



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:24 am BST

PDB ID : 4JD2  
Title : Crystal structure of Bos taurus Arp2/3 complex binding with Mus musculus GMF  
Authors : Nolen, B.J.; Luan, Q.  
Deposited on : 2013-02-22  
Resolution : 3.08 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

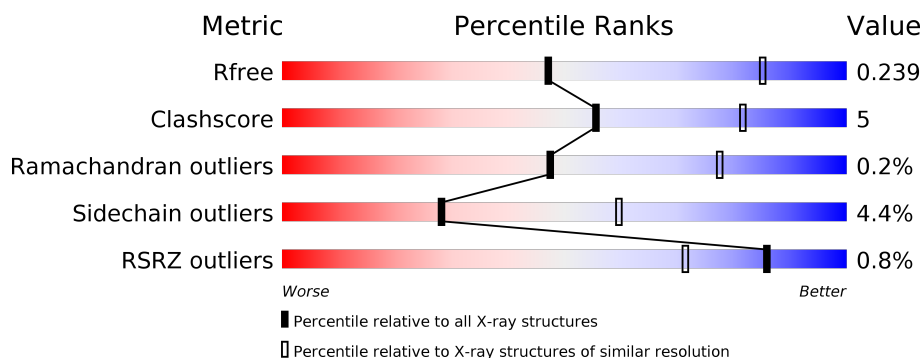
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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))
$R_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 on 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	418	<div> <div style="width: 83%;"></div> <div style="width: 11%;"></div> <div style="width: 5%;"></div> </div>
2	B	394	<div> <div style="width: 75%;"></div> <div style="width: 19%;"></div> <div style="width: 6%;"></div> </div>
3	C	372	<div> <div style="width: 81%;"></div> <div style="width: 10%;"></div> <div style="width: 8%;"></div> </div>
4	D	300	<div> <div style="width: 83%;"></div> <div style="width: 10%;"></div> <div style="width: 6%;"></div> </div>
5	E	178	<div> <div style="width: 84%;"></div> <div style="width: 11%;"></div> <div style="width: 5%;"></div> </div>
6	F	168	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	151	<div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
8	H	142	<div> <div></div> <div>85%</div> <div>10%</div> <div></div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16016 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3170	2034	531	591	14			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	377	Total	C	N	O	S	0	0	0
			2963	1898	507	542	16			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	342	Total	C	N	O	S	0	0	0
			2650	1681	464	486	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	283	Total	C	N	O	S	0	0	0
			2280	1447	395	430	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	170	Total	C	N	O	S	0	0	0
			1350	869	225	247	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	166	Total	C	N	O	S	0	0	0
			1356	866	237	244	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	139	Total	C	N	O	S	0	0	0
			1041	650	183	205	3			

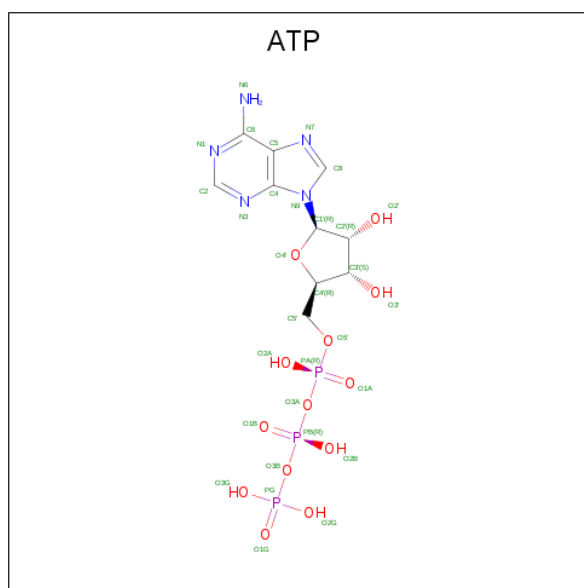
- Molecule 8 is a protein called Glia maturation factor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	713	188	208	7			

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

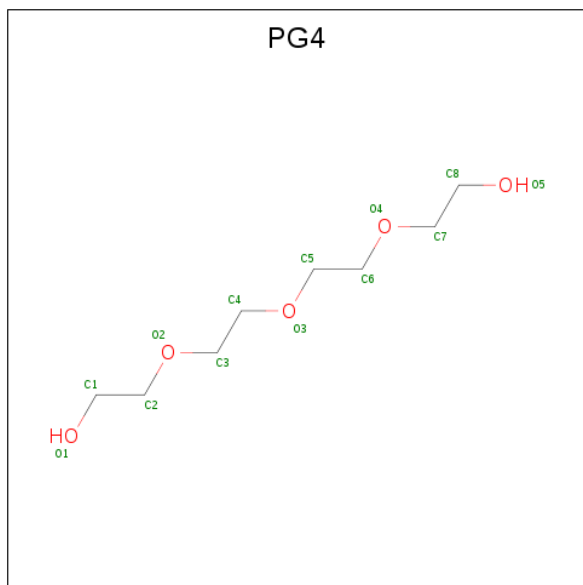
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	A	1	Total	Ca	0	0
			1	1		

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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
10	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
10	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).

