



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:37 PM UTC

PDB ID : 4JNE / pdb_00004jne
Title : Allosteric opening of the polypeptide-binding site when an Hsp70 binds ATP
Authors : Qi, R.; Sarbeng, E.B.; Liu, Q.; Le, K.Q.; Xu, X.; Xu, H.; Yang, J.; Wong, J.L.;
Vorvis, C.; Hendrickson, W.A.; Zhou, L.; Liu, Q.
Deposited on : 2013-03-15
Resolution : 1.96 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

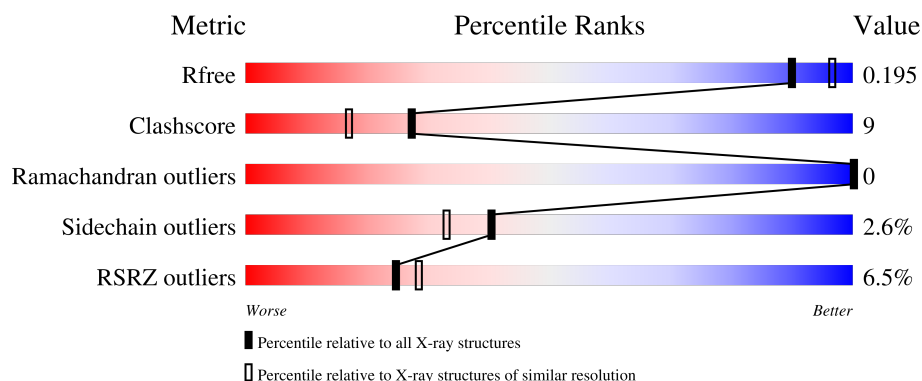
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	608	5% 83% 15% ..
1	B	608	8% 82% 15% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10677 atoms, of which 32 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 Hsp70 CHAPERONE DnaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4550	2828	791	915	16			
1	B	600	Total	C	N	O	S	0	0	0
			4550	2828	791	915	16			

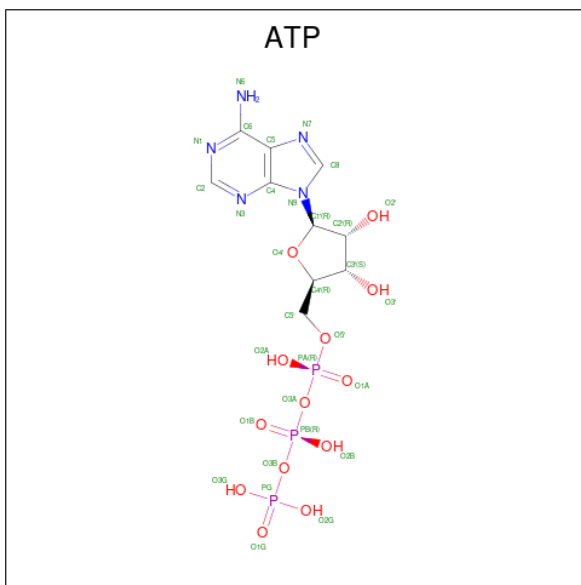
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P0A6Y8
A	199	ALA	THR	conflict	UNP P0A6Y8
A	?	-	THR	deletion	UNP P0A6Y8
A	?	-	ALA	deletion	UNP P0A6Y8
A	?	-	GLU	deletion	UNP P0A6Y8
A	?	-	ASP	deletion	UNP P0A6Y8
A	428	MET	ASN	engineered mutation	UNP P0A6Y8
A	429	GLY	GLN	engineered mutation	UNP P0A6Y8
A	430	GLY	SER	engineered mutation	UNP P0A6Y8
A	611	HIS	-	expression tag	UNP P0A6Y8
A	612	ALA	-	expression tag	UNP P0A6Y8
B	1	SER	-	expression tag	UNP P0A6Y8
B	199	ALA	THR	conflict	UNP P0A6Y8
B	?	-	THR	deletion	UNP P0A6Y8
B	?	-	ALA	deletion	UNP P0A6Y8
B	?	-	GLU	deletion	UNP P0A6Y8
B	?	-	ASP	deletion	UNP P0A6Y8
B	428	MET	ASN	engineered mutation	UNP P0A6Y8
B	429	GLY	GLN	engineered mutation	UNP P0A6Y8
B	430	GLY	SER	engineered mutation	UNP P0A6Y8
B	611	HIS	-	expression tag	UNP P0A6Y8
B	612	ALA	-	expression tag	UNP P0A6Y8

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	1
			10	8	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

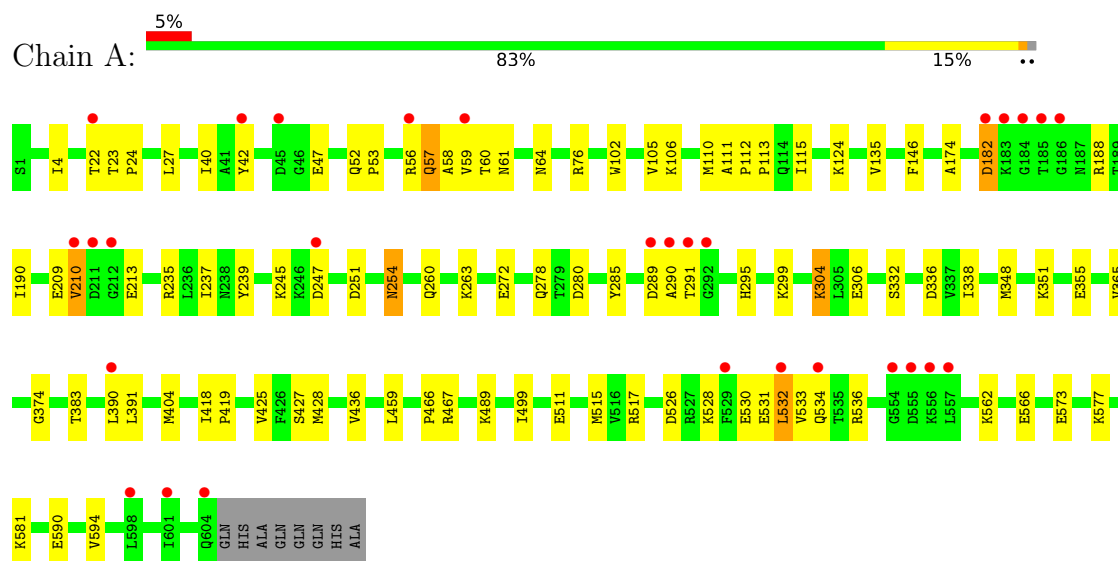
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	680	Total	O	0	0
			680	680		
6	B	717	Total	O	0	0
			717	717		

