



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:13 AM UTC

PDB ID : 2VWI / pdb_00002vwi
Title : Structure of the OSR1 kinase, a hypertension drug target
Authors : Villa, F.; Deak, M.; Alessi, D.R.; vanAalten, D.M.F.
Deposited on : 2008-06-25
Resolution : 2.15 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

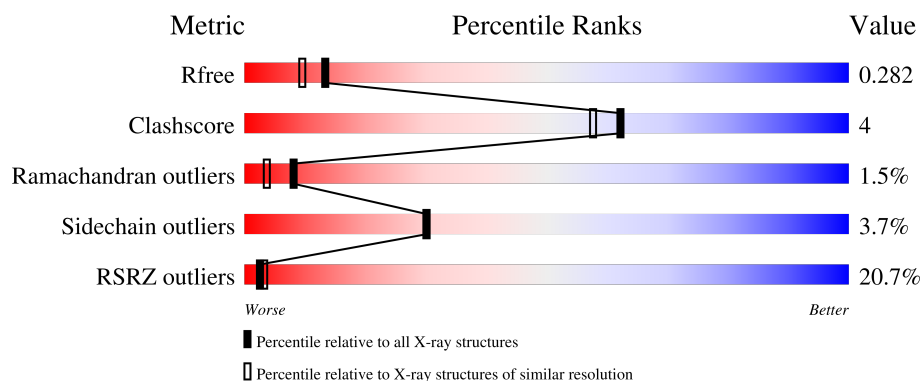
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	303	21% 66% 11% • 22%
1	B	303	27% 74% 11% • 13%
1	C	303	11% 79% 9% • 11%
1	D	303	13% 85% 8% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8508 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.

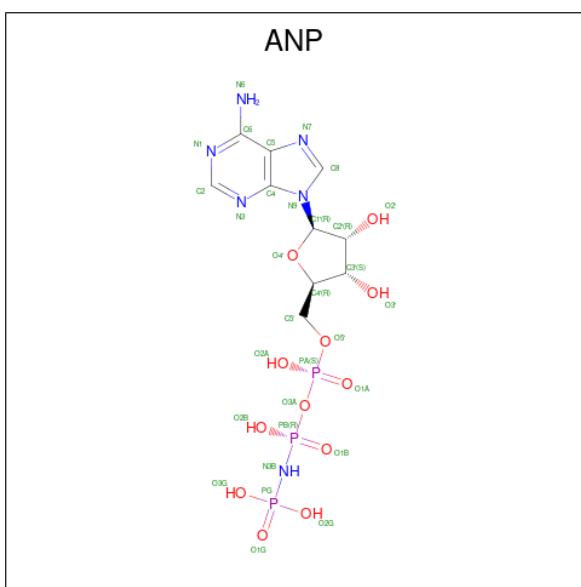
- Molecule 1 is a protein called SERINE/THREONINE-PROTEIN KINASE OSR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	1
			1792	1155	302	325	10			
1	B	264	Total	C	N	O	S	0	1	0
			2040	1306	343	378	13			
1	C	271	Total	C	N	O	S	0	0	1
			2106	1346	358	389	13			
1	D	284	Total	C	N	O	S	0	0	0
			2204	1406	374	410	14			

- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Au	0	0
			3	3		
2	B	4	Total	Au	0	0
			4	4		
2	C	2	Total	Au	0	0
			2	2		
2	D	2	Total	Au	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	32	Total	O	0	0
			32	32		

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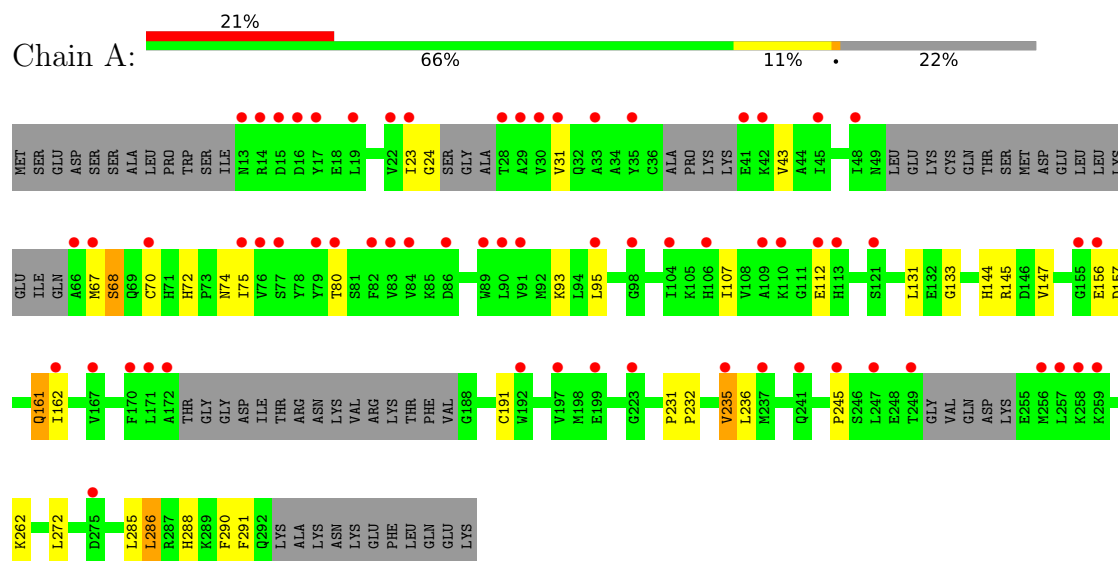
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	55	Total	O	0	0
			55	55		
5	D	91	Total	O	0	0
			91	91		

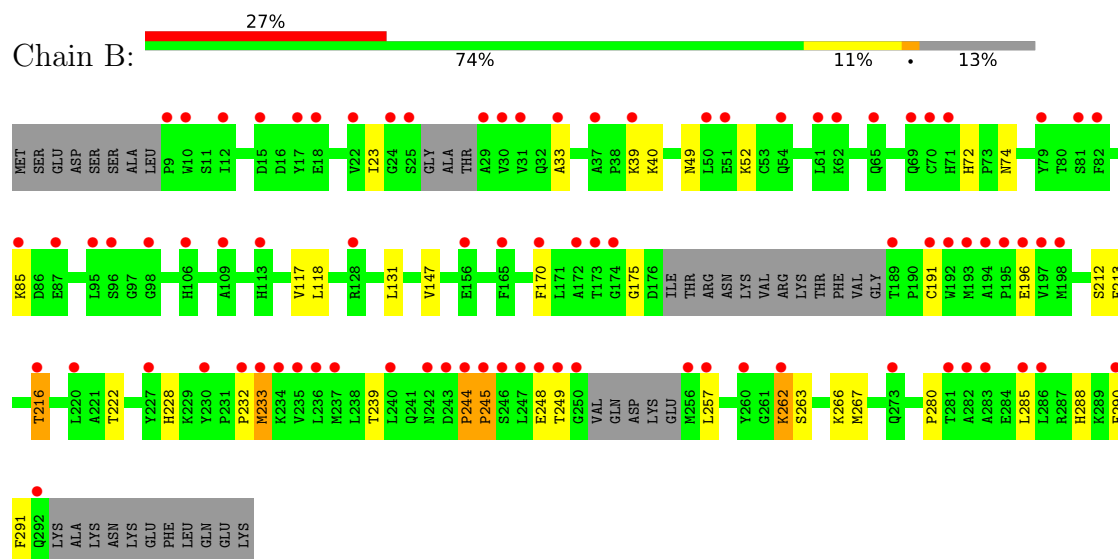
3 Residue-property plots [i](#)

