



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:34 AM UTC

PDB ID : 2QXL / pdb_00002qxl
Title : Crystal Structure Analysis of Sse1, a yeast Hsp110
Authors : Hendrickson, W.A.; Liu, Q.
Deposited on : 2007-08-12
Resolution : 2.41 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

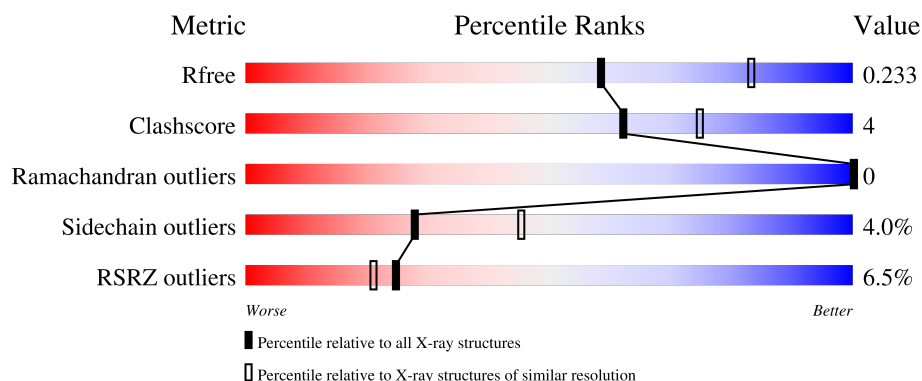
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	658	7% 83% 10% • 6%
1	B	658	5% 84% 10% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10060 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 Heat shock protein homolog SSE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			4802	3037	810	943	12			
1	B	625	Total	C	N	O	S	0	0	0
			4837	3058	818	949	12			

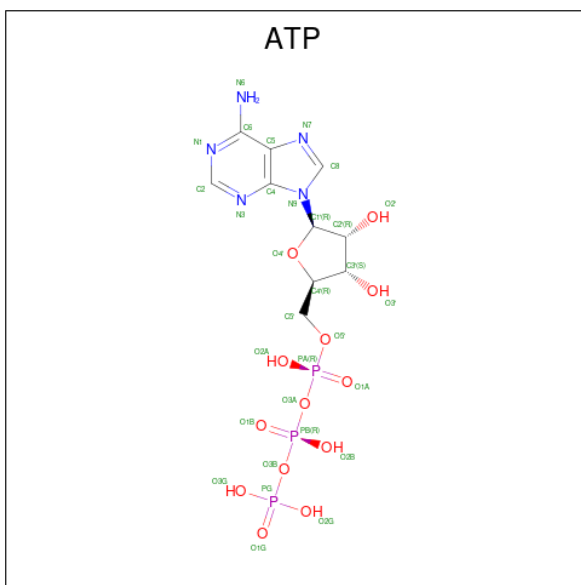
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

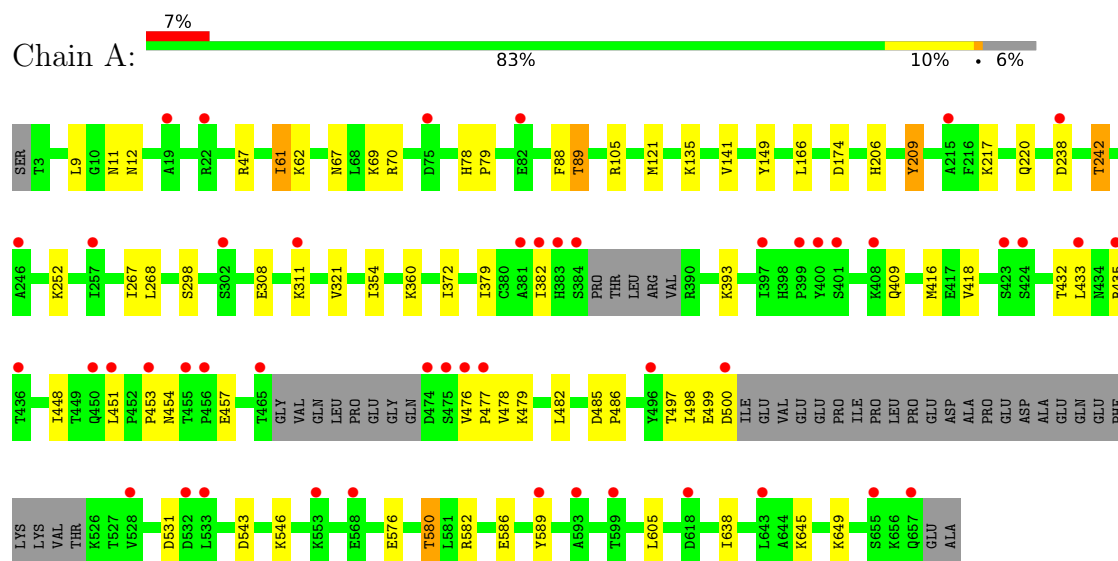
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0
5	B	229	Total O 229 229	0	0

