



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 04:13 PM JST

PDB ID : 9KCE / pdb_00009kce
Title : Crystal Structure of the ATP analog-bound closed state of *Thermotoga maritima* MutS2
Authors : Fukui, K.; Murakawa, T.; Yano, T.
Deposited on : 2024-11-01
Resolution : 2.49 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 Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

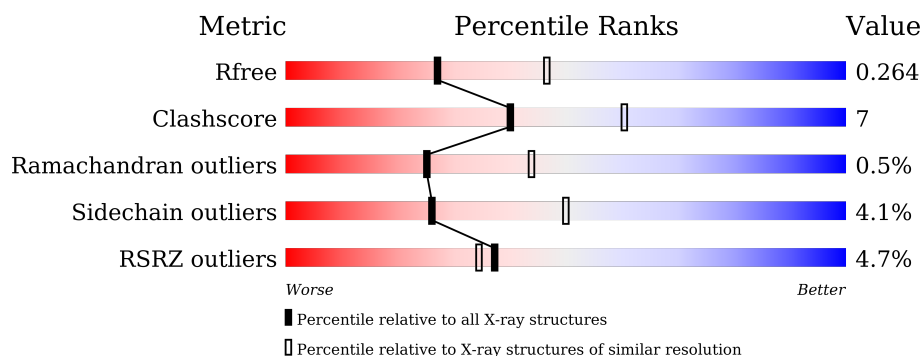
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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	497	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	B	497	<div> <div>6%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	C	497	<div> <div>4%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	497	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition [i](#)

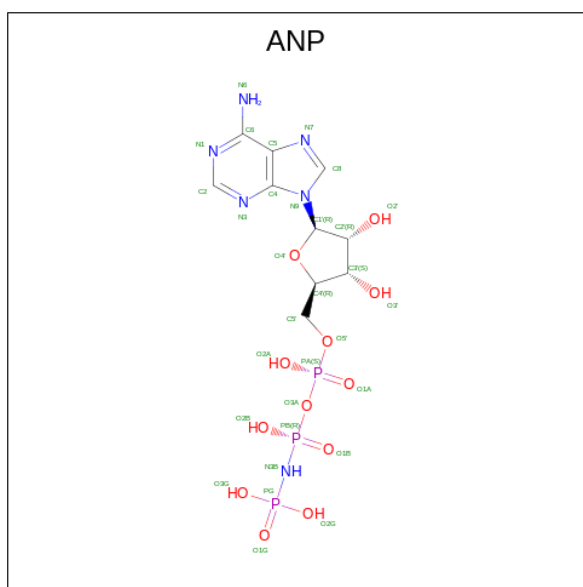
There are 6 unique types of molecules in this entry. The entry contains 15522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endonuclease MutS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	484	Total	C	N	O	S	0	0	0
			3723	2380	634	698	11			
1	C	490	Total	C	N	O	S	0	0	0
			3747	2397	640	698	12			
1	A	495	Total	C	N	O	S	0	0	0
			3847	2455	658	722	12			
1	D	494	Total	C	N	O	S	0	1	0
			3818	2437	663	706	12			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



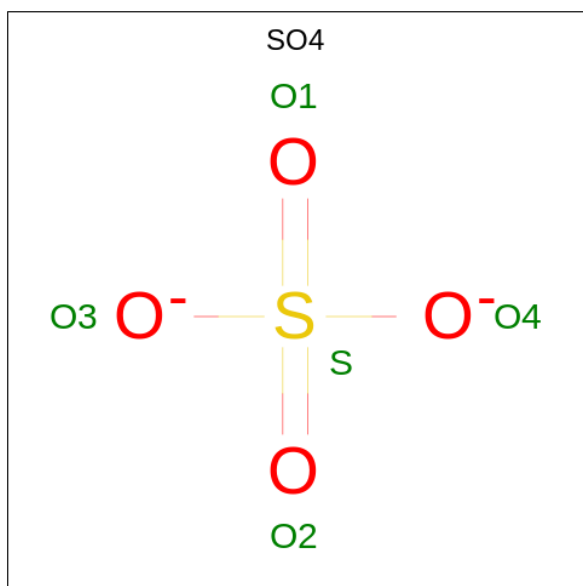
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



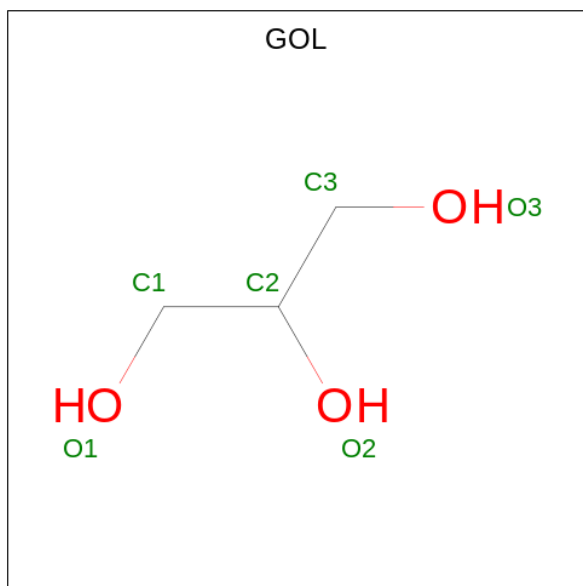
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

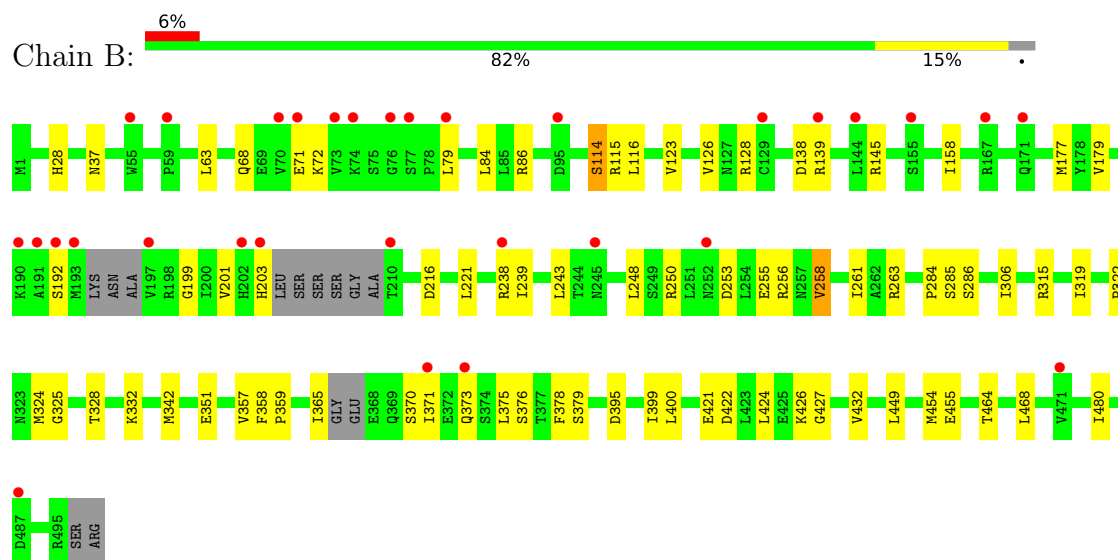
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	50	Total 50	O 50	0	0
6	C	67	Total 67	O 67	0	0
6	A	31	Total 31	O 31	0	0
6	D	40	Total 40	O 40	0	0

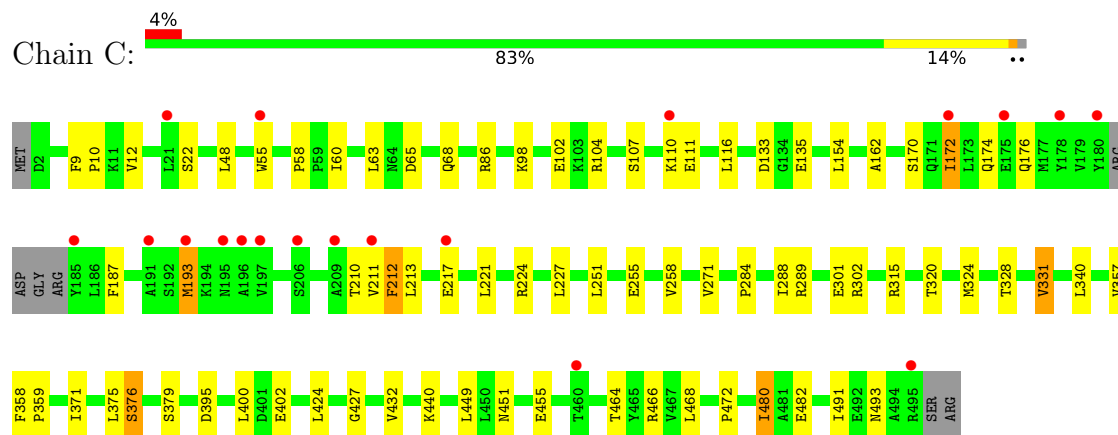
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

