



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:04 PM UTC

PDB ID : 9QN5 / pdb\_00009qn5  
Title : Crystal structure of human SUMO E1 with small unit cell parameters in the P1 21 1 space group.  
Authors : Vilorio, M.; Francois, R.M.M.; Didierjean, C.  
Deposited on : 2025-03-24  
Resolution : 1.97 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

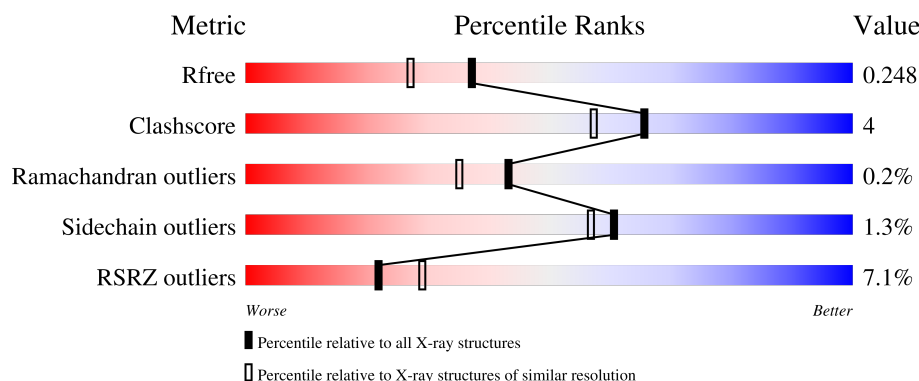
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	369	<div> <div>2%</div> <div>74%</div> <div>9%</div> <div>17%</div> </div>
1	C	369	<div> <div>6%</div> <div>73%</div> <div>10%</div> <div>16%</div> </div>
2	B	640	<div> <div>3%</div> <div>73%</div> <div>7%</div> <div>20%</div> </div>
2	D	640	<div> <div>11%</div> <div>68%</div> <div>11%</div> <div>20%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13159 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 SUMO-activating enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2411	1529	409	460	13			
1	C	309	Total	C	N	O	S	0	0	0
			2431	1542	413	463	13			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q9UBE0
A	-21	GLY	-	expression tag	UNP Q9UBE0
A	-20	SER	-	expression tag	UNP Q9UBE0
A	-19	SER	-	expression tag	UNP Q9UBE0
A	-18	HIS	-	expression tag	UNP Q9UBE0
A	-17	HIS	-	expression tag	UNP Q9UBE0
A	-16	HIS	-	expression tag	UNP Q9UBE0
A	-15	HIS	-	expression tag	UNP Q9UBE0
A	-14	HIS	-	expression tag	UNP Q9UBE0
A	-13	HIS	-	expression tag	UNP Q9UBE0
A	-12	SER	-	expression tag	UNP Q9UBE0
A	-11	SER	-	expression tag	UNP Q9UBE0
A	-10	GLY	-	expression tag	UNP Q9UBE0
A	-9	LEU	-	expression tag	UNP Q9UBE0
A	-8	VAL	-	expression tag	UNP Q9UBE0
A	-7	PRO	-	expression tag	UNP Q9UBE0
A	-6	ARG	-	expression tag	UNP Q9UBE0
A	-5	GLY	-	expression tag	UNP Q9UBE0
A	-4	SER	-	expression tag	UNP Q9UBE0
A	-3	HIS	-	expression tag	UNP Q9UBE0
A	-2	MET	-	expression tag	UNP Q9UBE0
A	-1	ALA	-	expression tag	UNP Q9UBE0
A	0	SER	-	expression tag	UNP Q9UBE0
C	-22	MET	-	initiating methionine	UNP Q9UBE0
C	-21	GLY	-	expression tag	UNP Q9UBE0

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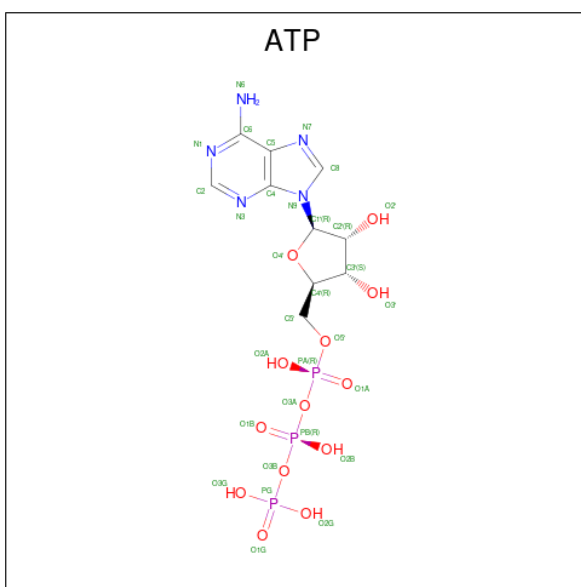
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	SER	-	expression tag	UNP Q9UBE0
C	-19	SER	-	expression tag	UNP Q9UBE0
C	-18	HIS	-	expression tag	UNP Q9UBE0
C	-17	HIS	-	expression tag	UNP Q9UBE0
C	-16	HIS	-	expression tag	UNP Q9UBE0
C	-15	HIS	-	expression tag	UNP Q9UBE0
C	-14	HIS	-	expression tag	UNP Q9UBE0
C	-13	HIS	-	expression tag	UNP Q9UBE0
C	-12	SER	-	expression tag	UNP Q9UBE0
C	-11	SER	-	expression tag	UNP Q9UBE0
C	-10	GLY	-	expression tag	UNP Q9UBE0
C	-9	LEU	-	expression tag	UNP Q9UBE0
C	-8	VAL	-	expression tag	UNP Q9UBE0
C	-7	PRO	-	expression tag	UNP Q9UBE0
C	-6	ARG	-	expression tag	UNP Q9UBE0
C	-5	GLY	-	expression tag	UNP Q9UBE0
C	-4	SER	-	expression tag	UNP Q9UBE0
C	-3	HIS	-	expression tag	UNP Q9UBE0
C	-2	MET	-	expression tag	UNP Q9UBE0
C	-1	ALA	-	expression tag	UNP Q9UBE0
C	0	SER	-	expression tag	UNP Q9UBE0

- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	513	Total	C	N	O	S	0	1	0
			4034	2563	694	757	20			
2	D	514	Total	C	N	O	S	1	1	0
			4041	2568	697	756	20			

- Molecule 3 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
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

