Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 06:16 PM JST

PDB ID	:	7EIV
Title	:	heterotetrameric glycyl-tRNA synthetase from Escherichia coli
Authors	:	Ju, Y.; Zhou, H.
Deposited on	:	2021-03-31
Resolution	:	2.68 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

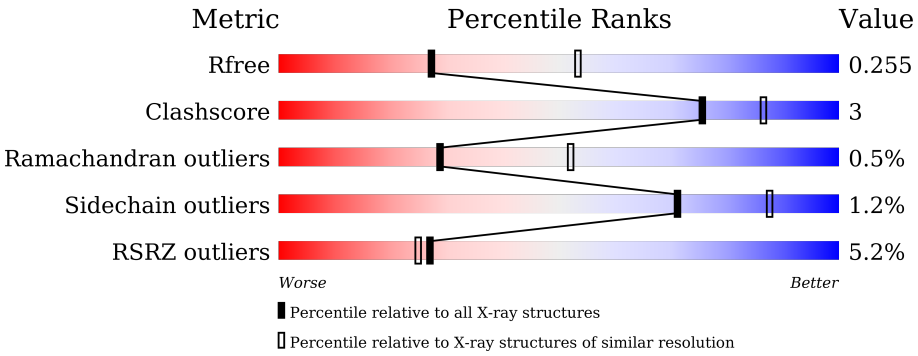
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	2% 91% 7%
1	B	303	4% 91% 8%
2	C	583	4% 85% 7% 8%
2	D	583	8% 88% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13407 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 Glycine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	1	0
			2421	1549	404	455	5	8			
1	B	300	Total	C	N	O	S	Se	0	0	0
			2418	1547	404	455	5	7			

- Molecule 2 is a protein called Glycine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	535	Total	C	N	O	S	Se	0	1	0
			4142	2629	723	777	2	11			
2	D	567	Total	C	N	O	S	Se	0	1	0
			4294	2717	748	815	3	11			

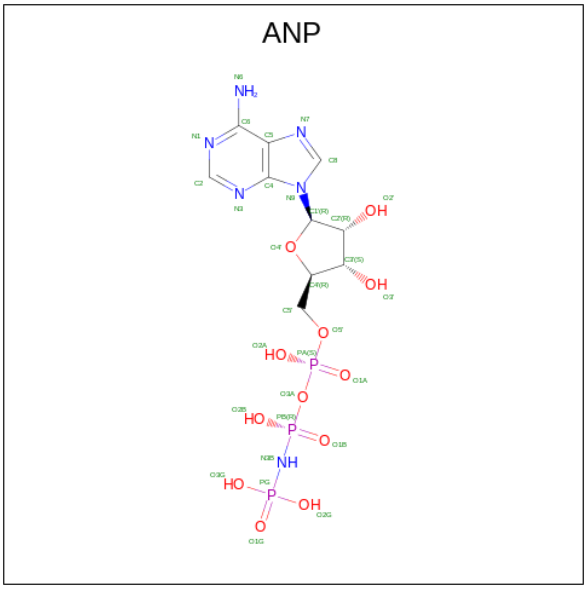
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	576	LEU	-	expression tag	UNP P00961
C	577	GLU	-	expression tag	UNP P00961
C	578	HIS	-	expression tag	UNP P00961
C	579	HIS	-	expression tag	UNP P00961
C	580	HIS	-	expression tag	UNP P00961
C	581	HIS	-	expression tag	UNP P00961
C	582	HIS	-	expression tag	UNP P00961
C	583	HIS	-	expression tag	UNP P00961
D	576	LEU	-	expression tag	UNP P00961
D	577	GLU	-	expression tag	UNP P00961
D	578	HIS	-	expression tag	UNP P00961
D	579	HIS	-	expression tag	UNP P00961
D	580	HIS	-	expression tag	UNP P00961
D	581	HIS	-	expression tag	UNP P00961
D	582	HIS	-	expression tag	UNP P00961
D	583	HIS	-	expression tag	UNP P00961

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

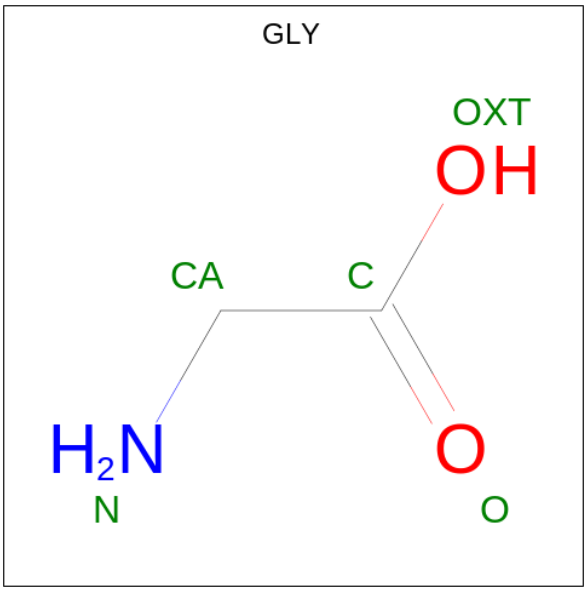
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 5 2 1 2	0	0
5	B	1	Total C N O 5 2 1 2	0	0

- Molecule 6 is water.

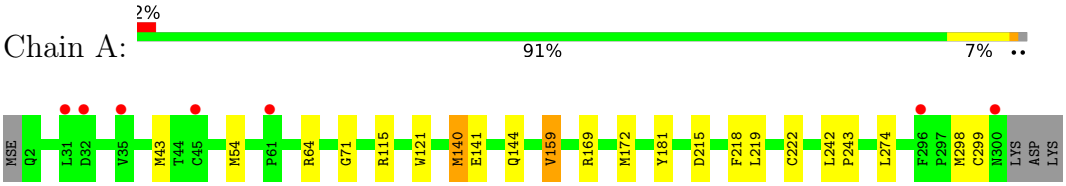
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	21	Total O 21 21	0	0
6	B	17	Total O 17 17	0	0
6	C	6	Total O 6 6	0	0
6	D	12	Total O 12 12	0	0

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.

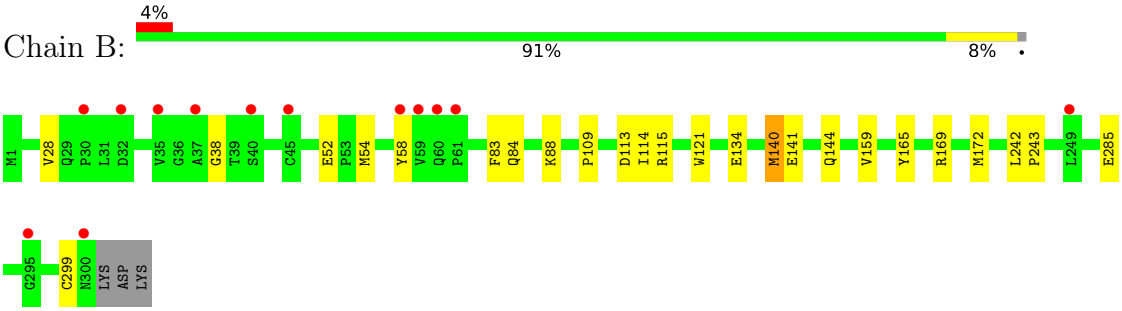
• Molecule 1: Glycine–tRNA ligase alpha subunit

Chain A:



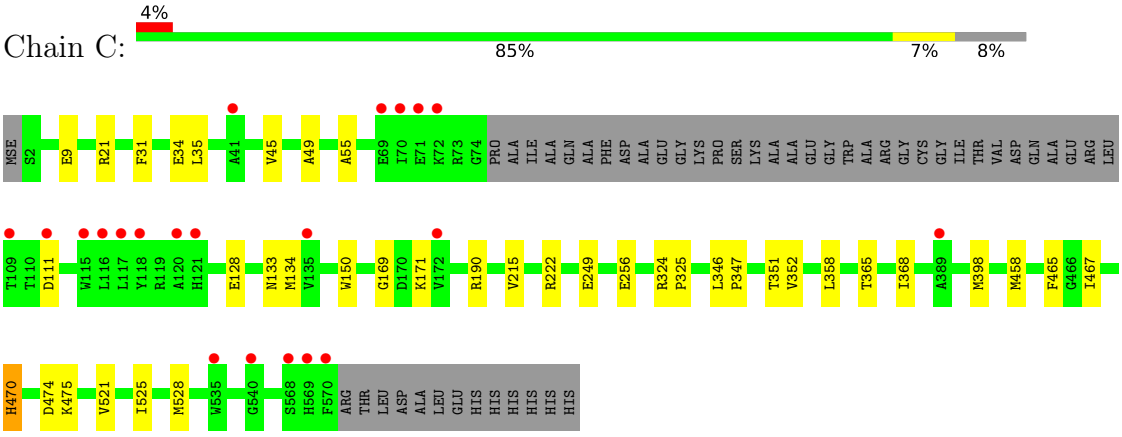
• Molecule 1: Glycine–tRNA ligase alpha subunit