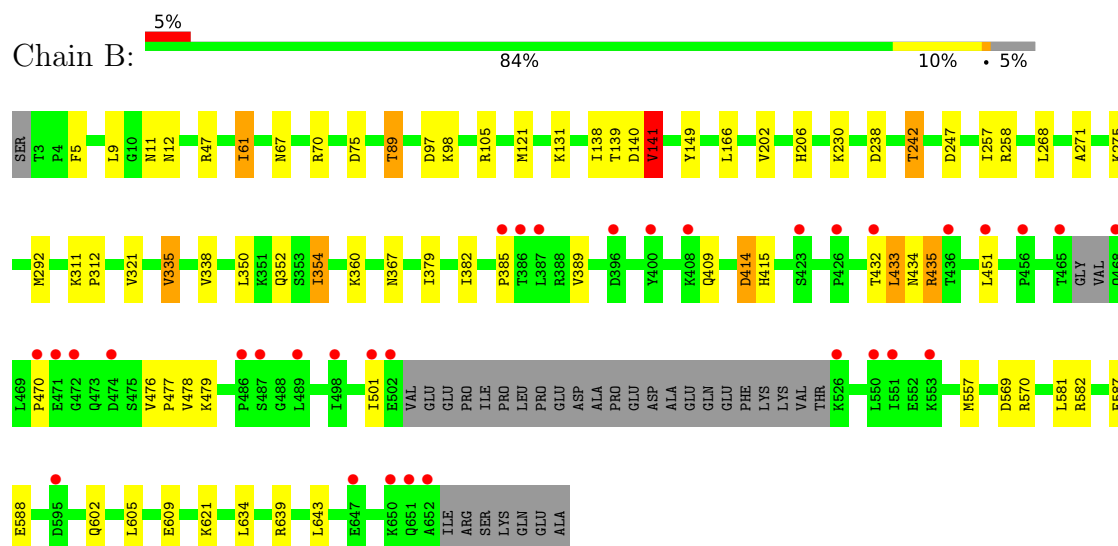
3 Residue-property plots [i](#)

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: Heat shock protein homolog SSE1



- Molecule 1: Heat shock protein homolog SSE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.04Å 125.33Å 74.71Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	29.49 – 2.41 29.49 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.49-2.41) 99.0 (29.49-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	37.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.235 0.193 , 0.233	Depositor DCC
R_{free} test set	3795 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, K, 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	0.66	5/4887 (0.1%)	0.83	3/6610 (0.0%)
1	B	0.81	3/4924 (0.1%)	0.86	4/6667 (0.1%)
All	All	0.74	8/9811 (0.1%)	0.85	7/13277 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	435	ARG	CZ-NH1	31.03	1.76	1.32
1	A	435	ARG	CZ-NH1	12.48	1.50	1.32
1	A	500	ASP	C-O	10.02	1.43	1.23
1	B	409	GLN	C-N	8.91	1.44	1.33
1	B	409	GLN	CD-NE2	6.54	1.47	1.33
1	A	409	GLN	C-N	6.07	1.41	1.33
1	A	409	GLN	CD-NE2	6.04	1.46	1.33
1	A	435	ARG	CZ-NH2	5.05	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	B	385	PRO	N-CA-CB	6.83	110.42	103.25
1	B	470	PRO	N-CA-CB	6.30	110.36	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	VAL	CB-CA-C	-5.76	100.39	110.71
1	B	61	ILE	N-CA-C	5.50	116.89	110.62
1	A	435	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	409	GLN	O-C-N	5.03	129.12	121.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	414	ASP	Peptide