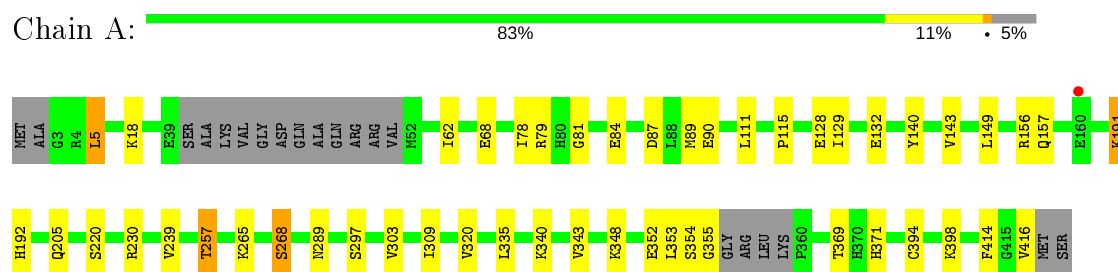


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			13	8	5		
11	F	1	Total	C	O	0	0
			13	8	5		

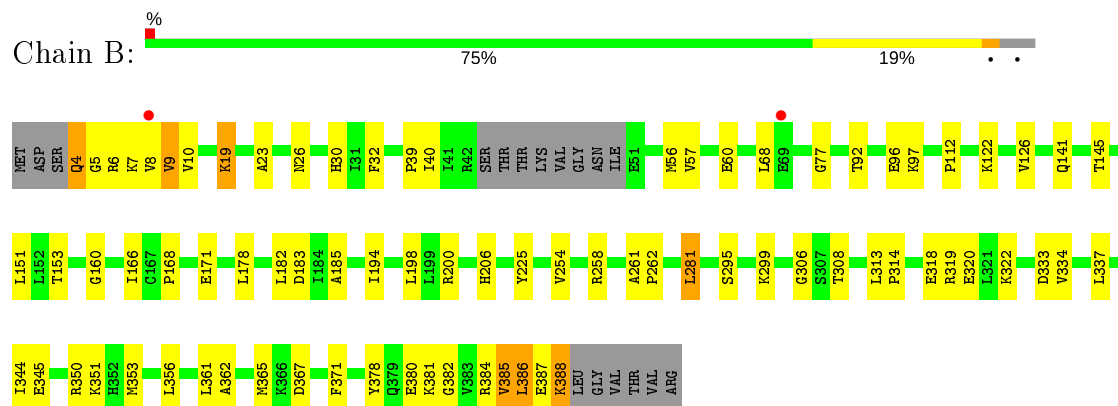
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

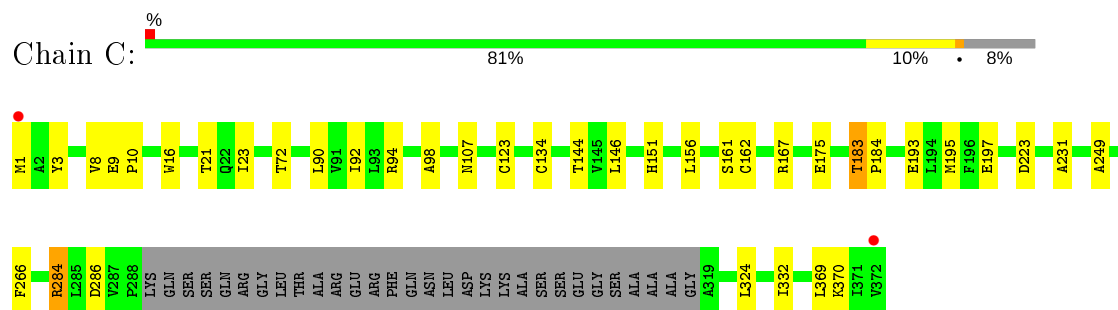
#### • Molecule 1: Actin-related protein 3



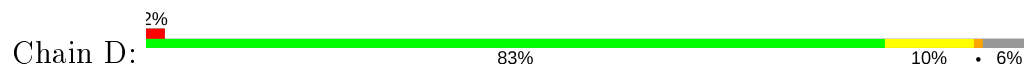
#### • Molecule 2: Actin-related protein 2

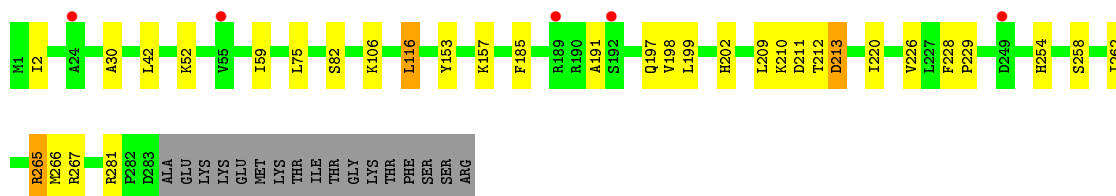


#### • Molecule 3: Actin-related protein 2/3 complex subunit 1B

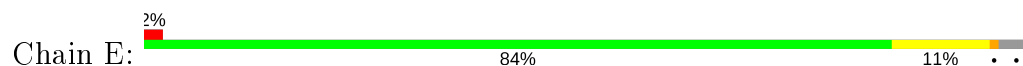


#### • Molecule 4: Actin-related protein 2/3 complex subunit 2

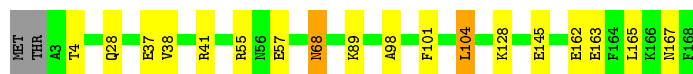




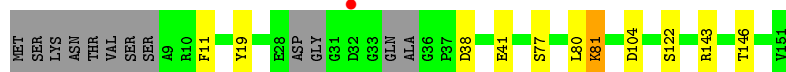
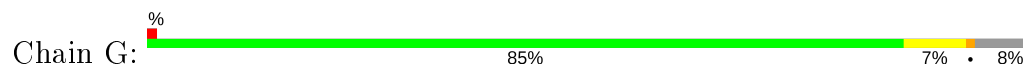
- Molecule 5: Actin-related protein 2/3 complex subunit 3



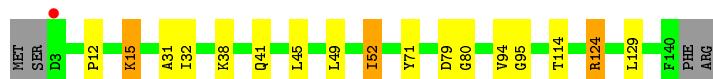
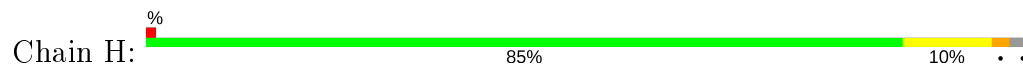
- Molecule 6: Actin-related protein 2/3 complex subunit 4



