



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 4UX9 / pdb_00004ux9
Title : Crystal structure of JNK1 bound to a MKK7 docking motif
Authors : Kragelj, J.; Palencia, A.; Nanao, M.H.; Maurin, D.; Bouvignies, G.; Blackledge, M.; Ringkjober-Jensen, M.
Deposited on : 2014-08-20
Resolution : 2.34 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:

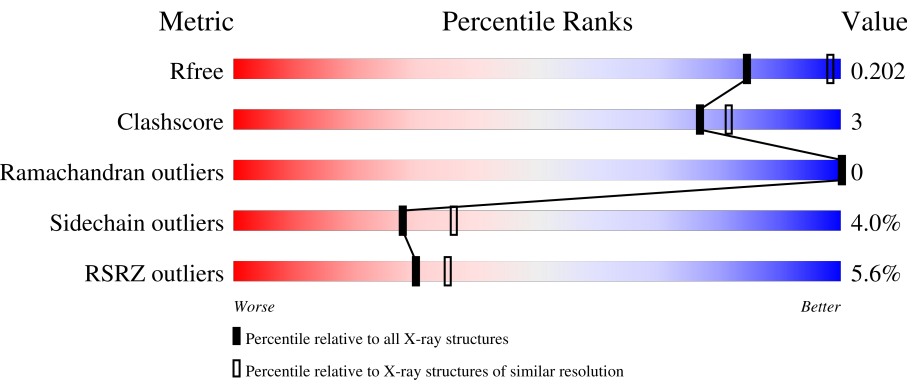
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.34 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.



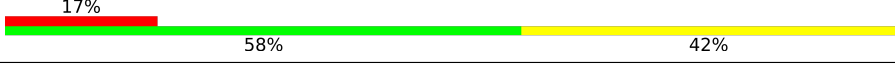
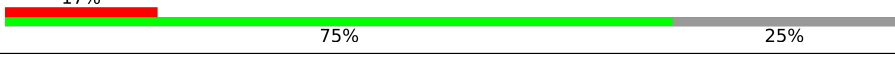
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	364	6% 80% 13% • 6%
1	B	364	5% 82% 7% • 10%
1	C	364	4% 79% 12% • 9%
1	D	364	4% 82% 11% • 5%
2	F	12	17% 75% 8% 17%

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Mol	Chain	Length	Quality of chain
2	G	12	
2	H	12	
2	I	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1365	-	-	X	-
4	SO4	C	1366	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11697 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.

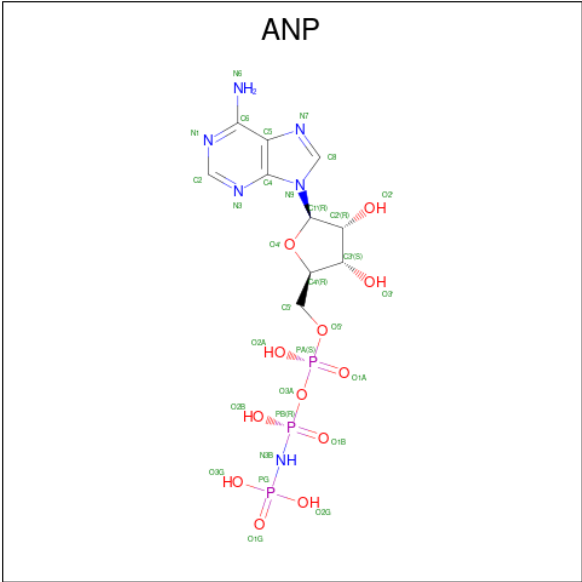
- Molecule 1 is a protein called MITOGEN-ACTIVATED PROTEIN KINASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2770	1782	466	502	20			
1	B	327	Total	C	N	O	S	0	1	0
			2643	1704	443	475	21			
1	C	333	Total	C	N	O	S	0	0	0
			2692	1737	452	483	20			
1	D	344	Total	C	N	O	S	0	1	0
			2802	1804	467	508	23			

- Molecule 2 is a protein called DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 7.

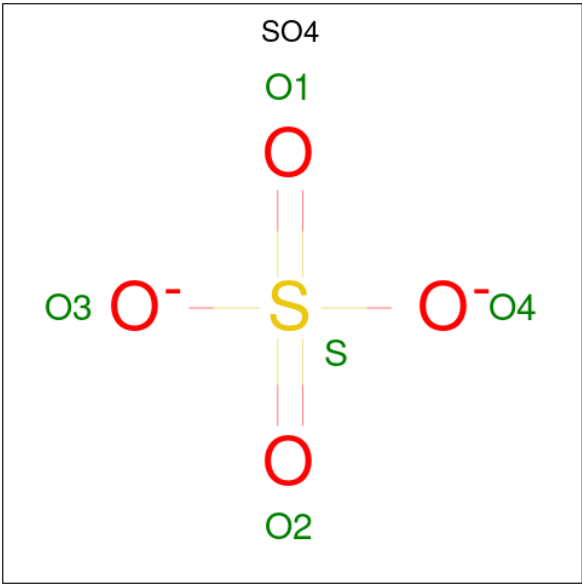
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			77	51	14	12			
2	G	8	Total	C	N	O	0	0	0
			59	40	9	10			
2	H	12	Total	C	N	O	0	0	0
			97	62	20	15			
2	I	9	Total	C	N	O	0	0	0
			77	49	17	11			

- 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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	79	Total O 79 79	0	0
5	B	66	Total O 66 66	0	0
5	C	61	Total O 61 61	0	0
5	D	69	Total O 69 69	0	0

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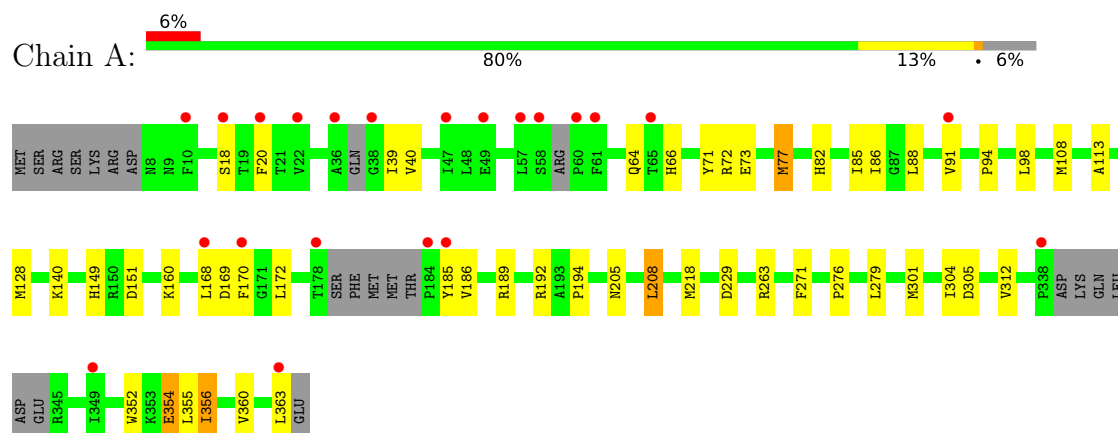
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	O	0	0
			1	1		

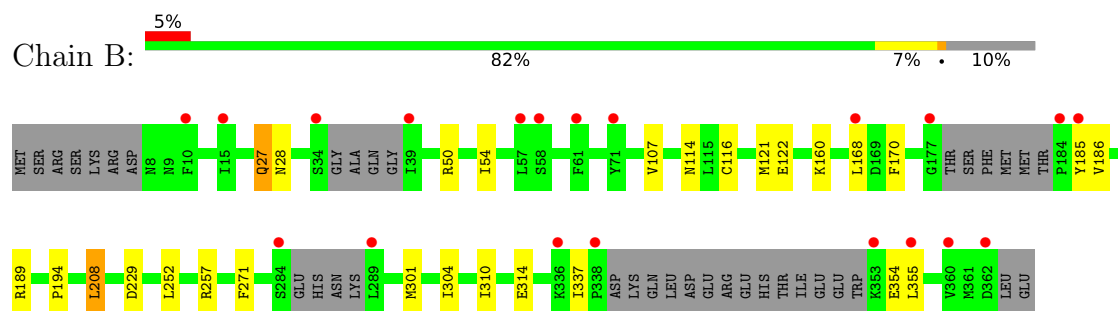
3 Residue-property plots [i](#)

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.