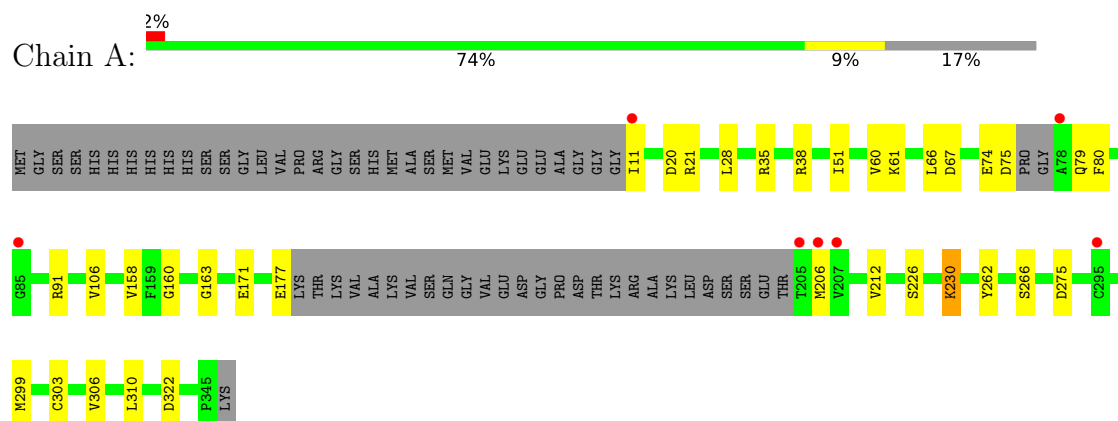
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total 47	O 47	0	0
6	B	69	Total 69	O 69	0	0
6	C	37	Total 37	O 37	0	0
6	D	23	Total 23	O 23	0	0

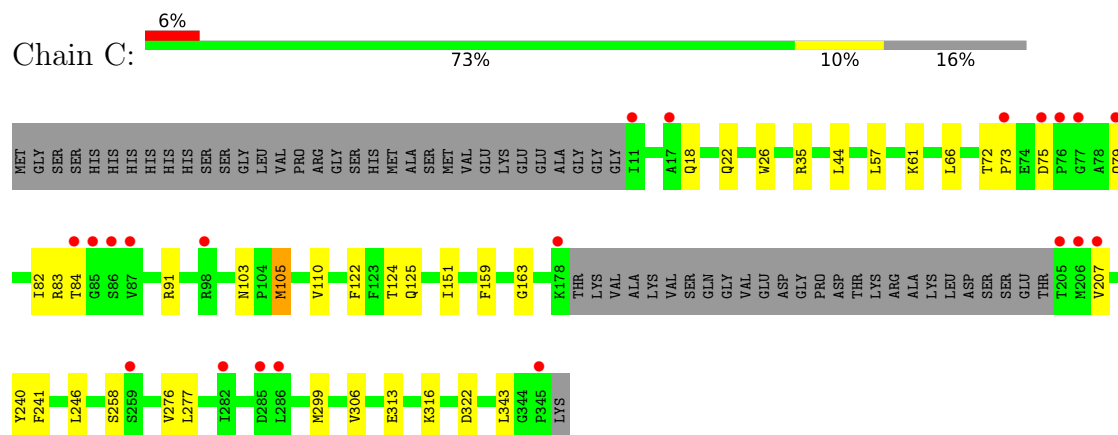
### 3 Residue-property plots [i](#)

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.

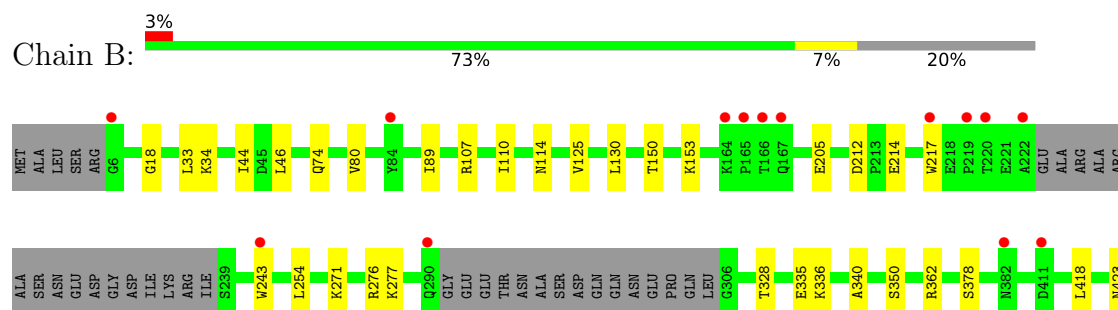
#### • Molecule 1: SUMO-activating enzyme subunit 1



#### • Molecule 1: SUMO-activating enzyme subunit 1



#### • Molecule 2: SUMO-activating enzyme subunit 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.47Å 115.56Å 98.57Å 90.00° 104.70° 90.00°	Depositor
Resolution (Å)	73.54 – 1.97 73.54 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.54-1.97) 95.4 (73.54-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.199 , 0.244 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	6555 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ZN

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	0.63	0/2452	1.03	2/3306 (0.1%)
1	C	0.60	0/2474	1.05	1/3337 (0.0%)
2	B	0.64	0/4112	1.07	4/5569 (0.1%)
2	D	0.60	0/4119	1.06	7/5578 (0.1%)
All	All	0.62	0/13157	1.06	14/17790 (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	A	0	1
2	B	0	2
2	D	0	3
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	58	ASN	CB-CA-C	6.23	120.31	109.65
2	D	117	ASP	CA-CB-CG	6.09	118.69	112.60
2	B	539	GLY	CA-C-O	-5.92	118.37	122.22
2	B	335	GLU	CB-CA-C	-5.69	101.35	110.79
2	B	74	GLN	N-CA-CB	5.58	118.11	110.01
2	D	203	ASP	CA-CB-CG	5.46	118.06	112.60
2	D	463	THR	CA-CB-OG1	-5.46	101.42	109.60
1	C	241	PHE	CA-CB-CG	-5.40	108.40	113.80
2	D	527	THR	CA-CB-OG1	-5.37	101.54	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LYS	CB-CA-C	-5.36	101.89	110.79
2	B	212	ASP	CA-CB-CG	5.25	117.84	112.60
1	A	275	ASP	CA-CB-CG	5.24	117.84	112.60
2	D	384	ILE	O-C-N	-5.19	118.10	121.37
2	D	212	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ARG	Sidechain
2	B	107	ARG	Sidechain
2	B	362	ARG	Sidechain
2	D	107	ARG	Sidechain
2	D	276	ARG	Sidechain
2	D	414	ARG	Sidechain