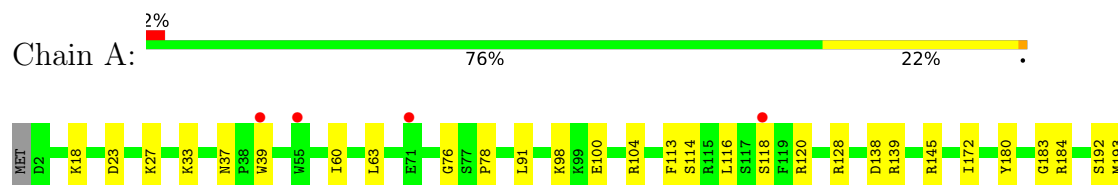
• Molecule 1: Endonuclease MutS2

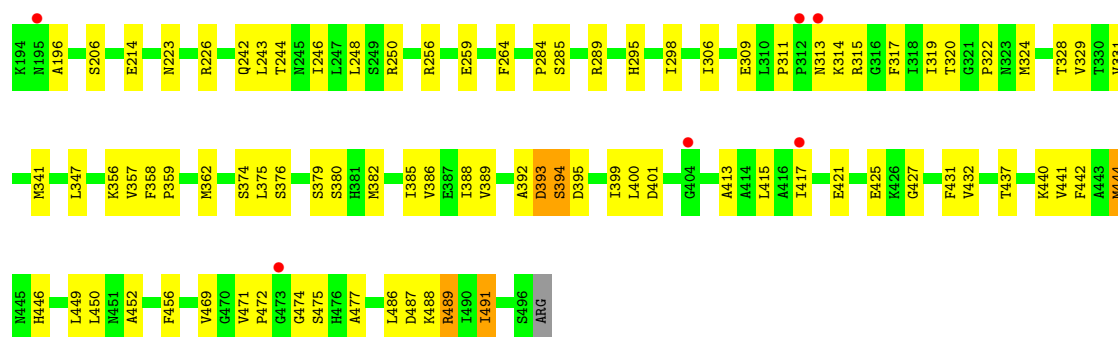


• Molecule 1: Endonuclease MutS2

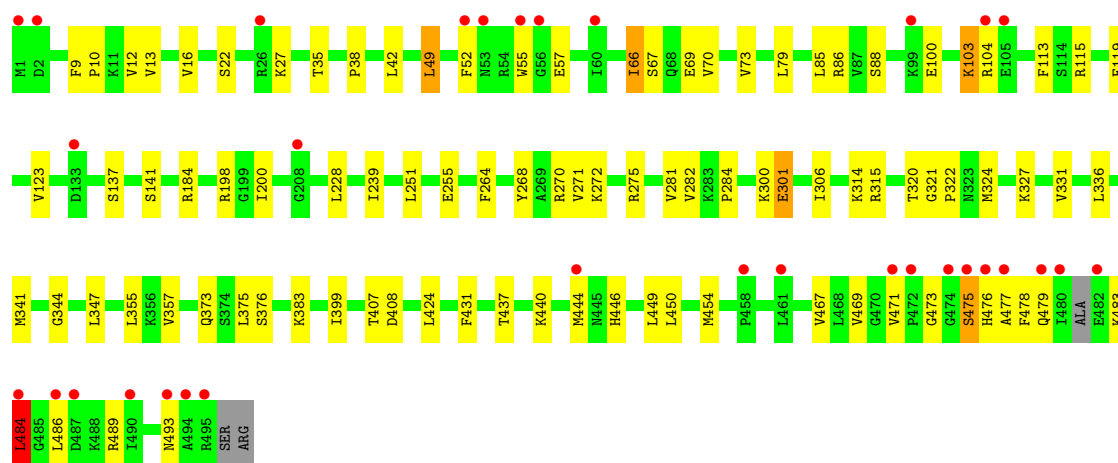
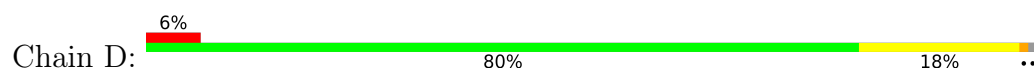


• Molecule 1: Endonuclease MutS2





• Molecule 1: Endonuclease MutS2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 142.85Å 139.42Å 90.00° 105.39° 90.00°	Depositor
Resolution (Å)	48.95 – 2.49 48.95 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-2.49) 100.0 (48.95-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.264 0.221 , 0.264	Depositor DCC
R_{free} test set	1682 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, GOL, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/3919	0.41	1/5312 (0.0%)
1	B	0.29	0/3791	0.47	1/5143 (0.0%)
1	C	0.24	0/3817	0.40	0/5181
1	D	0.26	0/3891	0.43	3/5271 (0.1%)
All	All	0.26	0/15418	0.43	5/20907 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	PHE	N-CA-C	-7.78	103.37	113.17
1	D	479	GLN	N-CA-C	-5.94	106.08	113.15
1	A	474	GLY	CA-C-O	-5.20	116.68	122.14
1	D	373	GLN	N-CA-C	-5.03	107.11	113.20
1	B	114	SER	N-CA-C	-5.03	105.50	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	ARG	Sidechain

