Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:06 PM JST

PDB ID	:	5GVP
Title	:	Plasmodium vivax SHMT bound with PLP-glycine and GS654
Authors	:	Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Schwertz, G.
Deposited on	:	2016-09-06
Resolution	:	2.26 Å(reported)

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

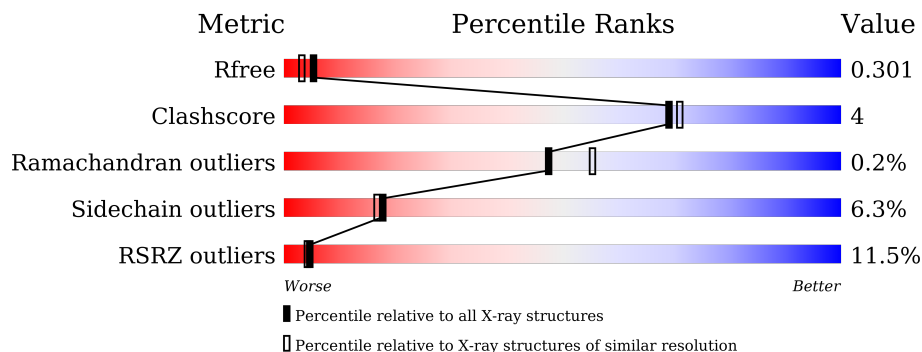|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.26 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	Percentile Ranks	Value
Rfree		0.301
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		6.3%
RSRZ outliers		11.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	442	11% — 85% — 14% •
1	B	442	13% — 86% — 14% •
1	C	442	10% — 84% — 15% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10819 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 Serine hydroxymethyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	B	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			
1	C	442	Total	C	N	O	S	0	0	0
			3458	2186	600	655	17			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).
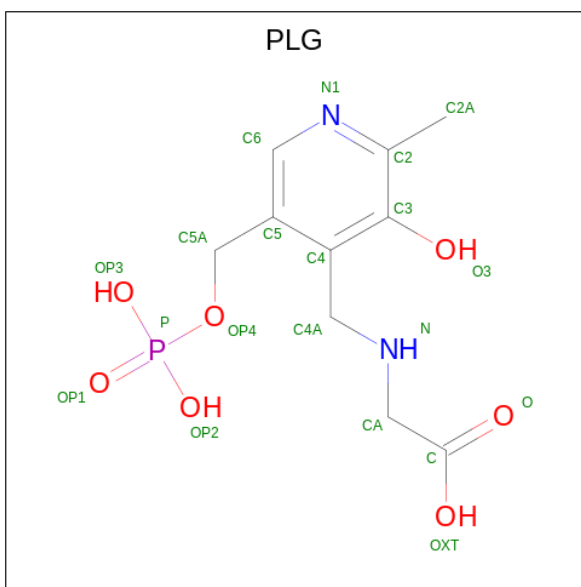
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 3-[3-[3-[(4 {S})-6-azanyl-5-cyano-3-methyl-4-propan-2-yl-2 {H}-pyrano[2,3
  -c]pyrazol-4-yl]-5-(trifluoromethyl)phenyl]phenyl]propanoic acid (three-letter code: GCF)
  (formula: $C_{27}H_{25}F_3N_4O_3$).
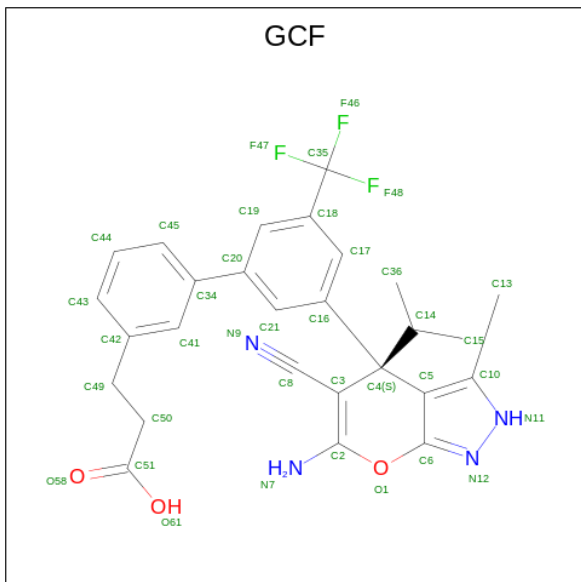
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			37	27	3	4	3		
3	A	1	Total	C	F	N	O	0	0
			37	27	3	4	3		
3	C	1	Total	C	F	N	O	0	0
			37	27	3	4	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	90	Total	O	0	0
			90	90		
5	C	84	Total	O	0	0
			84	84		

