



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:37 AM UTC

PDB ID : 2A19 / pdb_00002a19
Title : PKR kinase domain- eIF2alpha- AMP-PNP complex.
Authors : Dar, A.C.; Dever, T.E.; Sicheri, F.
Deposited on : 2005-06-19
Resolution : 2.50 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

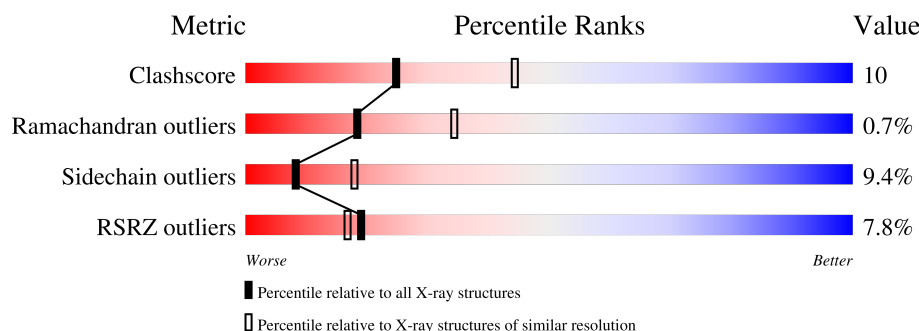
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
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	175	2% 73% 19% • 6%
2	B	284	4% 71% 19% • 7%
2	C	284	12% 50% 18% • 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5216 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 Eukaryotic translation initiation factor 2 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1342	862	220	254	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P20459
A	2	SER	-	cloning artifact	UNP P20459

- Molecule 2 is a protein called Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	P	S	0	0
			2137	1363	366	400	1	7		
2	C	203	Total	C	N	O	S	0	0	0
			1594	1027	265	297	5			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	cloning artifact	UNP P19525
B	256	ALA	-	cloning artifact	UNP P19525
B	257	HIS	-	cloning artifact	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	LEU	deletion	UNP P19525
B	?	-	GLU	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525

Continued on next page...

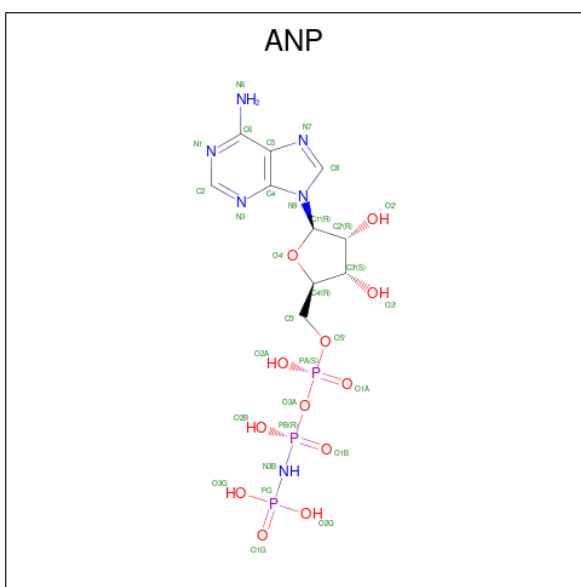
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	PRO	deletion	UNP P19525
B	?	-	GLU	deletion	UNP P19525
B	?	-	ASN	deletion	UNP P19525
B	412	ASN	HIS	engineered mutation	UNP P19525
B	446	TPO	THR	modified residue	UNP P19525
B	551	ALA	CYS	engineered mutation	UNP P19525
C	255	GLY	-	cloning artifact	UNP P19525
C	256	ALA	-	cloning artifact	UNP P19525
C	257	HIS	-	cloning artifact	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	LEU	deletion	UNP P19525
C	?	-	GLU	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	TYR	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	PRO	deletion	UNP P19525
C	?	-	GLU	deletion	UNP P19525
C	?	-	ASN	deletion	UNP P19525
C	412	ASN	HIS	engineered mutation	UNP P19525
C	446	TPO	THR	modified residue	UNP P19525
C	551	ALA	CYS	engineered mutation	UNP P19525

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

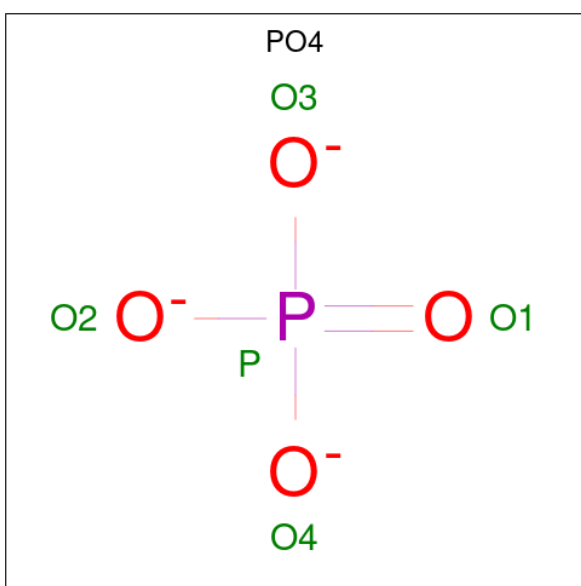
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

