



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 04:02 AM UTC

PDB ID : 9IF6 / pdb_00009if6
Title : Crystal structure of human SUMO E1 with large unit cell parameters in the P1 21 1 space group.
Authors : Vilorio, M.; Francois, R.M.M.; Didierjean, C.
Deposited on : 2025-02-17
Resolution : 2.51 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

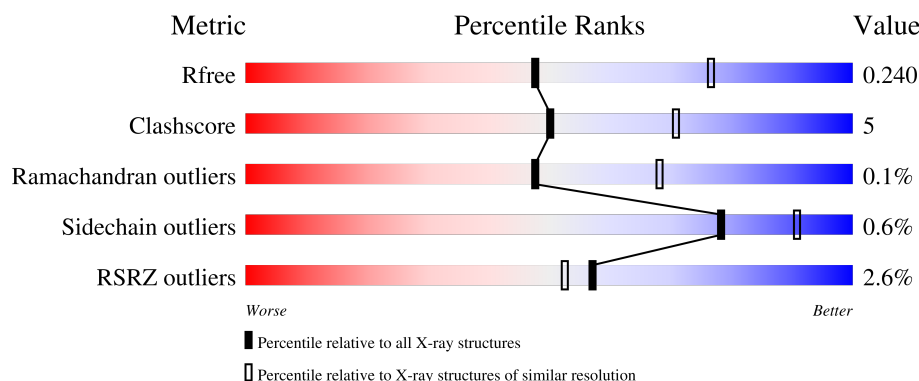
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	369	<div> <div>2%</div> <div>74%</div> <div>10%</div> <div>16%</div> </div>
1	C	369	<div> <div>2%</div> <div>74%</div> <div>10%</div> <div>16%</div> </div>
2	B	640	<div> <div>2%</div> <div>69%</div> <div>10%</div> <div>20%</div> </div>
2	D	640	<div> <div>2%</div> <div>68%</div> <div>11%</div> <div>21%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12960 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	311	Total	C	N	O	S	0	0	0
			2442	1548	415	466	13			
1	C	311	Total	C	N	O	S	0	0	0
			2442	1548	415	466	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

Continued on next page...

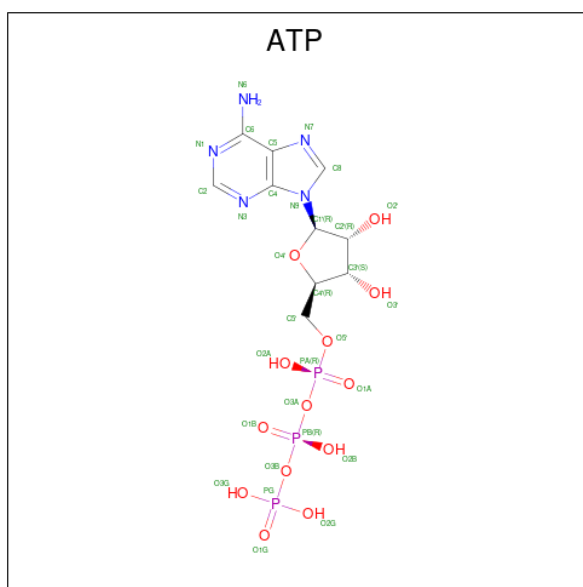
Continued from previous page...

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	509	Total	C	N	O	S	0	0	0
			3990	2535	688	747	20			
2	D	507	Total	C	N	O	S	0	0	0
			3979	2528	686	745	20			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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).

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	11	Total	O	0	0
			11	11		

Continued on next page...

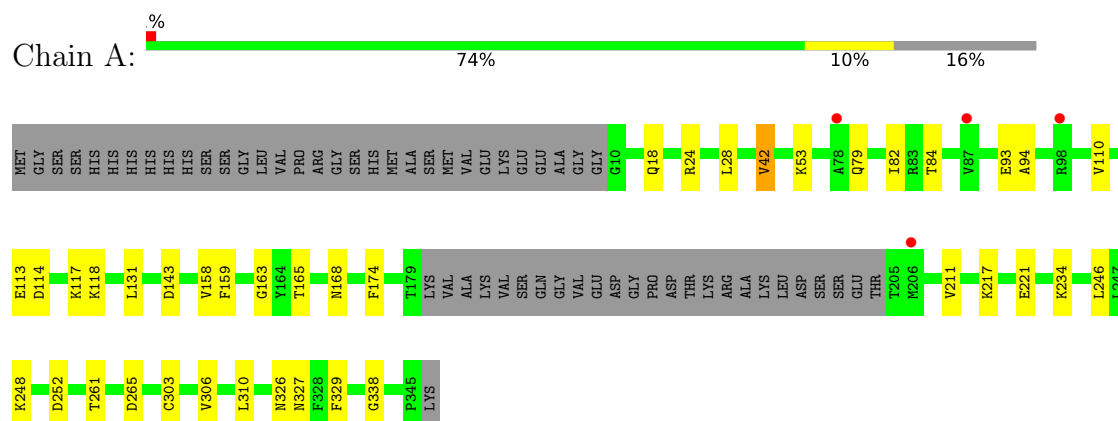
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total 11	O 11	0	0
6	C	11	Total 11	O 11	0	0
6	D	8	Total 8	O 8	0	0

