



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:01 AM UTC

PDB ID : 8K6R / pdb_00008k6r
Title : LnaB-Actin-PRUb ternary complex in the presence of AMPPNP
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2023-07-25
Resolution : 2.76 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

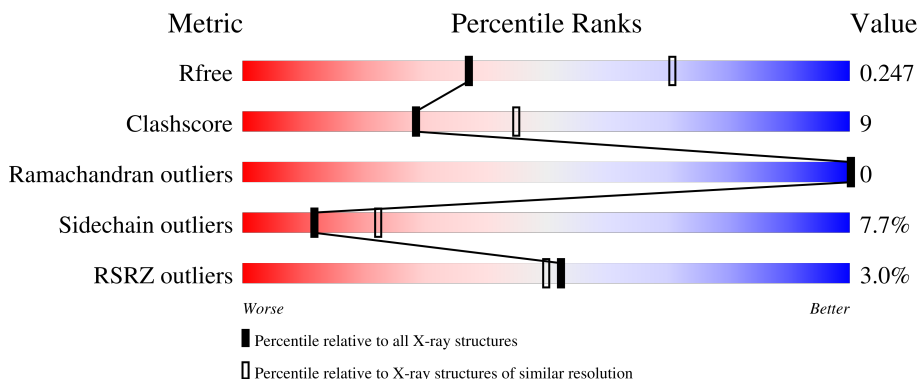
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

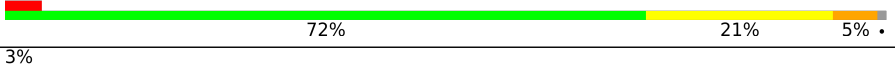
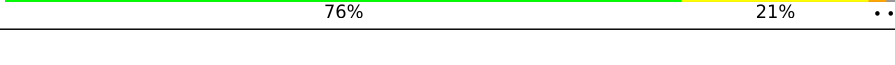
The reported resolution of this entry is 2.76 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	352	
2	C	76	
3	B	375	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6500 atoms, of which 21 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 LnaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2809	1792	461	551	5			

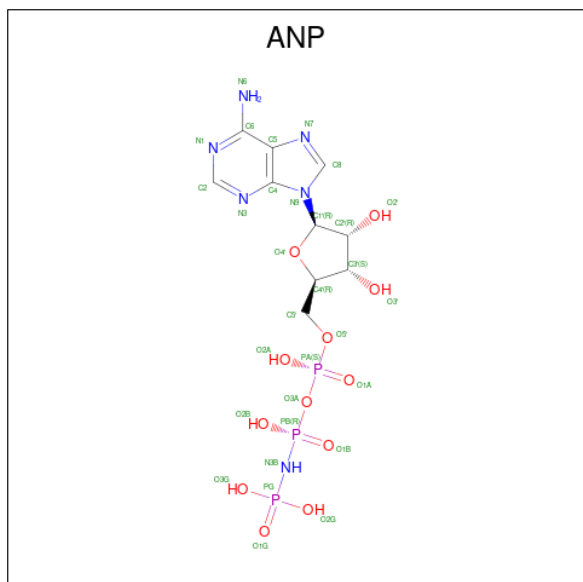
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is a protein called Actin gamma 1.

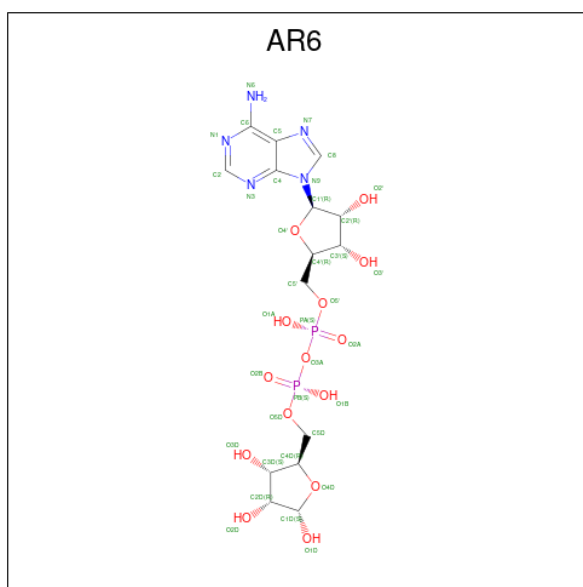
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	371	Total	C	N	O	S	0	0	0
			2894	1834	487	551	22			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

- Molecule 5 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL[HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	P	0	0
			22	5	8	8	1		