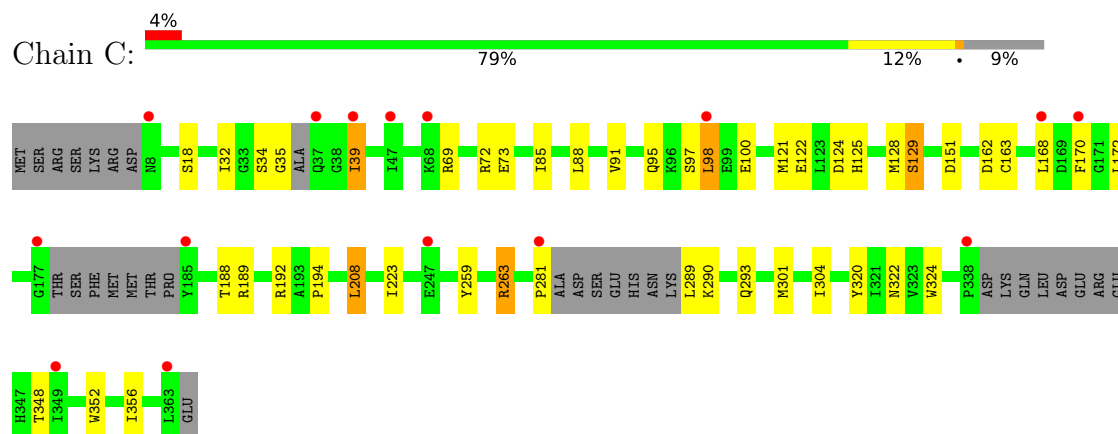
• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE 8



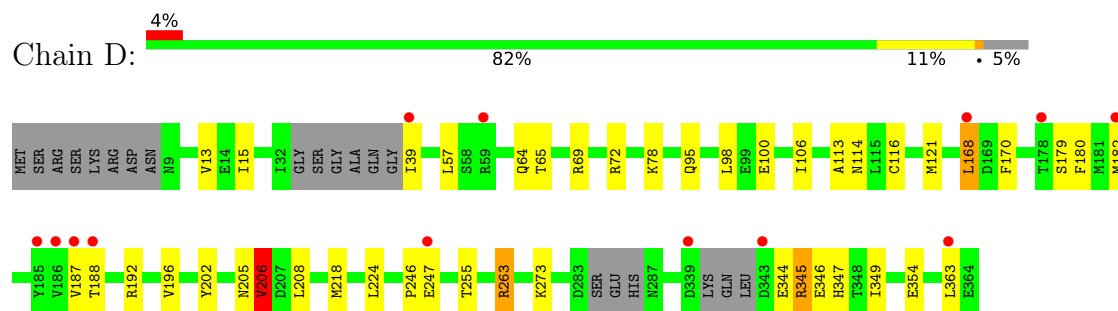
• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE 8



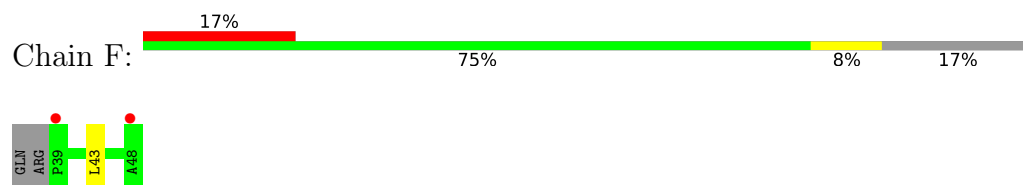
• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE 8



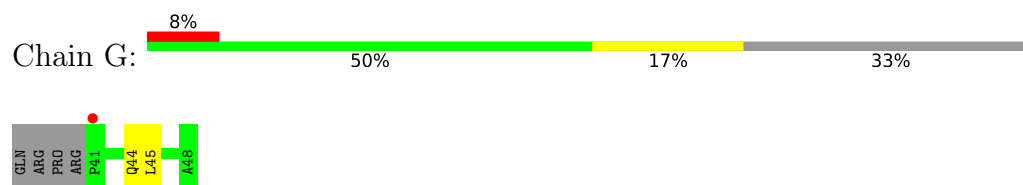
- Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE 8



- Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 7



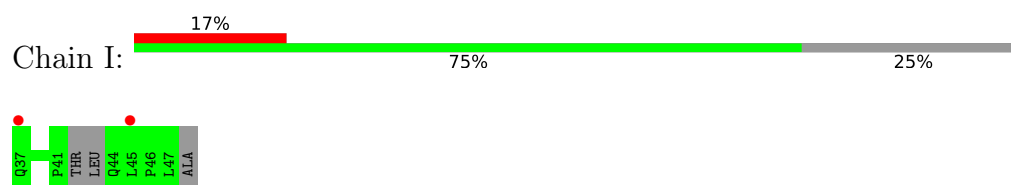
- Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 7



- Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 7



- Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 7



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 180.16Å 101.14Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	49.21 – 2.34 49.21 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.21-2.34) 98.4 (49.21-2.34)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.200 , 0.240 0.203 , 0.202	Depositor DCC
R_{free} test set	3796 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	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	0.96	EDS
Total number of atoms	11697	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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, SO4