## 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	2411	0	2401	18	0
1	C	2431	0	2425	22	0
2	B	4034	0	4063	21	0
2	D	4041	0	4075	41	0
3	B	31	0	12	0	0
3	D	31	0	12	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	47	0	0	1	0
6	B	69	0	0	1	0
6	C	37	0	0	0	0
6	D	23	0	0	2	0
All	All	13159	0	12988	98	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 (98) 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:456:VAL:HG11	2:D:511:ILE:O	1.82	0.80
1:A:177:GLU:OE1	1:A:206:MET:HA	1.82	0.78
2:D:250:ASP:OD2	2:D:253:LYS:HD3	1.86	0.75
1:A:79:GLN:HA	6:A:414:HOH:O	1.91	0.69
1:A:177:GLU:OE1	1:A:206:MET:CA	2.42	0.67
1:C:72:THR:OG1	1:C:73:PRO:HD2	1.98	0.64
1:C:105:MET:HA	1:C:105:MET:HE2	1.83	0.60
2:D:447:LYS:HE2	6:D:810:HOH:O	2.00	0.59
2:B:214:GLU:CD	2:B:276:ARG:HH22	2.10	0.59
1:A:171:GLU:HG2	1:A:212:VAL:HG22	1.84	0.58
1:A:163:GLY:HA3	1:A:306:VAL:HG21	1.85	0.58
2:D:54:VAL:HA	2:D:68:VAL:HG21	1.85	0.58
1:C:122:PHE:O	1:C:125:GLN:HG2	2.04	0.57
1:C:72:THR:HG22	1:C:75:ASP:CG	2.29	0.57
2:B:114:ASN:OD1	2:B:125:VAL:HG11	2.05	0.56
1:C:79:GLN:HB3	1:C:82:ILE:HD12	1.87	0.56
2:D:449:GLU:OE2	2:D:516:ARG:NH1	2.39	0.56
1:A:74:GLU:O	1:A:75:ASP:C	2.50	0.55
2:B:418:LEU:HD13	2:B:429:LEU:HD21	1.89	0.55
2:D:490:LEU:O	2:D:498:THR:OG1	2.26	0.54
2:D:18:GLY:HA3	2:D:110:ILE:HD13	1.90	0.53
2:D:208:PRO:HB3	2:D:266:LEU:HD12	1.91	0.52
2:D:461:VAL:HG22	2:D:490:LEU:HD22	1.92	0.51
1:C:83:ARG:NH2	1:C:84:THR:O	2.42	0.51
2:D:490:LEU:HD11	2:D:511:ILE:HD11	1.93	0.51
2:D:30:CYS:SG	2:D:62:LEU:HD12	2.51	0.51
2:B:453:ARG:NH1	2:B:545:GLU:OE2	2.44	0.50
2:D:265:TYR:C	2:D:265:TYR:CD1	2.89	0.50
1:A:51:ILE:HD11	1:A:310:LEU:HD23	1.93	0.50
1:C:159:PHE:CG	1:C:246:LEU:HD13	2.46	0.50
2:B:80:VAL:HG11	2:B:89:ILE:HD11	1.94	0.50
1:C:163:GLY:HA3	1:C:306:VAL:HG21	1.93	0.50
2:B:18:GLY:HA3	2:B:110:ILE:HD13	1.94	0.49
1:C:18:GLN:NE2	2:D:57:LEU:HD13	2.27	0.49
2:B:336:LYS:HE3	2:B:340:ALA:HB1	1.95	0.49
2:B:454:LEU:HD12	2:B:454:LEU:C	2.37	0.49
1:A:226:SER:O	1:A:230:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ILE:O	2:D:89:ILE:HA	2.14	0.48
2:B:130:LEU:O	2:B:153:LYS:HD2	2.13	0.48
2:D:250:ASP:OD2	2:D:253:LYS:CD	2.61	0.48
2:D:423:ASN:HB2	2:D:424:PRO:HD2	1.96	0.48
2:D:70:ARG:HH12	2:D:78:GLU:CD	2.22	0.48
2:D:470:LYS:O	2:D:474:ALA:HA	2.13	0.48
2:B:425:ARG:NH2	2:B:427:LYS:HD2	2.29	0.47
2:D:54:VAL:HA	2:D:68:VAL:CG2	2.43	0.47
2:D:110:ILE:HD12	2:D:406:LEU:HD22	1.96	0.47
1:A:262:TYR:O	1:A:266:SER:OG	2.21	0.47
1:A:11:ILE:HD12	1:A:28:LEU:HD11	1.97	0.46
1:A:66:LEU:C	1:A:66:LEU:HD23	2.40	0.46
2:B:243:TRP:CZ3	2:B:254:LEU:HD23	2.51	0.46
1:C:35:ARG:O	1:C:61:LYS:HB2	2.16	0.46
2:D:251:PRO:HB3	2:D:323:SER:HA	1.98	0.46
1:A:60:VAL:O	1:A:106:VAL:HG22	2.16	0.45
2:D:173:CYS:SG	2:D:209:ASP:OD2	2.74	0.45
1:A:160:GLY:O	1:A:299:MET:HG3	2.16	0.45
2:D:143:GLY:HA2	2:D:385:PRO:O	2.16	0.45
2:B:476:VAL:HG21	2:B:523:LEU:HD23	1.99	0.45
2:B:150:THR:O	6:B:801:HOH:O	2.21	0.45
2:B:490:LEU:HD11	2:B:511:ILE:HD11	1.99	0.45
2:D:50:ASP:HB3	2:D:72:LYS:HD2	1.99	0.45
2:D:307:LEU:HB2	2:D:310:GLN:HG2	1.99	0.45
2:D:65:LYS:C	2:D:67:HIS:H	2.25	0.45
2:D:307:LEU:HB2	2:D:310:GLN:CG	2.47	0.45
2:B:217:TRP:HA	2:B:271:LYS:HD2	1.99	0.44
1:C:57:LEU:HD11	2:D:61:PHE:HB3	1.98	0.44
1:C:22:GLN:HB3	1:C:26:TRP:CZ2	2.53	0.44
2:B:44:ILE:O	2:B:89:ILE:HA	2.18	0.44
1:C:72:THR:HG1	1:C:73:PRO:HD2	1.83	0.44
2:B:33:LEU:HD11	2:B:46:LEU:HD22	1.99	0.44
1:A:80:PHE:CD2	2:B:34:LYS:HD2	2.54	0.43
1:C:240:TYR:CD1	1:C:343:LEU:HD13	2.53	0.43
2:D:118:ASN:ND2	6:D:805:HOH:O	2.49	0.43
2:B:442:TYR:O	2:B:448:PRO:HB3	2.18	0.43
2:B:423:ASN:HD21	2:B:425:ARG:NH1	2.16	0.43
1:C:66:LEU:C	1:C:66:LEU:HD23	2.44	0.43
1:C:72:THR:OG1	1:C:73:PRO:CD	2.66	0.43
2:D:454:LEU:HD21	2:D:532:ILE:HD12	2.00	0.43
1:C:103:ASN:HA	2:D:57:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:LYS:HA	2:D:278:PRO:HD3	1.91	0.42
1:C:124:THR:HA	1:C:151:ILE:HD11	2.01	0.42
2:D:142:ALA:HA	2:D:384:ILE:CG2	2.49	0.42
1:C:299:MET:HB3	1:C:299:MET:HE2	1.87	0.42
2:D:450:VAL:HG11	2:D:473:PHE:CZ	2.55	0.41
1:A:67:ASP:OD2	1:A:91:ARG:HD2	2.20	0.41
2:D:496:GLY:HA2	2:D:499:GLU:CG	2.51	0.41
1:A:158:VAL:HG21	1:A:303:CYS:SG	2.61	0.41
2:D:166:THR:HG22	2:D:167:GLN:N	2.35	0.41
2:D:265:TYR:C	2:D:265:TYR:HD1	2.29	0.41
1:A:35:ARG:O	1:A:61:LYS:HB2	2.21	0.41
2:B:328:THR:HG21	2:B:350:SER:OG	2.20	0.41
2:D:218:GLU:OE1	2:D:220:THR:HG22	2.21	0.41
1:C:44:LEU:O	1:C:91:ARG:HD3	2.22	0.40
1:C:276:VAL:HG12	1:C:277:LEU:HD12	2.04	0.40
1:A:20:ASP:OD2	1:A:21:ARG:NH1	2.53	0.40
2:D:185:CYS:O	2:D:188:TRP:HB3	2.21	0.40
2:D:327:GLU:HG2	2:D:330:ARG:NH2	2.37	0.40
2:D:423:ASN:OD1	2:D:423:ASN:C	2.65	0.40
1:C:313:GLU:OE2	1:C:316:LYS:CE	2.70	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	300/369 (81%)	290 (97%)	9 (3%)	1 (0%)	36	27
1	C	305/369 (83%)	293 (96%)	11 (4%)	1 (0%)	36	27
2	B	508/640 (79%)	499 (98%)	9 (2%)	0	100	100
2	D	509/640 (80%)	483 (95%)	25 (5%)	1 (0%)	43	35
All	All	1622/2018 (80%)	1565 (96%)	54 (3%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	66	LYS
1	C	322	ASP
1	A	322	ASP