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: Serine hydroxymethyltransferase, putative
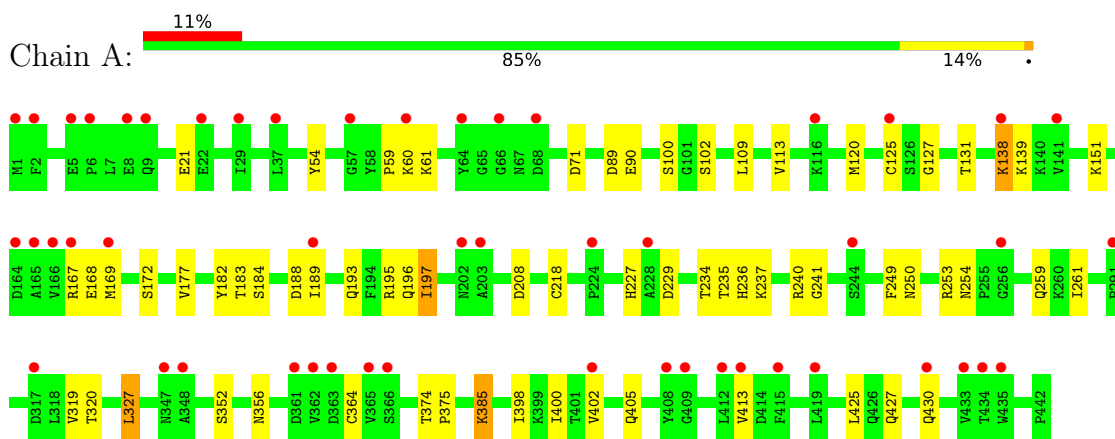
- Molecule 1: Serine hydroxymethyltransferase, putative
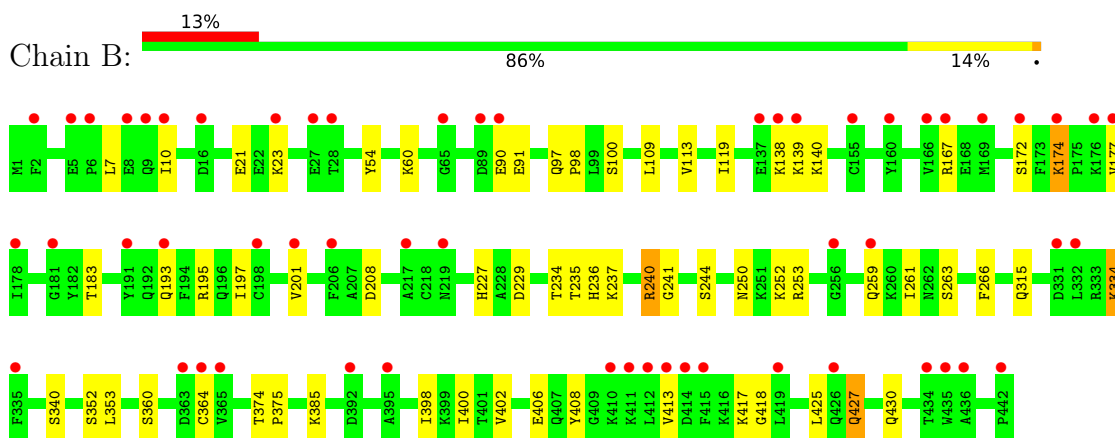
- Molecule 1: Serine hydroxymethyltransferase, putative