Chain B:



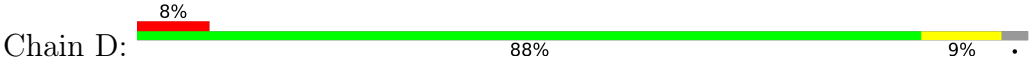
• Molecule 2: Glycine–tRNA ligase beta subunit

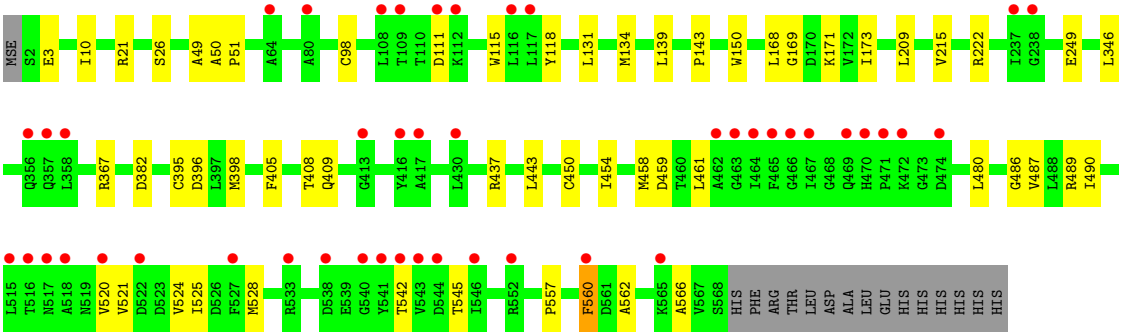
Chain C:



• Molecule 2: Glycine–tRNA ligase beta subunit

Chain D:




MSE S2 E3 I10 R21 S26 A49 A50 P51 A64 A80 C98 L108 T109 T110 D111 K112 W115 L116 L117 Y118 L131 M134 L139 P143 W150 L168 G169 D170 K171 V172 I173 L209 V215 R222 I237 G238 E249 L346
Q356 Q357 L358 R367 D382 C395 D396 L397 M398 F405 T408 Q409 G413 Y416 A417 L430 R437 L443 C450 I454 M458 D459 T460 L461 A462 G463 I464 F465 G466 I467 G468 Q469 H470 P471 K472 G473 D474 L480 G486 V487 L488 R489 I490
L515 T516 N517 A518 N519 V520 V521 D522 D523 V524 I525 D526 F527 M528 R533 D538 E539 G540 Y541 T542 V543 D544 T545 I546 R552 P557 F560 D561 A562 K565 A566 V567 S568 HIS PHE ARG THR LEU ASP ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	207.37Å 253.94Å 270.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.68 48.53 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.58-2.68) 99.8 (48.53-2.68)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.24 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.249 0.234 , 0.255	Depositor DCC
R_{free} test set	4996 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13407	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0870e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/2478	0.74	4/3360 (0.1%)
1	B	0.61	0/2475	0.72	1/3357 (0.0%)
2	C	0.64	0/4210	0.73	1/5694 (0.0%)
2	D	0.65	0/4365	0.75	1/5916 (0.0%)
All	All	0.63	0/13528	0.74	7/18327 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43[A]	MSE	CG-SE-CE	5.88	111.84	98.90
1	A	43[B]	MSE	CG-SE-CE	5.88	111.84	98.90
1	A	140	MSE	CG-SE-CE	5.85	111.77	98.90
1	B	140	MSE	CG-SE-CE	5.70	111.43	98.90
1	A	298	MSE	CG-SE-CE	5.55	111.12	98.90
2	C	134	MSE	CG-SE-CE	5.53	111.07	98.90
2	D	398	MSE	CG-SE-CE	5.08	110.06	98.90

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	2421	0	2330	14	0
1	B	2418	0	2327	15	0
2	C	4142	0	4075	20	0
2	D	4294	0	4139	29	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	31	0	13	5	0
4	B	31	0	13	2	0
5	A	5	0	2	1	0
5	B	5	0	2	1	0
6	A	21	0	0	1	0
6	B	17	0	0	0	0
6	C	6	0	0	0	0
6	D	12	0	0	0	0
All	All	13407	0	12901	80	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 (80) 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)
2:D:458:MSE:HE1	2:D:528:MSE:SE	2.31	0.79
1:B:140:MSE:HE1	1:B:172:MSE:SE	2.33	0.77
4:A:403:ANP:H5'2	5:A:404:GLY:OXT	1.91	0.70
2:C:458:MSE:SE	2:C:528:MSE:HE1	2.42	0.69
2:D:562:ALA:O	2:D:566:ALA:HB2	1.93	0.67
1:A:140:MSE:HE3	1:A:169:ARG:HB3	1.78	0.66
1:A:140:MSE:HE3	1:A:169:ARG:CB	2.30	0.61
2:C:352:VAL:HG21	2:C:398:MSE:HE1	1.84	0.59
2:D:458:MSE:HE3	2:D:487:VAL:HG21	1.85	0.58
2:D:405:PHE:O	2:D:408:THR:HG22	2.04	0.57
2:D:521:VAL:O	2:D:525:ILE:HG13	2.05	0.56
2:C:49:ALA:O	2:C:222:ARG:NH2	2.32	0.56
4:A:403:ANP:H5'1	4:A:403:ANP:H8	1.88	0.55
1:A:242:LEU:HB2	1:A:243:PRO:HD3	1.88	0.54
2:C:21:ARG:HD2	2:C:249:GLU:OE2	2.07	0.54
1:A:140:MSE:HE1	1:A:172:MSE:SE	2.57	0.54
2:C:365:THR:O	2:C:368:ILE:HG22	2.08	0.53
2:C:31:PHE:CD2	2:C:35:LEU:HD11	2.44	0.53
1:B:38:GLY:HA3	1:B:84:GLN:HG3	1.91	0.53
2:D:458:MSE:CE	2:D:487:VAL:HG11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:HB2	1:B:141:GLU:HG3	1.92	0.52
2:D:396:ASP:OD2	2:D:409:GLN:O	2.28	0.52
1:A:121:TRP:HB2	1:A:144:GLN:HE21	1.75	0.52
1:A:215:ASP:O	1:A:219:LEU:HD13	2.09	0.51
2:D:520:VAL:O	2:D:524:VAL:HG12	2.10	0.51
2:C:465:PHE:CE1	2:C:470:HIS:HB3	2.45	0.51
1:B:140:MSE:HE3	1:B:169:ARG:HB3	1.93	0.51
2:C:128:GLU:OE1	2:C:171:LYS:NZ	2.44	0.50
1:A:115:ARG:NH2	6:A:501:HOH:O	2.44	0.50
1:B:121:TRP:HB2	1:B:144:GLN:HE21	1.77	0.50
2:C:31:PHE:O	2:C:35:LEU:HD12	2.11	0.49
2:C:358:LEU:HG	2:C:467:ILE:HD11	1.94	0.49
2:D:49:ALA:O	2:D:222:ARG:NH2	2.37	0.49
2:D:557:PRO:HA	2:D:560:PHE:HB2	1.95	0.49
2:D:562:ALA:O	2:D:566:ALA:CB	2.61	0.48
1:B:242:LEU:HB2	1:B:243:PRO:HD3	1.94	0.48
2:D:346:LEU:HD12	2:D:395:CYS:SG	2.54	0.48
1:A:144:GLN:OE1	4:A:403:ANP:O2A	2.31	0.48
2:C:133[B]:ASN:O	2:C:133[B]:ASN:ND2	2.47	0.47
2:D:131:LEU:HD13	2:D:173:ILE:CD1	2.45	0.47
2:C:352:VAL:CG2	2:C:398:MSE:HE1	2.44	0.47
1:A:159:VAL:HG11	2:C:150:TRP:HA	1.95	0.47
1:B:113:ASP:OD2	1:B:115:ARG:NH2	2.46	0.47
2:D:443:LEU:HG	2:D:490:ILE:HD13	1.96	0.46
2:D:450:CYS:O	2:D:454:ILE:HG12	2.15	0.46
2:D:21:ARG:NH1	2:D:249:GLU:OE1	2.41	0.46
1:A:71:GLY:HA2	1:A:181:TYR:OH	2.15	0.46
1:A:141:GLU:OE1	4:A:403:ANP:O2A	2.33	0.46
2:C:31:PHE:O	2:C:34:GLU:N	2.49	0.46
1:B:83:PHE:HB3	1:B:165:TYR:HB2	1.98	0.45
2:D:367:ARG:HD2	2:D:459:ASP:OD1	2.16	0.45
2:C:346:LEU:N	2:C:347:PRO:HD2	2.31	0.45
2:D:524:VAL:O	2:D:528:MSE:HG3	2.17	0.45
2:C:324:ARG:HB3	2:C:325:PRO:HD3	1.98	0.45
2:D:486:GLY:O	2:D:490:ILE:HG12	2.18	0.44
1:A:64:ARG:NH1	4:A:403:ANP:O2B	2.47	0.44
2:D:168:LEU:HB2	2:D:173:ILE:HD11	2.00	0.44
1:B:109:PRO:HB3	1:B:114:ILE:HD12	2.00	0.44
1:A:215:ASP:O	1:A:219:LEU:CD1	2.66	0.43
2:C:45:VAL:O	2:C:45:VAL:HG23	2.18	0.43
2:D:98:CYS:HB3	2:D:118:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:CZ	1:A:222:CYS:SG	3.11	0.43
2:D:542:THR:HG22	2:D:545:THR:HB	2.01	0.43
4:B:403:ANP:H5'1	4:B:403:ANP:H8	2.01	0.43
2:C:521:VAL:O	2:C:525:ILE:HG12	2.19	0.43
1:B:140:MSE:HE3	1:B:169:ARG:HD2	2.01	0.43
2:D:454:ILE:HD13	2:D:487:VAL:HG23	1.99	0.42
2:D:26:SER:OG	2:D:143:PRO:HD3	2.20	0.42
2:D:10:ILE:HD11	2:D:139:LEU:HD11	2.02	0.42
2:C:215:VAL:HG13	2:C:256:GLU:HG2	2.01	0.42
1:B:28:VAL:HG22	1:B:58:TYR:HB3	2.01	0.42
1:B:140:MSE:CE	1:B:169:ARG:HB3	2.49	0.42
2:D:461:LEU:HD23	2:D:480:LEU:HG	2.02	0.41
1:B:159:VAL:HG21	2:D:150:TRP:HA	2.02	0.41
2:D:50:ALA:HB1	2:D:51:PRO:HD2	2.02	0.41
4:B:403:ANP:H5'2	5:B:404:GLY:OXT	2.21	0.40
1:B:134:GLU:OE1	1:B:141:GLU:OE1	2.38	0.40
2:D:209:LEU:HD22	2:D:215:VAL:HB	2.04	0.40
1:B:52:GLU:O	1:B:88:LYS:CE	2.70	0.40
2:C:9:GLU:HG3	2:C:55:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/303 (98%)	292 (98%)	6 (2%)	0	100	100
1	B	298/303 (98%)	288 (97%)	10 (3%)	0	100	100
2	C	532/583 (91%)	514 (97%)	14 (3%)	4 (1%)	19	40
2	D	566/583 (97%)	539 (95%)	23 (4%)	4 (1%)	22	44
All	All	1694/1772 (96%)	1633 (96%)	53 (3%)	8 (0%)	29	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	475	LYS
2	C	169	GLY
2	C	474	ASP
2	D	111	ASP
2	D	169	GLY
2	D	382	ASP
2	C	111	ASP
2	D	3	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/253 (102%)	253 (98%)	4 (2%)	62	83
1	B	256/253 (101%)	253 (99%)	3 (1%)	71	87
2	C	421/462 (91%)	418 (99%)	3 (1%)	84	93
2	D	421/462 (91%)	415 (99%)	6 (1%)	67	85
All	All	1355/1430 (95%)	1339 (99%)	16 (1%)	71	87