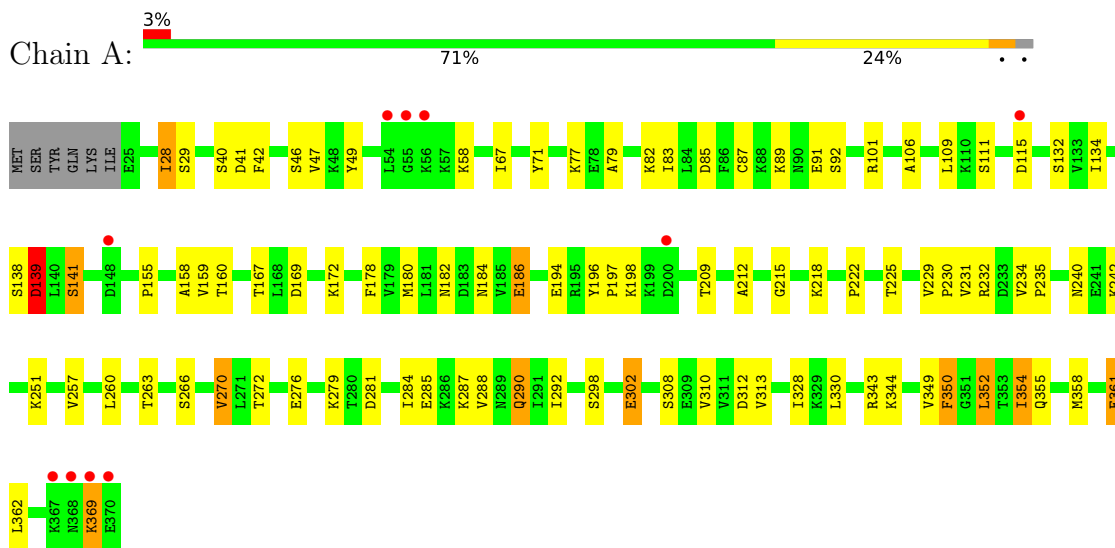
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	55	Total O 55 55	0	0
6	C	8	Total O 8 8	0	0
6	B	71	Total O 71 71	0	0

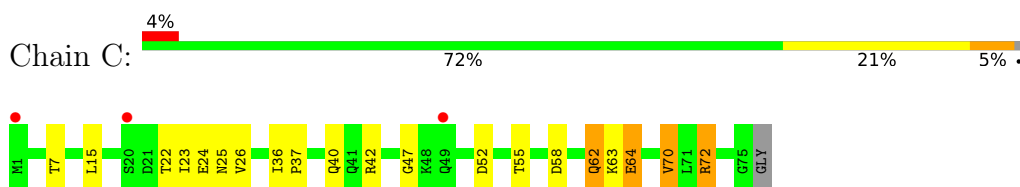
3 Residue-property plots [i](#)

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.

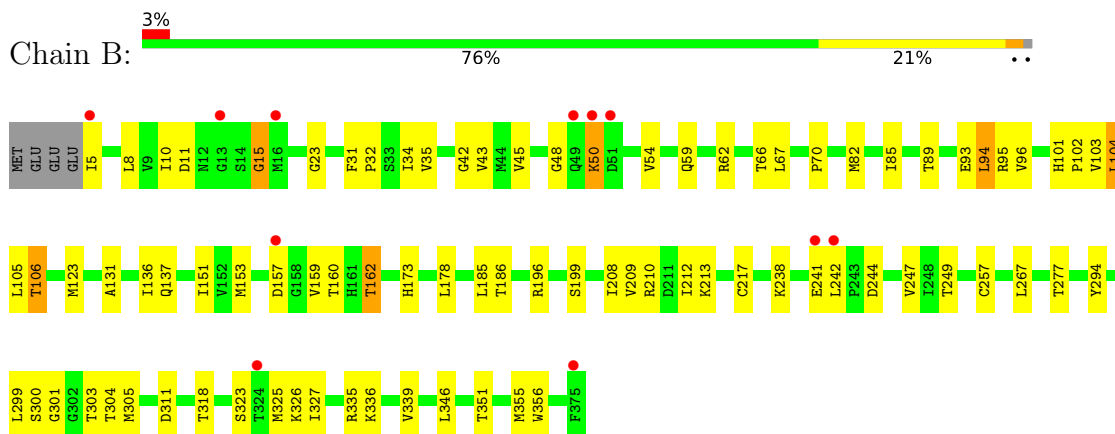
• Molecule 1: LnaB



• Molecule 2: Ubiquitin



• Molecule 3: Actin gamma 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	217.97Å 55.90Å 80.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.48 – 2.76 75.48 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (75.48-2.76) 97.1 (75.48-2.76)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.205 , 0.261 0.209 , 0.247	Depositor DCC
R_{free} test set	1997 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6500	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, AR6

