



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:42 AM UTC

PDB ID : 3D2F / pdb\_00003d2f  
Title : Crystal structure of a complex of Sse1p and Hsp70  
Authors : Polier, S.; Bracher, A.  
Deposited on : 2008-05-08  
Resolution : 2.30 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](mailto: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>.

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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

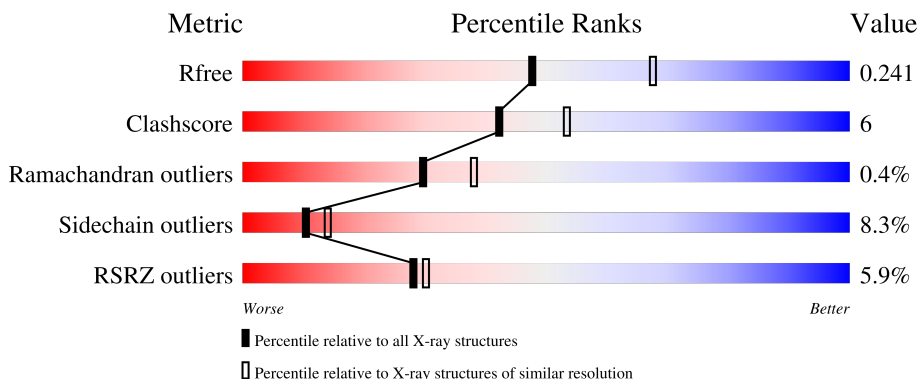
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	675	 2% 76% 13% • 7%
1	C	675	 4% 74% 16% •• 7%
2	B	382	 6% 87% 11% ••
2	D	382	 14% 81% 15% ••

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16199 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
			Total	C	N	O	S			
1	A	629	4874	3085	817	960	12	0	2	0
1	C	627	4828	3050	810	956	12	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	ALA	-	linker	UNP P32589
A	504	GLY	-	linker	UNP P32589
A	505	SER	-	linker	UNP P32589
A	506	ASP	-	linker	UNP P32589
C	503	ALA	-	linker	UNP P32589
C	504	GLY	-	linker	UNP P32589
C	505	SER	-	linker	UNP P32589
C	506	ASP	-	linker	UNP P32589

- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	379	2895	1824	505	559	7	0	1	0
2	D	379	2865	1806	490	562	7	0	3	0

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

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

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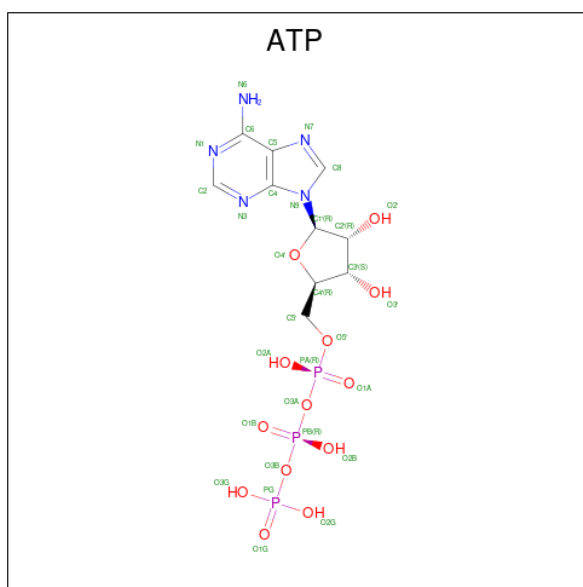
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0

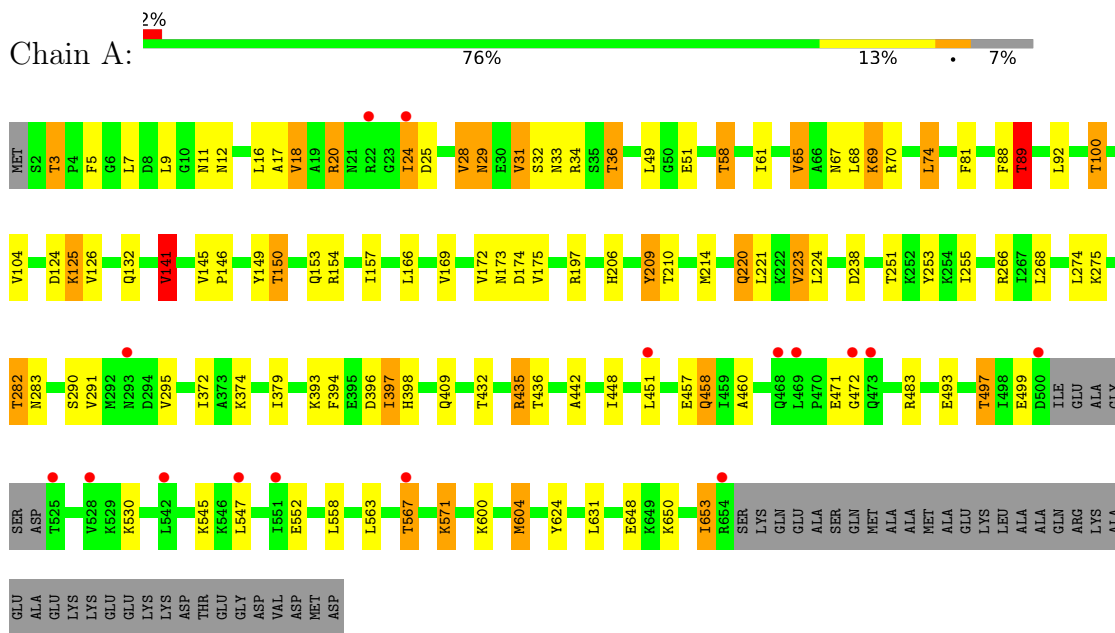
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	272	Total O 272 272	0	0
7	B	102	Total O 102 102	0	0
7	C	207	Total O 207 207	0	0
7	D	80	Total O 80 80	0	0

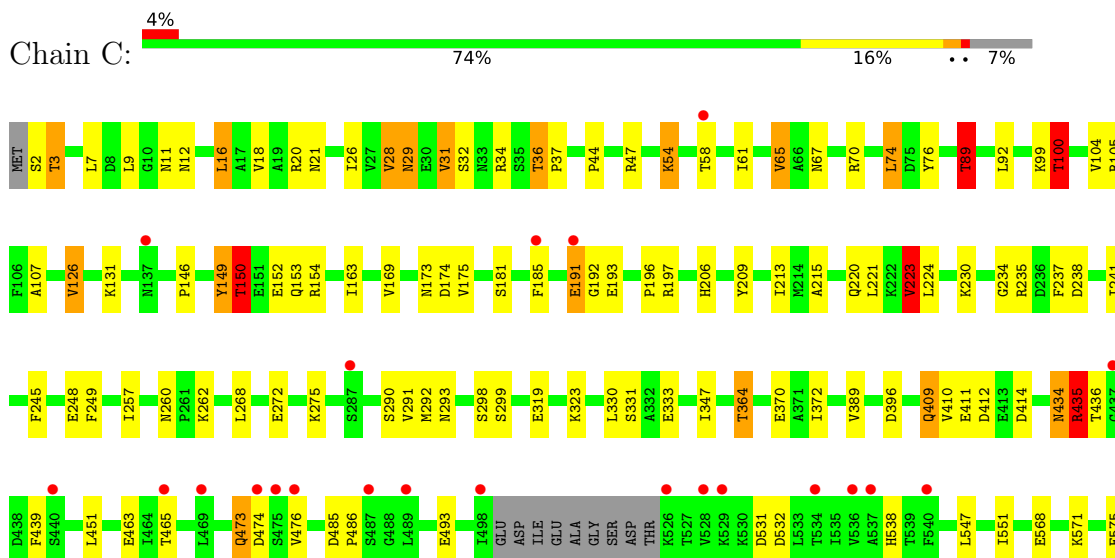
### 3 Residue-property plots [i](#)