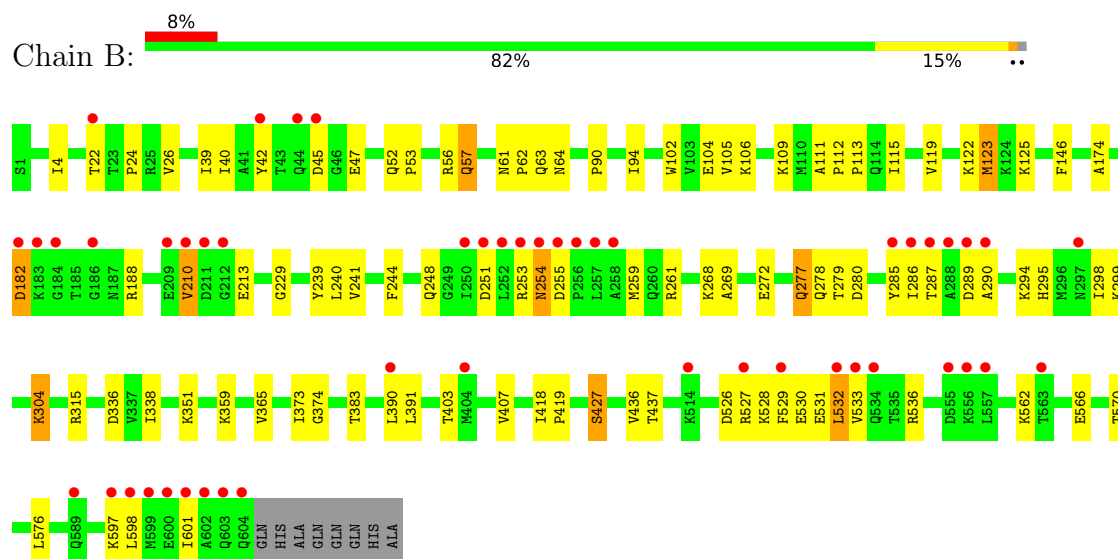
3 Residue-property plots [i](#)

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: Hsp70 CHAPERONE DnaK



• Molecule 1: Hsp70 CHAPERONE DnaK



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	290.68Å 290.68Å 99.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 1.96 29.97 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.97-1.96) 99.8 (29.97-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 1.97Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.173 , 0.201 0.168 , 0.195	Depositor DCC
R_{free} test set	7542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10677	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, SO4, 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	0.35	0/4602	0.69	0/6217
1	B	0.36	0/4602	0.70	0/6217
All	All	0.36	0/9204	0.69	0/12434

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

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	4550	0	4610	79	0
1	B	4550	0	4610	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	25	0	0	0	0
4	B	35	0	0	0	0
5	A	12	16	16	3	0
5	B	12	16	16	2	0
6	A	680	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	717	0	0	16	0
All	All	10645	32	9276	168	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 9.