4 Data and refinement statistics ⓘ

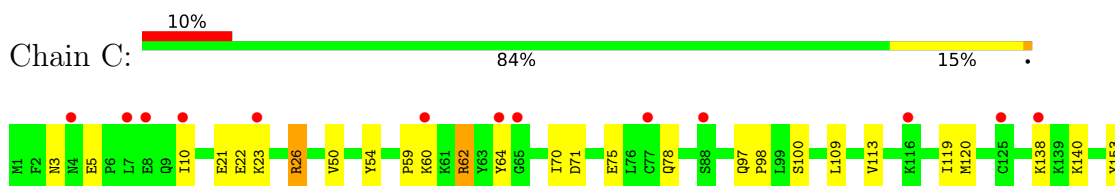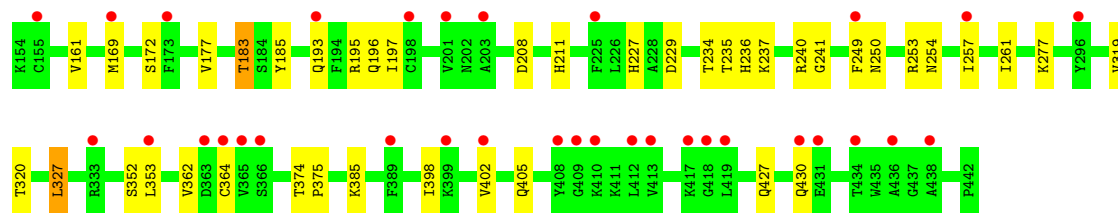| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.08Å 58.93Å 234.83Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	50.01 – 2.26 42.76 – 2.26	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.01-2.26) 95.8 (42.76-2.26)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.39 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.250 , 0.311 0.249 , 0.301	Depositor DCC
R_{free} test set	6374 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 16.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.470 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.478 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10819	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GCF, CL, PLG

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	0.55	0/3521	0.72	3/4754 (0.1%)
1	B	0.56	0/3521	0.72	2/4754 (0.0%)
1	C	0.54	0/3521	0.73	4/4754 (0.1%)
All	All	0.55	0/10563	0.72	9/14262 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	26	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	240	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	240	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	208	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	208	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	327	LEU	CA-CB-CG	5.25	127.38	115.30
1	C	240	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	327	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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	3458	0	3477	26	0
1	B	3458	0	3477	23	0
1	C	3458	0	3477	26	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
3	A	74	0	0	2	0
3	C	37	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	1	0
5	A	98	0	0	3	0
5	B	90	0	0	2	0
5	C	84	0	0	2	0
All	All	10819	0	10464	78	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 4.