### 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	265/315 (84%)	265 (100%)	0	100	100
1	C	267/315 (85%)	263 (98%)	4 (2%)	57	52
2	B	445/552 (81%)	442 (99%)	3 (1%)	76	73
2	D	444/552 (80%)	433 (98%)	11 (2%)	42	33
All	All	1421/1734 (82%)	1403 (99%)	18 (1%)	61	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	205	GLU
2	B	277	LYS
2	B	378	SER
1	C	105	MET
1	C	110	VAL
1	C	207	VAL
1	C	258	SER
2	D	49	LEU
2	D	70	ARG
2	D	117	ASP
2	D	205	GLU
2	D	275	LYS
2	D	276	ARG
2	D	350	SER
2	D	383	ILE
2	D	410	ILE
2	D	498	THR

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Mol	Chain	Res	Type
2	D	520	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
2	B	64	GLN
1	C	172	HIS
1	C	312	GLN
2	D	88	ASN
2	D	147	GLN
2	D	501	ASN

### 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	$\# Z  > 2$
3	ATP	B	701	4	32,33,33	1.04	2 (6%)	48,52,52	0.78	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	D	701	4	32,33,33	0.73	1 (3%)	48,52,52	0.82	1 (2%)

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	B	701	4	-	5/22/38/38	0/3/3/3
3	ATP	D	701	4	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ATP	PA-O3A	3.91	1.63	1.59
3	B	701	ATP	PB-O3A	2.83	1.62	1.59
3	D	701	ATP	PB-O3B	2.15	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	ATP	O3'-C3'-C2'	-2.57	103.58	111.82
3	B	701	ATP	O3B-PB-O1B	-2.15	104.24	110.70

There are no chirality outliers.

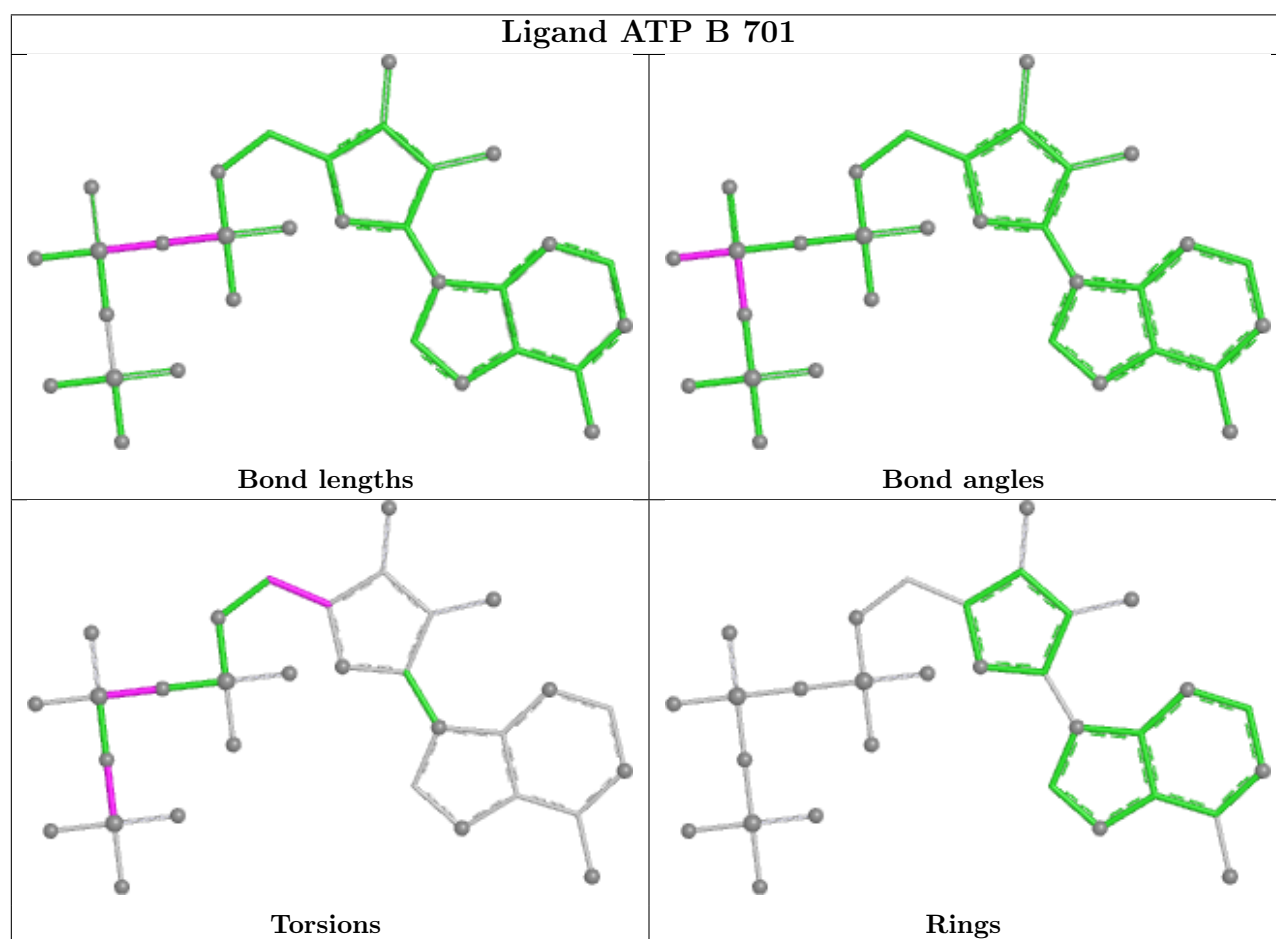
All (10) torsion outliers are listed below:

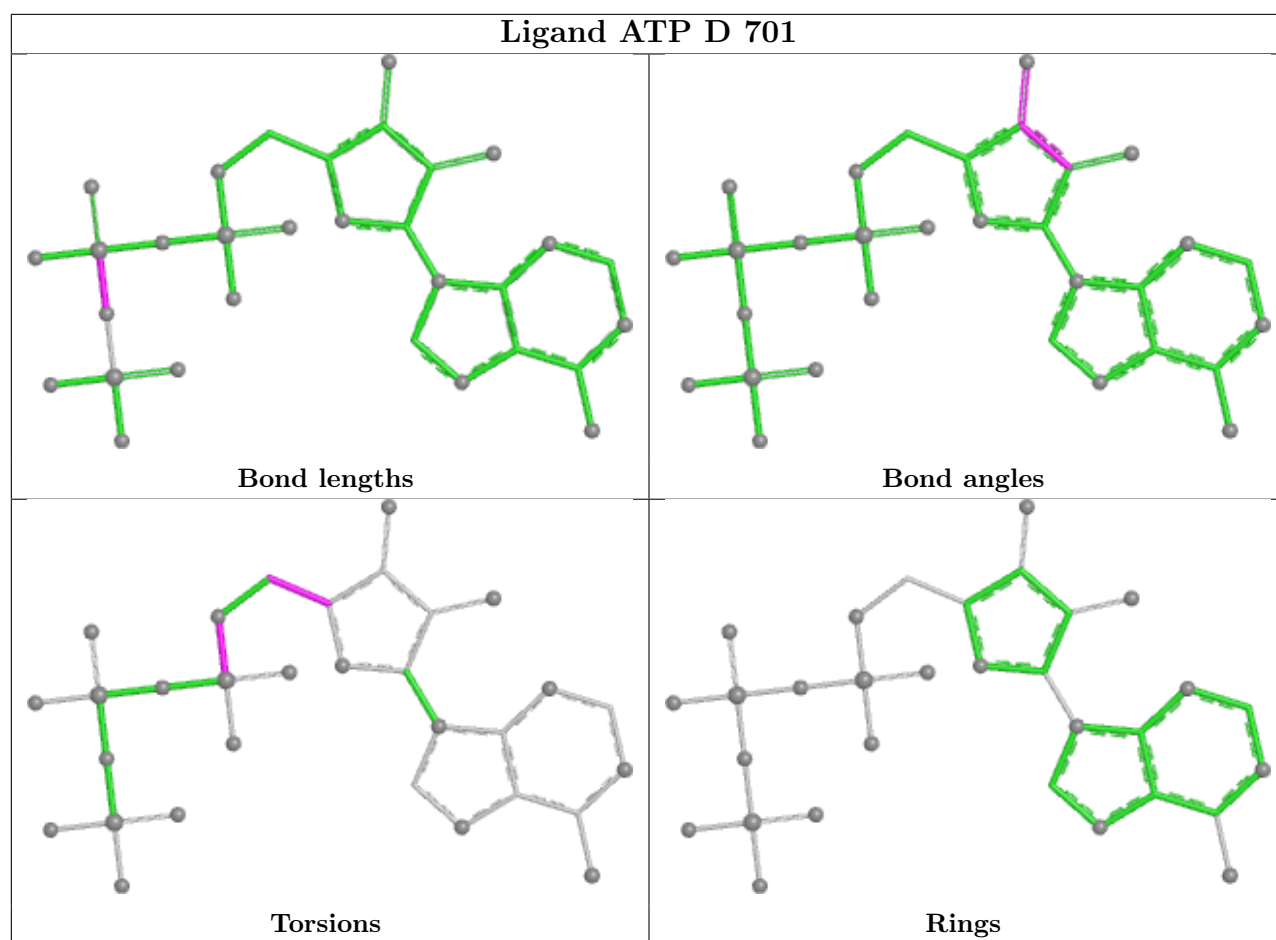
Mol	Chain	Res	Type	Atoms
3	B	701	ATP	PB-O3B-PG-O3G
3	D	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O3A
3	D	701	ATP	O4'-C4'-C5'-O5'
3	D	701	ATP	C3'-C4'-C5'-O5'
3	D	701	ATP	C5'-O5'-PA-O2A
3	B	701	ATP	PB-O3B-PG-O1G
3	B	701	ATP	PB-O3B-PG-O2G
3	B	701	ATP	O4'-C4'-C5'-O5'
3	B	701	ATP	PA-O3A-PB-O2B

