



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 5XIJ / pdb_00005xij
Title : Crystal Structure of Toxoplasma gondii Prolyl-tRNA Synthetase (TgPRS) in complex with Inhibitor 9
Authors : Jain, V.; Manickam, Y.; Sharma, A.
Deposited on : 2017-04-26
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

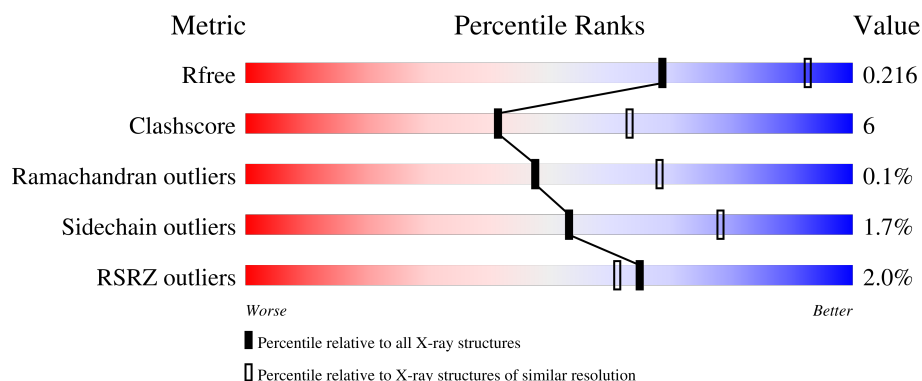
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	0% 84% 11% • •
1	B	500	3% 82% 12% • •
1	C	500	0% 80% 14% • 5%
1	D	500	2% 79% 14% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15971 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.

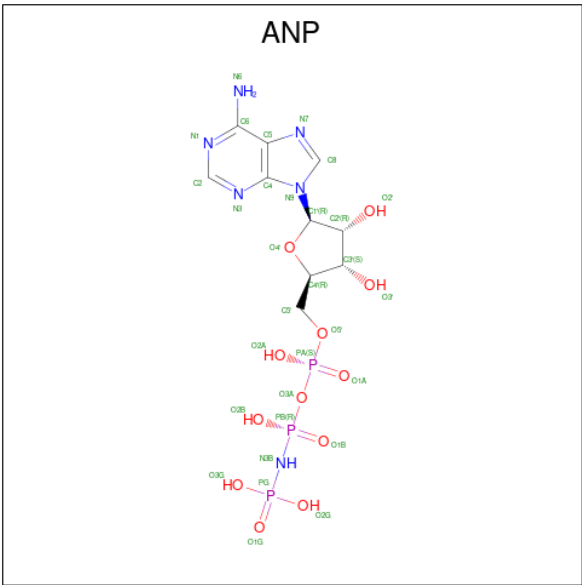
- Molecule 1 is a protein called Prolyl-tRNA synthetase (ProRS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3898	2505	663	708	22			
1	B	478	Total	C	N	O	S	0	0	0
			3831	2464	650	695	22			
1	C	477	Total	C	N	O	S	0	3	0
			3881	2496	665	698	22			
1	D	472	Total	C	N	O	S	0	2	0
			3807	2452	654	679	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP S8G8I1
A	332	ALA	-	expression tag	UNP S8G8I1
A	333	MET	-	expression tag	UNP S8G8I1
B	331	GLY	-	expression tag	UNP S8G8I1
B	332	ALA	-	expression tag	UNP S8G8I1
B	333	MET	-	expression tag	UNP S8G8I1
C	331	GLY	-	expression tag	UNP S8G8I1
C	332	ALA	-	expression tag	UNP S8G8I1
C	333	MET	-	expression tag	UNP S8G8I1
D	331	GLY	-	expression tag	UNP S8G8I1
D	332	ALA	-	expression tag	UNP S8G8I1
D	333	MET	-	expression tag	UNP S8G8I1

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

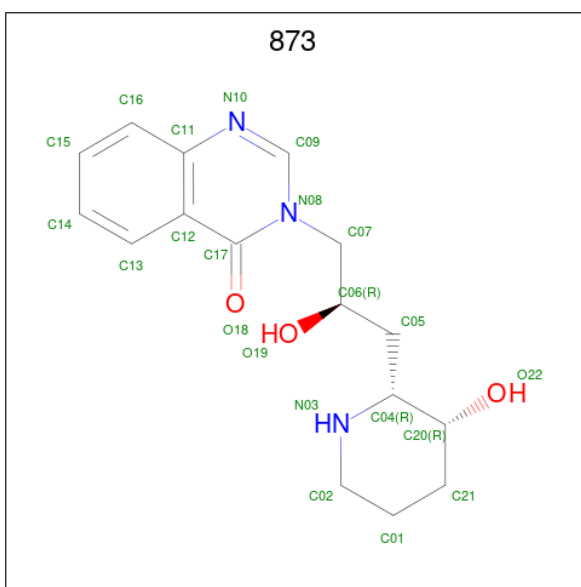


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is 3-[(2R)-2-oxidanyl-3-[(2R,3R)-3-oxidanylpiperidin-2-yl]propyl]quinazolin-4-one (CCD ID: 873) (formula: C₁₆H₂₁N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	3	3		
4	B	1	Total	C	N	O	0	0
			22	16	3	3		
4	C	1	Total	C	N	O	0	0
			22	16	3	3		
4	D	1	Total	C	N	O	0	0
			22	16	3	3		

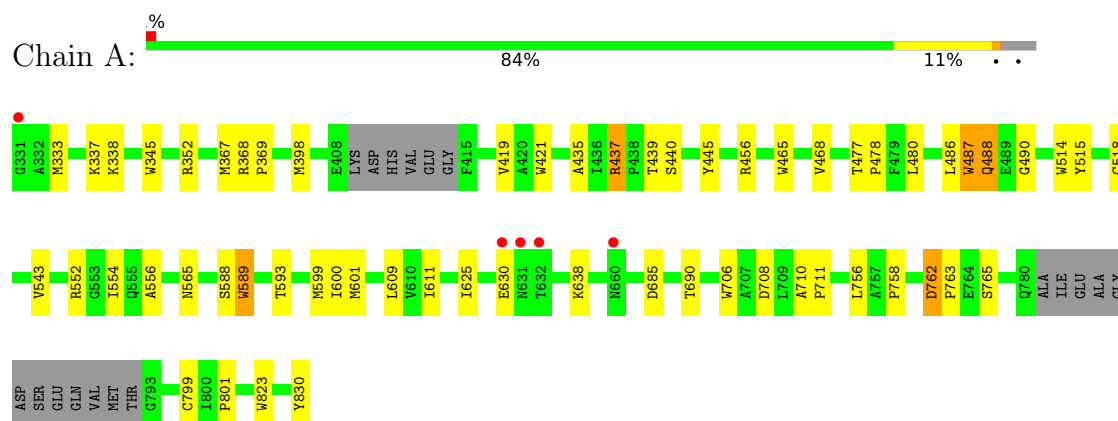
- Molecule 5 is water.

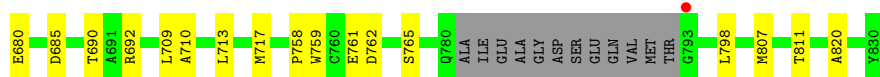
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	66	Total	O	0	2
			68	68		
5	C	77	Total	O	0	0
			77	77		
5	D	67	Total	O	0	1
			68	68		

3 Residue-property plots

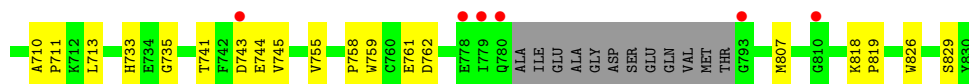
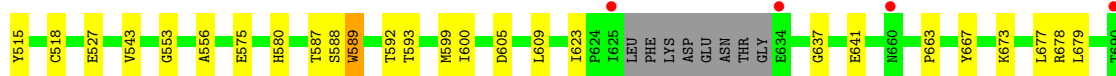
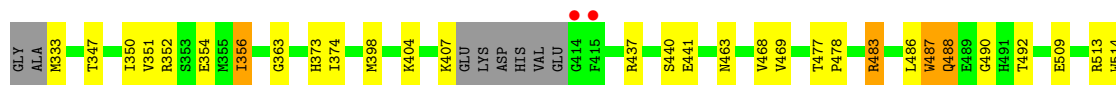
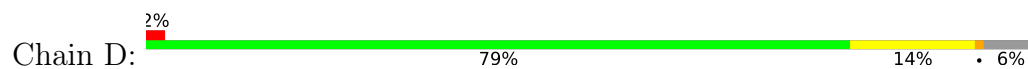
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Prolyl-tRNA synthetase (ProRS)





• Molecule 1: Prolyl-tRNA synthetase (ProRS)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 93.16Å 91.01Å 89.81° 104.52° 99.60°	Depositor
Resolution (Å)	40.36 – 2.50 40.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.36-2.50) 97.0 (40.36-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.240 (Not available) , 0.216	Depositor DCC
R_{free} test set	4043 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15971	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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, MG, 873

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	1.01	0/4007	1.07	9/5428 (0.2%)
1	B	0.92	0/3935	1.04	6/5334 (0.1%)
1	C	0.97	5/3994 (0.1%)	1.08	11/5402 (0.2%)
1	D	0.92	1/3917 (0.0%)	1.02	5/5304 (0.1%)
All	All	0.96	6/15853 (0.0%)	1.05	31/21468 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	611	ILE	N-CA	-6.12	1.41	1.46
1	C	443	ILE	C-O	-5.90	1.17	1.23
1	C	438	PRO	C-O	-5.24	1.17	1.24
1	C	416	SER	C-O	-5.20	1.19	1.24
1	C	543	VAL	C-O	-5.12	1.18	1.24
1	D	373	HIS	C-O	-5.03	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	745	VAL	N-CA-C	7.74	117.78	110.74
1	C	710	ALA	CA-C-N	-7.53	111.21	119.19
1	C	710	ALA	C-N-CA	-7.53	111.21	119.19
1	C	440	SER	N-CA-C	6.93	121.04	112.59
1	C	560	HIS	N-CA-C	6.87	120.64	109.59
1	C	543	VAL	CB-CA-C	6.81	119.61	110.42
1	A	437	ARG	N-CA-C	6.58	119.05	109.71
1	B	804	GLN	CA-C-N	-6.23	113.96	120.38
1	B	804	GLN	C-N-CA	-6.23	113.96	120.38
1	A	552	ARG	N-CA-C	6.14	118.96	109.07
1	A	419	VAL	N-CA-C	5.89	116.66	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	PRO	N-CA-C	5.80	121.77	113.47
1	C	344	GLU	N-CA-C	-5.57	105.36	111.82
1	D	762	ASP	CA-C-N	5.53	124.99	119.24
1	D	762	ASP	C-N-CA	5.53	124.99	119.24
1	B	657	ASP	N-CA-CB	-5.39	102.50	110.53
1	C	341	ASN	N-CA-C	-5.36	98.50	107.99
1	B	697	ASP	N-CA-C	5.33	117.09	111.28
1	D	356	ILE	N-CA-C	5.31	117.03	108.85
1	A	440	SER	N-CA-C	5.30	119.72	112.88
1	B	543	VAL	CB-CA-C	5.24	117.25	110.12
1	B	736	ILE	CB-CA-C	-5.20	104.23	110.99
1	A	630	GLU	N-CA-C	-5.18	98.83	107.99
1	C	437	ARG	N-CA-C	5.16	115.91	109.57
1	A	445	TYR	CA-C-N	-5.15	113.73	119.19
1	A	445	TYR	C-N-CA	-5.15	113.73	119.19
1	D	592	THR	N-CA-C	5.09	117.02	109.69
1	C	438	PRO	CA-C-N	5.03	131.45	122.09
1	C	438	PRO	C-N-CA	5.03	131.45	122.09
1	C	443	ILE	N-CA-C	-5.02	106.90	111.67
1	A	439	THR	N-CA-C	-5.01	100.10	108.07