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	1.11	0/2864	1.04	20/3865 (0.5%)
2	C	1.02	3/603 (0.5%)	0.88	1/811 (0.1%)
3	B	0.87	0/2957	0.85	8/4003 (0.2%)
All	All	0.99	3/6424 (0.0%)	0.94	29/8679 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	37	PRO	CA-C	6.88	1.58	1.52
2	C	36	ILE	CA-C	-6.69	1.47	1.53
2	C	62	GLN	CA-C	-5.02	1.46	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	N-CA-C	-13.43	87.39	109.96
1	A	313	VAL	N-CA-C	-9.51	104.19	111.90
1	A	215	GLY	N-CA-C	8.16	126.20	111.02
1	A	263	THR	N-CA-C	-8.00	103.53	113.28
1	A	138	SER	N-CA-C	7.26	120.25	108.34
3	B	199	SER	N-CA-C	6.76	119.70	108.96
1	A	182	ASN	N-CA-C	6.62	119.35	110.35
1	A	235	PRO	N-CA-C	6.51	120.63	110.80
1	A	106	ALA	N-CA-C	6.40	121.57	113.25
3	B	15	GLY	N-CA-C	6.37	122.15	113.99
3	B	23	GLY	N-CA-C	-6.37	106.76	113.58
1	A	184	ASN	N-CA-C	-6.19	98.23	108.07
3	B	301	GLY	N-CA-C	6.09	119.50	111.70
1	A	184	ASN	CA-C-O	-5.99	114.41	121.06
1	A	257	VAL	N-CA-C	-5.96	105.87	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LYS	N-CA-C	5.96	117.86	111.36
3	B	257	CYS	CA-C-N	-5.92	113.55	120.12
3	B	257	CYS	C-N-CA	-5.92	113.55	120.12
3	B	159	VAL	N-CA-C	5.80	116.00	108.35
1	A	260	LEU	N-CA-C	5.78	118.65	110.50
1	A	178	PHE	N-CA-C	-5.76	106.23	113.20
1	A	284	ILE	N-CA-C	5.68	116.41	110.62
1	A	257	VAL	CB-CA-C	5.66	116.52	111.71
1	A	350	PHE	N-CA-C	-5.51	105.27	111.28
3	B	335	ARG	N-CA-C	5.46	122.44	110.80
1	A	369	LYS	N-CA-C	-5.40	106.56	114.39
1	A	343	ARG	N-CA-C	5.29	117.96	111.82
1	A	194	GLU	N-CA-C	-5.19	106.97	113.72
2	C	72	ARG	N-CA-C	5.06	118.45	109.96

There are no chirality outliers.

There are no planarity outliers.

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	2809	0	2810	42	0
2	C	597	0	626	16	0
3	B	2894	0	2869	58	0
4	A	31	13	13	3	0
5	A	14	8	9	0	0
6	A	55	0	0	2	0
6	B	71	0	0	6	0
6	C	8	0	0	1	0
All	All	6479	21	6327	111	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 9.

