Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 11:21 AM EDT

PDB ID	:	4IPE
Title	:	Crystal structure of mitochondrial Hsp90 (TRAP1) with AMPPNP
Authors	:	Partridge, J.R.; Lavery, L.A.; Agard, D.A.
Deposited on	:	2013-01-09
Resolution	:	2.29 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 (i) 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 (i)) were used in the production of this report:

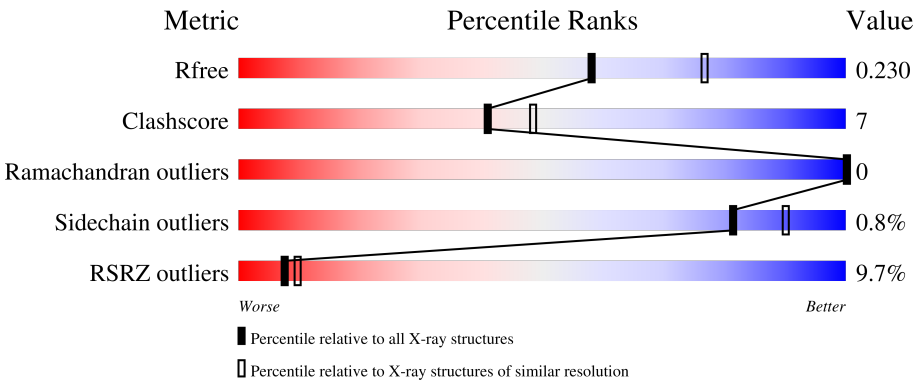
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	719	8% 67% 14% 18%
1	B	719	8% 71% 12% 16%

2 Entry composition (i)

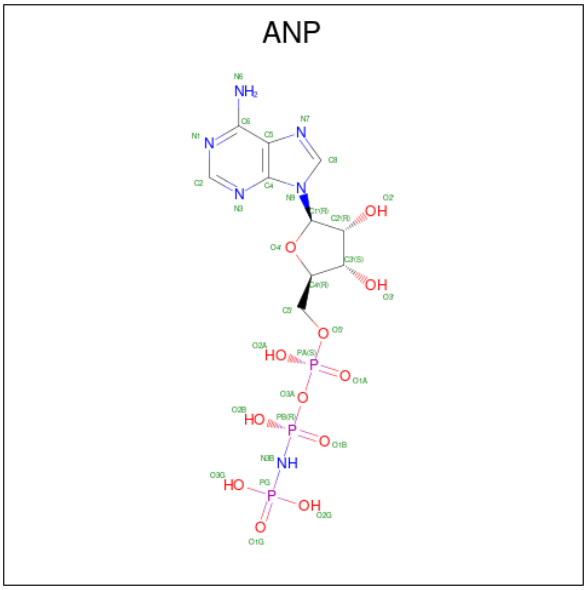
There are 5 unique types of molecules in this entry. The entry contains 9940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4720	2991	816	891	22	0	1	0
1	B	601	4872	3092	841	917	22	0	3	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Co		
4	A	2	2	2	0	0
			Total	Co		
4	B	2	2	2	0	0

- Molecule 5 is water.

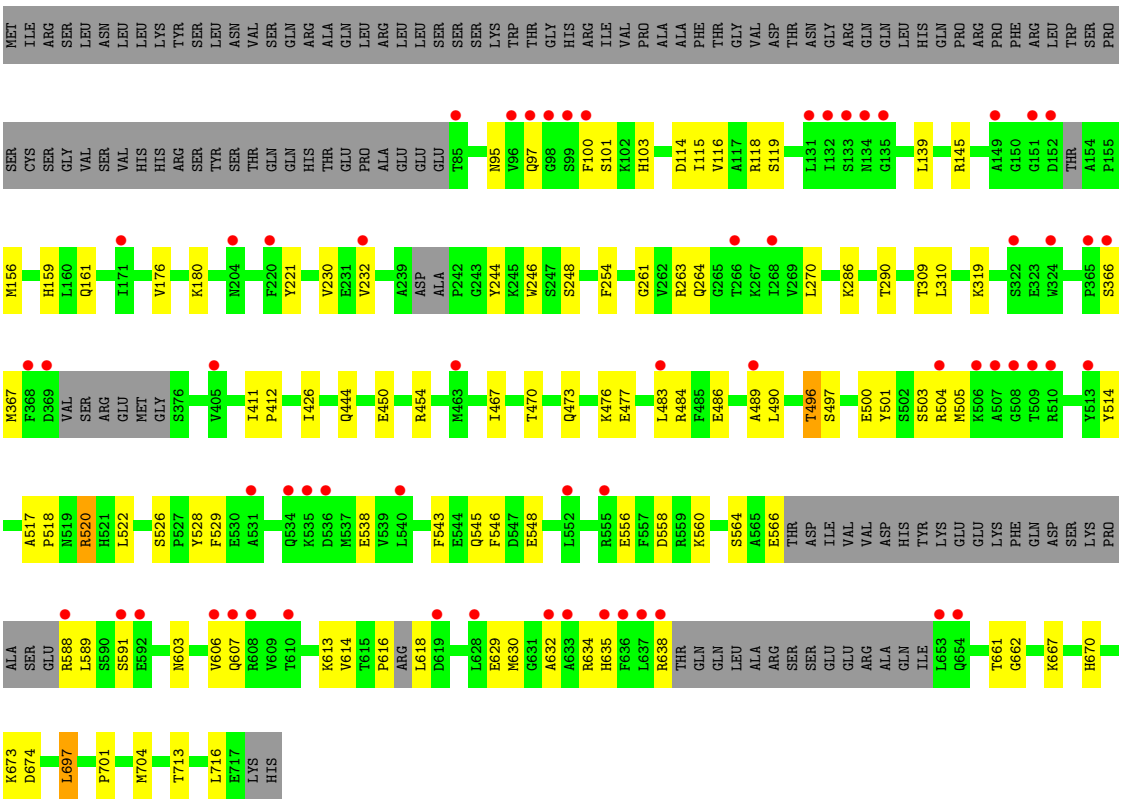
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	132	132	132	0	0
			Total	O		
5	B	148	148	148	0	0