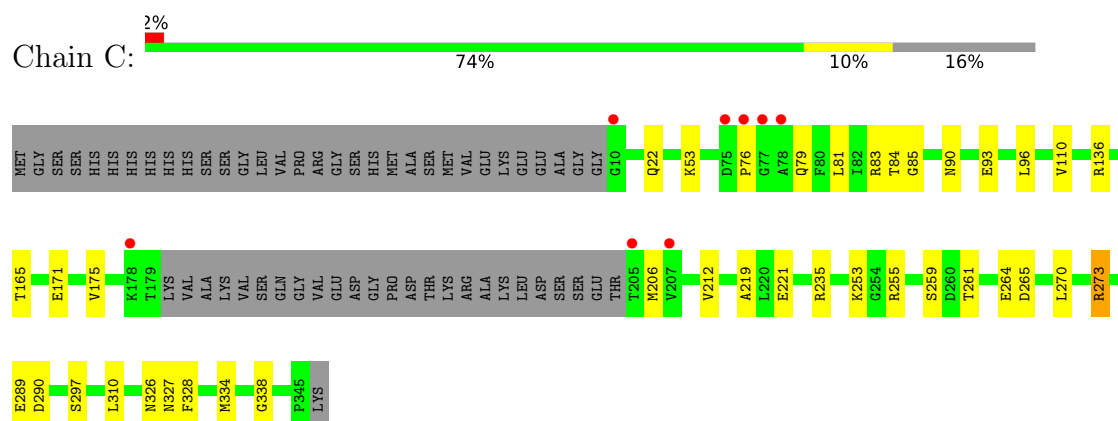
3 Residue-property plots [i](#)

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.

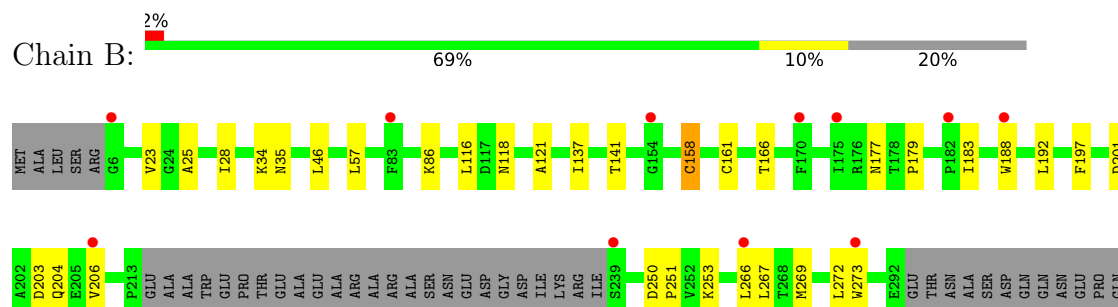
• Molecule 1: SUMO-activating enzyme subunit 1

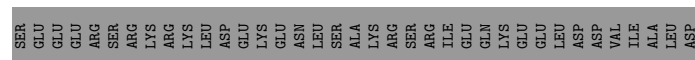
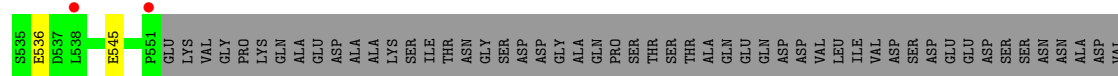


• Molecule 1: SUMO-activating enzyme subunit 1

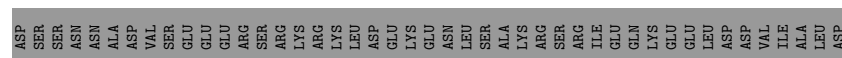
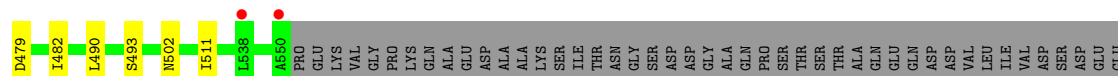
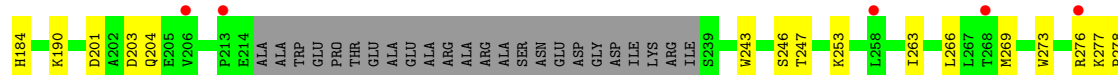


• Molecule 2: SUMO-activating enzyme subunit 2





• 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, α , β , γ	101.94Å 116.53Å 106.60Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	49.55 – 2.51 49.55 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.55-2.51) 92.7 (49.55-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.201 , 0.242 0.202 , 0.240	Depositor DCC
R_{free} test set	3971 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12960	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.07	0/2485	0.22	0/3352
1	C	0.16	0/2485	0.29	0/3352
2	B	0.11	0/4066	0.27	0/5503
2	D	0.11	0/4054	0.26	0/5486
All	All	0.12	0/13090	0.26	0/17693