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: SERINE/THREONINE-PROTEIN KINASE OSR1

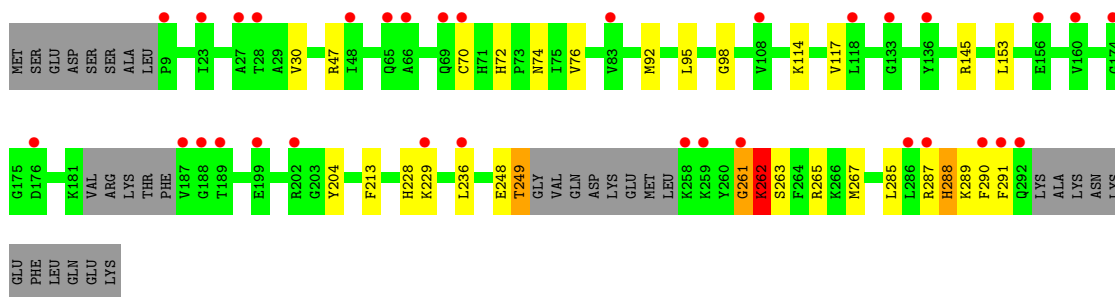


• Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1



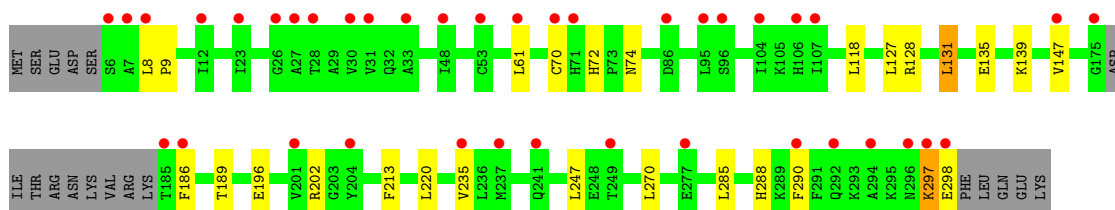
• Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1

Chain C:  11% 79% 9% 1%



• Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1

Chain D:  13% 85% 8% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.13Å 99.90Å 158.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.15 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.94-2.15) 98.5 (19.94-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.253 , 0.287 0.252 , 0.282	Depositor DCC
R_{free} test set	637 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8508	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% 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, AU, 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	0.48	1/1826 (0.1%)	0.84	0/2469
1	B	0.45	0/2083	0.81	3/2812 (0.1%)
1	C	0.47	1/2148 (0.0%)	0.79	0/2900
1	D	0.46	0/2247	0.79	2/3028 (0.1%)
All	All	0.47	2/8304 (0.0%)	0.81	5/11209 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	PHE	C-N	-7.08	1.23	1.33
1	A	291	PHE	C-N	-6.98	1.23	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	PRO	N-CA-C	6.84	119.04	110.70
1	B	244	PRO	CA-C-N	5.17	126.30	119.84
1	B	244	PRO	C-N-CA	5.17	126.30	119.84
1	D	189	THR	CA-C-N	5.05	126.15	119.84
1	D	189	THR	C-N-CA	5.05	126.15	119.84

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	1792	0	1761	20	0
1	B	2040	0	2031	22	0
1	C	2106	0	2124	17	0
1	D	2204	0	2225	10	0
2	A	3	0	0	3	0
2	B	4	0	0	1	0
2	C	2	0	0	0	0
2	D	2	0	0	1	0
3	A	31	0	13	0	0
3	B	31	0	12	0	0
3	C	31	0	13	0	0
3	D	31	0	13	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	50	0	0	0	0
5	B	32	0	0	1	0
5	C	55	0	0	0	0
5	D	91	0	0	0	0
All	All	8508	0	8192	68	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 4.

All (68) 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:A:67:MET:HA	1:A:68:SER:HB2	1.30	1.13
1:D:70:CYS:SG	2:D:1301:AU:AU	1.89	1.00
2:A:1293:AU:AU	1:C:70:CYS:SG	1.99	0.91
1:A:191:CYS:SG	2:A:1296:AU:AU	2.04	0.86
1:A:131:LEU:HD21	1:A:285:LEU:HB3	1.65	0.78
1:B:245:PRO:HD2	1:B:248:GLU:HB2	1.67	0.77
1:A:70:CYS:SG	2:A:1295:AU:AU	2.17	0.71
1:B:131:LEU:HD21	1:B:285:LEU:HB3	1.73	0.70
1:A:72:HIS:HB3	1:A:75:ILE:HD12	1.76	0.67
1:A:67:MET:HA	1:A:68:SER:CB	2.13	0.67
1:D:297:LYS:O	1:D:298:GLU:HB2	1.95	0.66
1:A:107:ILE:HG23	1:A:112:GLU:HG3	1.79	0.65
1:B:191:CYS:SG	2:B:1296:AU:AU	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:MET:HE3	1:B:291:PHE:HE2	1.63	0.62
1:B:213:PHE:CE1	1:B:267:MET:HE1	2.35	0.61
1:D:135:GLU:O	1:D:139:LYS:HG2	2.02	0.58
1:C:213:PHE:CE2	1:C:267:MET:HE1	2.39	0.58
1:C:30:VAL:HG13	1:C:47:ARG:HB2	1.85	0.57
1:A:288:HIS:HD2	1:A:290:PHE:H	1.50	0.57
1:B:213:PHE:HE1	1:B:267:MET:HE1	1.70	0.56
1:C:261:GLY:HA2	1:C:265:ARG:HE	1.69	0.56
1:C:213:PHE:HE2	1:C:267:MET:HE1	1.71	0.56
1:A:72:HIS:HD2	1:A:74:ASN:H	1.55	0.55
1:D:72:HIS:CD2	1:D:74:ASN:H	2.25	0.54
1:A:23:ILE:N	1:A:24:GLY:HA3	2.23	0.53
1:B:212:SER:O	1:B:216:THR:HG23	2.09	0.52
1:D:288:HIS:HD2	1:D:290:PHE:H	1.57	0.52
1:C:248:GLU:O	1:C:249:THR:HB	2.10	0.51
1:B:49:ASN:HD22	1:B:52:LYS:H	1.60	0.49
1:B:262:LYS:HG3	1:B:263:SER:H	1.76	0.49
1:C:76:VAL:HG11	1:C:92:MET:HE2	1.94	0.49
1:B:228:HIS:NE2	1:B:249:THR:HG23	2.27	0.49
1:D:72:HIS:HD2	1:D:74:ASN:H	1.59	0.49
1:D:288:HIS:CD2	1:D:290:PHE:H	2.31	0.48
1:A:72:HIS:CD2	1:A:74:ASN:H	2.32	0.48
1:C:95:LEU:HD22	1:C:153:LEU:HB3	1.96	0.48
1:D:131:LEU:HD21	1:D:285:LEU:HB3	1.95	0.47
1:B:72:HIS:CD2	1:B:74:ASN:H	2.31	0.47
1:B:288:HIS:CD2	1:B:290:PHE:H	2.33	0.47
1:C:72:HIS:CD2	1:C:74:ASN:H	2.33	0.47
1:C:288:HIS:HD2	1:C:290:PHE:H	1.62	0.46
1:B:213:PHE:HE1	1:B:267:MET:CE	2.28	0.46
1:D:118:LEU:HD12	1:D:220:LEU:HB3	1.98	0.46
1:A:75:ILE:HD11	1:A:133:GLY:O	2.16	0.45
1:A:95:LEU:HD21	1:A:161:GLN:CD	2.40	0.45
1:B:280:PRO:HG2	1:B:285:LEU:HG	1.98	0.45
1:A:288:HIS:CD2	1:A:290:PHE:H	2.33	0.45
1:C:267:MET:HE2	1:C:285:LEU:HD11	1.99	0.45
1:A:131:LEU:HD23	1:A:286:LEU:HD13	2.00	0.44
1:B:239:THR:HA	5:B:2026:HOH:O	2.18	0.44
1:B:267:MET:HE3	1:B:291:PHE:CE2	2.49	0.44
1:A:245:PRO:HB2	1:A:272:LEU:HD13	2.00	0.43
1:B:23:ILE:HD11	1:B:33:ALA:HB2	2.00	0.43
1:B:170:PHE:CZ	1:B:175:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:HB	1:B:249:THR:HG21	2.00	0.43
1:C:72:HIS:HD2	1:C:74:ASN:H	1.66	0.43
1:C:228:HIS:CE1	1:C:229:LYS:HG3	2.53	0.43
1:A:231:PRO:HG3	1:C:98:GLY:HA3	2.02	0.42
1:A:144:HIS:O	1:A:145:ARG:HB2	2.19	0.42
1:A:23:ILE:HD12	1:A:31:VAL:HG12	2.02	0.41
1:B:232:PRO:O	1:B:233:MET:CB	2.67	0.41
1:D:127:LEU:HB3	1:D:213:PHE:CZ	2.55	0.41
1:B:117:VAL:HG12	1:B:118:LEU:HD12	2.03	0.41
1:C:262:LYS:HB3	1:C:263:SER:H	1.66	0.41
1:B:244:PRO:HA	1:B:245:PRO:HD3	1.81	0.41
1:C:213:PHE:HE2	1:C:267:MET:CE	2.33	0.40
1:A:232:PRO:O	1:A:235:VAL:HG13	2.21	0.40
1:C:145:ARG:HE	1:C:204:TYR:HH	1.68	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	225/303 (74%)	211 (94%)	13 (6%)	1 (0%)	30	26
1	B	256/303 (84%)	236 (92%)	15 (6%)	5 (2%)	6	2
1	C	265/303 (88%)	251 (95%)	9 (3%)	5 (2%)	6	2
1	D	280/303 (92%)	266 (95%)	10 (4%)	4 (1%)	9	4
All	All	1026/1212 (85%)	964 (94%)	47 (5%)	15 (2%)	8	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	LYS