- Molecule 7: Actin-related protein 2/3 complex subunit 5



- Molecule 8: Glia maturation factor gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.54Å 231.54Å 109.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.82 – 3.08 35.82 – 3.08	Depositor EDS
% Data completeness (in resolution range)	97.6 (35.82-3.08) 97.6 (35.82-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.209 , 0.248 0.206 , 0.239	Depositor DCC
$R_{free}$ test set	3097 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: CA, PG4, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/3251	0.55	0/4413
2	B	0.35	0/3023	0.61	0/4093
3	C	0.35	0/2719	0.57	0/3692
4	D	0.34	0/2329	0.54	0/3146
5	E	0.33	0/1381	0.49	0/1863
6	F	0.38	0/1378	0.59	0/1849
7	G	0.36	0/1052	0.57	0/1415
8	H	0.34	0/1137	0.55	0/1536
All	All	0.35	0/16270	0.56	0/22007

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3170	0	3090	23	0
2	B	2963	0	2946	59	0
3	C	2650	0	2598	30	0
4	D	2280	0	2232	19	0
5	E	1350	0	1301	11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1356	0	1388	11	0
7	G	1041	0	1035	12	0
8	H	1116	0	1109	12	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	31	0	12	0	0
10	B	31	0	12	1	0
11	B	13	0	18	2	0
11	F	13	0	18	0	0
All	All	16016	0	15759	162	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 (162) 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)
7:G:77:SER:O	7:G:81:LYS:HD2	1.40	1.18
3:C:369:LEU:C	3:C:370:LYS:HD3	1.91	0.90
7:G:81:LYS:N	7:G:81:LYS:HE3	1.89	0.85
2:B:6:ARG:HB3	2:B:7:LYS:HA	1.62	0.81
2:B:382:GLY:O	2:B:385:VAL:HG23	1.84	0.76
2:B:6:ARG:HB3	2:B:7:LYS:CA	2.18	0.74
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.70	0.73
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.72	0.72
2:B:77:GLY:O	2:B:112:PRO:HG3	1.90	0.72
6:F:37:GLU:H	6:F:68:ASN:HD21	1.37	0.71
2:B:322:LYS:NZ	11:B:503:PG4:O3	2.25	0.69
2:B:386:LEU:HD13	2:B:388:LYS:HG2	1.74	0.69
2:B:388:LYS:HE3	2:B:388:LYS:CA	2.22	0.69
7:G:81:LYS:CA	7:G:81:LYS:HE3	2.24	0.68
8:H:49:LEU:HB2	8:H:52:ILE:HD11	1.76	0.68
5:E:9:MET:HE3	5:E:62:ASN:HB2	1.76	0.67
2:B:388:LYS:HE3	2:B:388:LYS:HA	1.77	0.66
1:A:348:LYS:HE3	1:A:352:GLU:OE1	1.96	0.65
3:C:193:GLU:HG2	3:C:195:MET:HE1	1.77	0.65
3:C:183:THR:HG22	3:C:184:PRO:HD2	1.77	0.65
5:E:37:LYS:HG3	5:E:38:ASP:H	1.60	0.65
3:C:144:THR:OG1	6:F:28:GLN:NE2	2.30	0.64
2:B:166:ILE:HD12	2:B:281:LEU:HD13	1.79	0.64
3:C:370:LYS:N	3:C:370:LYS:HD3	2.13	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:H	1:A:157:GLN:HA	1.61	0.64
2:B:8:VAL:HG12	2:B:9:VAL:N	2.13	0.64
2:B:385:VAL:O	2:B:385:VAL:HG12	1.99	0.63
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.81	0.62
5:E:37:LYS:CG	5:E:38:ASP:N	2.61	0.62
4:D:210:LYS:HG3	4:D:211:ASP:OD1	1.99	0.62
7:G:80:LEU:C	7:G:81:LYS:HE3	2.21	0.60
2:B:57:VAL:O	2:B:60:GLU:HG2	2.00	0.60
1:A:79:ARG:CG	1:A:84:GLU:HG3	2.32	0.59
3:C:146:LEU:HD11	3:C:162:CYS:SG	2.44	0.58
7:G:81:LYS:CA	7:G:81:LYS:CE	2.82	0.58
2:B:39:PRO:HA	2:B:68:LEU:HD23	1.87	0.56
5:E:37:LYS:CG	5:E:38:ASP:H	2.17	0.56
1:A:149:LEU:HD23	1:A:320:VAL:HG21	1.86	0.56