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 [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	306/369 (82%)	0.26	7 (2%) 61 70	28, 42, 75, 115	0
1	C	309/369 (83%)	0.49	21 (6%) 23 31	29, 47, 86, 114	0
2	B	513/640 (80%)	0.27	18 (3%) 47 57	16, 43, 78, 119	1 (0%)
2	D	514/640 (80%)	0.97	71 (13%) 6 9	18, 62, 101, 133	2 (0%)
All	All	1642/2018 (81%)	0.53	117 (7%) 22 29	16, 47, 90, 133	3 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	54	VAL	6.9
1	A	78	ALA	6.4
2	D	243	TRP	6.1
1	C	11	ILE	5.9
2	D	384	ILE	5.7
2	D	385	PRO	5.2
2	D	383	ILE	5.2
2	D	57	LEU	5.0
1	C	84	THR	4.4
2	D	6	GLY	3.9
1	C	85	GLY	3.8
2	D	282	LEU	3.8
2	D	217	TRP	3.7
2	D	380	ALA	3.7
1	A	11	ILE	3.7
1	A	205	THR	3.6
2	D	240	THR	3.6
2	B	166	THR	3.6
2	D	202	ALA	3.5
2	D	226	ALA	3.5
1	A	206	MET	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	84	TYR	3.4
2	D	219	PRO	3.3
2	D	222	ALA	3.2
2	D	58	ASN	3.2
2	D	503	HIS	3.2
2	B	222	ALA	3.2
2	D	254	LEU	3.1
2	B	164	LYS	3.1
2	D	166	THR	3.0
1	A	207	VAL	3.0
1	C	86	SER	3.0
1	C	76	PRO	3.0
2	D	498	THR	3.0
1	C	207	VAL	2.9
1	C	178	LYS	2.9
2	D	52	ILE	2.9
1	C	87	VAL	2.9
2	D	454	LEU	2.9
2	D	312	VAL	2.8
2	B	165	PRO	2.8
2	B	219	PRO	2.8
2	D	68	VAL	2.8
2	D	56	ASN	2.8
2	B	217	TRP	2.8
2	D	244	ALA	2.8
1	C	77	GLY	2.8
2	B	442	TYR	2.7
2	D	59	ARG	2.7
2	D	319	ALA	2.7
2	D	459	VAL	2.7
2	D	547	VAL	2.7
2	D	548	GLY	2.7
1	C	286	LEU	2.7
2	D	343	ILE	2.7
2	D	506	LEU	2.6
2	D	496	GLY	2.6
2	D	379	MET	2.6
2	D	284	TRP	2.6
1	C	285	ASP	2.5
2	D	462	LEU	2.5
2	D	532	ILE	2.5
2	D	315	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	542	VAL	2.5
2	D	540	LYS	2.5
2	D	306	GLY	2.5
1	C	17	ALA	2.5
2	B	496	GLY	2.4
2	D	273	TRP	2.4
2	D	344	TRP	2.4
1	C	79	GLN	2.4
2	B	290	GLN	2.4
2	D	509	PHE	2.4
2	D	183	ILE	2.4
2	D	307	LEU	2.4
2	D	285	ALA	2.4
1	C	73	PRO	2.3
2	D	289	SER	2.3
2	D	461	VAL	2.3
2	D	53	ASP	2.3
2	D	241	LYS	2.3
2	D	69	GLY	2.3
2	D	410	ILE	2.2
2	D	313	LEU	2.2
2	B	411	ASP	2.2
2	B	243	TRP	2.2
2	D	188	TRP	2.2
1	C	206	MET	2.2
1	A	295	CYS	2.2
2	D	144	TYR	2.2
2	D	442	TYR	2.2
2	D	175	ILE	2.2
2	D	337	GLY	2.2
2	D	171	PRO	2.2
2	D	477	ALA	2.2
2	D	170	PHE	2.1
2	D	387	ILE	2.1
2	D	511	ILE	2.1
1	C	75	ASP	2.1
1	A	85	GLY	2.1
1	C	98	ARG	2.1
2	B	540	LYS	2.1
2	D	374	PHE	2.1
2	D	544	PHE	2.1
1	C	282	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	205	THR	2.1
1	C	259	SER	2.1
2	D	538	LEU	2.1
2	B	549	ASP	2.1
2	D	249	TYR	2.1
2	B	6	GLY	2.1
2	D	456	VAL	2.1
2	B	167	GLN	2.1
2	B	382	ASN	2.0
1	C	345	PRO	2.0
2	D	193	PHE	2.0
2	B	220	THR	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](#)

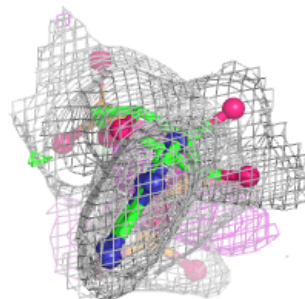
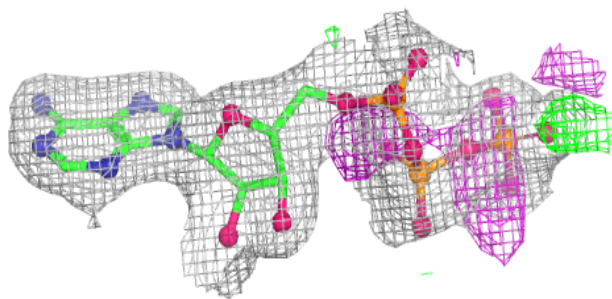
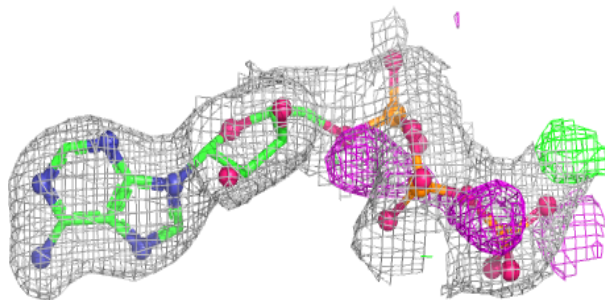
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	D	701	31/31	0.88	0.10	38,55,92,100	0
4	MG	B	702	1/1	0.88	0.09	63,63,63,63	0
3	ATP	B	701	31/31	0.92	0.09	35,45,81,89	0
4	MG	D	702	1/1	0.95	0.05	65,65,65,65	0
5	ZN	B	703	1/1	0.99	0.02	32,32,32,32	0
5	ZN	D	703	1/1	1.00	0.01	38,38,38,38	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 D 701:**

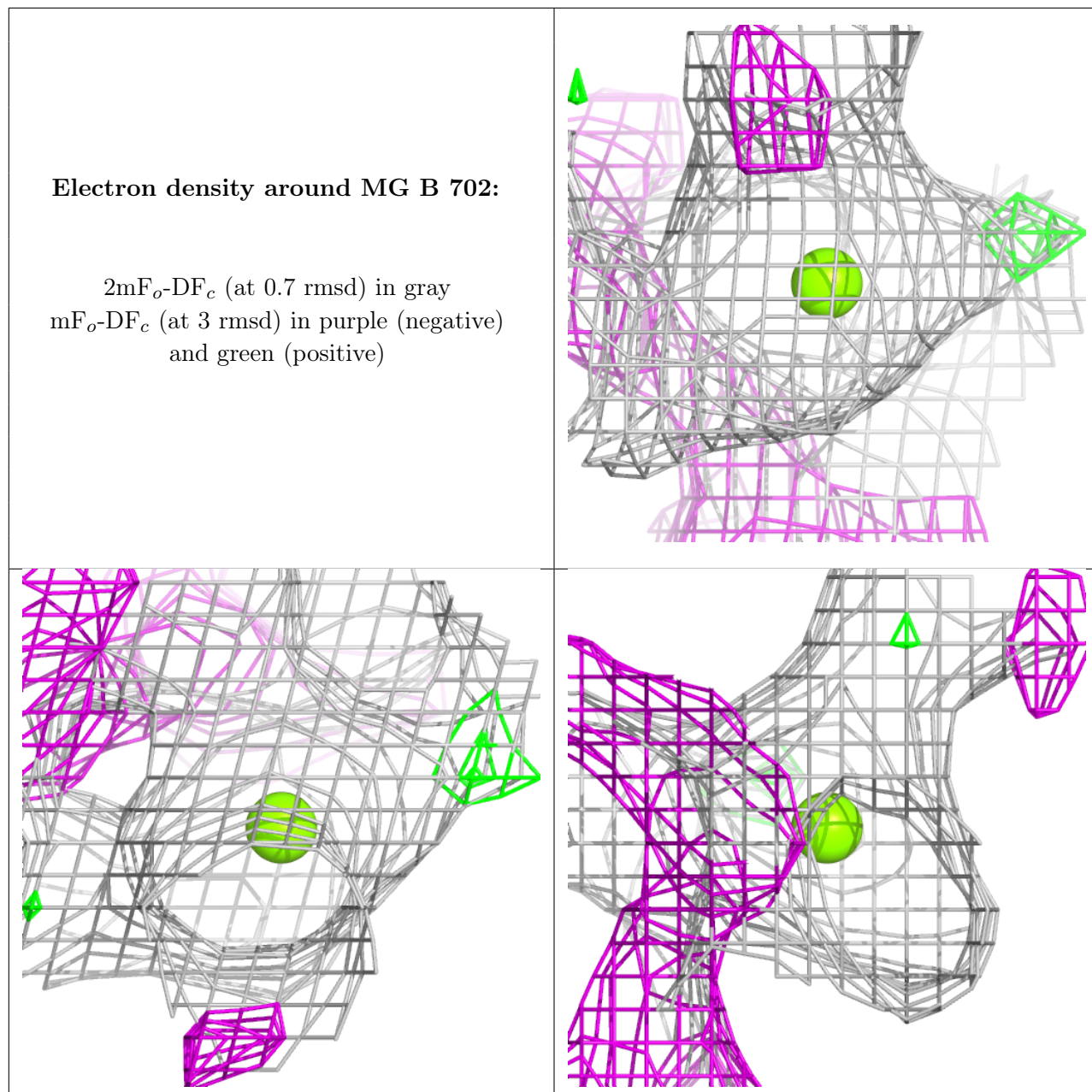
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