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

Mol	Chain	Res	Type
1	A	54	MSE
1	A	159	VAL
1	A	274	LEU
1	A	299	CYS
1	B	54	MSE
1	B	285	GLU
1	B	299	CYS
2	C	190	ARG
2	C	351	THR
2	C	470	HIS
2	D	115	TRP
2	D	134	MSE

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Mol	Chain	Res	Type
2	D	171	LYS
2	D	437	ARG
2	D	489	ARG
2	D	560	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	537	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GLY	A	404	-	1,4,4	0.07	0	0,4,4	0.00	-
5	GLY	B	404	-	1,4,4	0.11	0	0,4,4	0.00	-
4	ANP	A	403	3	29,33,33	1.23	4 (13%)	31,52,52	1.32	4 (12%)
4	ANP	B	403	3	29,33,33	1.27	3 (10%)	31,52,52	1.31	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLY	A	404	-	-	0/0/2/2	-
5	GLY	B	404	-	-	0/0/2/2	-
4	ANP	A	403	3	-	5/14/38/38	0/3/3/3
4	ANP	B	403	3	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	ANP	PG-O1G	3.62	1.51	1.46
4	A	403	ANP	PG-O1G	3.11	1.51	1.46
4	B	403	ANP	PB-O1B	2.90	1.50	1.46
4	A	403	ANP	PB-O1B	2.77	1.50	1.46
4	A	403	ANP	PB-O2B	-2.40	1.50	1.56
4	B	403	ANP	PB-O2B	-2.32	1.50	1.56
4	A	403	ANP	PG-O3G	-2.14	1.51	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	ANP	O1G-PG-N3B	-4.01	105.86	111.77
4	A	403	ANP	O2B-PB-O1B	3.94	118.18	109.92
4	B	403	ANP	O2B-PB-O1B	3.88	118.06	109.92
4	B	403	ANP	O3G-PG-O1G	-2.77	106.49	113.45
4	B	403	ANP	C3'-C2'-C1'	2.48	104.72	100.98
4	B	403	ANP	C5-C6-N6	2.34	123.92	120.35
4	A	403	ANP	C5-C6-N6	2.07	123.50	120.35
4	A	403	ANP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	ANP	PB-N3B-PG-O1G
4	A	403	ANP	PA-O3A-PB-O1B
4	A	403	ANP	PA-O3A-PB-O2B
4	B	403	ANP	PG-N3B-PB-O3A
4	B	403	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	B	403	ANP	PA-O3A-PB-O2B
4	A	403	ANP	O4'-C4'-C5'-O5'
4	B	403	ANP	O4'-C4'-C5'-O5'
4	A	403	ANP	PG-N3B-PB-O3A

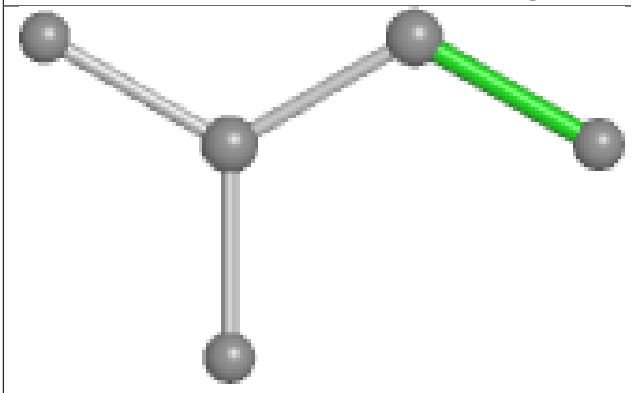
There are no ring outliers.

4 monomers are involved in 7 short contacts:

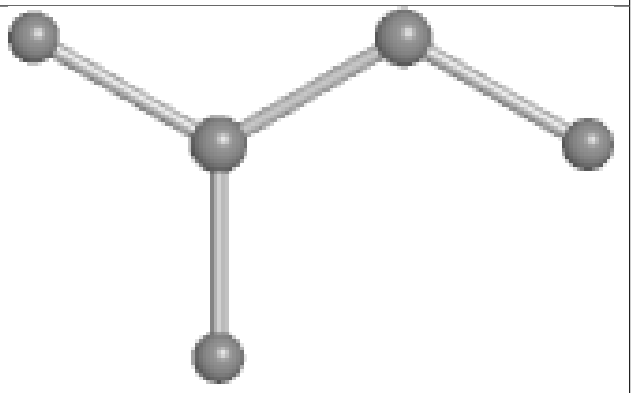
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	GLY	1	0
5	B	404	GLY	1	0
4	A	403	ANP	5	0
4	B	403	ANP	2	0

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 then 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.