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.

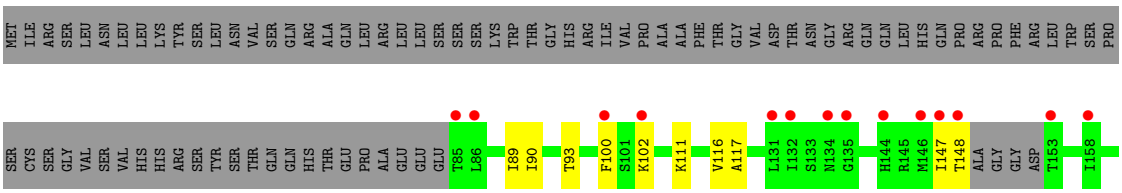
• Molecule 1: TNF receptor-associated protein 1

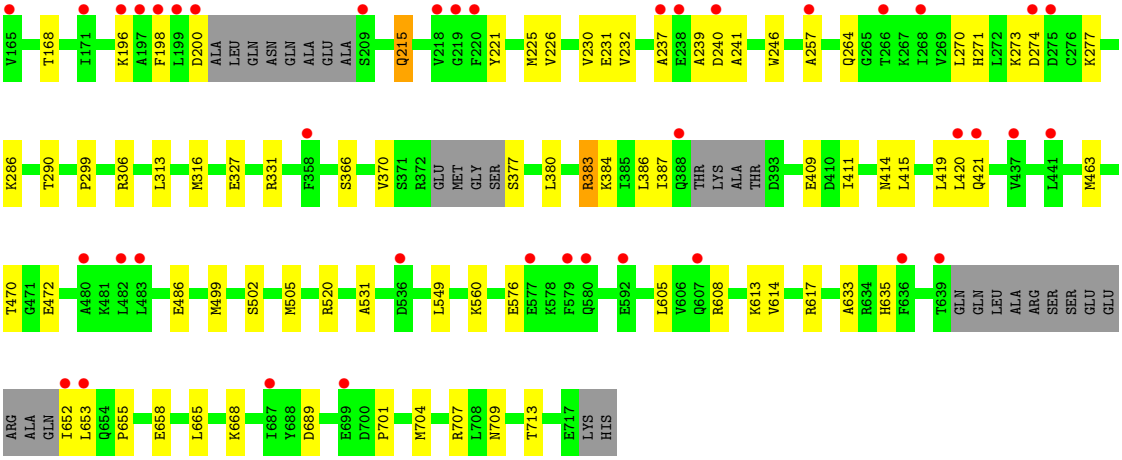
Chain A:



• Molecule 1: TNF receptor-associated protein 1

Chain B:




V165 T168 I171 K196 A197 F198 L199 D200 ALA LEU GLN ASN GLN ALA GLU ALA S209 Q215 V218 G219 F220 Y221 M225 V226 V230 E231 V232 A237 E238 A239 D240 A241 W246 A257 Q264 G265 T266 K267 I268 V269 L270 H271 L272 K273 D274 D275 C276 K277
K286 T290 P299 R306 L313 M316 E327 R331 F358 S366 V370 S371 R372 GLU MET GLY SER S377 L380 R383 K384 I385 L386 I387 Q388 THR LYS ALA THR D393 E409 D410 I411 N414 L415 L419 L420 Q421 V437 L441 M463
T470 G471 E472 A480 K481 L482 L483 E486 M499 S502 M505 R520 A531 D536 L549 K560 E576 E577 K578 F579 Q580 E592 L605 V606 Q607 R608 K613 V614 R617 A633 R634 H635 F636 T639 GLN GLN LEU ALA ARG SER SER GLU GLU
ARG ALA GLN I652 L653 Q654 P655 E658 L665 K668 I687 Y688 D689 E699 D700 P701 M704 R707 L708 N709 T713 E717 LYS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.98Å 96.36Å 125.15Å 90.00° 134.34° 90.00°	Depositor
Resolution (Å)	26.24 – 2.29 26.55 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (26.24-2.29) 92.1 (26.55-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1214)	Depositor
R, R_{free}	0.180 , 0.225 0.187 , 0.230	Depositor DCC
R_{free} test set	2001 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.006 for h,-k,-h-l 0.016 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CO, MG, ANP

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	0.41	0/4806	0.59	1/6473 (0.0%)
1	B	0.42	0/4970	0.58	1/6695 (0.0%)
All	All	0.41	0/9776	0.59	2/13168 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	GLY	N-CA-C	-7.71	93.83	113.10
1	B	215	GLN	N-CA-CB	-5.66	100.41	110.60

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	4720	0	4720	71	0
1	B	4872	0	4882	74	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	132	0	0	1	0
5	B	148	0	0	7	0
All	All	9940	0	9628	136	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 7.

