



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:43 pm BST

PDB ID : 1Q97
Title : The structure of the *Saccharomyces cerevisiae* SR protein kinase, Sky1p, with bound ATP
Authors : Nolen, B.; Ngo, J.; Chakrabarti, S.; Vu, D.; Adams, J.A.; Ghosh, G.
Deposited on : 2003-08-22
Resolution : 2.30 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 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

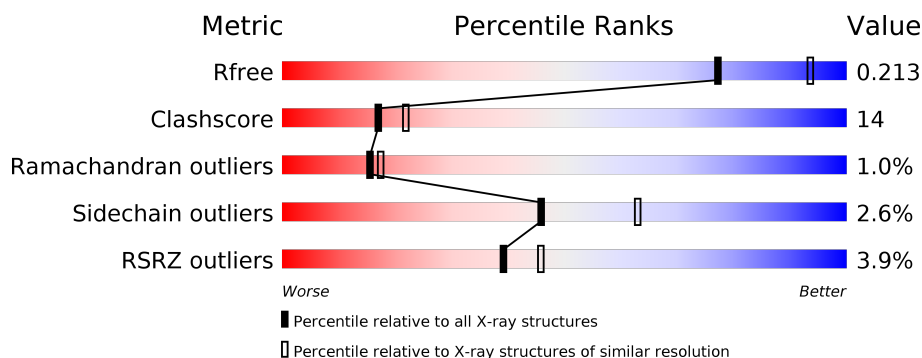
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	373	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• 6%</div> </div> </div>
1	B	373	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5940 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 SR protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2826	1816	480	518	12			
1	B	361	Total	C	N	O	S	0	0	0
			2906	1862	494	538	12			

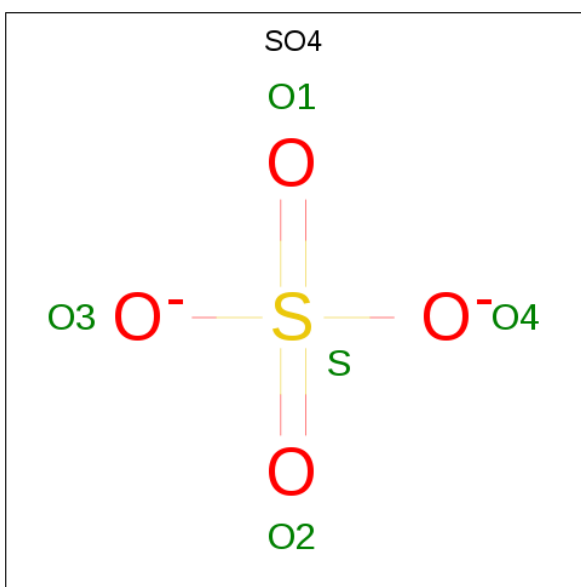
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	VAL	-	SEE REMARK 999	UNP Q03656
A	306	ASP	-	SEE REMARK 999	UNP Q03656
B	305	VAL	-	SEE REMARK 999	UNP Q03656
B	306	ASP	-	SEE REMARK 999	UNP Q03656

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

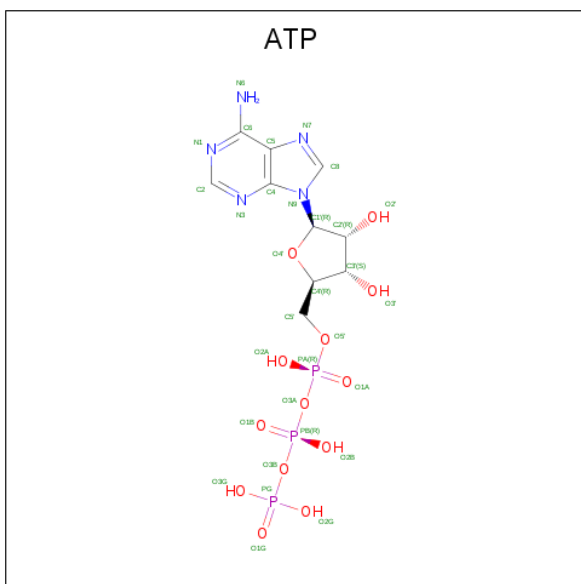
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

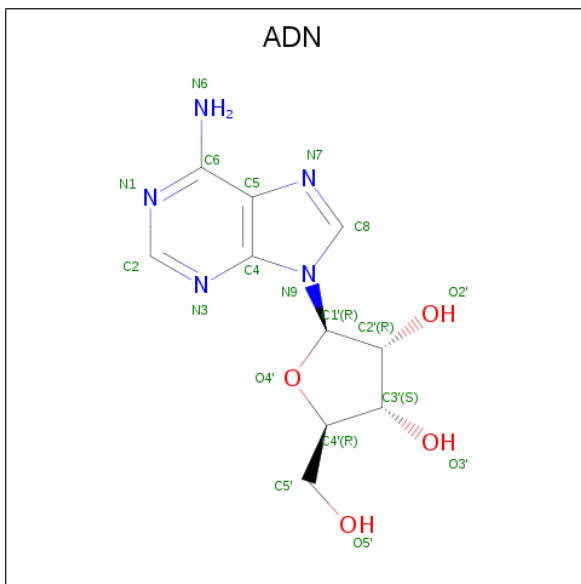


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ni 1 1	0	0

- Molecule 6 is ADENOSINE (three-letter code: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 19 10 5 4	0	0