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	0.90	2/2831 (0.1%)	1.30	16/3825 (0.4%)
1	B	0.92	3/2703 (0.1%)	1.29	7/3652 (0.2%)
1	C	0.88	0/2751	1.31	17/3718 (0.5%)
1	D	0.92	3/2867 (0.1%)	1.32	17/3876 (0.4%)
2	F	0.88	0/79	0.97	0/108
2	G	0.75	0/60	0.81	0/82
2	H	0.83	0/99	0.99	0/135
2	I	0.90	0/78	0.94	0/104
All	All	0.90	8/11468 (0.1%)	1.30	57/15500 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	TYR	CA-C	-13.23	1.34	1.52
1	B	185	TYR	C-O	7.87	1.34	1.23
1	B	186	VAL	N-CA	-6.35	1.39	1.46
1	D	247	GLU	N-CA	-5.80	1.38	1.46
1	A	168	LEU	CA-C	5.74	1.56	1.52
1	A	185	TYR	C-O	-5.59	1.16	1.24
1	D	246	PRO	C-O	-5.41	1.16	1.24
1	D	121	MET	SD-CE	-5.36	1.66	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	PRO	CA-C-O	8.10	131.12	118.89
1	D	168	LEU	N-CA-C	7.99	122.83	112.12
1	B	185	TYR	CA-C-N	7.50	130.74	120.46
1	B	185	TYR	C-N-CA	7.50	130.74	120.46
1	B	185	TYR	CA-C-O	6.87	127.39	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	ARG	N-CA-C	6.55	118.08	111.07
1	C	97	SER	CA-C-N	6.48	128.96	120.28
1	C	97	SER	C-N-CA	6.48	128.96	120.28
1	D	247	GLU	N-CA-CB	-6.20	101.02	110.26
1	A	305	ASP	CA-CB-CG	6.06	118.66	112.60
1	B	354	GLU	CA-C-N	5.74	128.44	120.29
1	B	354	GLU	C-N-CA	5.74	128.44	120.29
1	A	82	HIS	CA-C-N	5.74	128.76	120.38
1	A	82	HIS	C-N-CA	5.74	128.76	120.38
1	A	205	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	271	PHE	CA-CB-CG	-5.57	108.23	113.80
1	D	218	MET	CA-C-N	5.55	128.68	120.74
1	D	218	MET	C-N-CA	5.55	128.68	120.74
1	C	168	LEU	N-CA-C	5.46	119.62	112.13
1	A	356	ILE	CA-C-N	5.43	127.88	120.54
1	A	356	ILE	C-N-CA	5.43	127.88	120.54
1	A	66	HIS	CA-C-N	5.39	127.45	120.44
1	A	66	HIS	C-N-CA	5.39	127.45	120.44
1	C	162	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	170	PHE	CA-CB-CG	-5.31	108.49	113.80
1	D	179	SER	CA-C-N	5.30	128.37	120.95
1	D	179	SER	C-N-CA	5.30	128.37	120.95
1	C	98	LEU	CA-C-N	5.28	127.62	120.65
1	C	98	LEU	C-N-CA	5.28	127.62	120.65
1	A	94	PRO	CA-C-N	5.27	128.71	120.75
1	A	94	PRO	C-N-CA	5.27	128.71	120.75
1	A	168	LEU	N-CA-C	5.26	119.02	111.02
1	D	113	ALA	CA-C-N	5.26	132.60	122.03
1	D	113	ALA	C-N-CA	5.26	132.60	122.03
1	C	223	ILE	CA-C-N	5.24	127.57	120.44
1	C	223	ILE	C-N-CA	5.24	127.57	120.44
1	D	206	VAL	N-CA-C	-5.24	105.28	110.62
1	C	322	ASN	CA-CB-CG	5.23	117.83	112.60
1	C	128	MET	CA-C-N	5.22	127.22	120.44
1	C	128	MET	C-N-CA	5.22	127.22	120.44
1	C	290	LYS	CA-C-N	5.21	127.26	120.28
1	C	290	LYS	C-N-CA	5.21	127.26	120.28
1	A	354	GLU	CA-C-N	5.18	127.64	120.29
1	A	354	GLU	C-N-CA	5.18	127.64	120.29
1	B	170	PHE	CA-CB-CG	-5.17	108.63	113.80
1	C	188	THR	CA-C-N	5.17	129.41	121.19
1	C	188	THR	C-N-CA	5.17	129.41	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	THR	CA-C-N	5.17	127.76	120.42
1	D	255	THR	C-N-CA	5.17	127.76	120.42
1	D	187	VAL	CA-C-N	5.16	128.87	121.50
1	D	187	VAL	C-N-CA	5.16	128.87	121.50
1	D	205	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	113	ALA	CA-C-N	5.13	132.09	121.32
1	A	113	ALA	C-N-CA	5.13	132.09	121.32
1	A	271	PHE	CA-CB-CG	-5.07	108.73	113.80
1	C	348	THR	CA-C-N	5.05	127.65	120.53
1	C	348	THR	C-N-CA	5.05	127.65	120.53

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	2770	0	2792	23	0
1	B	2643	0	2682	11	0
1	C	2692	0	2721	21	0
1	D	2802	0	2825	11	0
2	F	77	0	87	0	0
2	G	59	0	67	1	0
2	H	97	0	107	3	0
2	I	77	0	83	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
3	C	31	0	13	1	0
3	D	31	0	13	0	0
4	A	20	0	0	2	0
4	B	20	0	0	1	0
4	C	20	0	0	2	0
4	D	15	0	0	0	0
4	H	5	0	0	0	0
5	A	79	0	0	0	0
5	B	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	61	0	0	1	0
5	D	69	0	0	1	0
5	F	1	0	0	0	0
All	All	11697	0	11416	67	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 3.

All (67) 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:208:LEU:HD21	1:A:312:VAL:HG22	1.79	0.64
1:A:276:PRO:HD2	1:A:279:LEU:HD12	1.81	0.62
1:C:88:LEU:HD11	1:C:91:VAL:HG23	1.83	0.61
1:A:189:ARG:HD3	4:A:1365:SO4:O1	2.02	0.60
1:D:57:LEU:HD21	1:D:106:ILE:HD12	1.84	0.59
1:A:208:LEU:HD12	1:A:301:MET:HE2	1.84	0.59
1:D:192:ARG:HD2	1:D:196:VAL:HG11	1.85	0.58
1:B:121:MET:HE1	2:G:45:LEU:HD22	1.86	0.57
1:A:208:LEU:HD21	1:A:312:VAL:CG2	2.35	0.56
1:D:202:TYR:HB2	1:D:206:VAL:HG21	1.87	0.55
1:C:125:HIS:O	1:C:129:SER:HB2	2.07	0.55
1:C:34:SER:HB3	1:C:39:ILE:HD12	1.90	0.54
1:A:352:TRP:O	1:A:356:ILE:HG12	2.07	0.54
1:C:151:ASP:HB2	1:C:172:LEU:HD12	1.89	0.53
1:A:192:ARG:NH2	4:A:1365:SO4:O1	2.42	0.52
1:A:128:MET:HE2	1:A:218:MET:HB3	1.92	0.52
1:C:35:GLY:HA3	3:C:1000:ANP:HNB1	1.76	0.51
1:A:208:LEU:CD2	1:A:312:VAL:HG22	2.41	0.51
1:B:54:ILE:HG12	1:B:107:VAL:HG22	1.93	0.51
1:B:189:ARG:HD3	4:B:1366:SO4:O1	2.11	0.50
1:D:95:GLN:HB3	1:D:100:GLU:O	2.12	0.50
1:C:129:SER:HB3	1:C:324:TRP:HE1	1.76	0.50
1:C:352:TRP:O	1:C:356:ILE:HG12	2.12	0.49
1:A:128:MET:HG3	1:A:218:MET:HE2	1.94	0.49
1:D:65:THR:O	1:D:69:ARG:HG3	2.11	0.49
1:B:194:PRO:HG2	1:B:304:ILE:HA	1.94	0.49
1:A:149:HIS:NE2	1:A:169:ASP:O	2.45	0.48
1:B:27:GLN:O	1:B:28:ASN:HB2	2.12	0.48
1:C:208:LEU:HD23	1:C:301:MET:HE2	1.96	0.48
1:C:194:PRO:HG2	1:C:304:ILE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HB2	1:A:172:LEU:HD12	1.95	0.47
1:A:98:LEU:HD11	1:A:354:GLU:HG3	1.96	0.47
1:C:95:GLN:HG2	1:C:100:GLU:O	2.14	0.47
1:C:163:CYS:HB2	2:H:43:LEU:O	2.14	0.47
1:D:346:GLU:HG2	1:D:347:HIS:N	2.29	0.46
1:A:88:LEU:HD11	1:A:91:VAL:CG2	2.46	0.46
1:C:189:ARG:HD3	4:C:1366:SO4:O2	2.15	0.46
1:C:192:ARG:NH2	4:C:1366:SO4:O2	2.41	0.46
1:C:263:ARG:HA	1:C:263:ARG:HD2	1.74	0.45
1:D:263:ARG:HD2	5:D:2055:HOH:O	2.16	0.45
1:A:71:TYR:CE1	1:A:355:LEU:HG	2.52	0.45
1:C:263:ARG:HD2	5:C:2042:HOH:O	2.16	0.45
1:D:78:LYS:HB2	1:D:363:LEU:HD21	1.98	0.45
1:A:73:GLU:O	1:A:77:MET:HB2	2.17	0.45
1:C:259:TYR:CZ	1:C:263:ARG:HD3	2.51	0.45
1:C:121:MET:HE1	2:H:45:LEU:HD22	2.00	0.44
1:A:85:ILE:HG23	1:A:170:PHE:CZ	2.53	0.44
1:C:289:LEU:N	1:C:293:GLN:OE1	2.51	0.43
1:D:64:GLN:HG3	1:D:349:ILE:HG13	2.01	0.43
1:A:189:ARG:HD2	1:A:229:ASP:C	2.43	0.43
1:C:124:ASP:HA	1:C:281:PRO:HB3	2.01	0.43
1:B:310:ILE:HG12	1:B:314:GLU:HB2	2.01	0.42
1:D:114:ASN:HB3	1:D:116:CYS:H	1.83	0.42
1:A:77:MET:HE3	1:A:86:ILE:HG23	2.01	0.42
1:B:252:LEU:HB2	1:B:257:ARG:HB2	2.01	0.42
2:H:39:PRO:C	2:H:41:PRO:HD3	2.44	0.42
1:B:208:LEU:HD23	1:B:301:MET:HE2	2.01	0.42
1:A:140:LYS:HA	1:A:140:LYS:HD2	1.89	0.42
1:D:98:LEU:HD21	1:D:354:GLU:HA	2.01	0.41
1:A:208:LEU:HD13	1:A:208:LEU:HA	1.87	0.41
1:C:85:ILE:HG23	1:C:170:PHE:CZ	2.55	0.41
1:B:189:ARG:HD2	1:B:229:ASP:C	2.46	0.41
1:B:114:ASN:HB3	1:B:116:CYS:H	1.86	0.41
1:C:129:SER:OG	1:C:320:TYR:O	2.38	0.41
1:A:194:PRO:HG2	1:A:304:ILE:HA	2.02	0.40
1:A:356:ILE:O	1:A:360:VAL:HG23	2.21	0.40
1:B:208:LEU:HD22	1:B:310:ILE:HG23	2.03	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	333/364 (92%)	323 (97%)	10 (3%)	0	100	100
1	B	318/364 (87%)	305 (96%)	13 (4%)	0	100	100
1	C	323/364 (89%)	316 (98%)	7 (2%)	0	100	100
1	D	337/364 (93%)	325 (96%)	12 (4%)	0	100	100
2	F	8/12 (67%)	6 (75%)	2 (25%)	0	100	100
2	G	6/12 (50%)	5 (83%)	1 (17%)	0	100	100
2	H	10/12 (83%)	10 (100%)	0	0	100	100
2	I	5/12 (42%)	5 (100%)	0	0	100	100
All	All	1340/1504 (89%)	1295 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/328 (94%)	294 (96%)	13 (4%)	26	34
1	B	295/328 (90%)	287 (97%)	8 (3%)	39	51
1	C	298/328 (91%)	287 (96%)	11 (4%)	30	39
1	D	313/328 (95%)	298 (95%)	15 (5%)	23	29
2	F	9/11 (82%)	8 (89%)	1 (11%)	6	4
2	G	7/11 (64%)	6 (86%)	1 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	11/11 (100%)	10 (91%)	1 (9%)	9	9
2	I	9/11 (82%)	9 (100%)	0	100	100
All	All	1249/1356 (92%)	1199 (96%)	50 (4%)	28	36