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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.50Å 141.90Å 151.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 99.8 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.30Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.244 0.196 , 0.241	Depositor DCC
$R_{free}$ test set	6248 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, GOL, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.77	2/4965 (0.0%)	0.99	10/6731 (0.1%)
1	C	0.92	15/4917 (0.3%)	1.00	15/6673 (0.2%)
2	B	0.72	0/2943	0.90	1/3988 (0.0%)
2	D	0.98	7/2913 (0.2%)	0.93	3/3958 (0.1%)
All	All	0.85	24/15738 (0.2%)	0.97	29/21350 (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	C	0	1
2	B	0	1
All	All	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	GLU	CD-OE1	32.20	1.86	1.25
1	C	435	ARG	CZ-NH1	18.77	1.59	1.32
1	C	434	ASN	CG-OD1	17.27	1.56	1.23
1	C	655	SER	C-O	12.63	1.48	1.23
1	C	414	ASP	CG-OD1	10.55	1.45	1.25
1	C	409	GLN	CD-NE2	9.26	1.52	1.33
1	C	411	GLU	CD-OE1	8.77	1.42	1.25
1	C	435	ARG	NE-CZ	8.58	1.42	1.33
1	A	471	GLU	C-O	8.35	1.34	1.24
2	D	99	ASP	CG-OD1	7.67	1.40	1.25
2	D	289	GLU	CD-OE2	-7.66	1.10	1.25
2	D	289	GLU	C-N	7.36	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	GLU	C-O	7.06	1.32	1.24
1	C	474	ASP	CG-OD2	6.97	1.38	1.25
1	C	434	ASN	C-O	6.83	1.32	1.24
1	C	412	ASP	CG-OD2	6.48	1.37	1.25
2	D	99	ASP	CG-OD2	6.47	1.37	1.25
1	C	473	GLN	C-N	6.27	1.42	1.33
2	D	290	GLY	C-O	6.18	1.32	1.24
1	A	65	VAL	CA-CB	6.15	1.61	1.54
1	C	414	ASP	CG-OD2	6.12	1.36	1.25
1	C	474	ASP	CG-OD1	5.39	1.35	1.25
1	C	410	VAL	CA-CB	5.38	1.60	1.54
2	D	254	SER	C-N	5.03	1.40	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	435	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	A	141	VAL	CB-CA-C	-8.06	97.80	110.69
1	C	409	GLN	OE1-CD-NE2	7.73	130.33	122.60
1	C	89	THR	N-CA-C	-7.20	104.76	113.97
2	D	289	GLU	CG-CD-OE2	7.01	134.53	118.40
1	A	65	VAL	CB-CA-C	6.79	120.07	110.84
2	D	80	ASP	CA-C-N	6.74	128.26	119.84
2	D	80	ASP	C-N-CA	6.74	128.26	119.84
1	A	89	THR	N-CA-C	-6.50	105.66	113.97
1	C	100	THR	N-CA-C	5.96	118.67	109.07
1	C	435	ARG	CD-NE-CZ	-5.89	116.16	124.40
1	C	3	THR	CB-CA-C	5.81	116.45	109.31
1	C	234	GLY	CA-C-N	5.80	128.32	120.38
1	C	234	GLY	C-N-CA	5.80	128.32	120.38
1	C	150	THR	N-CA-CB	-5.74	102.16	110.36
1	A	3	THR	CB-CA-C	5.73	116.23	109.47
1	A	69	LYS	CB-CA-C	-5.39	101.51	110.68
1	C	21	ASN	CB-CA-C	-5.38	110.35	116.54
1	A	493	GLU	N-CA-C	5.36	119.97	113.38
1	C	223	VAL	CB-CA-C	5.27	118.00	111.15
2	B	225	ASP	N-CA-C	-5.25	106.64	112.57
1	C	347	ILE	CA-C-N	5.22	124.67	119.24
1	C	347	ILE	C-N-CA	5.22	124.67	119.24
1	C	65	VAL	CB-CA-C	5.18	118.55	110.83
1	A	220	GLN	N-CA-C	5.18	116.94	108.76
1	A	68	LEU	CA-C-N	5.15	127.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LEU	C-N-CA	5.15	127.44	120.38
1	A	295	VAL	N-CA-C	5.10	115.11	107.51
1	C	220	GLN	N-CA-C	5.07	116.94	108.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	THR	Peptide
1	C	434	ASN	Sidechain

## 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	4874	0	4770	72	0
1	C	4828	0	4693	60	1
2	B	2895	0	2846	29	0
2	D	2865	0	2748	36	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	31	0	12	0	0
5	C	31	0	12	0	0
6	A	6	0	8	0	0
7	A	272	0	0	9	1
7	B	102	0	0	0	0
7	C	207	0	0	7	0
7	D	80	0	0	1	0
All	All	16199	0	15089	194	1

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 6.