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	273	ARG	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	2442	0	2435	26	0
1	C	2442	0	2435	29	0
2	B	3990	0	4029	42	0
2	D	3979	0	4019	51	0
3	B	31	0	12	0	0
3	D	31	0	12	2	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	11	0	0	0	0
6	B	11	0	0	0	0
6	C	11	0	0	0	0
6	D	8	0	0	0	0
All	All	12960	0	12942	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (138) 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:C:83:ARG:HG3	1:C:85:GLY:H	1.54	0.72
1:C:264:GLU:N	1:C:264:GLU:OE2	2.22	0.70
1:C:175:VAL:HG11	1:C:206:MET:CE	2.21	0.70
2:D:33:LEU:HD11	2:D:46:LEU:HD22	1.75	0.69
1:A:93:GLU:HG3	1:A:110:VAL:HG11	1.76	0.66
2:B:201:ASP:HB3	2:B:204:GLN:HB2	1.77	0.66
2:B:177:ASN:HA	2:B:266:LEU:HD11	1.79	0.65
2:D:181:GLU:H	2:D:184:HIS:HD2	1.45	0.65
1:C:175:VAL:CG1	1:C:206:MET:HE3	2.28	0.64
2:B:188:TRP:NE1	2:B:362:ARG:HH21	1.95	0.64
2:B:449:GLU:HG3	2:B:529:LEU:HB2	1.80	0.63
2:D:84:TYR:HD2	2:D:87:ALA:HB2	1.63	0.63
2:B:158:CYS:HB3	2:B:161:CYS:H	1.64	0.62
2:B:118:ASN:OD1	2:B:121:ALA:N	2.27	0.61
2:B:308:LYS:HD2	2:B:308:LYS:H	1.65	0.61
1:C:235:ARG:O	2:D:426:LYS:NZ	2.33	0.61
1:C:175:VAL:HG11	1:C:206:MET:HE1	1.83	0.61
1:C:175:VAL:HG11	1:C:206:MET:HE3	1.85	0.59
2:D:180:SER:H	2:D:184:HIS:HD2	1.51	0.59
2:B:201:ASP:OD1	2:B:203:ASP:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:SER:H	2:D:184:HIS:CD2	2.21	0.58
2:D:37:VAL:HG21	2:D:80:VAL:HG21	1.86	0.57
2:D:47:ILE:HG21	2:D:96:ILE:HD13	1.86	0.57
1:A:84:THR:HG21	2:B:86:LYS:HE2	1.86	0.57
1:C:175:VAL:CG1	1:C:206:MET:CE	2.83	0.57
2:D:181:GLU:H	2:D:184:HIS:CD2	2.21	0.57
1:C:90:ASN:HB3	1:C:93:GLU:HB2	1.87	0.57
1:C:76:PRO:HB2	1:C:84:THR:HA	1.88	0.55
2:D:490:LEU:HD21	2:D:511:ILE:HD11	1.89	0.55
1:C:171:GLU:HG2	1:C:212:VAL:HG13	1.87	0.55
1:A:174:PHE:HE1	1:A:211:VAL:HG23	1.71	0.55
1:C:261:THR:OG1	1:C:265:ASP:OD2	2.25	0.55
2:D:479:ASP:OD1	2:D:493:SER:N	2.39	0.54
2:D:58:ASN:OD1	2:D:59:ARG:NH1	2.40	0.54
2:B:476:VAL:HG21	2:B:523:LEU:HD23	1.91	0.52
1:C:136:ARG:NH2	1:C:221:GLU:OE2	2.42	0.52
1:C:253:LYS:HB3	1:C:255:ARG:HG2	1.92	0.52
2:B:534:HIS:CE1	2:B:536:GLU:HG2	2.45	0.52
2:D:482:ILE:HG13	2:D:490:LEU:HD11	1.92	0.52
1:A:248:LYS:NZ	1:A:252:ASP:OD2	2.30	0.51
2:B:28:ILE:HD11	2:B:141:THR:HG23	1.91	0.51
1:A:79:GLN:HG3	1:A:82:ILE:H	1.74	0.51
2:B:267:LEU:HA	2:B:273:TRP:HE1	1.74	0.51
2:B:158:CYS:HB3	2:B:161:CYS:N	2.26	0.50
1:C:259:SER:OG	1:C:297:SER:OG	2.22	0.50
2:D:277:LYS:HD2	2:D:278:PRO:HD2	1.93	0.50
2:B:161:CYS:HA	2:B:441:CYS:HB2	1.94	0.50
2:D:263:ILE:HA	2:D:266:LEU:HB2	1.93	0.50
2:B:456:VAL:HG12	2:B:507:SER:HB3	1.94	0.49
1:A:42:VAL:HG22	1:A:131:LEU:HA	1.95	0.49
2:B:251:PRO:HB3	2:B:323:SER:HA	1.94	0.49
2:B:322:PHE:O	2:B:326:ILE:HG13	2.12	0.49
2:D:360:ASN:HA	2:D:363:MET:HE3	1.95	0.49
2:D:467:LYS:HB3	2:D:467:LYS:HZ3	1.77	0.49
1:A:113:GLU:HB2	1:A:118:LYS:HE2	1.95	0.48
1:A:217:LYS:O	1:A:221:GLU:HG2	2.14	0.48
2:D:72:LYS:NZ	3:D:701:ATP:O2B	2.47	0.48
2:D:266:LEU:HA	2:D:269:MET:HE1	1.96	0.48
2:B:137:ILE:HG21	2:B:398:ILE:HG23	1.94	0.48
2:D:266:LEU:HD23	2:D:279:PRO:HG3	1.96	0.48
2:D:288:GLN:OE1	2:D:320:ARG:NE	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:MET:HB2	2:B:272:LEU:HD22	1.96	0.47
2:D:201:ASP:HB3	2:D:204:GLN:HG3	1.96	0.47
2:B:395:ALA:HA	2:B:398:ILE:HD12	1.96	0.47
2:B:486:LYS:HG2	2:B:487:GLY:N	2.29	0.47
2:D:463:THR:O	2:D:467:LYS:HB2	2.13	0.47
2:D:28:ILE:HD11	2:D:141:THR:HG23	1.96	0.47