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	20	PHE
1	A	39	ILE
1	A	40	VAL
1	A	64	GLN
1	A	72	ARG
1	A	77	MET
1	A	108	MET
1	A	160	LYS
1	A	186	VAL
1	A	208	LEU
1	A	263	ARG
1	A	363	LEU
1	B	27	GLN
1	B	50	ARG
1	B	122	GLU
1	B	160	LYS
1	B	168	LEU
1	B	208	LEU
1	B	337	ILE
1	B	355	LEU
1	C	18	SER
1	C	32	ILE
1	C	39	ILE
1	C	69	ARG
1	C	72	ARG
1	C	73	GLU
1	C	98	LEU
1	C	122	GLU
1	C	129	SER
1	C	208	LEU
1	C	263	ARG
1	D	13	VAL
1	D	15	ILE

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Mol	Chain	Res	Type
1	D	39	ILE
1	D	72	ARG
1	D	168	LEU
1	D	180	PHE
1	D	182	MET
1	D	188	THR
1	D	206	VAL
1	D	208	LEU
1	D	224	LEU
1	D	263	ARG
1	D	273	LYS
1	D	344	GLU
1	D	345	ARG
2	F	43	LEU
2	G	44	GLN
2	H	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	90	ASN
1	B	120	GLN
1	C	64	GLN
1	C	81	ASN
1	C	84	ASN
1	C	240	GLN
1	D	62	GLN
1	D	66	HIS
2	I	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	D	1365	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	A	1365	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	C	1366	-	4,4,4	0.23	0	6,6,6	0.18	0
4	SO4	D	1366	-	4,4,4	0.18	0	6,6,6	0.20	0
4	SO4	A	1367	-	4,4,4	0.35	0	6,6,6	0.13	0
3	ANP	B	1000	-	33,33,33	1.14	6 (18%)	45,52,52	0.70	0
4	SO4	B	1366	-	4,4,4	0.35	0	6,6,6	0.16	0
4	SO4	C	1365	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	A	1364	-	4,4,4	0.31	0	6,6,6	0.11	0
3	ANP	A	1000	-	33,33,33	0.92	3 (9%)	45,52,52	0.65	0
4	SO4	B	1365	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	B	1363	-	4,4,4	0.30	0	6,6,6	0.19	0
4	SO4	C	1364	-	4,4,4	0.26	0	6,6,6	0.23	0
3	ANP	C	1000	-	33,33,33	0.96	3 (9%)	45,52,52	0.76	1 (2%)
4	SO4	D	1367	-	4,4,4	0.27	0	6,6,6	0.07	0
3	ANP	D	1000	-	33,33,33	1.08	5 (15%)	45,52,52	0.65	0
4	SO4	H	1049	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	C	1367	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	B	1364	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	A	1366	-	4,4,4	0.29	0	6,6,6	0.17	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
3	ANP	B	1000	-	-	1/18/38/38	0/3/3/3
3	ANP	A	1000	-	-	4/18/38/38	0/3/3/3
3	ANP	D	1000	-	-	4/18/38/38	0/3/3/3
3	ANP	C	1000	-	-	5/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	ANP	PG-O1G	2.98	1.50	1.46
3	B	1000	ANP	PG-O1G	2.90	1.50	1.46
3	A	1000	ANP	PG-O1G	2.84	1.50	1.46
3	C	1000	ANP	PG-O1G	2.82	1.50	1.46
3	B	1000	ANP	PA-O3A	2.61	1.62	1.59
3	B	1000	ANP	PB-O3A	2.57	1.62	1.59
3	B	1000	ANP	PG-O3G	-2.52	1.50	1.56
3	D	1000	ANP	PG-O2G	-2.48	1.50	1.56
3	C	1000	ANP	PG-O2G	-2.38	1.50	1.56
3	C	1000	ANP	PG-O3G	-2.36	1.50	1.56
3	A	1000	ANP	PG-O2G	-2.35	1.50	1.56
3	B	1000	ANP	PG-O2G	-2.35	1.50	1.56
3	D	1000	ANP	PG-O3G	-2.31	1.50	1.56
3	A	1000	ANP	PG-O3G	-2.30	1.50	1.56
3	D	1000	ANP	PA-O3A	2.28	1.62	1.59
3	D	1000	ANP	PB-O1B	2.21	1.49	1.46
3	B	1000	ANP	PB-O1B	2.07	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	ANP	O1B-PB-N3B	-2.08	108.71	111.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	ANP	PB-N3B-PG-O1G
3	A	1000	ANP	PA-O3A-PB-O2B
3	B	1000	ANP	PB-N3B-PG-O1G
3	C	1000	ANP	PB-N3B-PG-O1G
3	C	1000	ANP	PG-N3B-PB-O1B
3	C	1000	ANP	PA-O3A-PB-O2B