All (111) 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)
3:B:31:PHE:HZ	3:B:89:THR:HG22	1.25	1.00
3:B:85:ILE:O	3:B:89:THR:HG23	1.72	0.88
1:A:358:MET:HA	3:B:351:THR:HG21	1.55	0.88
2:C:24:GLU:HG3	2:C:52:ASP:HB3	1.56	0.86
3:B:31:PHE:CZ	3:B:89:THR:HG22	2.13	0.84
2:C:22:THR:HG23	2:C:25:ASN:H	1.44	0.82
2:C:55:THR:HG23	2:C:58:ASP:H	1.45	0.81
3:B:210:ARG:HG3	6:B:467:HOH:O	1.88	0.74
3:B:153:MET:HE2	3:B:299:LEU:HD22	1.71	0.72
1:A:354:ILE:HD13	3:B:355:MET:HG2	1.72	0.70
3:B:106:THR:HG23	3:B:137:GLN:HG3	1.74	0.70
1:A:28:ILE:HD12	1:A:49:TYR:HB2	1.72	0.70
3:B:305:MET:HE2	3:B:336:LYS:HB2	1.74	0.68
3:B:104:LEU:HD12	3:B:105:LEU:N	2.09	0.67
1:A:234:VAL:HB	4:A:401:ANP:H2'	1.75	0.66
2:C:24:GLU:CG	2:C:52:ASP:HB3	2.26	0.66
1:A:167:THR:HG22	1:A:169:ASP:H	1.61	0.66
1:A:272:THR:O	1:A:276:GLU:HG2	1.97	0.64
2:C:22:THR:O	2:C:26:VAL:HG23	1.97	0.64
3:B:104:LEU:HD21	3:B:346:LEU:HD23	1.81	0.63
2:C:63:LYS:HG2	2:C:64:GLU:HG2	1.80	0.62
1:A:212:ALA:HB2	1:A:231:VAL:HG22	1.82	0.62
1:A:234:VAL:HB	4:A:401:ANP:C2'	2.30	0.61
3:B:105:LEU:HD11	3:B:123:MET:HE3	1.84	0.60
1:A:350:PHE:O	1:A:354:ILE:HG13	2.01	0.60
3:B:153:MET:HE2	3:B:299:LEU:CD2	2.31	0.60
3:B:131:ALA:HB1	3:B:356:TRP:HB3	1.84	0.59
1:A:218:LYS:HG2	4:A:401:ANP:O2A	2.02	0.59
1:A:285:GLU:HG3	1:A:328:ILE:HA	1.85	0.57
3:B:95:ARG:NH2	6:B:404:HOH:O	2.33	0.57
3:B:32:PRO:HB2	3:B:34:ILE:HG13	1.87	0.57
3:B:300:SER:H	3:B:304:THR:HG21	1.71	0.56
3:B:95:ARG:NE	6:B:404:HOH:O	2.27	0.55
3:B:35:VAL:HG22	3:B:54:VAL:HG22	1.89	0.54
3:B:137:GLN:HG2	3:B:339:VAL:HG11	1.90	0.54
2:C:55:THR:HG23	2:C:58:ASP:N	2.20	0.54
2:C:23:ILE:HB	2:C:52:ASP:HA	1.89	0.53
1:A:298:SER:O	1:A:302:GLU:HB2	2.08	0.53
1:A:159:VAL:HG23	2:C:47:GLY:HA3	1.89	0.53
2:C:55:THR:CG2	2:C:58:ASP:H	2.18	0.53
3:B:104:LEU:HD12	3:B:104:LEU:C	2.34	0.53
3:B:11:ASP:OD1	3:B:106:THR:HG21	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG21	1:A:67:ILE:HG21	1.91	0.52
3:B:106:THR:HG23	3:B:137:GLN:CG	2.38	0.52
1:A:79:ALA:O	1:A:83:ILE:HG13	2.09	0.52
1:A:222:PRO:HG2	1:A:352:LEU:HD11	1.90	0.52
3:B:50:LYS:C	3:B:50:LYS:HD2	2.35	0.52
1:A:354:ILE:HD12	1:A:355:GLN:N	2.26	0.51
1:A:358:MET:HA	3:B:351:THR:CG2	2.35	0.50
3:B:213:LYS:HA	3:B:217:CYS:SG	2.51	0.50
3:B:42:GLY:O	3:B:45:VAL:HG12	2.11	0.50
1:A:87:CYS:O	1:A:91:GLU:HG3	2.12	0.50
3:B:153:MET:CE	3:B:299:LEU:HD22	2.38	0.49
2:C:24:GLU:CD	2:C:52:ASP:HB3	2.37	0.49
3:B:311:ASP:O	6:B:401:HOH:O	2.20	0.49
3:B:8:LEU:HG	3:B:101:HIS:HB3	1.95	0.49
1:A:240:ASN:OD1	1:A:242:LYS:HE2	2.14	0.48
2:C:22:THR:HG22	2:C:25:ASN:HB2	1.96	0.47
2:C:42:ARG:HG3	2:C:72:ARG:HD2	1.96	0.47
3:B:62:ARG:HB3	3:B:67:LEU:HD11	1.96	0.47
3:B:318:THR:HA	3:B:327:ILE:CD1	2.45	0.47
1:A:85:ASP:O	1:A:89:LYS:HD2	2.15	0.47
3:B:95:ARG:CZ	6:B:404:HOH:O	2.63	0.46
3:B:153:MET:HE2	3:B:153:MET:HB3	1.77	0.46
3:B:31:PHE:CE2	3:B:93:GLU:HG3	2.50	0.46
3:B:101:HIS:O	3:B:103:VAL:HG23	2.15	0.46
3:B:102:PRO:HB3	3:B:131:ALA:HB3	1.98	0.46
3:B:136:ILE:HG13	6:B:405:HOH:O	2.16	0.46
1:A:308:SER:O	1:A:312:ASP:HB2	2.15	0.45
1:A:172:LYS:HE3	1:A:172:LYS:HB3	1.72	0.45
1:A:229:VAL:HB	1:A:230:PRO:HD2	1.99	0.45
6:A:514:HOH:O	3:B:173:HIS:HE1	1.99	0.45
3:B:106:THR:HG23	3:B:137:GLN:OE1	2.16	0.44
3:B:160:THR:HB	3:B:178:LEU:HB3	1.98	0.44
1:A:41:ASP:HB3	1:A:349:VAL:HG21	1.98	0.44
3:B:208:ILE:O	3:B:212:ILE:HG13	2.17	0.44
1:A:352:LEU:O	1:A:355:GLN:HB3	2.18	0.44
1:A:186:GLU:H	1:A:186:GLU:HG3	1.60	0.44
3:B:162:THR:HG21	3:B:277:THR:HG22	2.00	0.44
1:A:46:SER:OG	1:A:83:ILE:HD13	2.18	0.43
1:A:159:VAL:HG12	1:A:160:THR:O	2.18	0.43
2:C:7:THR:O	6:C:101:HOH:O	2.22	0.43
2:C:42:ARG:HB2	2:C:70:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.71	0.42
3:B:213:LYS:HE2	3:B:213:LYS:HB3	1.73	0.42
3:B:94:LEU:O	3:B:96:VAL:HG13	2.19	0.42
1:A:288:VAL:O	1:A:292:ILE:HG12	2.19	0.42
3:B:151:ILE:HG23	3:B:151:ILE:O	2.20	0.42
1:A:266:SER:O	1:A:270:VAL:HG12	2.19	0.42
3:B:294:TYR:CE2	3:B:325:MET:HE3	2.55	0.42
1:A:82:LYS:HE2	1:A:82:LYS:HB3	1.44	0.42
1:A:28:ILE:HD12	1:A:49:TYR:CB	2.46	0.42
3:B:105:LEU:CD1	3:B:123:MET:HE3	2.49	0.41
3:B:241:GLU:HG3	3:B:247:VAL:HG22	2.02	0.41
1:A:40:SER:HG	1:A:71:TYR:HH	1.67	0.41
1:A:42:PHE:CG	1:A:109:LEU:HD11	2.55	0.41
3:B:173:HIS:CD2	3:B:173:HIS:H	2.39	0.41
2:C:40:GLN:HG2	2:C:40:GLN:O	2.20	0.41
3:B:32:PRO:HB2	3:B:34:ILE:CD1	2.50	0.41
3:B:48:GLY:C	3:B:50:LYS:H	2.29	0.41
3:B:303:THR:O	3:B:303:THR:HG22	2.21	0.41
1:A:290:GLN:HG3	6:A:553:HOH:O	2.21	0.41
1:A:361:GLU:OE1	3:B:351:THR:HG22	2.21	0.41
1:A:139:ASP:C	1:A:141:SER:H	2.27	0.41
3:B:15:GLY:H	3:B:157:ASP:HB2	1.86	0.41
3:B:105:LEU:HD11	3:B:123:MET:CE	2.50	0.41
1:A:196:TYR:HB3	1:A:197:PRO:HD3	2.02	0.40
1:A:155:PRO:HD2	1:A:158:ALA:HB2	2.03	0.40
1:A:180:MET:HE2	1:A:180:MET:HB2	1.72	0.40
3:B:326:LYS:HD2	3:B:326:LYS:H	1.85	0.40
3:B:70:PRO:HB2	3:B:82:MET:HE2	2.04	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	344/352 (98%)	331 (96%)	13 (4%)	0	100	100
2	C	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
3	B	369/375 (98%)	353 (96%)	16 (4%)	0	100	100
All	All	786/803 (98%)	753 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/326 (98%)	290 (91%)	30 (9%)	8	16
2	C	68/68 (100%)	64 (94%)	4 (6%)	18	33
3	B	314/318 (99%)	294 (94%)	20 (6%)	16	29
All	All	702/712 (99%)	648 (92%)	54 (8%)	12	22