All (194) 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)
2:D:289:GLU:OE1	2:D:289:GLU:CD	1.86	1.18
2:B:311:ARG:HG2	2:B:311:ARG:HH21	1.13	1.09
1:A:17:ALA:HB1	1:A:24[A]:ILE:HD11	1.40	1.02
1:C:61:ILE:O	1:C:89:THR:HG23	1.65	0.95
2:B:194:ASN:H	2:B:332:HIS:HD2	1.15	0.89
1:C:150:THR:HG22	1:C:153:GLN:H	1.43	0.84
2:B:311:ARG:HH21	2:B:311:ARG:CG	1.92	0.82
1:A:61:ILE:O	1:A:89:THR:HG23	1.77	0.82
1:C:238:ASP:OD1	1:C:275:LYS:HE3	1.79	0.81
1:A:266:ARG:NH2	1:A:290:SER:O	2.17	0.77
1:C:463:GLU:OE1	1:C:538:HIS:HE1	1.66	0.77
1:A:150:THR:HG21	7:A:3030:HOH:O	1.84	0.77
1:C:150:THR:HG21	7:C:3030:HOH:O	1.85	0.76
1:A:20:ARG:HD2	1:A:25:ASP:OD2	1.85	0.76
1:C:11:ASN:HD21	1:C:67:ASN:HA	1.51	0.76
1:C:36:THR:HG22	7:C:3015:HOH:O	1.85	0.75
1:C:61:ILE:O	1:C:89:THR:CG2	2.34	0.75
2:B:311:ARG:HG2	2:B:311:ARG:NH2	1.92	0.74
2:D:364:ASN:C	2:D:364:ASN:HD22	1.96	0.74
2:D:205:PHE:HB3	2:D:225:ASP:HB3	1.69	0.74
2:D:151:ASN:H	2:D:154:GLN:HE21	1.35	0.73
1:A:58:THR:HG22	7:A:3178:HOH:O	1.88	0.73
1:A:563:LEU:O	1:A:567:THR:HG22	1.88	0.73
2:D:278:THR:OG1	2:D:279:GLN:NE2	2.21	0.73
1:A:238:ASP:OD1	1:A:275:LYS:HE2	1.90	0.72
2:B:194:ASN:H	2:B:332:HIS:CD2	2.06	0.71
1:A:497:THR:HG22	1:A:530:LYS:HB3	1.73	0.71
1:A:175:VAL:HG13	7:A:3094:HOH:O	1.92	0.69
1:A:11:ASN:HD21	1:A:67:ASN:HA	1.57	0.68
2:D:181:ILE:HD13	2:D:376:GLN:HE21	1.58	0.68
2:D:14:THR:HG22	2:D:15[A]:TYR:CD1	2.31	0.66
1:A:61:ILE:O	1:A:89:THR:CG2	2.43	0.65
1:C:58:THR:HG21	2:D:269:ARG:HH22	1.61	0.65
2:B:381:MET:HE3	2:B:381:MET:HA	1.78	0.65
1:A:31:VAL:HG13	1:A:51:GLU:HG3	1.79	0.64
1:A:49:LEU:HB2	1:A:125:LYS:HG3	1.80	0.64
2:D:310:PHE:CG	2:D:345:LYS:HG2	2.32	0.64
1:C:223:VAL:HG13	1:C:396:ASP:HA	1.80	0.62
1:A:150:THR:HG23	7:A:3144:HOH:O	1.99	0.62
1:A:150:THR:HG22	1:A:153:GLN:H	1.63	0.62
1:A:409:GLN:NE2	1:A:436:THR:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HH22	1:A:173:ASN:HD21	1.46	0.62
1:A:223:VAL:HG13	1:A:396:ASP:HA	1.82	0.62
1:A:5:PHE:CD1	1:A:141:VAL:HG13	2.35	0.61
1:A:11:ASN:ND2	1:A:67:ASN:HA	2.14	0.61
2:D:289:GLU:H	2:D:291:ILE:HD12	1.65	0.61
1:A:24[A]:ILE:HD12	1:A:374:LYS:HG2	1.82	0.61
1:C:11:ASN:ND2	1:C:67:ASN:HA	2.15	0.60
2:D:177:THR:O	2:D:181:ILE:HG23	2.00	0.60
2:D:14:THR:HG22	2:D:15[A]:TYR:HD1	1.65	0.60
1:C:150:THR:HG23	7:C:3145:HOH:O	2.00	0.60
1:A:571:LYS:HB2	1:A:624:TYR:CE1	2.37	0.60
1:C:206:HIS:O	1:C:235:ARG:HB2	2.02	0.60
1:A:29:ASN:HD22	1:A:29:ASN:C	2.09	0.60
2:D:364:ASN:ND2	2:D:366:ASP:H	1.99	0.60
2:B:235:ASN:ND2	2:B:264:ARG:HH22	2.00	0.59
1:C:181:SER:O	1:C:185:PHE:HB3	2.03	0.58
1:C:260:ASN:HB3	1:C:292:MET:HE2	1.84	0.58
2:D:364:ASN:HD22	2:D:366:ASP:H	1.50	0.57
2:B:11:LEU:HG	2:B:124:LEU:HD21	1.87	0.57
2:B:310:PHE:HB3	2:B:349:LEU:HD11	1.84	0.57
2:D:283:GLU:HG2	2:D:294:TYR:CD2	2.40	0.57
1:A:442:ALA:HB1	1:A:458:GLN:HE22	1.70	0.56
1:A:483:ARG:NH1	7:A:3233:HOH:O	2.06	0.56
2:B:211:THR:HG22	2:B:218:GLU:HB3	1.88	0.56
2:B:151:ASN:H	2:B:154:GLN:HE21	1.54	0.56
1:C:31:VAL:O	1:C:32:SER:HB2	2.06	0.55
1:C:28:VAL:HG13	1:C:32:SER:HA	1.89	0.55
1:C:154:ARG:HH22	1:C:173:ASN:HD21	1.54	0.55
1:A:24[A]:ILE:C	1:A:24[A]:ILE:HD13	2.32	0.54
1:C:34:ARG:NH1	1:C:370:GLU:OE2	2.41	0.54
1:C:174:ASP:HB2	1:C:372:ILE:HD13	1.88	0.54
1:A:124:ASP:OD2	1:A:558:LEU:HD11	2.08	0.53
1:A:28:VAL:HG13	1:A:32:SER:HA	1.90	0.53
1:A:563:LEU:O	1:A:567:THR:CG2	2.56	0.53
2:D:49:ARG:HD2	2:D:51:ILE:HD11	1.91	0.52
2:B:381:MET:HA	2:B:381:MET:CE	2.38	0.52
1:C:29:ASN:C	1:C:29:ASN:HD22	2.16	0.52
1:A:600:LYS:O	1:A:604:MET:HG2	2.10	0.52
1:C:485:ASP:HB2	1:C:486:PRO:CD	2.40	0.51
1:A:74:LEU:O	1:A:100:THR:HG23	2.10	0.51
1:A:282:THR:HG23	7:A:3166:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ARG:HH12	1:C:173:ASN:ND2	2.08	0.51
1:C:12:ASN:HB2	1:C:206:HIS:CG	2.46	0.51
1:A:24[A]:ILE:HD13	1:A:25:ASP:N	2.26	0.51
2:B:336:LEU:HD12	2:B:341:THR:HB	1.93	0.51
1:C:364:THR:HG23	1:C:364:THR:O	2.10	0.51
1:C:74:LEU:O	1:C:100:THR:HG22	2.10	0.51
1:C:196:PRO:HB2	1:C:215:ALA:HB1	1.92	0.50
1:A:17:ALA:CB	1:A:24[A]:ILE:HD11	2.27	0.50
1:A:18:VAL:HG13	1:A:20:ARG:HG2	1.93	0.50
1:C:257:ILE:HA	1:C:292:MET:CE	2.41	0.50
2:D:310:PHE:HB3	2:D:349:LEU:HD11	1.93	0.50
1:A:36:THR:HG22	7:A:3015:HOH:O	2.11	0.50
1:C:409:GLN:OE1	1:C:435:ARG:HG3	2.12	0.50
1:C:319:GLU:O	1:C:323:LYS:HG3	2.13	0.49
1:A:81:PHE:HE1	1:A:100:THR:HG21	1.78	0.49