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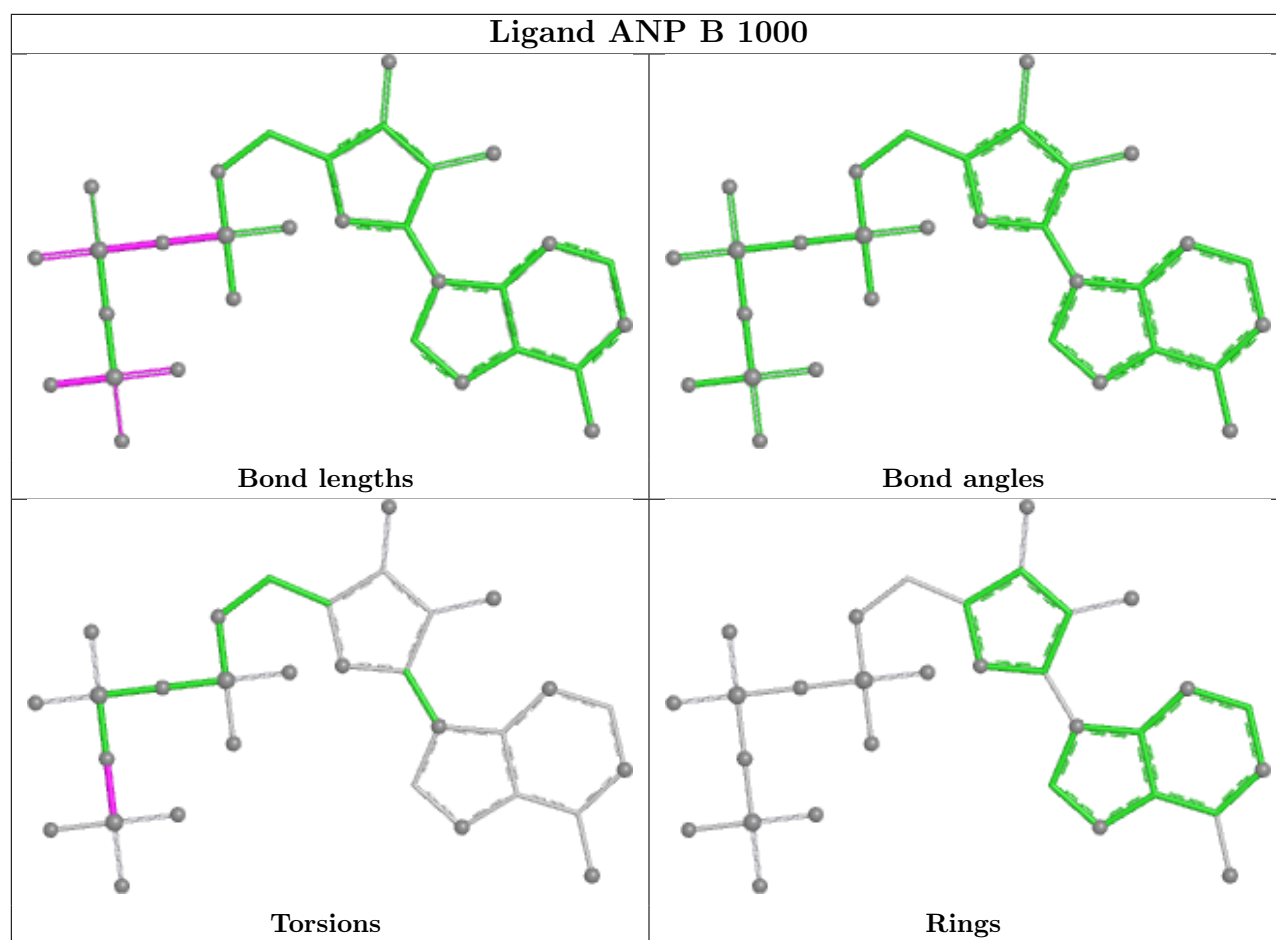
Mol	Chain	Res	Type	Atoms
3	D	1000	ANP	PB-N3B-PG-O1G
3	D	1000	ANP	PG-N3B-PB-O1B
3	D	1000	ANP	PB-O3A-PA-O5'
3	A	1000	ANP	PB-O3A-PA-O1A
3	C	1000	ANP	PB-O3A-PA-O1A
3	D	1000	ANP	O4'-C4'-C5'-O5'
3	A	1000	ANP	PB-O3A-PA-O2A
3	C	1000	ANP	PB-O3A-PA-O2A

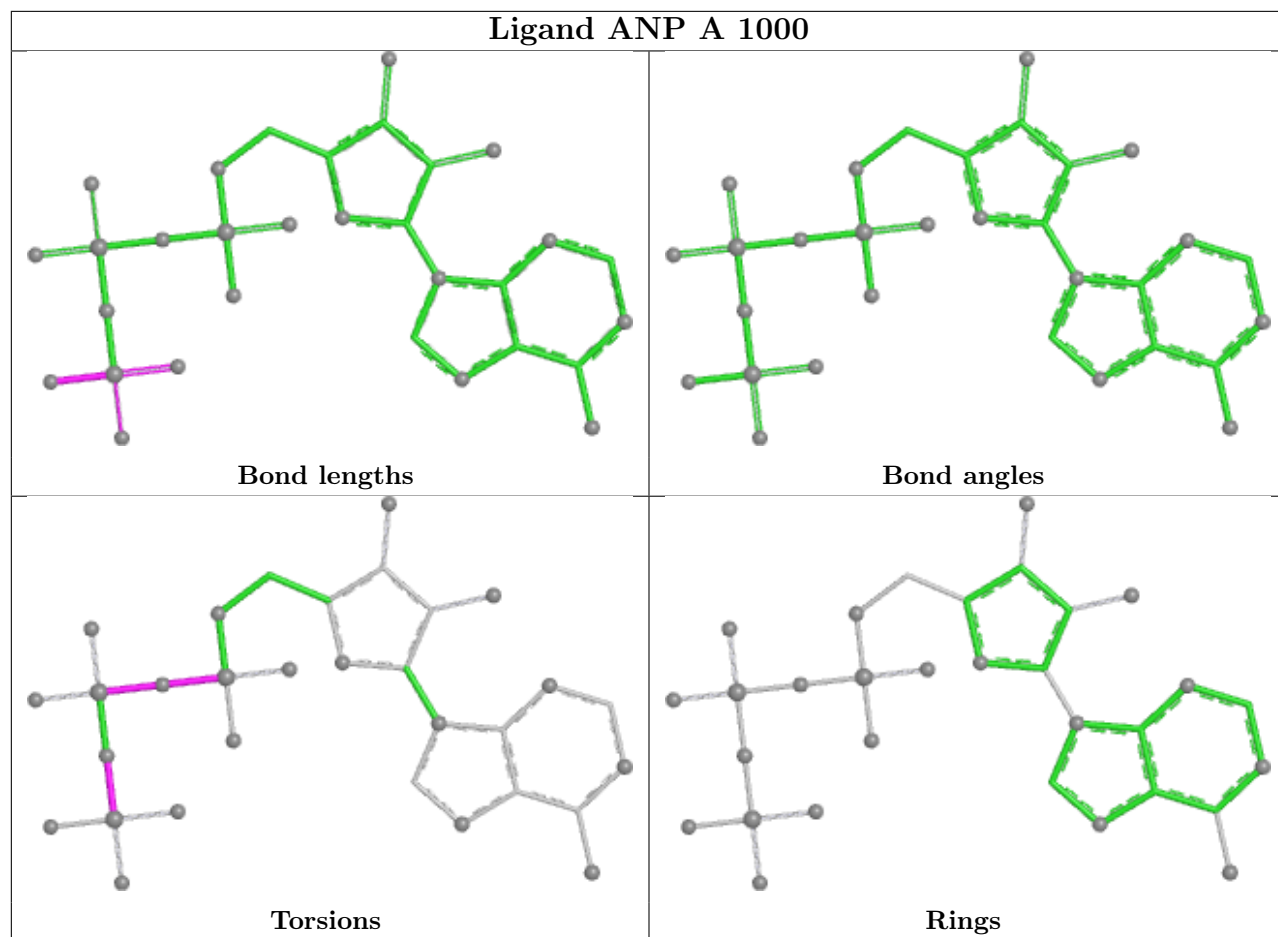
There are no ring outliers.