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	29	SER
1	A	58	LYS
1	A	77	LYS
1	A	92	SER
1	A	101	ARG
1	A	111	SER
1	A	115	ASP
1	A	132	SER
1	A	134	ILE
1	A	139	ASP
1	A	141	SER
1	A	186	GLU
1	A	198	LYS
1	A	209	THR

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Mol	Chain	Res	Type
1	A	225	THR
1	A	232	ARG
1	A	251	LYS
1	A	270	VAL
1	A	279	LYS
1	A	281	ASP
1	A	290	GLN
1	A	302	GLU
1	A	310	VAL
1	A	344	LYS
1	A	352	LEU
1	A	354	ILE
1	A	361	GLU
1	A	362	LEU
1	A	369	LYS
2	C	15	LEU
2	C	62	GLN
2	C	64	GLU
2	C	70	VAL
3	B	5	ILE
3	B	10	ILE
3	B	43	VAL
3	B	50	LYS
3	B	59	GLN
3	B	66	THR
3	B	94	LEU
3	B	104	LEU
3	B	106	THR
3	B	162	THR
3	B	185	LEU
3	B	186	THR
3	B	196	ARG
3	B	209	VAL
3	B	238	LYS
3	B	242	LEU
3	B	244	ASP
3	B	249	THR
3	B	267	LEU
3	B	323	SER