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Mol	Chain	Res	Type
1	B	40	LYS
1	D	8	LEU
1	B	233	MET
1	C	261	GLY
1	C	287	ARG
1	B	262	LYS
1	C	288	HIS
1	A	68	SER
1	C	262	LYS
1	B	245	PRO
1	D	186	PHE
1	D	297	LYS
1	C	117	VAL
1	D	9	PRO

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	183/260 (70%)	171 (93%)	12 (7%)	15	10
1	B	218/260 (84%)	212 (97%)	6 (3%)	38	40
1	C	227/260 (87%)	222 (98%)	5 (2%)	45	51
1	D	237/260 (91%)	228 (96%)	9 (4%)	29	29
All	All	865/1040 (83%)	833 (96%)	32 (4%)	30	30

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	80	THR
1	A	93	LYS
1	A	147	VAL
1	A	156	GLU
1	A	157	ASP
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	162	ILE
1	A	235	VAL
1	A	236	LEU
1	A	262	LYS
1	A	286	LEU
1	B	85	LYS
1	B	147	VAL
1	B	196	GLU
1	B	216	THR
1	B	257	LEU
1	B	266	LYS
1	C	114	LYS
1	C	236	LEU
1	C	249	THR
1	C	262	LYS
1	C	289	LYS
1	D	61	LEU
1	D	128	ARG
1	D	131	LEU
1	D	147	VAL
1	D	196	GLU
1	D	202	ARG
1	D	235	VAL
1	D	247	LEU
1	D	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	74	ASN
1	A	113	HIS
1	A	200	GLN
1	A	288	HIS
1	B	32	GLN
1	B	49	ASN
1	B	65	GLN
1	B	69	GLN
1	B	72	HIS
1	B	74	ASN
1	B	140	ASN
1	B	273	GLN

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Mol	Chain	Res	Type
1	B	288	HIS
1	C	69	GLN
1	C	72	HIS
1	C	140	ASN
1	C	151	ASN
1	C	180	ASN
1	C	228	HIS
1	D	72	HIS
1	D	142	GLN
1	D	273	GLN
1	D	288	HIS

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](#)

Of 18 ligands modelled in this entry, 14 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
3	ANP	B	1295	4	33,33,33	2.38	8 (24%)	45,52,52	1.98	11 (24%)
3	ANP	C	1294	4	33,33,33	2.36	6 (18%)	45,52,52	1.95	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	1294	-	33,33,33	2.36	9 (27%)	45,52,52	1.99	12 (26%)
3	ANP	D	1300	4	33,33,33	2.36	9 (27%)	45,52,52	1.95	11 (24%)