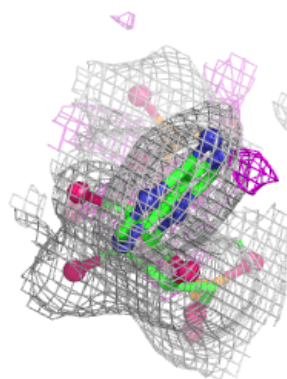
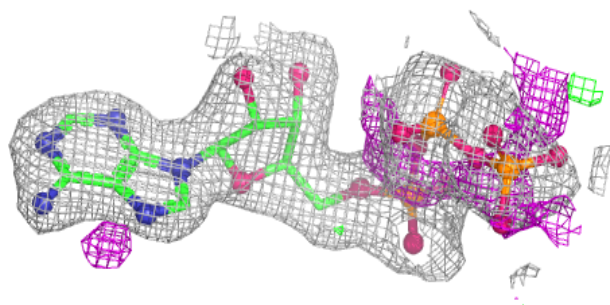
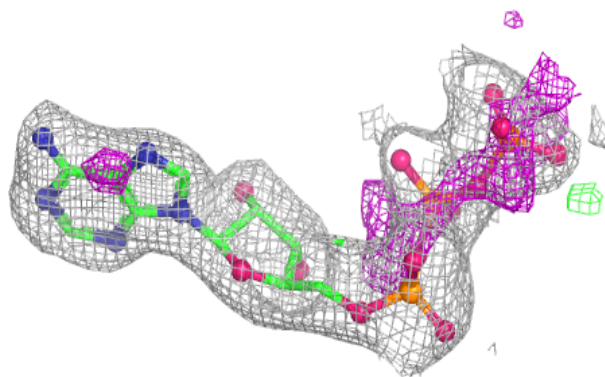
**Electron density around MG B 702:**

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



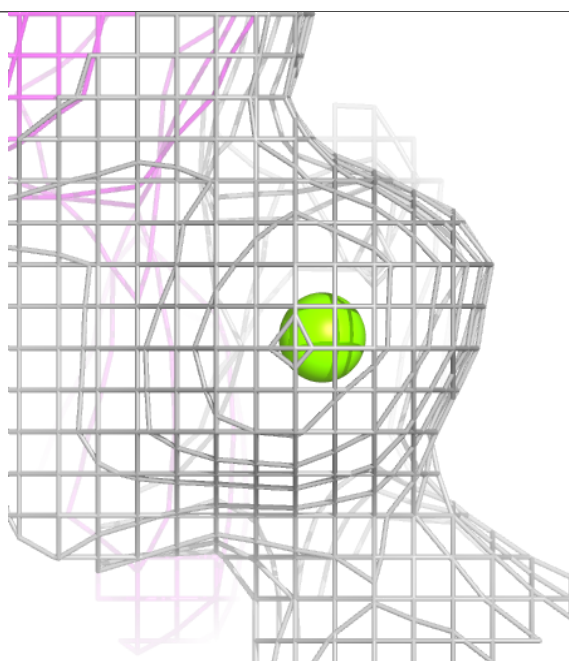
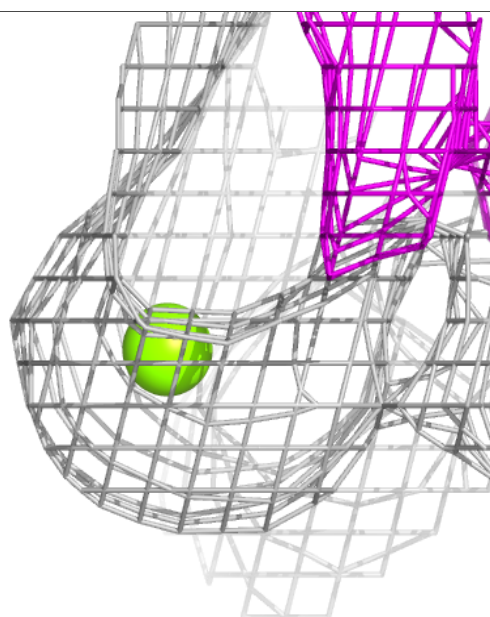
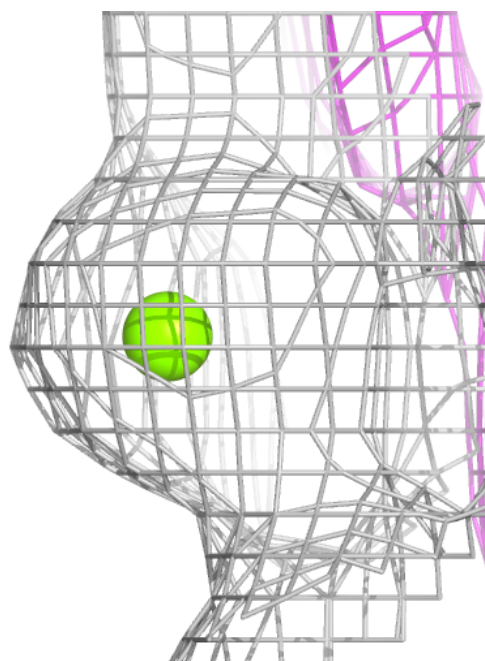
**Electron density around ATP B 701:**