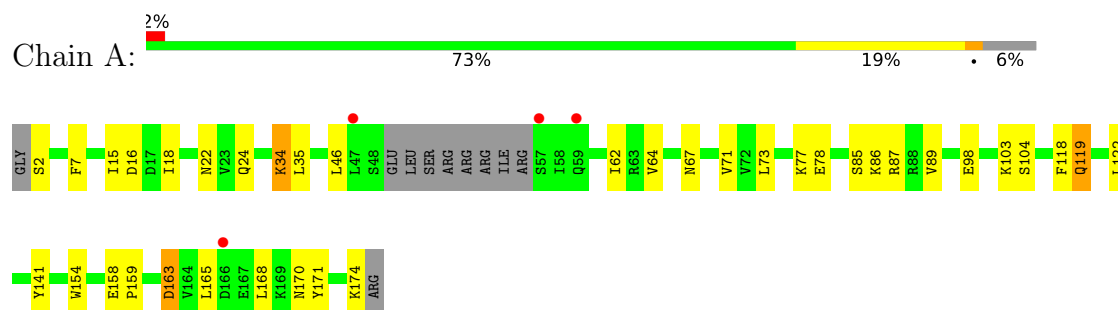
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	33	Total 33	O 33	0	0
6	C	7	Total 7	O 7	0	0

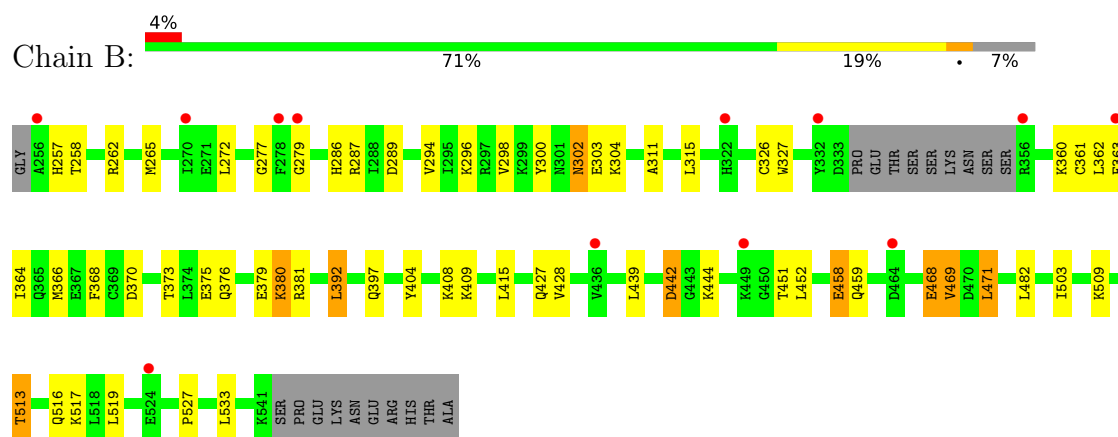
3 Residue-property plots [i](#)

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.

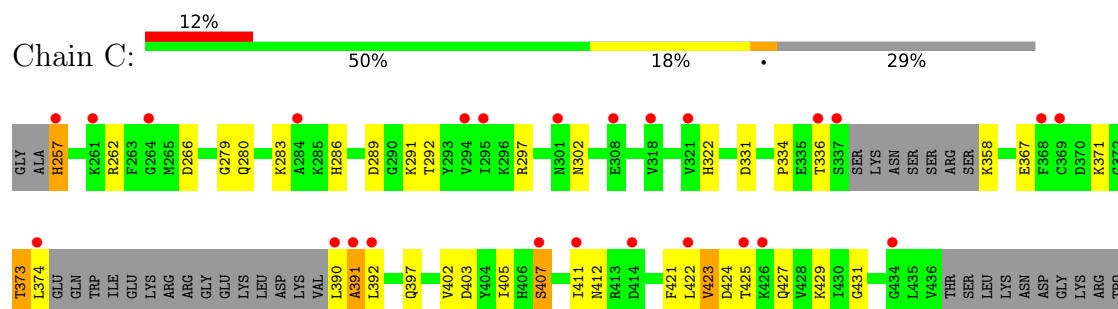
- Molecule 1: Eukaryotic translation initiation factor 2 alpha subunit

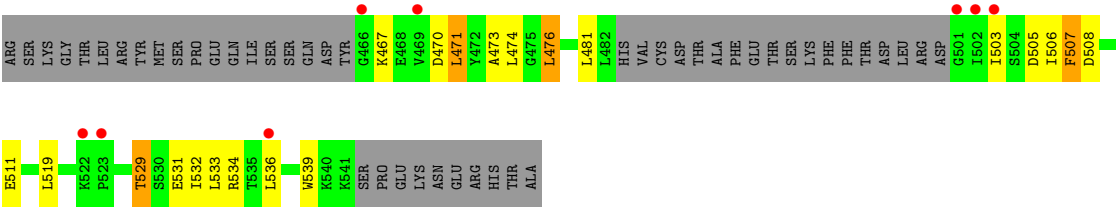


- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase



- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.66Å 48.75Å 133.43Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	27.33 – 2.50 27.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.33-2.50) 94.6 (27.33-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.228 , 0.286 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.7	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	0.92	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: ANP, PO4, TPO, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/1366	0.92	0/1839
2	B	0.65	0/2161	0.90	1/2895 (0.0%)
2	C	0.55	0/1618	0.88	1/2174 (0.0%)
All	All	0.63	0/5145	0.90	2/6908 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	279	GLY	N-CA-C	6.21	118.35	110.96
2	B	279	GLY	N-CA-C	5.18	117.86	110.46