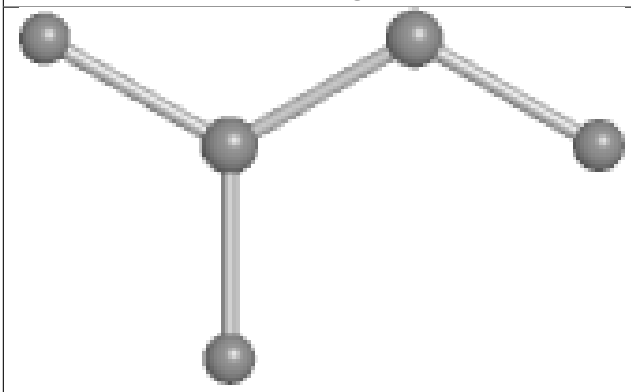
Ligand GLY A 404



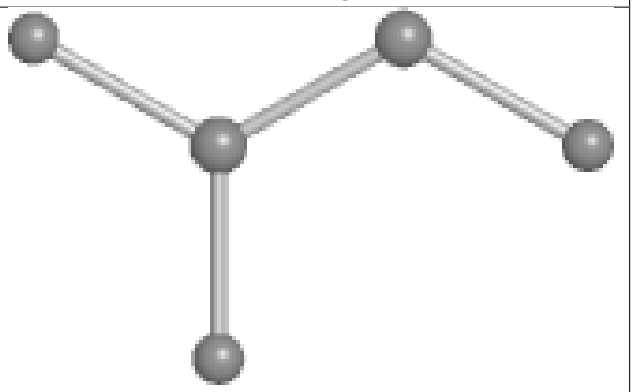
Bond lengths



Bond angles

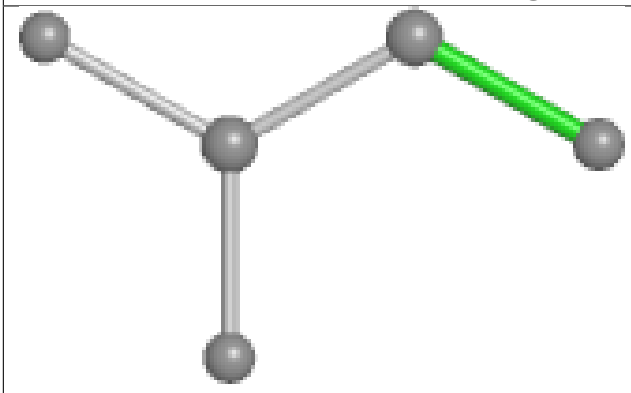


Torsions

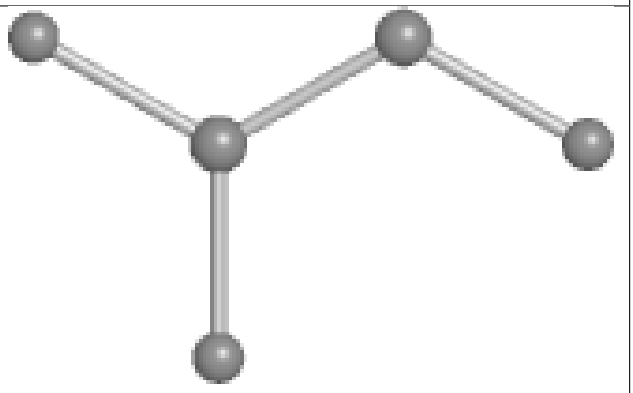


Rings

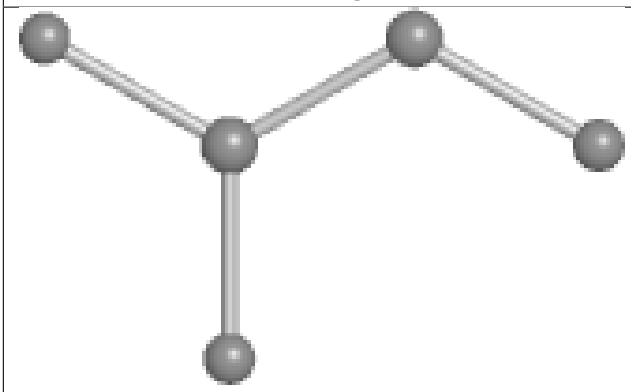
Ligand GLY B 404



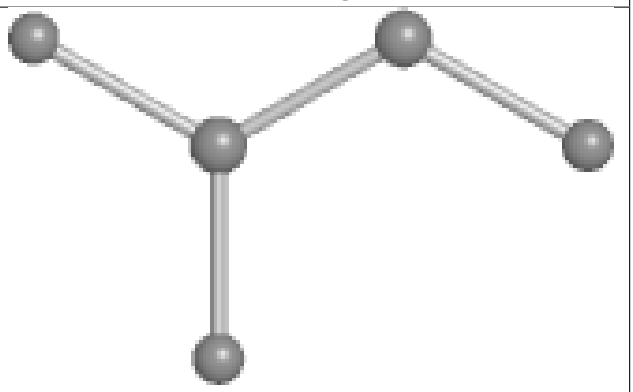
Bond lengths



Bond angles

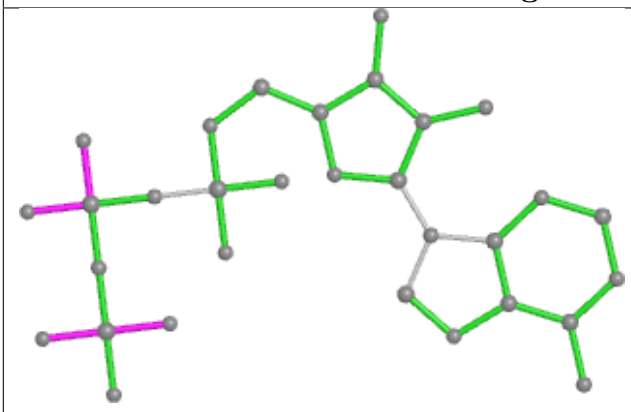


Torsions

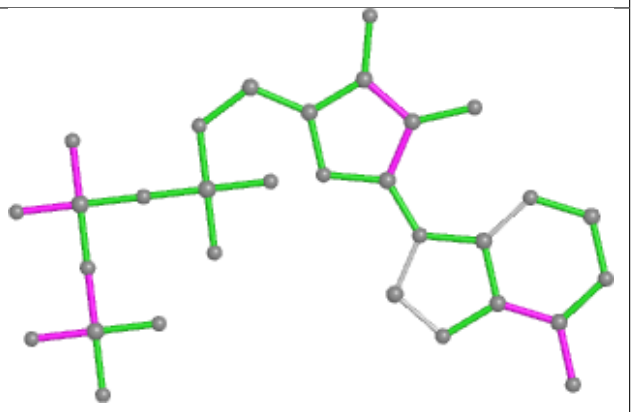


Rings

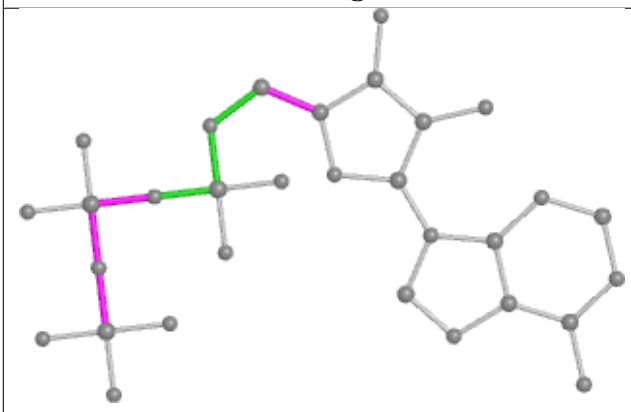
Ligand ANP A 403



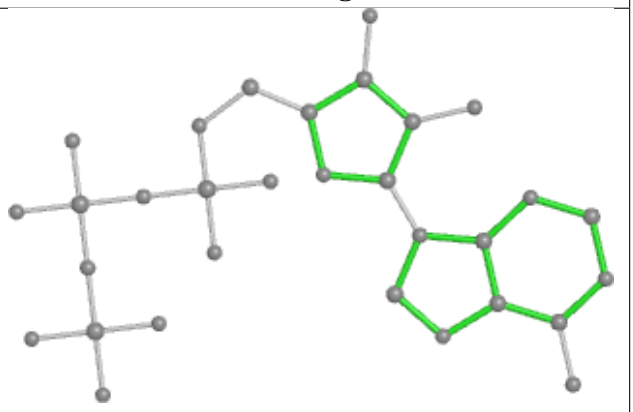
Bond lengths



Bond angles

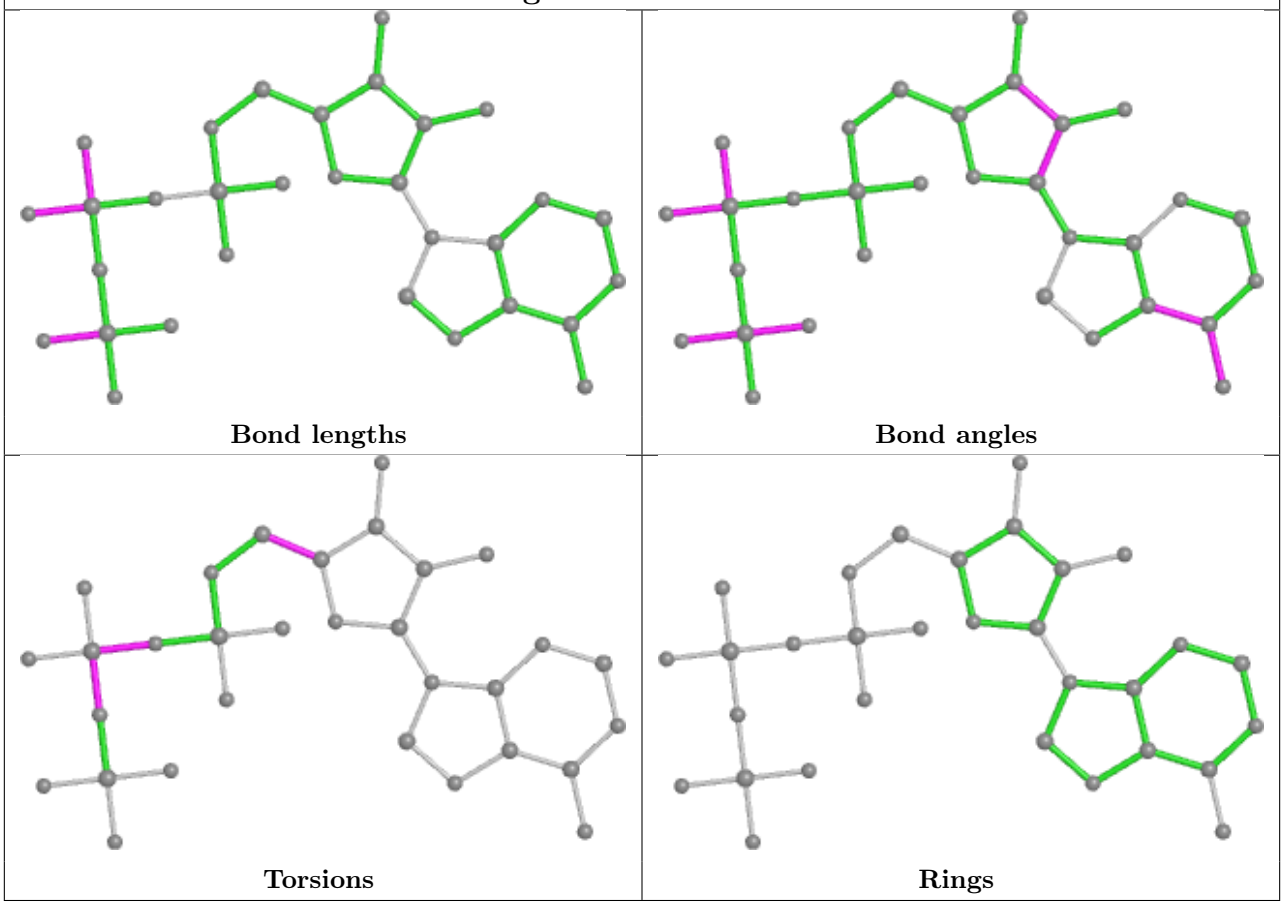


Torsions



Rings

Ligand ANP B 403



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, 95^{th} 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	292/303 (96%)	0.27	7 (2%)	59	59	44, 61, 94, 113	0
1	B	292/303 (96%)	0.41	13 (4%)	33	31	46, 61, 92, 120	0
2	C	524/583 (89%)	0.28	21 (4%)	38	36	50, 74, 118, 150	1 (0%)
2	D	556/583 (95%)	0.46	46 (8%)	11	9	49, 80, 130, 155	1 (0%)
All	All	1664/1772 (93%)	0.36	87 (5%)	27	25	44, 70, 117, 155	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	118	TYR	7.3
2	C	71	GLU	5.8
2	D	538	ASP	5.4
2	C	120	ALA	5.0
2	C	116	LEU	4.9
2	C	117	LEU	4.9
1	A	300	ASN	4.4
2	C	70	ILE	4.3
2	D	541	TYR	3.8
2	D	413	GLY	3.7
1	B	300	ASN	3.7
2	D	546	ILE	3.5
2	D	465	PHE	3.5
2	D	116	LEU	3.4
2	D	80	ALA	3.4