1:A:650:LYS:HA	1:A:653:ILE:HD12	1.95	0.48
1:A:67:ASN:HB2	1:A:88:PHE:CZ	2.49	0.48
1:C:237:PHE:O	1:C:241:ILE:HG13	2.14	0.48
1:A:49:LEU:CB	1:A:125:LYS:HG3	2.44	0.48
1:C:146:PRO:O	1:C:149:TYR:HB2	2.14	0.48
2:B:235:ASN:HD21	2:B:264:ARG:HH22	1.61	0.48
1:C:131:LYS:HE3	7:C:3113:HOH:O	2.13	0.47
1:C:74:LEU:HB3	1:C:100:THR:HG23	1.96	0.47
1:A:29:ASN:ND2	1:A:33:ASN:H	2.12	0.47
1:C:76:TYR:HD1	1:C:100:THR:HB	1.78	0.47
1:C:257:ILE:HG22	1:C:292:MET:HE3	1.97	0.47
2:D:78:PHE:N	2:D:99:ASP:O	2.47	0.47
2:B:22:GLN:NE2	2:B:134:TYR:OH	2.48	0.47
2:B:285:ASP:OD1	2:B:294:TYR:OH	2.22	0.47
1:C:435:ARG:HG2	1:C:439:PHE:CD1	2.50	0.46
1:A:31:VAL:HG22	1:A:33:ASN:ND2	2.29	0.46
1:A:571:LYS:HB2	1:A:624:TYR:CD1	2.49	0.46
2:D:310:PHE:CD1	2:D:345:LYS:HG2	2.50	0.46
1:A:458:GLN:NE2	1:A:460:ALA:O	2.48	0.46
1:A:175:VAL:HG11	1:A:210:THR:CG2	2.46	0.46
1:A:141:VAL:HG22	1:A:166:LEU:HB3	1.96	0.46
1:A:175:VAL:HG11	1:A:210:THR:HG21	1.97	0.46
2:D:68:PHE:HB2	7:D:1275:HOH:O	2.14	0.46
2:B:256:ASN:O	2:B:260:VAL:HG23	2.15	0.46
1:C:260:ASN:CB	1:C:292:MET:HE2	2.46	0.46
1:A:214:MET:HG2	1:A:223:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASN:ND2	1:C:70:ARG:HG2	2.31	0.45
1:C:163:ILE:HA	1:C:551:ILE:HG12	1.98	0.45
1:A:145:VAL:HB	1:A:146:PRO:HD2	1.97	0.45
1:C:330:LEU:HD12	1:C:331:SER:O	2.17	0.45
1:C:571:LYS:HE3	7:C:3205:HOH:O	2.17	0.45
1:C:44:PRO:O	1:C:107:ALA:HA	2.16	0.45
1:C:16:LEU:HD11	1:C:126:VAL:HG22	1.99	0.45
1:C:191:GLU:HB3	1:C:192:GLY:H	1.57	0.45
2:B:146:VAL:HB	2:B:150:PHE:CD1	2.51	0.45
1:C:154:ARG:HH12	1:C:173:ASN:HD21	1.63	0.45
1:A:31:VAL:O	1:A:32:SER:HB2	2.17	0.44
2:D:38:THR:HB	2:D:127:MET:HE1	1.99	0.44
2:D:143:VAL:HG11	2:D:173:ILE:HD12	1.98	0.44
1:C:37:PRO:HB3	1:C:54:LYS:HG3	1.99	0.44
2:D:364:ASN:HD22	2:D:365:PRO:N	2.15	0.44
1:A:409:GLN:HE22	1:A:435:ARG:HG3	1.83	0.44
2:B:292:ASP:HB3	2:B:294:TYR:CE2	2.53	0.44
1:A:24[A]:ILE:HD12	1:A:374:LYS:CG	2.48	0.44
2:B:46:ASP:O	2:B:108:LYS:HA	2.18	0.44
2:B:336:LEU:HD21	2:B:359:LEU:HD22	1.99	0.44
2:D:331:ILE:O	2:D:357:ARG:NH2	2.47	0.43
1:A:221:LEU:O	1:A:394:PHE:HA	2.18	0.43
1:A:397:ILE:HG13	1:A:398:HIS:N	2.33	0.43
1:C:26:ILE:HG13	1:C:370:GLU:CD	2.43	0.43
2:D:192:GLU:HA	2:D:212[A]:ILE:O	2.18	0.43
2:D:151:ASN:H	2:D:154:GLN:NE2	2.07	0.43
2:B:65:ASN:HA	2:B:105:VAL:HG22	2.01	0.43
2:B:12:GLY:HA3	2:B:15[B]:TYR:O	2.19	0.43
1:C:175:VAL:HG13	7:C:3093:HOH:O	2.17	0.43
1:A:648:GLU:HG3	7:A:3267:HOH:O	2.19	0.43
1:C:364:THR:O	1:C:364:THR:CG2	2.66	0.43
2:D:175:GLU:N	2:D:176:PRO:HD2	2.33	0.43
1:C:2:SER:N	7:C:3185:HOH:O	2.51	0.42
1:C:575:GLU:HG2	1:C:579:TYR:CE1	2.53	0.42
1:C:629:GLU:HA	1:C:629:GLU:OE1	2.19	0.42
2:D:303:GLU:HB3	2:D:345:LYS:HD2	2.00	0.42
1:A:11:ASN:ND2	1:A:70:ARG:HG2	2.33	0.42
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.54	0.42
1:C:568:GLU:HB3	2:D:279:GLN:NE2	2.35	0.42
1:A:31:VAL:O	1:A:31:VAL:HG23	2.19	0.42
1:A:253:TYR:HB2	1:A:255:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ILE:HD13	1:A:457:GLU:HA	2.00	0.42
1:C:248:GLU:OE1	1:C:299:SER:OG	2.37	0.42
2:B:128:LYS:O	2:B:132:GLU:HG3	2.19	0.42
2:B:197:ILE:N	2:B:197:ILE:HD12	2.34	0.42
1:A:34:ARG:HD3	7:A:3018:HOH:O	2.20	0.41
2:D:20:VAL:HG13	2:D:22:GLN:HG2	2.01	0.41
2:D:289:GLU:HG3	2:D:291:ILE:HD11	2.01	0.41
2:B:261:ARG:O	2:B:261:ARG:HD3	2.20	0.41
1:A:74:LEU:HB3	1:A:100:THR:HG23	2.01	0.41
1:A:238:ASP:OD1	1:A:275:LYS:CE	2.66	0.41
2:B:363:ILE:O	2:B:364:ASN:C	2.62	0.41
1:C:245:PHE:HB3	1:C:249:PHE:CE2	2.56	0.41
2:D:95:ILE:HG13	2:D:102:LYS:HB2	2.03	0.41
1:A:174:ASP:HB2	1:A:372:ILE:HD13	2.02	0.41
1:A:29:ASN:HD21	1:A:33:ASN:H	1.68	0.41
2:D:143:VAL:CG1	2:D:173:ILE:CD1	2.99	0.41
1:A:209:TYR:C	1:A:209:TYR:CD2	2.98	0.41
1:C:31:VAL:O	1:C:31:VAL:CG2	2.69	0.41
1:C:221:LEU:C	1:C:221:LEU:HD12	2.45	0.41
2:D:22:GLN:NE2	2:D:134:TYR:OH	2.52	0.41
1:A:221:LEU:C	1:A:221:LEU:HD12	2.45	0.41
1:A:497:THR:HG21	1:A:530:LYS:HD3	2.03	0.41
2:B:15[B]:TYR:CD2	2:B:15[B]:TYR:C	2.98	0.41
2:B:93:GLN:HE21	2:D:89:HIS:HD2	1.69	0.40
1:A:172:VAL:HG21	1:A:379:ILE:HD13	2.04	0.40
1:A:220:GLN:HA	1:A:393:LYS:O	2.21	0.40
1:C:36:THR:HA	1:C:37:PRO:HD3	1.97	0.40
1:A:157:ILE:HA	1:A:157:ILE:HD12	1.87	0.40
2:D:178:ALA:O	2:D:372:GLY:HA3	2.22	0.40
1:C:99:LYS:HE3	1:C:152:GLU:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ASN:OD1	7:A:3056:HOH:O[4_467]	2.13	0.07