2:D:34:LYS:NZ	2:D:35:ASN:OD1	2.48	0.47
2:D:243:TRP:O	2:D:246:SER:OG	2.22	0.47
1:A:114:ASP:HB3	1:A:117:LYS:HG3	1.98	0.46
2:B:197:PHE:HZ	2:B:326:ILE:HG23	1.81	0.46
1:A:338:GLY:O	2:B:428:LEU:N	2.40	0.46
1:C:96:LEU:HD13	1:C:110:VAL:HG23	1.97	0.46
2:D:84:TYR:CD2	2:D:87:ALA:HB2	2.49	0.46
1:A:18:GLN:HG3	2:B:57:LEU:HB2	1.97	0.46
2:D:460:THR:OG1	2:D:502:ASN:O	2.33	0.46
2:B:442:TYR:O	2:B:448:PRO:HB3	2.16	0.46
2:D:44:ILE:HB	2:D:89:ILE:HD13	1.97	0.46
2:B:414:ARG:HD2	2:B:431:PRO:HB2	1.97	0.46
2:B:513:ASN:HB2	2:B:534:HIS:HB3	1.97	0.45
2:D:161:CYS:HA	2:D:441:CYS:HB2	1.97	0.45
1:A:28:LEU:HD22	2:B:307:LEU:HG	1.98	0.45
2:B:25:ALA:HB2	2:B:46:LEU:HD11	1.98	0.45
2:B:453:ARG:NH1	2:B:545:GLU:OE2	2.48	0.45
1:C:53:LYS:NZ	2:D:31:GLU:OE2	2.28	0.45
1:C:219:ALA:HB1	1:C:328:PHE:CE2	2.52	0.45
2:B:23:VAL:HG12	2:B:116:LEU:HD21	1.98	0.45
1:C:219:ALA:HB1	1:C:328:PHE:HE2	1.81	0.45
2:D:282:LEU:HD12	2:D:282:LEU:HA	1.81	0.45
1:A:24:ARG:NH1	2:B:378:SER:OG	2.50	0.45
2:B:179:PRO:HD2	2:B:366:PHE:CE2	2.52	0.45
2:D:266:LEU:O	2:D:273:TRP:NE1	2.49	0.45
1:A:261:THR:OG1	1:A:265:ASP:OD2	2.35	0.44
1:C:22:GLN:HG2	2:D:387:ILE:HG22	1.99	0.44
2:D:37:VAL:HG13	2:D:84:TYR:CD2	2.52	0.44
1:A:24:ARG:HG2	2:B:374:PHE:CZ	2.52	0.44
1:A:143:ASP:OD1	1:A:168:ASN:ND2	2.43	0.44
1:C:76:PRO:CB	1:C:84:THR:HA	2.48	0.44
2:D:377:LYS:HG2	2:D:383:ILE:HD12	1.99	0.44
1:A:53:LYS:HE3	1:A:53:LYS:HB3	1.78	0.44
1:A:234:LYS:HE2	1:A:234:LYS:HB3	1.85	0.44
1:A:163:GLY:HA3	1:A:306:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:LYS:HD2	2:D:308:LYS:H	1.84	0.43
1:A:165:THR:OG1	1:A:329:PHE:HB3	2.18	0.43
1:C:83:ARG:HD2	1:C:84:THR:H	1.82	0.43
1:A:326:ASN:HA	1:A:327:ASN:HA	1.66	0.43
1:C:79:GLN:HG3	1:C:81:LEU:H	1.83	0.43
2:D:124:HIS:O	2:D:128:MET:HG2	2.19	0.43
2:B:371:LYS:HD3	2:B:379:MET:HE1	2.01	0.43
1:C:334:MET:HA	1:C:334:MET:HE2	2.00	0.43
1:C:326:ASN:HA	1:C:327:ASN:HA	1.65	0.43
2:B:423:ASN:HB2	2:B:424:PRO:HD2	2.01	0.43
2:B:34:LYS:NZ	2:B:35:ASN:OD1	2.51	0.43
2:B:250:ASP:HB3	2:B:253:LYS:HB2	2.01	0.42
1:C:165:THR:HB	1:C:310:LEU:HD13	2.00	0.42
2:D:56:ASN:ND2	3:D:701:ATP:O2B	2.52	0.42
2:B:346:LYS:H	2:B:346:LYS:HG3	1.61	0.42
2:D:203:ASP:N	2:D:203:ASP:OD1	2.52	0.42
1:C:338:GLY:O	2:D:428:LEU:N	2.40	0.42
2:D:179:PRO:O	2:D:276:ARG:NH2	2.44	0.42
2:D:77:LYS:HG3	2:D:89:ILE:HB	2.01	0.41
2:D:273:TRP:HZ3	2:D:276:ARG:HH11	1.67	0.41
1:A:159:PHE:CG	1:A:246:LEU:HD13	2.55	0.41
2:D:190:LYS:HE2	2:D:190:LYS:HB3	1.88	0.41
1:A:165:THR:HB	1:A:310:LEU:HD13	2.02	0.41
1:A:158:VAL:HG21	1:A:303:CYS:SG	2.60	0.41
1:C:270:LEU:HD21	1:C:289:GLU:HG2	2.03	0.41
2:D:160:GLU:CD	2:D:443:VAL:HG21	2.45	0.41
2:D:442:TYR:O	2:D:448:PRO:HB3	2.21	0.41
2:D:460:THR:HG23	2:D:463:THR:H	1.85	0.41
2:D:269:MET:HE3	2:D:269:MET:HB2	1.89	0.41
1:A:82:ILE:HG23	1:A:94:ALA:HB1	2.04	0.40
2:B:192:LEU:HD13	2:B:206:VAL:HG21	2.01	0.40
2:D:247:THR:HB	2:D:253:LYS:HD2	2.03	0.40
2:D:442:TYR:C	2:D:442:TYR:CD1	2.99	0.40
1:A:143:ASP:CG	1:A:168:ASN:HD22	2.28	0.40
2:B:183:ILE:HD12	2:B:183:ILE:H	1.85	0.40
1:C:83:ARG:HG3	1:C:85:GLY:N	2.30	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	307/369 (83%)	294 (96%)	13 (4%)	0	100	100
1	C	307/369 (83%)	290 (94%)	16 (5%)	1 (0%)	36	55
2	B	503/640 (79%)	491 (98%)	12 (2%)	0	100	100
2	D	501/640 (78%)	484 (97%)	16 (3%)	1 (0%)	43	63
All	All	1618/2018 (80%)	1559 (96%)	57 (4%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	ASP
2	D	8	PRO