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	74	GLN
1	A	90	ASN
1	A	290	GLN
2	C	62	GLN
3	B	73	HIS
3	B	173	HIS
3	B	263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	AR6	A	402	-	14,14,39	1.07	1 (7%)	19,21,60	1.31	2 (10%)
4	ANP	A	401	-	33,33,33	1.98	11 (33%)	45,52,52	2.06	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AR6	A	402	-	-	4/6/22/54	0/1/1/4
4	ANP	A	401	-	-	8/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ANP	PB-N3B	4.23	1.74	1.63
4	A	401	ANP	C5-C4	4.12	1.46	1.39
4	A	401	ANP	PG-N3B	4.09	1.74	1.63
4	A	401	ANP	PB-O1B	3.58	1.51	1.46
4	A	401	ANP	C5-N7	-3.18	1.33	1.39
5	A	402	AR6	PB-O2B	2.90	1.59	1.50
4	A	401	ANP	PG-O1G	2.70	1.50	1.46
4	A	401	ANP	PB-O2B	-2.66	1.49	1.56
4	A	401	ANP	C5-C6	2.38	1.47	1.41
4	A	401	ANP	PG-O2G	-2.31	1.50	1.56
4	A	401	ANP	PG-O3G	-2.21	1.50	1.56
4	A	401	ANP	PB-O3A	2.08	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ANP	C5-C4-N3	-5.96	118.51	126.72
4	A	401	ANP	N3-C4-N9	4.54	134.88	127.17
5	A	402	AR6	C1D-C2D-C3D	3.89	107.08	102.29
4	A	401	ANP	C4-C5-N7	-3.85	106.18	110.58
4	A	401	ANP	C2-N3-C4	3.84	121.20	111.83
4	A	401	ANP	O2B-PB-O1B	3.78	117.97	109.87
4	A	401	ANP	N3-C2-N1	-3.65	123.06	128.58
4	A	401	ANP	O1G-PG-N3B	-3.43	106.73	111.77
4	A	401	ANP	C5-N7-C8	3.31	108.66	103.45
5	A	402	AR6	O3A-PB-O1B	2.76	118.14	107.80
4	A	401	ANP	O2G-PG-O3G	2.69	114.82	107.59
4	A	401	ANP	O2B-PB-O3A	2.53	113.10	104.64
4	A	401	ANP	N9-C8-N7	-2.33	110.64	113.94
4	A	401	ANP	C2-N1-C6	2.14	122.25	118.73
4	A	401	ANP	C4-N9-C8	2.07	107.91	105.74
4	A	401	ANP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ANP	PB-N3B-PG-O1G
4	A	401	ANP	PG-N3B-PB-O1B
4	A	401	ANP	C5'-O5'-PA-O1A
4	A	401	ANP	C5'-O5'-PA-O3A
5	A	402	AR6	O4D-C4D-C5D-O5D
4	A	401	ANP	O4'-C4'-C5'-O5'
4	A	401	ANP	C3'-C4'-C5'-O5'
5	A	402	AR6	C3D-C4D-C5D-O5D
5	A	402	AR6	C5D-O5D-PB-O2B
5	A	402	AR6	C4D-C5D-O5D-PB
4	A	401	ANP	PA-O3A-PB-O2B
4	A	401	ANP	C4'-C5'-O5'-PA

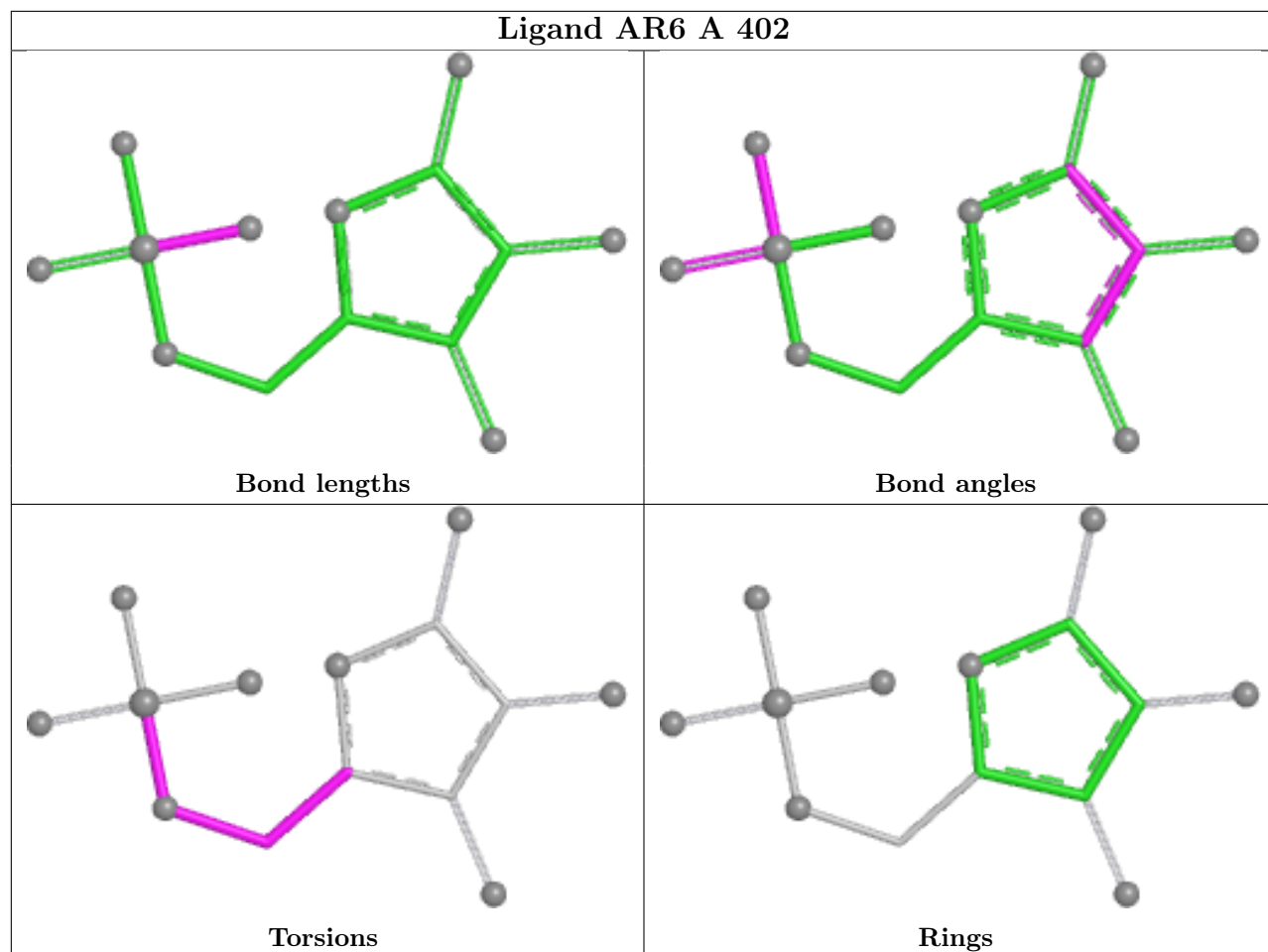
There are no ring outliers.