All (78) 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:B:315:GLN:O	1:B:334:LYS:NZ	1.77	1.15
1:B:427:GLN:HE21	1:B:427:GLN:HA	1.62	0.65
1:C:120:MET:SD	1:C:169:MET:HE3	2.39	0.63
1:C:195:ARG:HB2	1:C:227:HIS:HB3	1.84	0.60
1:A:120:MET:SD	1:A:169:MET:HE3	2.43	0.59
1:A:398:ILE:O	1:A:402:VAL:HG23	2.03	0.58
1:A:259:GLN:HG2	5:A:690:HOH:O	2.06	0.56
1:A:193:GLN:O	1:A:197:ILE:HG13	2.06	0.55
1:C:193:GLN:O	1:C:197:ILE:HG13	2.05	0.55
1:B:259:GLN:HG2	5:B:685:HOH:O	2.06	0.54
1:B:174:LYS:HD2	1:B:201:VAL:CG1	2.40	0.52
1:A:234:THR:HB	1:A:236:HIS:CE1	2.44	0.52
1:A:127:GLY:O	1:A:182:TYR:HB3	2.10	0.52
1:C:277:LYS:NZ	4:C:503:CL:CL	2.70	0.51
1:B:235:THR:O	1:B:241:GLY:N	2.42	0.51
1:A:400:ILE:HG21	1:A:425:LEU:HD21	1.92	0.50
1:C:249:PHE:HB3	1:C:261:ILE:HD12	1.92	0.50
1:C:229:ASP:OD1	1:C:253:ARG:HD2	2.12	0.50
1:A:195:ARG:HB2	1:A:227:HIS:HB3	1.92	0.50
1:C:234:THR:HB	1:C:236:HIS:CE1	2.47	0.50
1:C:183:THR:HA	1:C:211:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG1	1:A:177:VAL:HG23	2.43	0.49
1:B:234:THR:HB	1:B:236:HIS:CE1	2.47	0.49
1:C:235:THR:O	1:C:241:GLY:N	2.44	0.49
1:C:196:GLN:NE2	5:C:603:HOH:O	2.41	0.49
1:B:400:ILE:HG21	1:B:425:LEU:HD21	1.95	0.48
1:A:138:LYS:HA	1:A:138:LYS:HE2	1.96	0.48
1:C:3:ASN:OD1	1:C:5:GLU:HG3	2.13	0.48
1:A:229:ASP:OD1	1:A:253:ARG:HD2	2.13	0.47
1:A:89:ASP:OD1	1:A:89:ASP:C	2.53	0.47
1:A:249:PHE:HB3	1:A:261:ILE:HD12	1.97	0.46
1:A:218:CYS:SG	5:A:677:HOH:O	2.33	0.46
1:B:229:ASP:OD1	1:B:253:ARG:HD2	2.15	0.46
1:B:113:VAL:CG1	1:B:177:VAL:HG23	2.45	0.46
1:B:195:ARG:HB2	1:B:227:HIS:HB3	1.96	0.46
1:A:235:THR:O	1:A:241:GLY:N	2.48	0.46
3:A:503:GCF:C17	3:A:503:GCF:C8	2.94	0.45
1:B:427:GLN:HA	1:B:427:GLN:NE2	2.29	0.45
1:C:3:ASN:ND2	1:C:10:ILE:HD13	2.32	0.45
1:B:408:TYR:CZ	1:B:418:GLY:HA2	2.52	0.45
1:A:60:LYS:C	5:A:609:HOH:O	2.54	0.45
1:C:109:LEU:HD22	1:C:119:ILE:HG21	1.98	0.45
1:A:59:PRO:HA	1:A:71:ASP:OD1	2.16	0.45
1:B:60:LYS:C	5:B:612:HOH:O	2.55	0.45
1:B:109:LEU:HD22	1:B:119:ILE:HG21	1.99	0.45
1:C:22:GLU:OE1	1:C:26:ARG:NH2	2.46	0.45
1:C:319:VAL:HG12	1:C:320:THR:HG23	1.99	0.45
1:C:60:LYS:C	5:C:614:HOH:O	2.55	0.44
1:A:109:LEU:O	1:A:113:VAL:HG22	2.17	0.44
1:C:75:GLU:HA	1:C:78:GLN:OE1	2.17	0.44
1:B:374:THR:N	1:B:375:PRO:CD	2.81	0.44
1:B:7:LEU:HA	1:B:10:ILE:HG22	2.00	0.44
1:C:398:ILE:O	1:C:402:VAL:HG23	2.18	0.44
1:B:97:GLN:N	1:B:98:PRO:CD	2.81	0.43
3:A:502:GCF:C17	3:A:502:GCF:C8	2.96	0.43
1:C:50:VAL:CG2	1:C:70:ILE:CD1	2.96	0.43
1:A:319:VAL:HG12	1:A:320:THR:HG23	2.01	0.43
1:B:398:ILE:O	1:B:402:VAL:HG23	2.19	0.43
1:C:59:PRO:HA	1:C:71:ASP:OD1	2.17	0.42
1:A:374:THR:N	1:A:375:PRO:CD	2.82	0.42
1:C:374:THR:N	1:C:375:PRO:CD	2.82	0.42
1:B:263:SER:HA	1:B:266:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LYS:H	1:A:385:LYS:HE3	1.84	0.42
1:C:97:GLN:N	1:C:98:PRO:CD	2.83	0.42
1:C:161:VAL:HG23	1:C:185:TYR:CZ	2.55	0.42
1:C:153:TYR:HB3	1:C:169:MET:HE2	2.02	0.42
1:C:113:VAL:CG1	1:C:177:VAL:HG23	2.50	0.41
1:B:91:GLU:HG3	1:B:252:LYS:HB2	2.02	0.41
3:C:502:GCF:C17	3:C:502:GCF:C8	2.98	0.41
1:A:102:SER:HA	1:A:131:THR:HG21	2.02	0.41
1:B:193:GLN:O	1:B:197:ILE:HG13	2.21	0.41
1:A:385:LYS:H	1:A:385:LYS:CE	2.33	0.41
1:B:167:ARG:HB2	1:B:197:ILE:HD13	2.03	0.41
1:A:125:CYS:SG	1:A:364:CYS:HB2	2.61	0.41
1:A:167:ARG:HB2	1:A:197:ILE:HD13	2.02	0.41
1:C:62:ARG:HB3	1:C:64:TYR:O	2.22	0.40
1:A:188:ASP:OD1	1:A:189:ILE:N	2.51	0.40
1:B:174:LYS:HD2	1:B:201:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/442 (100%)	427 (97%)	12 (3%)	1 (0%)	47	55
1	B	440/442 (100%)	431 (98%)	8 (2%)	1 (0%)	47	55
1	C	440/442 (100%)	429 (98%)	10 (2%)	1 (0%)	47	55
All	All	1320/1326 (100%)	1287 (98%)	30 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	LYS