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	3847	0	3826	64	0
1	B	3723	0	3656	45	0
1	C	3747	0	3675	39	0
1	D	3818	0	3793	54	0
2	A	31	0	13	3	0
2	B	31	0	13	2	0
2	C	31	0	13	3	0
2	D	31	0	13	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
4	C	25	0	0	0	0
4	D	10	0	0	0	0
5	D	6	0	8	0	0
6	A	31	0	0	0	0
6	B	50	0	0	2	0
6	C	67	0	0	0	0
6	D	40	0	0	2	0
All	All	15522	0	15010	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (198) 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:376:SER:H	1:A:379:SER:HB3	1.40	0.85
1:C:324:MET:H	2:C:501:ANP:HNB1	1.24	0.82
1:D:324:MET:H	2:D:501:ANP:HNB1	1.29	0.79
1:B:324:MET:H	2:B:501:ANP:HNB1	1.31	0.77
1:A:477:ALA:HB2	1:D:407:THR:HG21	1.69	0.74
4:A:506:SO4:O1	1:D:184:ARG:NH2	2.20	0.74
1:C:376:SER:H	1:C:379:SER:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLU:OE2	1:C:493:ASN:ND2	2.23	0.71
1:A:450:LEU:HD21	1:A:469:VAL:HG23	1.75	0.69
1:D:73:VAL:HG22	1:D:79:LEU:HD11	1.74	0.69
1:A:118:SER:O	1:A:120:ARG:NH1	2.25	0.69
1:B:359:PRO:HD2	1:B:395:ASP:HB2	1.75	0.68
1:A:375:LEU:HD12	1:A:380:SER:HA	1.75	0.68
1:A:184:ARG:NH2	1:A:223:ASN:OD1	2.27	0.66
1:C:170:SER:HA	1:C:176:GLN:HE22	1.60	0.65
1:A:320:THR:HG21	1:A:440:LYS:HG2	1.78	0.65
1:B:332:LYS:HE3	1:B:365:ILE:HG21	1.79	0.64
1:A:446:HIS:CG	1:A:449:LEU:HD13	2.33	0.64
1:B:376:SER:H	1:B:379:SER:HB2	1.65	0.62
1:D:38:PRO:HB2	1:D:42:LEU:HD23	1.82	0.62
1:D:42:LEU:HD12	1:D:281:VAL:HG13	1.80	0.62
1:B:328:THR:HG22	1:B:332:LYS:HD2	1.81	0.62
1:D:320:THR:HG21	1:D:440:LYS:HD3	1.81	0.61
1:A:23:ASP:O	1:A:27:LYS:HG2	1.99	0.61
1:B:86:ARG:NH1	6:B:602:HOH:O	2.33	0.61
1:D:454:MET:HE1	1:D:467:VAL:HG22	1.81	0.61
1:D:321:GLY:HA2	1:D:473:GLY:HA3	1.82	0.61
1:A:421:GLU:O	1:A:425:GLU:HG2	2.01	0.61
2:D:501:ANP:O2G	2:D:501:ANP:O2B	2.19	0.61
1:D:27:LYS:NZ	6:D:604:HOH:O	2.33	0.60
1:B:371:ILE:HG22	1:B:375:LEU:HB2	1.83	0.60
1:D:322:PRO:HA	1:D:475:SER:HA	1.83	0.59
1:A:76:GLY:HA2	1:A:248:LEU:HD11	1.84	0.59
1:A:385:ILE:O	1:A:389:VAL:HG23	2.02	0.59
1:C:211:VAL:O	1:C:212:PHE:C	2.47	0.58
1:A:243:LEU:HA	1:A:246:ILE:HD12	1.87	0.56
1:B:455:GLU:HB2	1:B:468:LEU:HD23	1.88	0.56
1:C:455:GLU:HG3	1:C:468:LEU:HD11	1.89	0.55
1:A:78:PRO:HA	1:A:244:THR:HG21	1.89	0.54
1:A:138:ASP:HB3	1:A:145:ARG:HG3	1.87	0.54
1:A:322:PRO:HG3	1:A:456:PHE:HB2	1.90	0.54
1:C:482:GLU:HG3	1:C:491:ILE:HD13	1.90	0.54
1:A:331:VAL:HG22	1:A:399:ILE:HG23	1.88	0.54
1:A:98:LYS:HE2	1:A:114:SER:HA	1.90	0.54
1:B:371:ILE:HG23	1:B:373:GLN:H	1.74	0.52
1:B:128:ARG:NH1	1:B:139:ARG:O	2.43	0.52
1:C:400:LEU:HB2	1:C:432:VAL:HG22	1.92	0.52
1:D:141:SER:HB2	1:D:239:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:MET:O	1:A:386:VAL:HG23	2.09	0.52
1:A:317:PHE:HD2	1:A:319:ILE:HD11	1.75	0.52
1:A:331:VAL:HG23	1:A:431:PHE:HB3	1.91	0.52
1:C:466:ARG:HH11	1:C:466:ARG:HG3	1.74	0.52
1:D:282:VAL:HG23	1:D:341:MET:HG3	1.92	0.51
1:D:69:GLU:N	1:D:69:GLU:OE1	2.43	0.51
1:A:23:ASP:OD2	1:A:27:LYS:HD3	2.10	0.51
1:A:172:ILE:HG22	1:A:193:MET:HE2	1.92	0.51
1:B:422:ASP:O	1:B:426:LYS:HG2	2.10	0.51
1:C:102:GLU:HA	1:C:110:LYS:HE3	1.92	0.51
1:A:415:LEU:HD11	1:D:477:ALA:HB1	1.92	0.51
1:D:331:VAL:HG22	1:D:399:ILE:HG23	1.92	0.51
1:B:400:LEU:HB2	1:B:432:VAL:HG12	1.93	0.50
1:B:203:HIS:HE1	1:C:224:ARG:HG3	1.76	0.50
1:A:442:PHE:CZ	1:A:446:HIS:HD2	2.30	0.50
1:A:317:PHE:CD2	1:A:319:ILE:HD11	2.45	0.50
1:D:437:THR:HA	1:D:440:LYS:HG3	1.93	0.50
1:D:315:ARG:NH2	1:D:424:LEU:O	2.44	0.50
1:D:12:VAL:HG21	1:D:336:LEU:HD21	1.93	0.50
1:B:68:GLN:O	1:B:71:GLU:HG3	2.12	0.50
1:A:120:ARG:NH1	1:A:250:ARG:HH22	2.10	0.49
1:A:388:ILE:O	1:A:392:ALA:HB2	2.12	0.49
1:D:119:PHE:O	1:D:123:VAL:HG23	2.11	0.49
1:A:37:ASN:HA	1:A:39:TRP:CZ3	2.46	0.49
2:B:501:ANP:O2B	2:B:501:ANP:O3G	2.31	0.49
1:B:203:HIS:CE1	1:C:224:ARG:HG3	2.47	0.49
1:B:28:HIS:CE1	1:B:263:ARG:HG3	2.47	0.49
1:B:84:LEU:HD11	1:B:243:LEU:HB3	1.94	0.49
1:D:69:GLU:O	1:D:73:VAL:HG23	2.13	0.49
1:D:251:LEU:O	1:D:255:GLU:HG3	2.13	0.49
1:A:324:MET:H	2:A:501:ANP:HNB1	1.59	0.49
1:D:322:PRO:HA	1:D:475:SER:CA	2.42	0.49
1:C:172:ILE:HG13	1:C:193:MET:HB3	1.95	0.48
1:A:128:ARG:HA	1:A:139:ARG:HH21	1.79	0.48
1:D:55:TRP:HH2	1:D:104:ARG:HB3	1.78	0.48
1:D:331:VAL:HG23	1:D:431:PHE:HB3	1.94	0.48
1:C:48:LEU:HB3	1:C:271:VAL:HG21	1.95	0.48
1:D:486:LEU:O	1:D:489:ARG:N	2.44	0.48
1:B:284:PRO:HB3	1:B:357:VAL:HG23	1.95	0.48
1:B:324:MET:HE2	1:B:324:MET:HB3	1.70	0.48
1:A:284:PRO:HB3	1:A:357:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PRO:HD2	1:A:395:ASP:HB3	1.96	0.48
1:D:301:GLU:CD	1:D:301:GLU:H	2.22	0.47
1:A:374:SER:HA	2:D:501:ANP:O3'	2.15	0.47
1:A:328:THR:O	1:A:331:VAL:HG12	2.15	0.47
1:A:441:VAL:HA	1:A:444:MET:HE2	1.96	0.47
1:B:322:PRO:HG2	1:B:325:GLY:HA3	1.97	0.47
2:A:501:ANP:O2G	1:D:376:SER:OG	2.33	0.47
1:D:446:HIS:HB3	1:D:449:LEU:HB2	1.95	0.47
1:A:242:GLN:HA	1:A:242:GLN:HE21	1.79	0.47
1:B:138:ASP:HB3	1:B:145:ARG:HB3	1.96	0.47
1:C:315:ARG:HH12	1:C:427:GLY:HA2	1.78	0.47
1:D:57:GLU:OE1	1:D:268:TYR:OH	2.33	0.47
1:B:399:ILE:C	1:B:400:LEU:HD23	2.40	0.47
1:D:113:PHE:CE1	1:D:264:PHE:HB2	2.49	0.47
1:D:450:LEU:HD21	1:D:469:VAL:HG13	1.97	0.47
1:C:162:ALA:HA	1:C:187:PHE:HZ	1.81	0.46
1:D:282:VAL:HG22	1:D:347:LEU:HD23	1.97	0.46
1:C:359:PRO:HD2	1:C:395:ASP:HB3	1.97	0.46
1:B:72:LYS:HD3	1:B:79:LEU:HD23	1.98	0.46
1:B:250:ARG:HB3	1:B:253:ASP:HB2	1.98	0.46
1:A:120:ARG:H	1:A:120:ARG:CD	2.28	0.46
1:D:407:THR:HG22	1:D:408:ASP:H	1.79	0.46
1:C:424:LEU:HD11	1:C:449:LEU:HD21	1.96	0.46
1:B:342:MET:HE1	1:B:358:PHE:O	2.16	0.46
1:B:199:GLY:HA2	1:B:216:ASP:OD1	2.16	0.46
1:C:284:PRO:HB3	1:C:357:VAL:HG23	1.98	0.46
1:C:451:ASN:HD22	1:C:472:PRO:HG3	1.79	0.46
1:A:100:GLU:O	1:A:104:ARG:HG2	2.16	0.46
1:A:295:HIS:HB3	1:A:298:ILE:HG13	1.97	0.46
1:B:114:SER:C	1:B:116:LEU:N	2.73	0.45
1:A:311:PRO:HD2	1:A:314:LYS:HG3	1.98	0.45
1:A:486:LEU:HB3	1:A:491:ILE:HD11	1.97	0.45
1:D:42:LEU:HD22	1:D:344:GLY:HA2	1.97	0.45
1:D:327:LYS:O	1:D:331:VAL:HG12	2.17	0.45
1:A:319:ILE:HD13	1:A:452:ALA:HB3	1.98	0.45
1:C:217:GLU:O	1:C:221:LEU:HD13	2.17	0.45
1:A:437:THR:HA	1:A:440:LYS:HD3	1.99	0.45
1:B:84:LEU:HD12	1:B:126:VAL:HG22	1.99	0.45
1:B:255:GLU:O	1:B:258:VAL:HG12	2.17	0.45
1:A:256:ARG:O	1:A:259:GLU:HG2	2.17	0.45
1:A:341:MET:HB2	1:A:347:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLU:OE1	1:C:402:GLU:HA	2.17	0.44
1:D:484:LEU:HD12	1:D:484:LEU:HA	1.81	0.44
1:D:69:GLU:OE2	1:D:86:ARG:NH1	2.51	0.44
1:D:300:LYS:HD3	1:D:300:LYS:HA	1.77	0.44
1:A:184:ARG:HD3	1:A:214:GLU:OE2	2.18	0.44
1:B:454:MET:HE3	1:B:454:MET:HB3	1.84	0.44
1:B:468:LEU:HD13	1:B:468:LEU:HA	1.88	0.44
1:C:302:ARG:O	2:C:501:ANP:H2	2.17	0.44
1:D:100:GLU:O	1:D:104:ARG:HG2	2.17	0.43
1:B:315:ARG:NH2	1:B:427:GLY:HA2	2.33	0.43
1:C:255:GLU:O	1:C:258:VAL:HG12	2.17	0.43
2:C:501:ANP:O2G	2:C:501:ANP:O2B	2.37	0.43
1:A:37:ASN:OD1	1:A:39:TRP:HE3	2.01	0.43
1:A:113:PHE:CZ	1:A:264:PHE:HB2	2.53	0.43
1:B:378:PHE:HE2	1:C:480:ILE:HG22	1.83	0.43
1:C:98:LYS:NZ	1:C:116:LEU:O	2.42	0.43
1:C:107:SER:O	1:C:111:GLU:HG2	2.19	0.43
1:A:356:LYS:HD2	1:A:358:PHE:CZ	2.52	0.43
1:A:193:MET:HB3	1:A:196:ALA:HB2	2.01	0.43
1:A:289:ARG:HD3	1:A:309:GLU:OE1	2.18	0.43
1:D:383:LYS:HA	1:D:383:LYS:HD2	1.75	0.43
1:C:301:GLU:OE1	1:C:301:GLU:N	2.32	0.43
1:D:9:PHE:HB3	1:D:10:PRO:HD3	2.01	0.43
1:D:284:PRO:HB3	1:D:357:VAL:HG23	2.00	0.43
1:B:114:SER:C	1:B:116:LEU:H	2.27	0.42
1:C:455:GLU:HB3	1:C:464:THR:OG1	2.19	0.42
1:C:320:THR:HG21	1:C:440:LYS:HG2	2.02	0.42
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.78	0.42
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.86	0.42
1:A:329:VAL:HG21	2:A:501:ANP:H3'	2.02	0.42
1:B:315:ARG:NH2	1:B:424:LEU:O	2.52	0.42
1:D:115:ARG:HA	1:D:115:ARG:HD2	1.87	0.42
1:B:455:GLU:HB2	1:B:468:LEU:CD2	2.49	0.42
1:A:313:ASN:OD1	1:A:313:ASN:N	2.44	0.42
1:D:103:LYS:HE3	1:D:103:LYS:HB2	1.47	0.42
1:D:57:GLU:CD	1:D:272:LYS:HZ1	2.26	0.41
1:D:444:MET:HE3	1:D:444:MET:HB2	1.71	0.41
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.90	0.41
1:C:328:THR:O	1:C:331:VAL:HG12	2.20	0.41
1:D:440:LYS:NZ	1:D:473:GLY:O	2.53	0.41
1:B:158:ILE:HD11	1:B:221:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG11	1:C:340:LEU:HD11	2.02	0.41
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.86	0.41
1:D:314:LYS:NZ	6:D:602:HOH:O	2.31	0.41
1:B:238:ARG:HH21	1:B:239:ILE:HG12	1.85	0.41
1:B:455:GLU:HB3	1:B:464:THR:OG1	2.19	0.41
1:B:138:ASP:HB3	1:B:145:ARG:HD2	2.01	0.41
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.76	0.41
1:A:98:LYS:HE3	1:A:116:LEU:O	2.21	0.41
1:C:58:PRO:O	1:C:60:ILE:HG23	2.21	0.41
1:A:180:TYR:CZ	1:A:183:GLY:HA2	2.56	0.41
1:A:315:ARG:HH21	1:A:427:GLY:C	2.29	0.41
1:D:13:VAL:HA	1:D:16:VAL:HG12	2.03	0.41
1:D:52:PHE:HB3	1:D:275:ARG:HD3	2.03	0.41
1:C:288:ILE:HD11	1:C:358:PHE:HE2	1.86	0.41
1:A:184:ARG:CZ	1:D:200:ILE:HG23	2.51	0.41
1:A:362:MET:HE3	1:A:362:MET:HB2	1.84	0.41
1:A:413:ALA:O	1:A:417:ILE:HG12	2.21	0.41
1:B:351:GLU:OE1	1:B:351:GLU:N	2.25	0.41
1:C:55:TRP:NE1	1:C:104:ARG:HD2	2.36	0.41
1:A:393:ASP:HB2	1:A:394:SER:H	1.75	0.41
1:D:66:ILE:HD12	1:D:70:VAL:HG23	2.03	0.41
1:B:371:ILE:HG13	6:B:619:HOH:O	2.21	0.40
1:B:63:LEU:HD23	1:B:261:ILE:HG23	2.02	0.40
1:C:65:ASP:O	1:C:86:ARG:NH2	2.54	0.40
1:C:133:ASP:OD1	1:C:135:GLU:HG3	2.21	0.40
1:D:49:LEU:HD22	1:D:271:VAL:HG13	2.03	0.40
1:C:9:PHE:HB3	1:C:10:PRO:HD3	2.04	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	493/497 (99%)	476 (97%)	13 (3%)	4 (1%)	16	31
1	B	476/497 (96%)	457 (96%)	18 (4%)	1 (0%)	44	64
1	C	486/497 (98%)	470 (97%)	15 (3%)	1 (0%)	44	64
1	D	491/497 (99%)	460 (94%)	27 (6%)	4 (1%)	16	31
All	All	1946/1988 (98%)	1863 (96%)	73 (4%)	10 (0%)	25	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	SER
1	C	212	PHE
1	A	487	ASP
1	A	488	LYS
1	D	476	HIS
1	D	483	LYS
1	D	493	ASN
1	B	115	ARG
1	D	484	LEU
1	A	472	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	415/448 (93%)	399 (96%)	16 (4%)	27	52
1	B	395/448 (88%)	380 (96%)	15 (4%)	28	53
1	C	392/448 (88%)	376 (96%)	16 (4%)	26	50
1	D	405/448 (90%)	386 (95%)	19 (5%)	22	44
All	All	1607/1792 (90%)	1541 (96%)	66 (4%)	26	50