1	B	61	PRO	3.3
2	D	543	VAL	3.3
2	D	515	LEU	3.2
2	D	470	HIS	3.2
2	C	72	LYS	3.2
1	A	35	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	467	ILE	3.1
2	D	516	THR	3.1
2	D	565	LYS	3.0
2	D	356	GLN	3.0
2	D	471	PRO	3.0
2	D	358	LEU	3.0
2	D	540	GLY	2.9
2	D	109	THR	2.9
2	D	108	LEU	2.9
2	C	570	PHE	2.9
2	C	389	ALA	2.9
2	D	417	ALA	2.8
2	D	522	ASP	2.8
1	B	59	VAL	2.7
2	C	540	GLY	2.7
2	D	527	PHE	2.7
1	A	296	PHE	2.6
2	D	560	PHE	2.6
2	D	533	ARG	2.6
2	D	117	LEU	2.6
2	D	64	ALA	2.6
1	A	32	ASP	2.5
2	D	112	LYS	2.5
2	D	464	ILE	2.5
2	D	466	GLY	2.5
1	B	35	VAL	2.5
1	B	32	ASP	2.4
1	B	60	GLN	2.4
2	D	462	ALA	2.4
2	C	69	GLU	2.4
1	B	30	PRO	2.3
2	D	416	TYR	2.3
2	D	111	ASP	2.3
2	D	238	GLY	2.3
2	D	520	VAL	2.3
2	C	109	THR	2.3
1	B	45	CYS	2.3
2	C	569	HIS	2.3
2	D	472	LYS	2.3
1	B	295	GLY	2.3
2	C	535	TRP	2.3
2	D	518	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	172	VAL	2.3
2	D	517	ASN	2.3
2	D	544	ASP	2.3
1	B	37	ALA	2.2
2	C	115	TRP	2.2
1	A	45	CYS	2.2
2	D	542	THR	2.2
2	D	237	ILE	2.2
2	C	121	HIS	2.2
2	D	474	ASP	2.2
1	B	40	SER	2.2
1	A	61	PRO	2.2
2	D	463	GLY	2.1
2	D	552	ARG	2.1
1	B	58	TYR	2.1
2	C	135	VAL	2.1
1	A	31	LEU	2.1
2	C	111	ASP	2.1
1	B	249	LEU	2.0
2	D	357	GLN	2.0
2	D	469	GLN	2.0
2	C	41	ALA	2.0
2	C	568	SER	2.0
2	D	430	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

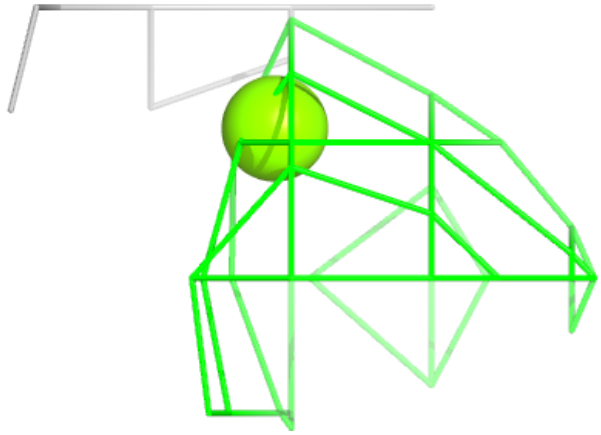
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