## 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	627/675 (93%)	600 (96%)	24 (4%)	3 (0%)	24	31
1	C	624/675 (92%)	594 (95%)	29 (5%)	1 (0%)	43	55
2	B	378/382 (99%)	365 (97%)	13 (3%)	0	100	100
2	D	380/382 (100%)	365 (96%)	11 (3%)	4 (1%)	11	13
All	All	2009/2114 (95%)	1924 (96%)	77 (4%)	8 (0%)	30	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	499	GLU
1	A	472	GLY
1	C	473	GLN
2	D	230	GLY
2	D	98	GLY
1	A	653	ILE
2	D	229	GLY
2	D	81	PRO

### 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	520/576 (90%)	470 (90%)	50 (10%)	8	10
1	C	512/576 (89%)	460 (90%)	52 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	301/315 (96%)	292 (97%)	9 (3%)	36	53
2	D	291/315 (92%)	266 (91%)	25 (9%)	10	13
All	All	1624/1782 (91%)	1488 (92%)	136 (8%)	10	14

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	LEU
1	A	9	LEU
1	A	16	LEU
1	A	18	VAL
1	A	20	ARG
1	A	24[A]	ILE
1	A	24[B]	ILE
1	A	28	VAL
1	A	29	ASN
1	A	31	VAL
1	A	36	THR
1	A	58	THR
1	A	65	VAL
1	A	69	LYS
1	A	74	LEU
1	A	89	THR
1	A	92	LEU
1	A	100	THR
1	A	104	VAL
1	A	125	LYS
1	A	126	VAL
1	A	132	GLN
1	A	141	VAL
1	A	149	TYR
1	A	150	THR
1	A	169	VAL
1	A	197	ARG
1	A	209	TYR
1	A	223	VAL
1	A	224	LEU
1	A	251	THR
1	A	268	LEU
1	A	274	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	282	THR
1	A	283	ASN
1	A	291	VAL
1	A	397	ILE
1	A	432	THR
1	A	435	ARG
1	A	451	LEU
1	A	458	GLN
1	A	497	THR
1	A	545	LYS
1	A	547	LEU
1	A	552	GLU
1	A	567	THR
1	A	571	LYS
1	A	604	MET
1	A	631	LEU
2	B	11	LEU
2	B	13	THR
2	B	61	LEU
2	B	100	LYS
2	B	105	VAL
2	B	228	LEU
2	B	279	GLN
2	B	311	ARG
2	B	381	MET
1	C	3	THR
1	C	7	LEU
1	C	9	LEU
1	C	16	LEU
1	C	18	VAL
1	C	20	ARG
1	C	28	VAL
1	C	29	ASN
1	C	31	VAL
1	C	36	THR
1	C	47	ARG
1	C	54	LYS
1	C	65	VAL
1	C	74	LEU
1	C	89	THR
1	C	92	LEU
1	C	100	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	104	VAL
1	C	105	ARG
1	C	126	VAL
1	C	149	TYR
1	C	150	THR
1	C	169	VAL
1	C	191	GLU
1	C	197	ARG
1	C	209	TYR
1	C	213	ILE
1	C	223	VAL
1	C	224	LEU
1	C	230	LYS
1	C	262	LYS
1	C	268	LEU
1	C	272	GLU
1	C	290	SER
1	C	291	VAL
1	C	298	SER
1	C	333	GLU
1	C	364	THR
1	C	389	VAL
1	C	435	ARG
1	C	436	THR
1	C	451	LEU
1	C	465	THR
1	C	476	VAL
1	C	493	GLU
1	C	531	ASP
1	C	532	ASP
1	C	547	LEU
1	C	588	GLU
1	C	600	LYS
1	C	601	LEU
1	C	631	LEU
2	D	11	LEU
2	D	13	THR
2	D	47	THR
2	D	51	ILE
2	D	58	GLN
2	D	61	LEU
2	D	64	GLN

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Mol	Chain	Res	Type
2	D	80	ASP
2	D	93	GLN
2	D	112	LYS
2	D	119	ILE
2	D	156	GLN
2	D	173	ILE
2	D	181	ILE
2	D	236	ARG
2	D	263	LEU
2	D	269	ARG
2	D	282	LEU
2	D	289	GLU
2	D	291	ILE
2	D	299	ARG
2	D	345	LYS
2	D	350	LEU
2	D	357	ARG
2	D	364	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	21	ASN
1	A	29	ASN
1	A	46	ASN
1	A	60	ASN
1	A	111	HIS
1	A	156	ASN
1	A	173	ASN
1	A	293	ASN
1	A	409	GLN
1	A	458	GLN
1	A	461	ASN
1	A	548	ASN
1	A	555	ASN
1	A	602	GLN
2	B	22	GLN
2	B	84	GLN
2	B	154	GLN
2	B	156	GLN
2	B	168	ASN

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Mol	Chain	Res	Type
2	B	235	ASN
2	B	256	ASN
2	B	332	HIS
2	B	376	GLN
1	C	11	ASN
1	C	29	ASN
1	C	60	ASN
1	C	83	GLN
1	C	111	HIS
1	C	117	GLN
1	C	156	ASN
1	C	173	ASN
1	C	283	ASN
1	C	352	GLN
1	C	454	ASN
1	C	538	HIS
1	C	548	ASN
1	C	555	ASN
1	C	602	GLN
2	D	22	GLN
2	D	64	GLN
2	D	89	HIS
2	D	154	GLN
2	D	156	GLN
2	D	194	ASN
2	D	279	GLN
2	D	364	ASN
2	D	376	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

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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
5	ATP	C	1001	4,3	32,33,33	1.48	4 (12%)	48,52,52	1.80	12 (25%)
5	ATP	A	1001	4,3	32,33,33	1.57	4 (12%)	48,52,52	1.85	13 (27%)
6	GOL	A	3002	-	5,5,5	0.66	0	5,5,5	0.82	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
5	ATP	C	1001	4,3	-	2/22/38/38	0/3/3/3
5	ATP	A	1001	4,3	-	1/22/38/38	0/3/3/3
6	GOL	A	3002	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	ATP	C5-C4	4.98	1.48	1.39
5	A	1001	ATP	PB-O3B	4.69	1.64	1.59
5	A	1001	ATP	C5-C4	4.66	1.47	1.39
5	C	1001	ATP	PB-O3B	3.95	1.63	1.59
5	A	1001	ATP	C5-C6	2.85	1.48	1.41
5	C	1001	ATP	C5-C6	2.82	1.48	1.41
5	C	1001	ATP	C8-N7	2.46	1.36	1.31
5	A	1001	ATP	C8-N7	2.13	1.35	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ATP	C5-C4-N3	-5.28	119.45	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1001	ATP	C5-C4-N3	-4.76	120.17	126.72
5	A	1001	ATP	N3-C4-N9	4.65	135.08	127.17
5	C	1001	ATP	N3-C4-N9	4.11	134.16	127.17
5	A	1001	ATP	C2-N3-C4	3.79	121.08	111.83
5	A	1001	ATP	N3-C2-N1	-3.79	122.85	128.58
5	A	1001	ATP	C4-N9-C8	3.68	109.60	105.74
5	C	1001	ATP	N3-C2-N1	-3.54	123.23	128.58
5	C	1001	ATP	C4-N9-C8	3.52	109.43	105.74
5	C	1001	ATP	C2-N3-C4	3.49	120.37	111.83
5	C	1001	ATP	C4-C5-N7	-3.36	106.74	110.58
5	A	1001	ATP	C4-C5-N7	-3.05	107.09	110.58
5	C	1001	ATP	C6-C5-N7	2.73	137.35	132.09
5	C	1001	ATP	C5-N7-C8	2.71	107.71	103.45
5	A	1001	ATP	O4'-C1'-N9	2.56	113.00	108.09
5	A	1001	ATP	C5-N7-C8	2.49	107.37	103.45
5	C	1001	ATP	N9-C8-N7	-2.46	110.45	113.94
5	A	1001	ATP	N9-C8-N7	-2.45	110.46	113.94
5	C	1001	ATP	O4'-C1'-N9	2.37	112.65	108.09
5	A	1001	ATP	O3G-PG-O2G	2.34	116.58	107.80
5	A	1001	ATP	C6-C5-N7	2.25	136.44	132.09
5	C	1001	ATP	C2-N1-C6	2.23	122.40	118.73
5	A	1001	ATP	C2-N1-C6	2.23	122.40	118.73
5	A	1001	ATP	O2A-PA-O3A	2.15	113.10	107.27
5	C	1001	ATP	O3A-PB-O1B	-2.07	104.47	110.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