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	4802	0	4732	40	0
1	B	4837	0	4730	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	126	0	0	1	0
5	B	229	0	0	1	0
All	All	10060	0	9486	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) 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:435:ARG:CZ	1:B:435:ARG:NH1	1.76	1.47
1:A:47:ARG:HD2	1:A:121:MET:HE3	1.29	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HD2	1:A:121:MET:CE	1.96	0.95
1:B:61:ILE:O	1:B:89:THR:HG23	1.80	0.80
1:A:141:VAL:HG21	1:A:166:LEU:HD13	1.63	0.79
1:B:238:ASP:O	1:B:242:THR:HG23	1.84	0.78
1:A:238:ASP:O	1:A:242:THR:HG23	1.85	0.76
1:B:242:THR:HG21	1:B:268:LEU:HA	1.71	0.73
1:A:645:LYS:O	1:A:649:LYS:HG2	1.90	0.72
1:A:61:ILE:O	1:A:89:THR:HG23	1.89	0.70
1:B:582:ARG:HG2	1:B:605:LEU:HD13	1.74	0.69
1:A:576:GLU:O	1:A:580:THR:HG23	1.93	0.68
1:A:308:GLU:HA	1:A:311:LYS:HE2	1.76	0.67
1:A:47:ARG:CD	1:A:121:MET:HE3	2.18	0.66
1:B:350:LEU:O	1:B:354:ILE:HG23	1.97	0.64
1:B:257:ILE:HG22	1:B:292:MET:HE2	1.80	0.64
1:B:433:LEU:HB3	1:B:435:ARG:HD3	1.81	0.63
1:B:432:THR:HG22	1:B:479:LYS:HG2	1.82	0.62
1:A:141:VAL:CG2	1:A:166:LEU:HD13	2.30	0.61
1:B:5:PHE:CD2	1:B:141:VAL:HG13	2.35	0.60
1:B:257:ILE:HG22	1:B:292:MET:CE	2.32	0.60
1:B:247:ASP:OD1	1:B:258:ARG:NH2	2.34	0.58
1:A:478:VAL:HG12	1:A:497:THR:HG22	1.86	0.58
1:B:335:VAL:O	1:B:360:LYS:HE2	2.03	0.57
1:A:11:ASN:HD21	1:A:67:ASN:HA	1.68	0.57
1:B:11:ASN:HD21	1:B:67:ASN:HA	1.70	0.56
1:A:242:THR:HG21	1:A:268:LEU:HA	1.87	0.56
1:B:311:LYS:HB3	1:B:312:PRO:HD3	1.88	0.55
1:B:11:ASN:ND2	1:B:67:ASN:HA	2.21	0.55
1:A:416:MET:HE3	1:A:418:VAL:HG22	1.90	0.54
1:B:121:MET:HE2	1:B:557:MET:HE1	1.89	0.54
1:A:11:ASN:ND2	1:A:67:ASN:HA	2.23	0.54
1:A:379:ILE:HA	1:A:382:ILE:HD12	1.91	0.53
1:B:242:THR:HG22	1:B:271:ALA:CB	2.40	0.52
1:A:432:THR:HG22	1:A:479:LYS:HG2	1.92	0.51
1:A:141:VAL:HG23	1:A:166:LEU:HB3	1.92	0.51
1:B:131:LYS:HG2	1:B:138:ILE:HG12	1.94	0.49
1:B:202:VAL:HG21	1:B:354:ILE:HD13	1.94	0.48
1:A:78:HIS:ND1	1:A:79:PRO:HD2	2.29	0.48
1:A:174:ASP:HB2	1:A:372:ILE:HD13	1.96	0.48
1:B:141:VAL:HG22	1:B:166:LEU:HB3	1.95	0.48
1:B:12:ASN:HB2	1:B:206:HIS:CG	2.49	0.47
1:B:587:GLU:C	5:B:1222:HOH:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:O	1:A:242:THR:CG2	2.60	0.47
1:B:569:ASP:OD2	1:B:570:ARG:NH1	2.48	0.47
1:A:485:ASP:HB2	1:A:486:PRO:CD	2.46	0.45
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.51	0.45
1:B:582:ARG:HH22	1:B:609:GLU:CD	2.24	0.45
1:B:11:ASN:ND2	1:B:70:ARG:HG2	2.31	0.45
1:A:582:ARG:HG2	1:A:605:LEU:HD13	1.99	0.45
1:B:47:ARG:NH1	1:B:121:MET:HG2	2.32	0.45
1:B:434:ASN:C	1:B:435:ARG:HD2	2.42	0.45
1:B:570:ARG:HG3	1:B:621:LYS:HG3	1.97	0.45
1:A:589:TYR:HB3	1:A:638:ILE:HG21	1.99	0.45
1:A:242:THR:HB	1:A:267:ILE:HG22	1.98	0.44
1:A:498:ILE:CG2	1:A:499:GLU:N	2.80	0.44
1:A:586:GLU:CD	1:B:367:ASN:HD22	2.25	0.44
1:B:414:ASP:OD1	1:B:415:HIS:HB2	2.18	0.44
1:A:67:ASN:HB2	1:A:88:PHE:CZ	2.53	0.43
1:A:69:LYS:HE2	5:A:1022:HOH:O	2.18	0.43
1:A:220:GLN:HA	1:A:393:LYS:O	2.18	0.43
1:B:275:LYS:HB3	1:B:275:LYS:HE2	1.85	0.43
1:A:453:PRO:O	1:A:454:ASN:HB2	2.18	0.43
1:A:242:THR:HG21	1:A:268:LEU:HD12	2.00	0.42
1:B:338:VAL:HG11	1:B:354:ILE:HD11	2.00	0.42
1:B:476:VAL:HA	1:B:477:PRO:HD3	1.89	0.42
1:B:257:ILE:HA	1:B:292:MET:HE1	2.02	0.42
1:A:476:VAL:HA	1:A:477:PRO:HD3	1.82	0.42
1:A:209:TYR:C	1:A:209:TYR:CD2	2.98	0.42
1:B:97:ASP:O	1:B:98:LYS:HB2	2.20	0.42
1:B:139:THR:HG23	1:B:140:ASP:OD2	2.20	0.41
1:B:581:LEU:HD23	1:B:605:LEU:HD21	2.02	0.41
1:A:543:ASP:OD1	1:A:546:LYS:HB2	2.20	0.41
1:A:11:ASN:ND2	1:A:70:ARG:HG2	2.36	0.41
1:A:379:ILE:O	1:A:382:ILE:HB	2.21	0.41
1:A:448:ILE:HD13	1:A:457:GLU:HA	2.03	0.41
1:A:217:LYS:HB2	1:A:220:GLN:HG2	2.02	0.41
1:B:379:ILE:O	1:B:382:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	609/658 (93%)	594 (98%)	15 (2%)	0	100	100
1	B	619/658 (94%)	599 (97%)	20 (3%)	0	100	100
All	All	1228/1316 (93%)	1193 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	514/567 (91%)	495 (96%)	19 (4%)	30	49
1	B	512/567 (90%)	490 (96%)	22 (4%)	26	42
All	All	1026/1134 (90%)	985 (96%)	41 (4%)	28	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	61	ILE
1	A	62	LYS
1	A	89	THR
1	A	105	ARG
1	A	135	LYS
1	A	149	TYR
1	A	209	TYR