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	3898	0	3798	44	0
1	B	3831	0	3698	50	0
1	C	3881	0	3816	50	0
1	D	3807	0	3713	45	0
2	A	31	0	13	2	0
2	B	31	0	13	7	0
2	C	31	0	13	1	0
2	D	31	0	13	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	22	0	0	1	0
4	B	22	0	0	4	0
4	C	22	0	0	2	0
4	D	22	0	0	2	0
5	A	121	0	0	1	0
5	B	68	0	0	1	0
5	C	77	0	0	2	0
5	D	68	0	0	2	0
All	All	15971	0	15077	197	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 6.

All (197) 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:C:547:ILE:HG21	1:C:601:MET:HE2	1.41	1.00
1:C:547:ILE:HG21	1:C:601:MET:CE	2.02	0.89
1:A:398:MET:HE1	1:B:398:MET:HE1	1.60	0.82
1:C:643:LYS:NZ	1:C:647:GLU:OE2	2.16	0.79
1:D:374:ILE:HD13	1:D:599:MET:HE1	1.66	0.77
2:B:1001:ANP:O3A	2:B:1001:ANP:H3'	1.86	0.76
1:C:515:TYR:CZ	1:C:556:ALA:HB1	2.20	0.76
1:C:547:ILE:CG2	1:C:601:MET:HE2	2.16	0.75
1:D:492:THR:OG1	1:D:587:THR:HB	1.88	0.74
1:B:567:ALA:HB1	1:B:583:LEU:HG	1.69	0.71
4:D:1004:873:N03	4:D:1004:873:O19	2.22	0.71
4:C:1004:873:O19	4:C:1004:873:N03	2.27	0.68
1:C:342:PHE:CE2	1:C:601:MET:HE3	2.29	0.67
1:D:515:TYR:CZ	1:D:556:ALA:HB1	2.31	0.66
4:A:1004:873:N03	4:A:1004:873:O19	2.29	0.66
1:B:567:ALA:CB	1:B:583:LEU:HG	2.26	0.65
1:C:807:MET:HE3	1:C:811:THR:HB	1.79	0.65
1:B:374:ILE:HG21	1:B:599:MET:HE1	1.79	0.65
1:D:350:ILE:HD12	1:D:356:ILE:HG12	1.80	0.64
1:A:710:ALA:N	1:A:711:PRO:HD2	2.13	0.64
1:D:486:LEU:HB2	1:D:593:THR:CG2	2.28	0.64
2:B:1001:ANP:O1A	4:B:1004:873:O22	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:ARG:HD3	5:D:1130:HOH:O	1.97	0.62
1:B:758:PRO:HB3	1:B:807:MET:HE1	1.82	0.61
1:B:529:SER:HB3	1:B:797:THR:HG21	1.82	0.61
1:A:480:LEU:HD22	1:A:554:ILE:CD1	2.31	0.60
1:A:543:VAL:HG23	1:A:556:ALA:HB3	1.82	0.60
1:A:486:LEU:HB2	1:A:593:THR:HG23	1.84	0.60
1:B:463:ASN:OD1	1:B:488:GLN:HG2	2.02	0.60
1:A:486:LEU:HB2	1:A:593:THR:CG2	2.33	0.59
1:A:398:MET:CE	1:B:398:MET:HE1	2.30	0.59
1:C:807:MET:CE	1:C:820:ALA:HB3	2.32	0.59
1:A:515:TYR:CZ	1:A:556:ALA:HB1	2.37	0.59
2:A:1001:ANP:O2G	5:A:1101:HOH:O	2.17	0.58
1:C:543:VAL:HG13	1:C:556:ALA:HB3	1.86	0.58
1:C:662:THR:HG22	1:C:664:GLY:N	2.19	0.57
1:D:486:LEU:HB2	1:D:593:THR:HG23	1.84	0.57
1:A:398:MET:HE1	1:B:398:MET:CE	2.32	0.57
1:D:515:TYR:CE2	1:D:556:ALA:HB1	2.39	0.57
1:C:680:GLU:OE1	1:C:692:ARG:HD3	2.04	0.56
1:D:741:THR:HB	1:D:744:GLU:HG3	1.87	0.56
1:C:512:ARG:HD3	1:C:525:LYS:HE3	1.87	0.56
1:C:528:LYS:NZ	1:C:544:GLU:OE2	2.38	0.55
2:A:1001:ANP:H3'	2:A:1001:ANP:O3A	2.07	0.55
1:B:568:LYS:HA	1:B:583:LEU:HD21	1.89	0.55
2:D:1001:ANP:O2A	4:D:1004:873:O22	2.25	0.55
1:B:669:HIS:O	1:B:672:VAL:HG12	2.06	0.54
1:A:708:ASP:O	1:A:711:PRO:HG2	2.08	0.54
1:C:398:MET:SD	1:D:398:MET:HE1	2.47	0.54
2:B:1001:ANP:PA	4:B:1004:873:O22	2.66	0.54
1:C:758:PRO:HB3	1:C:807:MET:HE1	1.88	0.54
1:C:523:VAL:CG2	1:C:543:VAL:HG22	2.38	0.53
1:B:543:VAL:CG1	1:B:557:ALA:HB3	2.38	0.53
1:B:635:ILE:HG23	1:B:681:LEU:HD23	1.91	0.53
1:B:514:TRP:O	1:B:518:CYS:HB2	2.09	0.53
1:B:437:ARG:HG2	1:B:437:ARG:O	2.08	0.52
1:D:553:GLY:O	1:D:829:SER:HA	2.09	0.52
1:D:818:LYS:HB3	1:D:819:PRO:CD	2.39	0.52
1:A:514:TRP:O	1:A:518:CYS:HB2	2.10	0.52
1:C:677:LEU:HD13	1:C:713:LEU:HD22	1.92	0.51
1:C:807:MET:HE1	1:C:820:ALA:HB3	1.91	0.51
1:A:490:GLY:O	1:A:588:SER:HA	2.11	0.51
1:A:708:ASP:O	1:A:711:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:LEU:HD11	1:C:709:LEU:HD21	1.92	0.51
1:C:437:ARG:HD3	5:C:1132:HOH:O	2.10	0.51
1:C:398:MET:HE1	1:D:469:VAL:CG2	2.40	0.50
1:C:487:TRP:C	1:C:487:TRP:CD1	2.89	0.50
1:D:543:VAL:HG23	1:D:556:ALA:HB3	1.92	0.50
1:C:342:PHE:CZ	1:C:601:MET:HE3	2.47	0.50
1:D:490:GLY:O	1:D:588:SER:HA	2.11	0.50
1:A:515:TYR:CE2	1:A:556:ALA:HB1	2.46	0.50
1:B:631:ASN:O	1:B:632:THR:C	2.55	0.50
1:D:741:THR:HG22	1:D:743:ASP:H	1.77	0.50
1:C:519:LEU:HD22	1:C:599:MET:HE3	1.94	0.50
1:C:342:PHE:HE2	1:C:601:MET:HE3	1.74	0.50
1:D:492:THR:HG1	1:D:587:THR:HB	1.75	0.50
1:A:333:MET:O	1:A:352:ARG:NH1	2.45	0.49
1:C:605:ASP:C	1:C:605:ASP:OD1	2.55	0.49
1:B:573:GLU:HG2	1:B:583:LEU:CD1	2.42	0.49
1:D:605:ASP:OD1	1:D:605:ASP:C	2.55	0.49
1:D:637:GLY:O	1:D:641:GLU:HG3	2.12	0.49
1:D:600:ILE:HG23	1:D:609:LEU:CD2	2.43	0.49
1:C:575:GLU:HA	1:C:580:HIS:O	2.12	0.49
2:C:1001:ANP:O3A	2:C:1001:ANP:H8	2.13	0.49
1:B:490:GLY:O	1:B:588:SER:HA	2.12	0.49
1:B:765:SER:O	1:B:769:ILE:HG13	2.13	0.48
1:B:472:GLU:O	1:B:483:ARG:NH1	2.32	0.48
1:D:333:MET:O	1:D:352:ARG:NH1	2.43	0.48
1:B:543:VAL:HG13	1:B:556:ALA:HB3	1.96	0.48
1:D:663:PRO:O	1:D:667:TYR:CD1	2.67	0.48
1:C:490:GLY:O	1:C:588:SER:HA	2.14	0.48
1:C:762:ASP:O	1:C:765:SER:OG	2.31	0.48
1:A:465:TRP:CE3	1:A:488:GLN:HB2	2.49	0.47
1:D:514:TRP:O	1:D:518:CYS:HB2	2.14	0.47
1:B:523:VAL:HG21	1:B:543:VAL:CG2	2.44	0.47
1:C:759:TRP:CZ3	1:C:761:GLU:HA	2.48	0.47
1:B:605:ASP:OD1	1:B:605:ASP:C	2.58	0.47
1:A:338:LYS:HG3	1:A:345:TRP:CD2	2.49	0.47
1:C:415:PHE:HB3	4:C:1004:873:C15	2.45	0.47
1:B:482:THR:H	2:B:1001:ANP:HN62	1.63	0.46