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	ASN

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Mol	Chain	Res	Type
1	B	123	VAL
1	B	177	MET
1	B	179	VAL
1	B	192	SER
1	B	201	VAL
1	B	256	ARG
1	B	258	VAL
1	B	285	SER
1	B	286	SER
1	B	306	ILE
1	B	319	ILE
1	B	370	SER
1	B	449	LEU
1	B	480	ILE
1	C	22	SER
1	C	63	LEU
1	C	68	GLN
1	C	154	LEU
1	C	172	ILE
1	C	174	GLN
1	C	193	MET
1	C	210	THR
1	C	213	LEU
1	C	227	LEU
1	C	251	LEU
1	C	289	ARG
1	C	331	VAL
1	C	371	ILE
1	C	376	SER
1	C	480	ILE
1	A	18	LYS
1	A	63	LEU
1	A	91	LEU
1	A	192	SER
1	A	206	SER
1	A	285	SER
1	A	306	ILE
1	A	393	ASP
1	A	394	SER
1	A	400	LEU
1	A	401	ASP
1	A	432	VAL

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Mol	Chain	Res	Type
1	A	444	MET
1	A	471	VAL
1	A	489	ARG
1	A	491	ILE
1	D	22	SER
1	D	35	THR
1	D	49	LEU
1	D	66	ILE
1	D	67	SER
1	D	85	LEU
1	D	88	SER
1	D	103	LYS
1	D	137	SER
1	D	198	ARG
1	D	228	LEU
1	D	270	ARG
1	D	301	GLU
1	D	306	ILE
1	D	355	LEU
1	D	375	LEU
1	D	471	VAL
1	D	475	SER
1	D	484	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	ASN
1	B	323	ASN
1	B	391	ASN
1	B	451	ASN
1	B	493	ASN
1	C	176	GLN
1	C	381	HIS
1	A	127	ASN
1	A	169	HIS
1	A	242	GLN
1	A	445	ASN
1	D	391	ASN
1	D	476	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
4	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.12	0
2	ANP	A	501	3	29,33,33	1.13	5 (17%)	31,52,52	0.92	3 (9%)
5	GOL	D	502	-	5,5,5	0.89	0	5,5,5	1.00	0
4	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.06	0
2	ANP	C	501	3	29,33,33	1.07	4 (13%)	31,52,52	1.05	2 (6%)
2	ANP	D	501	3	29,33,33	1.10	5 (17%)	31,52,52	1.10	3 (9%)
4	SO4	A	505	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	B	501	3	29,33,33	1.09	3 (10%)	31,52,52	1.07	3 (9%)

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
5	GOL	D	502	-	-	2/4/4/4	-
2	ANP	A	501	3	-	3/14/38/38	0/3/3/3
2	ANP	C	501	3	-	9/14/38/38	0/3/3/3
2	ANP	D	501	3	-	4/14/38/38	0/3/3/3
2	ANP	B	501	3	-	4/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ANP	PG-N3B	2.85	1.70	1.63
2	A	501	ANP	PG-N3B	2.85	1.70	1.63
2	D	501	ANP	PG-N3B	2.69	1.70	1.63
2	B	501	ANP	PG-O1G	2.62	1.50	1.46
2	C	501	ANP	PG-N3B	2.61	1.70	1.63
2	C	501	ANP	PG-O1G	2.60	1.50	1.46
2	A	501	ANP	PG-O1G	2.50	1.50	1.46
2	D	501	ANP	PG-O1G	2.38	1.49	1.46
2	B	501	ANP	PB-N3B	2.30	1.69	1.63
2	D	501	ANP	PB-O1B	2.26	1.49	1.46
2	A	501	ANP	PB-O3A	-2.25	1.56	1.59
2	A	501	ANP	PB-N3B	2.12	1.68	1.63
2	D	501	ANP	PB-N3B	2.10	1.68	1.63
2	D	501	ANP	PB-O3A	-2.09	1.56	1.59
2	C	501	ANP	PB-N3B	2.09	1.68	1.63
2	A	501	ANP	PB-O1B	2.06	1.49	1.46
2	C	501	ANP	PB-O1B	2.05	1.49	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ANP	PB-O3A-PA	-3.40	120.64	132.62
2	D	501	ANP	PB-O3A-PA	-3.27	121.11	132.62
2	A	501	ANP	PB-O3A-PA	-2.92	122.32	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ANP	PB-O3A-PA	-2.88	122.49	132.62
2	C	501	ANP	C5-C6-N6	2.33	123.89	120.35
2	B	501	ANP	C5-C6-N6	2.25	123.78	120.35
2	D	501	ANP	C5-C6-N6	2.24	123.75	120.35
2	A	501	ANP	O2G-PG-O1G	-2.18	107.98	113.45
2	A	501	ANP	C5-C6-N6	2.17	123.65	120.35
2	B	501	ANP	O2B-PB-O3A	2.16	111.85	104.64
2	D	501	ANP	O3G-PG-O1G	-2.13	108.10	113.45

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	ANP	PB-N3B-PG-O1G
2	B	501	ANP	PG-N3B-PB-O1B
2	B	501	ANP	PA-O3A-PB-O1B
2	B	501	ANP	PA-O3A-PB-O2B
2	C	501	ANP	PB-N3B-PG-O1G
2	C	501	ANP	PG-N3B-PB-O1B
2	C	501	ANP	PA-O3A-PB-O1B
2	C	501	ANP	PA-O3A-PB-O2B
2	C	501	ANP	C5'-O5'-PA-O1A
2	C	501	ANP	C5'-O5'-PA-O2A
2	C	501	ANP	C5'-O5'-PA-O3A
2	C	501	ANP	O4'-C4'-C5'-O5'
2	A	501	ANP	PB-N3B-PG-O1G
2	A	501	ANP	PA-O3A-PB-O1B
2	D	501	ANP	PB-N3B-PG-O1G
2	D	501	ANP	PG-N3B-PB-O1B
2	D	501	ANP	O4'-C4'-C5'-O5'
2	C	501	ANP	C3'-C4'-C5'-O5'
5	D	502	GOL	O1-C1-C2-C3
2	D	501	ANP	C3'-C4'-C5'-O5'
2	A	501	ANP	PA-O3A-PB-O2B
5	D	502	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