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Mol	Chain	Res	Type
1	A	242	THR
1	A	252	LYS
1	A	298	SER
1	A	321	VAL
1	A	354	ILE
1	A	360	LYS
1	A	433	LEU
1	A	451	LEU
1	A	482	LEU
1	A	531	ASP
1	A	580	THR
1	B	9	LEU
1	B	75	ASP
1	B	89	THR
1	B	105	ARG
1	B	141	VAL
1	B	149	TYR
1	B	230	LYS
1	B	242	THR
1	B	321	VAL
1	B	335	VAL
1	B	352	GLN
1	B	354	ILE
1	B	389	VAL
1	B	433	LEU
1	B	451	LEU
1	B	478	VAL
1	B	501	ILE
1	B	588	GLU
1	B	602	GLN
1	B	634	LEU
1	B	639	ARG
1	B	643	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	415	HIS
1	A	458	GLN
1	A	548	ASN
1	B	11	ASN

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Mol	Chain	Res	Type
1	B	111	HIS
1	B	167	ASN
1	B	260	ASN
1	B	293	ASN
1	B	473	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ATP	B	1001	3,2	32,33,33	1.43	7 (21%)	48,52,52	1.91	10 (20%)
4	ATP	A	1002	3,2	32,33,33	1.43	7 (21%)	48,52,52	1.92	12 (25%)