1:A:638:LYS:HE3	1:A:706:TRP:CZ3	2.50	0.46
1:A:480:LEU:HD11	1:A:601:MET:CE	2.45	0.46
1:A:710:ALA:N	1:A:711:PRO:CD	2.77	0.46
1:A:756:LEU:HD22	1:A:823:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:LYS:CA	1:B:583:LEU:HD21	2.45	0.46
1:B:379:GLN:O	1:B:383:ASP:HB2	2.16	0.46
1:D:477:THR:O	1:D:478:PRO:C	2.59	0.46
1:B:588:SER:C	1:B:589:TRP:CD1	2.94	0.46
1:B:437:ARG:NH2	1:B:466:CYS:HB2	2.31	0.46
1:A:625:ILE:HG22	1:A:625:ILE:O	2.16	0.45
1:A:685:ASP:HB3	1:A:690:THR:O	2.16	0.45
1:D:755:VAL:CG2	1:D:826:TRP:HB2	2.46	0.45
5:C:1123:HOH:O	1:D:404:LYS:HE2	2.16	0.45
1:B:487:TRP:CD1	1:B:487:TRP:C	2.94	0.45
1:C:677:LEU:HD12	1:C:717:MET:HE3	1.98	0.45
1:C:518:CYS:HA	1:C:614[B]:ARG:HG2	1.99	0.45
1:C:662:THR:HG22	1:C:664:GLY:H	1.82	0.45
1:C:668:ASN:O	1:C:672:VAL:HG23	2.16	0.45
1:D:588:SER:C	1:D:589:TRP:CD1	2.95	0.45
1:D:463:ASN:OD1	1:D:488:GLN:HG2	2.17	0.44
1:A:368:ARG:HB3	1:A:369:PRO:HD2	1.98	0.44
1:B:583:LEU:HD12	1:B:583:LEU:HA	1.77	0.44
1:C:576:ASP:OD2	1:C:582:ARG:NE	2.50	0.44
1:D:487:TRP:C	1:D:487:TRP:CD1	2.96	0.44
1:D:623:ILE:HD12	1:D:678:ARG:HD2	1.98	0.44
2:B:1001:ANP:O1B	5:B:1101:HOH:O	2.21	0.44
1:C:623:ILE:CD1	1:C:678:ARG:HG3	2.48	0.44
1:A:487:TRP:C	1:A:487:TRP:CD1	2.96	0.44
1:A:600:ILE:HG23	1:A:609:LEU:CD2	2.47	0.44
1:D:509:GLU:O	1:D:513:ARG:HG3	2.17	0.44
1:B:515:TYR:CE1	1:B:556:ALA:HB1	2.53	0.44
1:A:421:TRP:CZ3	1:A:435:ALA:HB2	2.53	0.44
1:B:523:VAL:CG2	1:B:543:VAL:HG22	2.47	0.44
1:C:350:ILE:HD12	1:C:356:ILE:HG12	1.98	0.44
1:D:587:THR:HG22	1:D:589:TRP:CD1	2.53	0.44
1:D:733:HIS:C	1:D:735:GLY:H	2.24	0.44
1:D:759:TRP:CZ3	1:D:761:GLU:HA	2.53	0.44
1:B:818:LYS:HB3	1:B:819:PRO:CD	2.48	0.44
1:A:762:ASP:O	1:A:765:SER:HB3	2.18	0.44
1:B:416:SER:HB2	1:B:417:PRO:HD3	2.00	0.44
1:C:399:PHE:CG	1:C:434:ILE:HD12	2.52	0.43
1:C:556:ALA:O	1:C:557:ALA:HB2	2.18	0.43
4:B:1004:873:O22	4:B:1004:873:C06	2.66	0.43
1:D:354:GLU:OE2	1:D:673:LYS:NZ	2.50	0.43
1:B:515:TYR:CZ	1:B:556:ALA:HB1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:C	1:A:589:TRP:CD1	2.97	0.43
1:B:576:ASP:OD1	1:B:580:HIS:N	2.52	0.43
1:D:758:PRO:HB3	1:D:807:MET:HE1	2.00	0.43
1:C:465:TRP:CE3	1:C:488:GLN:HB2	2.52	0.43
1:B:482:THR:N	2:B:1001:ANP:HN62	2.16	0.43
1:B:807:MET:CE	1:B:820:ALA:HB3	2.48	0.43
1:C:512:ARG:NH1	1:C:516:GLU:OE1	2.52	0.43
1:A:490:GLY:HA3	1:A:589:TRP:CZ3	2.52	0.43
1:A:337:LYS:HD3	1:A:337:LYS:HA	1.65	0.43
1:D:347:THR:O	1:D:351:VAL:HG23	2.18	0.43
1:D:363:GLY:HA3	1:D:483:ARG:HG3	2.00	0.43
1:D:818:LYS:HB3	1:D:819:PRO:HD2	2.01	0.43
1:A:599:MET:HE1	1:A:611:ILE:HD12	2.01	0.43
1:A:708:ASP:C	1:A:711:PRO:HD2	2.43	0.43
1:A:758:PRO:HD3	1:A:823:TRP:CZ3	2.54	0.43
1:A:480:LEU:HD11	1:A:601:MET:HE1	2.00	0.42
1:B:374:ILE:HG21	1:B:599:MET:CE	2.47	0.42
1:C:555:GLN:NE2	1:C:558:THR:HB	2.34	0.42
1:A:456:ARG:HD3	1:B:661:TYR:CE1	2.54	0.42
1:B:509:GLU:O	1:B:513:ARG:HG3	2.18	0.42
1:A:480:LEU:HD13	1:A:830:TYR:CE1	2.54	0.42
1:A:367:MET:HE2	1:A:367:MET:HB3	1.94	0.42
1:A:599:MET:O	1:A:600:ILE:C	2.61	0.42
1:D:677:LEU:HD13	1:D:713:LEU:HD22	2.02	0.42
1:B:523:VAL:HG21	1:B:543:VAL:HG22	2.02	0.42
1:B:651:ILE:O	1:B:653:VAL:HG23	2.20	0.42
1:D:440:SER:O	1:D:441:GLU:C	2.63	0.42
2:D:1001:ANP:O2G	5:D:1101:HOH:O	2.21	0.41
1:A:477:THR:O	1:A:478:PRO:C	2.63	0.41
1:B:746:MET:N	1:B:747:PRO:CD	2.83	0.41
1:D:710:ALA:HB3	1:D:711:PRO:CD	2.49	0.41
1:A:480:LEU:HD22	1:A:554:ILE:HD11	1.99	0.41
1:D:679:LEU:C	1:D:679:LEU:HD23	2.45	0.41
1:C:503:LEU:HD23	1:C:503:LEU:C	2.46	0.41
1:C:483:ARG:NH1	1:C:483:ARG:HG3	2.36	0.41
1:C:554:ILE:O	1:C:554:ILE:HG23	2.20	0.41
1:B:543:VAL:HG12	1:B:557:ALA:HB3	2.00	0.41
1:B:486:LEU:HB2	1:B:593:THR:HG23	2.02	0.41
1:A:799:CYS:O	1:A:801:PRO:HD3	2.21	0.41
1:C:599:MET:HE2	1:C:615:VAL:HG21	2.02	0.41
1:B:447:ALA:HB1	1:B:451:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:TYR:CE1	1:C:556:ALA:HB1	2.54	0.41
1:B:559:SER:HA	1:B:589:TRP:HB3	2.02	0.40
1:D:468:VAL:HG21	1:D:487:TRP:CE2	2.56	0.40
1:D:575:GLU:HA	1:D:580:HIS:O	2.21	0.40
1:A:468:VAL:HG21	1:A:487:TRP:CE2	2.57	0.40
1:B:678:ARG:O	1:B:693:VAL:HA	2.20	0.40
2:B:1001:ANP:O2A	4:B:1004:873:C06	2.69	0.40
1:C:685:ASP:HB3	1:C:690:THR:O	2.22	0.40
1:A:710:ALA:HB3	1:A:711:PRO:HD3	2.04	0.40
1:B:523:VAL:CG2	1:B:543:VAL:CG2	2.99	0.40
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.87	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	477/500 (95%)	457 (96%)	20 (4%)	0	100	100
1	B	470/500 (94%)	448 (95%)	22 (5%)	0	100	100
1	C	472/500 (94%)	461 (98%)	10 (2%)	1 (0%)	43	63
1	D	466/500 (93%)	448 (96%)	18 (4%)	0	100	100
All	All	1885/2000 (94%)	1814 (96%)	70 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	438	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	408/436 (94%)	402 (98%)	6 (2%)	57	80
1	B	396/436 (91%)	385 (97%)	11 (3%)	38	66
1	C	408/436 (94%)	404 (99%)	4 (1%)	68	86
1	D	395/436 (91%)	389 (98%)	6 (2%)	57	80
All	All	1607/1744 (92%)	1580 (98%)	27 (2%)	53	78