All (168) 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:B:123:MET:HA	1:B:123:MET:HE2	1.23	1.16
1:A:285:TYR:H	1:A:295:HIS:HD2	1.08	1.00
1:B:42:TYR:HD2	1:B:105:VAL:HG11	1.36	0.91
1:B:123:MET:SD	6:B:1210:HOH:O	2.28	0.90
1:B:531:GLU:HG3	6:B:1573:HOH:O	1.71	0.89
1:B:123:MET:HA	1:B:123:MET:CE	2.04	0.87
1:B:123:MET:HE2	1:B:123:MET:CA	2.05	0.84
1:B:280:ASP:OD1	1:B:299:LYS:HG2	1.78	0.83
1:A:285:TYR:H	1:A:295:HIS:CD2	1.94	0.82
1:A:42:TYR:HD2	1:A:105:VAL:HG11	1.43	0.80
1:A:534:GLN:HG3	6:A:1699:HOH:O	1.82	0.80
1:B:63:GLN:HA	6:B:1737:HOH:O	1.85	0.76
1:B:123:MET:CE	1:B:123:MET:CA	2.64	0.74
1:B:255:ASP:O	1:B:259:MET:HG2	1.88	0.74
1:B:64:ASN:HD22	1:B:106:LYS:HE2	1.53	0.72
1:B:285:TYR:H	1:B:295:HIS:HD2	1.37	0.72
1:B:285:TYR:H	1:B:295:HIS:CD2	2.07	0.72
1:A:57:GLN:HE22	1:A:61:ASN:HD22	1.37	0.71
1:A:280:ASP:OD1	1:A:299:LYS:HG2	1.90	0.70
1:B:390:LEU:HD23	1:B:391:LEU:N	2.06	0.70
1:A:278:GLN:OE1	1:B:536:ARG:HD2	1.90	0.70
1:A:245:LYS:HZ3	1:A:251:ASP:HB2	1.57	0.69
1:B:289:ASP:OD1	1:B:290:ALA:N	2.29	0.66
1:A:285:TYR:N	1:A:295:HIS:HD2	1.88	0.66
1:B:64:ASN:ND2	1:B:106:LYS:HE2	2.12	0.65
1:A:245:LYS:NZ	1:A:251:ASP:HB2	2.12	0.64
1:B:42:TYR:CD2	1:B:105:VAL:HG11	2.25	0.64
1:A:64:ASN:HD22	1:A:106:LYS:HE2	1.61	0.64
1:B:57:GLN:HE22	1:B:61:ASN:HD22	1.45	0.63
1:B:562:LYS:O	1:B:566:GLU:HG3	1.97	0.63
1:B:531:GLU:N	6:B:1573:HOH:O	2.22	0.62
1:A:27:LEU:HA	5:A:1008:GOL:H12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:119:VAL:HG23	1.81	0.61
1:A:64:ASN:ND2	1:A:106:LYS:HE2	2.15	0.61
1:B:123:MET:N	1:B:123:MET:HE3	2.16	0.61
1:A:526:ASP:O	1:A:530:GLU:HG3	2.01	0.61
1:A:190:ILE:HG22	1:A:336:ASP:HB2	1.83	0.60
1:B:40:ILE:N	1:B:40:ILE:HD12	2.17	0.60
1:A:390:LEU:HD23	1:A:391:LEU:N	2.17	0.59
1:A:511:GLU:O	1:A:515:MET:HG3	2.02	0.59
1:B:391:LEU:C	1:B:391:LEU:HD12	2.27	0.58
1:B:4:ILE:HD12	1:B:383:THR:HG23	1.86	0.58
1:B:94:ILE:HD13	1:B:104:GLU:HB2	1.86	0.57
1:A:562:LYS:O	1:A:566:GLU:HG3	2.03	0.57
6:A:1753:HOH:O	1:B:299:LYS:HE2	2.05	0.57
1:B:188:ARG:HD3	1:B:336:ASP:OD2	2.05	0.56
1:A:40:ILE:HD12	1:A:40:ILE:N	2.20	0.56
1:B:123:MET:CE	1:B:123:MET:N	2.69	0.56
1:A:304:LYS:HA	1:A:304:LYS:HE3	1.88	0.56
1:B:122:LYS:C	1:B:123:MET:HE3	2.31	0.56
1:A:338:ILE:HD12	1:A:365:VAL:HG21	1.88	0.56
1:B:248:GLN:HE21	1:B:294:LYS:HD2	1.69	0.56
1:A:209:GLU:O	1:A:209:GLU:HG3	2.06	0.56
1:A:289:ASP:HB3	1:A:291:THR:OG1	2.06	0.55
1:A:418:ILE:HA	1:A:419:PRO:C	2.32	0.55
1:B:90:PRO:C	6:B:1737:HOH:O	2.50	0.55
1:B:315:ARG:HH12	5:B:1010:GOL:H32	1.72	0.54
1:A:188:ARG:HD3	1:A:336:ASP:OD2	2.07	0.54
1:B:351:LYS:HE2	6:B:1768:HOH:O	2.06	0.54
1:A:254:ASN:H	1:A:254:ASN:HD22	1.55	0.54
1:A:532:LEU:HD22	1:A:581:LYS:HG3	1.89	0.54
1:B:94:ILE:HD12	1:B:109:LYS:HE3	1.90	0.53
1:B:526:ASP:O	1:B:530:GLU:HG3	2.09	0.53
1:A:254:ASN:HD22	1:A:254:ASN:N	2.07	0.53
1:B:536:ARG:NH1	1:B:576:LEU:O	2.41	0.53
1:B:64:ASN:ND2	6:B:1723:HOH:O	2.42	0.53
1:A:532:LEU:HD12	1:A:536:ARG:NE	2.24	0.52
1:B:268:LYS:HG3	6:B:1750:HOH:O	2.09	0.52
1:B:278:GLN:NE2	1:B:299:LYS:HD2	2.24	0.52
1:A:59:VAL:HG13	1:A:60:THR:HG23	1.92	0.52
1:A:573:GLU:O	1:A:577:LYS:HD3	2.10	0.52
1:B:533:VAL:HG23	6:B:1283:HOH:O	2.09	0.52
1:A:237:ILE:HD11	1:A:263:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HH22	5:B:1010:GOL:H2	1.75	0.51
1:A:532:LEU:HD12	1:A:536:ARG:HE	1.76	0.51
1:B:239:TYR:CZ	1:B:304:LYS:HD3	2.45	0.51
1:B:210:VAL:O	1:B:213:GLU:HG2	2.11	0.51
1:B:285:TYR:N	1:B:295:HIS:HD2	2.08	0.51
1:A:4:ILE:HD12	1:A:383:THR:HG23	1.94	0.50
1:A:489:LYS:HE2	6:A:1711:HOH:O	2.12	0.50
1:B:26:VAL:HG23	1:B:373:ILE:HD11	1.94	0.50
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.94	0.50
1:A:427:SER:HB2	1:A:436:VAL:CG2	2.42	0.49
1:A:533:VAL:HG23	6:A:1359:HOH:O	2.13	0.49
1:B:94:ILE:CD1	1:B:109:LYS:HG2	2.43	0.49
1:A:59:VAL:HA	1:A:260:GLN:HG3	1.95	0.49
1:A:210:VAL:O	1:A:213:GLU:HG2	2.13	0.49
1:B:359:LYS:HE3	6:B:1538:HOH:O	2.12	0.48
1:B:418:ILE:HA	1:B:419:PRO:C	2.38	0.48
1:A:351:LYS:O	1:A:355:GLU:HG3	2.13	0.48
1:B:277:GLN:HE21	1:B:277:GLN:HB3	1.54	0.48
1:B:286:ILE:HG23	1:B:287:THR:HG22	1.96	0.48
1:A:182:ASP:OD1	1:A:182:ASP:N	2.47	0.47
1:B:241:VAL:HG11	1:B:253:ARG:HG3	1.95	0.47
1:B:527:ARG:O	6:B:1573:HOH:O	2.20	0.47
1:A:210:VAL:O	1:A:210:VAL:HG12	2.14	0.47
1:B:528:LYS:C	6:B:1573:HOH:O	2.57	0.47
1:B:47:GLU:HB2	1:B:529:PHE:CZ	2.50	0.47
1:B:210:VAL:O	1:B:210:VAL:HG12	2.13	0.47
1:A:528:LYS:O	1:A:531:GLU:HG3	2.14	0.47
1:B:241:VAL:HG11	1:B:253:ARG:CZ	2.45	0.47
1:B:597:LYS:O	1:B:601:ILE:HG13	2.15	0.47
1:A:425:VAL:HG11	1:A:428:MET:CE	2.46	0.46
1:A:235:ARG:HH21	5:A:1009:GOL:H2	1.80	0.46
1:A:57:GLN:NE2	1:A:61:ASN:HD22	2.11	0.46
1:A:76:ARG:NH1	6:A:1313:HOH:O	2.45	0.46
1:A:391:LEU:C	1:A:391:LEU:HD12	2.39	0.46
1:B:40:ILE:HD11	1:B:119:VAL:CG2	2.46	0.46
1:B:532:LEU:HD12	1:B:536:ARG:HE	1.80	0.46
1:A:42:TYR:HA	1:A:47:GLU:O	2.15	0.46
1:B:62:PRO:C	6:B:1737:HOH:O	2.58	0.46
1:A:590:GLU:O	1:A:594:VAL:HG23	2.15	0.46
1:B:261:ARG:NH1	1:B:286:ILE:HA	2.30	0.46
1:A:459:LEU:HD21	1:A:499:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASP:OD1	1:B:182:ASP:N	2.47	0.46
1:B:240:LEU:HD22	1:B:298:ILE:HG21	1.98	0.46
1:B:254:ASN:ND2	1:B:254:ASN:C	2.74	0.45
1:B:527:ARG:HG3	6:B:1620:HOH:O	2.16	0.45
1:A:239:TYR:CZ	1:A:304:LYS:HD3	2.50	0.45
1:B:427:SER:HB3	1:B:436:VAL:CG2	2.46	0.45
1:A:52:GLN:N	1:A:53:PRO:CD	2.80	0.45
1:B:64:ASN:ND2	1:B:106:LYS:CE	2.77	0.45
1:B:532:LEU:O	1:B:536:ARG:HG3	2.17	0.45
1:B:248:GLN:NE2	1:B:294:LYS:HD2	2.31	0.45
1:A:110:MET:HE2	1:A:115:ILE:HD13	1.99	0.45
1:A:59:VAL:HA	1:A:260:GLN:CG	2.47	0.44
