.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (59.72-2.40) 99.6 (65.28-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.33 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/4591	0.55	0/6182
1	B	0.40	0/4567	0.52	0/6144
1	C	0.40	0/4551	0.53	0/6127
1	D	0.39	0/4548	0.53	0/6119
All	All	0.40	0/18257	0.53	0/24572

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	4554	0	4605	51	0
1	B	4534	0	4579	40	0
1	C	4515	0	4565	45	0
1	D	4515	0	4562	38	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	165	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 (165) 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:CA	1:A:185:THR:HB	1.44	1.47
1:A:184:GLY:HA2	1:A:185:THR:CB	1.43	1.38
1:A:184:GLY:HA3	1:A:188:ARG:HE	1.50	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
1:A:186:GLY:O	1:A:187:ASN:C	2.29	0.69
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:A:186:GLY:O	1:A:188:ARG:N	2.37	0.57
1:B:59:VAL:HG21	1:D:284:PRO:HG2	1.85	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:186:GLY:C	1:A:188:ARG:N	2.70	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:595:SER:O	1:B:599:MSE:HG2	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	47 62
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
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 (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	491/480 (102%)	490 (100%)	1 (0%)	93	97
1	B	489/480 (102%)	487 (100%)	2 (0%)	91	96
1	C	487/480 (102%)	485 (100%)	2 (0%)	91	96
1	D	487/480 (102%)	482 (99%)	5 (1%)	76	88
All	All	1954/1920 (102%)	1944 (100%)	10 (0%)	88	95

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

Mol	Chain	Res	Type
1	A	146	PHE
1	B	146	PHE
1	B	286	ILE
1	C	146	PHE
1	C	491	LYS
1	D	45	ASP
1	D	146	PHE
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	605	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	D	700	3	28,33,33	1.08	3 (10%)	34,52,52	1.23	2 (5%)
2	ATP	B	700	3	28,33,33	1.10	3 (10%)	34,52,52	1.33	4 (11%)
2	ATP	A	700	3	28,33,33	1.17	4 (14%)	34,52,52	1.21	3 (8%)
2	ATP	C	700	3	28,33,33	1.07	2 (7%)	34,52,52	1.59	9 (26%)

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	D	700	3	-	3/18/38/38	0/3/3/3
2	ATP	B	700	3	-	1/18/38/38	0/3/3/3
2	ATP	A	700	3	-	1/18/38/38	0/3/3/3
2	ATP	C	700	3	-	1/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ATP	PB-O3B	3.02	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	ATP	PB-O3B	3.01	1.62	1.59
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	D	700	ATP	PA-O3A	2.36	1.62	1.59
2	B	700	ATP	O4'-C1'	2.33	1.43	1.40
2	D	700	ATP	PB-O3B	2.24	1.61	1.59
2	A	700	ATP	PA-O3A	2.12	1.61	1.59
2	A	700	ATP	C2-N3	2.08	1.35	1.32
2	C	700	ATP	C2-N3	2.04	1.35	1.32
2	B	700	ATP	PB-O3A	2.01	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	700	ATP	N3-C2-N1	-4.11	123.09	128.67
2	C	700	ATP	N3-C2-N1	-4.01	123.22	128.67
2	A	700	ATP	N3-C2-N1	-3.22	124.30	128.67
2	A	700	ATP	C4-C5-N7	-3.20	105.95	109.34
2	B	700	ATP	N3-C2-N1	-3.15	124.40	128.67
2	B	700	ATP	C4-C5-N7	-2.80	106.38	109.34
2	C	700	ATP	C1'-N9-C4	-2.78	121.76	126.64
2	C	700	ATP	O4'-C1'-N9	2.57	112.16	108.75
2	C	700	ATP	C4-C5-N7	-2.55	106.64	109.34
2	D	700	ATP	C4-C5-N7	-2.49	106.70	109.34
2	C	700	ATP	O3'-C3'-C4'	-2.43	104.11	111.08
2	C	700	ATP	O2B-PB-O1B	2.36	123.41	112.44
2	A	700	ATP	O3G-PG-O2G	2.30	116.42	107.80
2	C	700	ATP	C4'-O4'-C1'	-2.27	107.84	109.92
2	C	700	ATP	O3G-PG-O2G	2.25	116.25	107.80
2	B	700	ATP	O2B-PB-O1B	2.18	122.60	112.44
2	C	700	ATP	O3A-PA-O1A	-2.11	104.37	110.70
2	B	700	ATP	C4'-O4'-C1'	-2.09	108.01	109.92

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

Continued on next page...