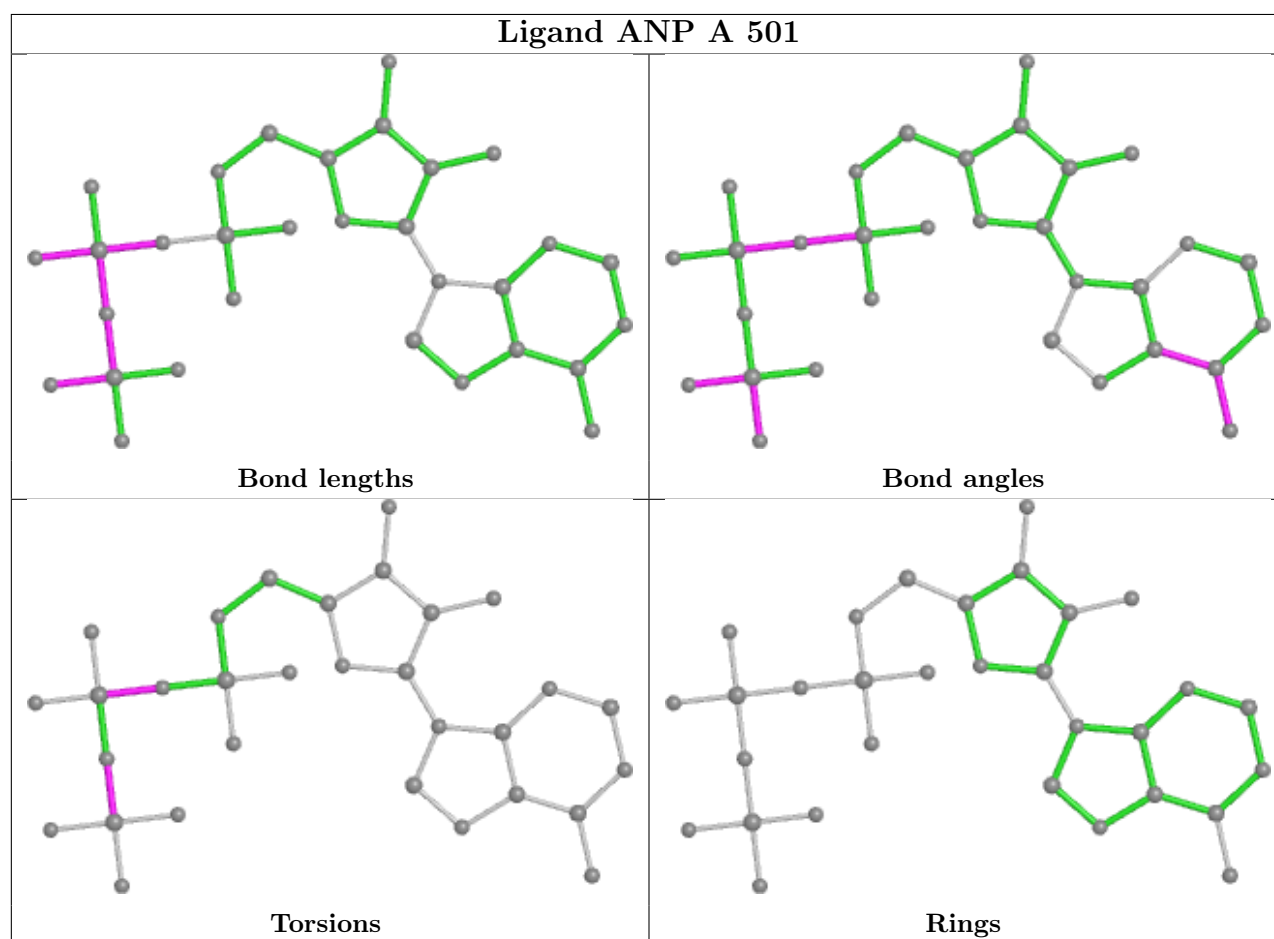
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ANP	3	0

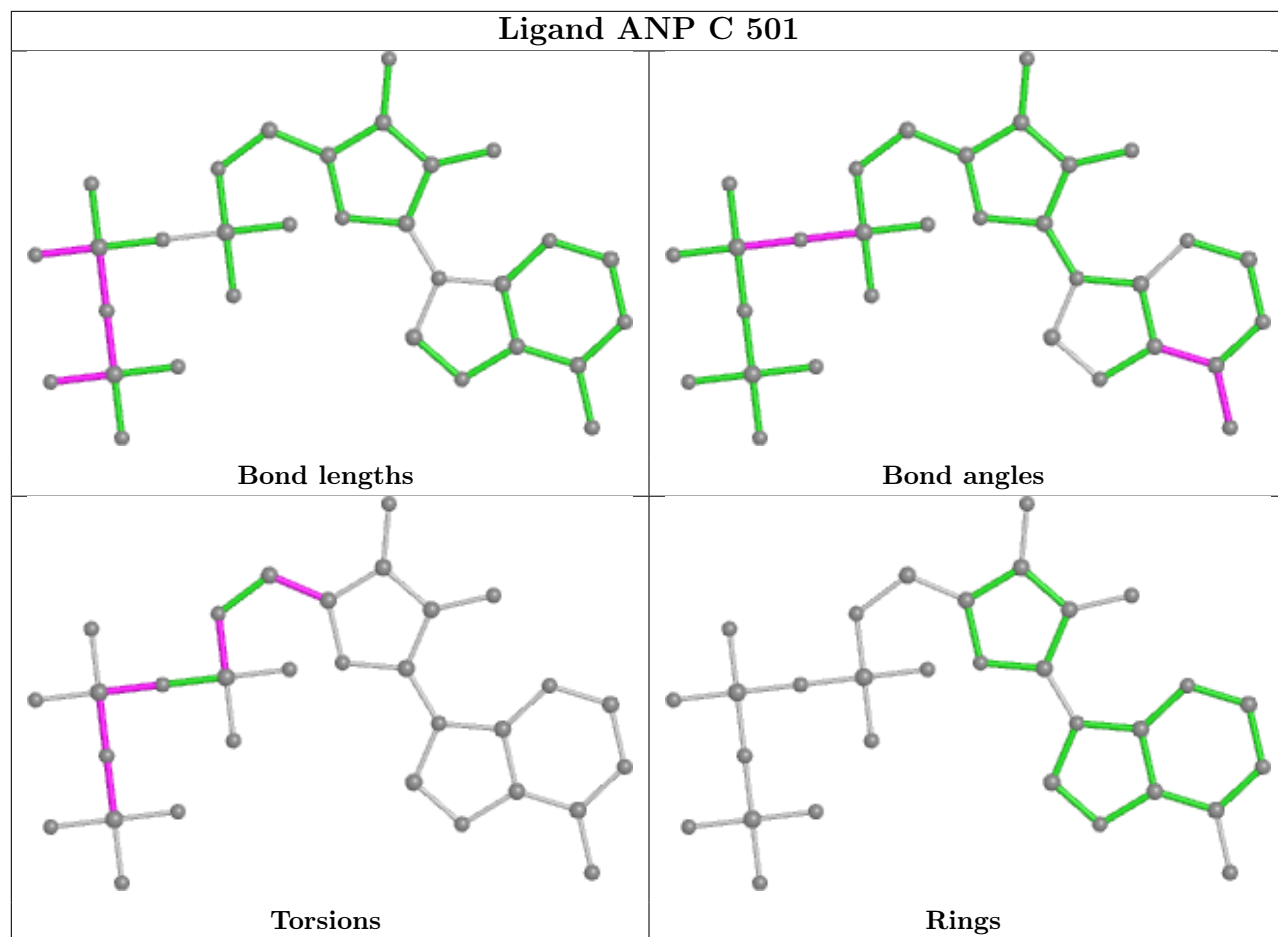
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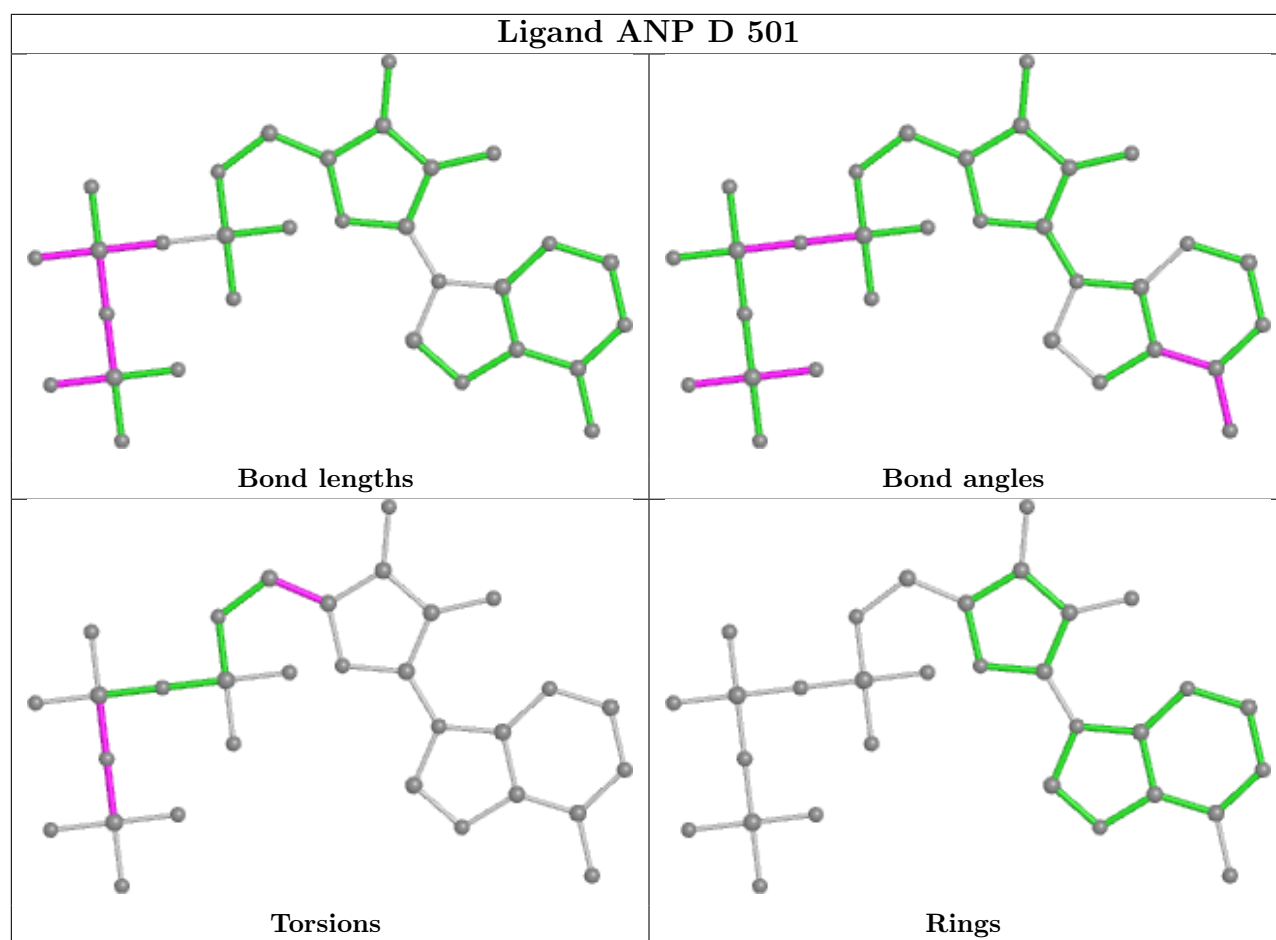
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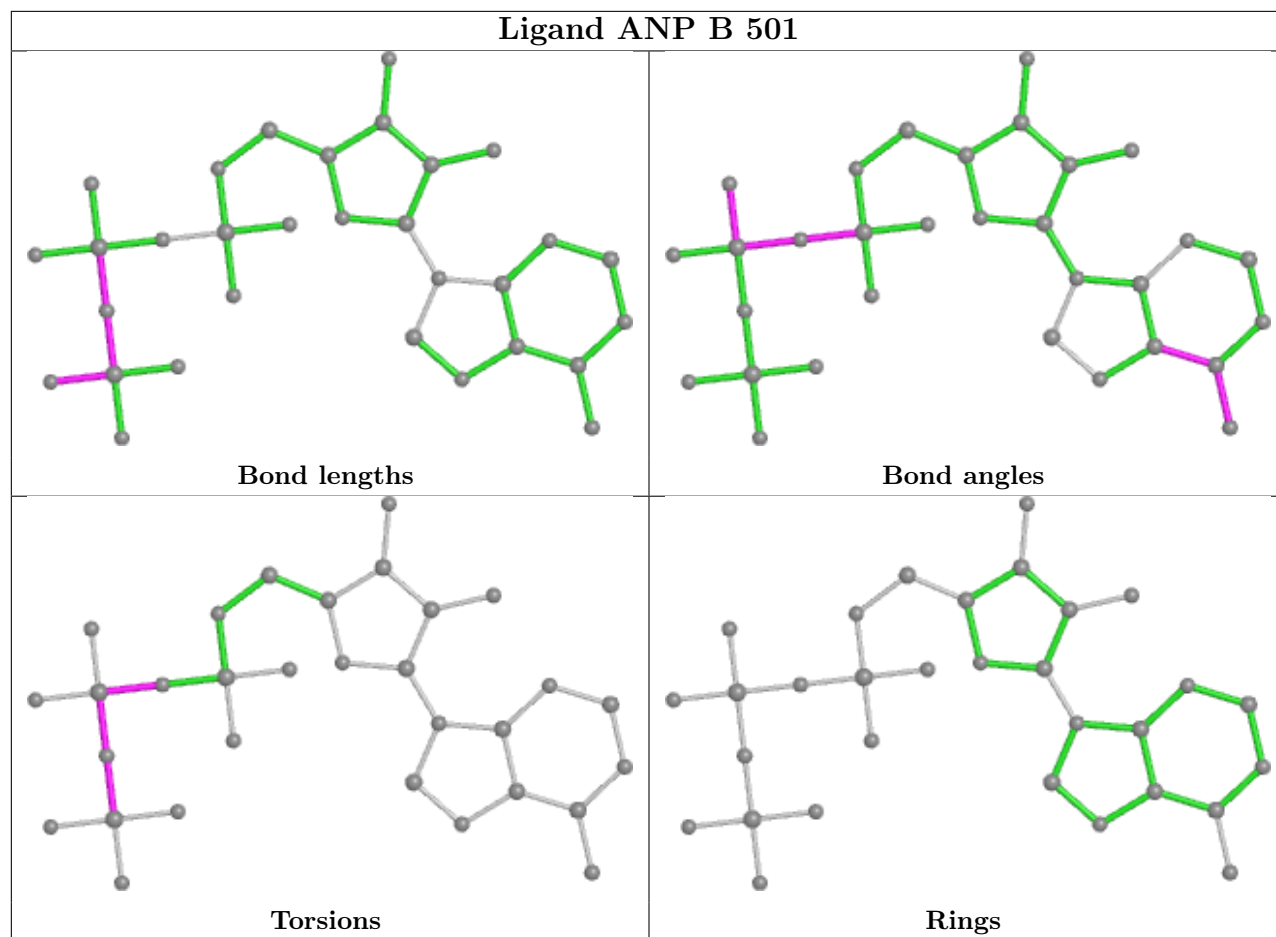
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	SO4	1	0
2	C	501	ANP	3	0
2	D	501	ANP	3	0
2	B	501	ANP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/497 (99%)	0.34	10 (2%) 64 62	36, 49, 70, 85	0
1	B	484/497 (97%)	0.57	31 (6%) 27 25	36, 53, 76, 110	0
1	C	490/497 (98%)	0.28	19 (3%) 44 40	36, 50, 75, 92	0
1	D	494/497 (99%)	0.47	32 (6%) 26 24	36, 50, 76, 108	1 (0%)
All	All	1963/1988 (98%)	0.41	92 (4%) 37 34	36, 50, 75, 110	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	60	ILE	4.8
1	B	193	MET	4.5
1	B	197	VAL	4.2
1	B	191	ALA	4.0
1	C	55	TRP	4.0
1	A	473	GLY	3.9
1	D	479	GLN	3.9
1	D	26[A]	ARG	3.9
1	D	477	ALA	3.8
1	B	245	ASN	3.8
1	B	252	ASN	3.8
1	D	471	VAL	3.6
1	B	203	HIS	3.6
1	D	472	PRO	3.6
1	D	484	LEU	3.5
1	D	476	HIS	3.4
1	D	461	LEU	3.4
1	D	55	TRP	3.3
1	B	144	LEU	3.3
1	D	56	GLY	3.3
1	C	209	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	404	GLY	3.2
1	C	195	ASN	3.2
1	C	175	GLU	3.2
1	D	487	ASP	3.2
1	B	77	SER	3.1
1	C	185	TYR	3.1
1	D	480	ILE	3.0
1	D	495	ARG	3.0
1	D	99	LYS	3.0
1	B	70	VAL	3.0
1	D	52	PHE	2.9
1	C	180	TYR	2.9
1	B	74	LYS	2.9
1	D	104	ARG	2.9
1	D	482	GLU	2.9
1	D	493	ASN	2.8
1	D	474	GLY	2.8
1	A	118	SER	2.8
1	D	494	ALA	2.8
1	C	495	ARG	2.7
1	B	76	GLY	2.7
1	D	2	ASP	2.7
1	D	1	MET	2.7
1	D	458	PRO	2.6
1	A	195	ASN	2.6
1	C	211	VAL	2.6
1	B	95	ASP	2.6
1	B	487	ASP	2.6
1	C	21	LEU	2.5
1	B	155	SER	2.5
1	B	71	GLU	2.5
1	B	373	GLN	2.5
1	B	192	SER	2.5
1	D	490	ILE	2.5
1	B	79	LEU	2.5
1	D	486	LEU	2.5
1	B	55	TRP	2.5
1	C	172	ILE	2.5
1	A	417	ILE	2.4
1	C	460	THR	2.4
1	C	191	ALA	2.4
1	B	139	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	313	ASN	2.4
1	B	190	LYS	2.4
1	C	196	ALA	2.4
1	B	238	ARG	2.3
1	A	39	TRP	2.3
1	B	171	GLN	2.3
1	B	471	VAL	2.3
1	B	129	CYS	2.3
1	D	53	ASN	2.3
1	C	178	TYR	2.3
1	B	210	THR	2.2
1	D	475	SER	2.2
1	B	202	HIS	2.2
1	B	59	PRO	2.2
1	D	133	ASP	2.2
1	A	55	TRP	2.2
1	C	193	MET	2.1
1	B	167	ARG	2.1
1	B	73	VAL	2.1
1	D	208	GLY	2.1
1	C	206	SER	2.1
1	C	197	VAL	2.1
1	D	105	GLU	2.1
1	D	444	MET	2.1
1	C	110	LYS	2.0
1	C	217	GLU	2.0
1	A	71	GLU	2.0
1	A	312	PRO	2.0
1	B	371	ILE	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

