



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 7EIV / pdb_00007eiv
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 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

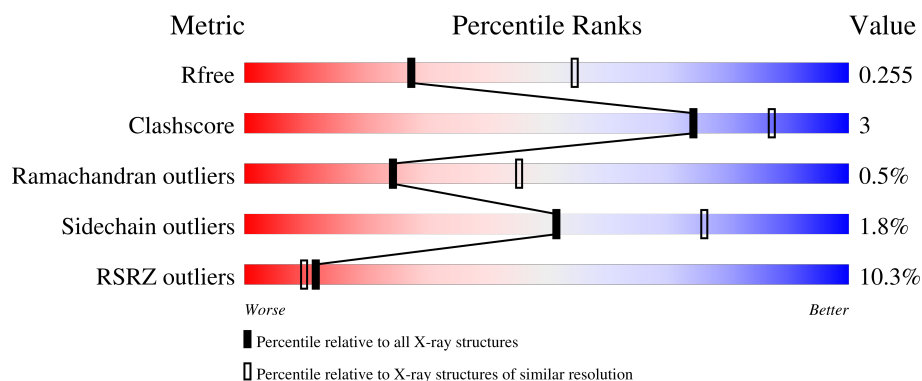
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	4% 91% 7% ..
1	B	303	5% 90% 8% ..
2	C	583	9% 84% 7% 8%
2	D	583	16% 88% 9% .

2 Entry composition

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			

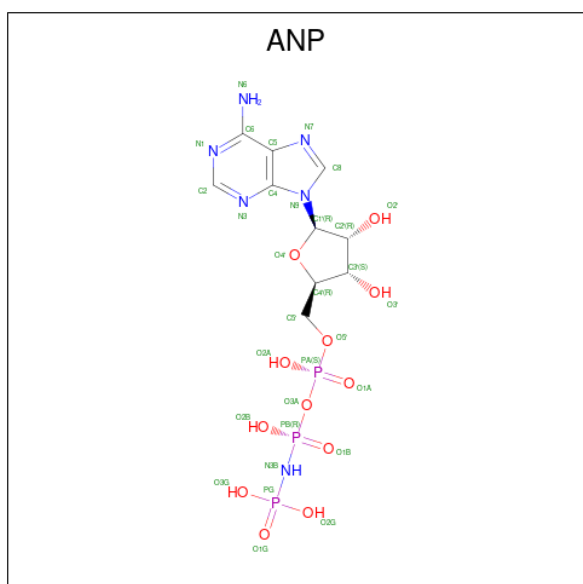
There are 16 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

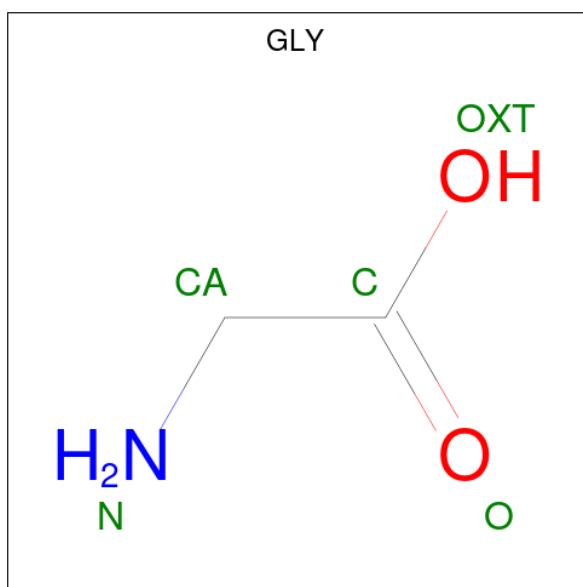
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



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

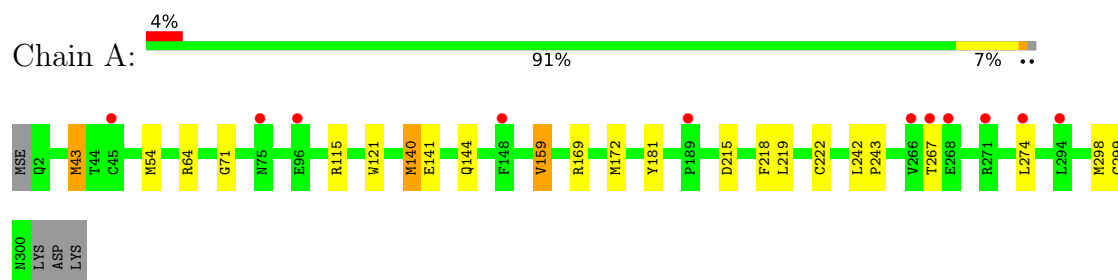
- Molecule 6 is water.

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

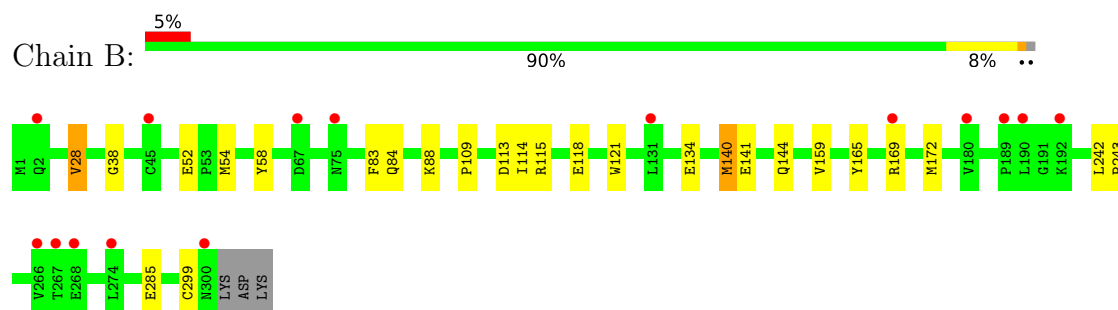
3 Residue-property plots

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.

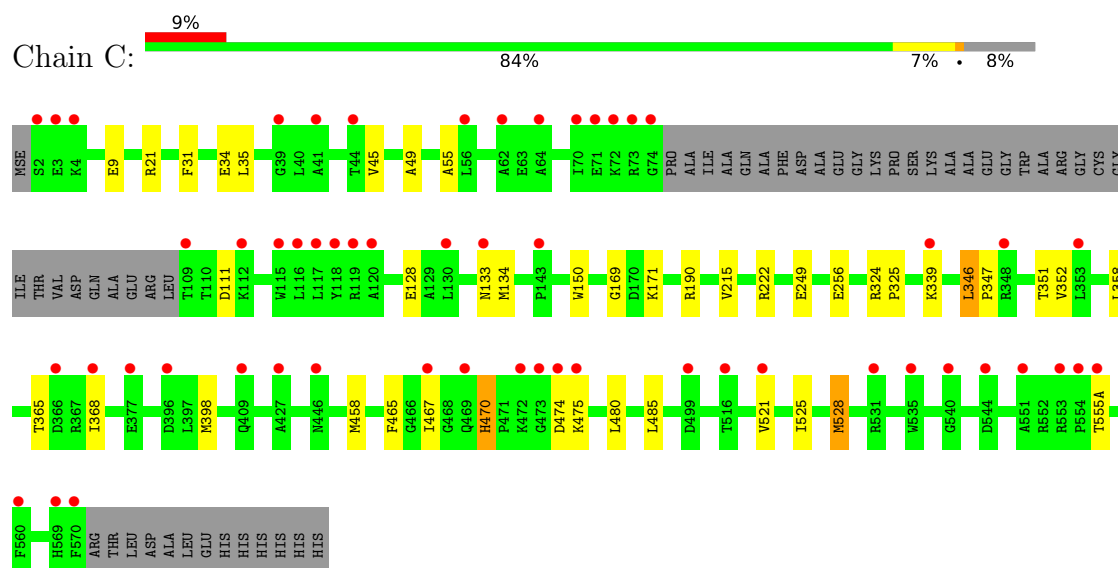
- Molecule 1: Glycine-tRNA ligase alpha subunit