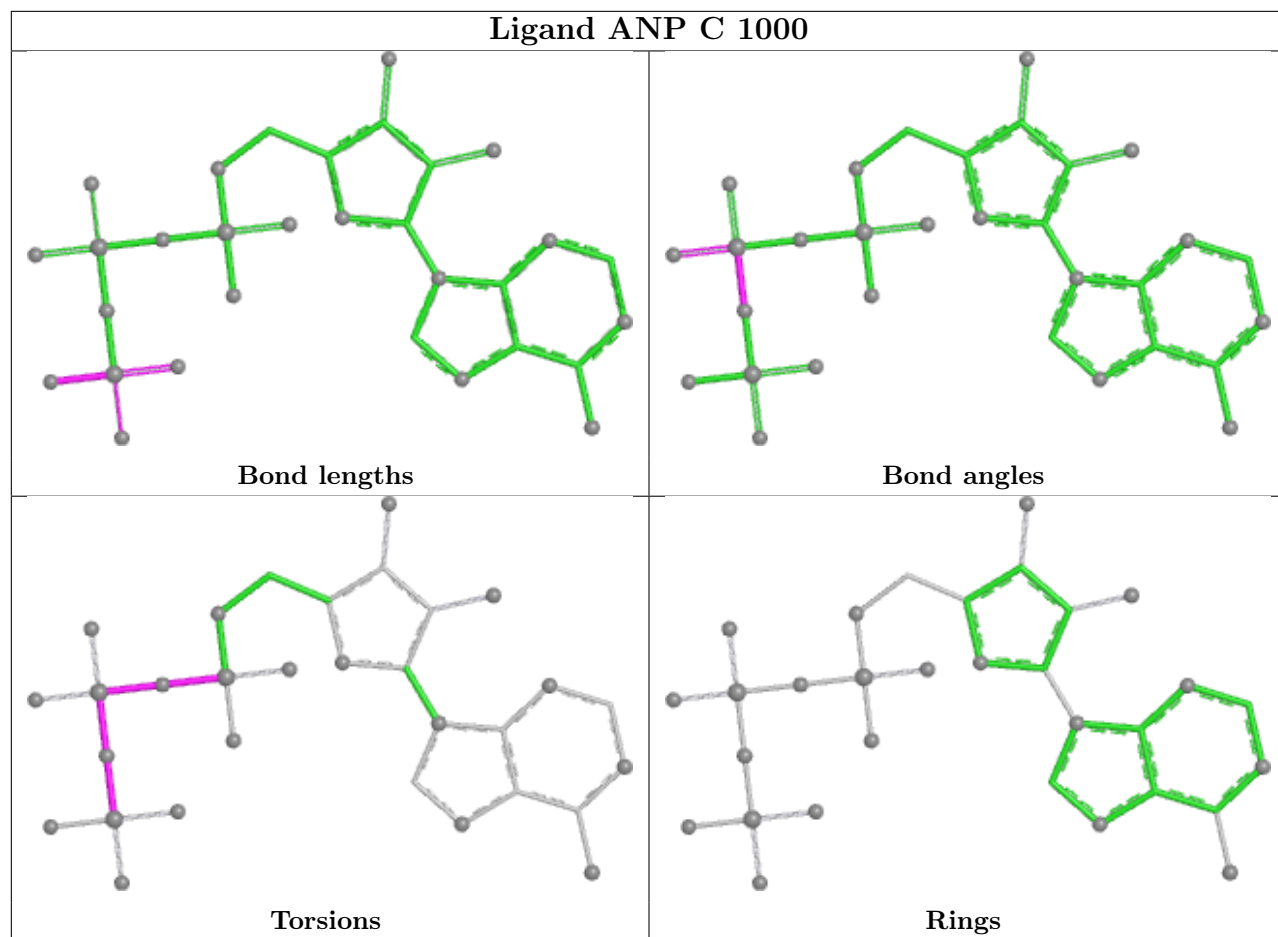
4 monomers are involved in 6 short contacts:

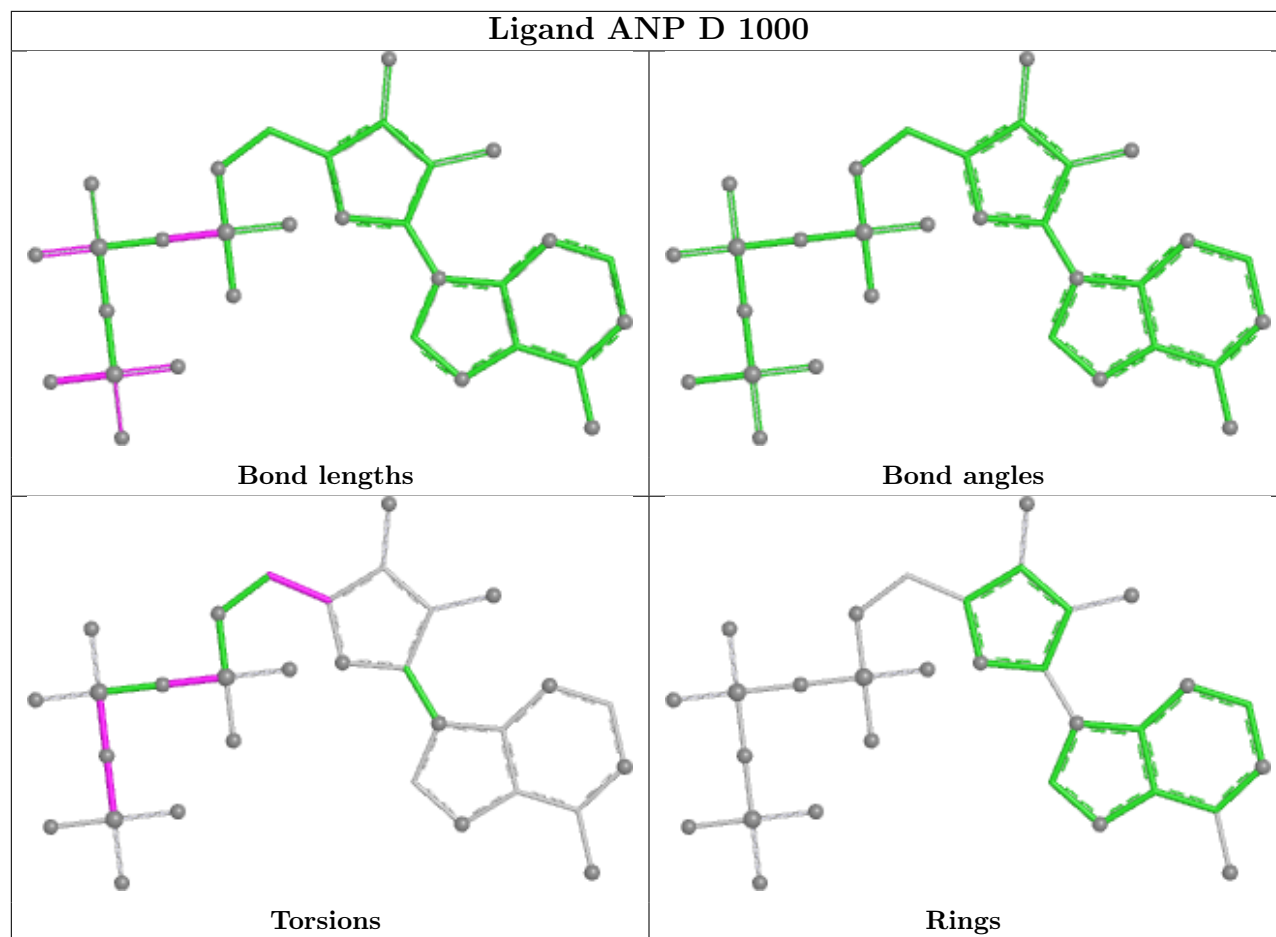
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1365	SO4	2	0
4	C	1366	SO4	2	0
4	B	1366	SO4	1	0
3	C	1000	ANP	1	0