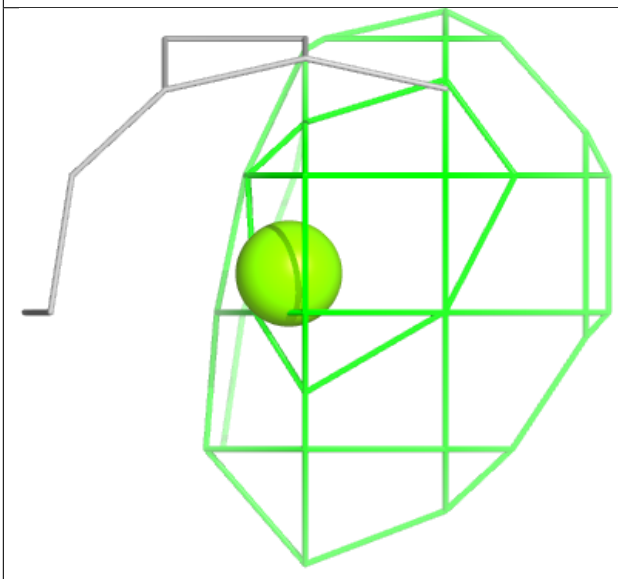
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	401	1/1	0.90	0.40	52,52,52,52	0
4	ANP	B	403	31/31	0.91	0.28	50,66,92,95	0
3	MG	B	402	1/1	0.92	0.51	50,50,50,50	0
4	ANP	A	403	31/31	0.93	0.26	50,63,90,98	0
3	MG	B	401	1/1	0.94	0.43	62,62,62,62	0
3	MG	A	402	1/1	0.95	0.42	54,54,54,54	0
5	GLY	B	404	5/5	0.96	0.23	51,55,57,57	0
5	GLY	A	404	5/5	0.98	0.22	50,53,55,58	0

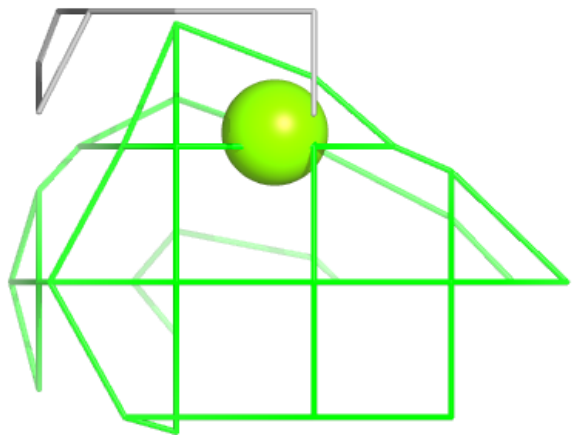
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG A 401:

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

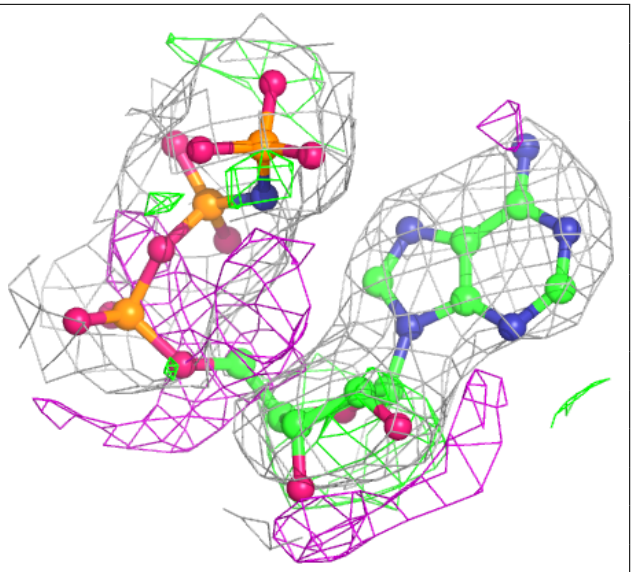


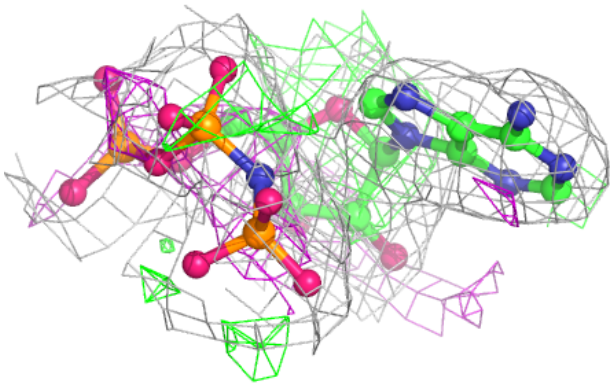


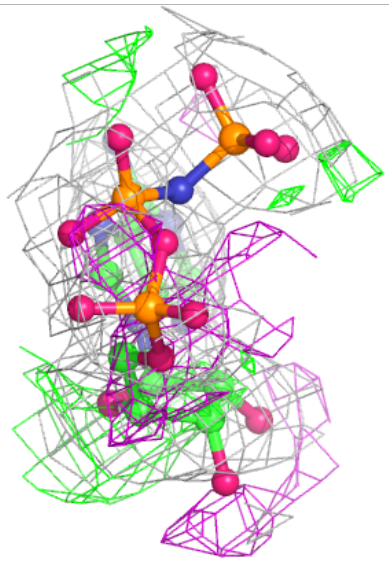


Electron density around ANP B 403:

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

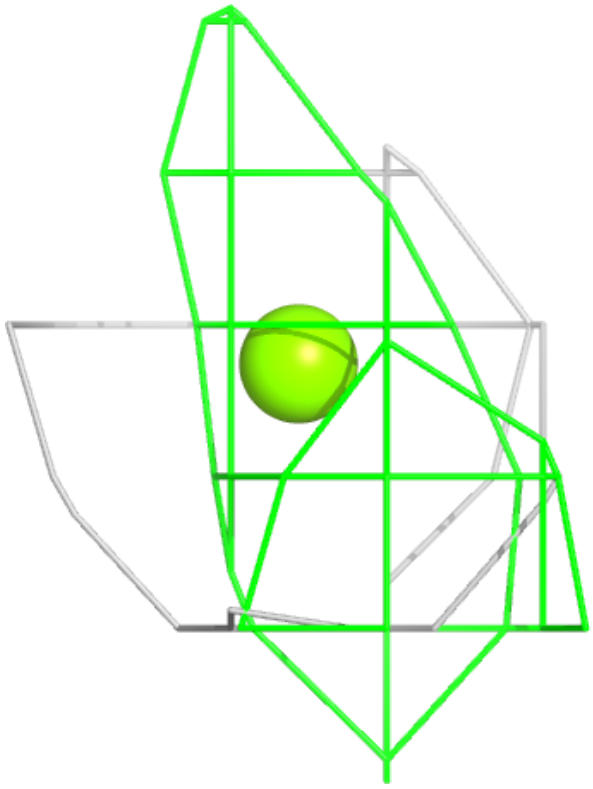


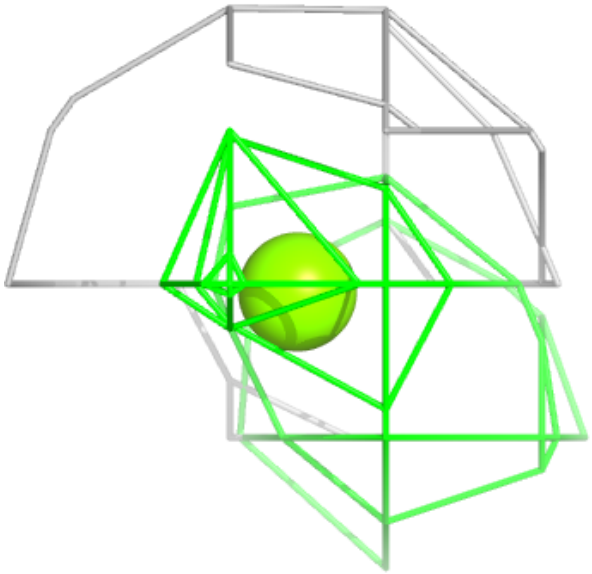


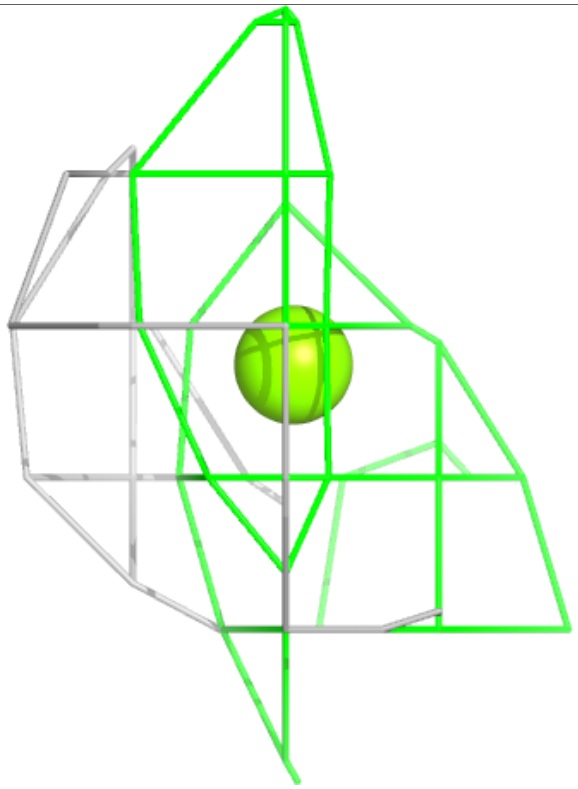


Electron density around MG B 402:

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

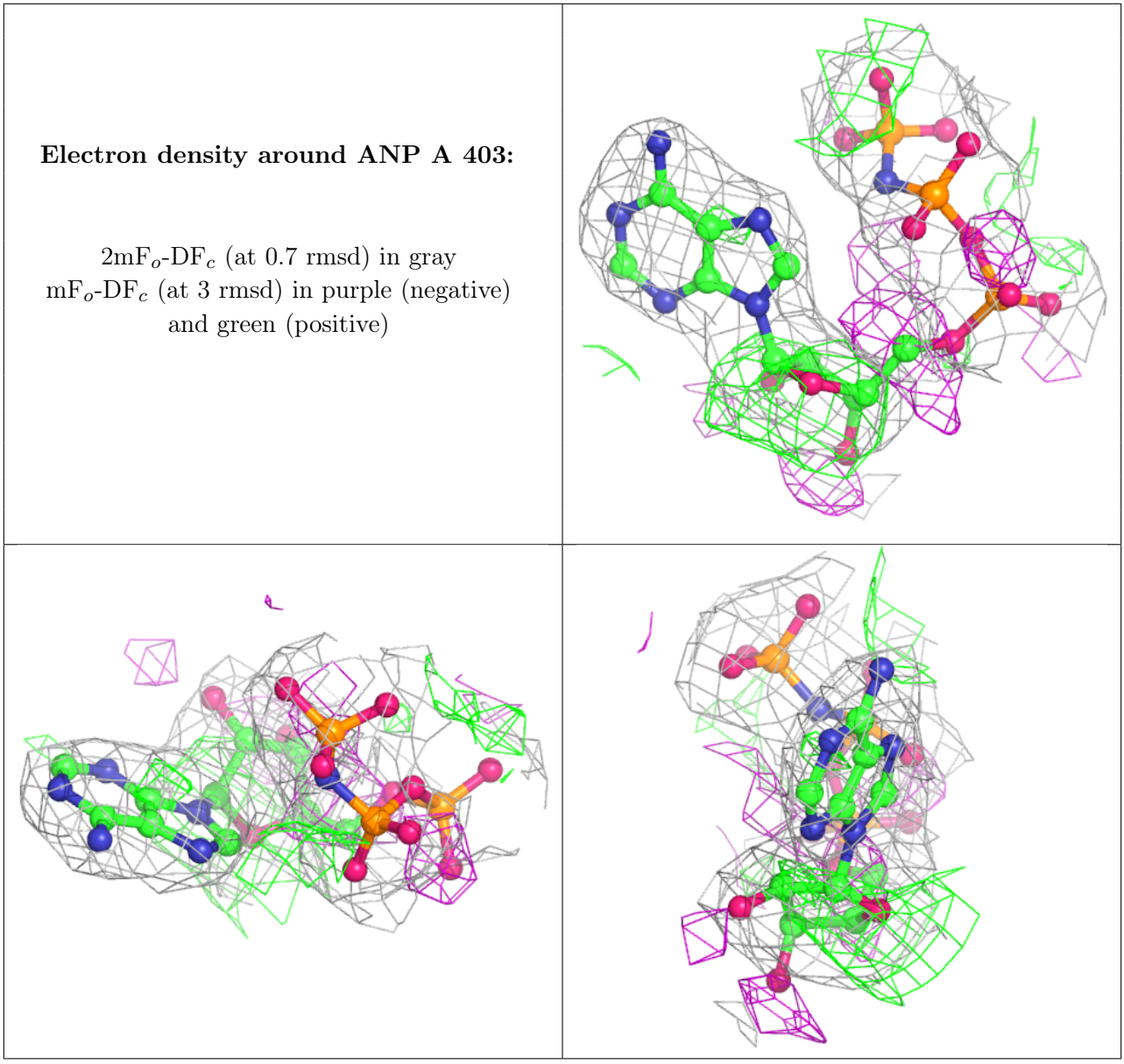






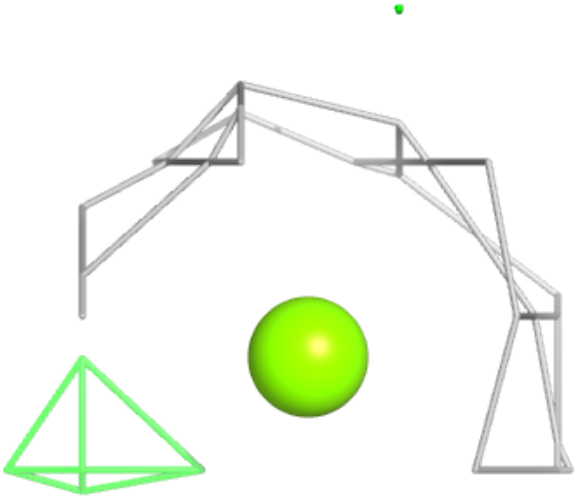
Electron density around ANP A 403:

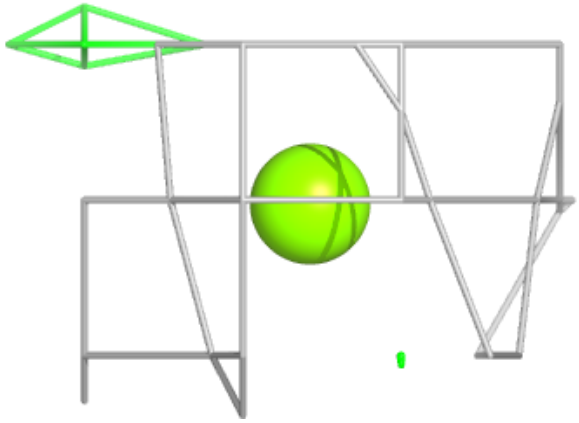
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

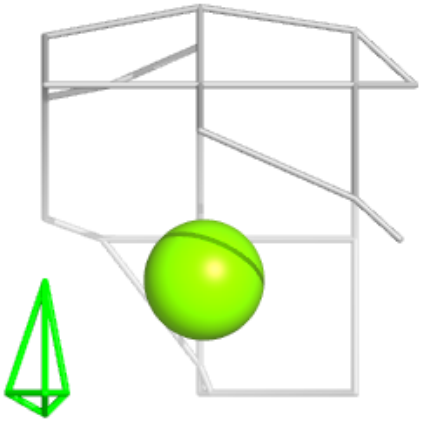


Electron density around MG B 401:

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

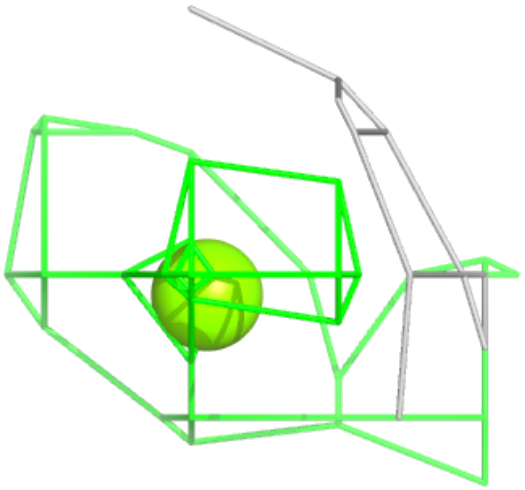


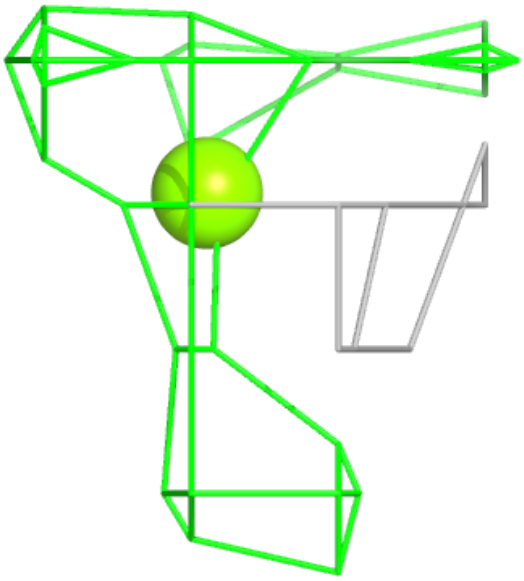


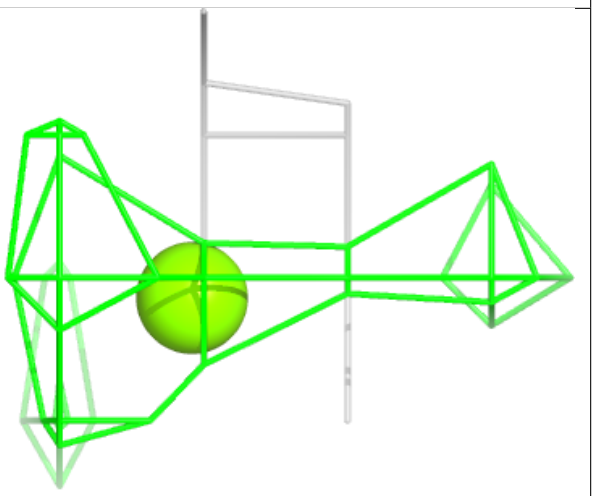


Electron density around MG A 402:

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

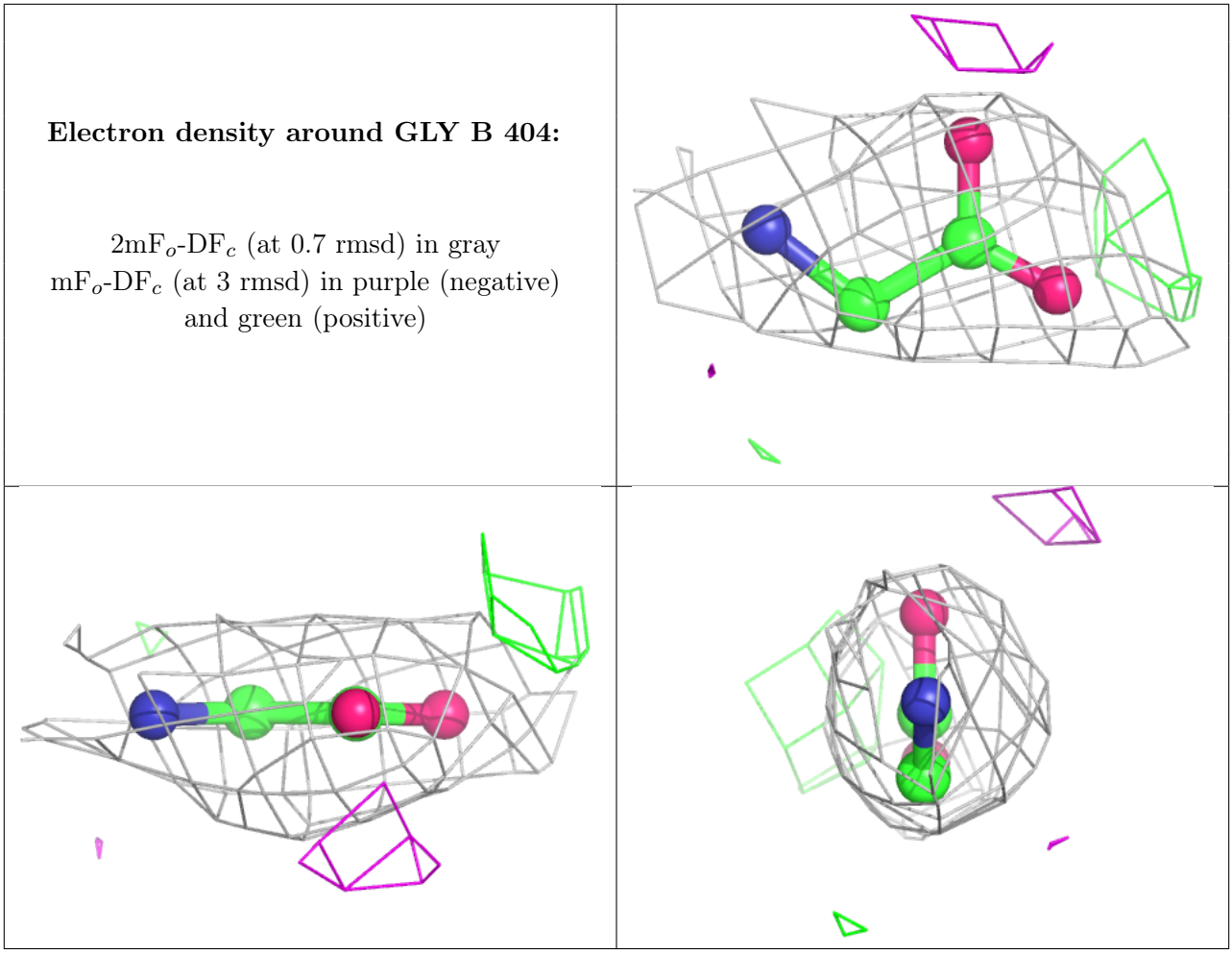






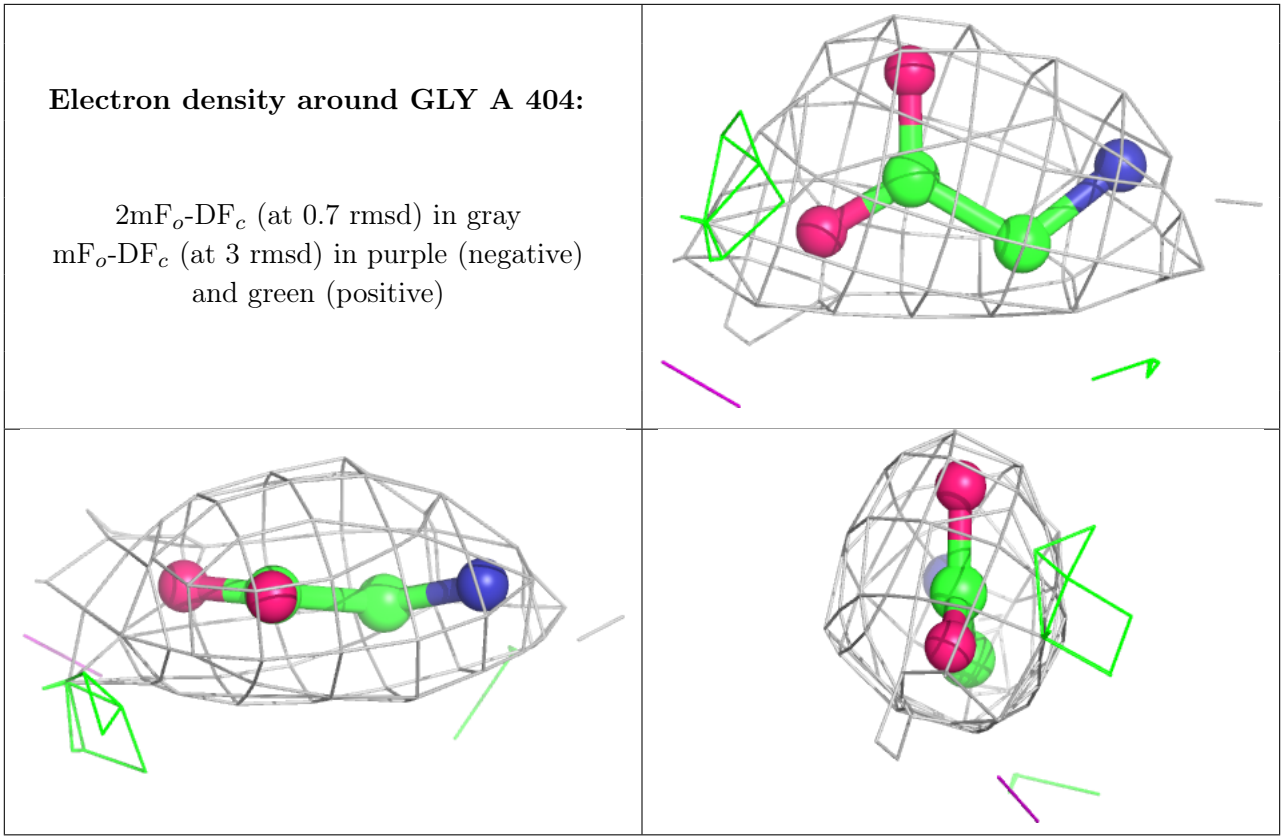
Electron density around GLY B 404:

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



Electron density around GLY A 404:

$2mF_o$-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.