1:B:39:ILE:C	1:B:40:ILE:HD12	2.43	0.44
1:A:278:GLN:OE1	1:B:536:ARG:CD	2.61	0.44
1:A:289:ASP:C	1:A:291:THR:N	2.76	0.44
1:B:174:ALA:O	1:B:374:GLY:HA3	2.18	0.44
1:A:517:ARG:NH2	6:A:1352:HOH:O	2.51	0.43
1:A:112:PRO:HB2	1:A:113:PRO:HD3	2.00	0.43
1:A:235:ARG:HH21	5:A:1009:GOL:C2	2.31	0.43
1:B:251:ASP:OD1	1:B:251:ASP:C	2.61	0.43
1:A:532:LEU:CD1	1:A:536:ARG:NE	2.81	0.43
1:A:52:GLN:HB3	1:A:53:PRO:HD3	2.01	0.43
1:A:533:VAL:HG13	1:B:278:GLN:HB2	2.01	0.43
1:B:24:PRO:HB2	1:B:373:ILE:HD12	2.00	0.43
1:B:52:GLN:HB3	1:B:53:PRO:HD3	2.00	0.43
1:B:244:PHE:CE1	1:B:248:GLN:HG3	2.53	0.43
1:A:40:ILE:HD13	1:A:115:ILE:HG22	2.01	0.43
1:A:56:ARG:NH1	1:B:272:GLU:OE1	2.51	0.43
1:A:404:MET:HE3	1:A:404:MET:HB3	1.78	0.43
1:A:174:ALA:O	1:A:374:GLY:HA3	2.19	0.42
1:B:112:PRO:HB2	1:B:113:PRO:HD3	2.01	0.42
1:B:45:ASP:C	1:B:45:ASP:OD1	2.62	0.42
1:B:52:GLN:HG2	6:B:1761:HOH:O	2.19	0.42
1:A:23:THR:HA	1:A:24:PRO:HD3	1.89	0.42
1:B:102:TRP:CZ2	1:B:111:ALA:HB2	2.55	0.42
1:A:102:TRP:CZ2	1:A:111:ALA:HB2	2.55	0.42
1:A:466:PRO:O	1:A:467:ARG:HB2	2.20	0.42
1:A:110:MET:HE2	1:A:115:ILE:CD1	2.50	0.41
1:A:124:LYS:HE2	1:A:135:VAL:O	2.20	0.41
1:B:90:PRO:HB2	6:B:1737:HOH:O	2.20	0.41
1:B:403:THR:OG1	1:B:407:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:HA	1:A:428:MET:HE2	2.02	0.41
1:B:338:ILE:HD12	1:B:365:VAL:HG21	2.02	0.41
1:B:532:LEU:HD12	1:B:536:ARG:NE	2.36	0.41
1:A:58:ALA:HB1	6:A:1554:HOH:O	2.21	0.41
1:A:289:ASP:OD1	1:A:290:ALA:N	2.54	0.41
1:A:306:GLU:HB3	1:A:348:MET:CE	2.50	0.41
1:B:94:ILE:HD11	1:B:109:LYS:HG2	2.02	0.41
1:A:272:GLU:OE2	1:B:56:ARG:NH1	2.49	0.40
1:B:269:ALA:HB1	1:B:279:THR:HG21	2.03	0.40
1:A:532:LEU:CD2	1:A:581:LYS:HB2	2.51	0.40
1:B:52:GLN:N	1:B:53:PRO:CD	2.84	0.40
1:A:532:LEU:O	1:A:536:ARG:HG3	2.22	0.40
1:B:229:GLY:HA3	3:B:1002:ATP:O3'	2.22	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	598/608 (98%)	592 (99%)	6 (1%)	0	100	100
1	B	598/608 (98%)	593 (99%)	5 (1%)	0	100	100
All	All	1196/1216 (98%)	1185 (99%)	11 (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	489/495 (99%)	479 (98%)	10 (2%)	48	43
1	B	489/495 (99%)	474 (97%)	15 (3%)	35	26
All	All	978/990 (99%)	953 (97%)	25 (3%)	40	33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	57	GLN
1	A	146	PHE
1	A	182	ASP
1	A	210	VAL
1	A	247	ASP
1	A	254	ASN
1	A	304	LYS
1	A	332	SER
1	A	532	LEU
1	B	22	THR
1	B	57	GLN
1	B	123	MET
1	B	125	LYS
1	B	146	PHE
1	B	182	ASP
1	B	210	VAL
1	B	254	ASN
1	B	277	GLN
1	B	304	LYS
1	B	427	SER
1	B	437	THR
1	B	532	LEU
1	B	570	THR
1	B	598	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	254	ASN
1	A	277	GLN
1	A	295	HIS
1	A	458	ASN
1	A	544	HIS
1	B	44	GLN
1	B	57	GLN
1	B	64	ASN
1	B	187	ASN
1	B	248	GLN
1	B	254	ASN
1	B	260	GLN
1	B	277	GLN
1	B	295	HIS
1	B	297	ASN
1	B	458	ASN
1	B	541	HIS
1	B	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	1004	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	A	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
5	GOL	A	1009	-	5,5,5	0.39	0	5,5,5	0.23	0
4	SO4	A	1007	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	B	1008[A]	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	B	1006	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	B	1003	-	4,4,4	0.24	0	6,6,6	0.13	0
3	ATP	A	1002	2	32,33,33	1.53	8 (25%)	48,52,52	1.72	11 (22%)
4	SO4	B	1007	-	4,4,4	0.24	0	6,6,6	0.07	0
5	GOL	B	1010	-	5,5,5	0.36	0	5,5,5	0.25	0
5	GOL	A	1008	-	5,5,5	0.41	0	5,5,5	0.38	0
4	SO4	B	1004	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	1008[B]	-	4,4,4	0.22	0	6,6,6	0.08	0
5	GOL	B	1009	-	5,5,5	0.36	0	5,5,5	0.28	0
3	ATP	B	1002	2	32,33,33	1.37	5 (15%)	48,52,52	1.72	10 (20%)
4	SO4	A	1003	-	4,4,4	0.22	0	6,6,6	0.07	0
4	SO4	A	1006	-	4,4,4	0.27	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1002	2	-	1/22/38/38	0/3/3/3
5	GOL	B	1010	-	-	2/4/4/4	-
5	GOL	A	1008	-	-	2/4/4/4	-
5	GOL	B	1009	-	-	2/4/4/4	-
3	ATP	B	1002	2	-	1/22/38/38	0/3/3/3
5	GOL	A	1009	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ATP	C5-C4	4.52	1.47	1.39
3	B	1002	ATP	C5-C4	4.31	1.46	1.39
3	A	1002	ATP	PB-O3B	3.41	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	ATP	C5-C6	2.62	1.48	1.41
3	A	1002	ATP	C8-N7	2.48	1.36	1.31
3	A	1002	ATP	C5-C6	2.37	1.47	1.41
3	B	1002	ATP	C5-N7	-2.26	1.35	1.39
3	B	1002	ATP	C8-N7	2.21	1.35	1.31
3	A	1002	ATP	C4-N9	-2.20	1.33	1.37
3	A	1002	ATP	C5-N7	-2.18	1.35	1.39
3	B	1002	ATP	C4-N9	-2.17	1.33	1.37
3	A	1002	ATP	PA-O3A	2.12	1.61	1.59
3	A	1002	ATP	PB-O3A	2.03	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	ATP	C5-C4-N3	-4.96	119.89	126.72
3	A	1002	ATP	C5-C4-N3	-4.87	120.02	126.72
3	A	1002	ATP	N3-C4-N9	4.29	134.46	127.17
3	B	1002	ATP	N3-C4-N9	4.26	134.41	127.17
3	A	1002	ATP	C4-N9-C8	3.90	109.84	105.74
3	B	1002	ATP	C4-N9-C8	3.68	109.61	105.74
3	B	1002	ATP	N3-C2-N1	-3.52	123.25	128.58
3	A	1002	ATP	N3-C2-N1	-3.46	123.35	128.58
3	B	1002	ATP	C2-N3-C4	3.45	120.27	111.83
3	A	1002	ATP	C2-N3-C4	3.33	119.97	111.83
3	B	1002	ATP	C4-C5-N7	-3.21	106.92	110.58
3	A	1002	ATP	C4-C5-N7	-3.02	107.13	110.58
3	B	1002	ATP	N9-C8-N7	-2.70	110.11	113.94
3	B	1002	ATP	C5-N7-C8	2.68	107.66	103.45
3	A	1002	ATP	N9-C8-N7	-2.68	110.13	113.94
3	A	1002	ATP	C5-N7-C8	2.50	107.38	103.45
3	A	1002	ATP	O2A-PA-O1A	2.18	122.60	112.44
3	B	1002	ATP	C6-C5-N7	2.18	136.30	132.09
3	A	1002	ATP	C2-N1-C6	2.12	122.21	118.73
3	B	1002	ATP	C2-N1-C6	2.12	122.21	118.73
3	A	1002	ATP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1008	GOL	O1-C1-C2-O2
5	A	1008	GOL	O1-C1-C2-C3