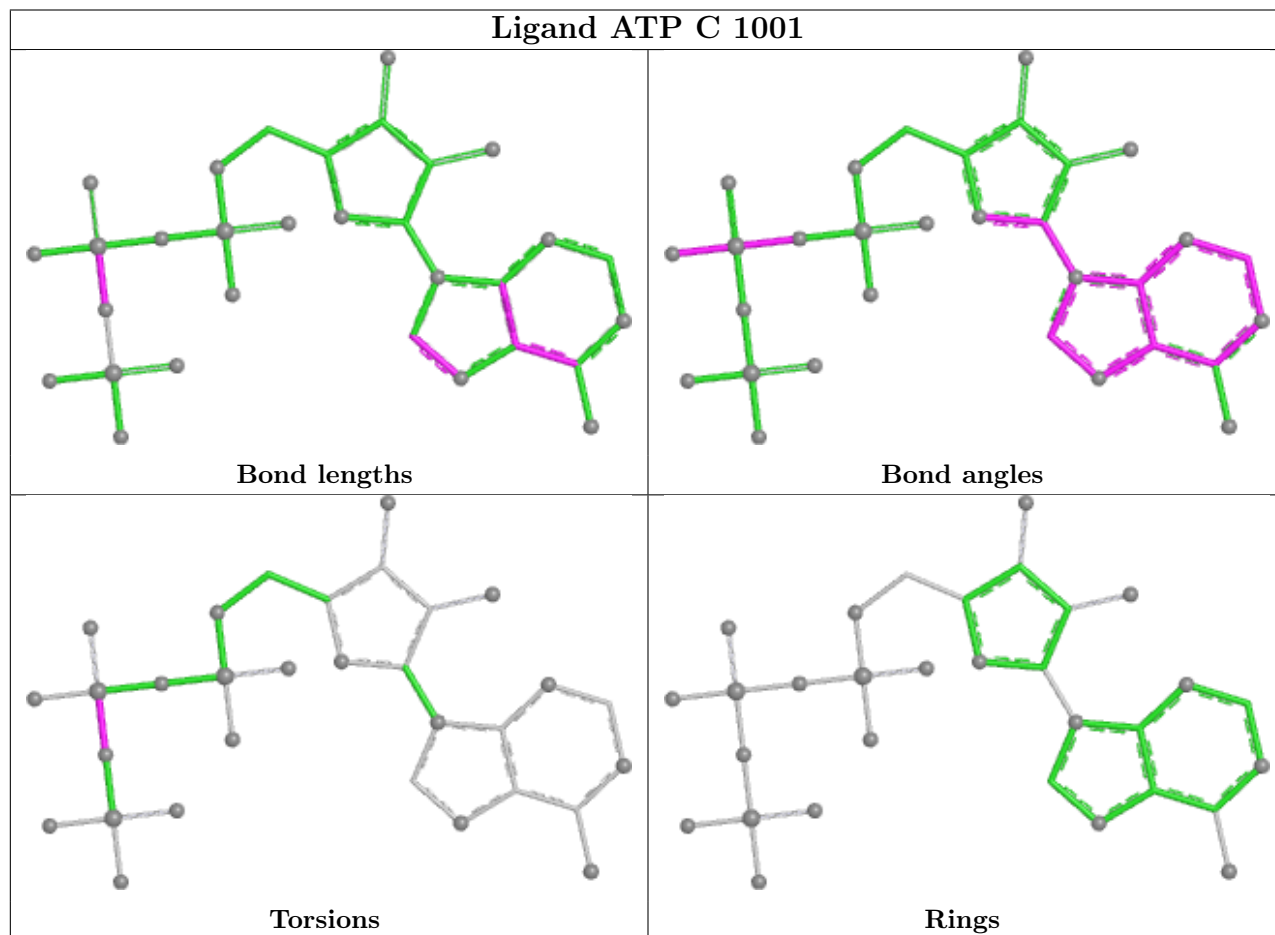
Mol	Chain	Res	Type	Atoms
6	A	3002	GOL	C1-C2-C3-O3
6	A	3002	GOL	O2-C2-C3-O3
5	A	1001	ATP	PG-O3B-PB-O2B
5	C	1001	ATP	PG-O3B-PB-O2B
5	C	1001	ATP	PG-O3B-PB-O1B