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
3	ANP	B	1295	4	-	3/18/38/38	0/3/3/3
3	ANP	C	1294	4	-	5/18/38/38	0/3/3/3
3	ANP	A	1294	-	-	4/18/38/38	0/3/3/3
3	ANP	D	1300	4	-	3/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1294	ANP	PG-O1G	11.07	1.62	1.46
3	D	1300	ANP	PG-O1G	11.07	1.62	1.46
3	B	1295	ANP	PG-O1G	10.91	1.62	1.46
3	A	1294	ANP	PG-O1G	10.85	1.62	1.46
3	D	1300	ANP	C5-N7	-3.23	1.33	1.39
3	A	1294	ANP	C5-N7	-3.19	1.33	1.39
3	C	1294	ANP	PB-O2B	-3.18	1.48	1.56
3	A	1294	ANP	PB-O2B	-3.17	1.48	1.56
3	B	1295	ANP	C5-N7	-3.17	1.33	1.39
3	B	1295	ANP	PB-O2B	-3.10	1.48	1.56
3	D	1300	ANP	PB-O2B	-3.07	1.48	1.56
3	C	1294	ANP	C5-N7	-3.05	1.33	1.39
3	B	1295	ANP	PG-O3G	-2.99	1.48	1.56
3	B	1295	ANP	PB-O3A	2.91	1.62	1.59
3	D	1300	ANP	PG-O3G	-2.91	1.49	1.56
3	A	1294	ANP	PG-O3G	-2.91	1.49	1.56
3	B	1295	ANP	PA-O3A	2.87	1.62	1.59
3	C	1294	ANP	PG-O3G	-2.81	1.49	1.56
3	A	1294	ANP	PB-O3A	2.56	1.62	1.59
3	A	1294	ANP	PA-O3A	2.55	1.62	1.59
3	C	1294	ANP	PG-O2G	2.36	1.63	1.56
3	D	1300	ANP	PA-O3A	2.25	1.61	1.59
3	A	1294	ANP	PG-O2G	2.22	1.62	1.56
3	D	1300	ANP	PB-O3A	2.16	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1300	ANP	PG-O2G	2.13	1.62	1.56
3	D	1300	ANP	C8-N9	-2.11	1.34	1.37
3	A	1294	ANP	C8-N9	-2.08	1.34	1.37
3	C	1294	ANP	C4-N9	-2.06	1.33	1.37
3	B	1295	ANP	C8-N9	-2.03	1.34	1.37
3	A	1294	ANP	C4-N9	-2.02	1.33	1.37
3	B	1295	ANP	C4-N9	-2.01	1.33	1.37
3	D	1300	ANP	C4-N9	-2.00	1.33	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1295	ANP	C5-C4-N3	-5.46	119.20	126.72
3	A	1294	ANP	C5-C4-N3	-5.41	119.27	126.72
3	C	1294	ANP	C5-C4-N3	-5.21	119.55	126.72
3	D	1300	ANP	C5-C4-N3	-5.20	119.56	126.72
3	D	1300	ANP	N3-C2-N1	-4.76	121.38	128.58
3	C	1294	ANP	N3-C2-N1	-4.73	121.43	128.58
3	B	1295	ANP	N3-C2-N1	-4.64	121.55	128.58
3	A	1294	ANP	N3-C2-N1	-4.56	121.67	128.58
3	C	1294	ANP	O2B-PB-O1B	4.50	119.51	109.87
3	B	1295	ANP	O2B-PB-O1B	4.37	119.24	109.87
3	D	1300	ANP	O2B-PB-O1B	4.30	119.09	109.87
3	A	1294	ANP	O2B-PB-O1B	4.18	118.84	109.87
3	A	1294	ANP	N3-C4-N9	3.76	133.56	127.17
3	B	1295	ANP	N3-C4-N9	3.76	133.56	127.17
3	D	1300	ANP	N3-C4-N9	3.72	133.50	127.17
3	C	1294	ANP	N3-C4-N9	3.64	133.36	127.17
3	B	1295	ANP	C2-N3-C4	3.63	120.70	111.83
3	B	1295	ANP	O2G-PG-O1G	-3.62	104.36	113.45
3	D	1300	ANP	O2G-PG-O1G	-3.59	104.44	113.45
3	A	1294	ANP	C2-N3-C4	3.59	120.59	111.83
3	C	1294	ANP	C2-N3-C4	3.57	120.56	111.83
3	D	1300	ANP	C2-N3-C4	3.55	120.49	111.83
3	A	1294	ANP	O2G-PG-O1G	-3.47	104.74	113.45
3	A	1294	ANP	O1G-PG-N3B	-3.28	106.94	111.77
3	C	1294	ANP	O2G-PG-O1G	-3.27	105.24	113.45
3	A	1294	ANP	O1B-PB-N3B	-3.24	107.00	111.77
3	D	1300	ANP	N9-C8-N7	-3.21	109.38	113.94
3	C	1294	ANP	N9-C8-N7	-3.18	109.43	113.94
3	B	1295	ANP	N9-C8-N7	-3.10	109.54	113.94
3	A	1294	ANP	N9-C8-N7	-3.05	109.61	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1294	ANP	O1G-PG-N3B	-2.98	107.39	111.77
3	B	1295	ANP	O1B-PB-N3B	-2.88	107.53	111.77
3	D	1300	ANP	C5-N7-C8	2.86	107.94	103.45
3	B	1295	ANP	C5-N7-C8	2.83	107.90	103.45
3	C	1294	ANP	O1B-PB-N3B	-2.77	107.69	111.77
3	A	1294	ANP	C5-N7-C8	2.76	107.79	103.45
3	C	1294	ANP	C5-N7-C8	2.75	107.77	103.45
3	B	1295	ANP	C4-C5-N7	-2.71	107.48	110.58
3	A	1294	ANP	C4-C5-N7	-2.62	107.58	110.58
3	D	1300	ANP	O1G-PG-N3B	-2.58	107.97	111.77
3	D	1300	ANP	C4-C5-N7	-2.57	107.64	110.58
3	B	1295	ANP	O1G-PG-N3B	-2.56	108.00	111.77
3	C	1294	ANP	C4-C5-N7	-2.53	107.69	110.58
3	D	1300	ANP	C4-N9-C8	2.24	108.09	105.74
3	C	1294	ANP	C4-N9-C8	2.17	108.02	105.74
3	A	1294	ANP	C4-N9-C8	2.01	107.85	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

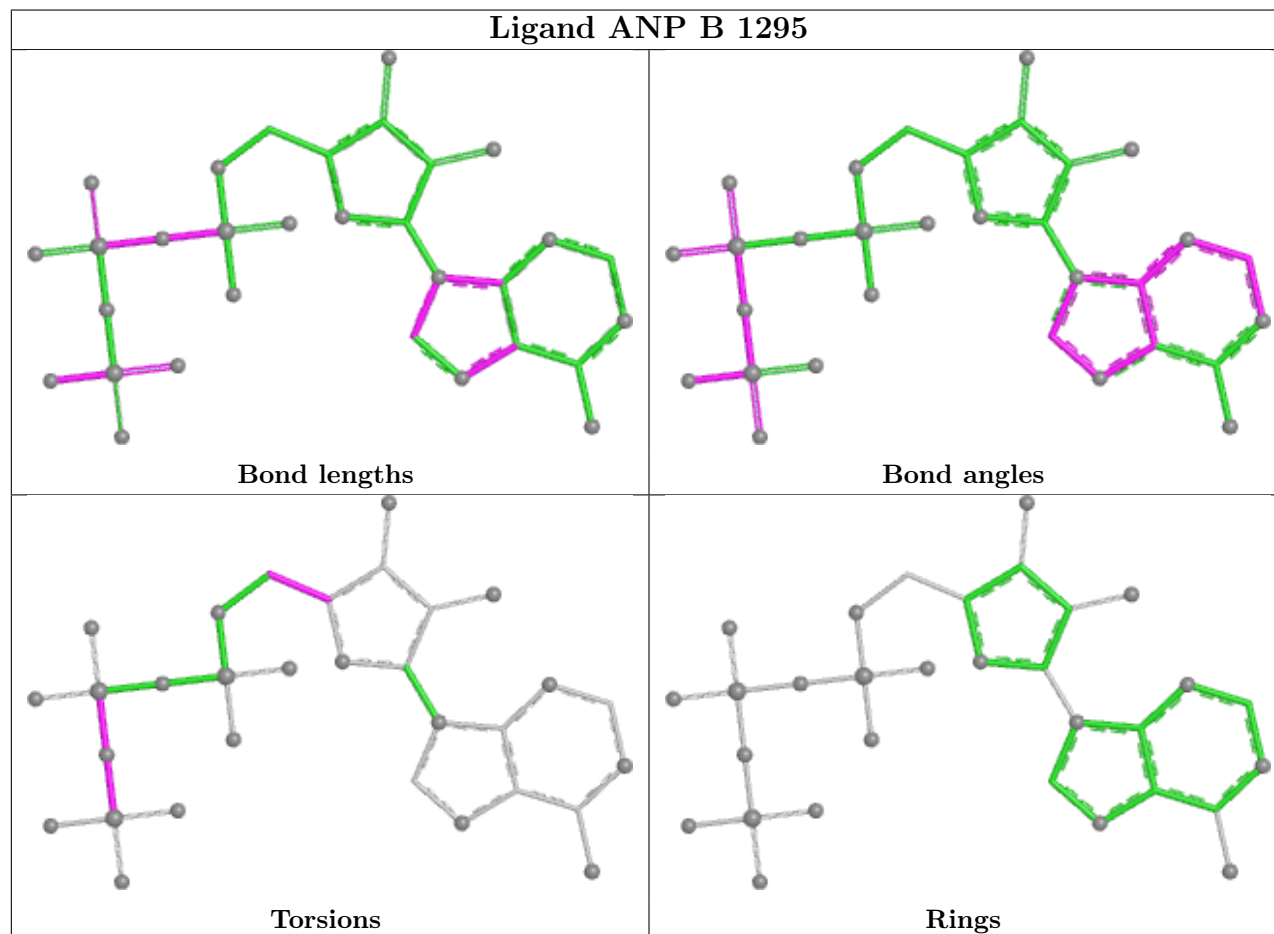
Mol	Chain	Res	Type	Atoms
3	A	1294	ANP	PB-N3B-PG-O1G
3	A	1294	ANP	PG-N3B-PB-O1B
3	A	1294	ANP	PA-O3A-PB-O1B
3	B	1295	ANP	PB-N3B-PG-O1G
3	B	1295	ANP	PG-N3B-PB-O3A
3	C	1294	ANP	PB-N3B-PG-O1G
3	D	1300	ANP	PB-N3B-PG-O1G
3	D	1300	ANP	PG-N3B-PB-O3A
3	D	1300	ANP	C5'-O5'-PA-O3A
3	B	1295	ANP	O4'-C4'-C5'-O5'
3	C	1294	ANP	PG-N3B-PB-O1B
3	C	1294	ANP	PB-O3A-PA-O2A
3	A	1294	ANP	PG-N3B-PB-O3A
3	C	1294	ANP	PG-N3B-PB-O3A
3	C	1294	ANP	PB-O3A-PA-O1A