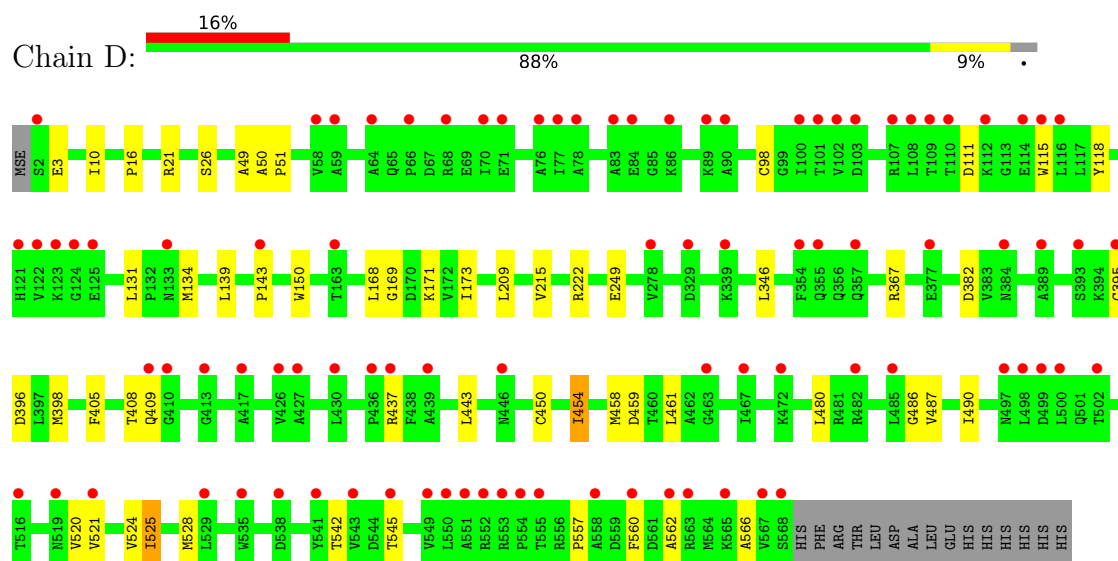
- Molecule 1: Glycine-tRNA ligase alpha subunit



- Molecule 2: Glycine-tRNA ligase beta subunit



● Molecule 2: Glycine-tRNA ligase beta subunit



4 Data and refinement statistics

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 48.58 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.58-2.68) 99.9 (48.58-2.68)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.01%)	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)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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, 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	0.94	0/2478	1.40	4/3360 (0.1%)
1	B	0.94	0/2475	1.39	1/3357 (0.0%)
2	C	0.99	0/4210	1.48	1/5694 (0.0%)
2	D	1.01	0/4365	1.52	1/5916 (0.0%)
All	All	0.98	0/13528	1.46	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(°)	Ideal(°)
1	A	140	MSE	CG-SE-CE	5.84	111.77	98.92
1	B	140	MSE	CG-SE-CE	5.69	111.43	98.92
1	A	298	MSE	CG-SE-CE	5.54	111.12	98.92
2	C	134	MSE	CG-SE-CE	5.52	111.07	98.92
1	A	43[A]	MSE	CG-SE-CE	5.14	110.24	98.92
1	A	43[B]	MSE	CG-SE-CE	5.14	110.24	98.92
2	D	398	MSE	CG-SE-CE	5.07	110.06	98.92

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	16	0
2	C	4142	0	4075	20	0
2	D	4294	0	4139	30	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	81	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 (81) 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
1:B:118:GLU:CD	2:D:16:PRO:HB3	2.44	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%)	16	34
2	D	566/583 (97%)	539 (95%)	23 (4%)	4 (1%)	18	37
All	All	1694/1772 (96%)	1633 (96%)	53 (3%)	8 (0%)	24	45

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%)	250 (97%)	7 (3%)	39	67
1	B	256/253 (101%)	252 (98%)	4 (2%)	55	78
2	C	421/462 (91%)	412 (98%)	9 (2%)	47	73
2	D	421/462 (91%)	415 (99%)	6 (1%)	59	80
All	All	1355/1430 (95%)	1329 (98%)	26 (2%)	51	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	MSE
1	A	43[B]	MSE
1	A	54	MSE
1	A	159	VAL
1	A	267	THR
1	A	274	LEU
1	A	299	CYS
1	B	28	VAL
1	B	54	MSE
1	B	285	GLU
1	B	299	CYS
2	C	190	ARG

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Mol	Chain	Res	Type
2	C	339	LYS
2	C	346	LEU
2	C	351	THR
2	C	470	HIS
2	C	480	LEU
2	C	485	LEU
2	C	528	MSE
2	C	555(A)	THR
2	D	115	TRP
2	D	134	MSE
2	D	171	LYS
2	D	437	ARG
2	D	454	ILE
2	D	525	ILE

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

Mol	Chain	Res	Type
1	A	144	GLN
1	A	202	ASN
1	A	206	GLN
1	B	29	GLN
1	B	202	ASN
1	B	253	HIS
2	C	433	GLN
2	C	435	GLN
2	C	537	GLN
2	D	121	HIS
2	D	300	ASN
2	D	345	ASN
2	D	537	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	ANP	A	403	3	33,33,33	1.16	5 (15%)	45,52,52	1.04	2 (4%)
4	ANP	B	403	3	33,33,33	1.21	3 (9%)	45,52,52	1.02	2 (4%)
5	GLY	B	404	-	4,4,4	1.06	1 (25%)	3,4,4	1.56	0
5	GLY	A	404	-	4,4,4	1.21	1 (25%)	3,4,4	1.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	403	3	-	4/18/38/38	0/3/3/3
4	ANP	B	403	3	-	2/18/38/38	0/3/3/3
5	GLY	B	404	-	-	0/2/2/2	-
5	GLY	A	404	-	-	0/2/2/2	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	ANP	PG-O1G	3.77	1.51	1.46
4	A	403	ANP	PG-O1G	3.24	1.51	1.46
4	B	403	ANP	PB-O1B	3.02	1.50	1.46
4	A	403	ANP	PB-O1B	2.88	1.50	1.46
4	A	403	ANP	PB-O2B	-2.45	1.50	1.56
4	B	403	ANP	PB-O2B	-2.37	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	GLY	OXT-C	-2.36	1.23	1.30
4	A	403	ANP	PG-O3G	-2.19	1.51	1.56
5	B	404	GLY	OXT-C	-2.05	1.24	1.30
4	A	403	ANP	PA-O3A	2.00	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	ANP	O1G-PG-N3B	-4.01	105.86	111.77
4	A	403	ANP	O2B-PB-O1B	3.88	118.18	109.87
4	B	403	ANP	O2B-PB-O1B	3.82	118.06	109.87
4	B	403	ANP	O3G-PG-O1G	-2.78	106.49	113.45

There are no chirality outliers.