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	ARG
1	A	487	TRP
1	A	488	GLN
1	A	565	ASN
1	A	589	TRP
1	A	762	ASP
1	B	403	HIS
1	B	437	ARG
1	B	487	TRP
1	B	488	GLN
1	B	583	LEU
1	B	589	TRP
1	B	599	MET
1	B	607	LYS
1	B	645	MET
1	B	765	SER
1	B	821	LYS
1	C	487	TRP
1	C	488	GLN
1	C	565	ASN
1	C	589	TRP
1	D	407	LYS
1	D	483	ARG
1	D	487	TRP

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Mol	Chain	Res	Type
1	D	488	GLN
1	D	527	GLU
1	D	589	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	586	GLN
1	A	669	HIS
1	A	750	ASN
1	A	780	GLN
1	B	565	ASN
1	B	750	ASN
1	C	555	GLN
1	C	565	ASN
1	C	585	HIS
1	C	586	GLN
1	C	750	ASN
1	D	660	ASN
1	D	668	ASN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ANP	A	1001	3	33,33,33	1.74	4 (12%)	45,52,52	1.01	3 (6%)
4	873	C	1004	-	24,24,24	1.62	4 (16%)	27,33,33	1.24	4 (14%)
4	873	D	1004	-	24,24,24	0.62	0	27,33,33	1.34	5 (18%)
4	873	A	1004	-	24,24,24	1.10	1 (4%)	27,33,33	1.39	4 (14%)
2	ANP	B	1001	3	33,33,33	1.54	2 (6%)	45,52,52	0.84	1 (2%)
2	ANP	D	1001	3	33,33,33	1.55	2 (6%)	45,52,52	0.88	1 (2%)
4	873	B	1004	-	24,24,24	1.61	3 (12%)	27,33,33	1.25	4 (14%)
2	ANP	C	1001	3	33,33,33	2.07	4 (12%)	45,52,52	0.92	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	1001	3	-	3/18/38/38	0/3/3/3
4	873	C	1004	-	-	3/8/19/19	1/3/3/3
4	873	D	1004	-	-	1/8/19/19	1/3/3/3
4	873	A	1004	-	-	2/8/19/19	1/3/3/3
2	ANP	B	1001	3	-	3/18/38/38	0/3/3/3
2	ANP	D	1001	3	-	5/18/38/38	0/3/3/3
4	873	B	1004	-	-	2/8/19/19	1/3/3/3
2	ANP	C	1001	3	-	7/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ANP	PB-O1B	6.77	1.56	1.46
2	C	1001	ANP	PB-O1B	6.77	1.56	1.46
2	C	1001	ANP	PG-O1G	6.74	1.56	1.46
2	A	1001	ANP	PG-O1G	6.72	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ANP	PG-O1G	6.70	1.56	1.46
4	B	1004	873	C20-C04	6.15	1.58	1.52
4	C	1004	873	C20-C04	4.71	1.57	1.52
2	C	1001	ANP	PG-O3G	-3.95	1.46	1.56
2	D	1001	ANP	PG-O3G	-3.93	1.46	1.56
2	A	1001	ANP	PG-O3G	-3.92	1.46	1.56
2	B	1001	ANP	PB-O2B	-3.92	1.46	1.56
2	C	1001	ANP	PB-O2B	-3.92	1.46	1.56
2	A	1001	ANP	PB-O3A	3.77	1.63	1.59
4	C	1004	873	C04-N03	-3.59	1.42	1.47
2	A	1001	ANP	PA-O3A	3.50	1.63	1.59
4	C	1004	873	C07-N08	-3.00	1.43	1.47
4	B	1004	873	C01-C21	2.92	1.60	1.53
4	B	1004	873	C07-N08	2.26	1.49	1.47
4	C	1004	873	C05-C04	2.16	1.56	1.53
4	A	1004	873	C12-C17	-2.03	1.43	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	873	C12-C17-N08	4.90	116.67	113.76
4	D	1004	873	C06-C05-C04	-3.32	109.49	115.62
4	A	1004	873	C09-N08-C17	-3.19	119.50	121.89
2	C	1001	ANP	O2G-PG-O1G	-3.16	105.54	113.45
2	A	1001	ANP	O2G-PG-O1G	-3.15	105.55	113.45
2	D	1001	ANP	O2G-PG-O1G	-3.13	105.60	113.45
4	B	1004	873	C12-C17-N08	3.09	115.60	113.76
4	D	1004	873	C09-N08-C17	-3.01	119.64	121.89
4	D	1004	873	C12-C17-N08	2.92	115.49	113.76
4	B	1004	873	C09-N08-C17	-2.88	119.74	121.89
2	A	1001	ANP	C5'-C4'-C3'	-2.82	105.06	115.21
4	C	1004	873	C06-C05-C04	-2.74	110.55	115.62
4	C	1004	873	C09-N08-C17	-2.74	119.84	121.89
4	C	1004	873	C12-C17-N08	2.63	115.32	113.76
2	B	1001	ANP	O1G-PG-N3B	-2.55	108.02	111.77
4	D	1004	873	C11-N10-C09	2.51	119.24	116.69
4	B	1004	873	C11-N10-C09	2.38	119.12	116.69
4	C	1004	873	C11-N10-C09	2.35	119.09	116.69
4	A	1004	873	C12-C11-N10	-2.28	119.48	122.51
2	A	1001	ANP	C4'-O4'-C1'	-2.23	104.55	109.47
4	B	1004	873	C12-C11-N10	-2.09	119.73	122.51
4	A	1004	873	C16-C11-N10	2.03	120.75	118.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1004	873	C12-C11-N10	-2.03	119.82	122.51

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ANP	PB-N3B-PG-O1G
2	B	1001	ANP	PG-N3B-PB-O1B
2	C	1001	ANP	PB-N3B-PG-O1G
2	C	1001	ANP	PG-N3B-PB-O1B
2	C	1001	ANP	PG-N3B-PB-O3A
2	C	1001	ANP	C5'-O5'-PA-O1A
2	D	1001	ANP	PB-N3B-PG-O1G
2	D	1001	ANP	C5'-O5'-PA-O2A
2	D	1001	ANP	C5'-O5'-PA-O3A
4	A	1004	873	N03-C04-C05-C06
4	B	1004	873	C05-C06-C07-N08
4	C	1004	873	N03-C04-C05-C06
4	D	1004	873	N03-C04-C05-C06
2	C	1001	ANP	O4'-C4'-C5'-O5'
4	B	1004	873	O19-C06-C07-N08
2	A	1001	ANP	O4'-C4'-C5'-O5'
2	B	1001	ANP	C5'-O5'-PA-O1A
2	D	1001	ANP	C5'-O5'-PA-O1A
2	A	1001	ANP	C4'-C5'-O5'-PA
2	B	1001	ANP	C4'-C5'-O5'-PA
2	C	1001	ANP	C4'-C5'-O5'-PA
4	C	1004	873	O19-C06-C07-N08
4	A	1004	873	C20-C04-C05-C06
4	C	1004	873	C20-C04-C05-C06
2	C	1001	ANP	C3'-C4'-C5'-O5'
2	D	1001	ANP	C4'-C5'-O5'-PA

All (4) ring outliers are listed below:

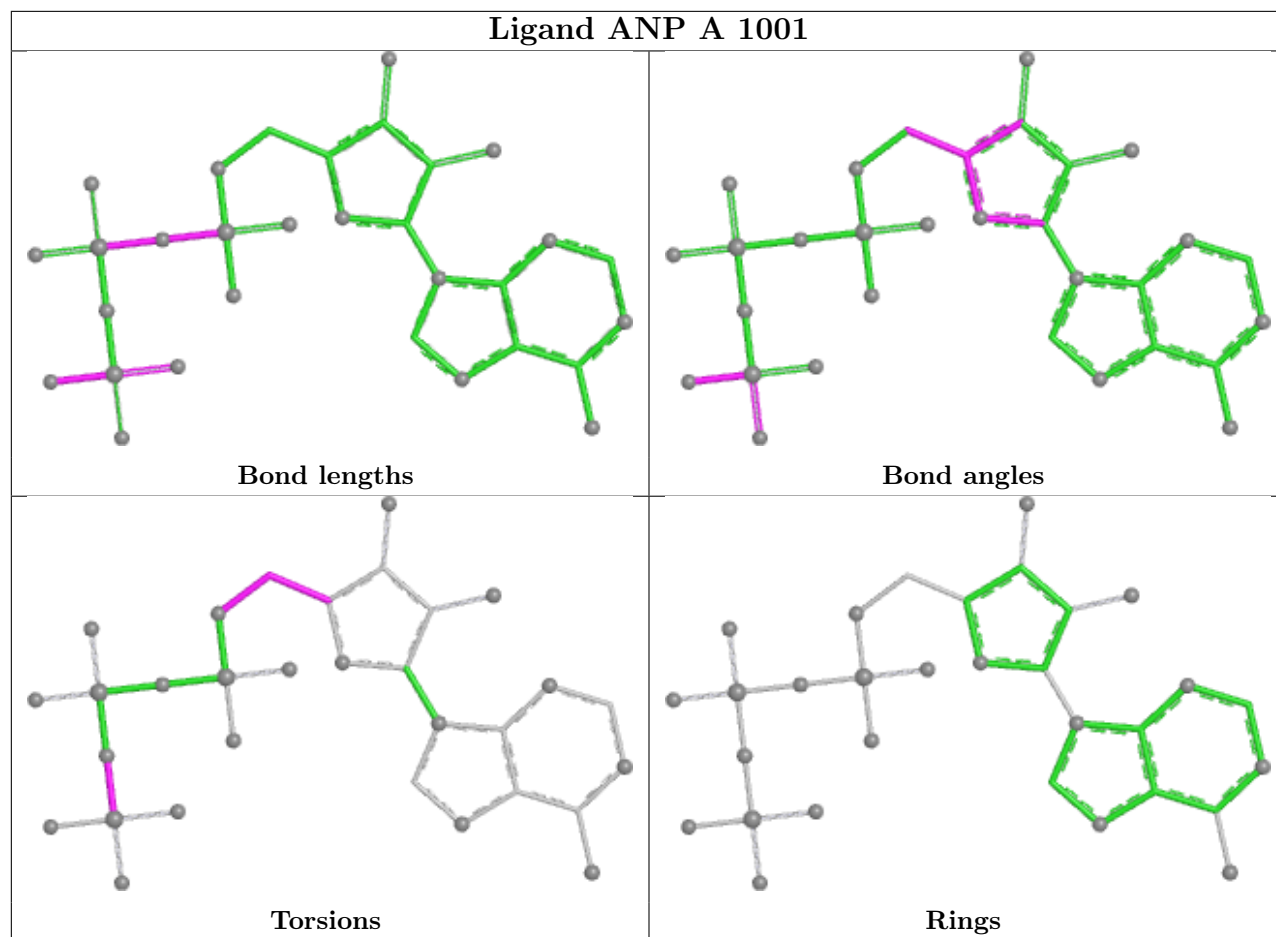
Mol	Chain	Res	Type	Atoms
4	B	1004	873	C01-C02-C04-C20-C21-N03
4	C	1004	873	C01-C02-C04-C20-C21-N03
4	D	1004	873	C01-C02-C04-C20-C21-N03
4	A	1004	873	C01-C02-C04-C20-C21-N03

8 monomers are involved in 17 short contacts:

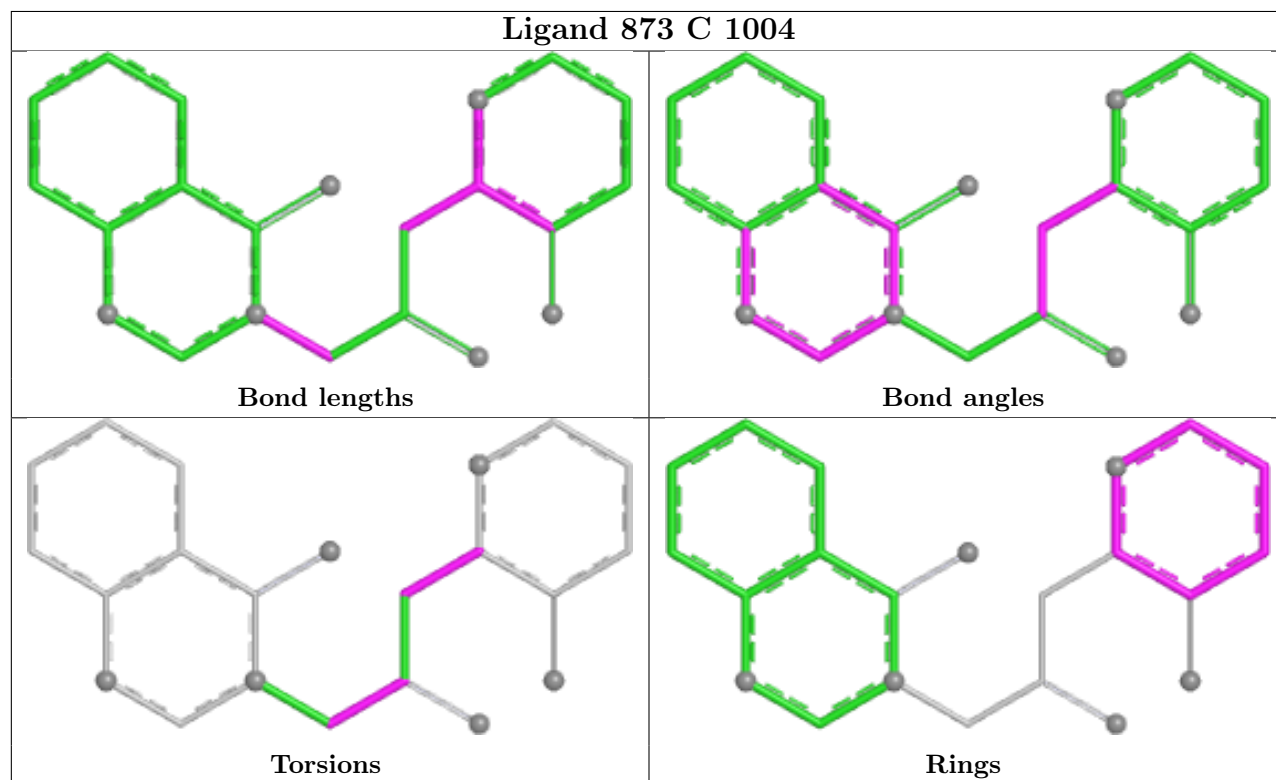
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ANP	2	0
4	C	1004	873	2	0
4	D	1004	873	2	0
4	A	1004	873	1	0
2	B	1001	ANP	7	0
2	D	1001	ANP	2	0
4	B	1004	873	4	0
2	C	1001	ANP	1	0