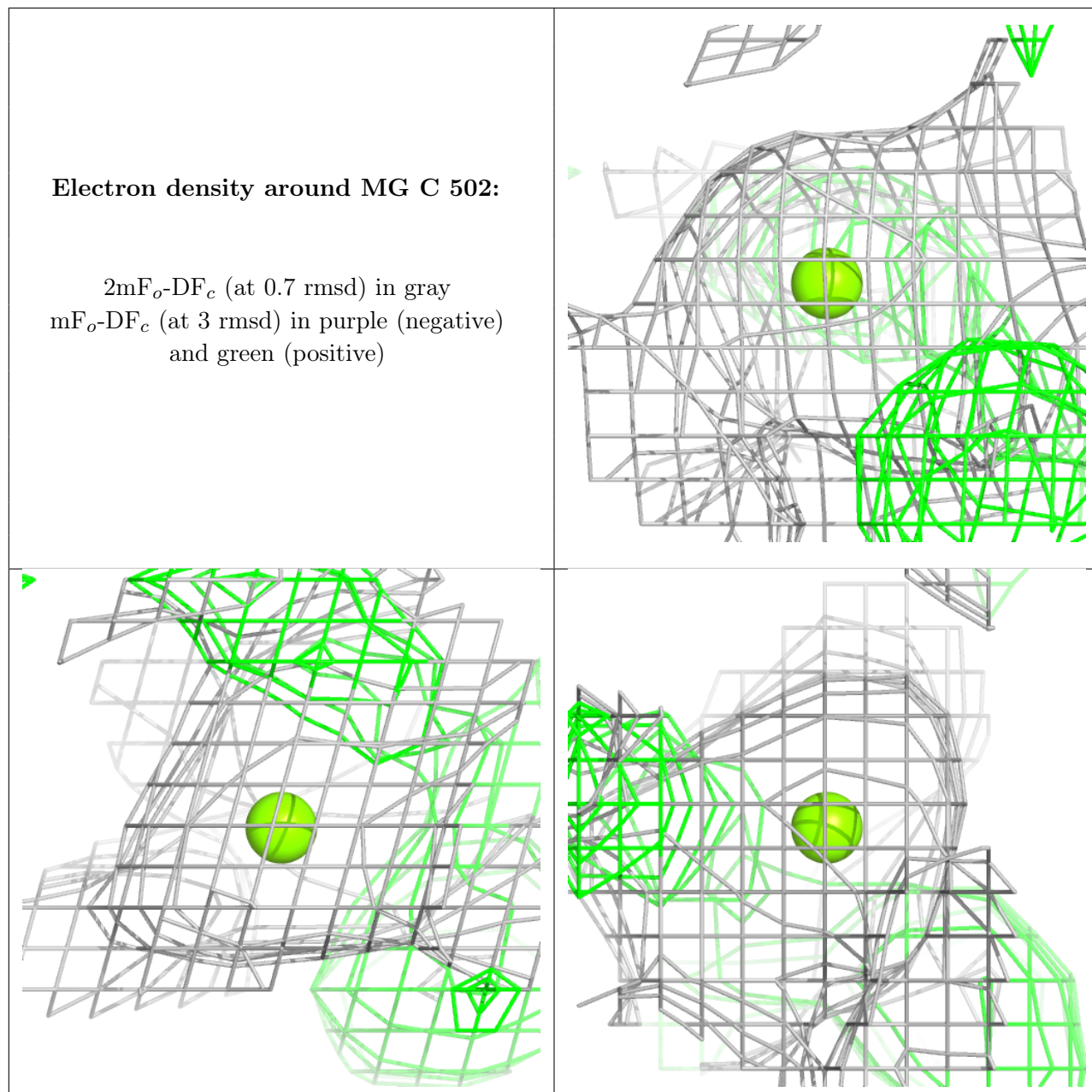
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	506	5/5	0.86	0.10	78,90,94,110	0
4	SO4	C	504	5/5	0.87	0.13	71,72,81,87	0
4	SO4	C	505	5/5	0.88	0.16	77,80,86,106	0
5	GOL	D	502	6/6	0.88	0.17	41,51,55,60	0
4	SO4	D	504	5/5	0.90	0.11	54,86,87,90	0
4	SO4	A	505	5/5	0.91	0.10	73,73,80,89	0
4	SO4	B	503	5/5	0.92	0.10	57,61,74,78	0
4	SO4	B	504	5/5	0.92	0.15	60,70,79,93	0
3	MG	C	502	1/1	0.93	0.09	46,46,46,46	0
4	SO4	A	506	5/5	0.93	0.12	49,52,56,62	0
4	SO4	D	503	5/5	0.94	0.13	40,58,72,72	0
4	SO4	B	505	5/5	0.94	0.12	65,69,75,83	0
2	ANP	D	501	31/31	0.94	0.11	42,58,65,80	0
3	MG	A	503	1/1	0.95	0.07	52,52,52,52	0
3	MG	B	502	1/1	0.95	0.06	37,37,37,37	0
2	ANP	B	501	31/31	0.95	0.09	34,37,52,54	0
3	MG	A	502	1/1	0.95	0.13	44,44,44,44	0
2	ANP	C	501	31/31	0.96	0.09	35,42,55,57	0
4	SO4	C	507	5/5	0.96	0.10	49,60,64,69	0
4	SO4	A	504	5/5	0.96	0.08	60,62,77,79	0
2	ANP	A	501	31/31	0.96	0.09	35,36,54,60	0
4	SO4	C	503	5/5	0.97	0.10	38,50,62,63	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.