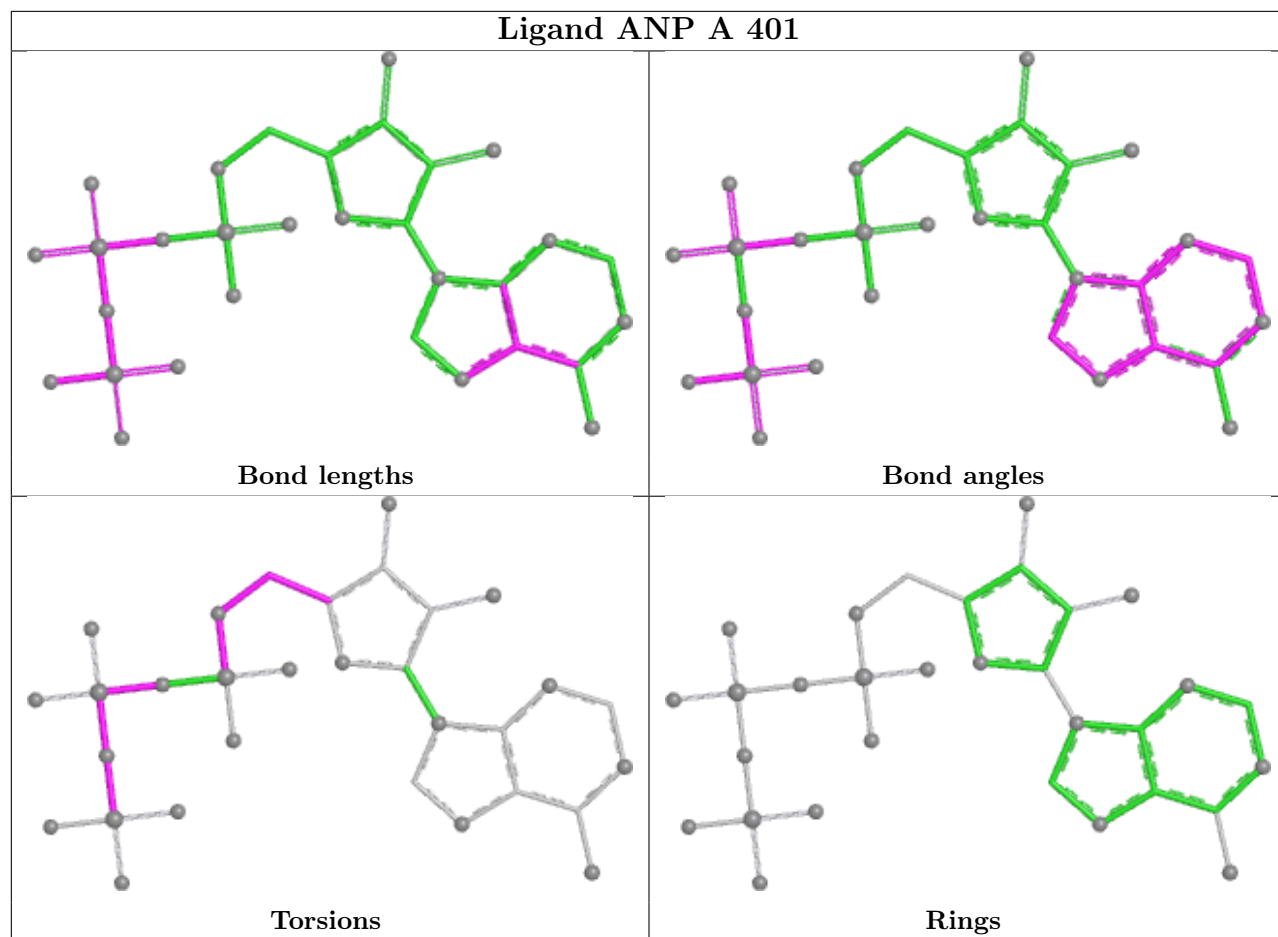
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	ANP	3	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.