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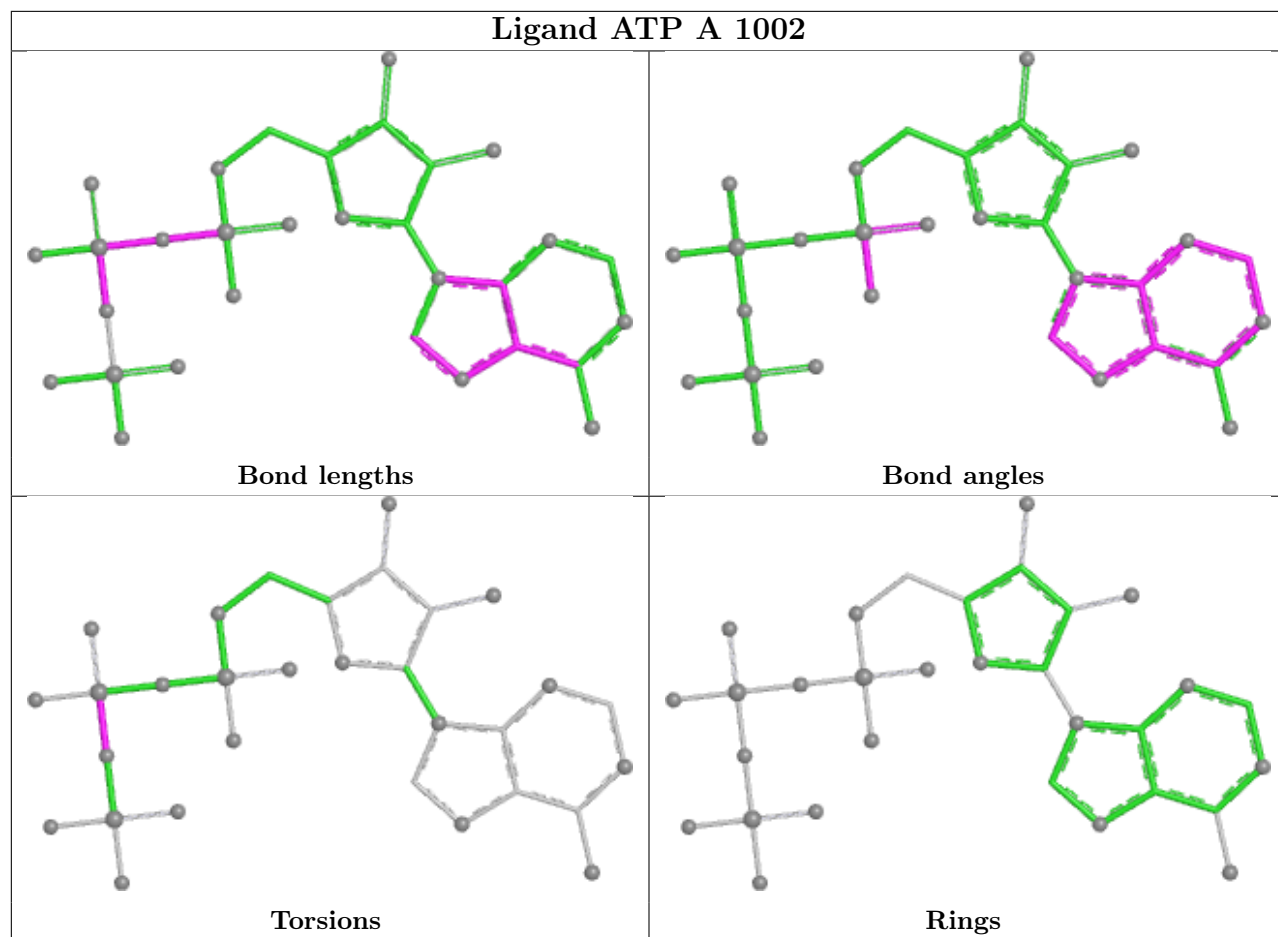
Mol	Chain	Res	Type	Atoms
5	A	1009	GOL	O1-C1-C2-C3
5	B	1009	GOL	C1-C2-C3-O3
5	B	1010	GOL	O1-C1-C2-C3
5	A	1009	GOL	O1-C1-C2-O2
5	B	1010	GOL	O1-C1-C2-O2
5	B	1009	GOL	O2-C2-C3-O3
3	A	1002	ATP	PG-O3B-PB-O2B
3	B	1002	ATP	PG-O3B-PB-O2B