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



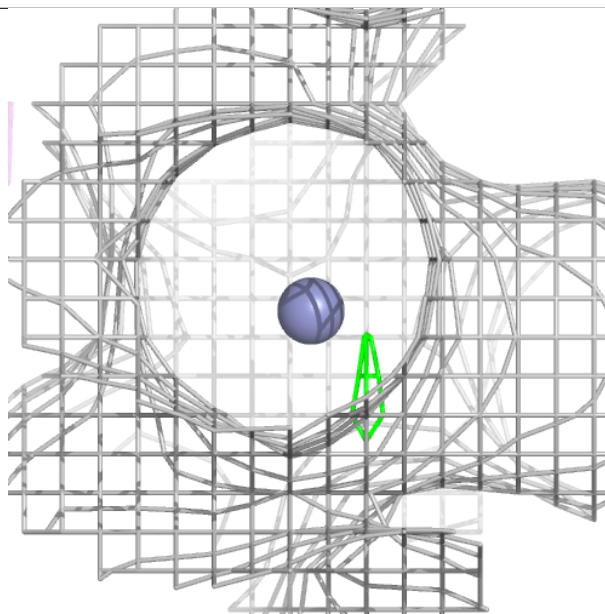
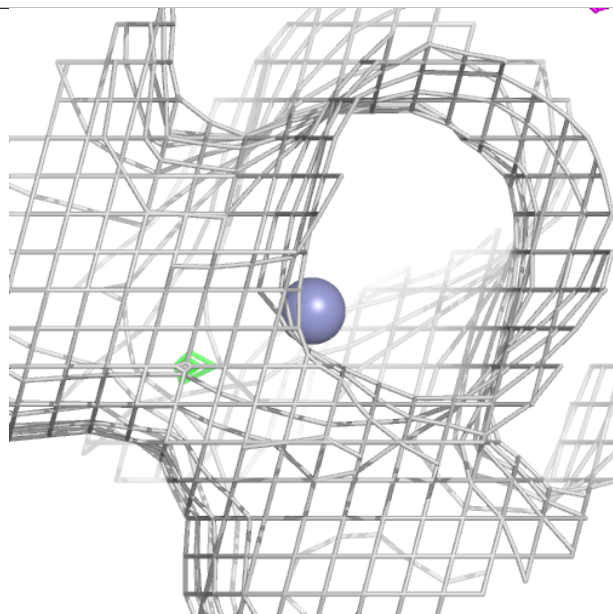
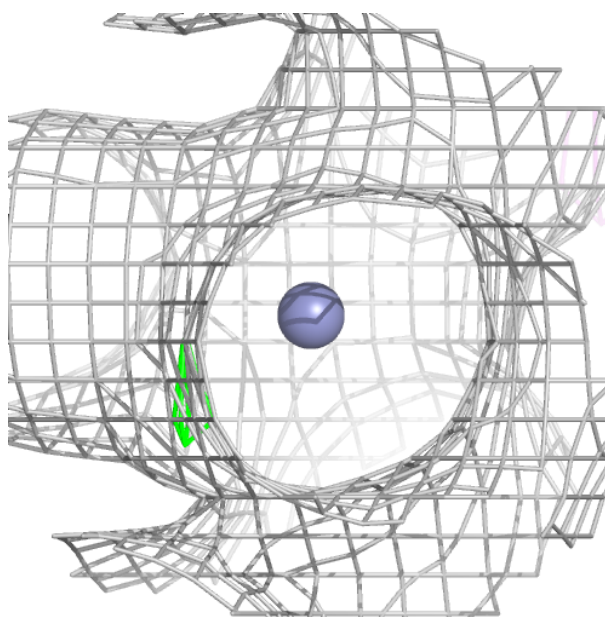
**Electron density around MG D 702:**

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



**Electron density around ZN B 703:**

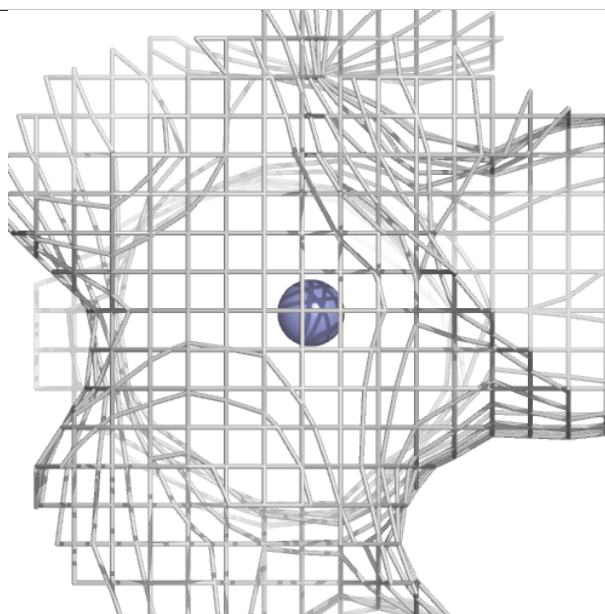
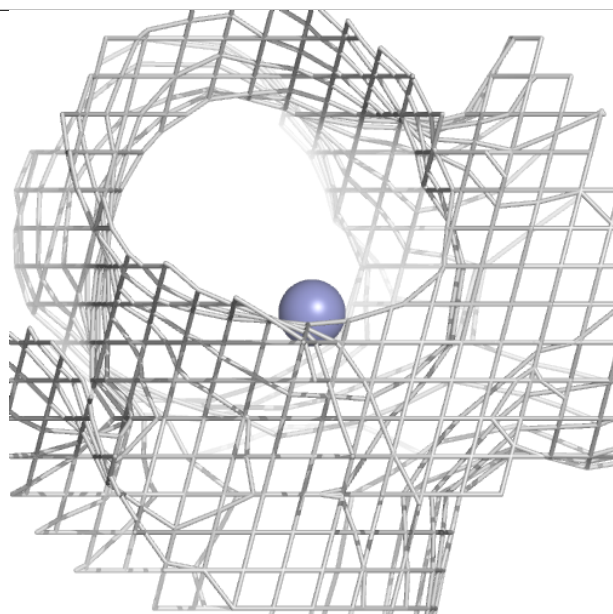
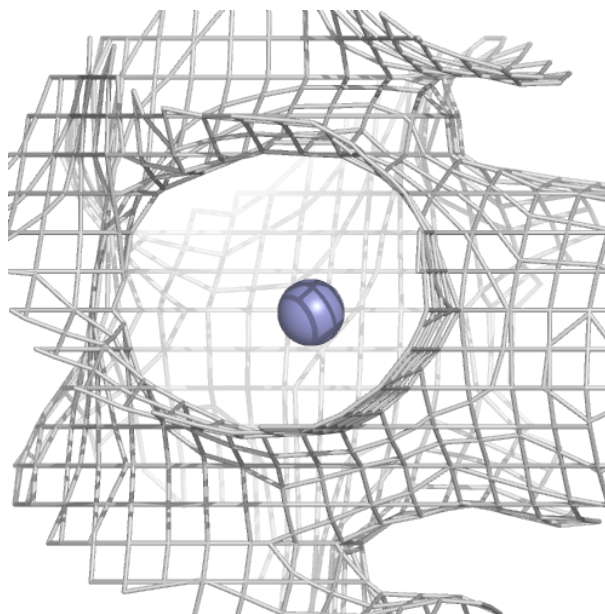
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN D 703:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.