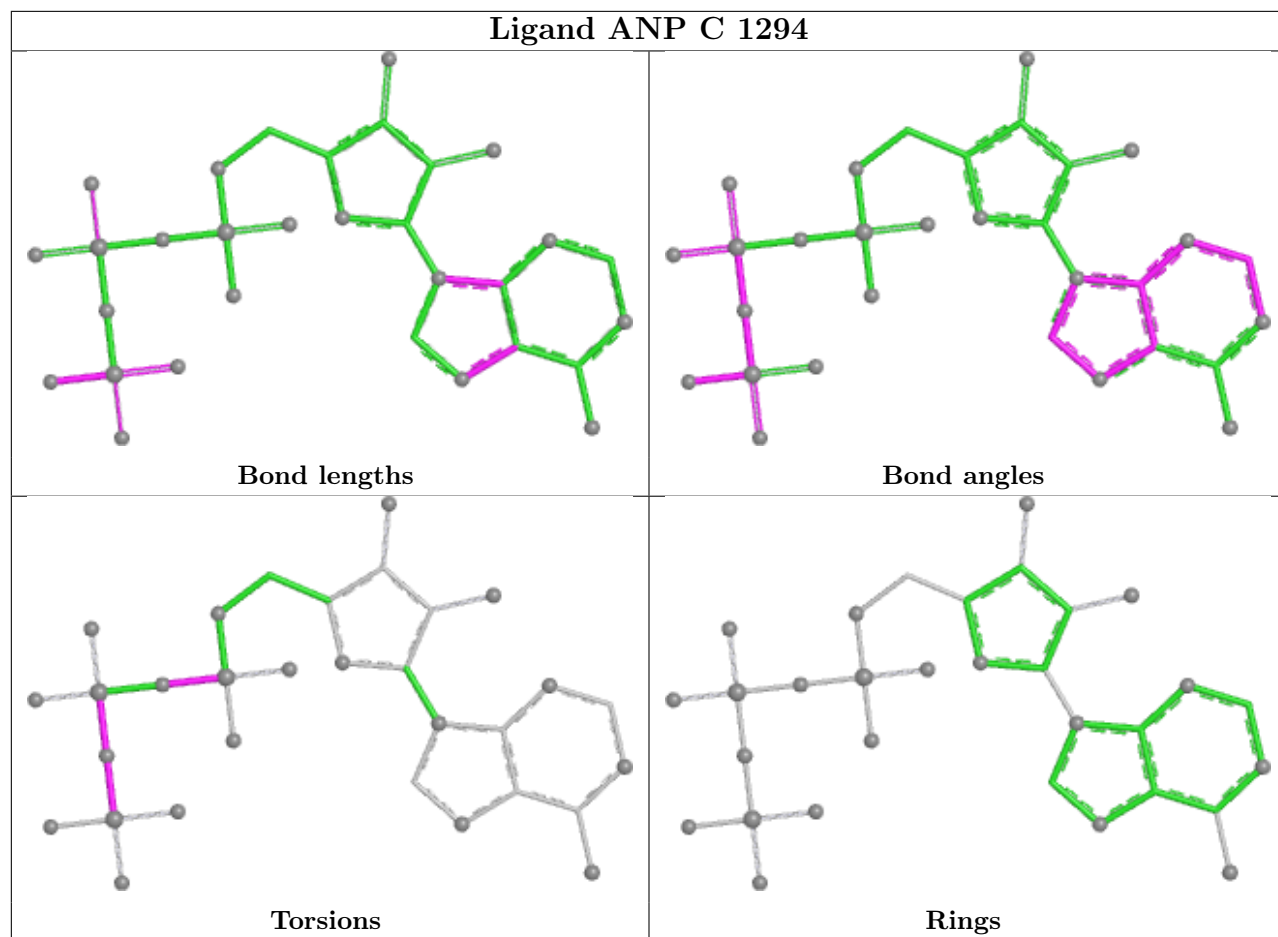
There are no ring outliers.