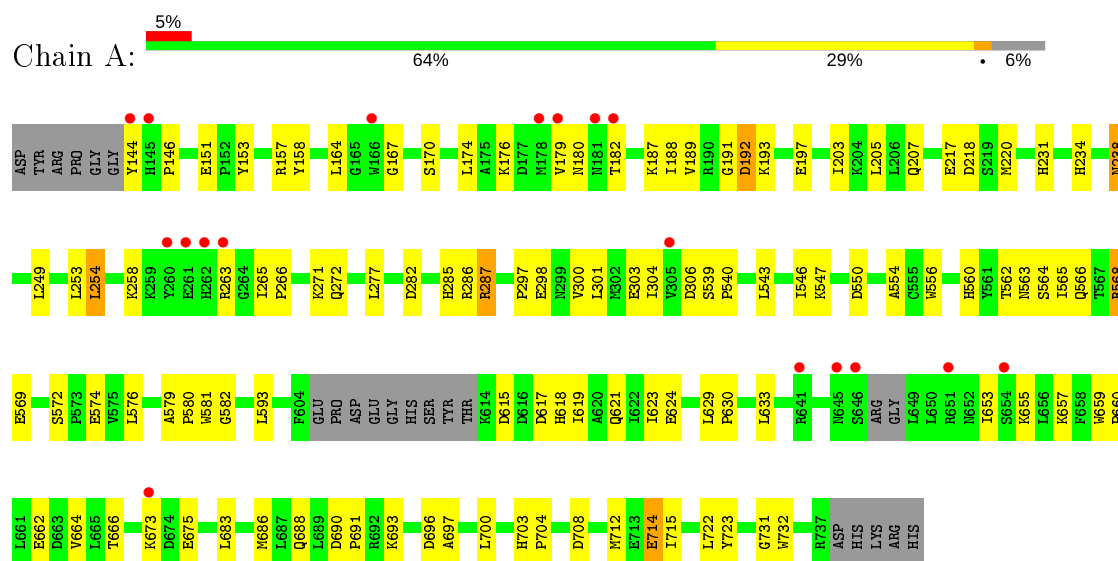
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	63	Total O 63 63	0	0
7	B	82	Total O 82 82	0	0

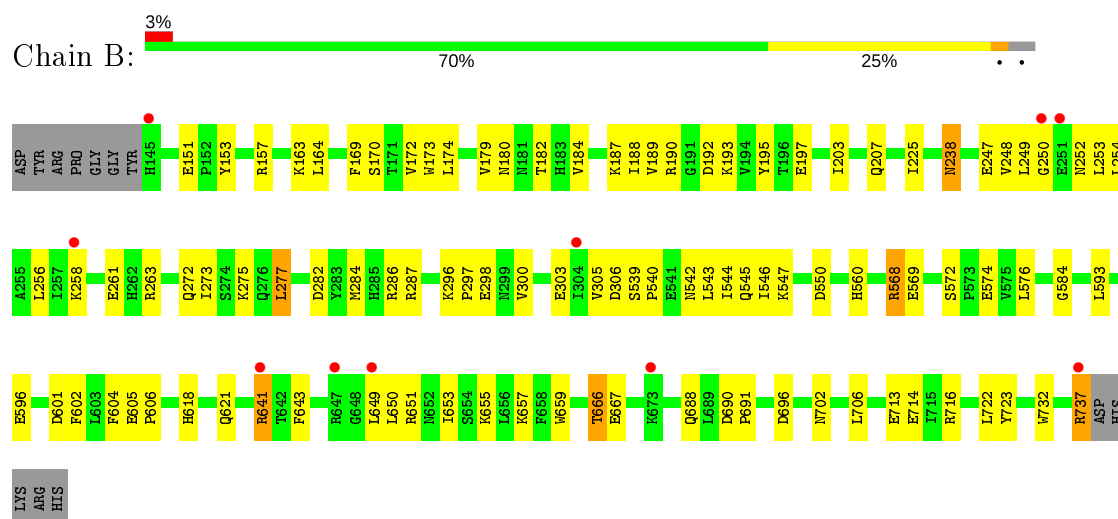
3 Residue-property plots [i](#)

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: SR protein kinase



• Molecule 1: SR protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.82Å 88.69Å 133.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.30 48.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.0 (19.89-2.30) 80.9 (48.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.215 , 0.264 0.210 , 0.213	Depositor DCC
R_{free} test set	1551 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5940	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2990e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, NI, MG, SO4, 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	0.33	0/2891	0.57	0/3910
1	B	0.34	0/2975	0.57	0/4027
All	All	0.34	0/5866	0.57	0/7937

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

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	2826	0	2797	94	1
1	B	2906	0	2874	69	1
2	A	2	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	31	0	12	2	0
5	B	1	0	0	0	0
6	B	19	0	13	0	0
7	A	63	0	0	3	0
7	B	82	0	0	4	0
All	All	5940	0	5696	161	1

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 14.