Continued from previous page...

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

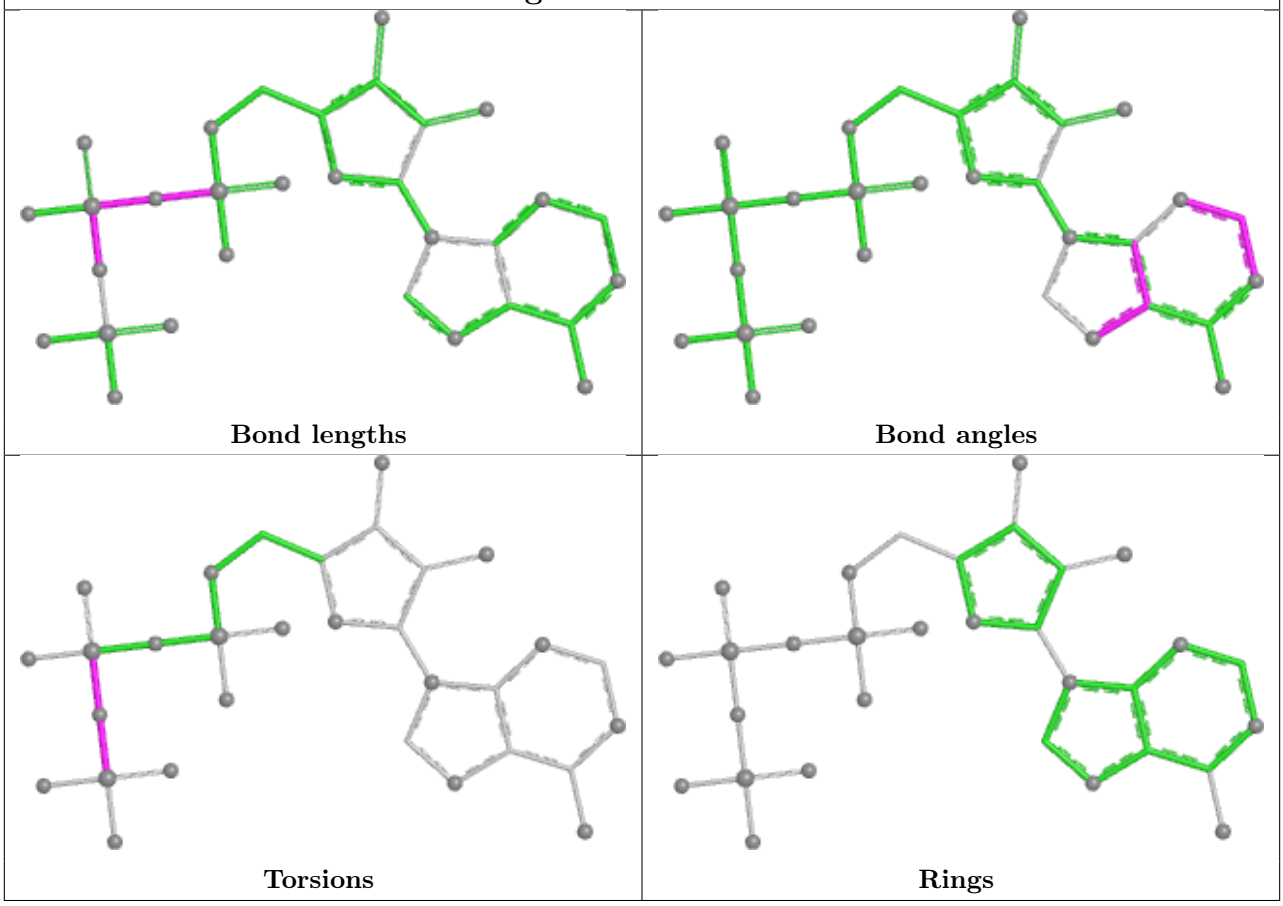
There are no ring outliers.