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	1342	0	1350	24	0
2	B	2137	0	2160	35	0
2	C	1594	0	1588	37	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	B	31	0	13	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	31	0	13	0	0
5	C	5	0	0	0	0
6	A	32	0	0	0	0
6	B	33	0	0	1	0
6	C	7	0	0	0	0
All	All	5216	0	5124	101	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 10.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:PHE:H	2:C:507:PHE:HD1	1.04	1.01
4:B:1640:ANP:HNB1	4:B:1640:ANP:H5'2	1.33	0.93
2:B:373:THR:H	2:B:376:GLN:HE21	1.22	0.85
4:B:1640:ANP:HNB1	4:B:1640:ANP:C5'	1.90	0.83
4:B:1640:ANP:H5'2	4:B:1640:ANP:N3B	1.92	0.83
1:A:119:GLN:HE21	1:A:119:GLN:HA	1.44	0.81
4:B:1640:ANP:H8	4:B:1640:ANP:O5'	1.86	0.75
2:B:286:HIS:HD2	2:B:289:ASP:H	1.36	0.71
2:B:397:GLN:HE22	2:B:427:GLN:HA	1.56	0.71
2:C:507:PHE:CD1	2:C:507:PHE:N	2.55	0.64
1:A:15:ILE:O	1:A:16:ASP:HB2	1.96	0.64
2:C:507:PHE:HD1	2:C:507:PHE:N	1.85	0.64
2:C:322:HIS:HB3	2:C:367:GLU:HB3	1.80	0.63
2:B:300:TYR:HB2	2:B:362:LEU:HB2	1.79	0.62
2:B:366:MET:HE2	4:B:1640:ANP:HN61	1.64	0.62
2:B:381:ARG:HB3	6:B:59:HOH:O	1.99	0.61
2:B:503:ILE:HG13	2:B:516:GLN:HG2	1.83	0.61
2:C:424:ASP:OD1	2:C:425:THR:N	2.35	0.59
2:C:529:THR:HA	2:C:532:ILE:HD12	1.83	0.59
1:A:2:SER:N	1:A:122:LEU:H	2.01	0.59
2:B:509:LYS:O	2:B:513:THR:HG23	2.03	0.58
2:B:442:ASP:HB3	2:B:444:LYS:H	1.68	0.58
2:C:507:PHE:HB2	2:C:511:GLU:OE2	2.04	0.58
2:C:331:ASP:O	2:C:358:LYS:HA	2.03	0.57
2:B:262:ARG:HG2	2:B:327:TRP:CD1	2.40	0.56
2:C:390:LEU:HG	2:C:391:ALA:H	1.69	0.56
1:A:119:GLN:HE21	1:A:119:GLN:CA	2.17	0.56
2:C:397:GLN:HE22	2:C:427:GLN:HA	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:GLN:HE21	2:C:297:ARG:HH11	1.52	0.56
2:C:286:HIS:CD2	2:C:289:ASP:H	2.24	0.55
4:B:1640:ANP:C5'	4:B:1640:ANP:N3B	2.60	0.54
2:B:368:PHE:CE2	2:B:370:ASP:HB3	2.42	0.54
2:C:286:HIS:HD2	2:C:289:ASP:H	1.55	0.54
2:C:390:LEU:C	2:C:392:LEU:H	2.15	0.53
2:C:423:VAL:HG23	2:C:427:GLN:HB3	1.89	0.53
2:C:473:ALA:O	2:C:476:LEU:HB2	2.10	0.51
1:A:171:TYR:O	1:A:174:LYS:HG2	2.09	0.51
2:B:326:CYS:HA	2:B:363:PHE:O	2.10	0.51
1:A:154:TRP:HH2	1:A:168:LEU:HD11	1.75	0.51
2:B:458:GLU:CD	2:B:458:GLU:H	2.19	0.51
2:B:517:LYS:HB3	2:B:527:PRO:HD3	1.93	0.51
1:A:22:ASN:HD22	1:A:67:ASN:ND2	2.09	0.50
2:B:409:LYS:HD2	2:B:439:LEU:HD23	1.93	0.50
2:B:392:LEU:HD13	2:B:482:LEU:HD21	1.93	0.50
2:B:397:GLN:NE2	2:B:428:VAL:H	2.10	0.49
2:B:404:TYR:O	2:B:408:LYS:HG2	2.12	0.49
1:A:18:ILE:HD13	1:A:71:VAL:HG22	1.94	0.49
2:C:402:VAL:HA	2:C:405:ILE:HD12	1.94	0.49
2:C:471:LEU:HA	2:C:474:LEU:HD12	1.95	0.49
2:C:291:LYS:HG2	2:C:292:THR:N	2.28	0.48
2:C:423:VAL:HG11	2:C:429:LYS:HD2	1.95	0.48
2:B:265:MET:O	2:B:287:ARG:HD2	2.13	0.48
2:B:257:HIS:CE1	2:B:272:LEU:HD22	2.48	0.48
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.22	0.48
2:C:291:LYS:HG2	2:C:292:THR:H	1.78	0.48
1:A:22:ASN:HD22	1:A:67:ASN:HD22	1.60	0.47
1:A:24:GLN:NE2	1:A:34:LYS:HD3	2.29	0.47
2:C:280:GLN:NE2	2:C:297:ARG:HH11	2.12	0.47
1:A:86:LYS:O	1:A:87:ARG:C	2.55	0.47
1:A:154:TRP:CH2	1:A:168:LEU:CD1	2.97	0.47
1:A:159:PRO:HG3	1:A:165:LEU:HB2	1.95	0.47
2:B:380:LYS:HA	2:B:380:LYS:HE3	1.97	0.47
2:C:297:ARG:HD3	2:C:334:PRO:HG3	1.97	0.47
2:C:411:ILE:HG13	2:C:411:ILE:O	2.15	0.47
2:B:468:GLU:CD	2:B:468:GLU:H	2.22	0.47
1:A:154:TRP:CH2	1:A:168:LEU:HD11	2.50	0.46
2:B:311:ALA:O	2:B:315:LEU:HG	2.16	0.46
2:B:302:ASN:O	2:B:304:LYS:N	2.49	0.46
2:B:302:ASN:HD22	2:B:302:ASN:N	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:HIS:HD2	2:C:289:ASP:N	2.13	0.45
1:A:103:LYS:HG2	1:A:141:TYR:CG	2.51	0.45
2:C:531:GLU:HA	2:C:534:ARG:HD2	1.98	0.45
1:A:24:GLN:CD	1:A:34:LYS:HD3	2.42	0.45
1:A:103:LYS:HG2	1:A:141:TYR:CD2	2.51	0.45
2:B:459:GLN:HB2	2:B:469:VAL:HG22	1.99	0.45
2:C:421:PHE:CE1	2:C:431:GLY:HA3	2.52	0.44
2:B:262:ARG:NH2	2:C:266:ASP:OD1	2.48	0.44
1:A:71:VAL:HG23	1:A:89:VAL:HG22	1.99	0.44
2:B:373:THR:H	2:B:376:GLN:NE2	2.02	0.44
4:B:1640:ANP:HNB1	4:B:1640:ANP:H5'1	1.79	0.43
2:C:257:HIS:O	2:C:297:ARG:NH2	2.35	0.43
1:A:15:ILE:O	1:A:16:ASP:CB	2.65	0.43
2:B:366:MET:HE2	4:B:1640:ANP:N6	2.31	0.43
2:C:421:PHE:HE1	2:C:431:GLY:HA3	1.82	0.43
1:A:118:PHE:CE2	1:A:163:ASP:HB3	2.54	0.43
2:B:468:GLU:HA	2:B:471:LEU:HD22	2.01	0.43
2:B:262:ARG:HG2	2:B:327:TRP:NE1	2.33	0.43
1:A:87:ARG:C	1:A:89:VAL:H	2.27	0.42
2:C:539:TRP:CD1	2:C:539:TRP:N	2.87	0.42
2:B:375:GLU:O	2:B:379:GLU:HG3	2.19	0.42
2:B:370:ASP:OD1	2:B:370:ASP:N	2.50	0.42
1:A:7:PHE:CD2	1:A:104:SER:HB3	2.55	0.42
1:A:73:LEU:HD11	1:A:85:SER:HB2	2.01	0.42
2:C:411:ILE:CG2	2:C:467:LYS:HB3	2.50	0.41
2:C:403:ASP:O	2:C:407:SER:HB2	2.20	0.41
2:C:467:LYS:HD3	2:C:467:LYS:H	1.85	0.41
2:B:302:ASN:HD22	2:B:302:ASN:H	1.68	0.41
2:C:373:THR:HG23	2:C:374:LEU:N	2.35	0.41
2:B:296:LYS:HB3	2:B:364:ILE:HB	2.02	0.41
2:C:412:ASN:O	2:C:470:ASP:OD1	2.39	0.41
2:C:373:THR:CG2	2:C:374:LEU:N	2.84	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	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	B	259/284 (91%)	250 (96%)	7 (3%)	2 (1%)	16	31
2	C	193/284 (68%)	177 (92%)	14 (7%)	2 (1%)	12	24
All	All	613/743 (82%)	578 (94%)	31 (5%)	4 (1%)	18	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	303	GLU
2	B	277	GLY
2	C	371	LYS
2	C	391	ALA