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
4	ATP	B	1001	3,2	-	1/22/38/38	0/3/3/3
4	ATP	A	1002	3,2	-	4/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	ATP	C5-C4	4.45	1.47	1.39
4	A	1002	ATP	C5-C4	4.29	1.46	1.39
4	A	1002	ATP	PA-O3A	3.10	1.62	1.59
4	B	1001	ATP	C8-N7	3.00	1.37	1.31
4	B	1001	ATP	PB-O3B	2.63	1.62	1.59
4	B	1001	ATP	PA-O3A	2.49	1.62	1.59
4	A	1002	ATP	C5-C6	2.39	1.47	1.41
4	A	1002	ATP	C4-N9	-2.23	1.33	1.37
4	B	1001	ATP	C5-C6	2.20	1.47	1.41
4	A	1002	ATP	C8-N7	2.19	1.35	1.31
4	B	1001	ATP	C4-N9	-2.07	1.33	1.37
4	A	1002	ATP	PB-O3A	2.05	1.61	1.59
4	B	1001	ATP	C5-N7	-2.05	1.35	1.39
4	A	1002	ATP	PB-O3B	2.00	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	ATP	N3-C2-N1	-5.50	120.25	128.58
4	B	1001	ATP	C5-C4-N3	-5.21	119.54	126.72
4	A	1002	ATP	C5-C4-N3	-4.86	120.03	126.72
4	A	1002	ATP	N3-C4-N9	4.59	134.97	127.17
4	A	1002	ATP	N3-C2-N1	-4.56	121.67	128.58
4	B	1001	ATP	C2-N3-C4	4.32	122.38	111.83
4	A	1002	ATP	C4-N9-C8	4.27	110.22	105.74
4	B	1001	ATP	O4'-C1'-N9	4.02	115.81	108.09
4	B	1001	ATP	N3-C4-N9	3.94	133.87	127.17
4	A	1002	ATP	C2-N3-C4	3.90	121.37	111.83
4	B	1001	ATP	C2-N1-C6	3.45	124.40	118.73
4	A	1002	ATP	N9-C8-N7	-2.93	109.77	113.94
4	B	1001	ATP	C4-C5-N7	-2.69	107.50	110.58
4	B	1001	ATP	C6-C5-N7	2.55	137.01	132.09
4	A	1002	ATP	C2-N1-C6	2.53	122.89	118.73
4	A	1002	ATP	C4-C5-N7	-2.48	107.75	110.58
4	A	1002	ATP	C5-N7-C8	2.42	107.26	103.45
4	B	1001	ATP	C4-N9-C8	2.35	108.20	105.74
4	A	1002	ATP	C2'-C1'-N9	-2.24	107.73	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	ATP	O3G-PG-O2G	2.20	116.06	107.80
4	A	1002	ATP	O4'-C1'-N9	2.18	112.28	108.09
4	A	1002	ATP	C6-C5-N7	2.13	136.19	132.09

There are no chirality outliers.

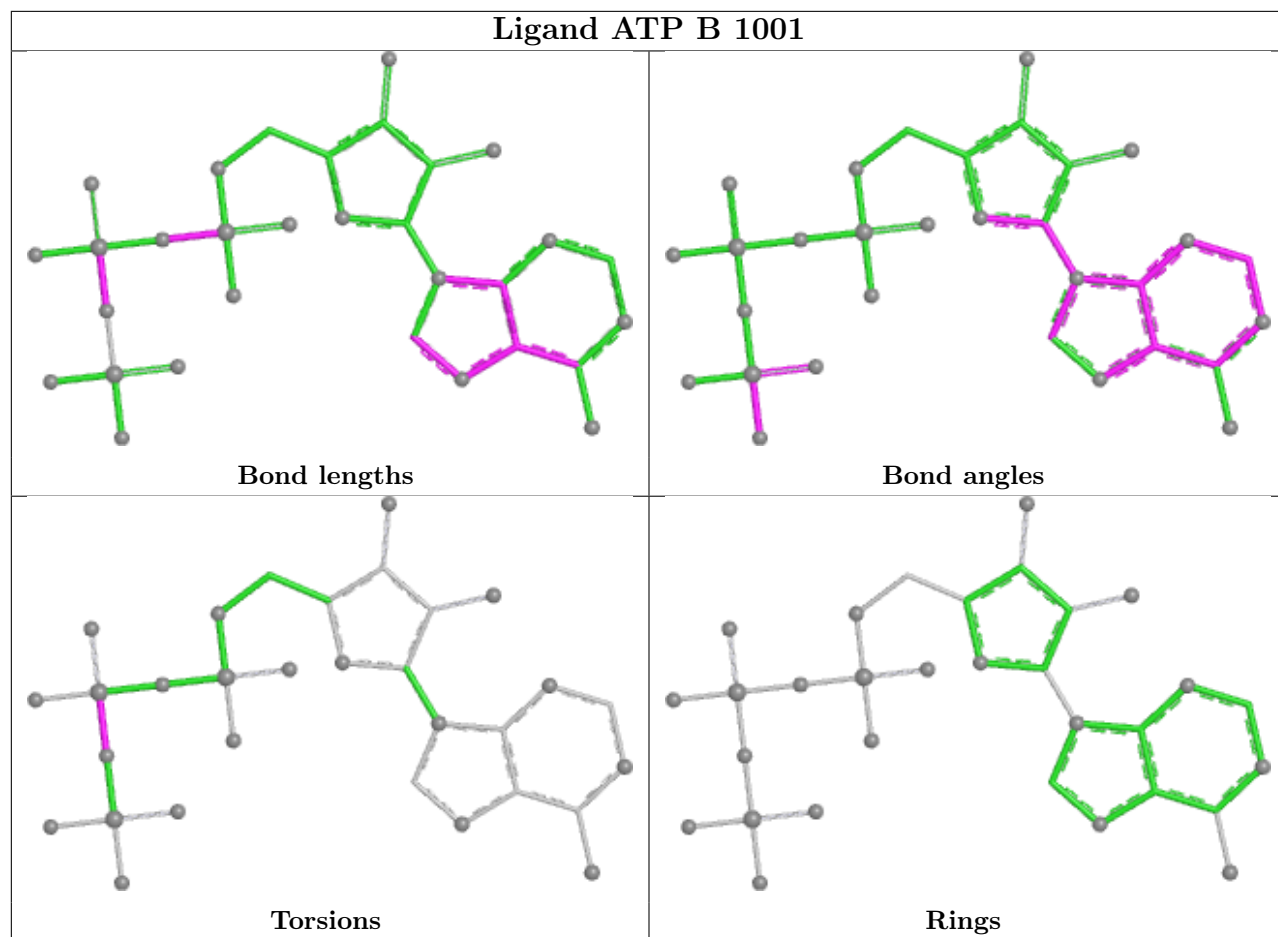
All (5) torsion outliers are listed below:

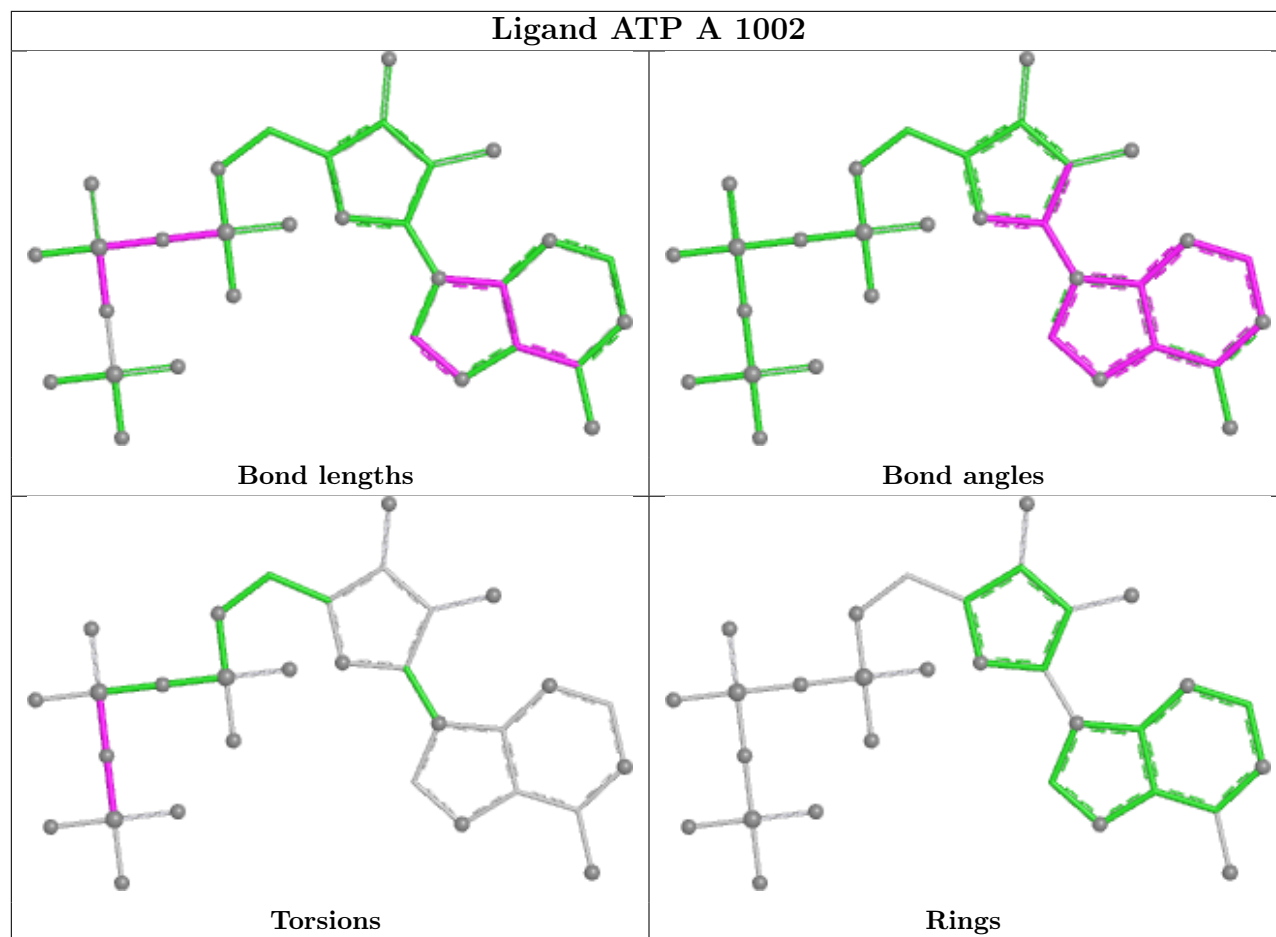
Mol	Chain	Res	Type	Atoms
4	A	1002	ATP	PB-O3B-PG-O2G
4	A	1002	ATP	PB-O3B-PG-O3G
4	B	1001	ATP	PG-O3B-PB-O1B
4	A	1002	ATP	PG-O3B-PB-O1B
4	A	1002	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	617/658 (93%)	0.84	48 (7%) 19 15	46, 58, 67, 74	0
1	B	625/658 (94%)	0.26	33 (5%) 32 28	36, 46, 61, 72	0
All	All	1242/1316 (94%)	0.55	81 (6%) 25 21	36, 53, 66, 74	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	ASP	4.6
1	B	387	LEU	4.5
1	B	465	THR	4.1
1	B	652	ALA	3.9
1	B	474	ASP	3.8
1	B	385	PRO	3.8
1	A	383	HIS	3.6
1	A	500	ASP	3.5
1	B	498	ILE	3.4
1	A	433	LEU	3.4
1	B	502	GLU	3.3
1	A	657	GLN	3.3
1	A	533	LEU	3.2
1	A	528	VAL	3.2
1	B	471	GLU	3.1
1	A	451	LEU	3.1
1	A	19	ALA	3.1
1	A	401	SER	3.1
1	B	651	GLN	3.0
1	B	472	GLY	3.0
1	A	400	TYR	2.9
1	A	456	PRO	2.8
1	A	381	ALA	2.8
1	A	455	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	595	ASP	2.8
1	A	382	ILE	2.7
1	B	553	LYS	2.7
1	B	470	PRO	2.7
1	B	486	PRO	2.7
1	A	423	SER	2.7
1	A	599	THR	2.6
1	A	215	ALA	2.6
1	A	496	TYR	2.6
1	A	435	ARG	2.5
1	A	399	PRO	2.5
1	A	408	LYS	2.5
1	B	386	THR	2.5
1	A	22	ARG	2.5
1	A	655	SER	2.5
1	A	397	ILE	2.4
1	A	450	GLN	2.4
1	A	465	THR	2.4
1	B	526	LYS	2.4
1	A	532	ASP	2.3
1	A	618	ASP	2.3
1	A	568	GLU	2.3
1	A	384	SER	2.3
1	A	257	ILE	2.3
1	B	396	ASP	2.3
1	A	82	GLU	2.3
1	A	477	PRO	2.3
1	A	475	SER	2.2
1	A	593	ALA	2.2
1	B	451	LEU	2.2
1	B	550	LEU	2.2
1	B	501	ILE	2.2
1	A	453	PRO	2.2
1	B	426	PRO	2.2
1	A	436	THR	2.2
1	B	436	THR	2.2
1	B	456	PRO	2.2
1	A	643	LEU	2.2
1	B	647	GLU	2.2
1	A	246	ALA	2.1
1	B	400	TYR	2.1
1	B	551	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	ASP	2.1
1	A	424	SER	2.1
1	A	553	LYS	2.1
1	B	489	LEU	2.1
1	A	311	LYS	2.1
1	B	650	LYS	2.1
1	B	487	SER	2.1
1	B	432	THR	2.1
1	A	589	TYR	2.1
1	B	423	SER	2.1
1	B	468	GLN	2.0
1	B	408	LYS	2.0
1	A	75	ASP	2.0
1	A	476	VAL	2.0
1	A	302	SER	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.