8:H:15:LYS:NZ	8:H:15:LYS:HB3	2.20	0.56
2:B:308:THR:HA	2:B:313:LEU:HD22	1.87	0.56
2:B:141:GLN:O	2:B:145:THR:HG23	2.05	0.56
2:B:384:ARG:HA	2:B:385:VAL:HB	1.87	0.55
4:D:212:THR:O	4:D:213:ASP:OD1	2.24	0.55
7:G:81:LYS:CE	7:G:81:LYS:HA	2.36	0.55
6:F:4:THR:HG23	6:F:55:ARG:HE	1.73	0.54
2:B:30:HIS:CD2	2:B:97:LYS:HE3	2.41	0.54
2:B:151:LEU:HD21	8:H:124:ARG:HD3	1.90	0.54
2:B:153:THR:HG22	2:B:171:GLU:H	1.71	0.54
3:C:123:CYS:SG	3:C:134:CYS:CB	2.96	0.54
7:G:81:LYS:HE3	7:G:81:LYS:HA	1.89	0.54
2:B:388:LYS:N	2:B:388:LYS:CD	2.70	0.53
8:H:79:ASP:OD1	8:H:80:GLY:N	2.40	0.53
2:B:8:VAL:HG12	2:B:9:VAL:H	1.74	0.53
2:B:381:LYS:CB	2:B:382:GLY:CA	2.87	0.53
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.91	0.53
2:B:96:GLU:O	2:B:97:LYS:HD2	2.09	0.53
2:B:387:GLU:N	2:B:388:LYS:HD2	2.24	0.52
1:A:79:ARG:HG2	1:A:84:GLU:HG3	1.91	0.52
4:D:191:ALA:HB2	6:F:162:GLU:HG2	1.91	0.52
1:A:156:ARG:N	1:A:157:GLN:HA	2.24	0.52
5:E:110:GLY:CA	5:E:111:PHE:C	2.78	0.52
4:D:2:ILE:HG21	6:F:163:GLU:HG2	1.92	0.52
4:D:265:ARG:NH1	6:F:145:GLU:OE2	2.43	0.52
3:C:266:PHE:CD1	3:C:284:ARG:HG3	2.45	0.52
5:E:152:GLN:N	5:E:153:ASN:HA	2.24	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:PRO:HG2	2:B:178:LEU:HB3	1.93	0.51
2:B:32:PHE:HZ	2:B:92:THR:HG22	1.76	0.51
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.46	0.51
1:A:340:LYS:HA	1:A:343:VAL:HG12	1.92	0.50
2:B:388:LYS:HD2	2:B:388:LYS:N	2.26	0.50
2:B:350:ARG:HA	2:B:353:MET:HG2	1.92	0.50
2:B:6:ARG:CB	2:B:7:LYS:HA	2.33	0.50
2:B:378:TYR:HA	2:B:385:VAL:HG21	1.94	0.50
2:B:306:GLY:HA2	2:B:351:LYS:HG3	1.94	0.49
3:C:72:THR:HA	3:C:98:ALA:HB1	1.94	0.49
3:C:123:CYS:SG	3:C:134:CYS:HB2	2.52	0.49
3:C:92:ILE:HG22	3:C:92:ILE:O	2.12	0.49
4:D:185:PHE:HB3	4:D:198:VAL:HG11	1.94	0.49
2:B:380:GLU:N	2:B:381:LYS:HA	2.27	0.49
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.52	0.49
2:B:8:VAL:HG11	2:B:362:ALA:HB1	1.94	0.49
2:B:387:GLU:H	2:B:388:LYS:HD2	1.77	0.49
2:B:382:GLY:O	2:B:384:ARG:HA	2.12	0.49
4:D:202:HIS:O	4:D:220:ILE:O	2.30	0.49
2:B:6:ARG:HB3	2:B:7:LYS:CB	2.43	0.48
3:C:193:GLU:CG	3:C:195:MET:HE1	2.42	0.48
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.96	0.48
2:B:334:VAL:HG21	7:G:19:TYR:CE2	2.48	0.47
8:H:12:PRO:O	8:H:15:LYS:HB2	2.15	0.47
2:B:194:ILE:HD13	2:B:206:HIS:HA	1.97	0.47
3:C:16:TRP:CZ2	3:C:23:ILE:HD12	2.49	0.47
4:D:197:GLN:HB3	4:D:226:VAL:HB	1.96	0.47
2:B:26:ASN:O	2:B:356:LEU:HD11	2.15	0.47
3:C:9:GLU:HB3	3:C:10:PRO:HD2	1.97	0.47
1:A:354:SER:CB	1:A:355:GLY:CA	2.93	0.47
3:C:123:CYS:SG	3:C:134:CYS:HB3	2.55	0.46
3:C:3:TYR:HB2	3:C:324:LEU:HD23	1.95	0.46
2:B:345:GLU:OE2	8:H:124:ARG:NH1	2.48	0.46
2:B:4:GLN:N	2:B:6:ARG:O	2.47	0.46
6:F:163:GLU:O	6:F:167:ASN:ND2	2.48	0.46
4:D:30:ALA:HB2	4:D:52:LYS:HD3	1.97	0.46
6:F:38:VAL:O	6:F:41:ARG:NH1	2.48	0.46
5:E:43:ASP:OD1	5:E:143:ARG:NH1	2.49	0.46
2:B:56:MET:HG3	2:B:68:LEU:HD11	1.97	0.46
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.96	0.46
2:B:8:VAL:HG11	2:B:23:ALA:HB2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:GLY:O	2:B:384:ARG:CA	2.65	0.45