All (6) 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-O2B
4	B	403	ANP	PG-N3B-PB-O3A
4	B	403	ANP	PA-O3A-PB-O2B
4	A	403	ANP	O4'-C4'-C5'-O5'
4	A	403	ANP	PG-N3B-PB-O3A

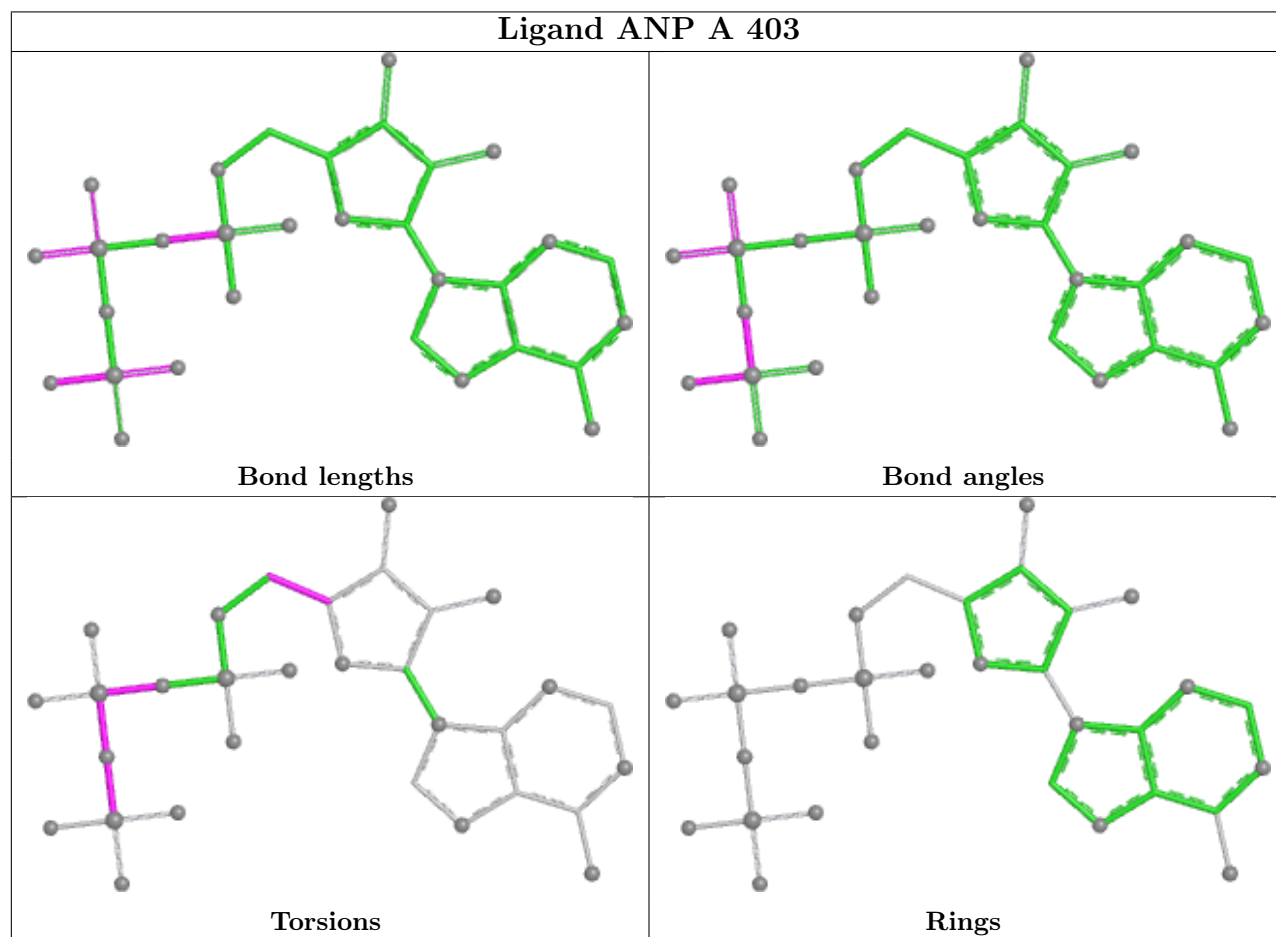
There are no ring outliers.

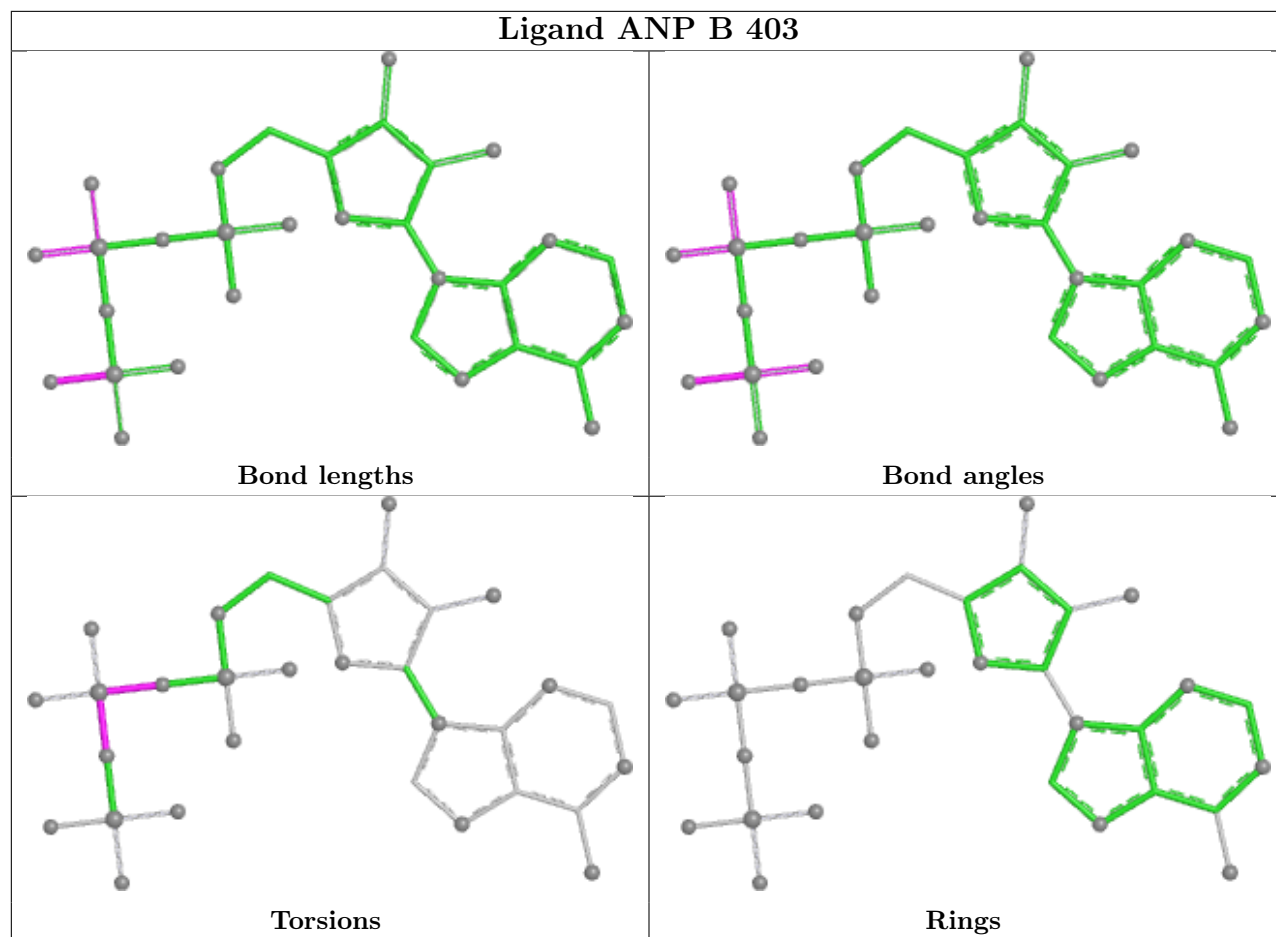
4 monomers are involved in 7 short contacts:

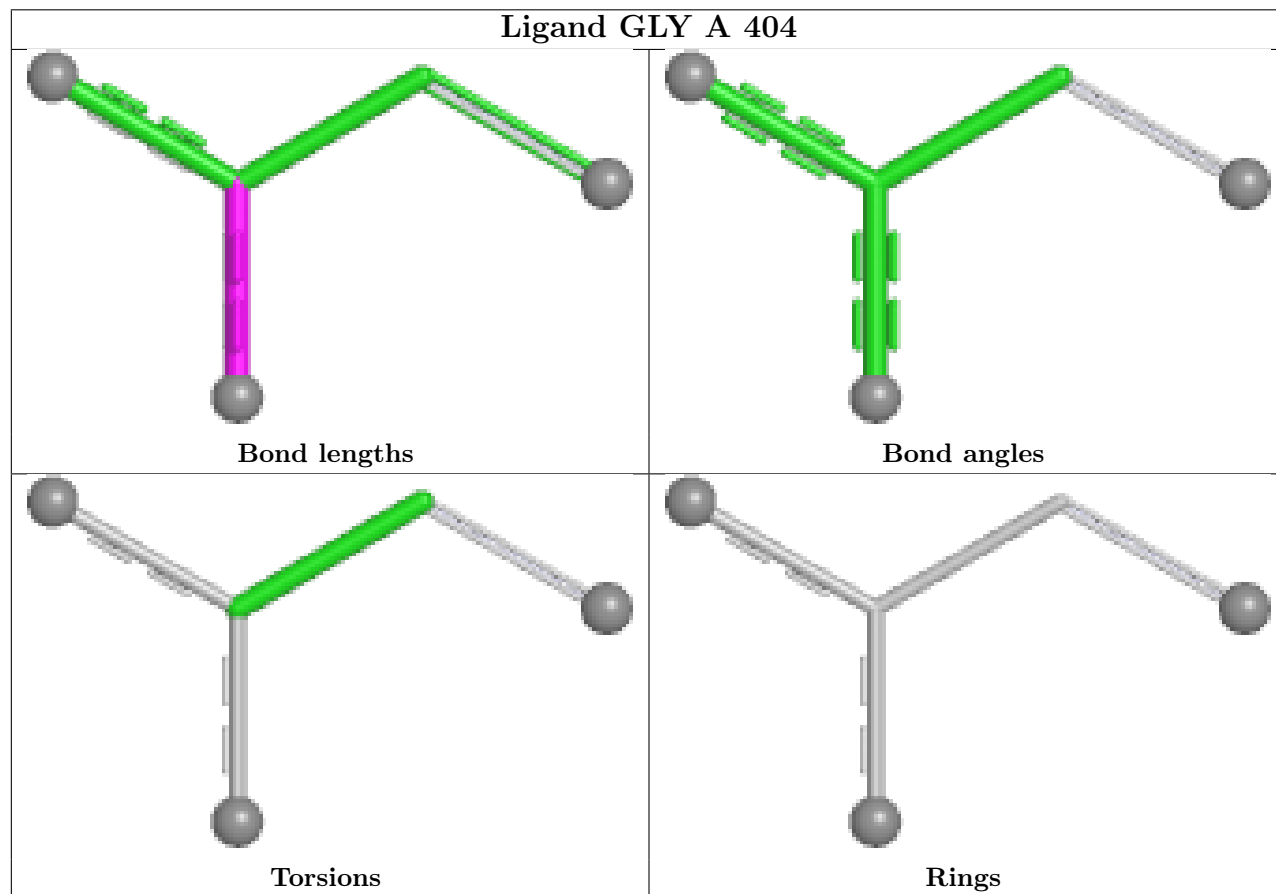
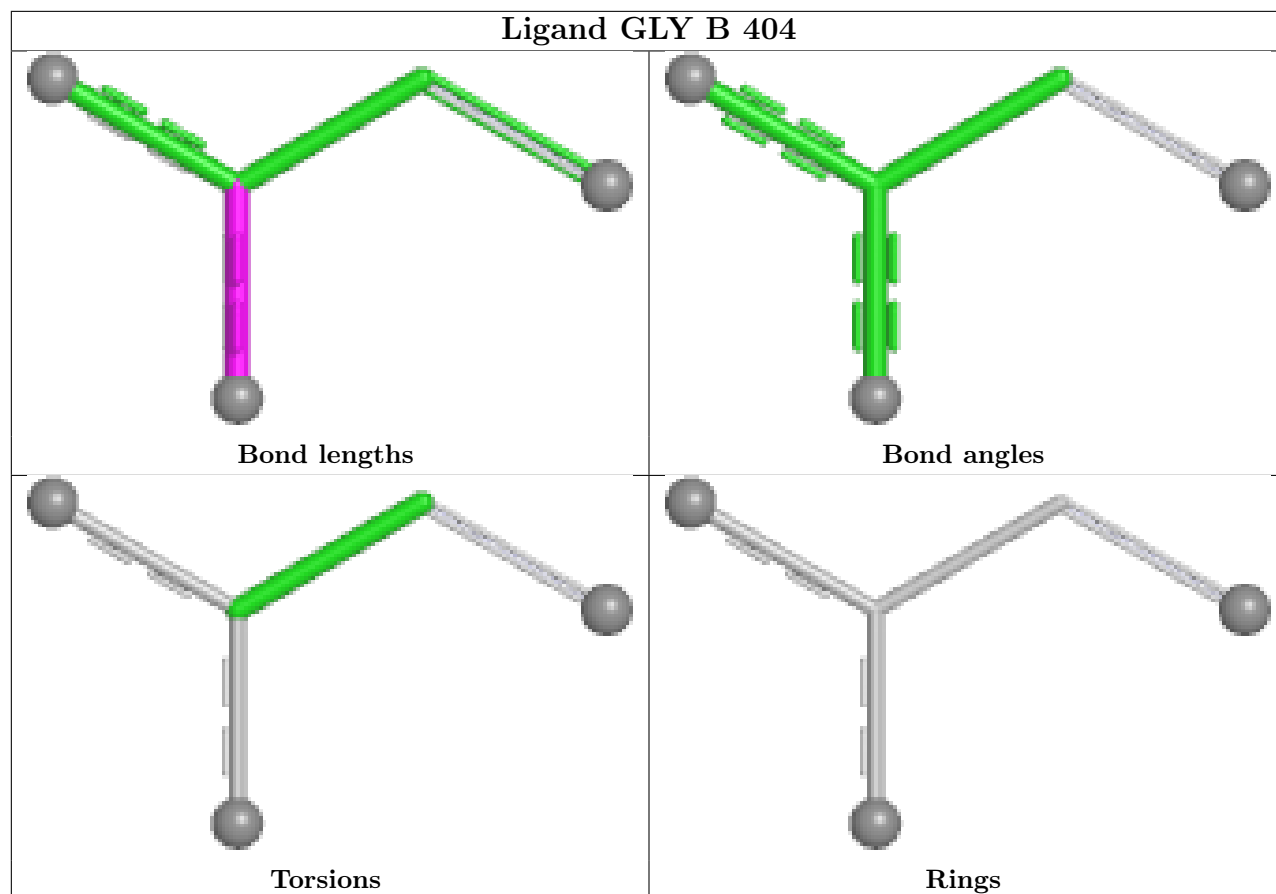
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	ANP	5	0
4	B	403	ANP	2	0
5	B	404	GLY	1	0
5	A	404	GLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	292/303 (96%)	0.42	11 (3%) 44 39	44, 61, 94, 113	0
1	B	292/303 (96%)	0.52	15 (5%) 33 29	46, 61, 92, 120	0
2	C	524/583 (89%)	0.85	55 (10%) 11 9	40, 74, 118, 150	2 (0%)
2	D	556/583 (95%)	1.09	91 (16%) 4 3	37, 80, 130, 155	2 (0%)
All	All	1664/1772 (93%)	0.80	172 (10%) 12 10	37, 70, 117, 155	4 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	568	SER	7.6
2	C	71	GLU	7.3
2	C	74	GLY	6.4
1	B	266	VAL	6.3
2	C	2	SER	6.2
2	C	570	PHE	5.6
2	C	115	TRP	5.2
2	D	357	GLN	4.9
2	D	115	TRP	4.8
2	C	569	HIS	4.7
2	D	499	ASP	4.6
2	D	413	GLY	4.6
2	D	2	SER	4.6
2	D	550	LEU	4.5
2	D	543	VAL	4.5
1	B	75	ASN	4.4
2	D	502	THR	4.2
2	D	563	ARG	4.2
2	C	474	ASP	4.1
2	D	554	PRO	4.0
2	C	120	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	355	GLN	4.0
2	C	472	LYS	3.9
1	A	267	THR	3.9
2	C	475	LYS	3.9
2	C	133[A]	ASN	3.9
2	D	567	VAL	3.9
2	D	90	ALA	3.8
2	D	497	ASN	3.8
1	B	45	CYS	3.7
2	D	555	THR	3.7
1	B	267	THR	3.7
2	D	77	ILE	3.7
2	D	68	ARG	3.7
2	D	439	ALA	3.7
2	D	560	PHE	3.6
2	D	109	THR	3.5
2	C	554	PRO	3.5
2	D	467	ILE	3.4
2	D	78	ALA	3.4
2	D	472	LYS	3.3
2	D	116	LEU	3.3
1	B	190	LEU	3.3
1	B	274	LEU	3.3
2	D	553	ARG	3.3
2	C	366	ASP	3.3
2	D	84	GLU	3.3
1	A	148	PHE	3.2
2	C	555(A)	THR	3.2
2	C	41	ALA	3.2
2	D	562	ALA	3.2
1	A	266	VAL	3.2
2	C	72	LYS	3.2
2	D	565	LYS	3.2
2	C	540	GLY	3.1
2	C	560	PHE	3.1
2	C	117	LEU	3.1
2	D	498	LEU	3.1
2	C	116	LEU	3.1
2	C	377	GLU	3.0
2	C	4	LYS	3.0
2	C	516	THR	3.0
1	B	169	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	64	ALA	3.0
2	D	417	ALA	3.0
2	D	125	GLU	3.0
1	B	189	PRO	3.0
2	D	107	ARG	3.0
2	C	551	ALA	3.0
1	A	274	LEU	2.9
2	C	409	GLN	2.9
1	A	294	LEU	2.9
2	D	101	THR	2.9
2	D	110	THR	2.9
2	D	122	VAL	2.9
2	D	89	LYS	2.9
2	D	133[A]	ASN	2.9
2	D	114	GLU	2.9
2	C	118	TYR	2.9
2	C	109	THR	2.8
2	D	430	LEU	2.8
2	D	545	THR	2.8
2	D	71	GLU	2.8
2	D	112	LYS	2.8
2	C	339	LYS	2.8
2	C	499	ASP	2.8
2	D	395	CYS	2.7
2	D	535	TRP	2.7
2	C	427	ALA	2.7
2	D	549	VAL	2.7
2	D	552	ARG	2.7
1	A	45	CYS	2.7
2	C	467	ILE	2.7
1	A	75	ASN	2.7
2	D	558	ALA	2.7
2	D	463	GLY	2.7
2	D	86	LYS	2.7
2	C	130	LEU	2.6
1	B	192	LYS	2.6
2	C	112	LYS	2.6
2	D	393	SER	2.6
2	C	70	ILE	2.6
2	D	108	LEU	2.5
1	A	189	PRO	2.5
2	D	427	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	368	ILE	2.5
2	D	339	LYS	2.5
2	C	553	ARG	2.5
2	D	482	ARG	2.5
2	D	410	GLY	2.5
2	C	143	PRO	2.5
2	D	64	ALA	2.5
2	D	485	LEU	2.5
2	C	544	ASP	2.5
2	D	436	PRO	2.5
2	D	354	PHE	2.5
2	D	70	ILE	2.4
2	C	535	TRP	2.4
2	C	353	LEU	2.4
2	D	426	VAL	2.4
2	C	39	GLY	2.4
2	D	551	ALA	2.4
2	D	102	VAL	2.4
2	D	121	HIS	2.3
2	C	119	ARG	2.3
2	D	500	LEU	2.3
2	D	538	ASP	2.3
2	C	469	GLN	2.3
2	D	529	LEU	2.3
1	A	96	GLU	2.3
2	C	73	ARG	2.3
2	D	409	GLN	2.3
2	D	83	ALA	2.3
2	D	541	TYR	2.3
1	A	271	ARG	2.3
2	D	143	PRO	2.3
2	D	124	GLY	2.3
1	B	131	LEU	2.3
2	C	62	ALA	2.2
2	C	348	ARG	2.2
2	C	531	ARG	2.2
2	C	521	VAL	2.2
1	B	268	GLU	2.2
2	C	44	THR	2.2
2	D	163	THR	2.2
2	C	446	ASN	2.2
1	B	2	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	76	ALA	2.2
2	D	437	ARG	2.2
2	D	66	PRO	2.2
2	D	103	ASP	2.2
1	B	180	VAL	2.2
2	C	396	ASP	2.2
2	D	519	ASN	2.1
2	D	278	VAL	2.1
2	D	377	GLU	2.1
2	D	384	ASN	2.1
1	B	67	ASP	2.1
2	D	59	ALA	2.1
2	D	516	THR	2.1
2	C	3	GLU	2.1
2	D	100	ILE	2.1
2	D	329	ASP	2.0
2	C	56	LEU	2.0
2	D	446	ASN	2.0
2	C	473	GLY	2.0
1	A	268	GLU	2.0
2	D	123	LYS	2.0
2	D	389	ALA	2.0
1	B	300	ASN	2.0
2	D	58	VAL	2.0
2	D	521	VAL	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](#)