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	343/364 (94%)	0.41	22 (6%)	25 30	38, 59, 107, 123	0
1	B	327/364 (89%)	0.51	20 (6%)	27 32	33, 61, 109, 135	1 (0%)
1	C	333/364 (91%)	0.50	15 (4%)	38 44	40, 61, 105, 122	0
1	D	344/364 (94%)	0.35	13 (3%)	44 50	34, 59, 96, 129	1 (0%)
2	F	10/12 (83%)	1.15	2 (20%)	3 3	60, 83, 99, 110	0
2	G	8/12 (66%)	1.17	1 (12%)	8 9	69, 83, 97, 103	0
2	H	12/12 (100%)	0.91	2 (16%)	4 5	66, 70, 95, 102	0
2	I	9/12 (75%)	1.35	2 (22%)	2 2	57, 74, 91, 106	0
All	All	1386/1504 (92%)	0.46	77 (5%)	30 35	33, 61, 106, 135	2 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	PRO	4.9
1	D	187	VAL	4.7
1	B	184	PRO	4.7
1	A	184	PRO	4.3
1	C	363	LEU	4.3
1	C	177	GLY	4.2
1	B	185	TYR	4.2
1	B	338	PRO	4.1
1	A	58	SER	3.8
1	B	34	SER	3.8
1	A	178	THR	3.7
1	B	353	LYS	3.7
1	C	98	LEU	3.7
1	D	363	LEU	3.7
1	A	363	LEU	3.7
1	D	339	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	185	TYR	3.6
1	C	349	ILE	3.6
1	B	61	PHE	3.5
1	A	338	PRO	3.5
1	A	60	PRO	3.4
1	C	185	TYR	3.4
2	H	48	ALA	3.4
1	B	39	ILE	3.3
1	B	355	LEU	3.2
1	B	57	LEU	3.2
1	A	36	ALA	3.2
1	B	362	ASP	3.1
1	B	177	GLY	3.1
2	I	37	GLN	3.0
1	D	186	VAL	2.9
1	C	170	PHE	2.8
1	A	57	LEU	2.8
1	A	91	VAL	2.7
1	C	37	GLN	2.7
1	A	185	TYR	2.7
2	G	41	PRO	2.7
1	A	349	ILE	2.6
2	F	48	ALA	2.6
1	D	343	ASP	2.6
1	D	188	THR	2.6
1	C	39	ILE	2.6
1	A	170	PHE	2.5
1	B	360	VAL	2.5
1	A	20	PHE	2.4
1	B	168	LEU	2.4
2	F	39	PRO	2.4
1	D	178	THR	2.4
1	D	168	LEU	2.4
1	A	10	PHE	2.3
1	A	18	SER	2.3
1	D	247	GLU	2.3
1	D	39	ILE	2.3
1	C	168	LEU	2.3
2	I	45	LEU	2.3
2	H	42	THR	2.3
1	A	49	GLU	2.3
1	A	22	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	59	ARG	2.2
1	A	38	GLY	2.2
1	D	182	MET	2.2
1	B	336	LYS	2.2
1	B	58	SER	2.2
1	C	8	ASN	2.2
1	C	247	GLU	2.2
1	B	284	SER	2.2
1	B	15	ILE	2.1
1	B	71	TYR	2.1
1	A	47	ILE	2.1
1	B	289	LEU	2.1
1	C	47	ILE	2.1
1	A	61	PHE	2.1
1	C	281	PRO	2.1
1	A	168	LEU	2.0
1	B	10	PHE	2.0
1	C	68	LYS	2.0
1	A	65	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

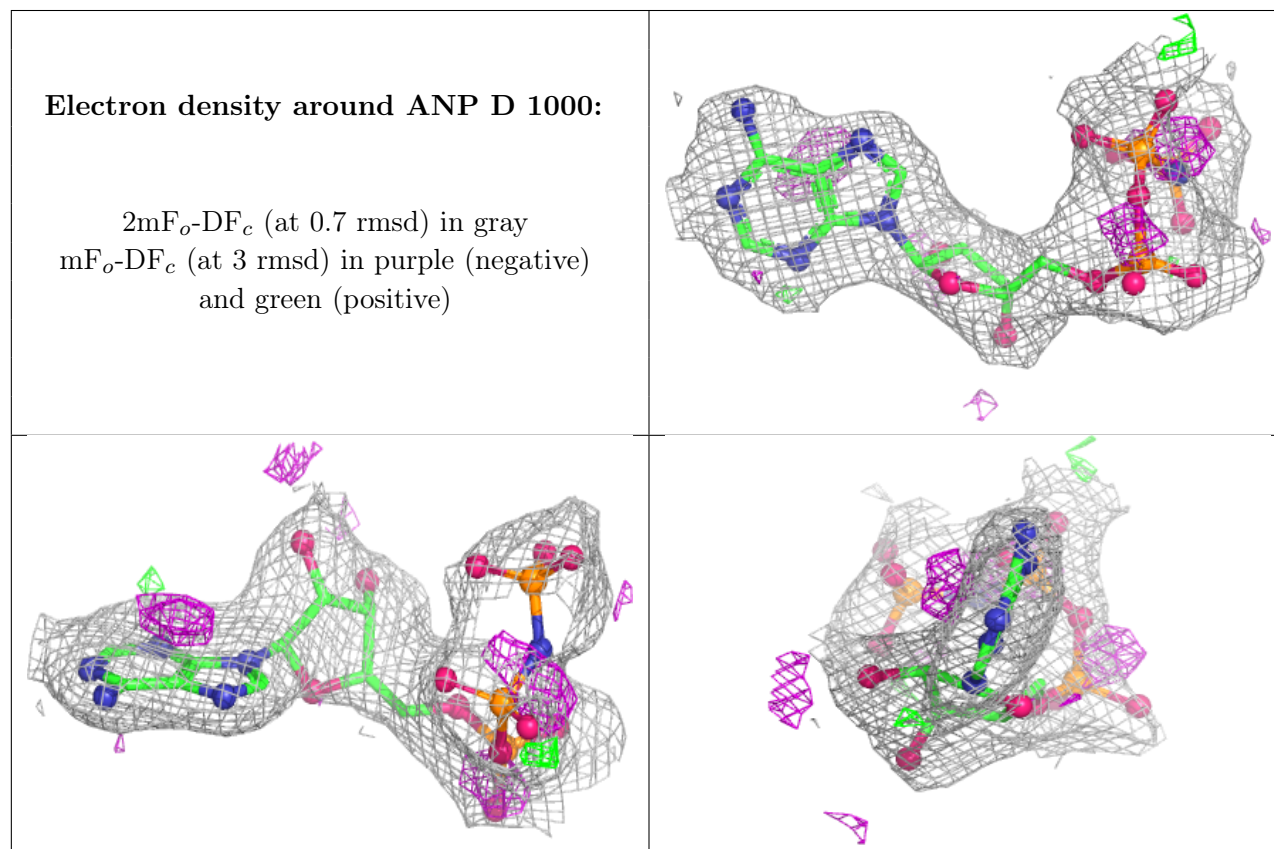
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	1365	5/5	0.58	0.11	145,145,146,146	0
4	SO4	B	1365	5/5	0.60	0.10	145,145,146,146	0
4	SO4	C	1365	5/5	0.68	0.14	147,147,147,147	0
4	SO4	A	1366	5/5	0.71	0.14	124,124,125,126	0