3:C:370:LYS:N	3:C:370:LYS:CD	2.80	0.45
8:H:31:ALA:HB2	8:H:71:TYR:HD1	1.81	0.45
5:E:37:LYS:HG2	5:E:38:ASP:N	2.32	0.45
3:C:266:PHE:CE1	3:C:284:ARG:HG3	2.51	0.45
4:D:153:TYR:CD2	4:D:209:LEU:HD22	2.53	0.44
2:B:4:GLN:CB	2:B:5:GLY:HA3	2.47	0.44
1:A:348:LYS:HE3	1:A:352:GLU:CD	2.37	0.44
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.98	0.44
1:A:78:ILE:HD11	1:A:89:MET:HE1	1.99	0.44
4:D:59:ILE:HG21	4:D:116:LEU:HD22	2.00	0.44
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.17	0.44
2:B:122:LYS:O	2:B:126:VAL:HG23	2.18	0.44
3:C:284:ARG:HD3	3:C:286:ASP:O	2.18	0.44
1:A:257:THR:HG22	1:A:268:SER:HB3	2.00	0.44
2:B:318:GLU:CG	2:B:344:ILE:HD12	2.46	0.44
2:B:19:LYS:NZ	10:B:502:ATP:O1B	2.50	0.44
8:H:124:ARG:HA	8:H:124:ARG:HD2	1.73	0.44
4:D:262:ILE:O	4:D:266:MET:HG3	2.18	0.44
4:D:191:ALA:CB	6:F:162:GLU:HG2	2.47	0.44
3:C:156:LEU:HD22	3:C:195:MET:HG3	2.00	0.43
4:D:210:LYS:HA	4:D:211:ASP:HA	1.69	0.43
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.99	0.43
2:B:365:MET:HG2	2:B:371:PHE:CG	2.53	0.43
4:D:228:PHE:HB3	4:D:229:PRO:HD2	2.00	0.43
7:G:81:LYS:N	7:G:81:LYS:CE	2.72	0.43
4:D:254:HIS:O	4:D:258:SER:HB2	2.19	0.43
1:A:191:LYS:HE2	1:A:303:VAL:HG22	2.01	0.43
1:A:309:ILE:HD12	2:B:40:ILE:CD1	2.49	0.43
5:E:9:MET:CE	5:E:64:ALA:H	2.32	0.43
7:G:104:ASP:OD2	7:G:143:ARG:NE	2.49	0.43
3:C:1:MET:HA	3:C:324:LEU:HD21	2.01	0.42
3:C:184:PRO:HB2	3:C:231:ALA:HB3	2.01	0.42
3:C:94:ARG:HD2	8:H:94:VAL:HG23	2.00	0.42
3:C:151:HIS:HB2	3:C:156:LEU:HB2	2.02	0.42
8:H:32:ILE:HG23	8:H:45:LEU:CD1	2.50	0.42
1:A:18:LYS:N	1:A:18:LYS:CD	2.82	0.42
3:C:94:ARG:HD3	8:H:95:GLY:HA3	2.01	0.42
2:B:385:VAL:CG1	2:B:385:VAL:O	2.67	0.41
8:H:15:LYS:HE3	8:H:114:THR:HG23	2.01	0.41
1:A:5:LEU:HB3	4:D:42:LEU:HD13	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:HA	3:C:324:LEU:CD2	2.50	0.41
6:F:98:ALA:O	6:F:101:PHE:O	2.38	0.41
6:F:101:PHE:HB3	6:F:104:LEU:HB2	2.02	0.41
2:B:322:LYS:CE	11:B:503:PG4:H82	2.50	0.41
4:D:75:LEU:C	4:D:75:LEU:HD23	2.41	0.41
1:A:111:LEU:C	1:A:111:LEU:HD23	2.41	0.41
1:A:90:GLU:HG3	1:A:129:ILE:HG23	2.02	0.41
2:B:160:GLY:O	2:B:185:ALA:HB1	2.21	0.41
5:E:150:ASP:HA	5:E:151:PRO:HD3	1.93	0.41
1:A:205:GLN:HE21	1:A:220:SER:HB3	1.85	0.41
1:A:81:GLY:O	1:A:115:PRO:HG3	2.21	0.40
2:B:8:VAL:CG1	2:B:9:VAL:N	2.81	0.40
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.51	0.40
2:B:225:TYR:CZ	2:B:319:ARG:HD2	2.56	0.40
1:A:128:GLU:O	1:A:132:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/418 (94%)	372 (95%)	20 (5%)	0	100	100
2	B	373/394 (95%)	348 (93%)	24 (6%)	1 (0%)	41	71
3	C	338/372 (91%)	318 (94%)	20 (6%)	0	100	100
4	D	281/300 (94%)	266 (95%)	15 (5%)	0	100	100
5	E	162/178 (91%)	149 (92%)	12 (7%)	1 (1%)	25	57
6	F	164/168 (98%)	157 (96%)	7 (4%)	0	100	100
7	G	133/151 (88%)	124 (93%)	8 (6%)	1 (1%)	19	52
8	H	136/142 (96%)	130 (96%)	6 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1979/2123 (93%)	1864 (94%)	112 (6%)	3 (0%)	47 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	385	VAL
7	G	11	PHE
5	E	16	ILE