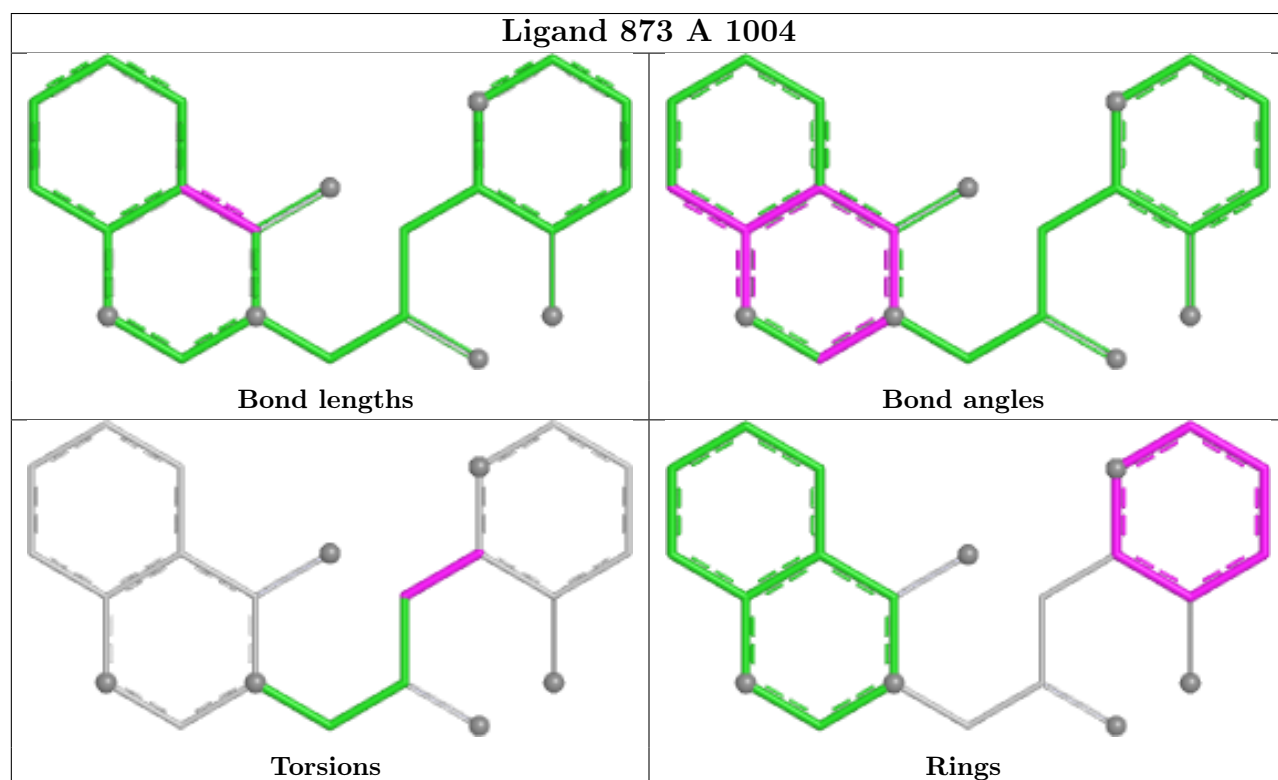
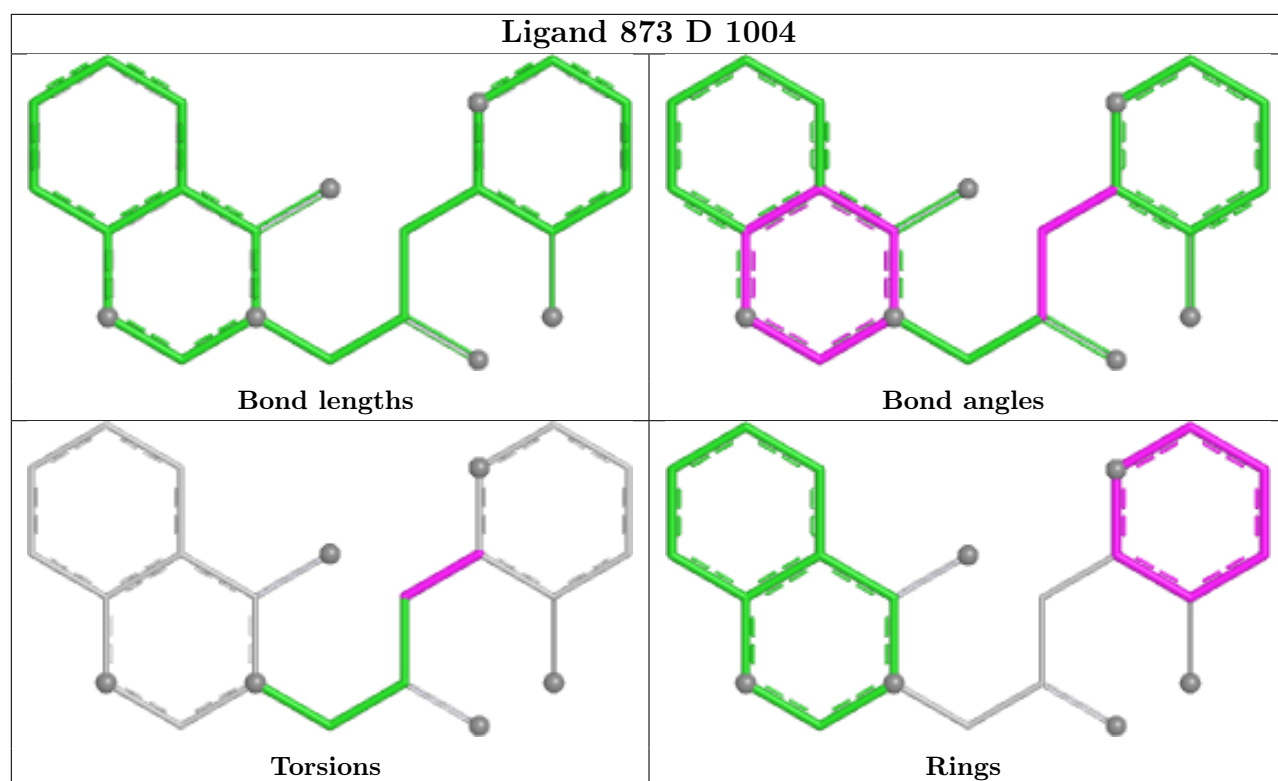
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