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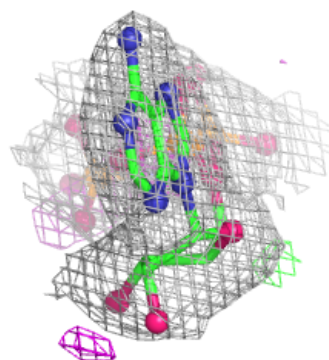
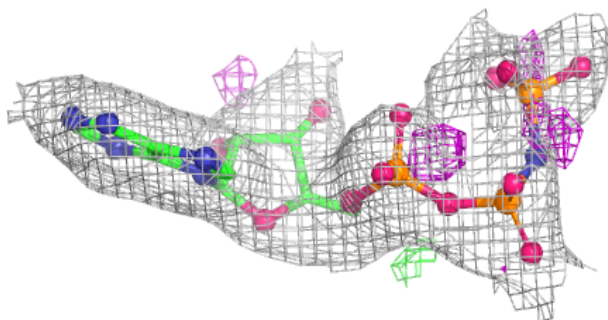
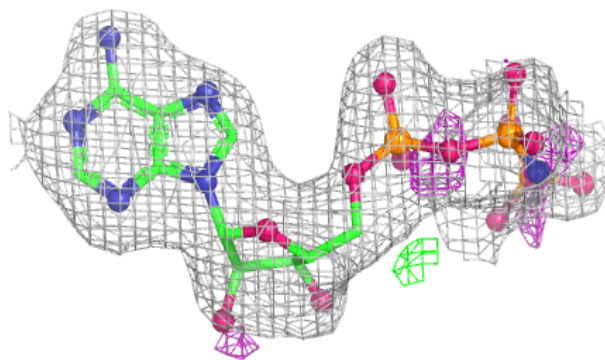
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1364	5/5	0.73	0.14	134,134,135,136	0
4	SO4	H	1049	5/5	0.75	0.09	136,137,137,137	0
3	ANP	D	1000	31/31	0.78	0.13	64,95,144,145	0
4	SO4	A	1367	5/5	0.78	0.18	121,121,123,124	0
4	SO4	B	1364	5/5	0.79	0.12	155,156,156,156	0
4	SO4	B	1363	5/5	0.82	0.11	113,114,115,115	0
4	SO4	C	1367	5/5	0.83	0.10	129,130,130,130	0
3	ANP	B	1000	31/31	0.85	0.11	59,86,136,136	0
4	SO4	D	1367	5/5	0.86	0.10	126,126,126,126	0
4	SO4	C	1364	5/5	0.88	0.09	99,100,100,102	0
3	ANP	A	1000	31/31	0.89	0.10	55,72,133,134	0
3	ANP	C	1000	31/31	0.90	0.09	58,76,122,124	0
4	SO4	D	1366	5/5	0.95	0.07	78,78,79,80	0
4	SO4	A	1365	5/5	0.97	0.06	51,51,52,54	0
4	SO4	C	1366	5/5	0.98	0.06	44,48,50,54	0
4	SO4	B	1366	5/5	0.98	0.06	41,45,48,49	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.

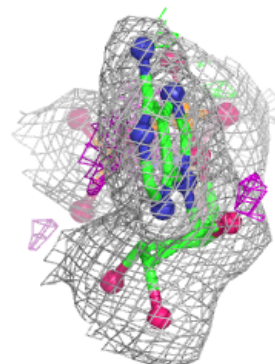
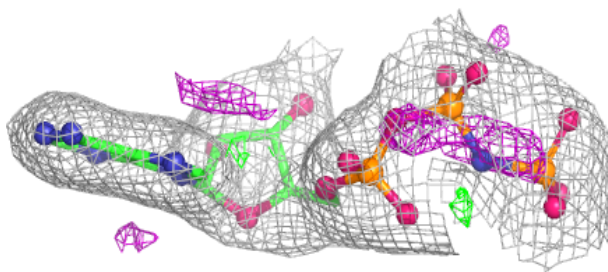
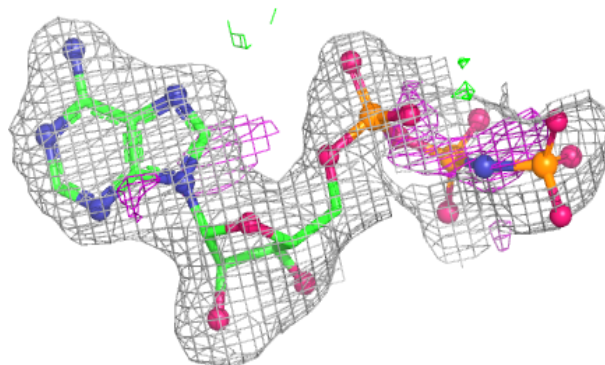


Electron density around ANP B 1000:

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

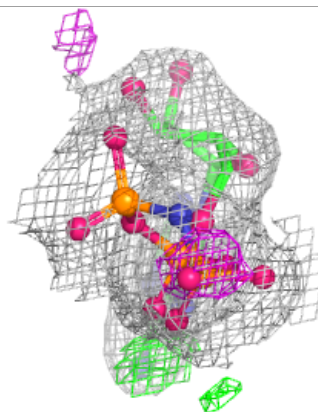
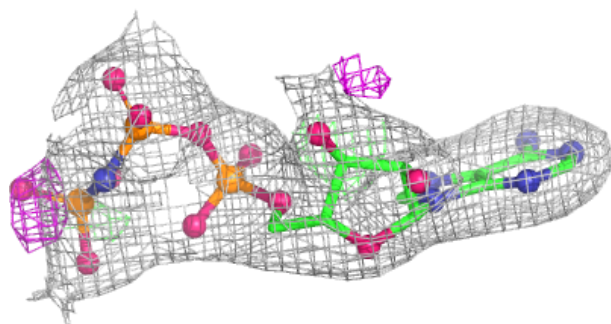
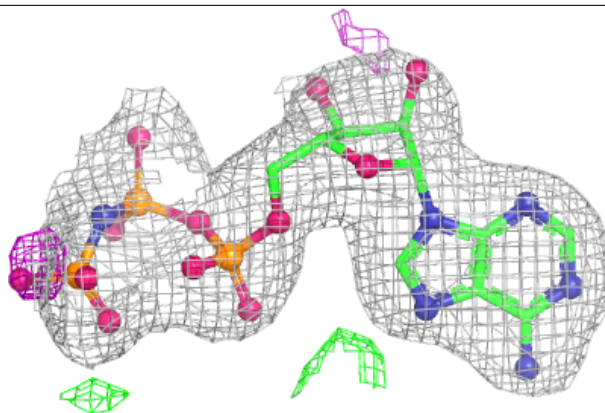
**Electron density around ANP A 1000:**

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



Electron density around ANP C 1000:

$2mF_o-DF_c$ (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.