### 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	342/363 (94%)	323 (94%)	19 (6%)	21 51
2	B	315/345 (91%)	297 (94%)	18 (6%)	20 50
3	C	289/313 (92%)	281 (97%)	8 (3%)	43 71
4	D	247/264 (94%)	239 (97%)	8 (3%)	39 68
5	E	141/159 (89%)	133 (94%)	8 (6%)	20 50
6	F	151/155 (97%)	145 (96%)	6 (4%)	31 63
7	G	109/123 (89%)	107 (98%)	2 (2%)	59 80
8	H	123/134 (92%)	117 (95%)	6 (5%)	25 56
All	All	1717/1856 (92%)	1642 (96%)	75 (4%)	28 59

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	62	ILE
1	A	68	GLU
1	A	143	VAL
1	A	191	LYS
1	A	192	HIS
1	A	230	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	257	THR
1	A	265	LYS
1	A	268	SER
1	A	289	ASN
1	A	297	SER
1	A	335	LEU
1	A	353	LEU
1	A	369	THR
1	A	371	HIS
1	A	398	LYS
1	A	414	PHE
1	A	416	VAL
2	B	4	GLN
2	B	9	VAL
2	B	10	VAL
2	B	19	LYS
2	B	182	LEU
2	B	183	ASP
2	B	198	LEU
2	B	200	ARG
2	B	281	LEU
2	B	295	SER
2	B	299	LYS
2	B	320	GLU
2	B	333	ASP
2	B	337	LEU
2	B	361	LEU
2	B	367	ASP
2	B	386	LEU
2	B	388	LYS
3	C	8	VAL
3	C	21	THR
3	C	90	LEU
3	C	107	ASN
3	C	161	SER
3	C	175	GLU
3	C	183	THR
3	C	284	ARG
4	D	82	SER
4	D	106	LYS
4	D	116	LEU
4	D	157	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	199	LEU
4	D	213	ASP
4	D	265	ARG
4	D	281	ARG
5	E	62	ASN
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	130	ARG
5	E	144	LEU
5	E	145	CYS
5	E	152	GLN
6	F	57	GLU
6	F	68	ASN
6	F	89	LYS
6	F	104	LEU
6	F	128	LYS
6	F	165	LEU
7	G	81	LYS
7	G	122	SER
8	H	15	LYS
8	H	38	LYS
8	H	41	GLN
8	H	52	ILE
8	H	124	ARG
8	H	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	205	GLN
1	A	318	ASN
2	B	30	HIS
2	B	205	ASN
2	B	267	GLN
2	B	284	ASN
2	B	323	GLN
3	C	22	GLN
3	C	40	ASN
3	C	107	ASN
4	D	140	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	231	HIS
5	E	62	ASN
6	F	28	GLN
6	F	68	ASN
6	F	125	GLN
6	F	167	ASN
7	G	56	GLN
7	G	96	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
10	ATP	A	502	9	26,33,33	0.98	1 (3%)	31,52,52	1.36	5 (16%)
10	ATP	B	502	9	26,33,33	0.97	2 (7%)	31,52,52	1.47	5 (16%)
11	PG4	B	503	-	12,12,12	0.71	0	11,11,11	0.64	0
11	PG4	F	201	-	12,12,12	0.58	0	11,11,11	0.20	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
10	ATP	A	502	9	-	2/18/38/38	0/3/3/3
10	ATP	B	502	9	-	0/18/38/38	0/3/3/3
11	PG4	B	503	-	-	4/10/10/10	-
11	PG4	F	201	-	-	3/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	502	ATP	C5-C4	2.36	1.47	1.40
10	B	502	ATP	O4'-C1'	2.16	1.44	1.41
10	B	502	ATP	C5-C4	2.11	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	ATP	PA-O3A-PB	-3.39	121.19	132.83
10	B	502	ATP	PB-O3B-PG	-3.15	122.01	132.83
10	A	502	ATP	C4-C5-N7	-3.14	106.12	109.40
10	A	502	ATP	N3-C2-N1	-2.82	124.27	128.68
10	B	502	ATP	N3-C2-N1	-2.78	124.34	128.68
10	A	502	ATP	PB-O3B-PG	-2.71	123.54	132.83
10	A	502	ATP	PA-O3A-PB	-2.51	124.21	132.83
10	B	502	ATP	C4-C5-N7	-2.32	106.98	109.40
10	A	502	ATP	O4'-C1'-C2'	-2.27	103.61	106.93
10	B	502	ATP	O2A-PA-O1A	2.14	122.80	112.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	502	ATP	PB-O3B-PG-O2G
11	B	503	PG4	O1-C1-C2-O2
10	A	502	ATP	PB-O3B-PG-O1G
11	F	201	PG4	O2-C3-C4-O3
11	B	503	PG4	C6-C5-O3-C4
11	B	503	PG4	C3-C4-O3-C5
11	F	201	PG4	C8-C7-O4-C6

*Continued on next page...*

*Continued from previous page...*

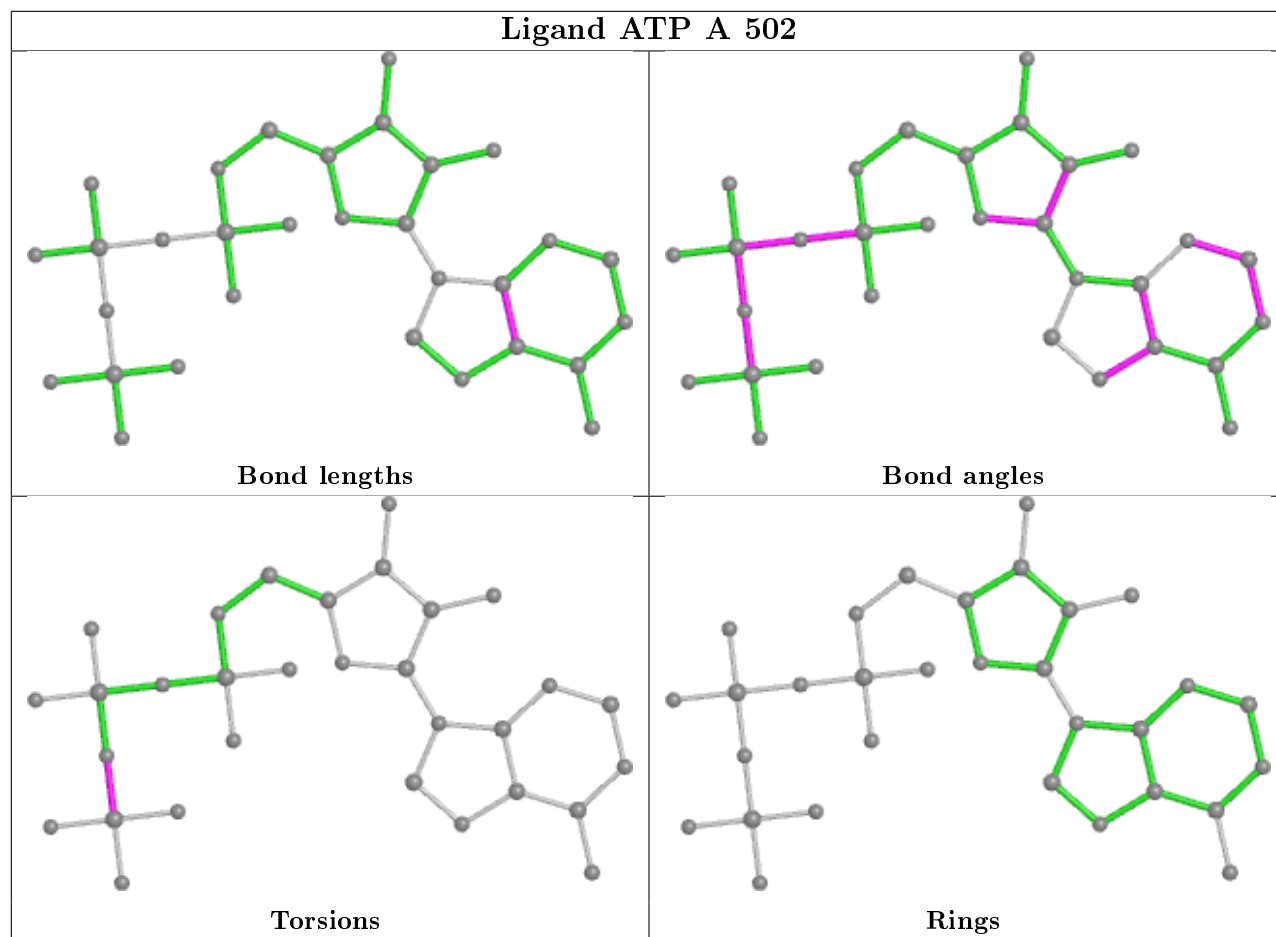
Mol	Chain	Res	Type	Atoms
11	F	201	PG4	O1-C1-C2-O2
11	B	503	PG4	C8-C7-O4-C6