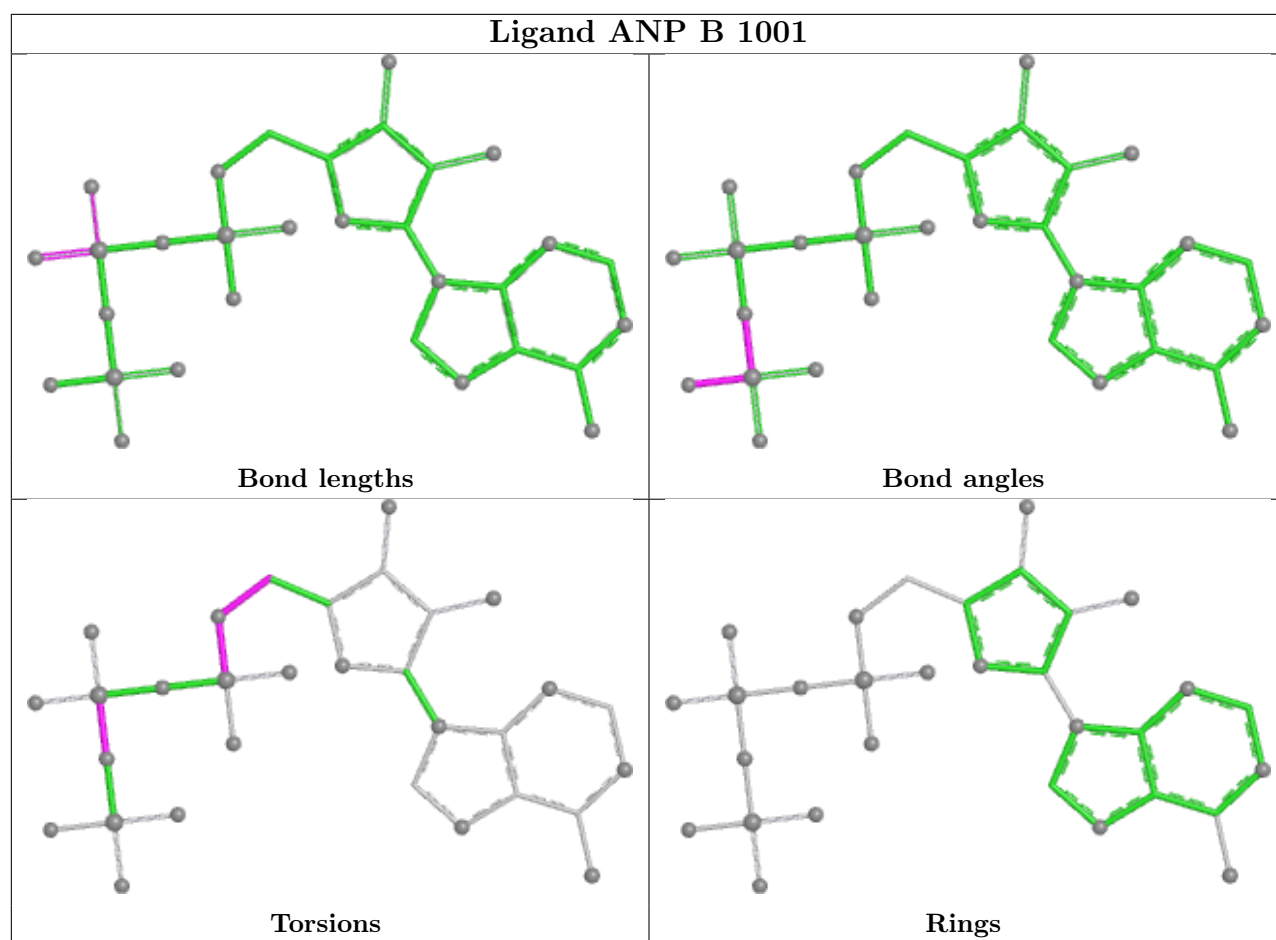
Ligand ANP A 1001



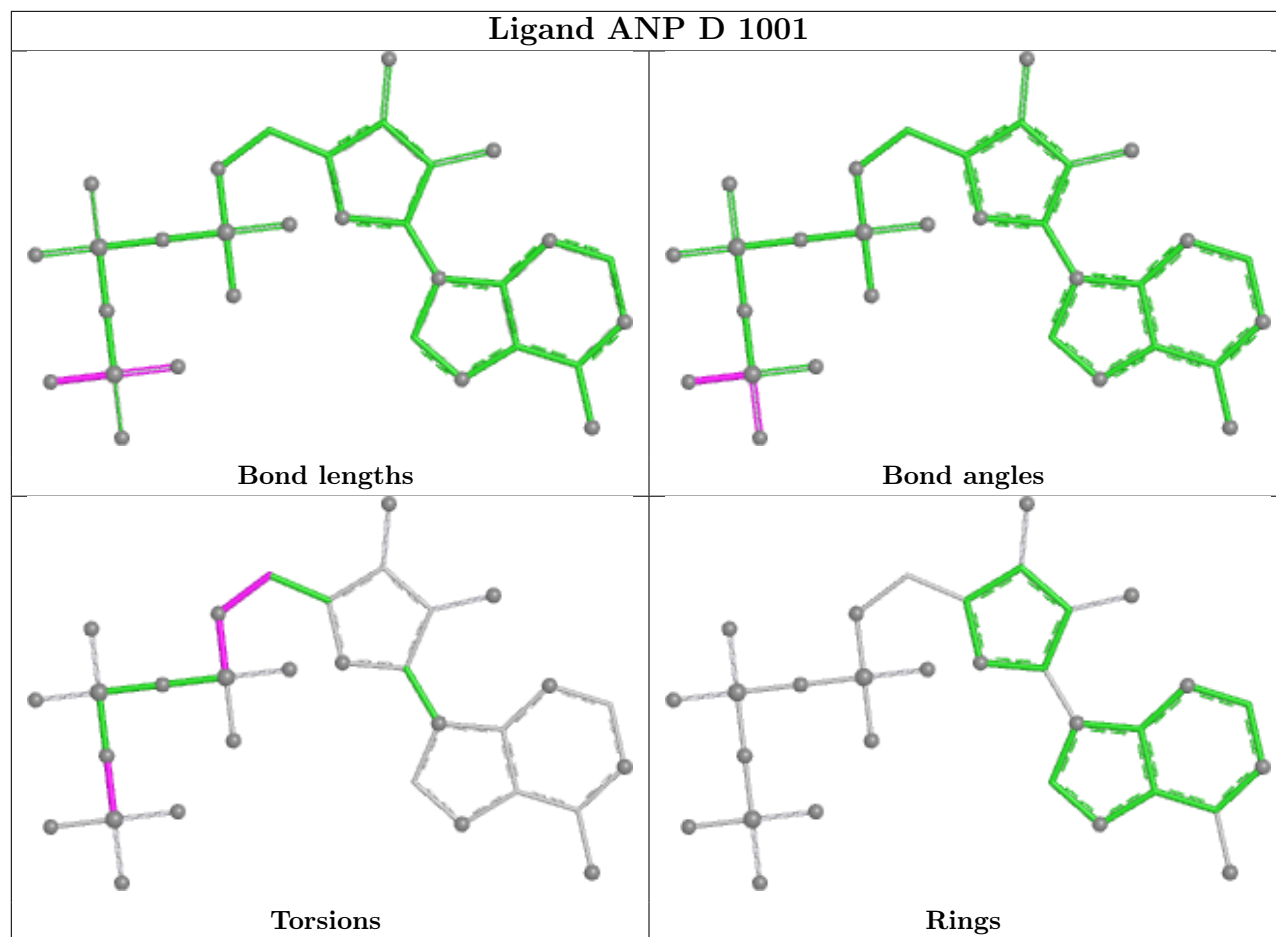
Ligand 873 C 1004



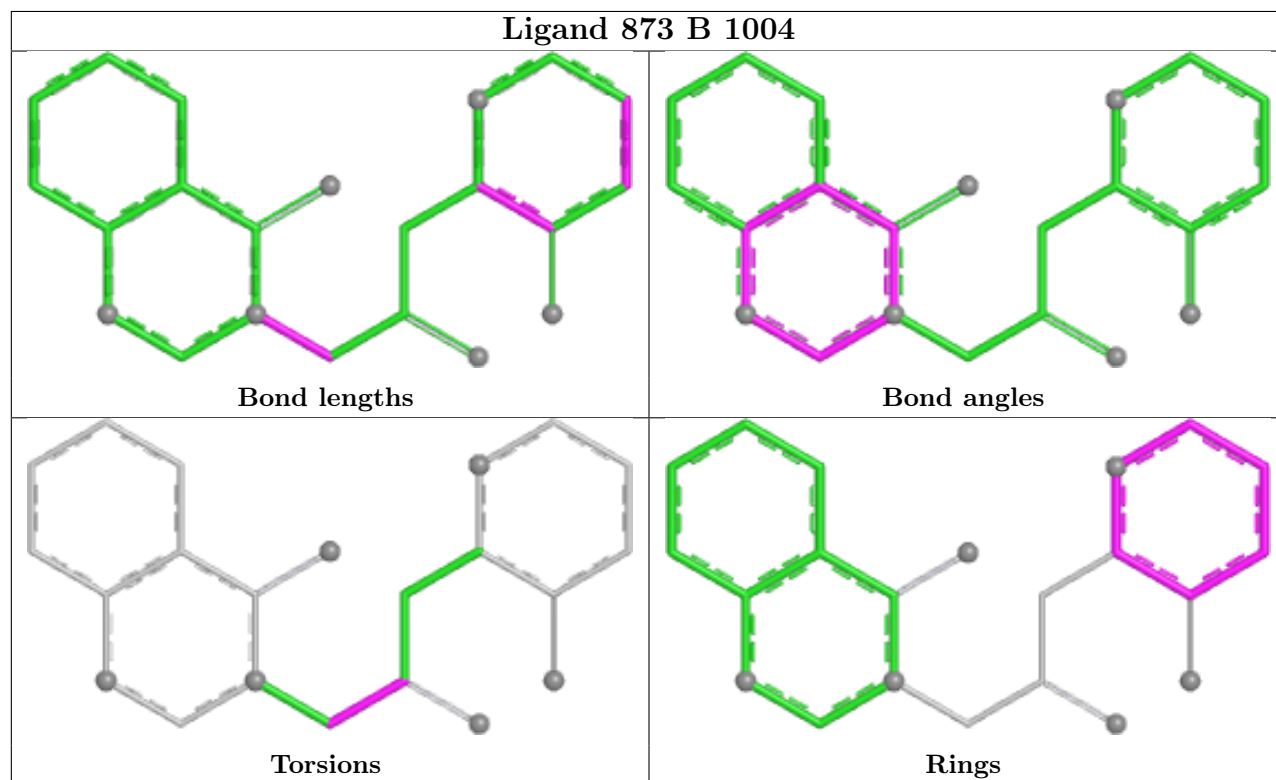


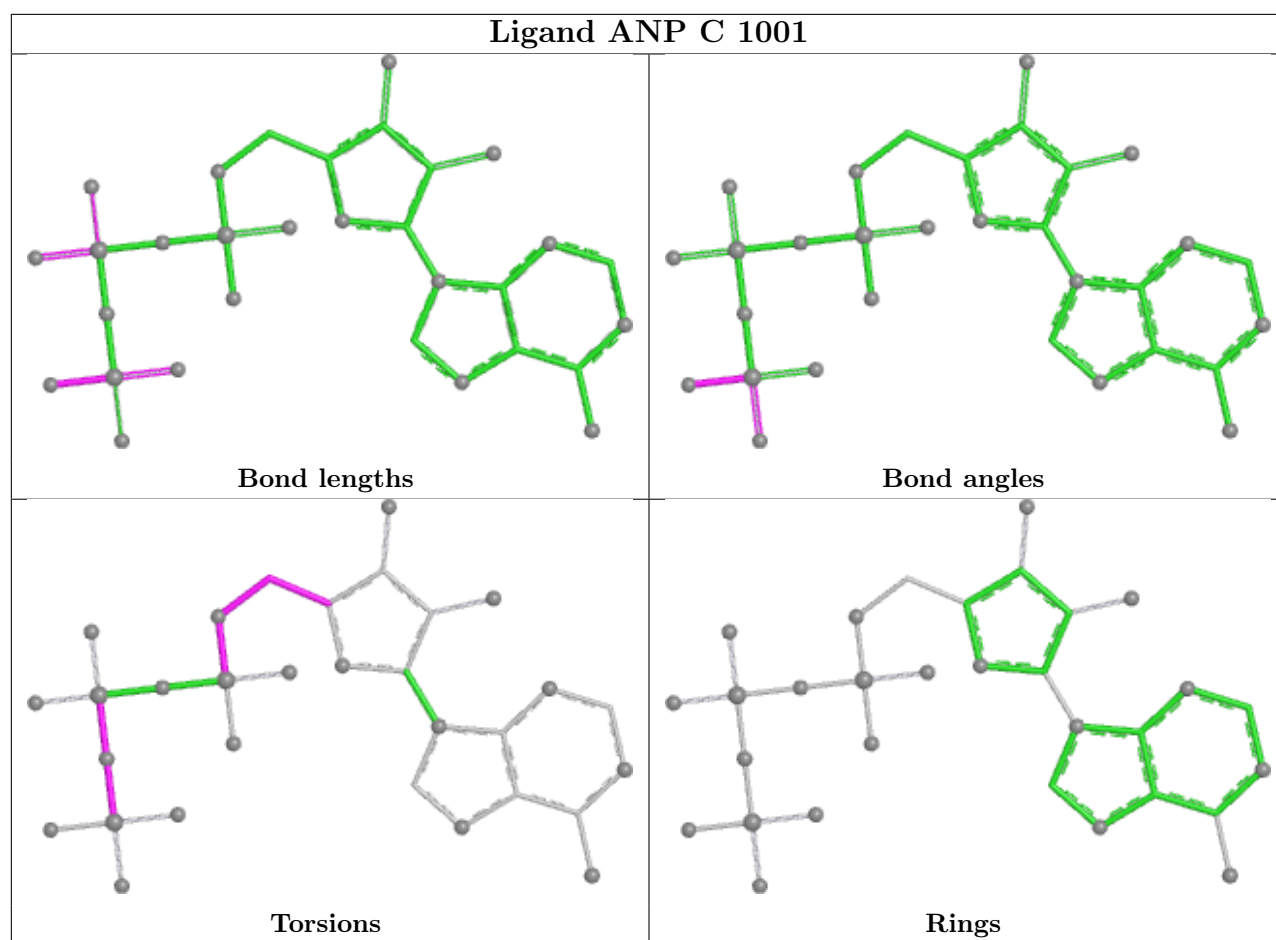


Ligand ANP D 1001



Ligand 873 B 1004





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	482/500 (96%)	-0.40	5 (1%) 79 76	16, 29, 54, 91	3 (0%)
1	B	478/500 (95%)	-0.13	15 (3%) 51 47	15, 37, 70, 95	1 (0%)
1	C	477/500 (95%)	-0.26	6 (1%) 75 71	13, 34, 62, 80	4 (0%)
1	D	472/500 (94%)	-0.14	12 (2%) 58 54	17, 38, 69, 98	2 (0%)
All	All	1909/2000 (95%)	-0.23	38 (1%) 65 61	13, 34, 66, 98	10 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	780	GLN	4.3
1	B	762	ASP	3.9
1	B	780	GLN	3.8
1	B	793	GLY	3.6
1	B	763	PRO	3.5
1	B	407	LYS	3.4
1	B	811	THR	3.4
1	C	632	THR	3.3
1	D	414	GLY	3.3
1	B	779	ILE	3.2
1	A	631	ASN	3.2
1	D	779	ILE	3.0
1	B	764	GLU	2.9
1	A	660	ASN	2.9
1	D	793	GLY	2.9
1	C	627	PHE	2.9
1	A	630	GLU	2.7
1	D	743	ASP	2.6
1	B	706	TRP	2.5
1	C	343	SER	2.4
1	D	810	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	625	ILE	2.4
1	C	580	HIS	2.4
1	C	793	GLY	2.3
1	B	687	ALA	2.3
1	A	632	THR	2.3
1	D	660	ASN	2.2
1	B	577	GLU	2.2
1	D	415	PHE	2.2
1	D	634	GLU	2.2
1	D	778	GLU	2.1
1	B	684	LYS	2.1
1	B	685	ASP	2.1
1	B	686	LEU	2.0
1	C	341	ASN	2.0
1	A	331	GLY	2.0
1	B	414	GLY	2.0
1	D	690	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	873	D	1004	22/22	0.84	0.12	24,26,30,34	0
4	873	C	1004	22/22	0.90	0.10	26,28,32,32	0