All (161) 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:238:ASN:H	1:B:238:ASN:HD22	1.20	0.84
1:A:205:LEU:HD13	1:A:554:ALA:HB3	1.60	0.84
1:A:238:ASN:H	1:A:238:ASN:HD22	1.30	0.80
1:B:164:LEU:HD21	1:B:174:LEU:HB2	1.64	0.79
1:B:737:ARG:NE	1:B:737:ARG:H	1.80	0.78
1:A:203:ILE:O	1:A:207:GLN:HG3	1.84	0.78
1:A:655:LYS:HD3	1:A:657:LYS:NZ	1.99	0.77
1:B:737:ARG:HE	1:B:737:ARG:H	1.32	0.77
1:B:297:PRO:HD3	1:B:593:LEU:HD13	1.68	0.75
1:A:238:ASN:ND2	1:A:238:ASN:H	1.85	0.75
1:B:238:ASN:H	1:B:238:ASN:ND2	1.84	0.74
1:B:688:GLN:HE21	1:B:690:ASP:H	1.35	0.74
1:B:702:ASN:OD1	1:B:716:ARG:HB2	1.87	0.74
1:A:623:ILE:CD1	1:A:629:LEU:HD13	2.19	0.73
1:A:297:PRO:HD3	1:A:593:LEU:HD13	1.71	0.73
1:A:624:GLU:HG3	1:A:657:LYS:O	1.88	0.72
1:A:170:SER:HB2	1:A:188:ILE:O	1.91	0.70
1:B:172:VAL:HG22	1:B:187:LYS:HG2	1.74	0.69
1:A:282:ASP:OD1	1:A:286:ARG:HD3	1.93	0.69
1:B:170:SER:HB2	1:B:188:ILE:O	1.93	0.69
1:B:650:LEU:HD23	1:B:653:ILE:HB	1.77	0.67
1:A:623:ILE:HD13	1:A:629:LEU:HD13	1.76	0.67
1:A:272:GLN:HE22	1:A:543:LEU:HA	1.61	0.66
1:A:562:THR:HG22	1:A:564:SER:H	1.60	0.66
1:A:655:LYS:HD3	1:A:657:LYS:HZ1	1.60	0.66
1:A:569:GLU:CD	1:A:569:GLU:H	1.99	0.66
1:B:252:ASN:OD1	1:B:254:LEU:HB2	1.96	0.66
1:A:238:ASN:N	1:A:238:ASN:HD22	1.92	0.64
1:A:254:LEU:HD22	1:A:258:LYS:HE2	1.78	0.64
1:A:304:ILE:N	1:A:304:ILE:HD12	2.14	0.63
1:B:192:ASP:HB3	1:B:195:TYR:HB2	1.81	0.62
1:A:617:ASP:OD1	1:A:653:ILE:HD11	2.00	0.62
1:B:170:SER:HB3	1:B:189:VAL:HA	1.81	0.62
1:B:272:GLN:HE22	1:B:543:LEU:HA	1.64	0.62
1:B:282:ASP:OD1	1:B:286:ARG:HD3	2.00	0.61
1:B:254:LEU:HD12	1:B:298:GLU:HG3	1.82	0.61
1:B:254:LEU:CD1	1:B:298:GLU:HG3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:ILE:O	1:A:623:ILE:HG12	2.01	0.59
1:A:306:ASP:OD2	1:A:540:PRO:HD2	2.02	0.59
1:A:560:HIS:HE1	7:A:746:HOH:O	1.86	0.58
1:A:568:ARG:HB3	1:A:569:GLU:OE2	2.02	0.58
1:A:164:LEU:HD21	1:A:174:LEU:HB2	1.86	0.58
1:B:722:LEU:O	1:B:723:TYR:HB2	2.04	0.58
1:A:170:SER:HB3	1:A:189:VAL:HA	1.87	0.57
1:A:254:LEU:HG	1:A:298:GLU:OE2	2.05	0.56
1:B:737:ARG:CD	1:B:737:ARG:H	2.18	0.56
1:B:272:GLN:HE22	1:B:544:ILE:H	1.52	0.56
1:A:180:ASN:O	1:A:182:THR:HG23	2.06	0.56
1:B:655:LYS:HD2	1:B:657:LYS:HE3	1.88	0.56
1:A:144:TYR:CE1	1:A:146:PRO:HB3	2.41	0.55
1:B:584:GLY:HA3	7:B:772:HOH:O	2.07	0.55
1:B:569:GLU:HG2	1:B:602:PHE:CD2	2.41	0.55
1:A:675:GLU:HA	1:A:675:GLU:OE2	2.07	0.55
1:A:712:MET:HB3	1:A:715:ILE:HD12	1.89	0.55