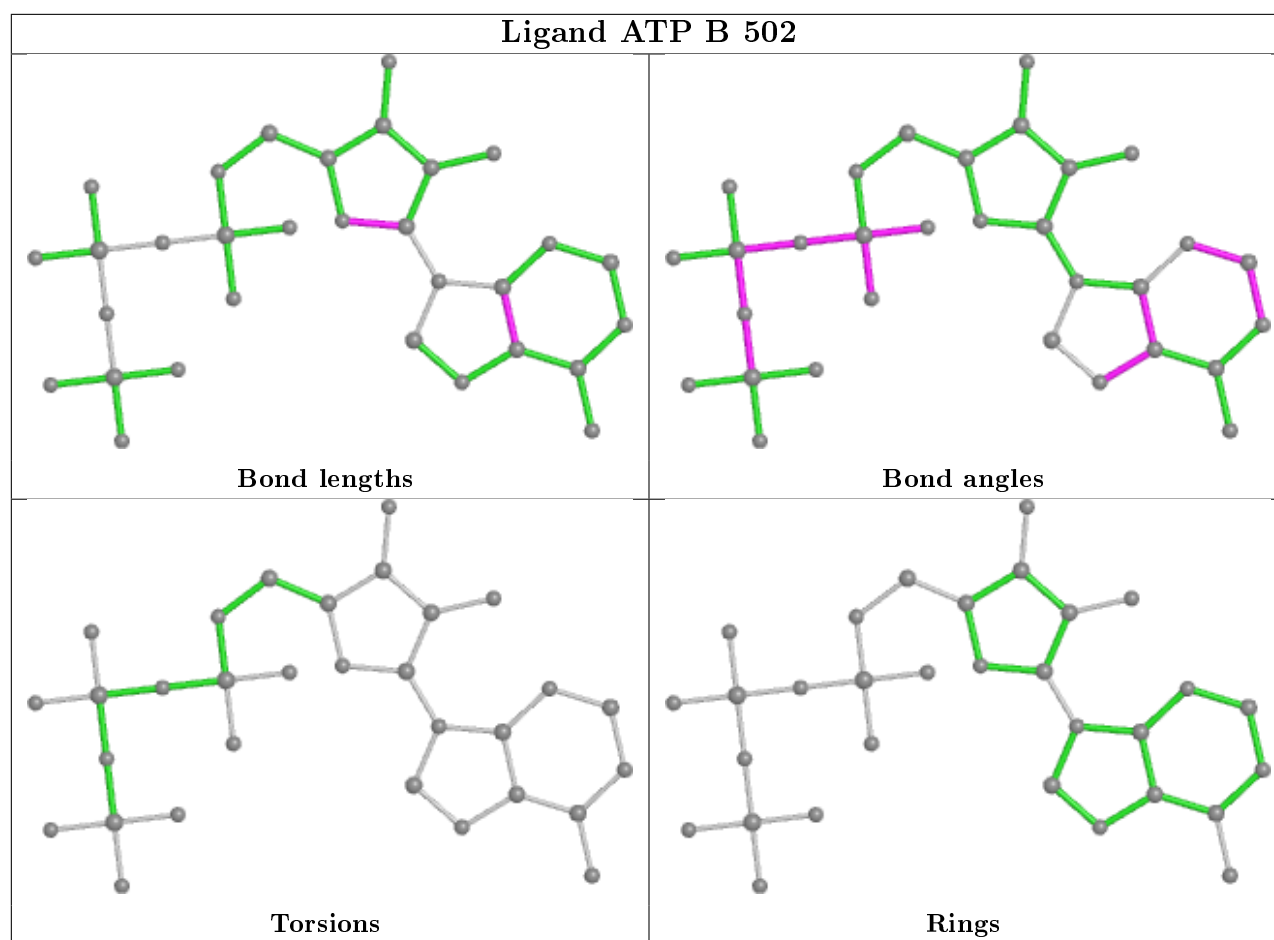
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	502	ATP	1	0
11	B	503	PG4	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, 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	398/418 (95%)	-0.39	1 (0%) 94 87	57, 83, 126, 163	0
2	B	377/394 (95%)	-0.38	2 (0%) 91 80	53, 92, 141, 160	0
3	C	342/372 (91%)	-0.41	2 (0%) 89 77	56, 75, 113, 143	0
4	D	283/300 (94%)	-0.17	5 (1%) 68 46	61, 97, 142, 162	0
5	E	170/178 (95%)	0.00	4 (2%) 59 35	94, 145, 183, 200	0
6	F	166/168 (98%)	-0.54	0 100 100	52, 69, 94, 109	0
7	G	139/151 (92%)	-0.28	1 (0%) 87 74	62, 98, 131, 155	0
8	H	138/142 (97%)	-0.20	1 (0%) 87 74	82, 120, 164, 186	0
All	All	2013/2123 (94%)	-0.32	16 (0%) 86 71	52, 90, 154, 200	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	192	SER	3.3
3	C	1	MET	2.8
8	H	3	ASP	2.7
5	E	21	LEU	2.6
4	D	189	ARG	2.5
3	C	372	VAL	2.4
5	E	10	ASP	2.3
7	G	32	ASP	2.3
5	E	17	GLY	2.1
1	A	160	GLU	2.1
4	D	24	ALA	2.1
5	E	11	PRO	2.1
2	B	69	GLU	2.1
4	D	55	VAL	2.1
2	B	8	VAL	2.0
4	D	249	ASP	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