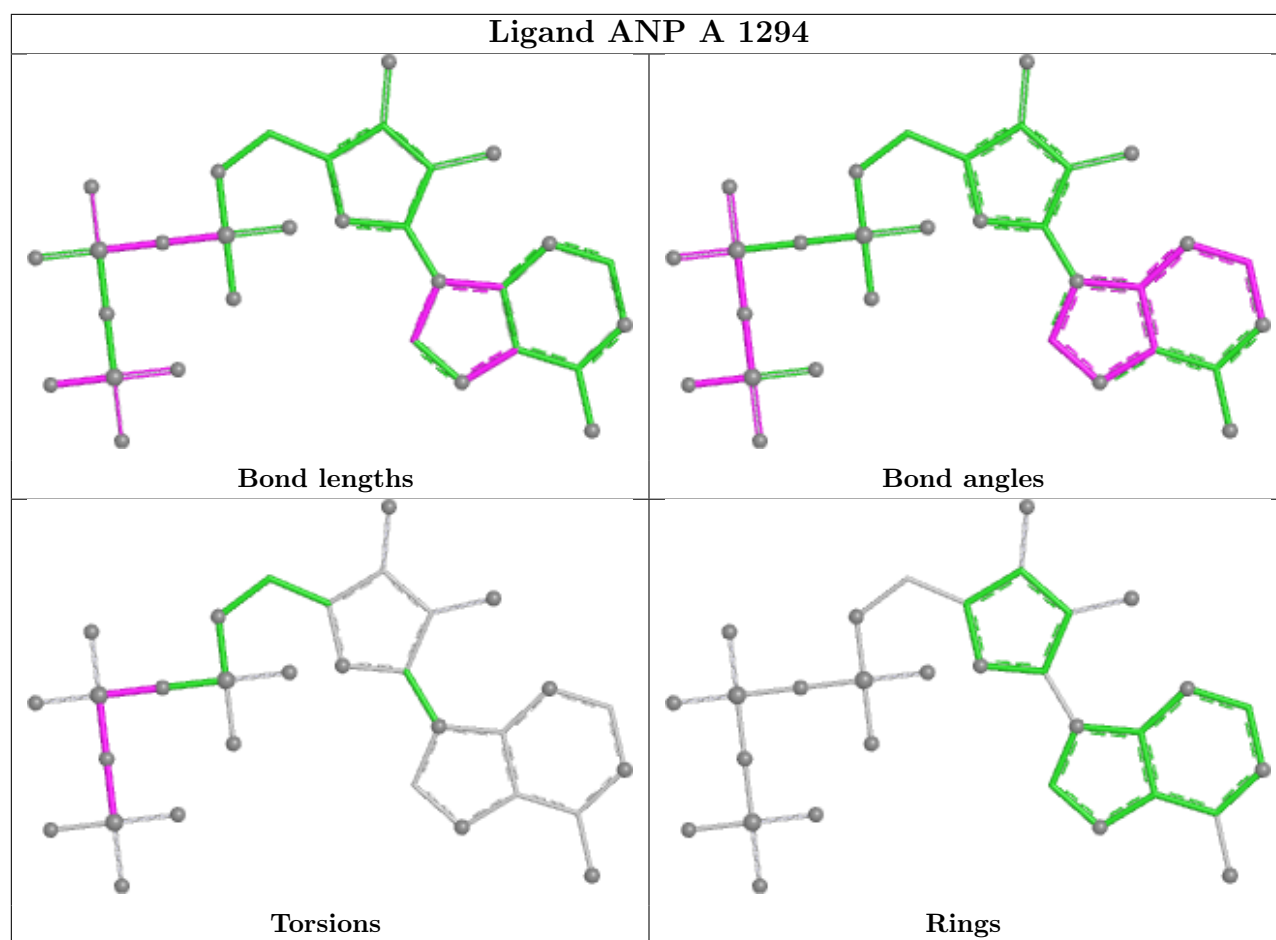
No monomer is involved in short contacts.

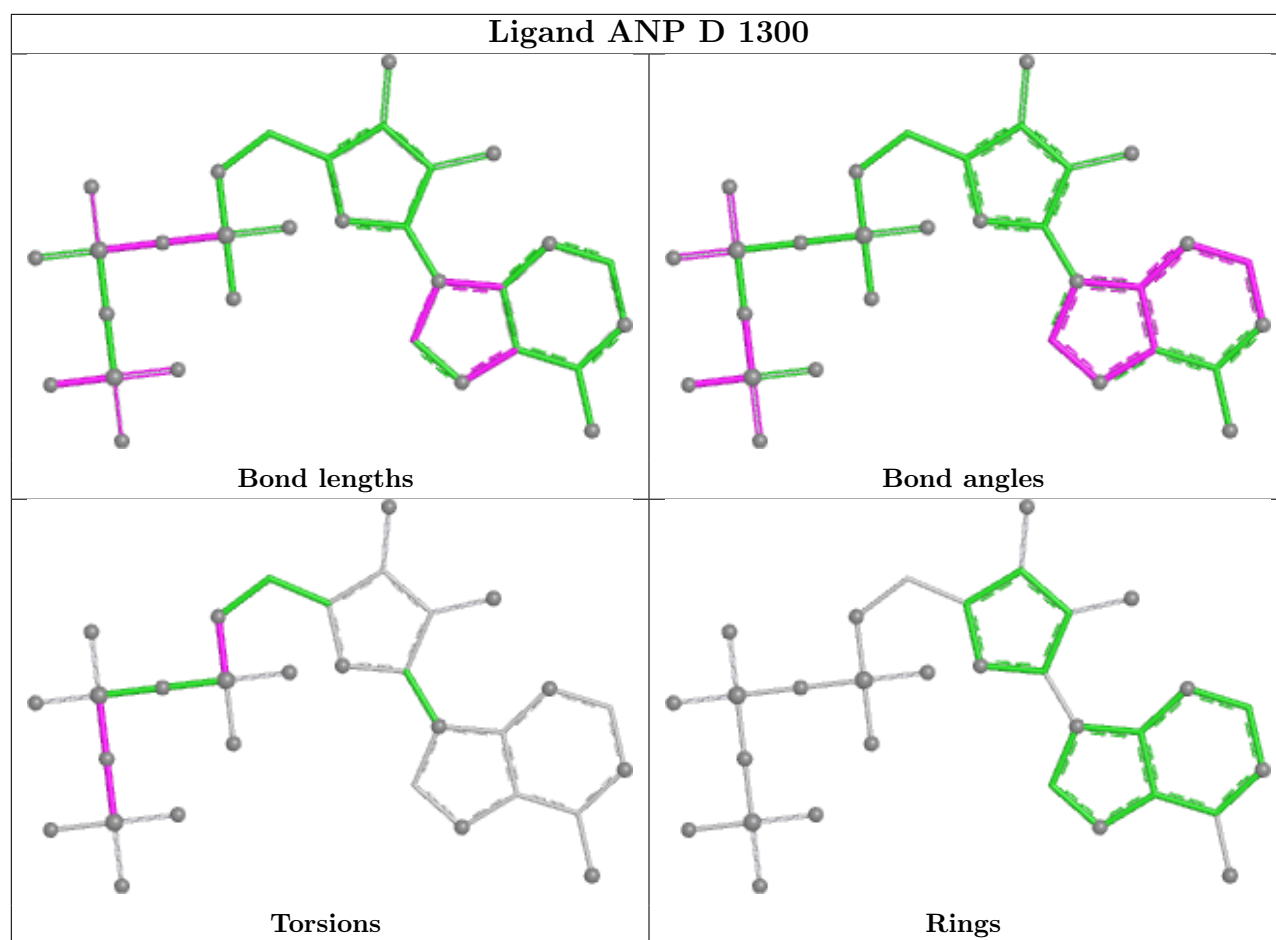
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	291:PHE	C	292:GLN	N	3.44

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	237/303 (78%)	1.70	64 (27%) ⓘ ⓘ	38, 50, 65, 67	0
1	B	264/303 (87%)	1.72	83 (31%) ⓘ ⓘ	37, 53, 66, 78	1 (0%)
1	C	271/303 (89%)	1.18	33 (12%) ⓘ ⓘ	39, 49, 56, 58	0
1	D	284/303 (93%)	1.29	39 (13%) ⓘ ⓘ	37, 50, 61, 66	0
All	All	1056/1212 (87%)	1.46	219 (20%) ⓘ ⓘ	37, 51, 64, 78	1 (0%)