1:A:722:LEU:O	1:A:723:TYR:HB2	2.08	0.54
1:A:655:LYS:HD3	1:A:657:LYS:HZ2	1.72	0.54
1:A:683:LEU:HA	1:A:686:MET:HE3	1.89	0.54
1:B:275:LYS:HD2	1:B:706:LEU:HB3	1.89	0.54
1:B:546:ILE:C	1:B:546:ILE:HD12	2.28	0.54
1:B:605:GLU:H	1:B:621:GLN:HE22	1.56	0.54
1:A:683:LEU:HD23	1:A:686:MET:CE	2.38	0.54
1:B:272:GLN:NE2	1:B:544:ILE:H	2.06	0.53
1:B:203:ILE:O	1:B:207:GLN:HG3	2.09	0.53
1:A:167:GLY:HA3	4:A:485:ATP:O2B	2.07	0.53
1:A:253:LEU:HD13	1:A:300:VAL:O	2.09	0.53
1:A:254:LEU:CD2	1:A:258:LYS:HE2	2.40	0.52
1:B:542:ASN:HA	7:B:818:HOH:O	2.10	0.52
1:B:238:ASN:N	1:B:238:ASN:ND2	2.51	0.52
1:A:655:LYS:HG3	1:B:659:TRP:CZ2	2.45	0.51
1:A:688:GLN:HE21	1:A:690:ASP:H	1.57	0.51
1:A:546:ILE:C	1:A:546:ILE:HD12	2.31	0.51
1:B:249:LEU:HD22	1:B:303:GLU:OE1	2.10	0.51
1:A:539:SER:HB3	1:A:540:PRO:HD3	1.93	0.51
1:B:157:ARG:HG3	1:B:179:VAL:HG23	1.93	0.51
1:A:696:ASP:HA	1:A:732:TRP:CH2	2.45	0.51
1:B:572:SER:HB2	1:B:574:GLU:OE2	2.11	0.51
1:A:683:LEU:HD23	1:A:686:MET:HE1	1.93	0.50
1:A:158:TYR:HA	1:A:176:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD23	1:A:301:LEU:CB	2.40	0.50
1:B:180:ASN:O	1:B:182:THR:HG23	2.11	0.50
1:B:574:GLU:HG2	1:B:691:PRO:HG3	1.94	0.49
1:B:737:ARG:N	1:B:737:ARG:HE	2.07	0.49
1:B:273:ILE:O	1:B:277:LEU:HB2	2.12	0.49
1:A:712:MET:CB	1:A:715:ILE:HD12	2.43	0.48
1:A:285:HIS:HD2	7:A:758:HOH:O	1.95	0.48
1:B:238:ASN:N	1:B:238:ASN:HD22	1.90	0.48
1:A:205:LEU:HD13	1:A:554:ALA:CB	2.37	0.48
1:B:254:LEU:O	1:B:258:LYS:HG3	2.12	0.48
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.79	0.48
1:A:662:GLU:O	1:A:666:THR:HG23	2.13	0.48
1:A:187:LYS:HE3	4:A:485:ATP:O1B	2.14	0.48
1:A:191:GLY:O	1:A:192:ASP:HB2	2.14	0.48
1:A:271:LYS:NZ	1:A:708:ASP:OD1	2.47	0.47
1:A:217:GLU:O	1:A:220:MET:HB2	2.15	0.47
1:A:630:PRO:HD2	1:A:633:LEU:HD12	1.96	0.47
1:B:261:GLU:O	1:B:263:ARG:HG3	2.15	0.47
1:B:666:THR:HG22	1:B:667:GLU:N	2.29	0.47
1:A:157:ARG:HG3	1:A:179:VAL:HG23	1.97	0.46
1:A:249:LEU:HD23	1:A:301:LEU:HB2	1.97	0.46
1:A:265:ILE:HG23	1:A:266:PRO:HD2	1.97	0.46
1:A:615:ASP:O	1:A:619:ILE:HG13	2.16	0.46
1:A:144:TYR:O	1:A:146:PRO:HD3	2.16	0.46
1:A:234:HIS:HD2	3:A:745:SO4:O2	1.99	0.46
1:A:249:LEU:O	1:A:303:GLU:HB3	2.15	0.46
1:B:305:VAL:CG2	1:B:545:GLN:HB2	2.46	0.46
1:A:287:ARG:HH11	1:A:287:ARG:HG3	1.81	0.45
1:A:298:GLU:CD	1:A:298:GLU:H	2.19	0.45
1:A:562:THR:HG22	1:A:563:ASN:H	1.82	0.45
1:A:304:ILE:HD12	1:A:304:ILE:H	1.81	0.45