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	149/161 (92%)	137 (92%)	12 (8%)	11	23
2	B	232/254 (91%)	213 (92%)	19 (8%)	10	23
2	C	170/254 (67%)	149 (88%)	21 (12%)	4	9
All	All	551/669 (82%)	499 (91%)	52 (9%)	8	18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	35	LEU
1	A	46	LEU
1	A	62	ILE
1	A	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	77	LYS
1	A	78	GLU
1	A	98	GLU
1	A	119	GLN
1	A	158	GLU
1	A	163	ASP
1	A	170	ASN
2	B	258	THR
2	B	294	VAL
2	B	298	VAL
2	B	302	ASN
2	B	360	LYS
2	B	361	CYS
2	B	380	LYS
2	B	392	LEU
2	B	415	LEU
2	B	442	ASP
2	B	451	THR
2	B	452	LEU
2	B	458	GLU
2	B	468	GLU
2	B	469	VAL
2	B	471	LEU
2	B	513	THR
2	B	519	LEU
2	B	533	LEU
2	C	257	HIS
2	C	262	ARG
2	C	283	LYS
2	C	302	ASN
2	C	336	THR
2	C	373	THR
2	C	407	SER
2	C	422	LEU
2	C	423	VAL
2	C	471	LEU
2	C	476	LEU
2	C	481	LEU
2	C	503	ILE
2	C	505	ASP
2	C	506	ILE
2	C	507	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	508	ASP
2	C	519	LEU
2	C	529	THR
2	C	533	LEU
2	C	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	24	GLN
1	A	119	GLN
2	B	286	HIS
2	B	302	ASN
2	B	319	ASN
2	B	322	HIS
2	B	324	ASN
2	B	376	GLN
2	B	397	GLN
2	C	280	GLN
2	C	286	HIS
2	C	302	ASN
2	C	319	ASN
2	C	322	HIS
2	C	397	GLN
2	C	406	HIS
2	C	528	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	TPO	B	446	2	8,10,11	0.85	0	10,14,16	1.19	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
2	TPO	B	446	2	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	C	901	-	4,4,4	0.89	0	6,6,6	0.59	0
4	ANP	C	2640	3	33,33,33	2.07	10 (30%)	45,52,52	1.88	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	B	1640	3	33,33,33	2.04	9 (27%)	45,52,52	2.13	13 (28%)