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	THR	6.9
1	C	187	VAL	6.1
1	B	243[A]	ASP	5.5
1	A	172	ALA	5.2
1	A	22	VAL	5.1
1	B	249	THR	5.0
1	A	30	VAL	5.0
1	C	261	GLY	4.9
1	A	19	LEU	4.7
1	B	39	LYS	4.6
1	A	89	TRP	4.5
1	C	28	THR	4.4
1	D	297	LYS	4.2
1	D	27	ALA	4.2
1	A	84	VAL	4.2
1	B	250	GLY	4.1
1	B	192	TRP	4.1
1	D	7	ALA	4.1
1	B	156	GLU	4.0
1	B	191	CYS	4.0
1	A	13	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	3.8
1	A	29	ALA	3.8
1	D	28	THR	3.8
1	B	232	PRO	3.7
1	A	259	LYS	3.7
1	B	235	VAL	3.7
1	D	186	PHE	3.7
1	B	173	THR	3.7
1	A	86	ASP	3.7
1	A	23	ILE	3.6
1	A	171	LEU	3.6
1	B	244	PRO	3.6
1	A	42	LYS	3.6
1	B	257	LEU	3.5
1	D	292	GLN	3.5
1	D	8	LEU	3.5
1	B	98	GLY	3.5
1	B	242	ASN	3.5
1	D	296	ASN	3.5
1	B	71	HIS	3.4
1	A	33	ALA	3.4
1	B	248	GLU	3.4
1	A	112	GLU	3.4
1	B	233	MET	3.4
1	A	31	VAL	3.3
1	A	170	PHE	3.3
1	A	257	LEU	3.3
1	A	35	TYR	3.2
1	B	17	TYR	3.2
1	A	249	THR	3.2
1	B	70	CYS	3.2
1	A	75	ILE	3.2
1	A	66	ALA	3.1
1	A	167	VAL	3.1
1	B	31	VAL	3.1
1	B	194	ALA	3.1
1	A	247	LEU	3.1
1	C	229	LYS	3.1
1	B	87	GLU	3.1
1	B	51	GLU	3.1
1	B	69	GLN	3.1
1	C	27	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	121	SER	3.0
1	B	195	PRO	3.0
1	B	245	PRO	3.0
1	C	291	PHE	3.0
1	A	237	MET	3.0
1	B	25	SER	3.0
1	D	298	GLU	3.0
1	C	69	GLN	3.0
1	B	33	ALA	2.9
1	A	91	VAL	2.9
1	B	165	PHE	2.9
1	A	192	TRP	2.9
1	D	30	VAL	2.9
1	B	113	HIS	2.9
1	D	235	VAL	2.9
1	A	79	TYR	2.9
1	A	275	ASP	2.8
1	D	237	MET	2.8
1	B	96	SER	2.8
1	C	136	TYR	2.8
1	A	95	LEU	2.8
1	B	61	LEU	2.8
1	A	45	ILE	2.8
1	B	292	GLN	2.8
1	B	283	ALA	2.8
1	A	197	VAL	2.8
1	C	70	CYS	2.8
1	B	29	ALA	2.8
1	B	109	ALA	2.7
1	A	162	ILE	2.7
1	A	155	GLY	2.7
1	A	156	GLU	2.7
1	B	15	ASP	2.7
1	A	82	PHE	2.7
1	B	237	MET	2.7
1	A	113	HIS	2.6
1	B	106	HIS	2.6
1	D	106	HIS	2.6
1	D	96	SER	2.6
1	B	85	LYS	2.6
1	B	197	VAL	2.6
1	D	277	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	189	THR	2.6
1	B	82	PHE	2.6
1	A	16	ASP	2.6
1	D	61	LEU	2.6
1	D	6	SER	2.6
1	D	104	ILE	2.6
1	B	256	MET	2.6
1	C	176	ASP	2.6
1	B	285	LEU	2.6
1	C	292	GLN	2.5
1	D	204	TYR	2.5
1	B	240	LEU	2.5
1	A	41	GLU	2.5
1	D	290	PHE	2.5
1	D	71	HIS	2.5
1	C	9	PRO	2.5
1	D	95	LEU	2.5
1	B	262	LYS	2.5
1	C	290	PHE	2.5
1	C	65	GLN	2.4
1	B	260	TYR	2.4
1	D	185	THR	2.4
1	D	294	ALA	2.4
1	B	50	LEU	2.4
1	B	62	LYS	2.4
1	B	30	VAL	2.4
1	B	246	SER	2.4
1	B	9	PRO	2.4
1	A	109	ALA	2.4
1	B	286	LEU	2.4
1	C	23	ILE	2.4
1	A	67	MET	2.4
1	B	230	TYR	2.4
1	B	281	THR	2.4
1	C	189	THR	2.4
1	C	259	LYS	2.4
1	C	236	LEU	2.4
1	B	196	GLU	2.4
1	B	65	GLN	2.4
1	A	235	VAL	2.4
1	D	70	CYS	2.4
1	C	118	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	31	VAL	2.3
1	A	245	PRO	2.3
1	A	48	ILE	2.3
1	A	83	VAL	2.3
1	D	53	CYS	2.3
1	D	33	ALA	2.3
1	A	14	ARG	2.3
1	C	174	GLY	2.3
1	B	216	THR	2.3
1	B	282	ALA	2.3
1	D	86	ASP	2.3
1	A	256	MET	2.3
1	B	236	LEU	2.3
1	D	23	ILE	2.2
1	C	108	VAL	2.2
1	B	24	GLY	2.2
1	B	198	MET	2.2
1	D	26	GLY	2.2
1	B	95	LEU	2.2
1	A	199	GLU	2.2
1	B	81	SER	2.2
1	B	170	PHE	2.2
1	B	12	ILE	2.2
1	D	107	ILE	2.2
1	B	174	GLY	2.2
1	B	37	ALA	2.2
1	B	79	TYR	2.2
1	B	227	TYR	2.2
1	C	202	ARG	2.2
1	A	80	THR	2.2
1	A	104	ILE	2.2
1	A	223	GLY	2.2
1	B	18	GLU	2.2
1	B	220	LEU	2.2
1	B	247	LEU	2.2
1	C	156	GLU	2.1
1	C	199	GLU	2.1
1	B	22	VAL	2.1
1	B	54	GLN	2.1
1	B	273	GLN	2.1
1	C	188	GLY	2.1
1	D	175	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	70	CYS	2.1
1	A	258	LYS	2.1
1	C	258	LYS	2.1
1	D	12	ILE	2.1
1	D	201	VAL	2.1
1	A	90	LEU	2.1
1	A	15	ASP	2.1
1	A	241	GLN	2.1
1	A	106	HIS	2.1
1	D	48	ILE	2.1
1	C	160	VAL	2.1
1	D	147	VAL	2.1
1	D	241	GLN	2.1
1	B	128	ARG	2.1
1	C	133	GLY	2.1
1	C	83	VAL	2.1
1	B	10	TRP	2.1
1	A	77	SER	2.1
1	C	66	ALA	2.1
1	C	286	LEU	2.0
1	C	287	ARG	2.0
1	A	98	GLY	2.0
1	C	48	ILE	2.0
1	A	76	VAL	2.0
1	B	290	PHE	2.0
1	B	193	MET	2.0
1	B	172	ALA	2.0
1	A	110	LYS	2.0
1	B	234	LYS	2.0
1	D	249	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