1 monomer is involved in 1 short contact:

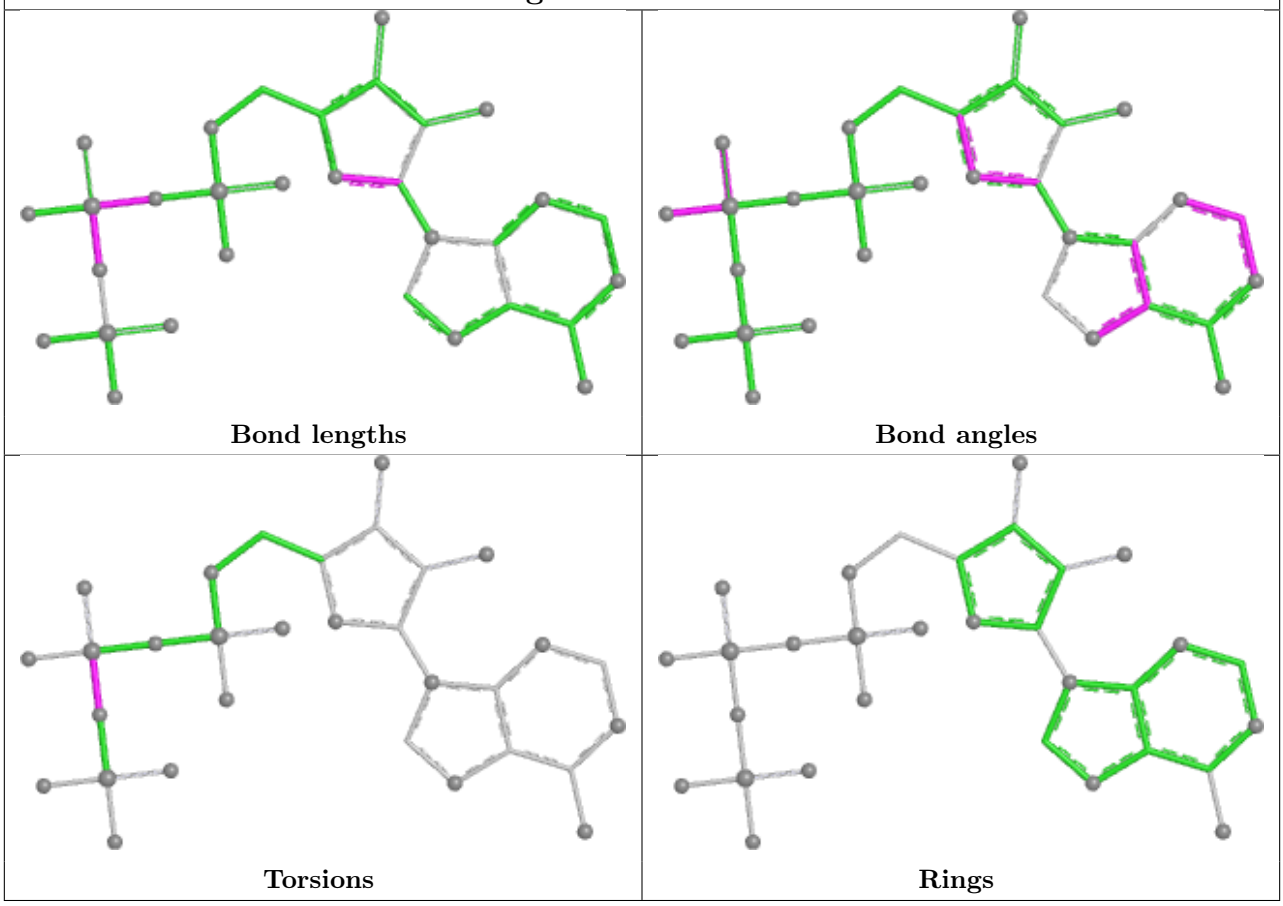
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	ATP	1	0

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 then 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.