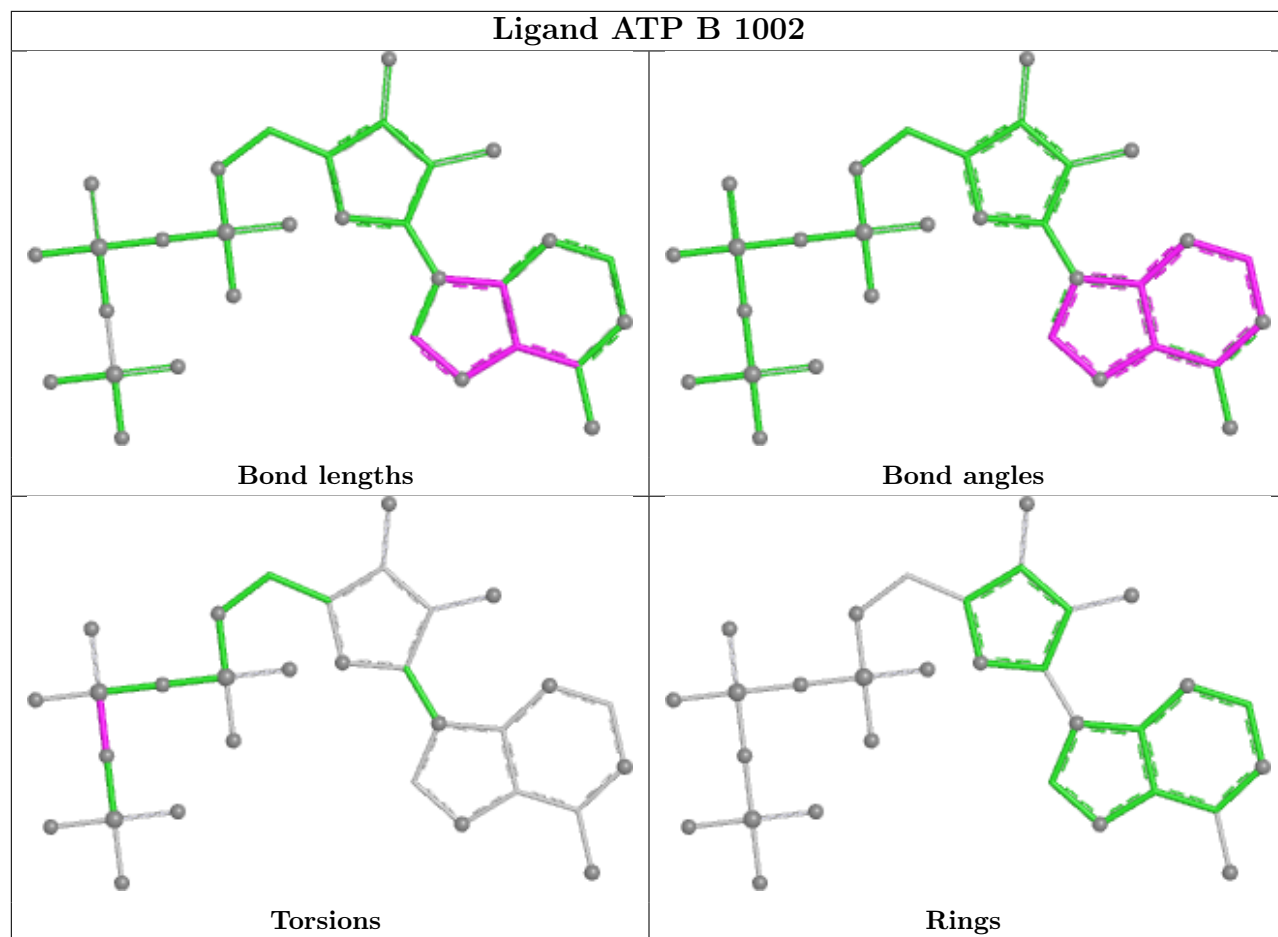
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	GOL	2	0
5	B	1010	GOL	2	0
5	A	1008	GOL	1	0
3	B	1002	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	600/608 (98%)	-0.11	29 (4%)	35 41	13, 26, 60, 112	0
1	B	600/608 (98%)	0.01	49 (8%)	17 20	11, 26, 69, 119	0
All	All	1200/1216 (98%)	-0.05	78 (6%)	25 28	11, 26, 62, 119	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	VAL	8.3
1	A	210	VAL	7.8
1	B	598	LEU	6.3
1	A	42	TYR	5.9
1	B	288	ALA	5.3
1	A	289	ASP	5.1
1	B	253	ARG	4.6
1	B	604	GLN	4.5
1	B	251	ASP	4.2
1	A	604	GLN	4.1
1	A	184	GLY	4.1
1	B	601	ILE	4.1
1	B	556	LYS	4.1
1	A	390	LEU	4.1
1	A	290	ALA	4.0
1	B	532	LEU	4.0
1	B	183	LYS	4.0
1	B	254	ASN	4.0
1	A	185	THR	4.0
1	A	532	LEU	3.9
1	B	289	ASP	3.9
1	A	601	ILE	3.8
1	B	533	VAL	3.8
1	B	390	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	3.6
1	B	286	ILE	3.6
1	B	212	GLY	3.5
1	A	291	THR	3.4
1	A	598	LEU	3.3
1	A	529	PHE	3.3
1	A	212	GLY	3.3
1	B	527	ARG	3.2
1	A	183	LYS	3.2
1	B	404	MET	3.2
1	B	209	GLU	3.1
1	B	534	GLN	3.1
1	B	22	THR	3.1
1	A	555	ASP	3.0
1	B	42	TYR	3.0
1	B	256	PRO	3.0
1	B	557	LEU	2.9
1	B	258	ALA	2.9
1	B	602	ALA	2.8
1	B	287	THR	2.8
1	B	45	ASP	2.7
1	B	182	ASP	2.7
1	A	182	ASP	2.6
1	B	529	PHE	2.6
1	A	211	ASP	2.6
1	A	247	ASP	2.6
1	A	557	LEU	2.5
1	A	186	GLY	2.5
1	B	186	GLY	2.5
1	B	297	ASN	2.5
1	B	285	TYR	2.5
1	A	22	THR	2.5
1	B	44	GLN	2.4
1	B	599	MET	2.4
1	B	211	ASP	2.3
1	A	556	LYS	2.3
1	B	563	THR	2.3
1	B	597	LYS	2.3
1	A	554	GLY	2.2
1	B	290	ALA	2.2
1	B	600	GLU	2.2
1	B	589	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLY	2.2
1	A	56	ARG	2.2
1	A	534	GLN	2.2
1	B	603	GLN	2.2
1	B	252	LEU	2.2
1	B	257	LEU	2.2
1	B	514	LYS	2.1
1	A	45	ASP	2.1
1	B	255	ASP	2.1
1	B	555	ASP	2.1
1	A	59	VAL	2.0
1	B	250	ILE	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.