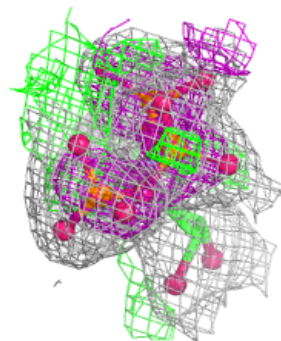
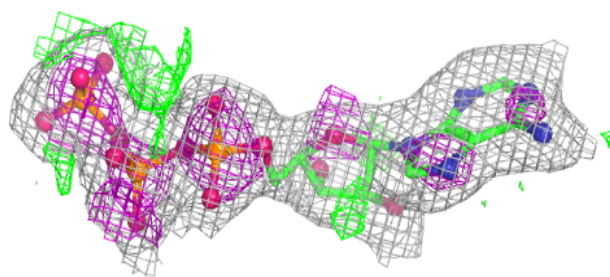
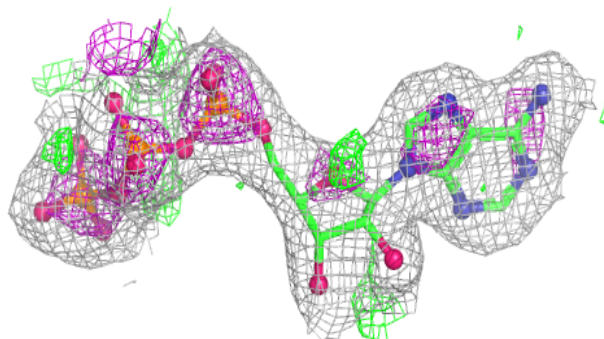
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1004	1/1	0.86	0.14	45,45,45,45	0
4	ATP	A	1002	31/31	0.96	0.10	35,38,43,44	0
3	K	A	1005	1/1	0.97	0.20	48,48,48,48	0
4	ATP	B	1001	31/31	0.97	0.09	25,28,30,30	0
2	MG	B	1003	1/1	0.98	0.12	28,28,28,28	0
3	K	B	1006	1/1	0.99	0.17	36,36,36,36	0