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	268/315 (85%)	267 (100%)	1 (0%)	84	93
1	C	268/315 (85%)	267 (100%)	1 (0%)	84	93
2	B	441/552 (80%)	438 (99%)	3 (1%)	76	89
2	D	440/552 (80%)	436 (99%)	4 (1%)	70	87
All	All	1417/1734 (82%)	1408 (99%)	9 (1%)	78	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
2	B	158	CYS
2	B	166	THR
2	B	346	LYS
1	C	273	ARG
2	D	308	LYS
2	D	411	ASP
2	D	441	CYS
2	D	476	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	274	ASN
2	B	108	GLN
2	B	364	HIS
2	B	501	ASN
2	B	534	HIS
1	C	18	GLN
1	C	103	ASN
1	C	172	HIS
1	C	271	GLN
1	C	320	GLN
2	D	184	HIS
2	D	311	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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	0.31	0	48,52,52	0.39	0
3	ATP	D	701	4	32,33,33	0.27	0	48,52,52	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	701	4	-	7/22/38/38	0/3/3/3
3	ATP	D	701	4	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

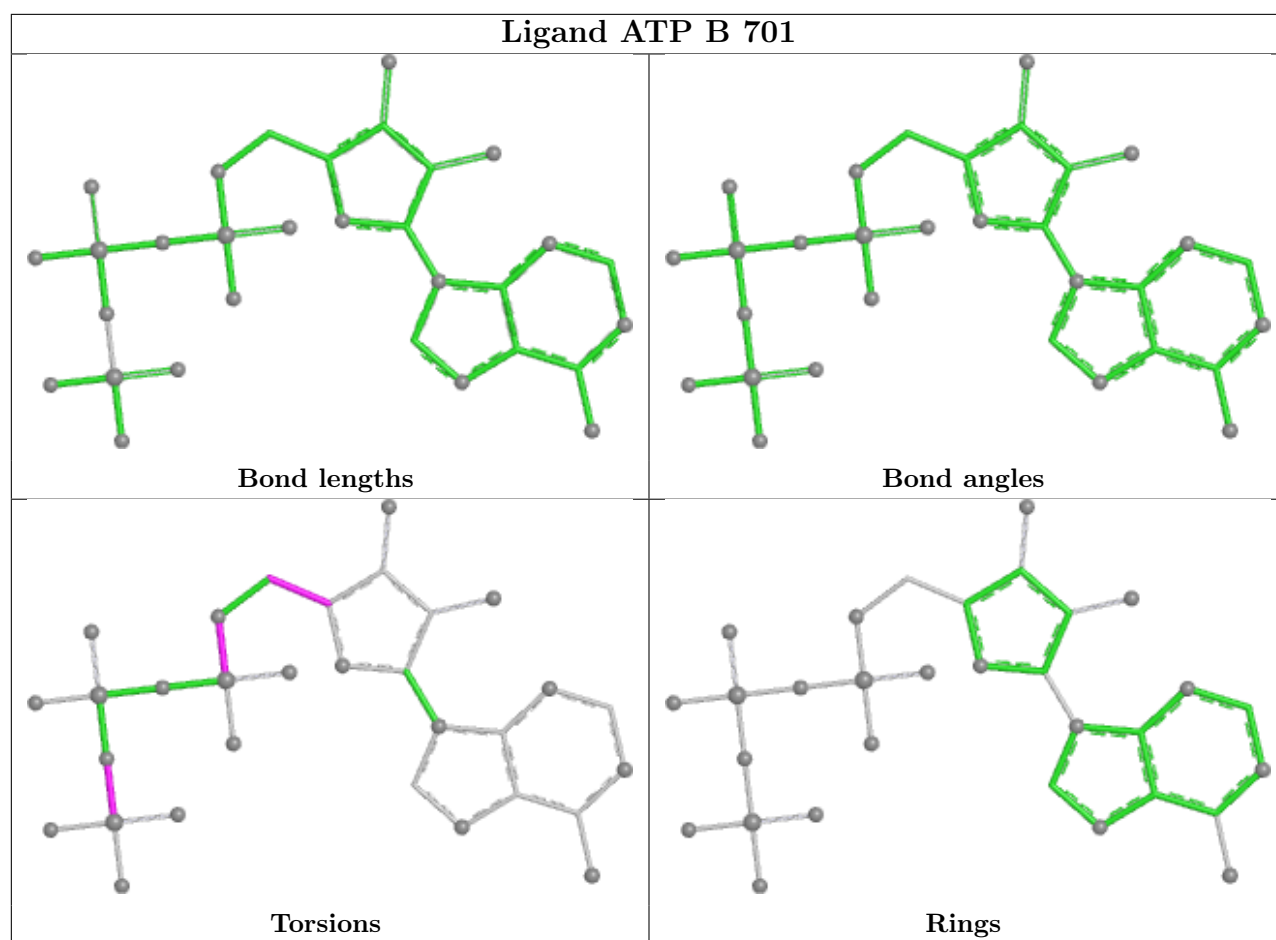
Mol	Chain	Res	Type	Atoms
3	B	701	ATP	PB-O3B-PG-O2G