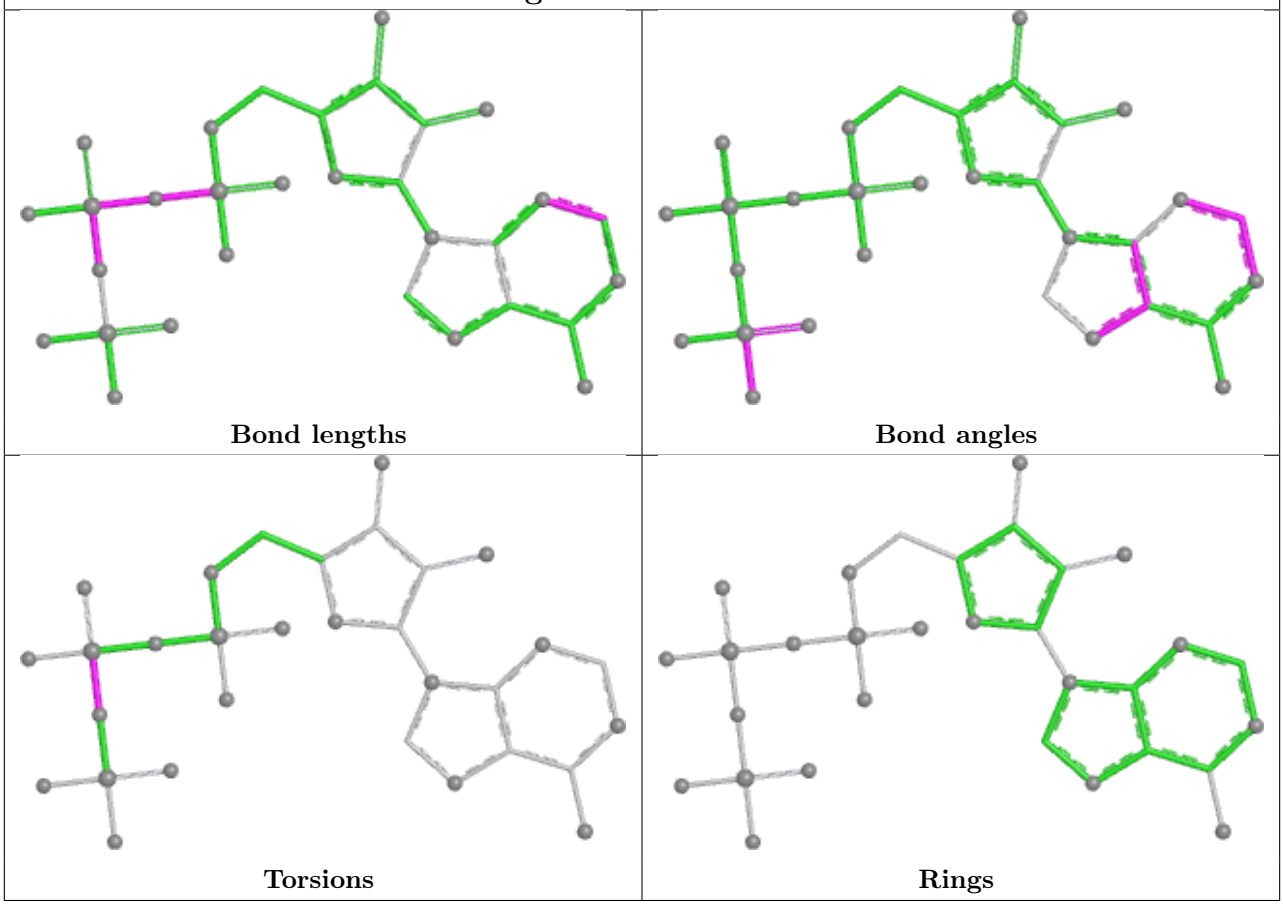
Ligand ATP D 700



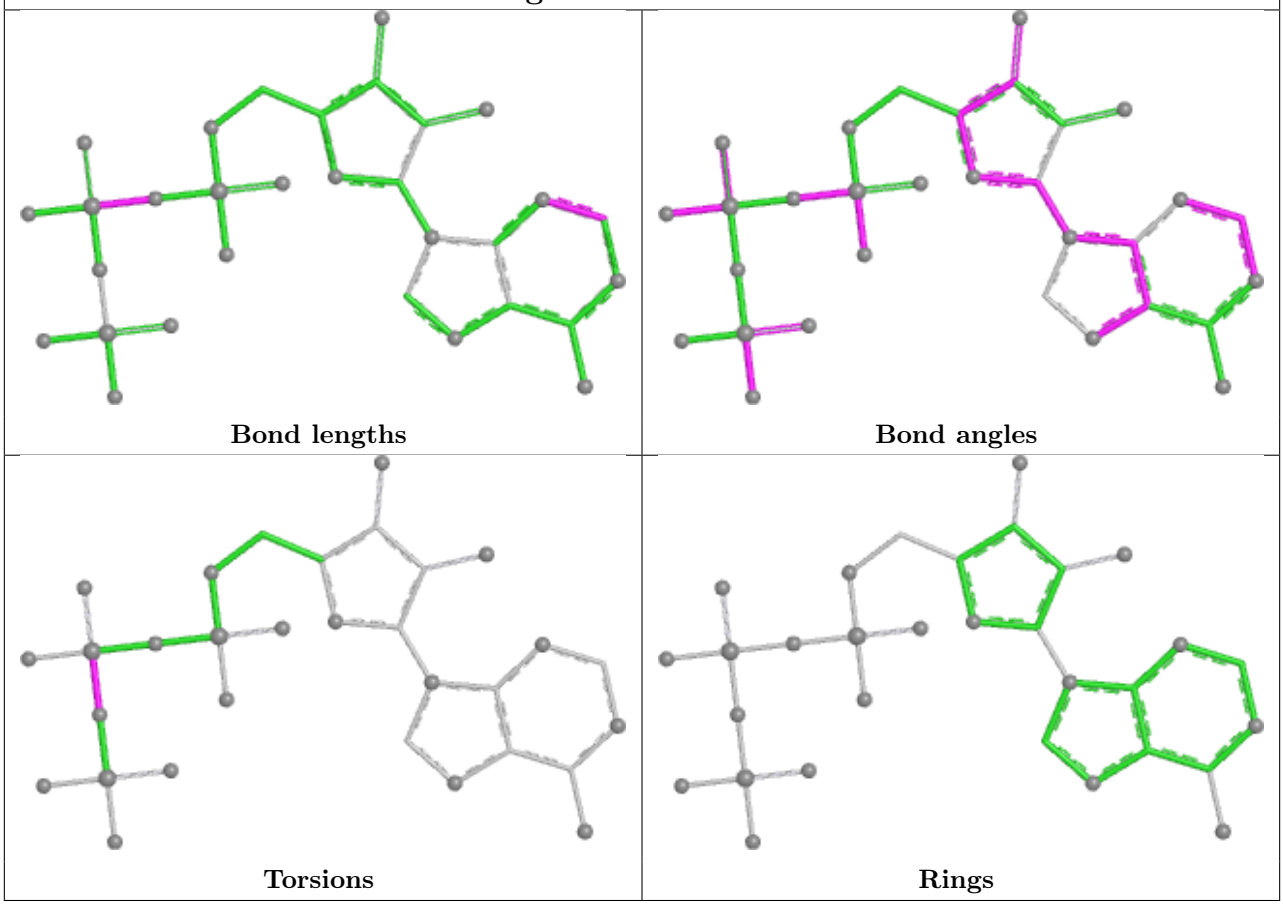
Ligand ATP B 700



Ligand ATP A 700



Ligand ATP C 700



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.47	36 (6%)	21	20	29, 60, 123, 196	0
1	B	583/605 (96%)	0.47	37 (6%)	20	18	31, 64, 130, 172	0
1	C	581/605 (96%)	0.48	42 (7%)	15	14	32, 66, 134, 168	0
1	D	581/605 (96%)	0.35	29 (4%)	28	27	34, 65, 115, 155	0
All	All	2332/2420 (96%)	0.44	144 (6%)	20	19	29, 64, 127, 196	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	9.0
1	D	462	ILE	7.1
1	A	472	ILE	6.4
1	A	435	ALA	5.7
1	C	550	VAL	5.7
1	B	598	LEU	5.6
1	C	597	LYS	5.6
1	C	557	LEU	5.5
1	C	562	LYS	5.2
1	B	597	LYS	5.2
1	C	567	SER	5.1
1	C	559	ALA	5.0
1	D	492	ASN	5.0
1	C	563	THR	5.0
1	B	600	GLU	4.9
1	A	432	ASN	4.8
1	A	490	ASP	4.6
1	A	470	PRO	4.5
1	B	472	ILE	4.5
1	A	494	GLY	4.5
1	B	471	GLN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	565	ILE	4.3
1	B	432	ASN	4.3
1	A	503	ALA	4.3
1	C	434	SER	4.2
1	B	431	ASP	4.1
1	C	491	LYS	4.1