1:A:297:PRO:CD	1:A:593:LEU:HD13	2.45	0.45
1:B:737:ARG:NE	1:B:737:ARG:N	2.56	0.45
1:A:205:LEU:HD23	1:A:556:TRP:CZ2	2.53	0.44
1:A:218:ASP:OD1	1:A:287:ARG:HG2	2.17	0.44
1:A:562:THR:HG22	1:A:563:ASN:N	2.31	0.44
1:B:151:GLU:HG2	1:B:153:TYR:CE1	2.52	0.44
1:A:582:GLY:HA3	1:A:731:GLY:O	2.17	0.44
1:A:617:ASP:O	1:A:621:GLN:HG3	2.17	0.44
1:B:596:GLU:HA	1:B:601:ASP:O	2.18	0.44
1:B:649:LEU:HD12	1:B:649:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ARG:HH21	1:B:618:HIS:HD2	1.66	0.44
1:A:151:GLU:HG2	1:A:153:TYR:CE1	2.54	0.43
1:A:304:ILE:CD1	1:A:304:ILE:N	2.81	0.43
1:A:568:ARG:HH21	1:A:576:LEU:HD21	1.84	0.43
1:A:659:TRP:CH2	1:B:655:LYS:HG2	2.53	0.43
1:B:560:HIS:HE1	7:B:748:HOH:O	1.99	0.43
1:B:643:PHE:O	1:B:651:ARG:HG2	2.19	0.43
1:A:714:GLU:HG2	7:A:754:HOH:O	2.18	0.43
1:B:253:LEU:HD22	1:B:300:VAL:HB	2.01	0.43
1:A:170:SER:CB	1:A:189:VAL:HA	2.48	0.43
1:B:296:LYS:HB2	1:B:297:PRO:HD2	1.98	0.43
1:A:579:ALA:HB1	1:A:580:PRO:HD2	2.01	0.43
1:A:574:GLU:HG2	1:A:691:PRO:HG3	1.99	0.43
1:B:193:LYS:O	1:B:197:GLU:HG3	2.19	0.43
1:B:604:PHE:O	1:B:606:PRO:HD3	2.19	0.43
1:A:297:PRO:HD3	1:A:593:LEU:CD1	2.45	0.42
1:A:249:LEU:CD2	1:A:547:LYS:HB2	2.49	0.42
1:B:249:LEU:HD11	1:B:547:LYS:HD2	2.01	0.42
1:B:696:ASP:HA	1:B:732:TRP:CH2	2.54	0.42
1:B:666:THR:HG22	1:B:667:GLU:HG3	2.01	0.42
1:A:673:LYS:HB3	1:A:673:LYS:HE2	1.84	0.42
1:B:247:GLU:HG2	7:B:811:HOH:O	2.19	0.42
1:B:225:ILE:HD11	1:B:284:MET:HG3	2.01	0.42
1:A:572:SER:HB2	1:A:574:GLU:OE2	2.20	0.42
1:A:565:ILE:HD13	1:A:581:TRP:CH2	2.55	0.42
1:B:641:ARG:HA	1:B:641:ARG:HE	1.84	0.42
1:A:193:LYS:O	1:A:197:GLU:HG3	2.20	0.41
1:A:703:HIS:CG	1:A:704:PRO:HD2	2.54	0.41
1:B:163:LYS:HG2	1:B:173:TRP:CE2	2.54	0.41
1:A:629:LEU:HA	1:A:630:PRO:HD3	1.94	0.41
1:A:660:PRO:O	1:A:664:VAL:HG23	2.19	0.41
1:B:189:VAL:HG12	1:B:190:ARG:N	2.36	0.41
1:B:539:SER:N	1:B:540:PRO:CD	2.83	0.41
1:A:301:LEU:O	1:A:546:ILE:HA	2.20	0.41
1:B:539:SER:HB2	1:B:540:PRO:HD3	2.01	0.41
1:A:688:GLN:CG	1:A:693:LYS:HB2	2.50	0.41
1:A:697:ALA:HA	1:A:700:LEU:HD12	2.03	0.41
1:A:688:GLN:HG2	1:A:693:LYS:HB2	2.02	0.41
1:B:306:ASP:OD1	1:B:540:PRO:HD2	2.21	0.40
1:A:203:ILE:HD13	1:A:231:HIS:CD2	2.56	0.40
1:B:170:SER:OG	1:B:187:LYS:HE3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:VAL:HA	1:B:248:VAL:HG23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:GLU:OE1	1:B:713:GLU:OE2[2_654]	2.15	0.05