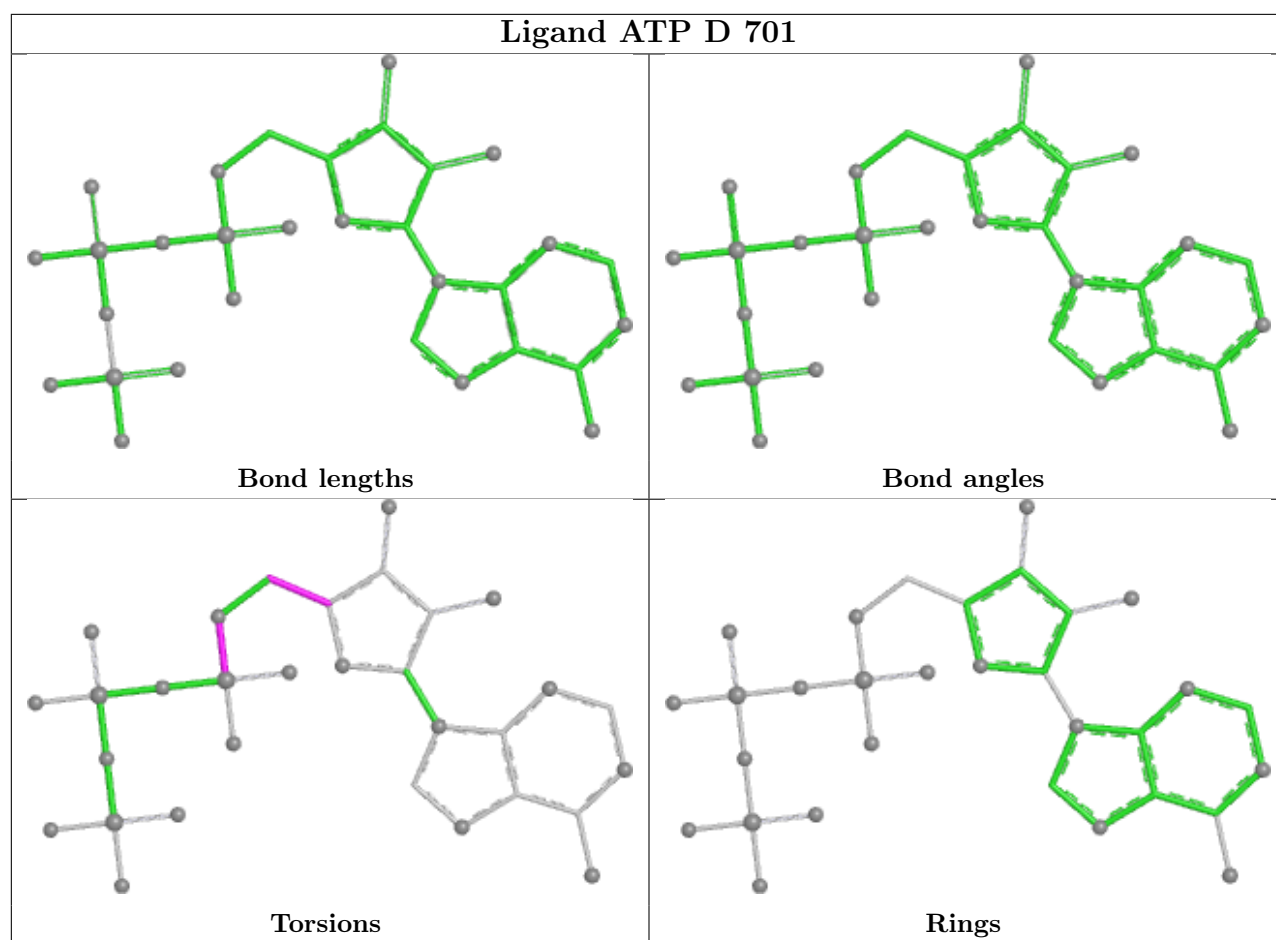
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	ATP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/369 (84%)	0.06	4 (1%) 75 71	48, 68, 103, 138	0
1	C	311/369 (84%)	0.17	8 (2%) 57 52	47, 69, 116, 139	0
2	B	509/640 (79%)	0.33	15 (2%) 53 49	45, 77, 127, 157	0
2	D	507/640 (79%)	0.39	16 (3%) 50 46	45, 84, 131, 161	0
All	All	1638/2018 (81%)	0.27	43 (2%) 57 52	45, 75, 126, 161	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	550	ALA	3.4
1	C	78	ALA	3.4
2	B	206	VAL	3.2
2	D	6	GLY	3.1
1	C	75	ASP	3.1
2	B	170	PHE	3.0
2	B	6	GLY	3.0
1	C	10	GLY	2.9
2	B	175	ILE	2.8
2	B	551	PRO	2.8
2	D	158	CYS	2.8
2	B	182	PRO	2.8
1	C	77	GLY	2.7
2	B	188	TRP	2.7
2	B	266	LEU	2.7
2	D	305	LEU	2.7
2	D	206	VAL	2.6
1	C	178	LYS	2.6
2	D	276	ARG	2.5
2	B	154	GLY	2.5
2	D	258	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	538	LEU	2.5
1	C	76	PRO	2.4
2	D	213	PRO	2.4
2	D	282	LEU	2.4
1	A	87	VAL	2.4
2	B	538	LEU	2.4
1	C	205	THR	2.3
2	B	273	TRP	2.3
2	B	305	LEU	2.3
2	B	83	PHE	2.3
1	C	207	VAL	2.2
2	D	366	PHE	2.2
2	D	280	VAL	2.2
2	D	442	TYR	2.1
1	A	98	ARG	2.1
2	D	117	ASP	2.0
1	A	206	MET	2.0
2	B	239	SER	2.0
2	D	180	SER	2.0
1	A	78	ALA	2.0
2	D	268	THR	2.0
2	B	442	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	702	1/1	0.89	0.20	66,66,66,66	0

Continued on next page...