All (136) 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:B:411:ILE:CG2	1:B:420:LEU:HD22	1.63	1.28
1:B:411:ILE:HG21	1:B:420:LEU:HD22	1.15	1.08
1:B:240:ASP:H	1:B:241:ALA:HB2	1.32	0.94
1:A:588:ARG:HD3	1:A:662:GLY:HA3	1.51	0.91
1:B:411:ILE:HG21	1:B:420:LEU:CD2	2.05	0.84
1:B:411:ILE:HG22	1:B:420:LEU:HD22	1.58	0.83
1:A:505:MET:SD	1:A:560:LYS:NZ	2.50	0.83
1:B:147:ILE:H	1:B:148:THR:HA	1.43	0.81
1:A:588:ARG:HD3	1:A:662:GLY:CA	2.12	0.79
1:A:119:SER:HA	1:B:421:GLN:HE22	1.49	0.77
1:A:716:LEU:O	1:B:668:LYS:NZ	2.20	0.73
1:B:377:SER:N	5:B:1004:HOH:O	2.21	0.73
1:A:116:VAL:HG11	1:A:221:TYR:HB2	1.73	0.70
1:B:116:VAL:HG11	1:B:221:TYR:HB2	1.73	0.70
1:A:616:PRO:O	1:A:618:LEU:N	2.25	0.70
1:B:383:ARG:HH21	1:B:409:GLU:HG2	1.57	0.68
1:A:101:SER:OG	1:A:103:HIS:NE2	2.21	0.67
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.77	0.67
1:B:232:VAL:HB	1:B:246:TRP:HB3	1.76	0.67
1:B:414:ASN:ND2	1:B:419:LEU:HB2	2.11	0.66
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.27	0.65
1:B:701:PRO:O	1:B:704:MET:HG2	1.98	0.64
1:B:531:ALA:O	1:B:617:ARG:NH2	2.31	0.63
1:A:119:SER:O	1:B:415:LEU:N	2.32	0.62
1:B:499:MET:HG2	5:B:1016:HOH:O	2.00	0.62
1:B:327:GLU:OE1	1:B:331:ARG:NH2	2.33	0.61
1:A:486:GLU:OE1	1:A:520:ARG:NH1	2.35	0.60
1:B:414:ASN:ND2	1:B:419:LEU:HD12	2.17	0.60
1:B:605:LEU:HD23	1:B:608:ARG:HH21	1.69	0.58
1:B:414:ASN:HD22	1:B:419:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:OG	1:A:367:MET:N	2.38	0.57
1:B:168:THR:HG22	5:B:954:HOH:O	2.05	0.57
1:B:709:ASN:O	1:B:713:THR:HG23	2.05	0.57
1:A:606:VAL:HG12	1:A:607:GLN:HG3	1.87	0.57
1:A:100:PHE:HB3	1:B:257:ALA:HB2	1.86	0.56
1:B:117:ALA:O	1:B:225:MET:HG2	2.06	0.56
1:A:139:LEU:HD22	1:A:156:MET:HB3	1.88	0.55
1:A:114:ASP:OD2	1:A:118:ARG:NH2	2.41	0.55
1:A:309:THR:O	1:A:309:THR:HG22	2.07	0.54
1:A:489:ALA:CB	1:A:538:GLU:HG3	2.37	0.54
1:A:558:ASP:O	1:A:560:LYS:HG3	2.07	0.54
1:B:502:SER:HA	1:B:505:MET:HE3	1.90	0.54
1:A:518:PRO:HD2	1:A:630:MET:HE2	1.90	0.54
1:B:239:ALA:H	1:B:241:ALA:HB2	1.73	0.54
1:B:313:LEU:HA	1:B:316:MET:HE2	1.88	0.53
1:A:232:VAL:HB	1:A:246:TRP:HB3	1.90	0.53
1:A:263:ARG:NH1	5:A:997:HOH:O	2.36	0.53
1:A:319:LYS:H	1:A:319:LYS:HE2	1.74	0.52
1:B:240:ASP:N	1:B:241:ALA:HB2	2.13	0.52
1:B:274:ASP:HA	1:B:277:LYS:HE3	1.91	0.52
1:B:502:SER:HA	1:B:505:MET:CE	2.39	0.52
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.91	0.51
1:B:470:THR:HG22	1:B:472:GLU:H	1.75	0.51
1:B:380:LEU:HD13	1:B:420:LEU:HD11	1.92	0.51
1:B:383:ARG:O	1:B:384:LYS:HB2	2.11	0.51
1:B:652:ILE:N	5:B:999:HOH:O	2.44	0.50
1:B:240:ASP:HB2	1:B:241:ALA:HA	1.94	0.50
1:B:633:ALA:HB1	1:B:653:LEU:HD11	1.94	0.49
1:B:652:ILE:HG22	1:B:653:LEU:N	2.27	0.49
1:B:380:LEU:CD1	1:B:420:LEU:HD11	2.43	0.49
1:B:147:ILE:N	1:B:148:THR:HA	2.11	0.49
1:B:198:PHE:O	1:B:200:ASP:HA	2.12	0.49
1:A:501:TYR:O	1:A:505:MET:HG3	2.12	0.49
1:B:230:VAL:HG22	1:B:270:LEU:HD22	1.94	0.49
1:A:286:LYS:O	1:A:290:THR:HG23	2.13	0.48
1:B:237:ALA:HB2	1:B:264:GLN:HE22	1.77	0.48
1:A:450:GLU:HG3	1:A:454:ARG:HH21	1.78	0.48
1:B:226:VAL:O	1:B:273:LYS:HG2	2.13	0.48
1:B:100:PHE:CE1	1:B:102:LYS:HE3	2.49	0.47
1:A:713:THR:HG22	1:B:665:LEU:HB2	1.95	0.47
1:A:489:ALA:HB2	1:A:538:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PRO:HD2	1:A:630:MET:CE	2.45	0.47
1:A:483:LEU:O	1:A:484:ARG:HD3	2.14	0.47
1:B:689:ASP:OD2	1:B:707:ARG:NH2	2.43	0.47
1:A:119:SER:CA	1:B:421:GLN:HE22	2.24	0.46
1:A:522:LEU:HD11	1:A:697:LEU:HD13	1.97	0.46