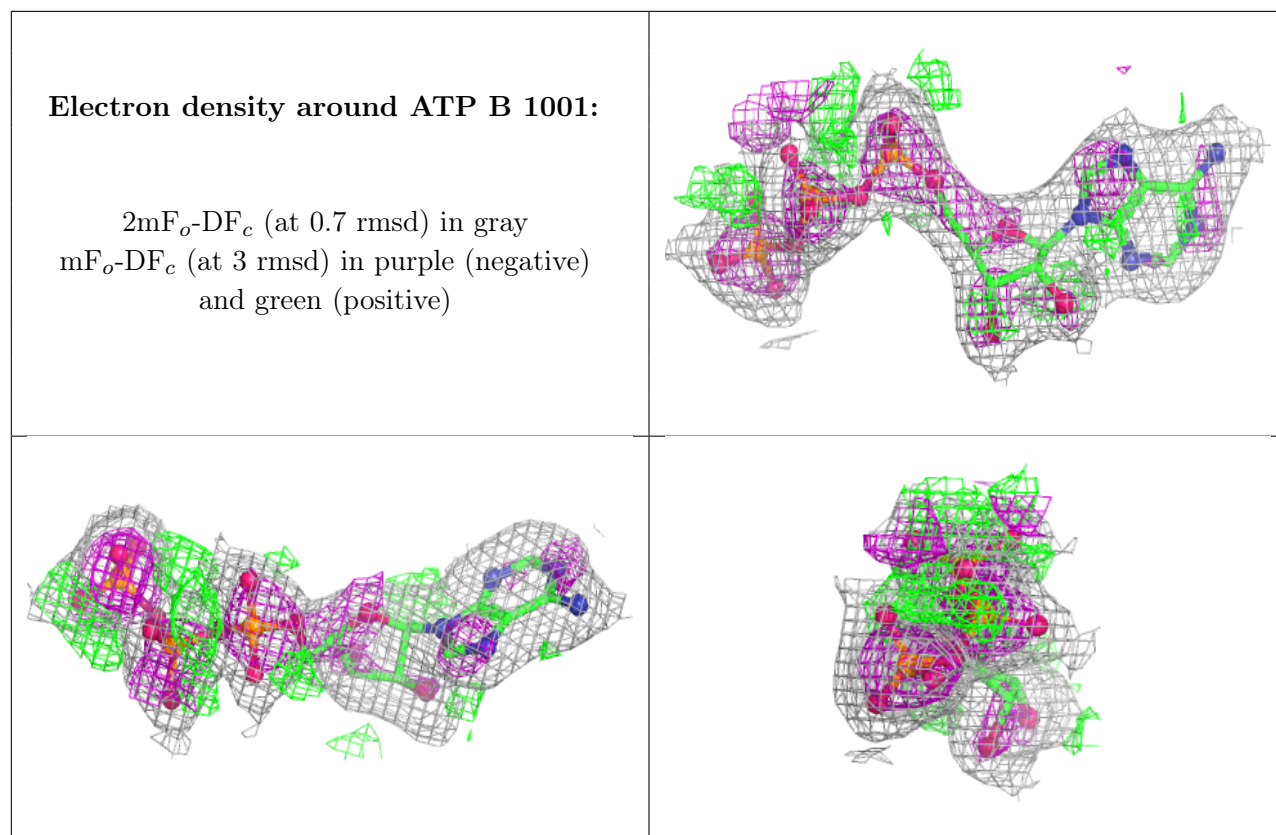
The following is a graphical depiction of the model fit to experimental electron density of all

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

Electron density around ATP A 1002:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.