4	873	A	1004	22/22	0.92	0.09	23,27,28,29	0
4	873	B	1004	22/22	0.92	0.08	20,24,27,31	0
2	ANP	A	1001	31/31	0.92	0.11	17,19,21,22	0
2	ANP	B	1001	31/31	0.92	0.10	20,23,26,30	0

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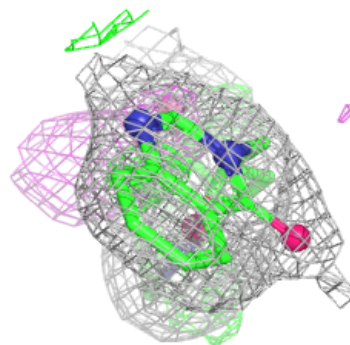
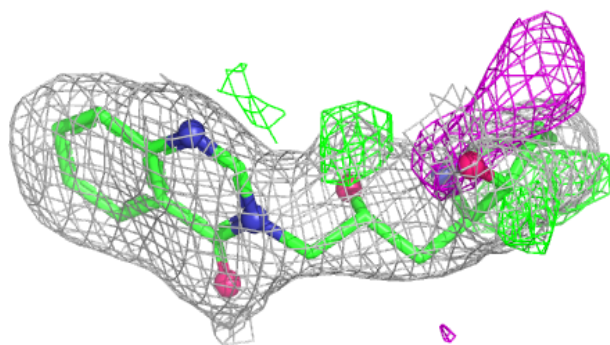
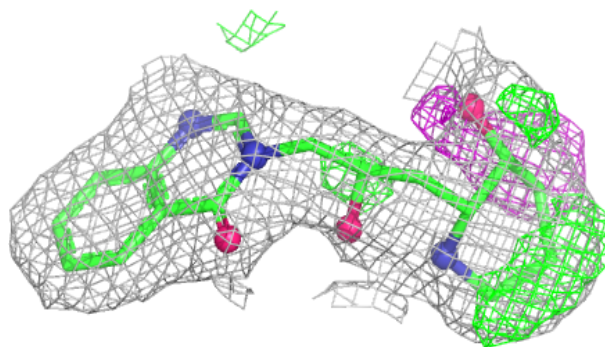
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1002	1/1	0.93	0.06	21,21,21,21	0
2	ANP	C	1001	31/31	0.95	0.07	22,24,28,31	0
2	ANP	D	1001	31/31	0.96	0.08	23,25,30,34	0
3	MG	D	1003	1/1	0.96	0.05	38,38,38,38	0
3	MG	D	1002	1/1	0.98	0.04	22,22,22,22	0
3	MG	A	1003	1/1	0.98	0.03	37,37,37,37	0
3	MG	B	1003	1/1	0.98	0.03	38,38,38,38	0
3	MG	B	1002	1/1	0.99	0.03	24,24,24,24	0
3	MG	C	1002	1/1	1.00	0.02	23,23,23,23	0
3	MG	C	1003	1/1	1.00	0.02	42,42,42,42	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.

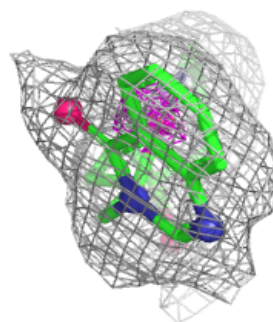
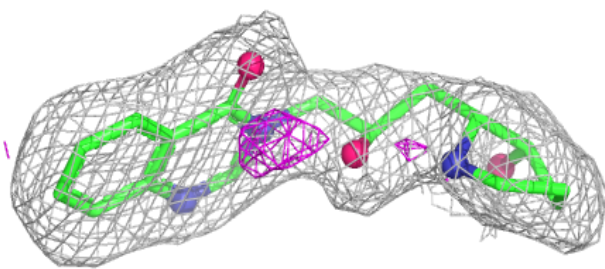
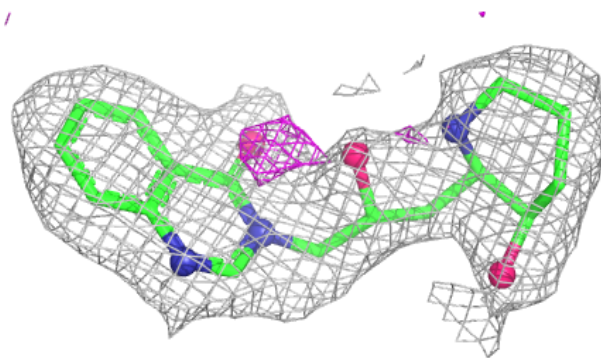
Electron density around 873 D 1004:

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

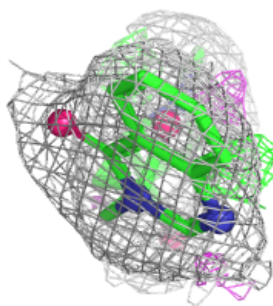
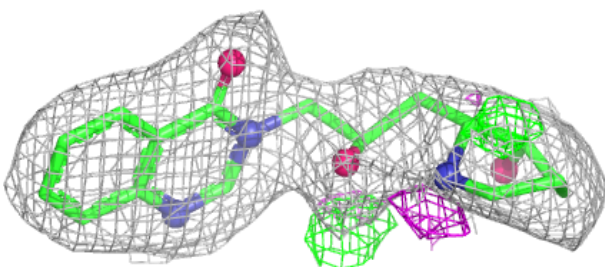
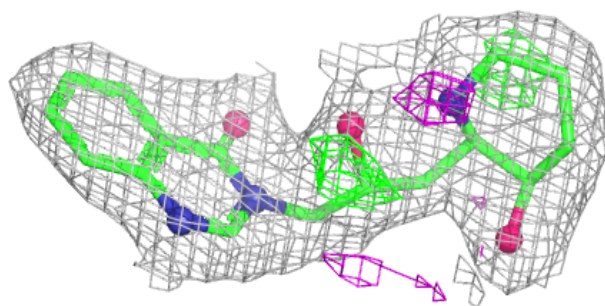


Electron density around 873 C 1004:

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

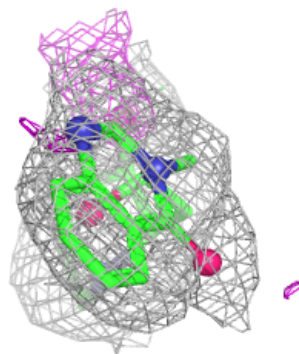
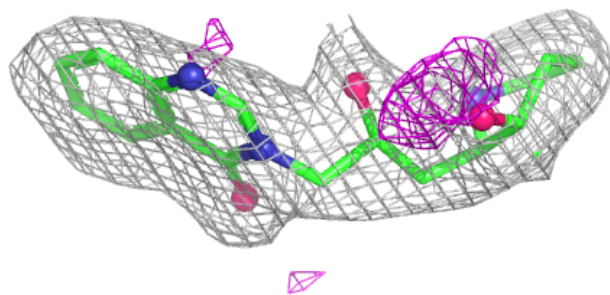
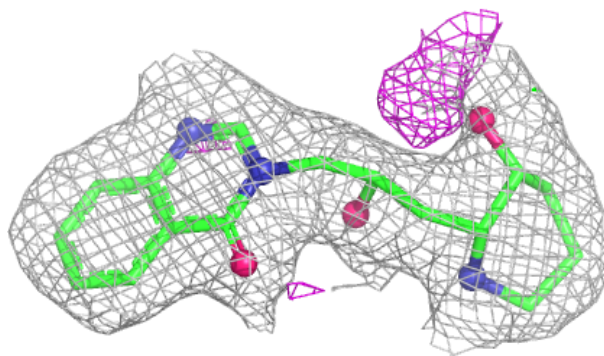
**Electron density around 873 A 1004:**