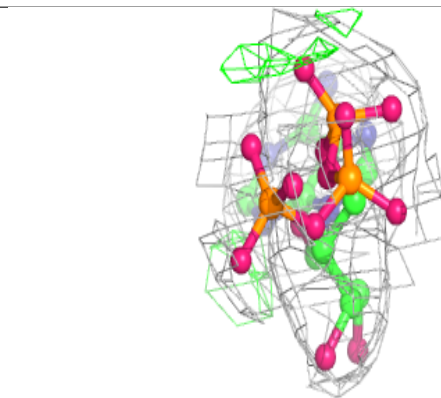
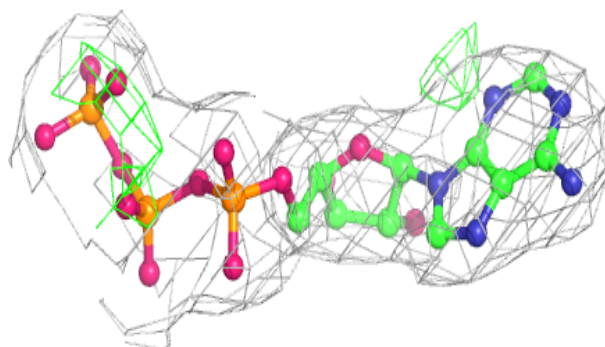
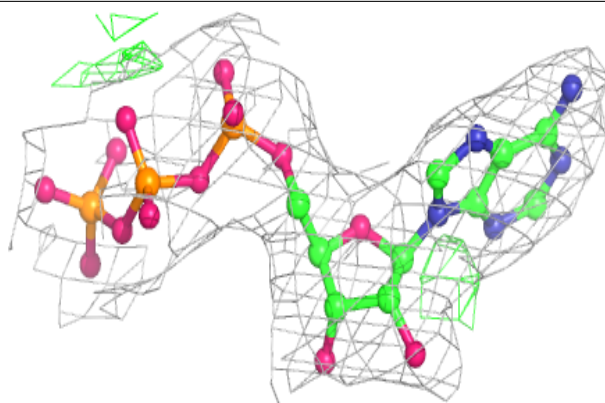
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
11	PG4	B	503	13/13	0.85	0.26	83,100,104,104	0
11	PG4	F	201	13/13	0.86	0.18	93,97,99,101	0
10	ATP	B	502	31/31	0.96	0.18	66,71,90,95	0
10	ATP	A	502	31/31	0.96	0.18	60,71,82,84	0
9	CA	B	501	1/1	0.97	0.41	77,77,77,77	0
9	CA	A	501	1/1	0.99	0.36	64,64,64,64	0

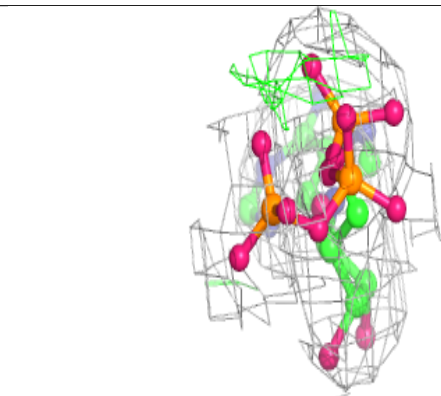
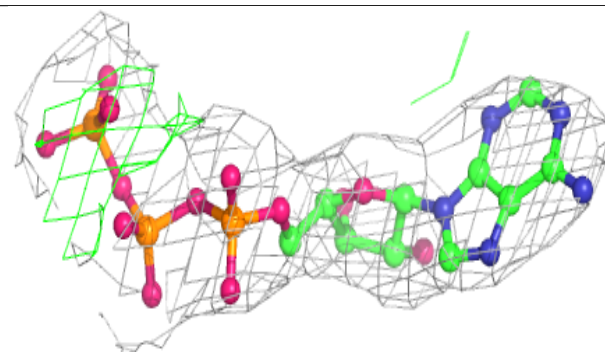
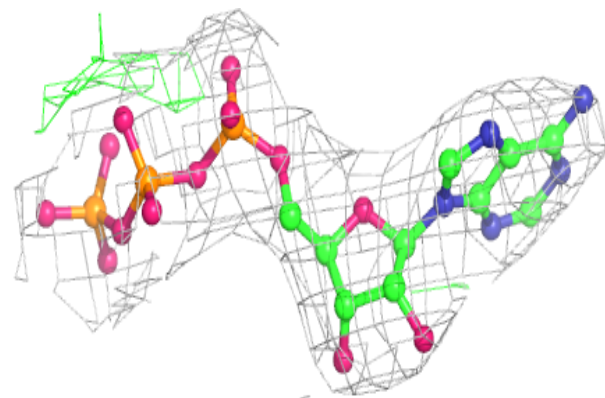
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 502:**

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

**Electron density around ATP A 502:**

$2mF_o-DF_c$  (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.