1	B	555	ASP	4.1
1	D	322	VAL	4.0
1	A	464	PRO	4.0
1	C	429	ALA	3.9
1	C	462	ILE	3.9
1	B	470	PRO	3.8
1	C	598	LEU	3.6
1	D	213	GLU	3.5
1	A	427	SER	3.5
1	B	460	ASP	3.5
1	C	595	SER	3.5
1	C	472	ILE	3.5
1	B	591	LEU	3.4
1	B	406	GLY	3.4
1	A	428	THR	3.4
1	C	564	ALA	3.4
1	B	560	ASP	3.4
1	A	185	THR	3.4
1	D	447	ARG	3.4
1	C	553	ALA	3.4
1	B	290	ALA	3.3
1	A	431	ASP	3.3
1	B	435	ALA	3.2
1	D	431	ASP	3.2
1	B	572	LEU	3.2
1	B	461	GLY	3.2
1	C	560	ASP	3.2
1	D	433	GLN	3.2
1	A	405	GLY	3.1
1	B	595	SER	3.1
1	A	437	THR	3.1
1	C	389	VAL	3.1
1	D	428	THR	3.0
1	A	463	ASN	3.0
1	B	495	LYS	3.0
1	B	564	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	246	LYS	2.9
1	A	434	SER	2.9
1	C	430	GLU	2.9
1	B	462	ILE	2.9
1	B	557	LEU	2.9
1	C	570	THR	2.9
1	D	491	LYS	2.9
1	C	594	VAL	2.9
1	D	461	GLY	2.8
1	C	286	ILE	2.8
1	D	448	ALA	2.8
1	B	254	ASN	2.8
1	C	601	ILE	2.8
1	D	430	GLU	2.8
1	A	407	VAL	2.7
1	A	462	ILE	2.7
1	D	498	LYS	2.7
1	A	447	ARG	2.7
1	C	447	ARG	2.7
1	B	426	PHE	2.7
1	A	488	ALA	2.6
1	B	565	ILE	2.6
1	A	184	GLY	2.6
1	C	591	LEU	2.6