1:B:100:PHE:HE1	1:B:102:LYS:HE3	1.80	0.46
1:A:588:ARG:HD3	1:A:662:GLY:HA2	1.96	0.46
1:B:237:ALA:HB2	1:B:264:GLN:NE2	2.30	0.46
1:B:411:ILE:HG22	1:B:420:LEU:CD2	2.38	0.46
1:B:605:LEU:HD23	1:B:608:ARG:NH2	2.29	0.46
1:A:248:SER:HB2	1:A:254:PHE:HB3	1.97	0.46
1:A:528:TYR:CD1	1:A:566:GLU:HA	2.51	0.46
1:B:505:MET:HE1	1:B:560:LYS:HD3	1.98	0.46
1:A:470:THR:O	1:A:476:LYS:HE3	2.16	0.46
1:B:111:LYS:NZ	5:B:1041:HOH:O	2.48	0.46
1:A:500:GLU:O	1:A:503:SER:HB3	2.16	0.46
1:A:548:GLU:OE1	1:A:634:ARG:NH1	2.49	0.46
1:A:591:SER:O	1:A:591:SER:OG	2.34	0.45
1:A:500:GLU:O	1:A:504:ARG:HG3	2.16	0.45
1:A:634:ARG:HB3	1:A:638:ARG:HH21	1.82	0.45
1:B:286:LYS:O	1:B:290:THR:HG23	2.16	0.45
1:B:411:ILE:CG2	1:B:420:LEU:CD2	2.60	0.45
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.52	0.45
1:A:603:ASN:O	1:A:606:VAL:HG23	2.17	0.45
1:A:613:LYS:HG2	1:A:614:VAL:H	1.81	0.45
1:A:145:ARG:HE	1:A:176:VAL:HG21	1.82	0.44
1:B:386:LEU:HD11	5:B:1048:HOH:O	2.17	0.44
1:A:526:SER:HB3	1:A:529:PHE:HB3	2.00	0.44
1:A:514:TYR:CE1	1:A:564:SER:HB3	2.53	0.44
1:A:517:ALA:O	1:A:543:PHE:HA	2.17	0.44
1:B:486:GLU:OE1	1:B:520:ARG:HD3	2.17	0.44
1:B:653:LEU:C	1:B:655:PRO:HD3	2.37	0.44
1:A:566:GLU:OE2	1:A:629:GLU:HA	2.18	0.44
1:A:564:SER:O	1:A:566:GLU:N	2.51	0.44
1:A:497:SER:OG	1:A:500:GLU:HG3	2.18	0.43
1:A:632:ALA:O	1:A:635:HIS:N	2.51	0.43
1:B:196:LYS:NZ	1:B:215:GLN:HA	2.32	0.43
1:B:386:LEU:O	1:B:387:ILE:HD13	2.18	0.43
1:B:633:ALA:HB1	1:B:653:LEU:CD1	2.48	0.43
1:B:652:ILE:O	1:B:653:LEU:HG	2.19	0.43
1:A:670:HIS:O	1:A:673:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:HG2	1:A:546:PHE:CD2	2.54	0.42
1:A:263:ARG:HG2	1:A:264:GLN:N	2.35	0.42
1:A:467:ILE:O	1:A:476:LYS:HE2	2.19	0.42
1:B:299:PRO:HB3	1:B:306:ARG:CZ	2.49	0.42
1:B:549:LEU:HD13	1:B:635:HIS:CE1	2.55	0.42
1:B:576:GLU:N	1:B:576:GLU:OE2	2.53	0.42
1:A:95:ASN:O	1:A:97:GLN:HG2	2.20	0.42
1:A:589:LEU:HB3	1:A:661:THR:HB	2.01	0.42
1:A:489:ALA:HB3	1:A:538:GLU:HG3	2.02	0.41
1:A:412:PRO:HD2	1:A:426:ILE:HD11	2.01	0.41
1:A:473:GLN:NE2	1:A:556:GLU:O	2.53	0.41
1:A:473:GLN:O	1:A:477:GLU:HG3	2.21	0.41
1:B:331:ARG:HD2	5:B:1017:HOH:O	2.20	0.41
1:B:613:LYS:O	1:B:658:GLU:HA	2.19	0.41
1:A:159:HIS:CE1	1:B:89:ILE:HD13	2.56	0.41
1:A:701:PRO:O	1:A:704:MET:HG2	2.21	0.41
1:A:490:LEU:HD11	1:A:496:THR:HG21	2.03	0.41
1:A:115:ILE:CG2	1:B:415:LEU:HD22	2.50	0.41
1:A:673:LYS:NZ	1:A:674:ASP:OD2	2.47	0.41
1:A:161:GLN:HB2	1:B:90:ILE:HD12	2.03	0.40
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.90	0.40
1:B:366:SER:O	1:B:370:VAL:HG23	2.21	0.40
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.69	0.40
1:B:505:MET:HE1	1:B:560:LYS:CD	2.52	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	575/719 (80%)	545 (95%)	30 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	592/719 (82%)	568 (96%)	24 (4%)	0	100	100
All	All	1167/1438 (81%)	1113 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	516/634 (81%)	512 (99%)	4 (1%)	81	90
1	B	537/634 (85%)	533 (99%)	4 (1%)	84	91
All	All	1053/1268 (83%)	1045 (99%)	8 (1%)	81	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	A	496	THR
1	A	520	ARG
1	A	697	LEU
1	B	93	THR
1	B	383	ARG
1	B	463	MET
1	B	614	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	421	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
2	ANP	B	802	3	29,33,33	1.23	5 (17%)	31,52,52	1.08	5 (16%)
2	ANP	A	801	3	29,33,33	1.20	3 (10%)	31,52,52	0.92	2 (6%)