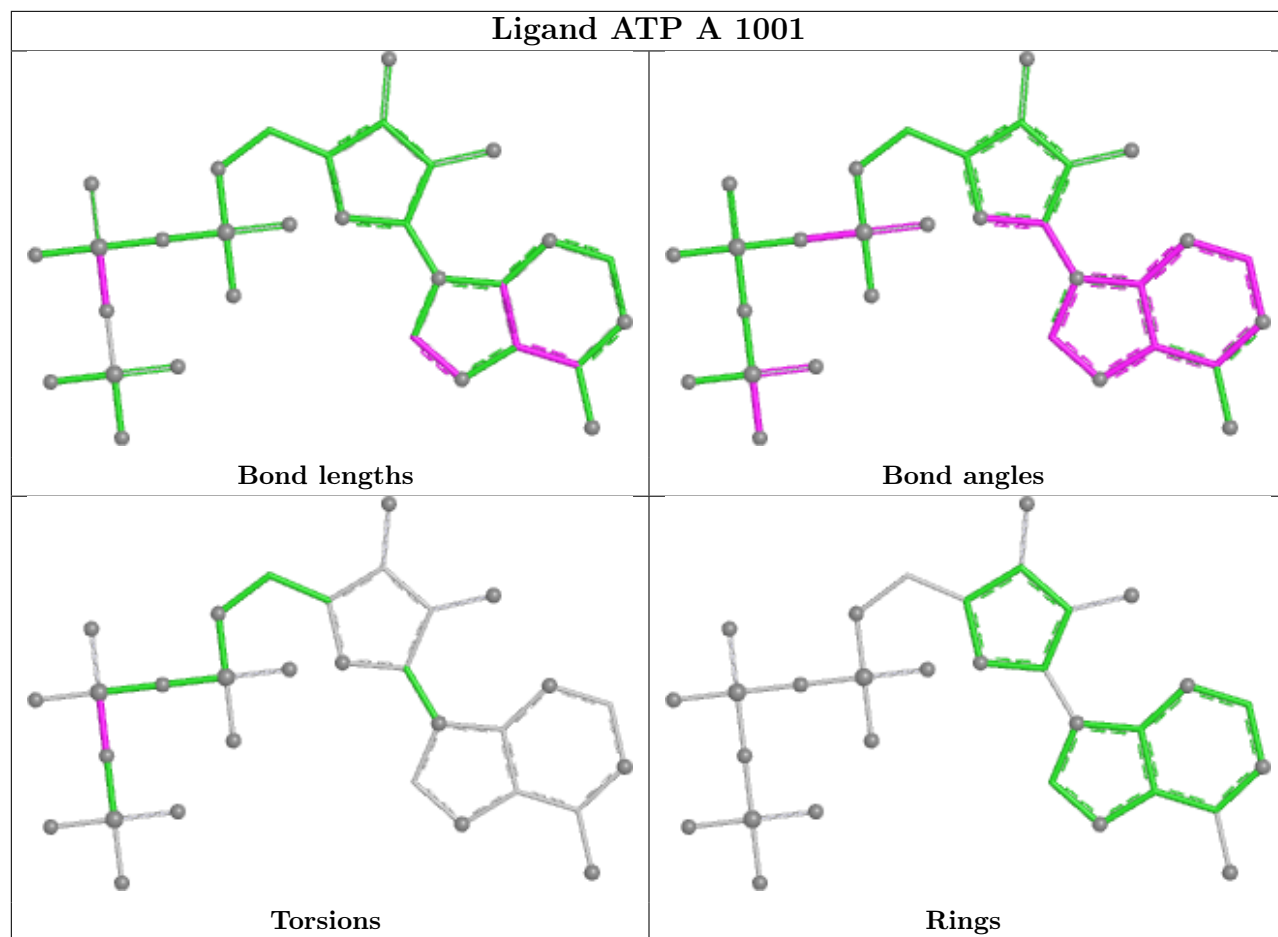
There are no ring outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	629/675 (93%)	0.12	16 (2%) 58 60	24, 43, 54, 68	2 (0%)
1	C	627/675 (92%)	0.36	27 (4%) 40 41	28, 44, 55, 76	1 (0%)
2	B	379/382 (99%)	0.33	22 (5%) 29 31	22, 44, 54, 79	1 (0%)
2	D	379/382 (99%)	1.01	54 (14%) 6 7	20, 45, 52, 72	3 (0%)
All	All	2014/2114 (95%)	0.40	119 (5%) 28 30	20, 44, 54, 79	7 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	GLY	5.5
1	C	655	SER	4.8
2	B	228	LEU	4.7
2	D	226	THR	4.6
1	C	654	ARG	4.5
2	D	255	GLN	4.5
1	A	473	GLN	4.3
2	D	4	ALA	4.3
2	D	256	ASN	4.3
2	D	229	GLY	4.3
2	D	300	ALA	4.0
2	D	227	HIS	4.0
2	B	227	HIS	3.6
2	B	226	THR	3.6
1	A	525	THR	3.5
2	D	258	ARG	3.5
1	A	472	GLY	3.5
1	C	526	LYS	3.4
2	D	278	THR	3.4
1	C	475	SER	3.3
1	C	487	SER	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	228	LEU	3.2
1	A	528	VAL	3.1
1	A	469	LEU	3.1
2	D	15[A]	TYR	3.1
2	D	250	LYS	3.1
2	D	34	GLY	3.0
1	C	652	ALA	3.0
1	C	536	VAL	3.0
1	C	653	ILE	3.0
2	B	229	GLY	2.9
2	D	203	GLY	2.9
1	C	540	PHE	2.9
2	B	278	THR	2.9
1	A	293	ASN	2.9
1	C	191	GLU	2.9
1	C	58	THR	2.9
1	A	500	ASP	2.9
2	D	230	GLY	2.8
1	C	137	ASN	2.8
2	D	355	ASN	2.8
1	C	437	GLY	2.8
2	D	131	ALA	2.8
1	A	22	ARG	2.8
2	D	299	ARG	2.8
2	D	287	LEU	2.7
1	A	654	ARG	2.7
1	C	537	ALA	2.7
1	C	185	PHE	2.7
1	A	547	LEU	2.7
2	D	5	ALA	2.7
2	D	279	GLN	2.7
2	B	275	SER	2.7
2	D	231	GLU	2.6
2	D	187[A]	ARG	2.6
2	B	202	GLY	2.6
2	D	202	GLY	2.6
2	D	274	LEU	2.6
2	D	288	PHE	2.6
2	D	26	VAL	2.6
1	C	650	LYS	2.6
2	D	137	TYR	2.5
2	B	274	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	136	GLY	2.5
2	D	138	PRO	2.5
1	C	528	VAL	2.5
1	C	474	ASP	2.5
2	D	225	ASP	2.5
2	D	259	ALA	2.5
2	B	250	LYS	2.4
2	B	276	SER	2.4
2	B	288	PHE	2.4
2	D	7	ILE	2.4
2	D	260	VAL	2.4
1	C	469	LEU	2.4
2	D	245	PHE	2.4
2	D	99	ASP	2.3
2	D	276	SER	2.3
1	C	498	ILE	2.3
2	B	336	LEU	2.3
2	D	135	LEU	2.3
2	B	298	THR	2.3
2	B	299	ARG	2.3
1	A	24[A]	ILE	2.3
2	D	134	TYR	2.3
2	D	6	ALA	2.3
2	D	142	ALA	2.3
2	B	233	PHE	2.2
2	D	28	ILE	2.2
2	D	20	VAL	2.2
2	D	262	ARG	2.2
1	A	468	GLN	2.2
2	B	300	ALA	2.2
2	D	298	THR	2.2
1	C	489	LEU	2.2
2	D	291	ILE	2.2
2	B	203	GLY	2.2
1	C	440	SER	2.2
2	D	30	ALA	2.2
2	D	275	SER	2.2
1	A	551	ILE	2.1
2	D	133	ALA	2.1
2	B	258	ARG	2.1
1	A	451	LEU	2.1
2	D	58	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	567	THR	2.1
1	C	534	THR	2.1
2	D	280	ALA	2.1
2	B	225	ASP	2.1
1	C	287	SER	2.1
1	C	465	THR	2.1
1	C	529	LYS	2.1
2	B	289	GLU	2.1
1	A	542	LEU	2.1
2	D	119	ILE	2.1
2	D	127	MET	2.0
2	D	320	ALA	2.0
2	B	15[A]	TYR	2.0
1	C	476	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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.