1	B	556	LYS	2.6
1	A	495	LYS	2.6
1	B	474	VAL	2.6
1	D	598	LEU	2.6
1	A	460	ASP	2.6
1	C	437	THR	2.5
1	D	594	VAL	2.5
1	A	459	LEU	2.5
1	A	600	GLU	2.5
1	A	429	ALA	2.4
1	B	603	GLN	2.4
1	D	436	VAL	2.4
1	A	492	ASN	2.4
1	D	329	LEU	2.4
1	C	446	LYS	2.4
1	A	291	THR	2.4
1	B	285	TYR	2.3
1	B	559	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	602	ALA	2.3
1	C	254	ASN	2.3
1	A	247	ASP	2.3
1	A	430	GLU	2.3
1	D	429	ALA	2.3
1	D	596	GLN	2.3
1	D	338	ILE	2.3
1	C	295	HIS	2.3
1	C	495	LYS	2.3
1	B	554	GLY	2.3
1	C	285	TYR	2.3
1	D	412	ILE	2.2
1	B	407	VAL	2.2
1	C	283	LEU	2.2
1	A	250	ILE	2.2
1	C	428	THR	2.2
1	C	59	VAL	2.2
1	C	574	THR	2.2
1	B	571	ALA	2.1
1	C	261	ARG	2.1
1	D	554	GLY	2.1
1	B	562	LYS	2.1
1	D	489	LYS	2.1
1	B	467	ARG	2.1
1	D	460	ASP	2.1
1	A	466	PRO	2.1
1	A	496	GLU	2.1
1	D	245	LYS	2.1
1	A	210	VAL	2.1
1	D	388	ASP	2.1
1	C	459	LEU	2.1
1	B	430	GLU	2.1
1	B	210	VAL	2.1
1	D	604	GLN	2.0
1	C	436	VAL	2.0
1	A	489	LYS	2.0
1	D	605	GLN	2.0
1	C	211	ASP	2.0
1	C	213	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