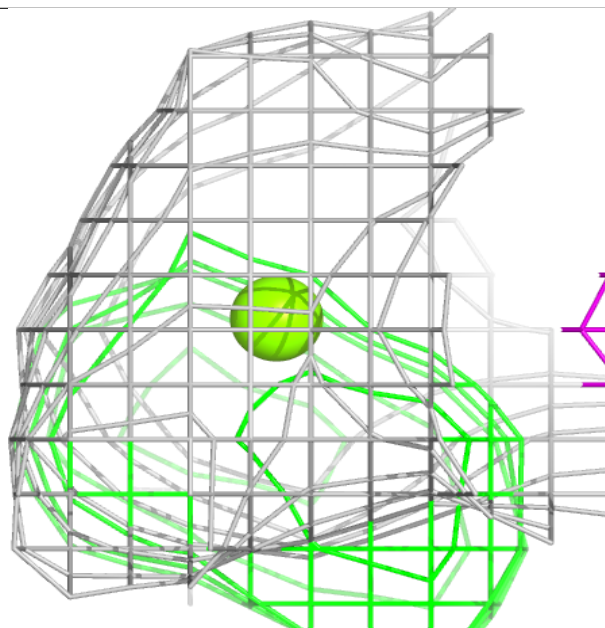
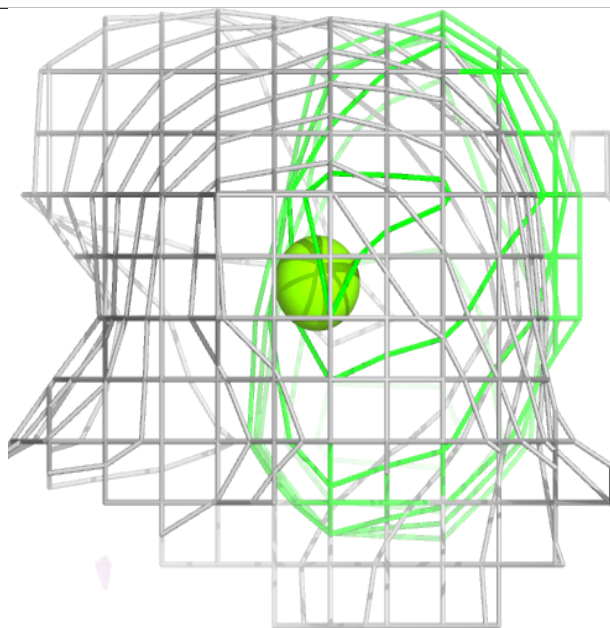
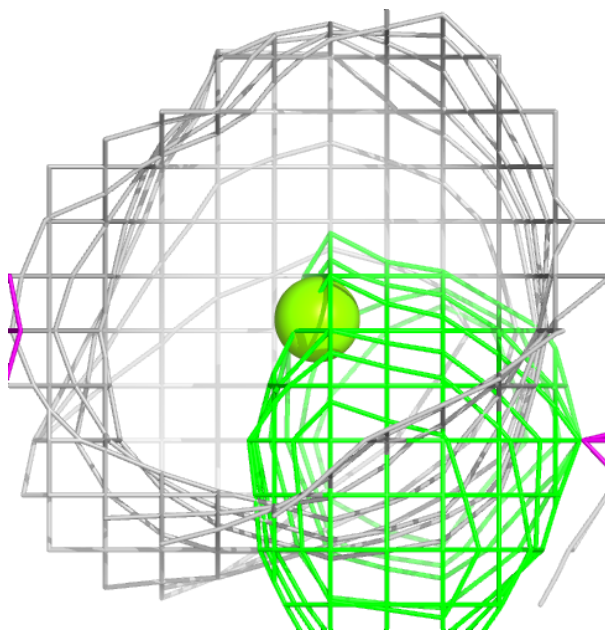
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	A	401	1/1	0.81	0.19	52,52,52,52	0
3	MG	B	402	1/1	0.88	0.20	50,50,50,50	0
4	ANP	B	403	31/31	0.90	0.13	50,66,92,95	0
4	ANP	A	403	31/31	0.91	0.13	50,63,90,98	0
3	MG	B	401	1/1	0.93	0.10	62,62,62,62	0
5	GLY	B	404	5/5	0.93	0.17	51,55,57,57	0
5	GLY	A	404	5/5	0.95	0.13	50,53,55,58	0
3	MG	A	402	1/1	0.95	0.15	54,54,54,54	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.