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	ANP	B	802	3	-	2/14/38/38	0/3/3/3
2	ANP	A	801	3	-	2/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-O1G	3.11	1.50	1.46
2	B	802	ANP	PG-N3B	2.86	1.70	1.63
2	A	801	ANP	PG-N3B	2.67	1.70	1.63
2	A	801	ANP	PB-O1B	2.66	1.50	1.46
2	B	802	ANP	PG-O1G	2.58	1.50	1.46
2	B	802	ANP	PB-O1B	2.43	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	ANP	PB-O3A	-2.20	1.56	1.59
2	B	802	ANP	PB-N3B	2.04	1.68	1.63

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	ANP	O1G-PG-N3B	-2.75	107.72	111.77
2	B	802	ANP	O2G-PG-O1G	-2.53	107.11	113.45
2	B	802	ANP	C5-C6-N6	2.42	124.00	120.31
2	A	801	ANP	C5-C6-N6	2.35	123.89	120.31
2	B	802	ANP	O3A-PB-N3B	2.19	112.67	106.59
2	A	801	ANP	O2B-PB-O3A	2.04	111.45	104.64
2	B	802	ANP	O1B-PB-N3B	-2.02	108.79	111.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

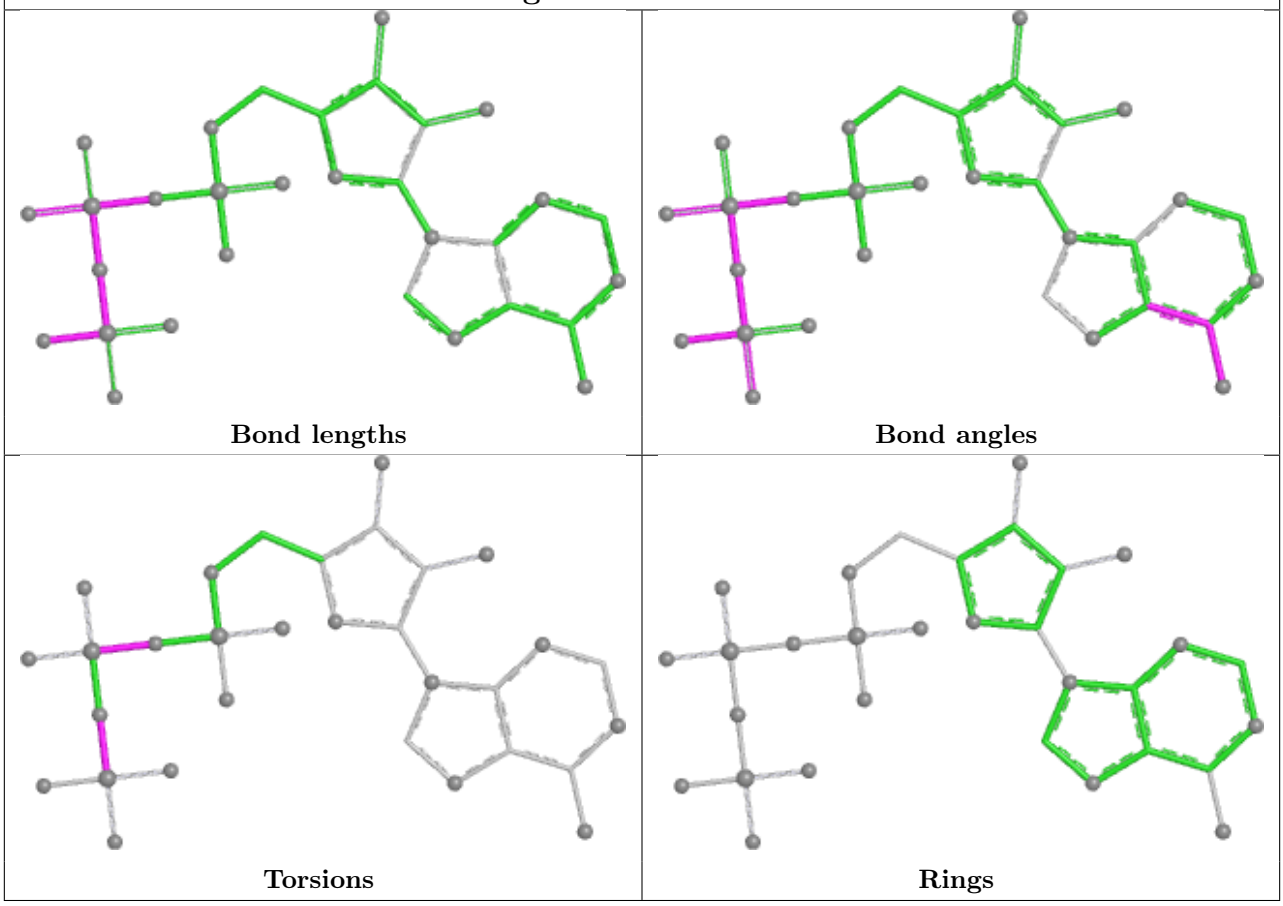
Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PA-O3A-PB-O2B
2	B	802	ANP	PB-N3B-PG-O1G
2	B	802	ANP	PA-O3A-PB-O2B

There are no ring outliers.

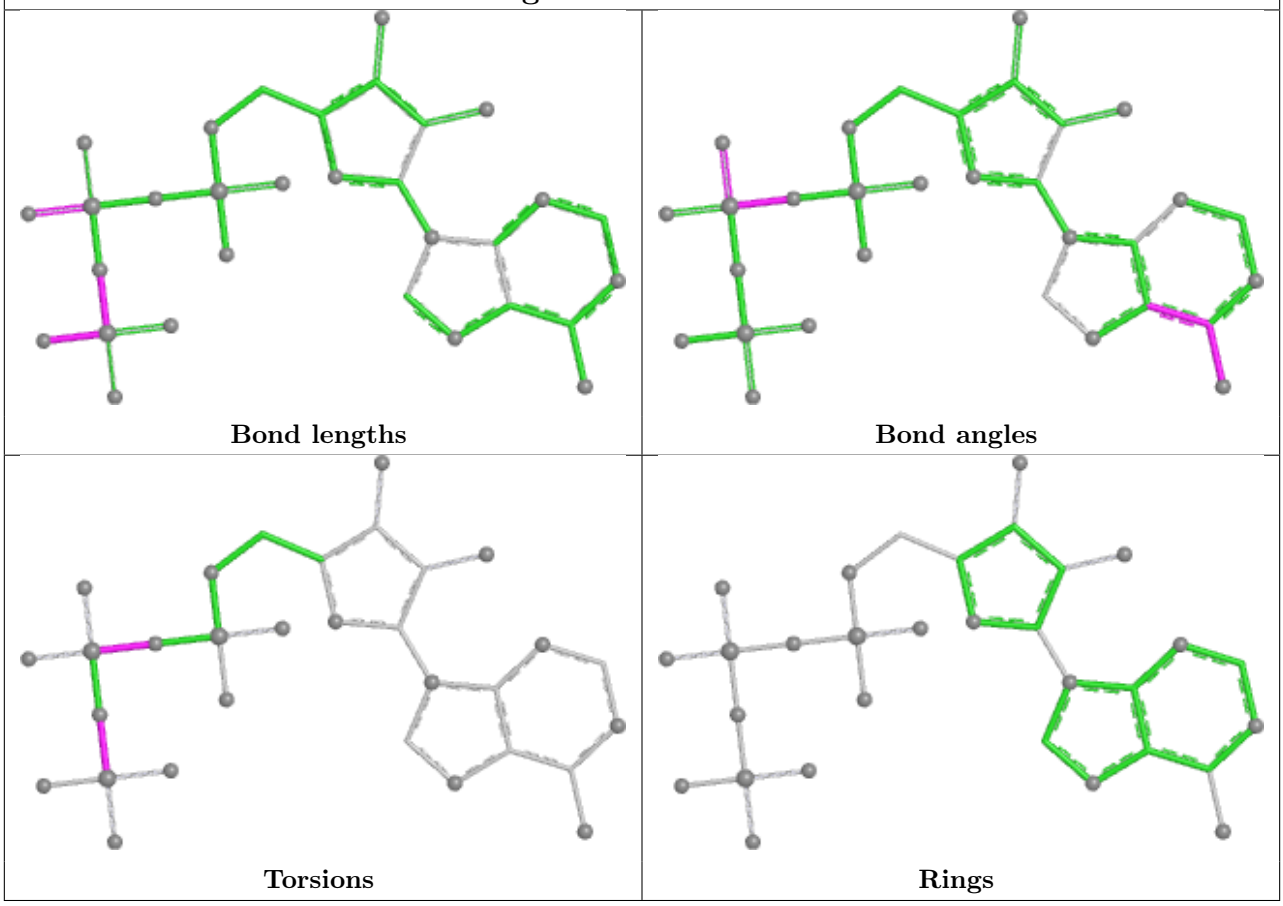
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 ANP B 802