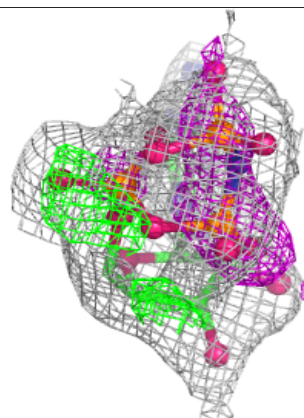
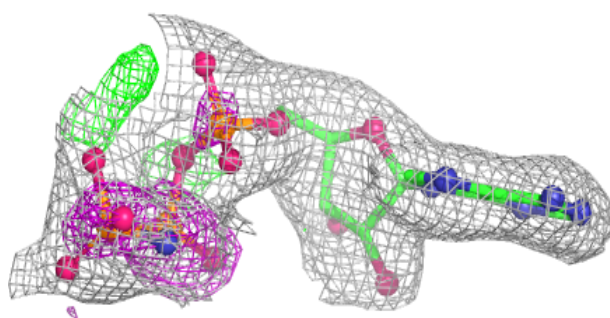
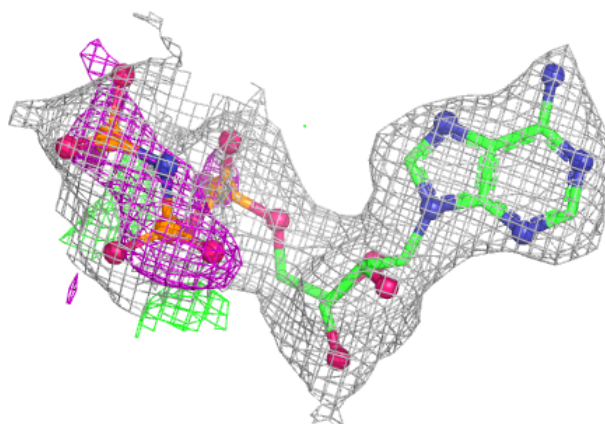
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	B	1295	31/31	0.78	0.13	55,57,65,65	0
3	ANP	A	1294	31/31	0.79	0.12	63,64,70,70	0
3	ANP	D	1300	31/31	0.79	0.13	39,41,57,58	0
4	MG	B	1293	1/1	0.82	0.12	58,58,58,58	0
3	ANP	C	1294	31/31	0.87	0.11	26,29,45,46	0
2	AU	C	1295	1/1	0.90	0.09	65,65,65,65	1
4	MG	C	1293	1/1	0.91	0.13	40,40,40,40	0
4	MG	D	1299	1/1	0.93	0.07	42,42,42,42	0
2	AU	B	1297	1/1	0.94	0.16	78,78,78,78	1
2	AU	B	1296	1/1	0.96	0.17	55,55,55,55	1
2	AU	B	1298	1/1	0.96	0.08	69,69,69,69	1
2	AU	D	1301	1/1	0.98	0.07	36,36,36,36	1
2	AU	A	1295	1/1	0.98	0.07	56,56,56,56	1
2	AU	A	1296	1/1	0.98	0.09	47,47,47,47	1
2	AU	C	1296	1/1	0.98	0.15	57,57,57,57	1
2	AU	B	1294	1/1	0.99	0.07	39,39,39,39	1
2	AU	D	1302	1/1	0.99	0.10	53,53,53,53	1
2	AU	A	1293	1/1	0.99	0.06	35,35,35,35	1

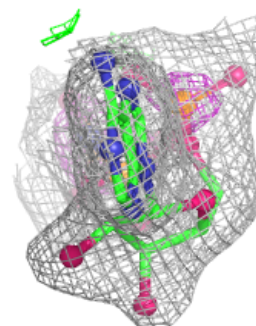
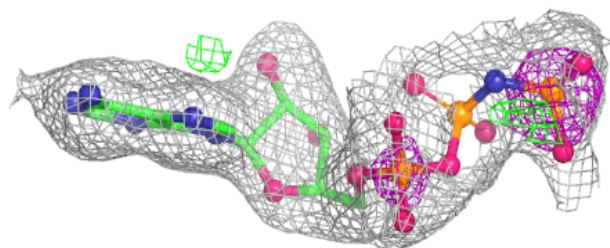
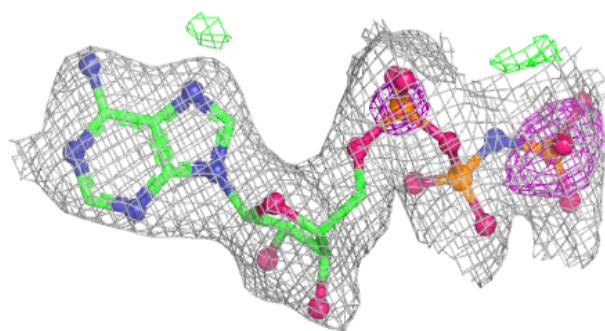
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 1295:

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

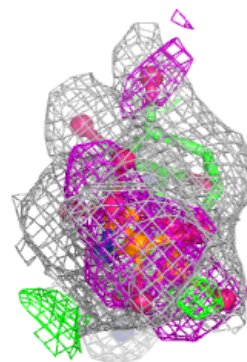
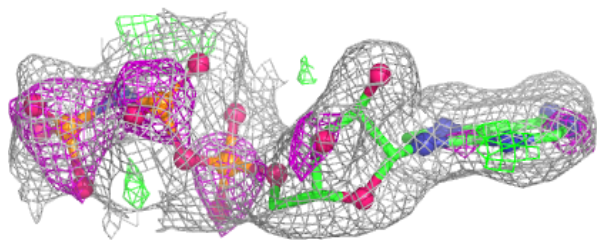
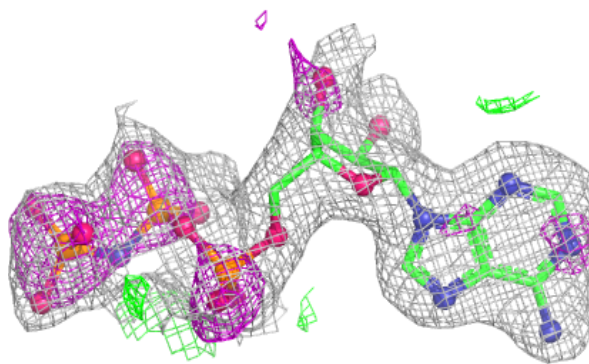
**Electron density around ANP A 1294:**

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

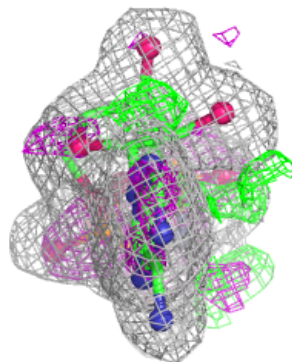
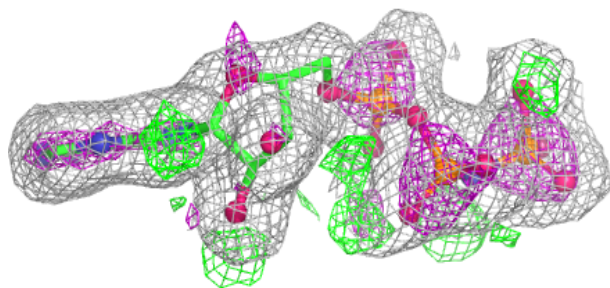
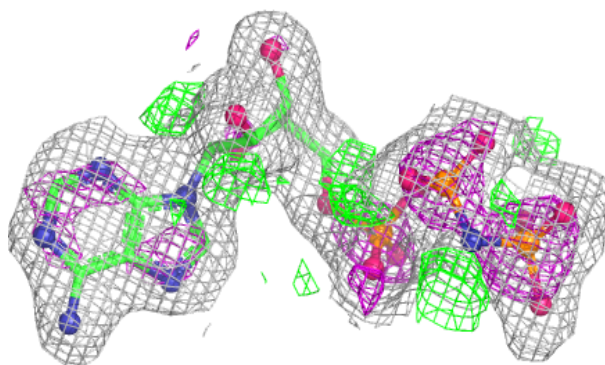


Electron density around ANP D 1300:

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

**Electron density around ANP C 1294:**

$2mF_o-DF_c$ (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.