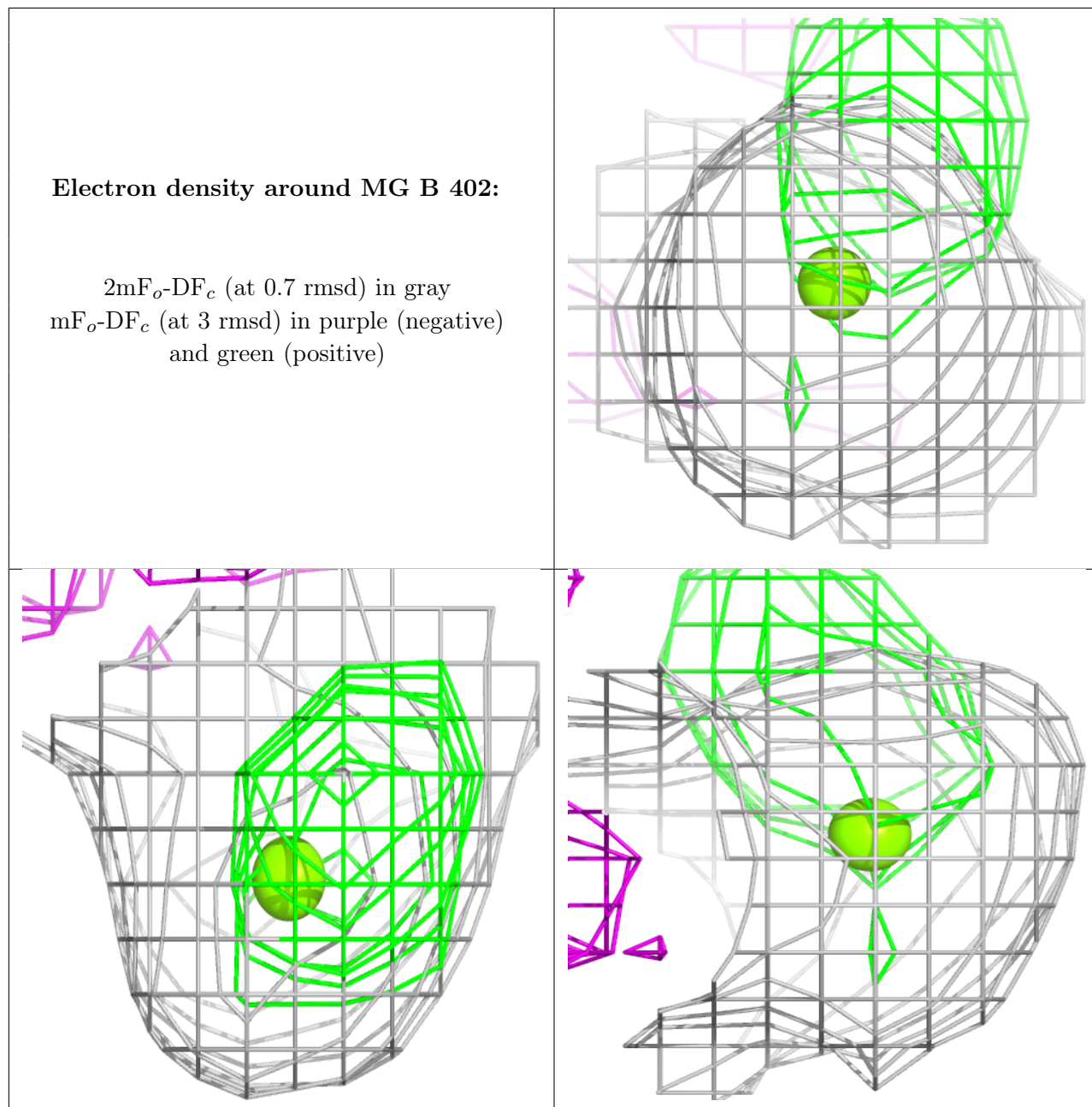
Electron density around MG A 401:

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



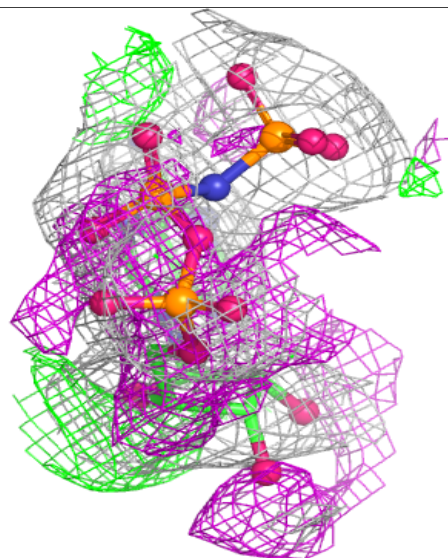
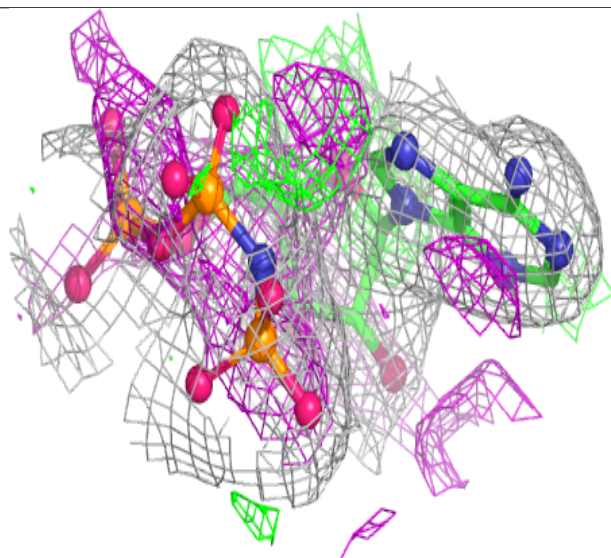
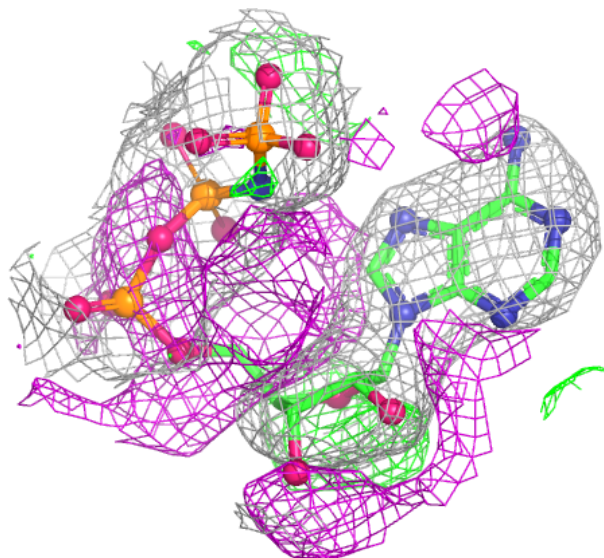
Electron density around MG B 402:

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and green (positive)



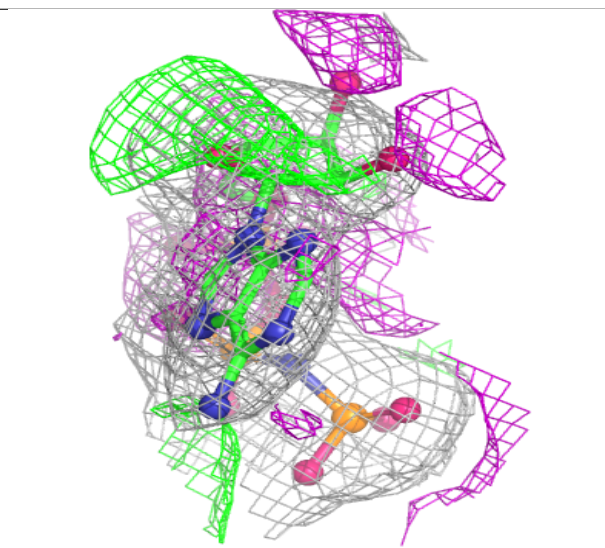
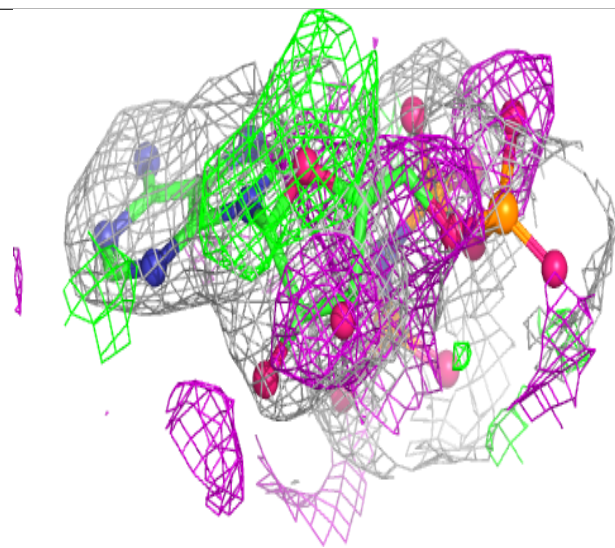
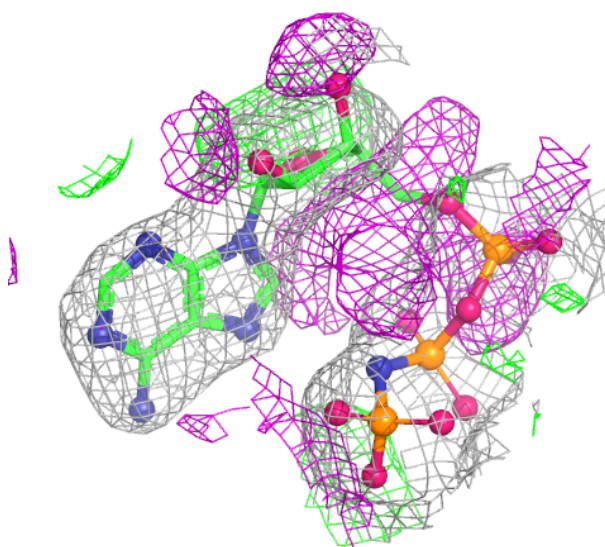
Electron density around ANP B 403:

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and green (positive)



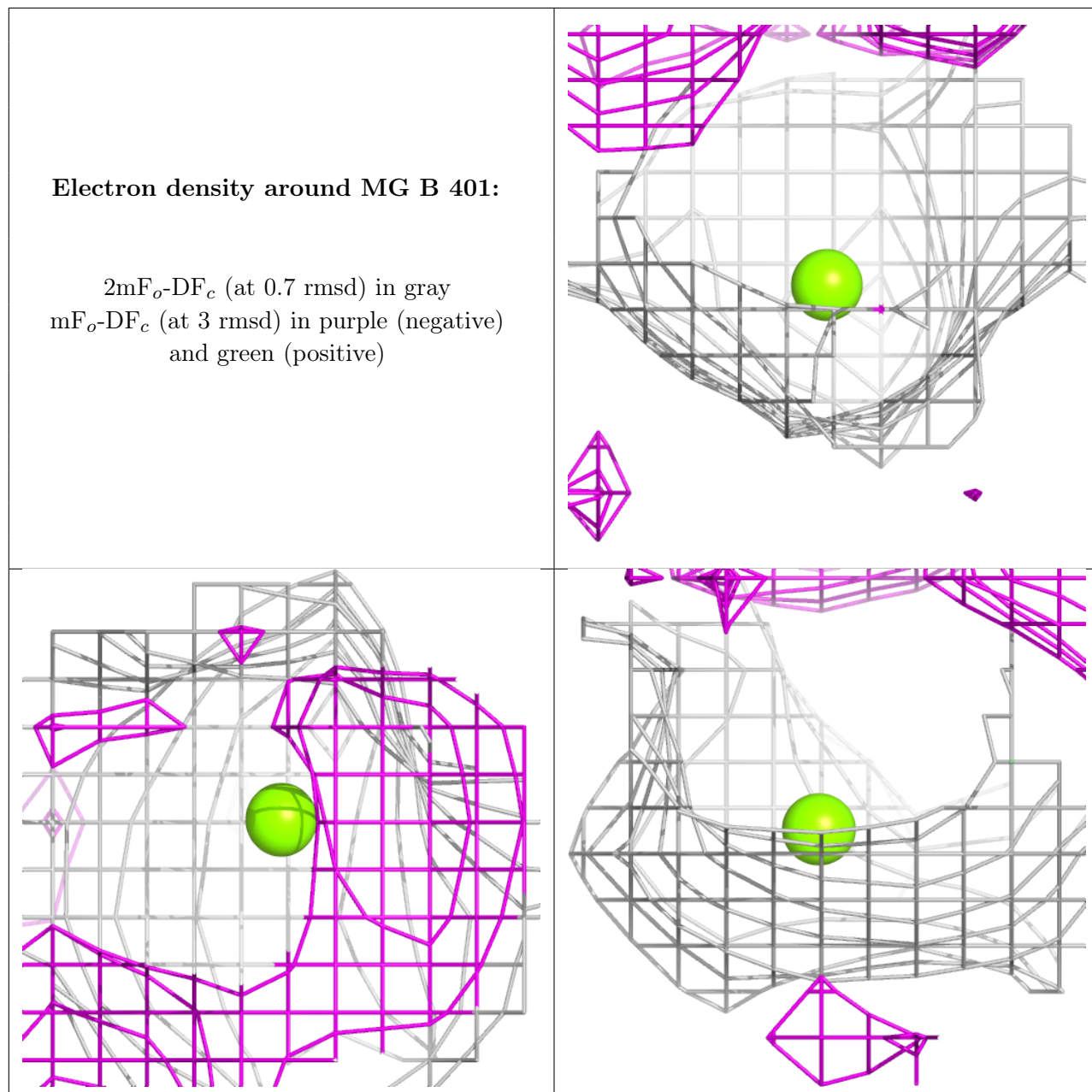
Electron density around ANP A 403:

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



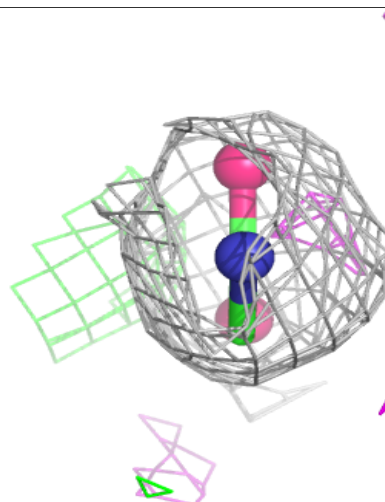
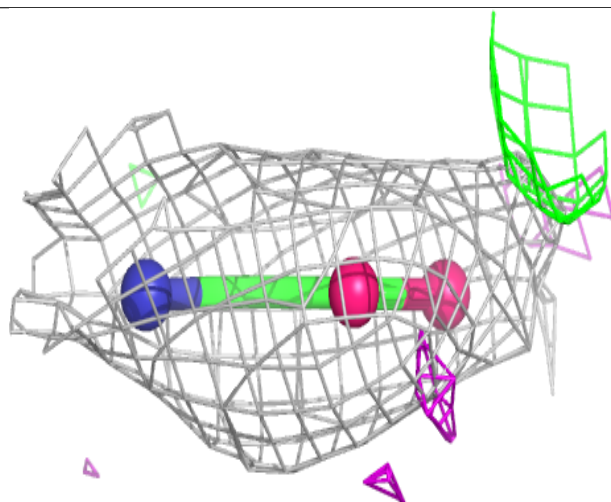
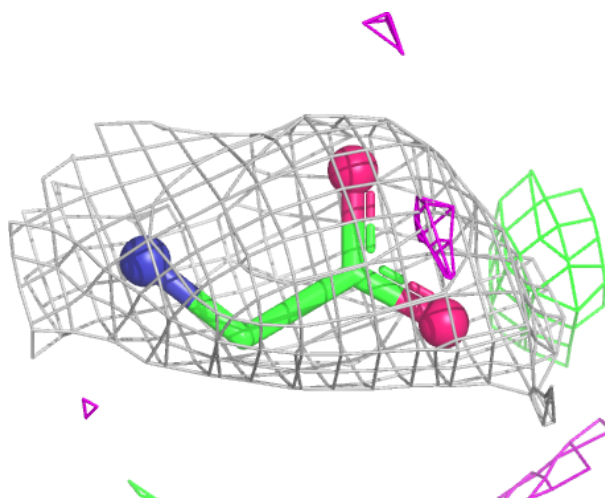
Electron density around MG B 401:

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



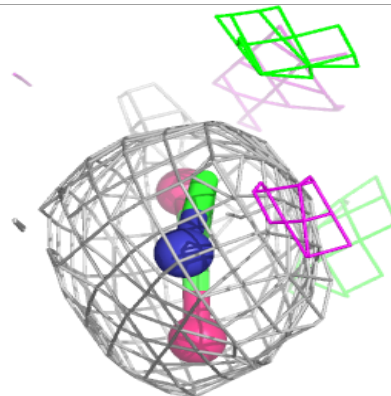
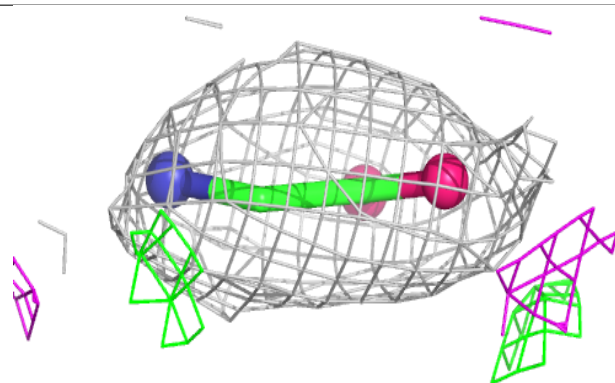
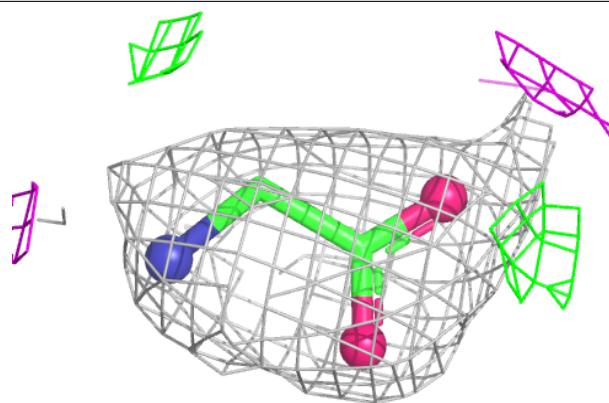
Electron density around GLY B 404:

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



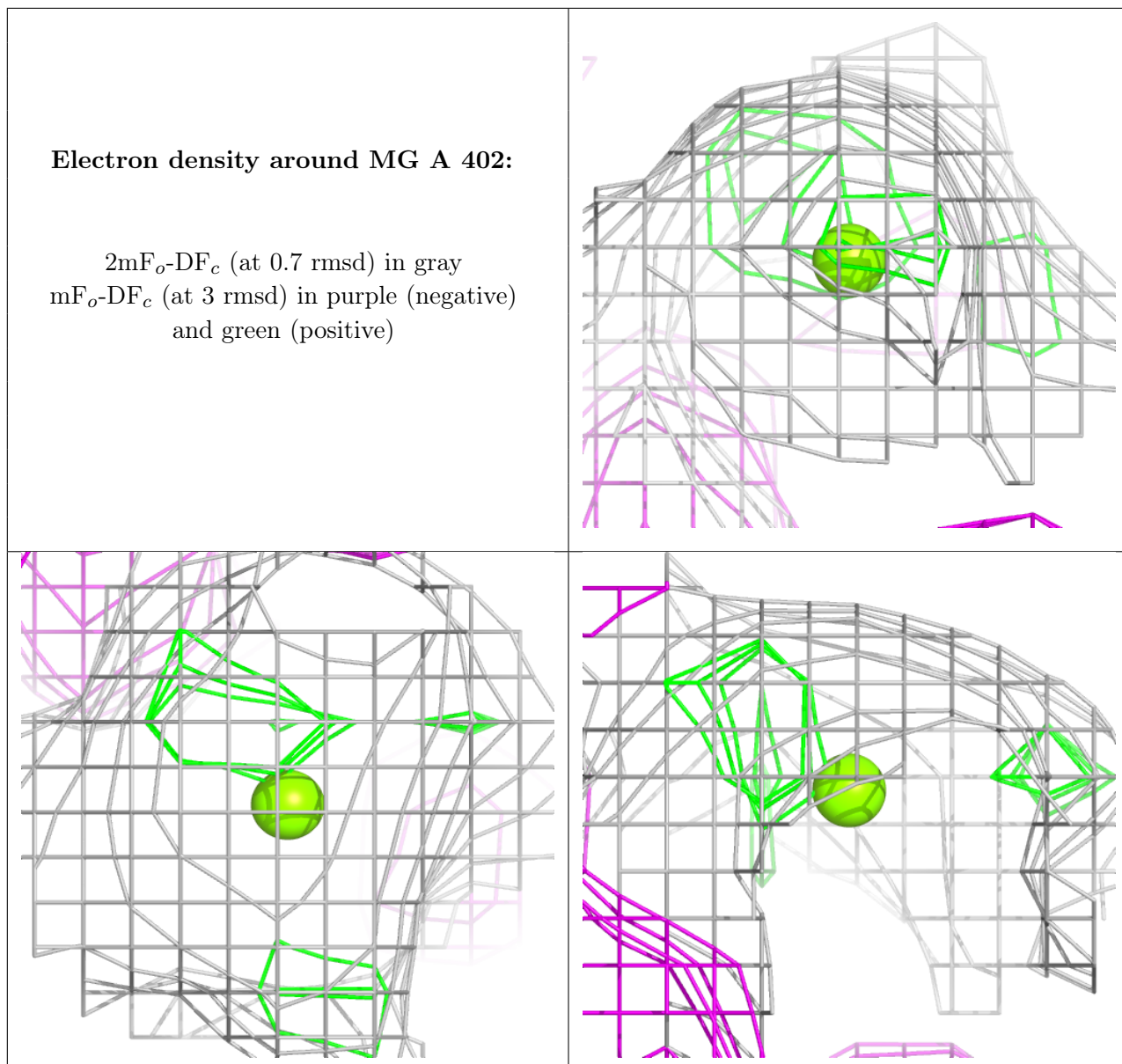
Electron density around GLY A 404:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.