Ligand ANP A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	588/719 (81%)	0.41	61 (10%) 6 8	38, 71, 126, 186	0
1	B	601/719 (83%)	0.30	54 (8%) 9 12	40, 66, 108, 145	0
All	All	1189/1438 (82%)	0.35	115 (9%) 7 10	38, 68, 119, 186	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	9.9
1	B	607	GLN	7.0
1	B	652	ILE	6.8
1	A	508	GLY	6.8
1	A	588	ARG	6.6
1	A	607	GLN	6.5
1	A	534	GLN	6.1
1	A	152	ASP	5.0
1	A	535	LYS	5.0
1	A	96	VAL	5.0
1	B	131	LEU	4.9
1	B	653	LEU	4.8
1	A	507	ALA	4.8
1	B	198	PHE	4.6
1	B	146	MET	4.5
1	B	482	LEU	4.5
1	B	420	LEU	4.5
1	A	628	LEU	4.4
1	A	608	ARG	4.4
1	A	636	PHE	4.4
1	A	368	PHE	4.3
1	B	147	ILE	4.2
1	A	638	ARG	4.2
1	B	268	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	ILE	4.0
1	B	238	GLU	4.0
1	A	131	LEU	3.9
1	B	577	GLU	3.9
1	B	86	LEU	3.9
1	A	100	PHE	3.9
1	A	632	ALA	3.8
1	B	421	GLN	3.8
1	A	266	THR	3.7
1	A	510	ARG	3.7
1	A	635	HIS	3.7
1	A	268	ILE	3.7
1	B	639	THR	3.7
1	A	531	ALA	3.6
1	B	85	THR	3.6
1	B	257	ALA	3.5
1	A	324	TRP	3.5
1	B	220	PHE	3.4
1	A	592	GLU	3.3
1	B	153	THR	3.3
1	B	199	LEU	3.3
1	A	132	ILE	3.2
1	B	171	ILE	3.2
1	A	85	THR	3.2
1	B	165	VAL	3.2
1	A	369	ASP	3.2
1	B	148	THR	3.2
1	A	99	SER	3.2
1	B	196	LYS	3.1
1	B	135	GLY	3.1
1	A	506	LYS	3.1
1	A	220	PHE	3.1
1	B	209	SER	3.1
1	A	97	GLN	3.0
1	A	619	ASP	3.0
1	B	144	HIS	2.8
1	A	366	SER	2.7
1	A	637	LEU	2.7
1	A	509	THR	2.7
1	A	232	VAL	2.7
1	B	100	PHE	2.7
1	B	441	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	322	SER	2.7
1	A	591	SER	2.7
1	B	699	GLU	2.7
1	B	200	ASP	2.7
1	B	237	ALA	2.6
1	A	653	LEU	2.6
1	B	437	VAL	2.6
1	B	197	ALA	2.6
1	A	151	GLY	2.5
1	A	555	ARG	2.5
1	A	540	LEU	2.5
1	B	219	GLY	2.5
1	A	365	PRO	2.5
1	A	489	ALA	2.5
1	A	133	SER	2.4
1	A	204	ASN	2.4
1	A	149	ALA	2.4
1	A	610	THR	2.4
1	A	483	LEU	2.4
1	B	536	ASP	2.4
1	B	134	ASN	2.4
1	B	358	PHE	2.4
1	A	134	ASN	2.4
1	A	513	TYR	2.4
1	B	483	LEU	2.4
1	B	579	PHE	2.4
1	B	275	ASP	2.3
1	B	158	ILE	2.3
1	B	274	ASP	2.3
1	B	636	PHE	2.3
1	A	552	LEU	2.3
1	B	580	GLN	2.3
1	A	606	VAL	2.3
1	A	405	VAL	2.2
1	A	504	ARG	2.2
1	A	135	GLY	2.2
1	B	132	ILE	2.2
1	B	592	GLU	2.2
1	A	654	GLN	2.2
1	B	240	ASP	2.1
1	B	266	THR	2.1
1	B	388	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	218	VAL	2.1
1	B	687	ILE	2.1
1	B	102	LYS	2.1
1	A	98	GLY	2.0
1	B	480	ALA	2.0
1	A	463	MET	2.0
1	A	633	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