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Mol	Chain	Res	Type
1	B	237	LYS
1	C	237	LYS

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	381/381 (100%)	357 (94%)	24 (6%)	18	17
1	B	381/381 (100%)	354 (93%)	27 (7%)	14	13
1	C	381/381 (100%)	360 (94%)	21 (6%)	21	21
All	All	1143/1143 (100%)	1071 (94%)	72 (6%)	18	17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	54	TYR
1	A	61	LYS
1	A	90	GLU
1	A	100	SER
1	A	138	LYS
1	A	139	LYS
1	A	151	LYS
1	A	168	GLU
1	A	172	SER
1	A	183	THR
1	A	184	SER
1	A	196	GLN
1	A	197	ILE
1	A	250	ASN
1	A	254	ASN
1	A	327	LEU
1	A	352	SER
1	A	356	ASN
1	A	385	LYS

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Mol	Chain	Res	Type
1	A	405	GLN
1	A	413	VAL
1	A	427	GLN
1	A	430	GLN
1	B	21	GLU
1	B	23	LYS
1	B	54	TYR
1	B	90	GLU
1	B	100	SER
1	B	138	LYS
1	B	139	LYS
1	B	140	LYS
1	B	172	SER
1	B	174	LYS
1	B	183	THR
1	B	240	ARG
1	B	244	SER
1	B	250	ASN
1	B	261	ILE
1	B	334	LYS
1	B	340	SER
1	B	352	SER
1	B	353	LEU
1	B	360	SER
1	B	364	CYS
1	B	385	LYS
1	B	406	GLU
1	B	413	VAL
1	B	417	LYS
1	B	427	GLN
1	B	430	GLN
1	C	21	GLU
1	C	23	LYS
1	C	54	TYR
1	C	62	ARG
1	C	100	SER
1	C	138	LYS
1	C	140	LYS
1	C	172	SER
1	C	183	THR
1	C	250	ASN
1	C	254	ASN