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
4	ANP	C	2640	3	-	4/18/38/38	0/3/3/3
4	ANP	B	1640	3	-	3/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2640	ANP	PG-N3B	5.04	1.76	1.63
4	C	2640	ANP	PB-N3B	4.95	1.76	1.63
4	C	2640	ANP	C5-C4	4.69	1.47	1.39
4	B	1640	ANP	C5-C4	4.44	1.47	1.39
4	B	1640	ANP	PG-N3B	4.27	1.74	1.63
4	B	1640	ANP	PB-N3B	4.17	1.74	1.63
4	B	1640	ANP	PG-O1G	4.17	1.52	1.46
4	C	2640	ANP	PB-O1B	3.81	1.51	1.46
4	B	1640	ANP	PB-O1B	3.50	1.51	1.46
4	C	2640	ANP	PG-O1G	3.49	1.51	1.46
4	B	1640	ANP	C5-N7	-2.76	1.34	1.39
4	B	1640	ANP	PA-O3A	2.66	1.62	1.59
4	C	2640	ANP	C5-C6	2.60	1.48	1.41
4	B	1640	ANP	C5-C6	2.45	1.47	1.41
4	C	2640	ANP	C8-N7	2.41	1.36	1.31
4	C	2640	ANP	C5-N7	-2.34	1.34	1.39
4	C	2640	ANP	C4-N9	-2.33	1.32	1.37
4	B	1640	ANP	PG-O2G	-2.09	1.51	1.56
4	C	2640	ANP	PG-O2G	-2.06	1.51	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1640	ANP	C5-C4-N3	-6.30	118.04	126.72
4	B	1640	ANP	N3-C4-N9	5.27	136.13	127.17
4	C	2640	ANP	C5-C4-N3	-5.14	119.65	126.72
4	B	1640	ANP	O2B-PB-O1B	5.03	120.65	109.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2640	ANP	N3-C4-N9	4.12	134.17	127.17
4	B	1640	ANP	C2-N3-C4	4.04	121.69	111.83
4	C	2640	ANP	O2B-PB-O1B	3.88	118.20	109.87
4	C	2640	ANP	O1G-PG-N3B	-3.73	106.27	111.77
4	C	2640	ANP	N3-C2-N1	-3.67	123.02	128.58
4	C	2640	ANP	C2-N3-C4	3.63	120.70	111.83
4	B	1640	ANP	N3-C2-N1	-3.59	123.15	128.58
4	B	1640	ANP	O1G-PG-N3B	-3.26	106.97	111.77
4	C	2640	ANP	C4-C5-N7	-3.14	107.00	110.58
4	B	1640	ANP	O2G-PG-O3G	2.99	115.61	107.59
4	C	2640	ANP	C4-N9-C8	2.87	108.75	105.74
4	B	1640	ANP	C4-C5-N7	-2.76	107.43	110.58
4	B	1640	ANP	O3A-PA-O1A	-2.68	102.64	110.70
4	C	2640	ANP	C6-C5-N7	2.44	136.80	132.09
4	B	1640	ANP	C5-N7-C8	2.24	106.97	103.45
4	C	2640	ANP	C2-N1-C6	2.23	122.40	118.73
4	C	2640	ANP	C5-N7-C8	2.21	106.92	103.45
4	B	1640	ANP	C2'-C1'-N9	-2.19	107.86	113.30
4	B	1640	ANP	C4-N9-C8	2.09	107.93	105.74
4	B	1640	ANP	O4'-C1'-N9	2.04	112.01	108.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1640	ANP	PB-N3B-PG-O1G
4	B	1640	ANP	PG-N3B-PB-O1B
4	C	2640	ANP	PG-N3B-PB-O1B
4	C	2640	ANP	PG-N3B-PB-O3A
4	C	2640	ANP	PB-O3A-PA-O2A
4	C	2640	ANP	C4'-C5'-O5'-PA
4	B	1640	ANP	PA-O3A-PB-O1B