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	345/373 (92%)	324 (94%)	17 (5%)	4 (1%)	13	14
1	B	359/373 (96%)	337 (94%)	19 (5%)	3 (1%)	19	23
All	All	704/746 (94%)	661 (94%)	36 (5%)	7 (1%)	15	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	GLY
1	A	568	ARG
1	B	568	ARG
1	B	550	ASP
1	A	192	ASP
1	A	550	ASP
1	A	566	GLN

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	304/327 (93%)	298 (98%)	6 (2%)	55	72
1	B	314/327 (96%)	304 (97%)	10 (3%)	39	54
All	All	618/654 (94%)	602 (97%)	16 (3%)	46	63

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	254	LEU
1	A	277	LEU
1	A	287	ARG
1	A	618	HIS
1	A	714	GLU
1	B	169	PHE
1	B	238	ASN
1	B	256	LEU
1	B	277	LEU
1	B	287	ARG
1	B	576	LEU
1	B	641	ARG
1	B	666	THR
1	B	714	GLU
1	B	737	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	231	HIS
1	A	234	HIS
1	A	238	ASN
1	A	262	HIS
1	A	272	GLN
1	A	285	HIS
1	A	560	HIS
1	A	688	GLN
1	B	145	HIS

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Mol	Chain	Res	Type
1	B	234	HIS
1	B	238	ASN
1	B	272	GLN
1	B	285	HIS
1	B	618	HIS
1	B	621	GLN
1	B	688	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 7 ligands modelled in this entry, 3 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	$\# Z > 2$
6	ADN	B	486	-	18,21,21	1.45	1 (5%)	18,31,31	1.65	2 (11%)
3	SO4	B	744	-	4,4,4	0.30	0	6,6,6	0.05	0
3	SO4	A	745	-	4,4,4	0.28	0	6,6,6	0.08	0
4	ATP	A	485	2	26,33,33	1.38	2 (7%)	31,52,52	1.49	4 (12%)

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
6	ADN	B	486	-	-	0/2/22/22	0/3/3/3
4	ATP	A	485	2	-	6/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	485	ATP	O4'-C1'	5.32	1.48	1.41
6	B	486	ADN	O4'-C1'	4.77	1.47	1.41
4	A	485	ATP	PG-O3G	2.01	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	486	ADN	N3-C2-N1	-5.44	120.17	128.68
4	A	485	ATP	N3-C2-N1	-5.30	120.40	128.68
4	A	485	ATP	PB-O3B-PG	-3.26	121.65	132.83
4	A	485	ATP	PA-O3A-PB	-2.96	122.67	132.83
6	B	486	ADN	C5'-C4'-C3'	-2.95	107.97	115.09
4	A	485	ATP	O2G-PG-O1G	2.03	118.63	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

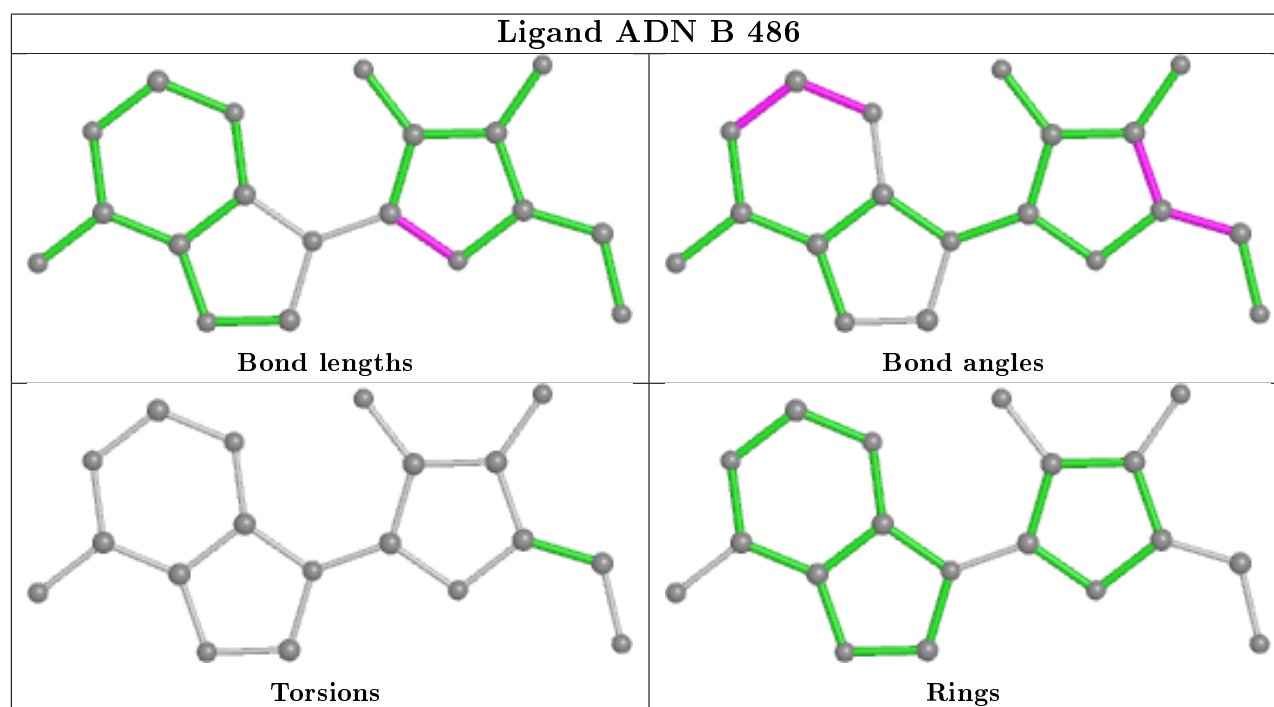
Mol	Chain	Res	Type	Atoms
4	A	485	ATP	C5'-O5'-PA-O1A
4	A	485	ATP	C5'-O5'-PA-O3A
4	A	485	ATP	PA-O3A-PB-O1B
4	A	485	ATP	PB-O3B-PG-O2G
4	A	485	ATP	PB-O3A-PA-O2A
4	A	485	ATP	C5'-O5'-PA-O2A