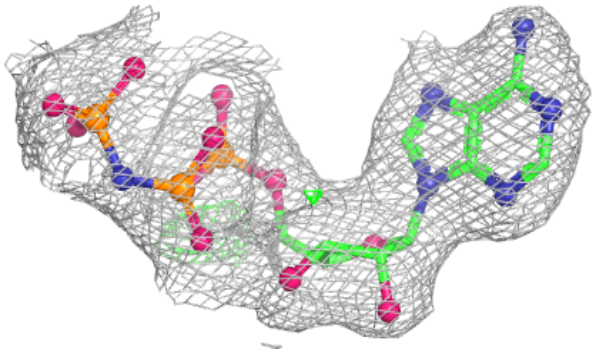
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

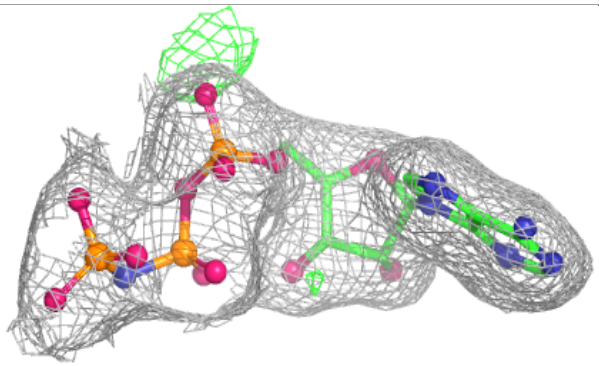
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CO	B	804	1/1	0.71	0.14	99,99,99,99	1
4	CO	A	804	1/1	0.87	0.05	88,88,88,88	1
3	MG	A	802	1/1	0.89	0.20	42,42,42,42	0
4	CO	A	803	1/1	0.89	0.05	127,127,127,127	0
3	MG	B	803	1/1	0.96	0.17	53,53,53,53	0
4	CO	B	801	1/1	0.98	0.09	89,89,89,89	0
2	ANP	B	802	31/31	0.98	0.21	47,54,60,62	0
2	ANP	A	801	31/31	0.99	0.20	35,43,48,52	0

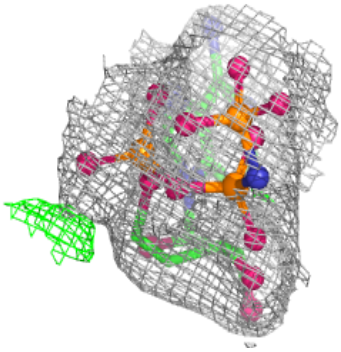
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 802:

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

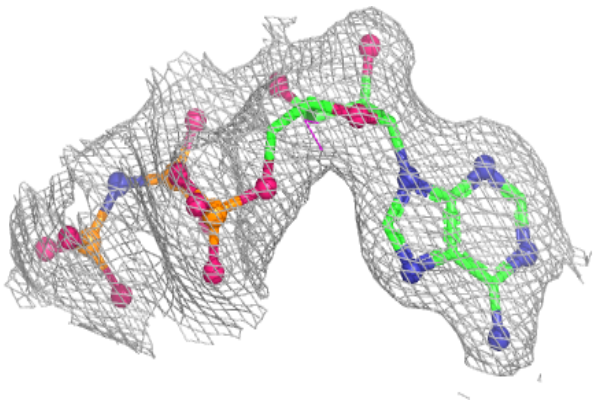


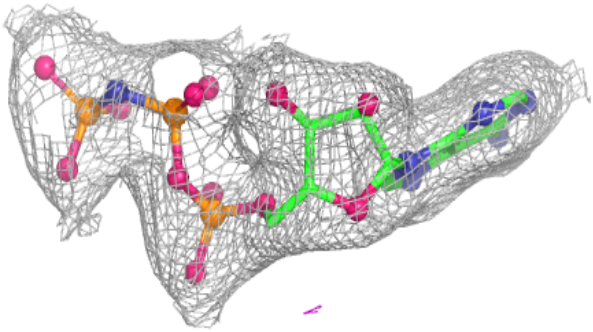


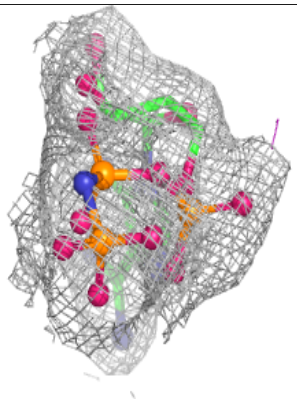


Electron density around ANP A 801:

$2mF_o$-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.