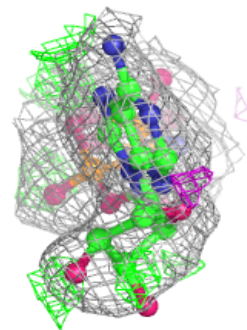
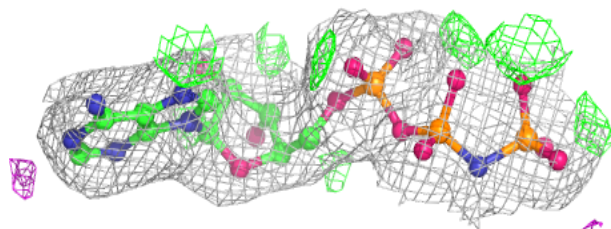
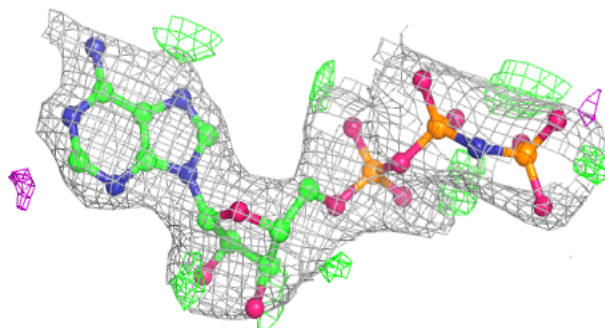
Electron density around MG C 502:

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



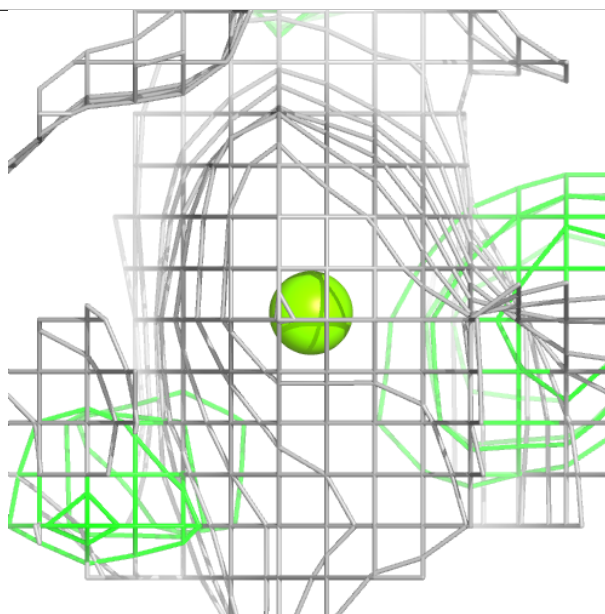
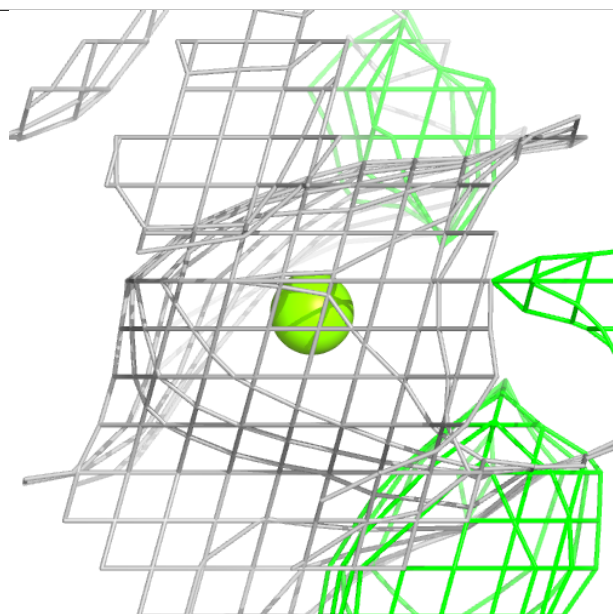
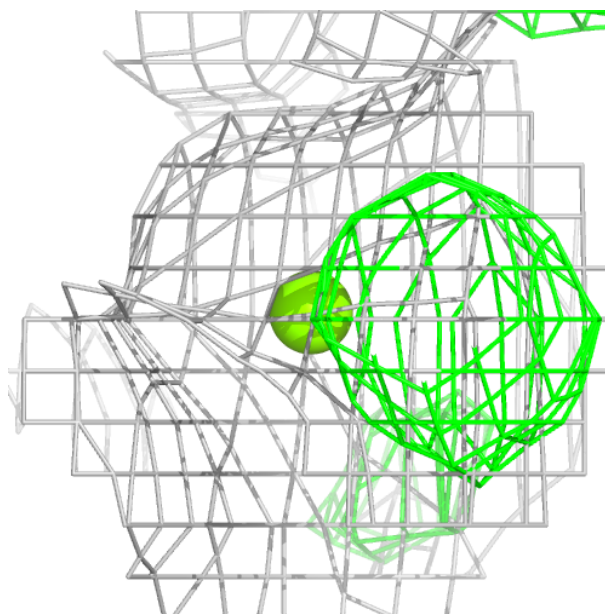
Electron density around ANP D 501:

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



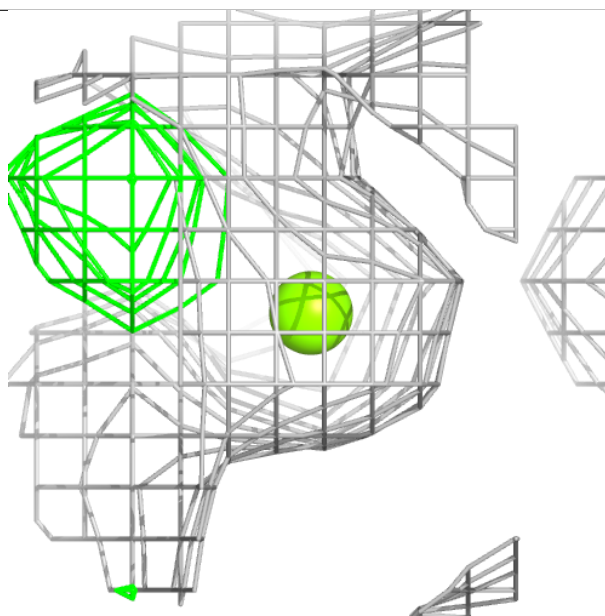
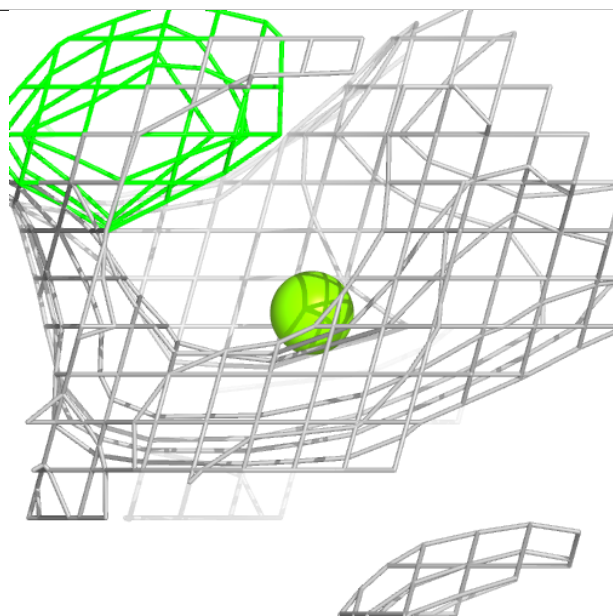
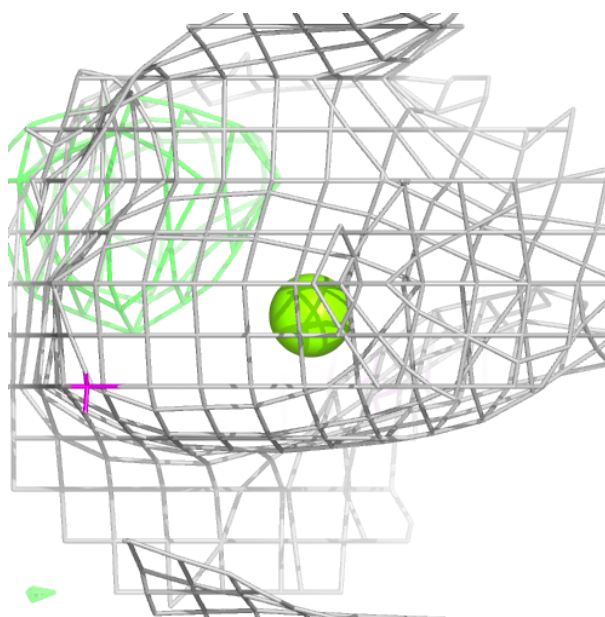
Electron density around MG A 503:

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



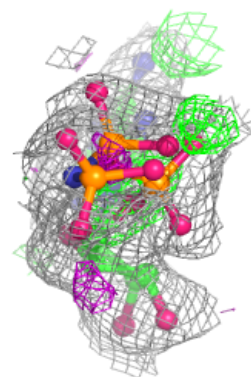
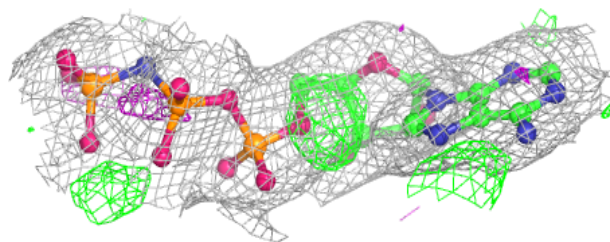
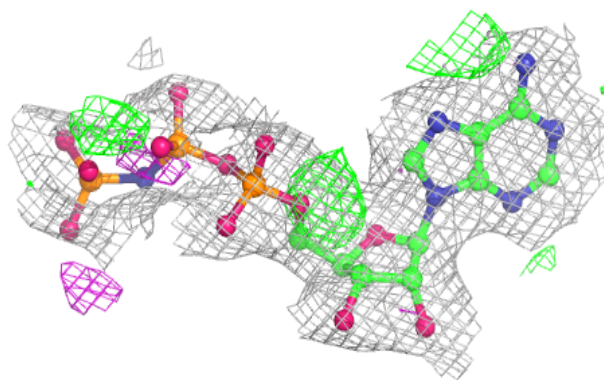
Electron density around MG B 502:

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



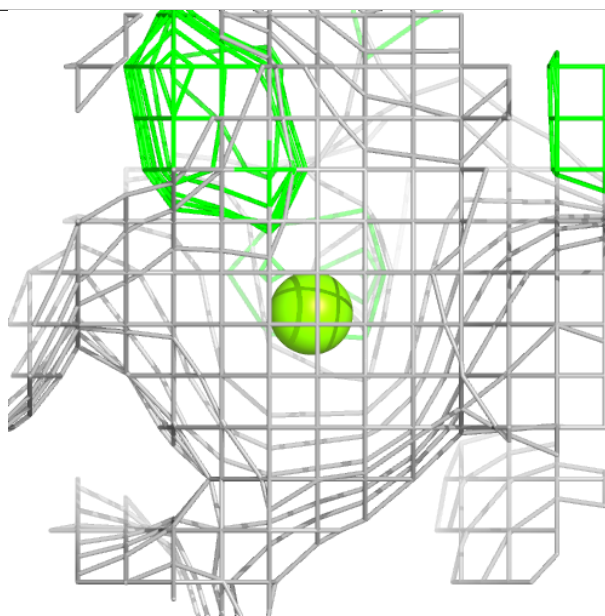
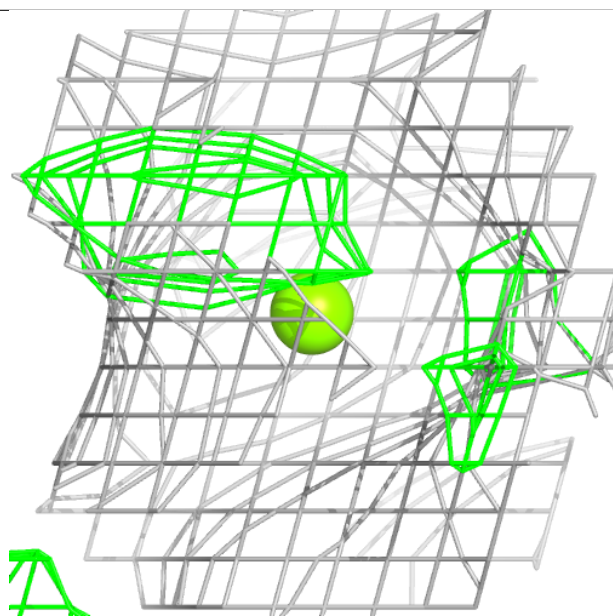
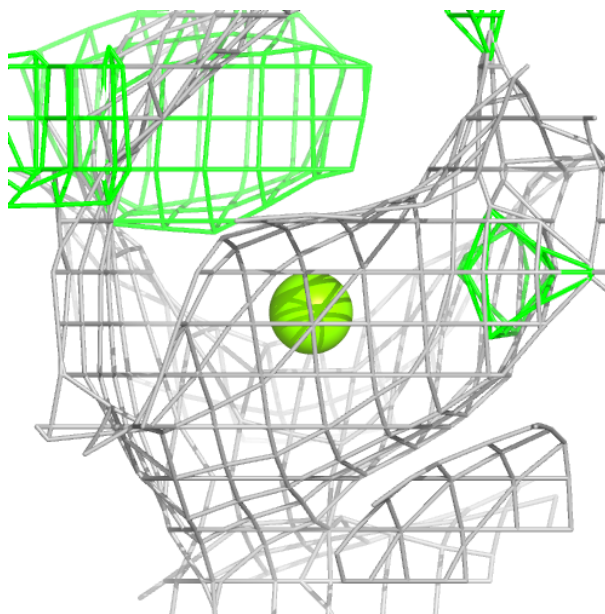
Electron density around ANP B 501:

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



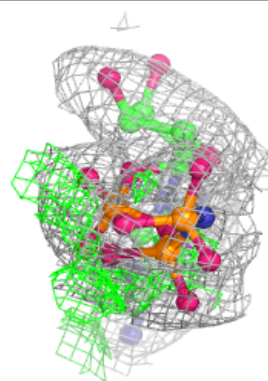
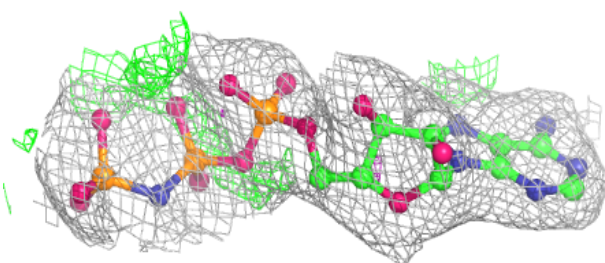
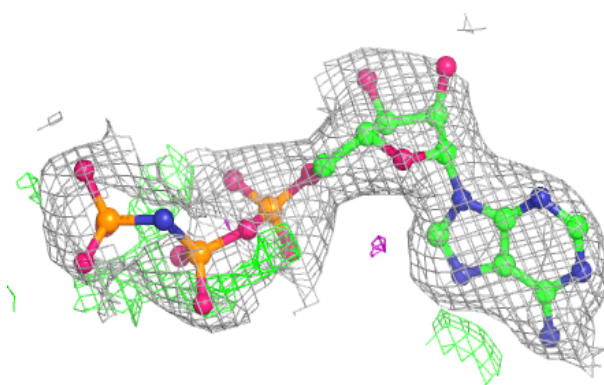
Electron density around MG A 502:

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

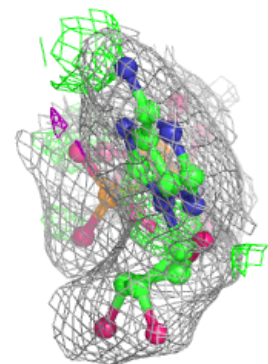
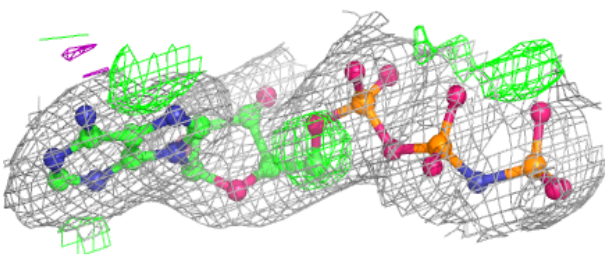
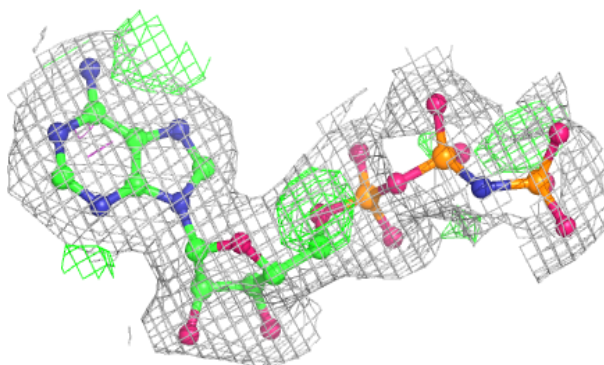


Electron density around ANP C 501:

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

**Electron density around ANP A 501:**

$2mF_o-DF_c$ (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.