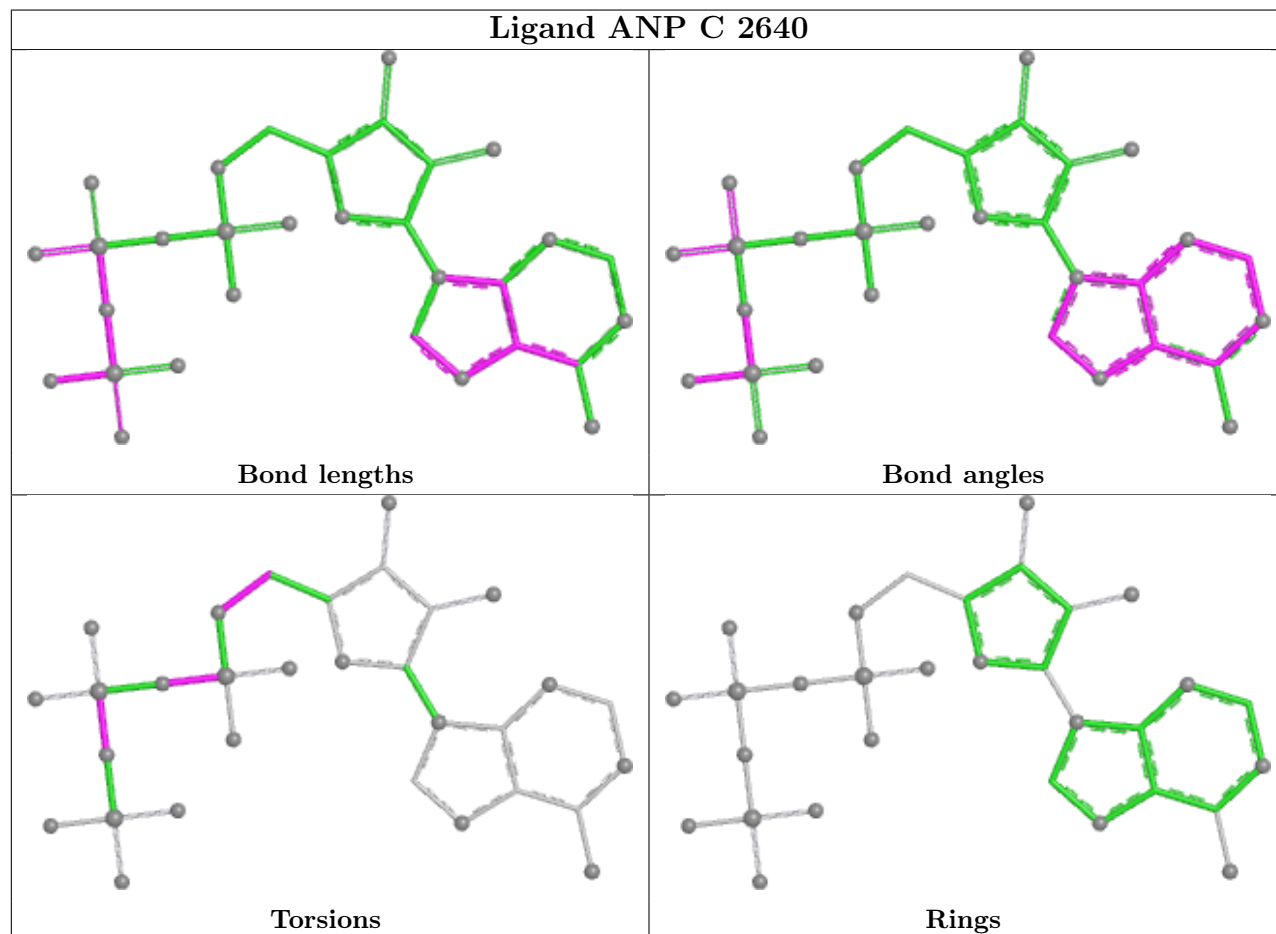
There are no ring outliers.