Ligand AR6 A 402





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	346/352 (98%)	0.18	10 (2%) 53 52	8, 20, 46, 78	0
2	C	75/76 (98%)	0.59	3 (4%) 42 40	14, 35, 55, 58	0
3	B	371/375 (98%)	0.05	11 (2%) 52 50	6, 19, 42, 63	0
All	All	792/803 (98%)	0.16	24 (3%) 52 50	6, 21, 49, 78	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	49	GLN	3.7
3	B	5	ILE	3.7
3	B	13	GLY	3.3
1	A	56	LYS	3.1
3	B	157	ASP	2.9
1	A	368	ASN	2.7
3	B	51	ASP	2.6
1	A	54	LEU	2.5
3	B	375	PHE	2.5
3	B	50	LYS	2.5
2	C	20	SER	2.4
1	A	148	ASP	2.4
1	A	55	GLY	2.4
2	C	1	MET	2.3
3	B	241	GLU	2.3
3	B	324	THR	2.3
1	A	115	ASP	2.3
1	A	370	GLU	2.3
3	B	242	LEU	2.2
3	B	16	MET	2.2
1	A	200	ASP	2.1
1	A	369	LYS	2.1
1	A	367	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	49	GLN	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](#)

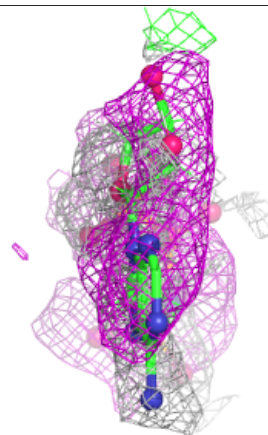
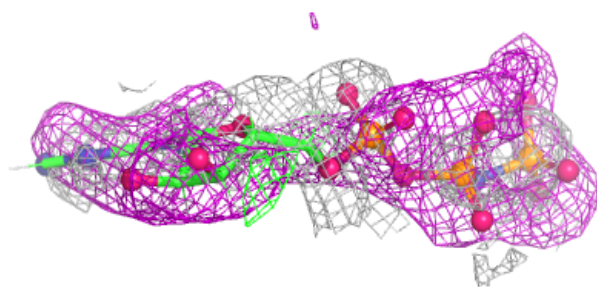
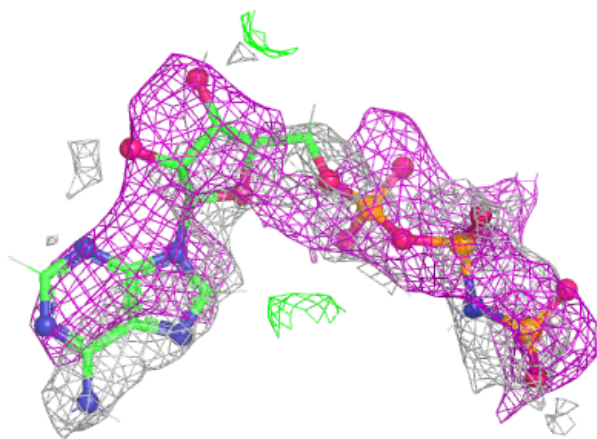
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ANP	A	401	31/31	0.66	0.20	30,50,66,92	0
5	AR6	A	402	14/36	0.90	0.19	9,33,39,44	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.

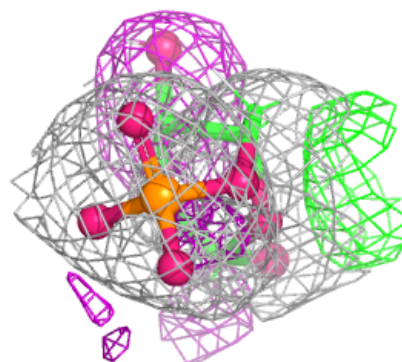
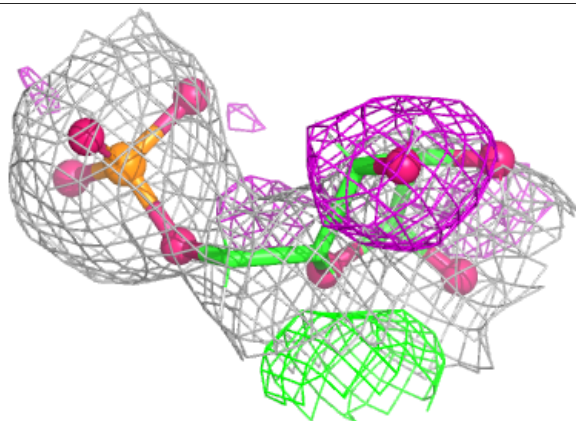
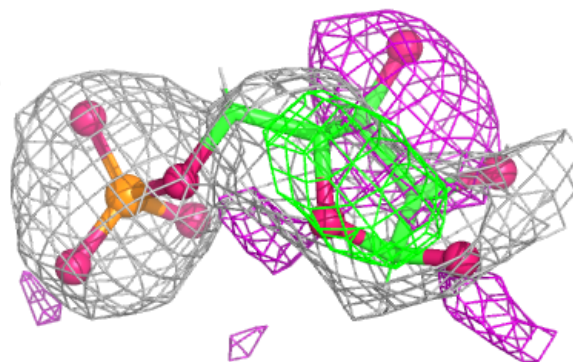
Electron density around ANP A 401:

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



Electron density around AR6 A 402:

$2mF_o-DF_c$ (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.