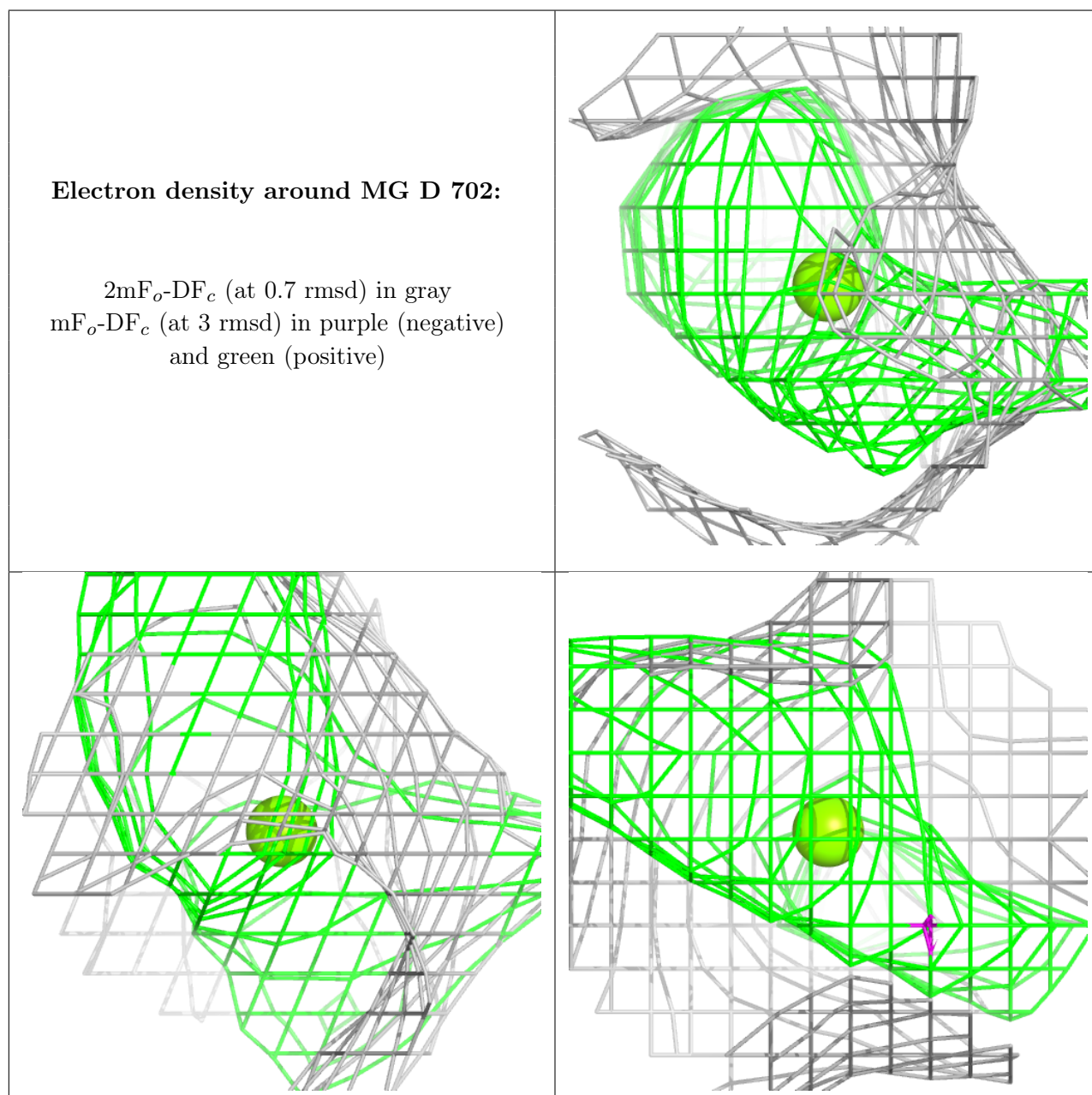
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	B	701	31/31	0.90	0.10	58,77,97,107	0
3	ATP	D	701	31/31	0.91	0.11	58,82,101,121	0
4	MG	B	702	1/1	0.92	0.13	73,73,73,73	0
5	ZN	D	703	1/1	0.93	0.07	65,65,65,65	0
5	ZN	B	703	1/1	0.98	0.04	55,55,55,55	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.

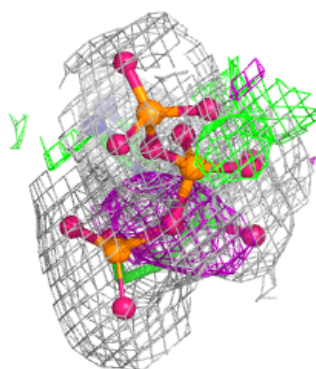
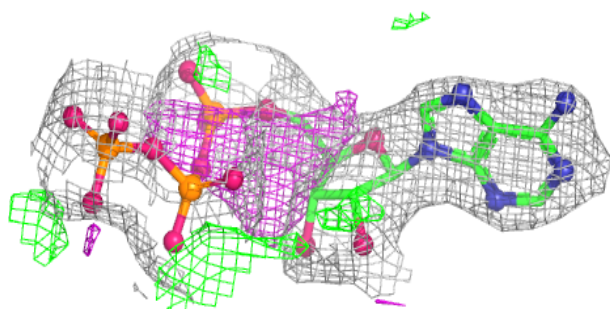
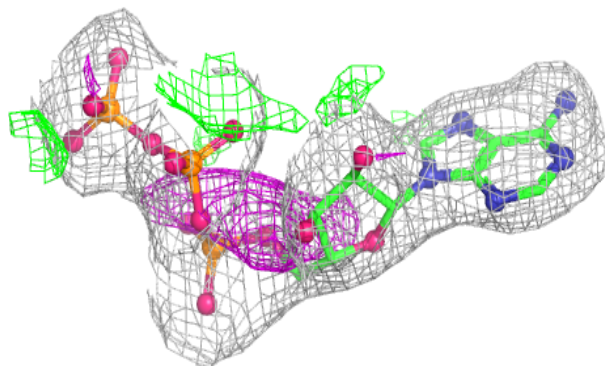
Electron density around MG D 702:

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

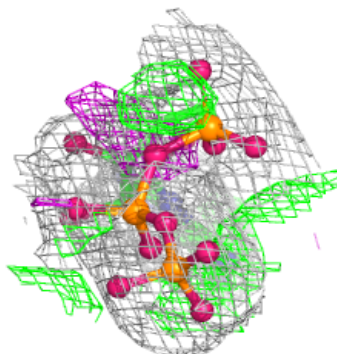
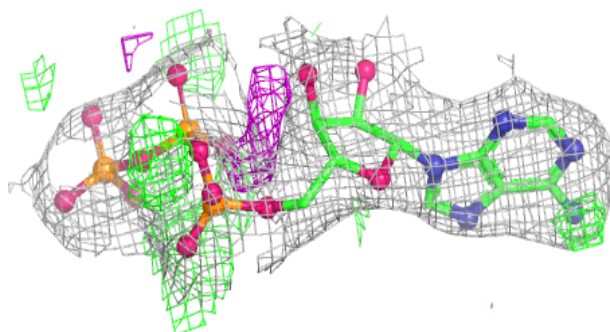
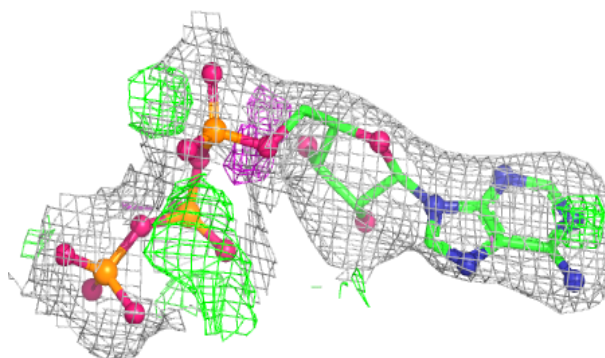


Electron density around ATP B 701:

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

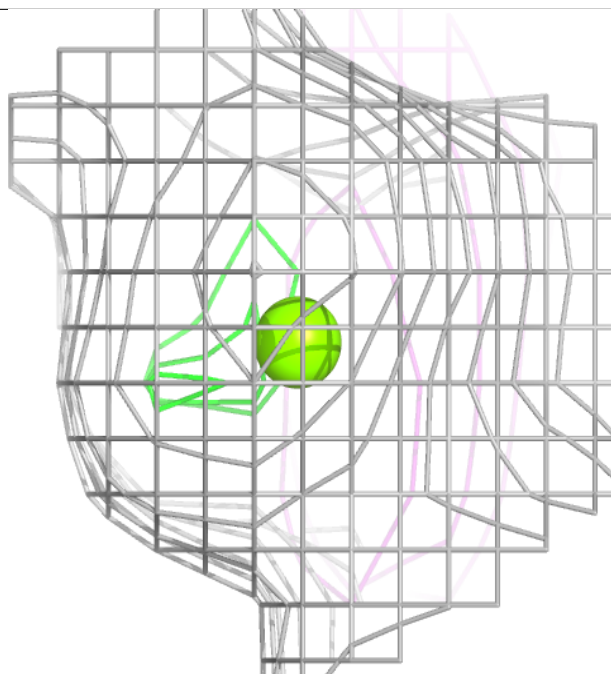
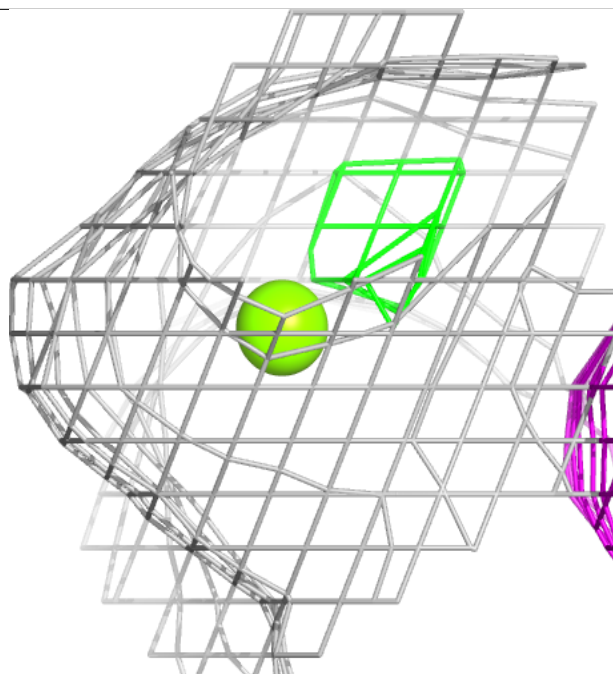
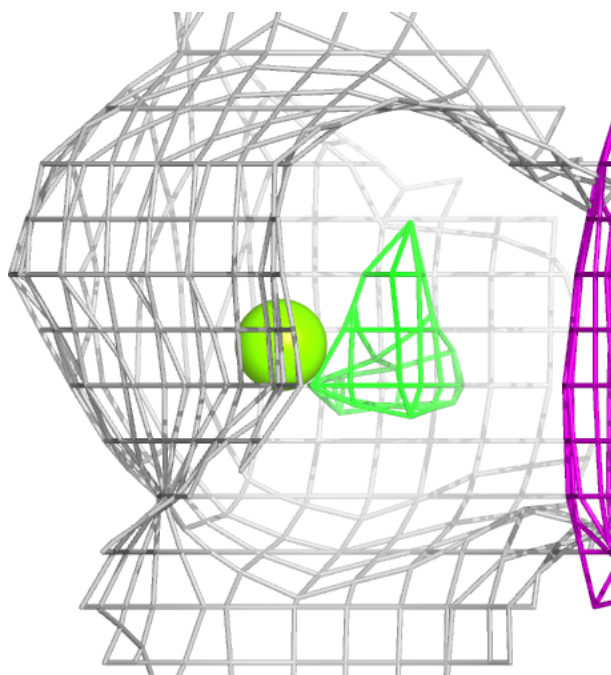
**Electron density around ATP D 701:**

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.