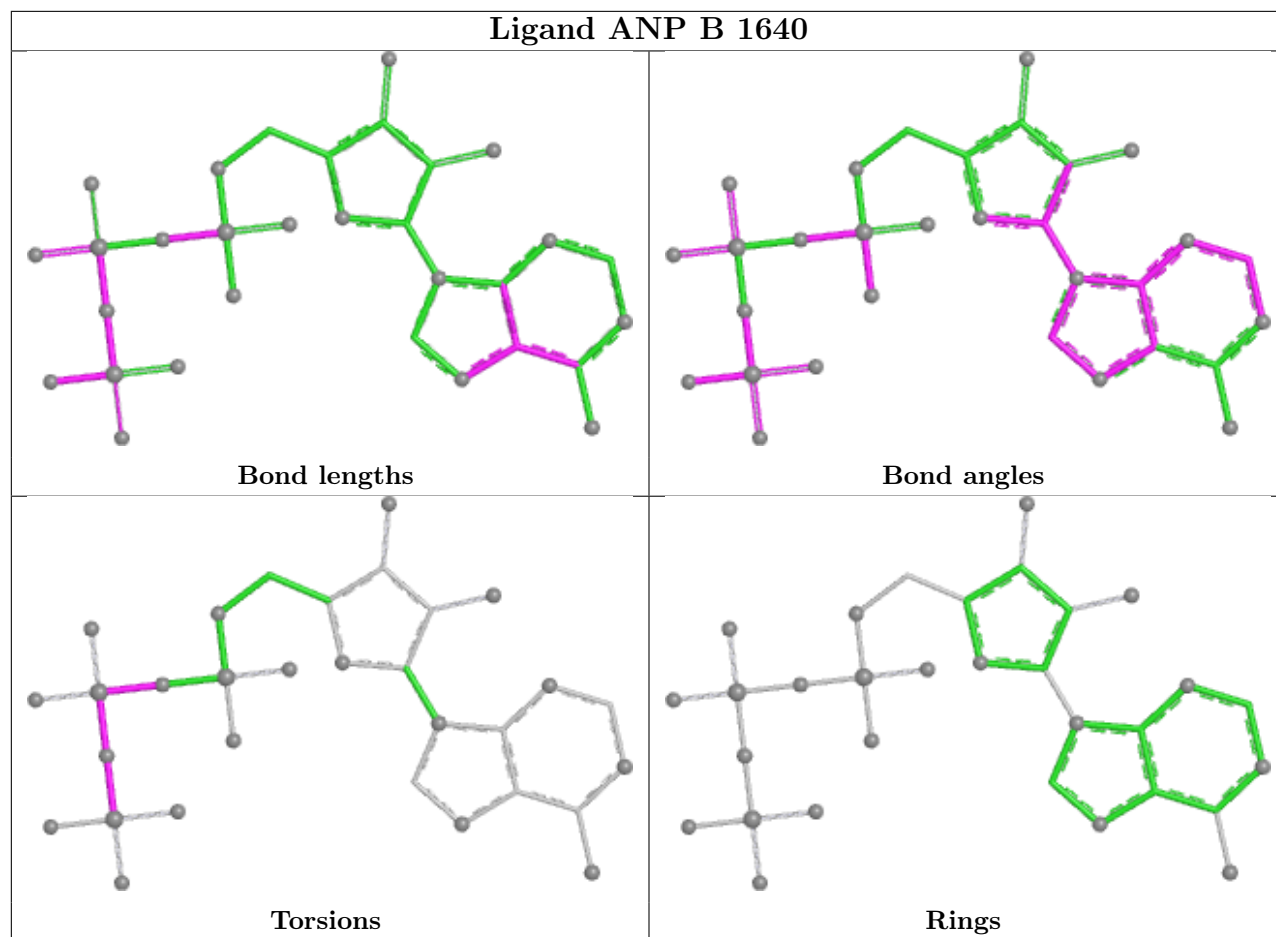
1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1640	ANP	8	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	165/175 (94%)	0.43	4 (2%) 59 55	43, 51, 65, 71	0
2	B	263/284 (92%)	0.58	12 (4%) 37 33	45, 57, 77, 86	0
2	C	203/284 (71%)	1.31	33 (16%) 4 3	52, 67, 79, 82	0
All	All	631/743 (84%)	0.78	49 (7%) 19 17	43, 59, 77, 86	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	390	LEU	6.8
2	C	434	GLY	6.0
2	B	279	GLY	5.2
2	C	501	GLY	4.9
2	C	523	PRO	4.6
1	A	59	GLN	3.8
2	B	278	PHE	3.8
2	C	257	HIS	3.7
2	C	407	SER	3.5
2	C	261	LYS	3.3
2	C	374	LEU	3.1
2	C	294	VAL	3.1
2	C	466	GLY	3.0
2	C	369	CYS	2.9
2	B	449	LYS	2.8
2	C	411	ILE	2.7
2	C	301	ASN	2.7
2	C	318	VAL	2.7
2	C	368	PHE	2.7
2	B	356	ARG	2.7
2	C	536	LEU	2.6
2	C	425	THR	2.6
2	C	414	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	332	TYR	2.6
2	C	391	ALA	2.5
2	C	469	VAL	2.5
2	C	264	GLY	2.5
2	C	308	GLU	2.4
2	C	426	LYS	2.4
2	C	295	ILE	2.4
1	A	57	SER	2.4
2	C	502	ILE	2.4
2	C	321	VAL	2.3
2	C	392	LEU	2.3
2	B	524	GLU	2.3
2	C	503	ILE	2.2
2	B	436	VAL	2.2
2	B	322	HIS	2.2
2	B	464	ASP	2.2
2	B	256	ALA	2.2
2	B	270	ILE	2.2
1	A	166	ASP	2.2
2	B	363	PHE	2.2
2	C	337	SER	2.1
2	C	522	LYS	2.1
2	C	284	ALA	2.1
1	A	47	LEU	2.1
2	C	336	THR	2.1
2	C	422	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	B	446	11/12	0.93	0.08	51,54,57,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