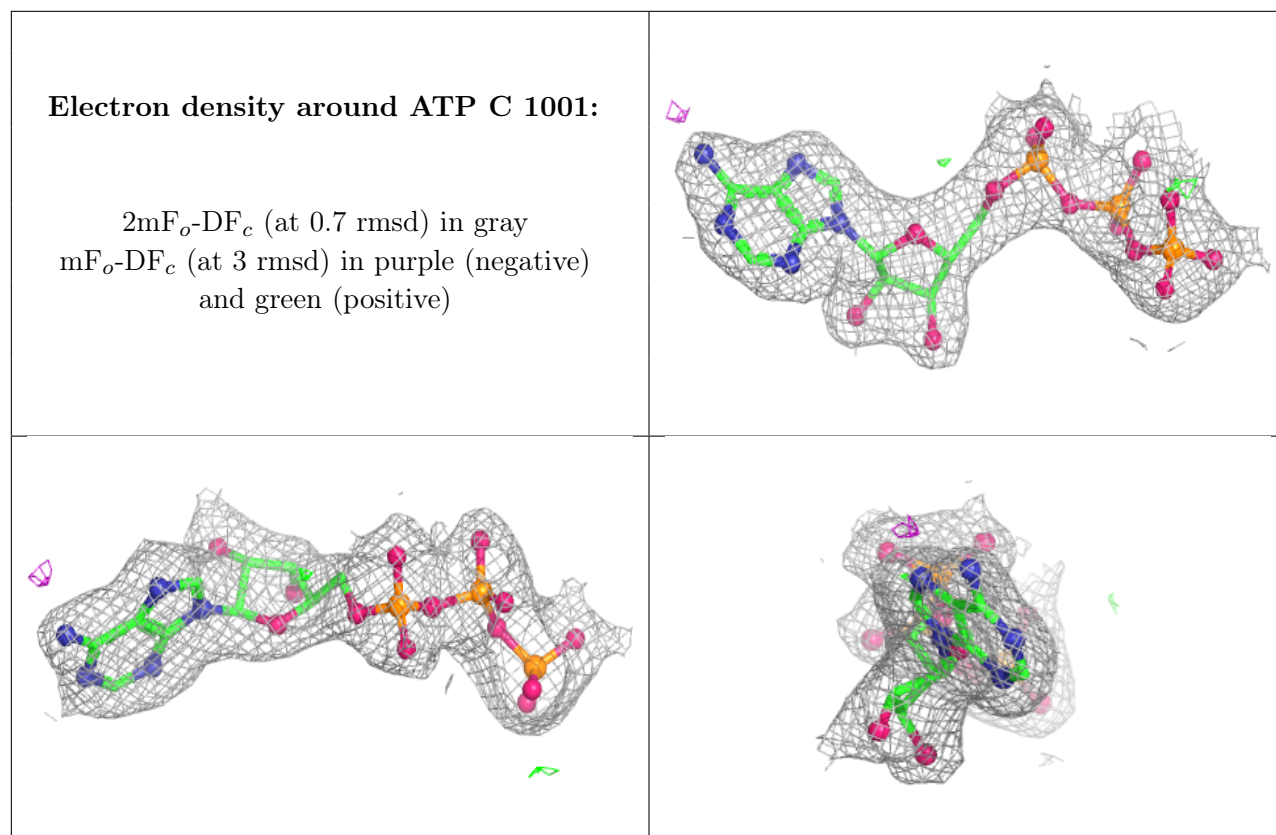
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	3002	6/6	0.79	0.19	57,60,61,62	0
3	MG	D	2001	1/1	0.89	0.09	33,33,33,33	0
3	MG	B	2001	1/1	0.92	0.15	37,37,37,37	0
3	MG	C	2002	1/1	0.92	0.07	29,29,29,29	0
3	MG	A	2002	1/1	0.94	0.06	42,42,42,42	0
4	K	C	3001	1/1	0.98	0.05	45,45,45,45	0
5	ATP	C	1001	31/31	0.98	0.05	36,41,43,44	0
3	MG	C	2001	1/1	0.98	0.05	40,40,40,40	0
5	ATP	A	1001	31/31	0.99	0.05	40,42,45,47	0

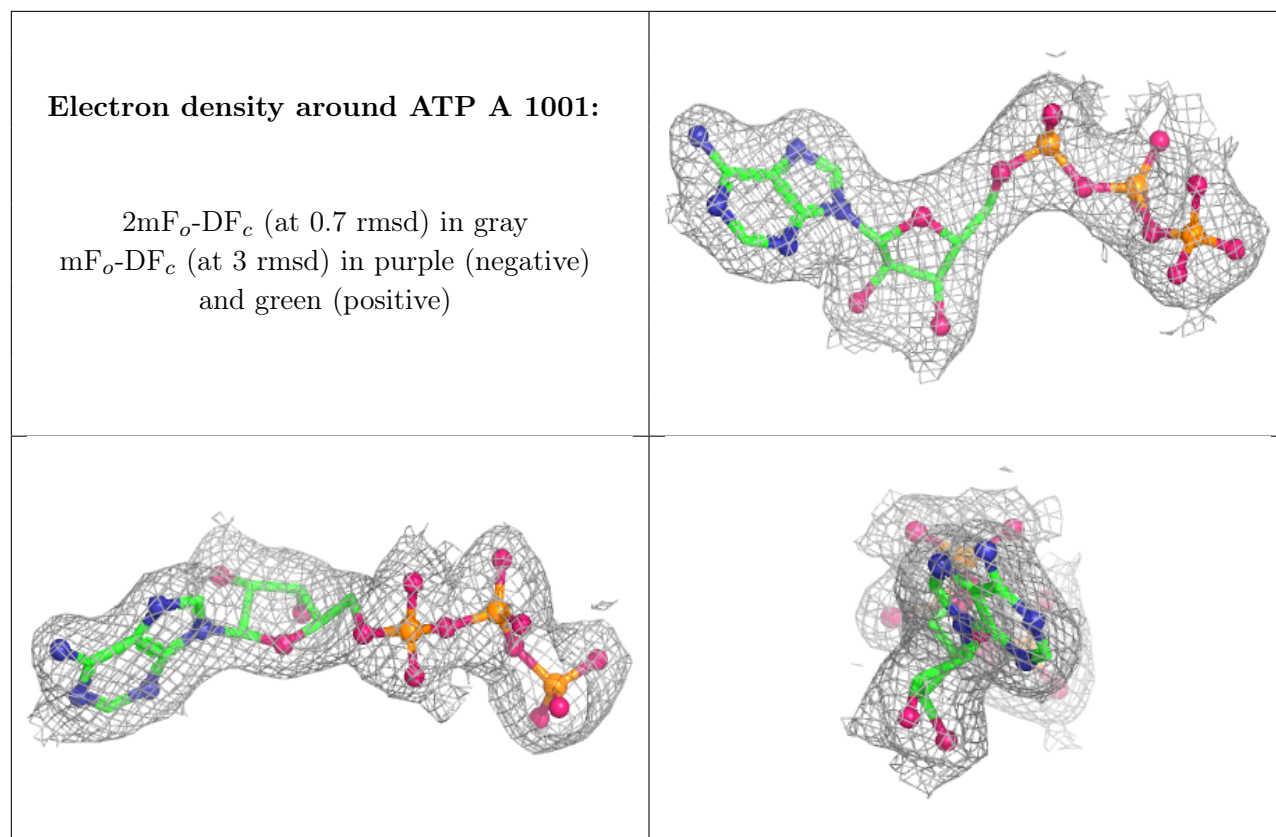
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	A	3001	1/1	0.99	0.05	44,44,44,44	0
3	MG	A	2001	1/1	0.99	0.02	40,40,40,40	0

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 [i](#)

There are no such residues in this entry.