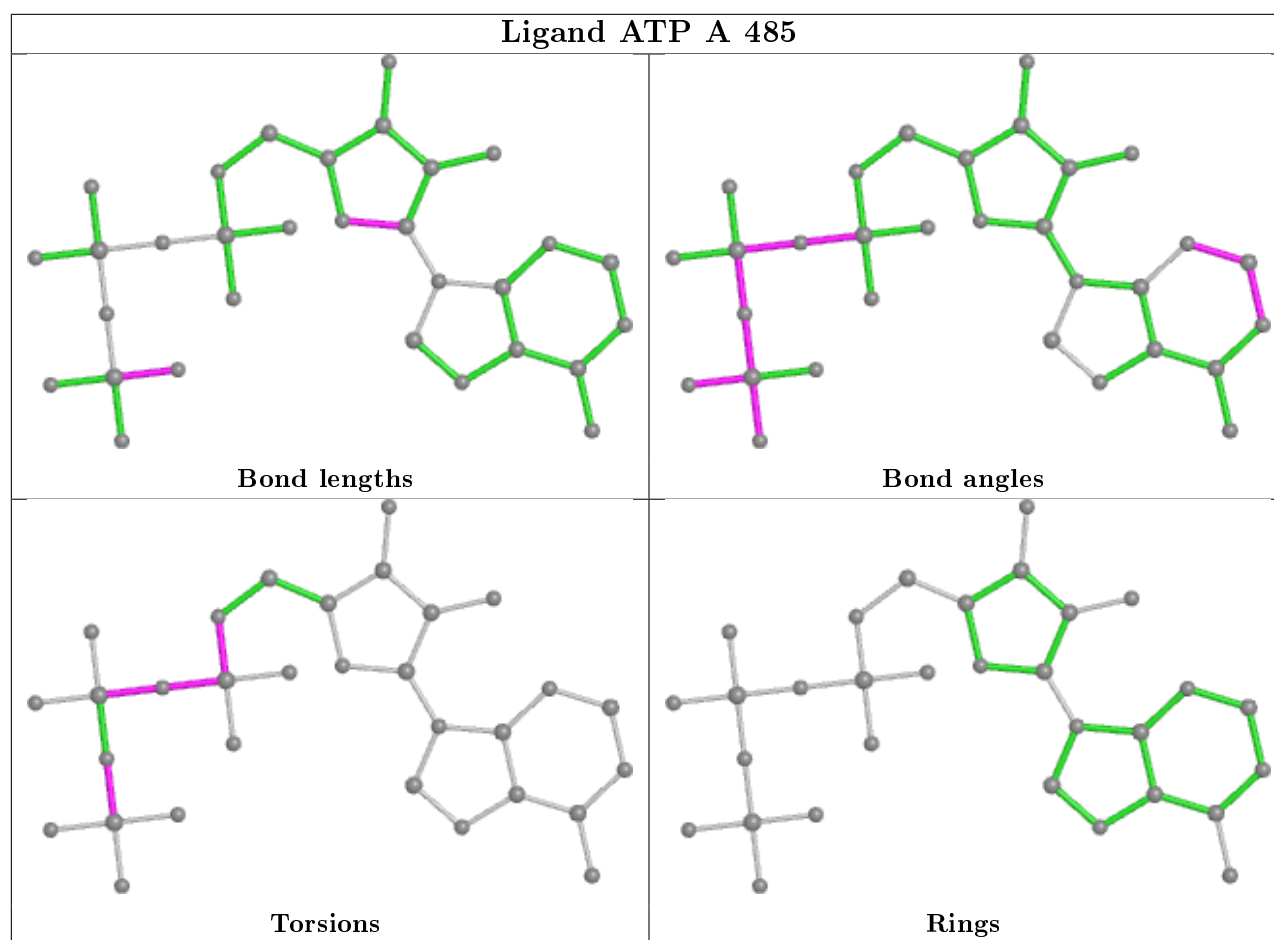
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	745	SO4	1	0
4	A	485	ATP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	351/373 (94%)	0.17	18 (5%)	28 35	19, 35, 58, 84	0
1	B	361/373 (96%)	0.03	10 (2%)	53 60	15, 32, 52, 64	0
All	All	712/746 (95%)	0.10	28 (3%)	39 46	15, 34, 56, 84	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	SER	7.5
1	A	145	HIS	6.5
1	A	144	TYR	3.9
1	B	641	ARG	3.9
1	B	304	ILE	3.8
1	A	641	ARG	3.8
1	A	645	ASN	3.6
1	B	649	LEU	3.1
1	A	181	ASN	3.1
1	A	262	HIS	3.0
1	A	651	ARG	2.9
1	A	305	VAL	2.9
1	B	145	HIS	2.8
1	B	647	ARG	2.8
1	B	250	GLY	2.7
1	B	737	ARG	2.6
1	B	673	LYS	2.5
1	A	654	SER	2.5
1	A	263	ARG	2.5
1	A	260	TYR	2.5
1	A	166	TRP	2.4
1	A	178	MET	2.4
1	A	179	VAL	2.4
1	B	251	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	673	LYS	2.1
1	A	261	GLU	2.1
1	B	258	LYS	2.1
1	A	182	THR	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