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



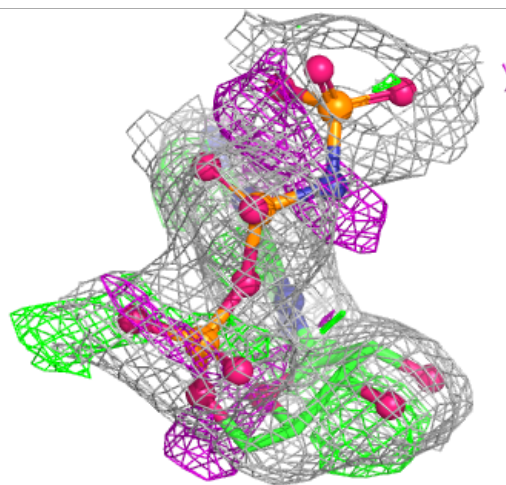
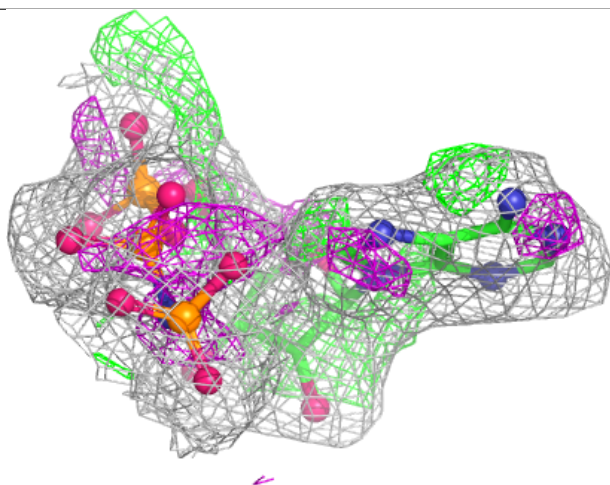
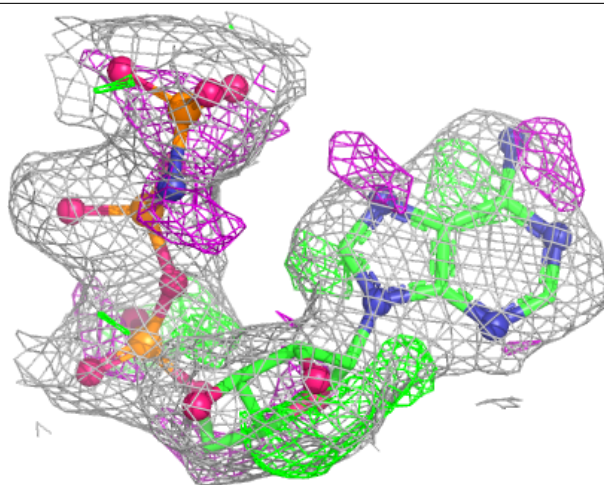
Electron density around 873 B 1004:

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



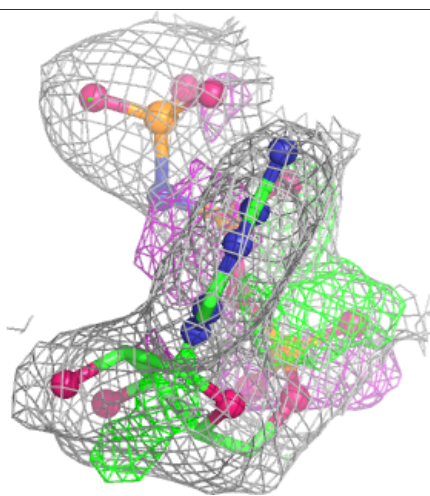
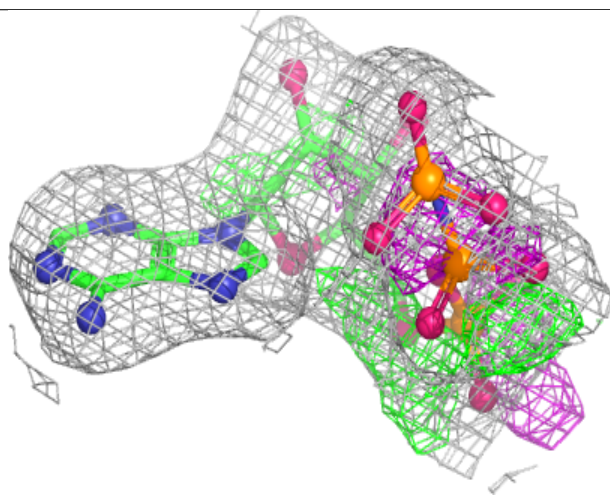
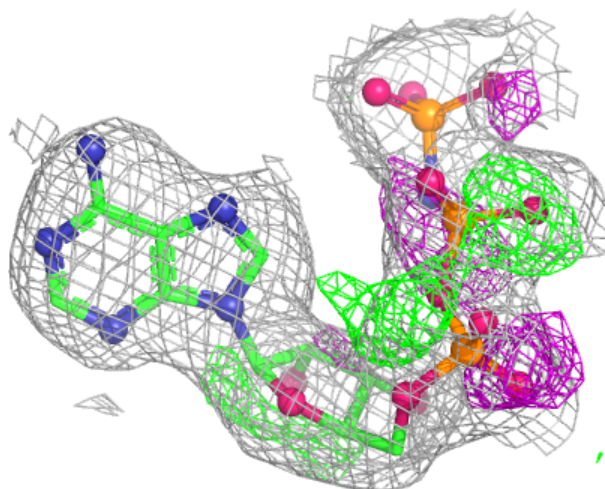
Electron density around ANP A 1001:

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



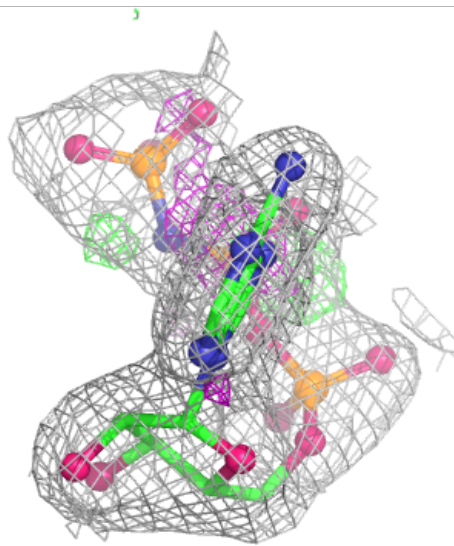
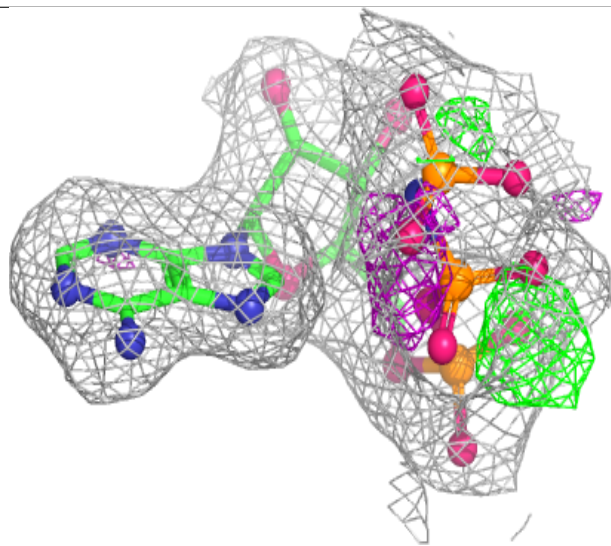
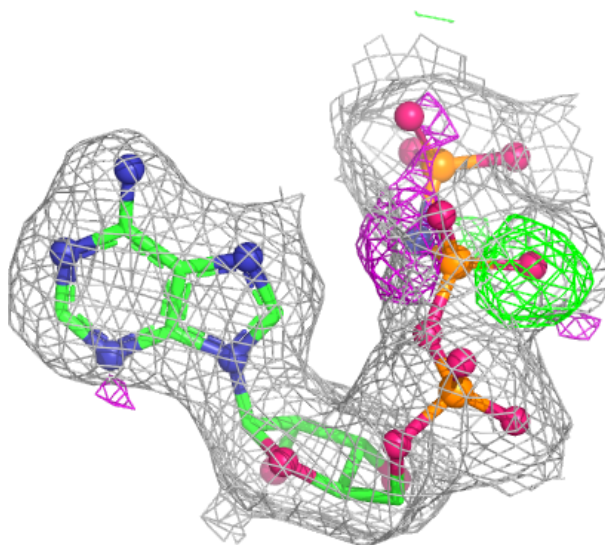
Electron density around ANP B 1001:

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and green (positive)



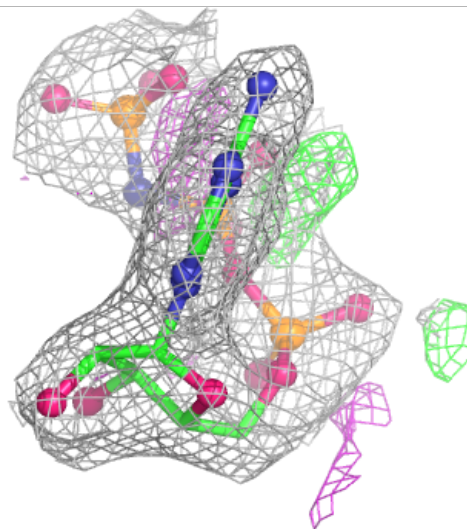
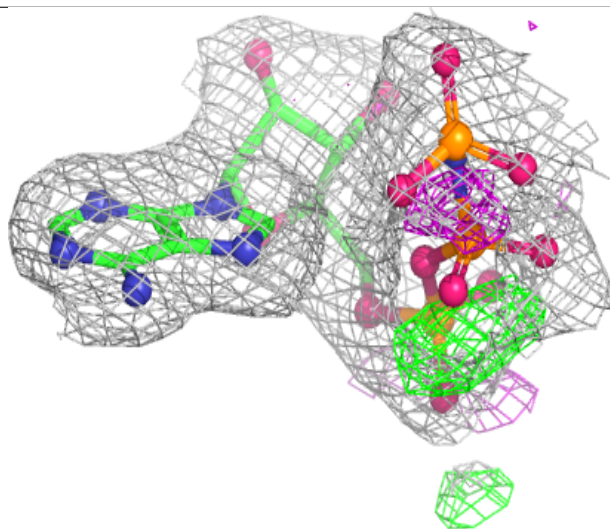
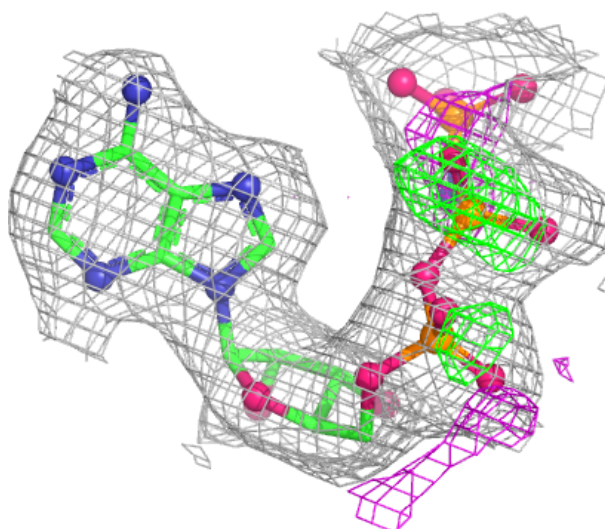
Electron density around ANP C 1001:

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



Electron density around ANP D 1001:

$2mF_o-DF_c$ (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.