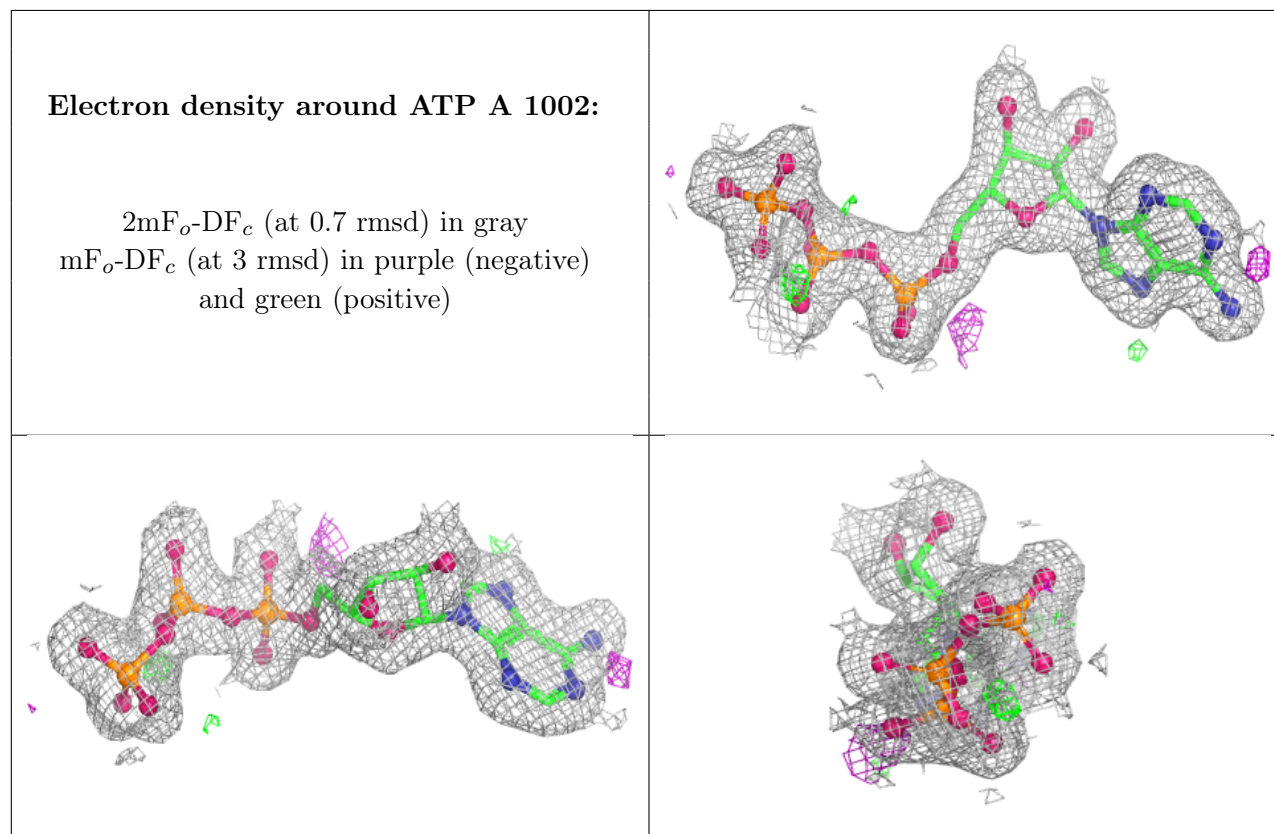
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	1009	6/6	0.82	0.14	68,82,92,94	0
5	GOL	B	1010	6/6	0.83	0.13	42,60,72,82	0
4	SO4	A	1005	5/5	0.86	0.12	73,75,77,84	0
4	SO4	B	1005	5/5	0.88	0.12	71,79,79,85	0
4	SO4	A	1004	5/5	0.90	0.12	60,74,78,88	0
4	SO4	B	1007	5/5	0.90	0.12	53,54,59,67	0
4	SO4	B	1004	5/5	0.91	0.11	70,72,74,80	0
4	SO4	B	1008[A]	5/5	0.92	0.16	29,41,42,52	5
4	SO4	B	1008[B]	5/5	0.92	0.16	39,41,43,44	5
5	GOL	A	1008	6/6	0.92	0.14	27,46,56,56	0
4	SO4	B	1006	5/5	0.92	0.10	31,43,69,74	0