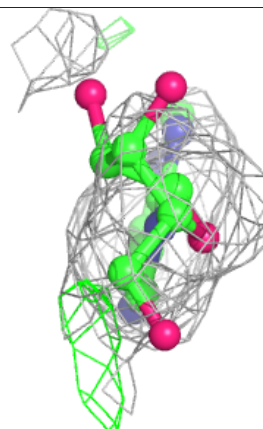
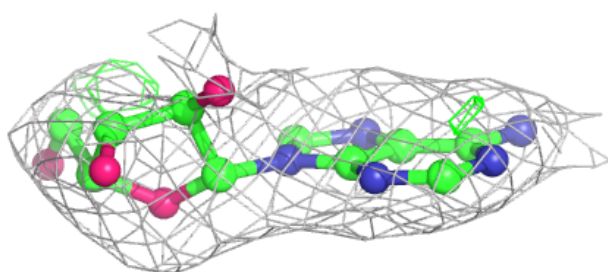
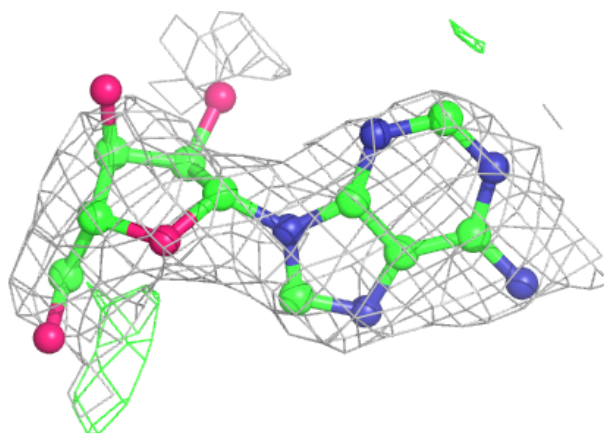
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	744	1/1	0.75	0.17	59,59,59,59	0
6	ADN	B	486	19/19	0.77	0.20	72,75,79,80	0
2	MG	A	743	1/1	0.78	0.10	46,46,46,46	0
3	SO4	B	744	5/5	0.81	0.17	86,87,88,89	0
3	SO4	A	745	5/5	0.89	0.15	62,64,66,66	0
4	ATP	A	485	31/31	0.94	0.14	32,47,66,67	0
5	NI	B	743	1/1	0.97	0.06	59,59,59,59	0

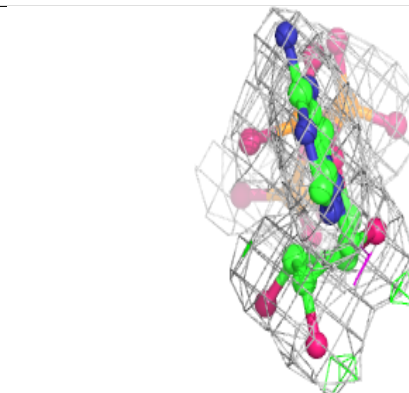
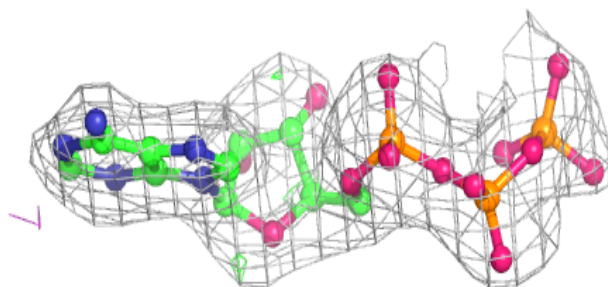
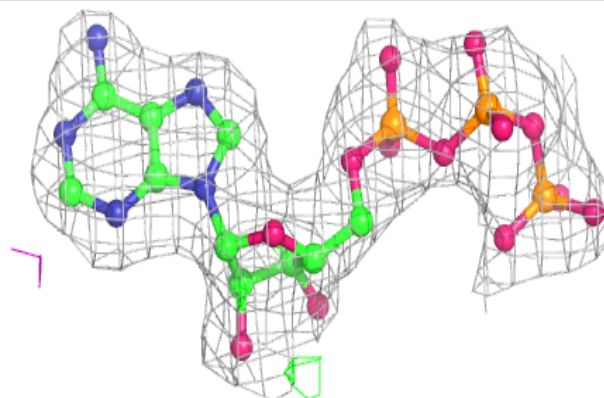
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN B 486:

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

**Electron density around ATP A 485:**

$2mF_o-DF_c$ (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.