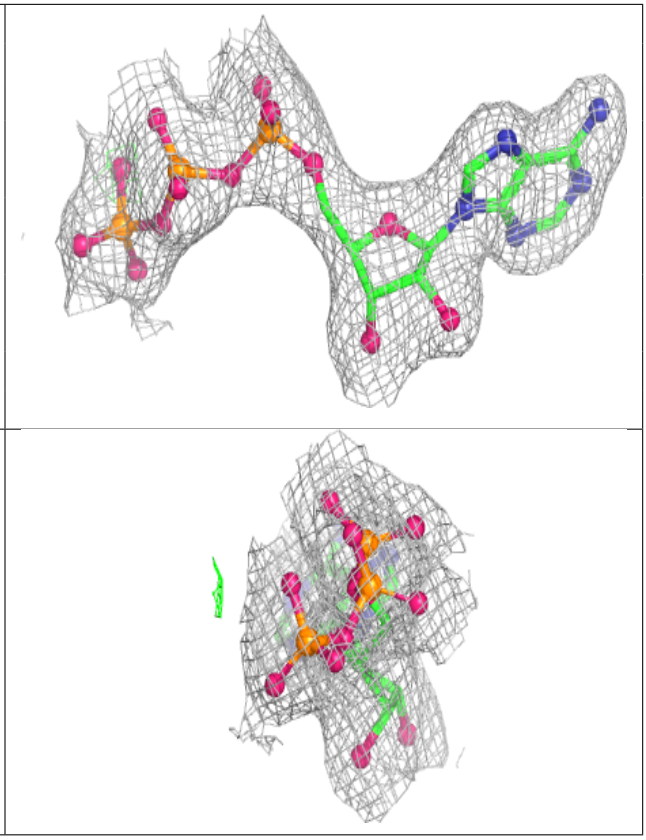
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	701	1/1	0.97	0.09	33,33,33,33	0
3	MG	C	701	1/1	0.97	0.06	33,33,33,33	0
2	ATP	C	700	31/31	0.98	0.16	22,42,65,75	0
2	ATP	D	700	31/31	0.98	0.14	30,55,72,73	0
3	MG	A	701	1/1	0.99	0.06	35,35,35,35	0
2	ATP	A	700	31/31	0.99	0.15	21,37,48,53	0
2	ATP	B	700	31/31	0.99	0.16	22,39,55,61	0
3	MG	D	701	1/1	0.99	0.11	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.

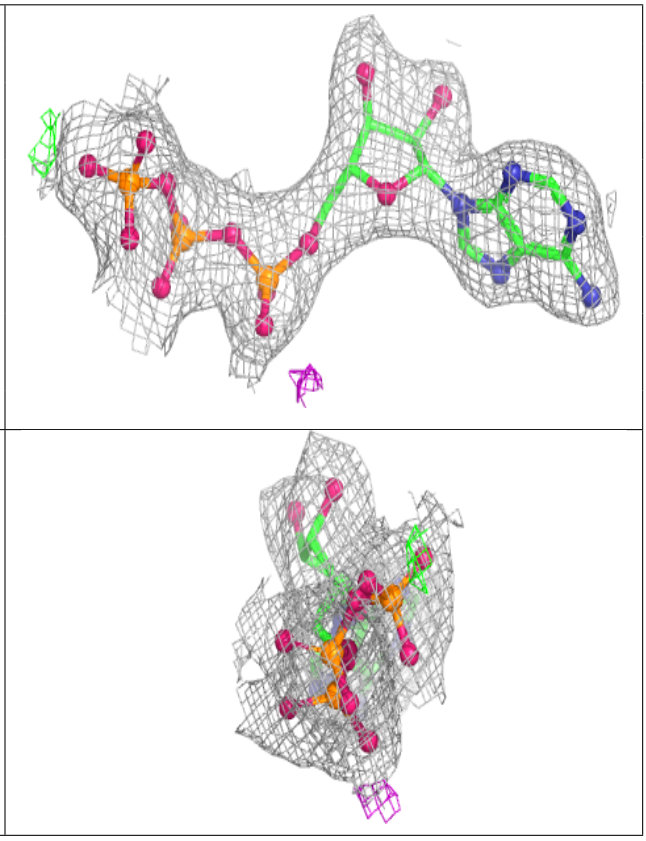
Electron density around ATP C 700:

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



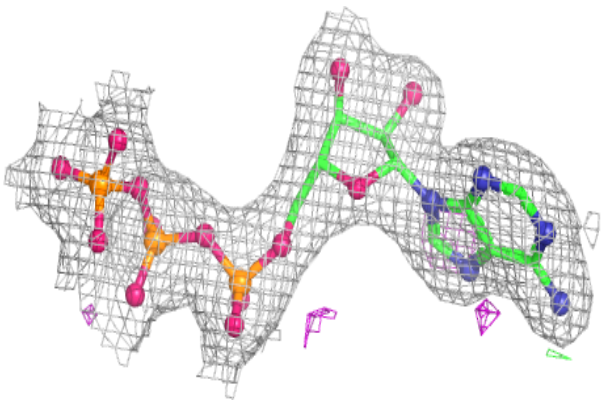
Electron density around ATP D 700:

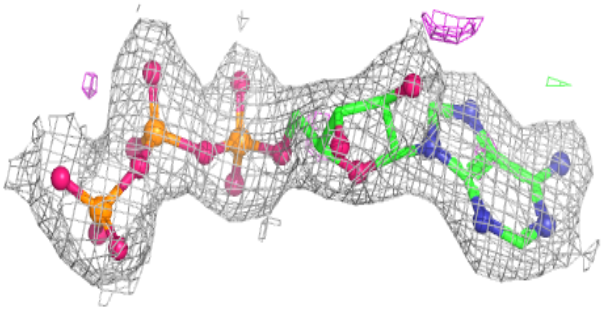
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

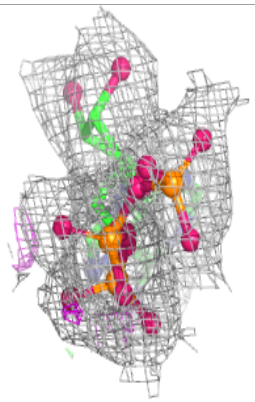


Electron density around ATP A 700:

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

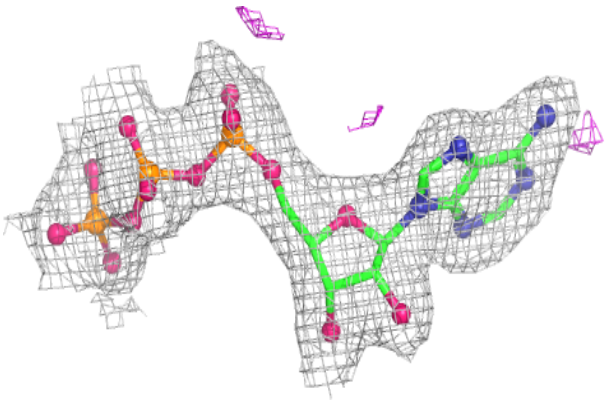


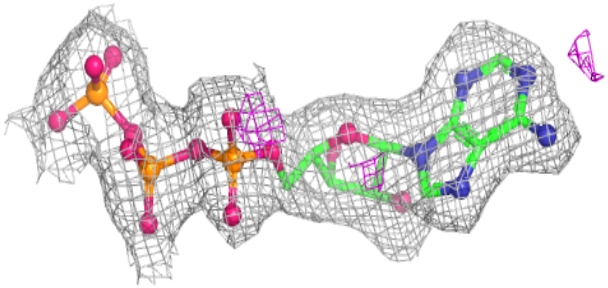


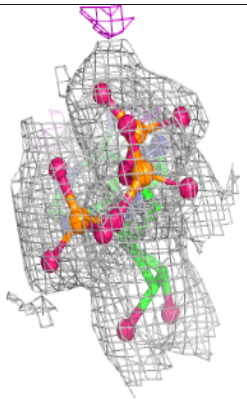


Electron density around ATP B 700:

$2mF_o$-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.