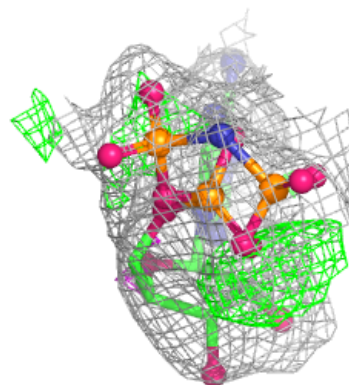
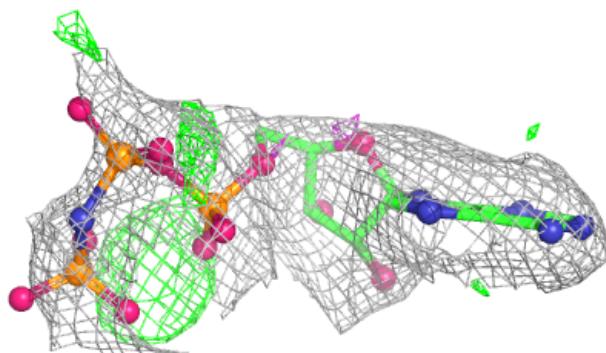
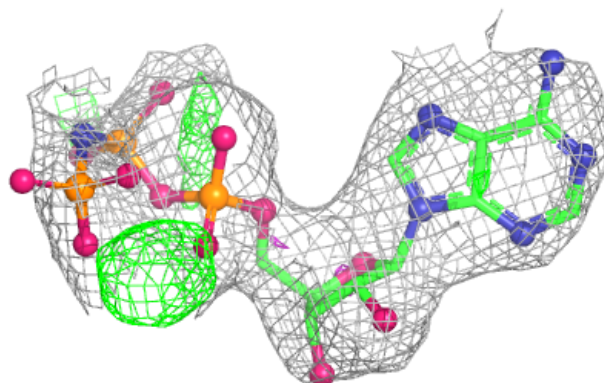
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	C	901	5/5	0.57	0.11	108,108,108,108	0
4	ANP	C	2640	31/31	0.64	0.17	75,77,79,80	12
4	ANP	B	1640	31/31	0.79	0.13	70,76,90,91	0
3	MG	C	2641	1/1	0.85	0.10	75,75,75,75	0
3	MG	B	1641	1/1	0.86	0.16	63,63,63,63	0
3	MG	C	2642	1/1	0.92	0.07	79,79,79,79	0
3	MG	B	1642	1/1	0.95	0.06	44,44,44,44	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.

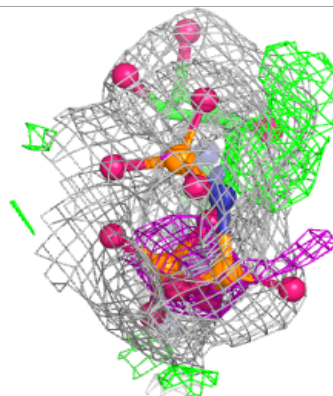
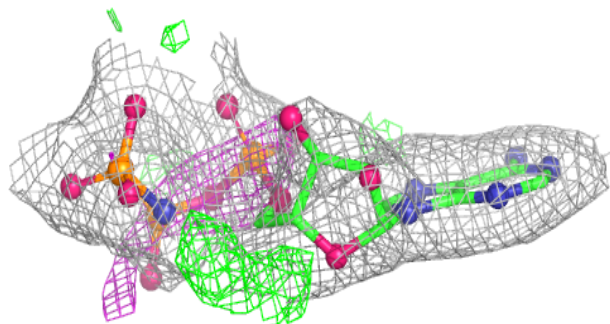
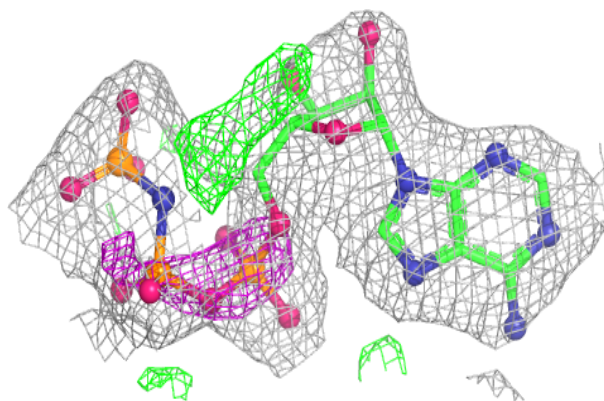
Electron density around ANP C 2640:

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 ANP B 1640:

$2mF_o-DF_c$ (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.