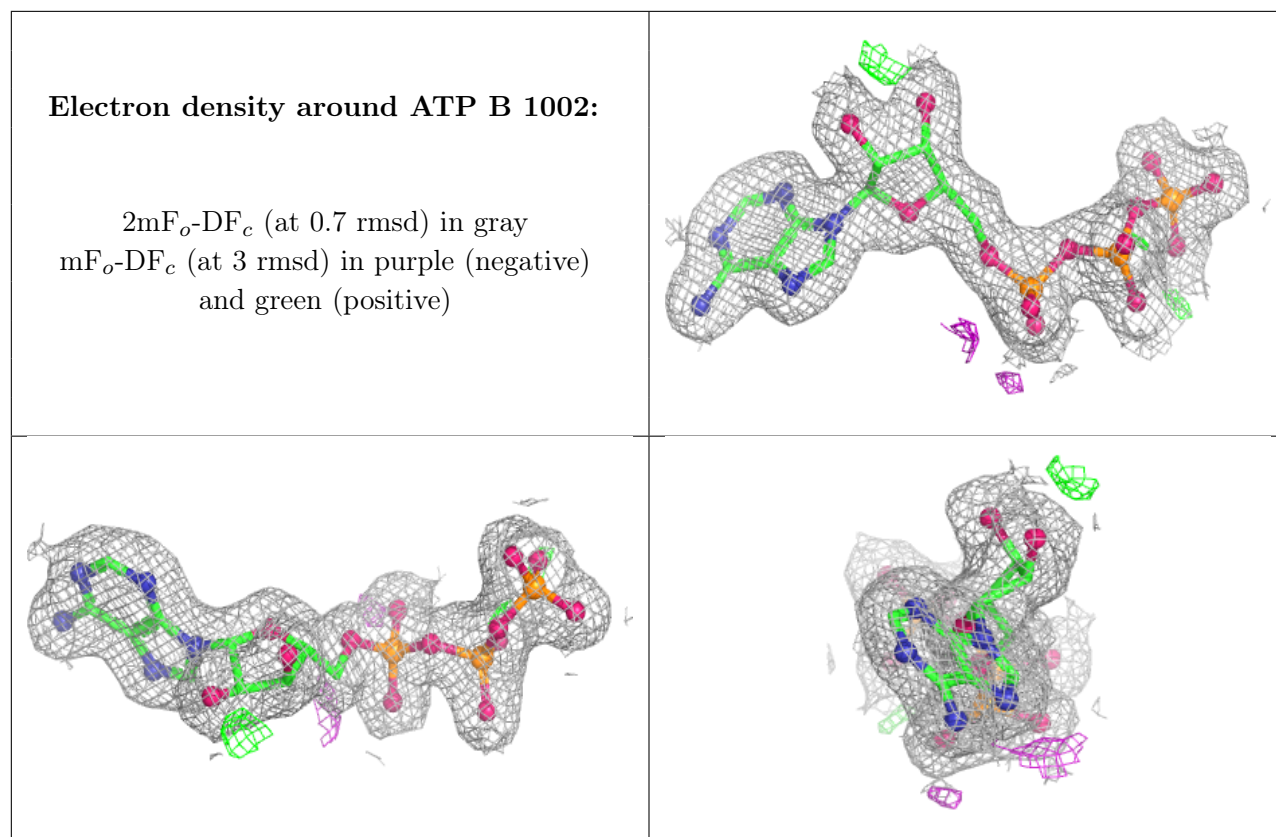
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1006	5/5	0.92	0.10	29,41,70,76	0
4	SO4	A	1003	5/5	0.97	0.09	38,42,48,50	0
4	SO4	A	1007	5/5	0.97	0.16	41,44,45,53	0
5	GOL	B	1009	6/6	0.97	0.07	22,31,39,39	0
4	SO4	B	1003	5/5	0.97	0.09	37,38,39,47	0
2	MG	A	1001	1/1	0.99	0.05	18,18,18,18	0
2	MG	B	1001	1/1	0.99	0.07	18,18,18,18	0
3	ATP	A	1002	31/31	0.99	0.03	11,16,21,22	0
3	ATP	B	1002	31/31	0.99	0.03	10,14,19,21	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.