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Mol	Chain	Res	Type
1	C	257	ILE
1	C	327	LEU
1	C	352	SER
1	C	353	LEU
1	C	362	VAL
1	C	364	CYS
1	C	385	LYS
1	C	405	GLN
1	C	427	GLN
1	C	430	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	427	GLN
1	B	427	GLN
1	B	430	GLN
1	C	196	GLN
1	C	227	HIS
1	C	250	ASN
1	C	424	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PLG	B	501	-	20,20,20	2.89	4 (20%)	25,28,28	2.59	9 (36%)
2	PLG	C	501	-	20,20,20	2.58	3 (15%)	25,28,28	2.33	6 (24%)
3	GCF	A	502	-	35,40,40	2.34	4 (11%)	48,61,61	1.47	10 (20%)
3	GCF	C	502	-	35,40,40	2.40	4 (11%)	48,61,61	1.59	9 (18%)
3	GCF	A	503	-	35,40,40	2.36	4 (11%)	48,61,61	1.58	9 (18%)
2	PLG	A	501	-	20,20,20	2.70	3 (15%)	25,28,28	2.44	9 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	B	501	-	-	5/12/12/12	0/1/1/1
2	PLG	C	501	-	-	5/12/12/12	0/1/1/1
3	GCF	A	502	-	-	3/27/49/49	0/4/4/4
3	GCF	C	502	-	-	3/27/49/49	0/4/4/4
3	GCF	A	503	-	-	6/27/49/49	0/4/4/4
2	PLG	A	501	-	-	3/12/12/12	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	GCF	C8-C3	-11.38	1.27	1.42
3	A	503	GCF	C8-C3	-11.12	1.27	1.42
3	A	502	GCF	C8-C3	-10.96	1.27	1.42
2	B	501	PLG	C3-C2	9.04	1.49	1.40
2	A	501	PLG	C3-C2	8.04	1.48	1.40
2	C	501	PLG	C3-C2	7.37	1.48	1.40
3	A	502	GCF	O1-C2	6.88	1.44	1.36
3	C	502	GCF	O1-C2	6.69	1.44	1.36
2	A	501	PLG	C5-C4	6.58	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GCF	O1-C2	6.56	1.44	1.36
2	C	501	PLG	C5-C4	6.24	1.49	1.40
2	B	501	PLG	C5-C4	6.20	1.49	1.40
2	B	501	PLG	C3-C4	5.64	1.48	1.40
2	C	501	PLG	C3-C4	5.35	1.48	1.40
2	A	501	PLG	C3-C4	5.00	1.47	1.40
3	A	503	GCF	C17-C16	2.53	1.43	1.39
3	C	502	GCF	N12-N11	2.35	1.42	1.37
3	C	502	GCF	C17-C16	2.22	1.43	1.39
3	A	502	GCF	N12-N11	2.20	1.41	1.37
2	B	501	PLG	OXT-C	-2.15	1.23	1.30
3	A	502	GCF	C17-C16	2.12	1.42	1.39
3	A	503	GCF	N12-N11	2.10	1.41	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	PLG	C4A-N-CA	9.33	122.32	112.58
2	A	501	PLG	C4A-N-CA	7.57	120.49	112.58
2	C	501	PLG	C4A-N-CA	7.56	120.47	112.58
3	C	502	GCF	O1-C2-N7	5.31	114.03	110.22
3	A	502	GCF	O1-C2-N7	4.66	113.57	110.22
3	A	503	GCF	O1-C2-N7	4.52	113.47	110.22
2	A	501	PLG	C4A-C4-C5	3.97	124.12	119.71
2	C	501	PLG	OP4-C5A-C5	3.62	116.26	109.35
3	C	502	GCF	C3-C2-N7	-3.52	123.95	127.47
2	A	501	PLG	OP4-C5A-C5	3.44	115.91	109.35
2	B	501	PLG	OP4-C5A-C5	3.36	115.76	109.35
3	A	503	GCF	F46-C35-C18	-3.25	105.78	112.93
3	A	503	GCF	C5-C4-C3	3.23	110.92	104.34
2	C	501	PLG	OP3-P-OP4	-3.20	98.21	106.73
2	A	501	PLG	C3-C4-C5	-3.12	115.73	118.72
2	C	501	PLG	C6-N1-C2	3.08	124.87	119.17
2	B	501	PLG	OP3-P-OP2	3.06	119.33	107.64
3	A	503	GCF	C6-O1-C2	3.01	121.64	118.38
3	A	502	GCF	C5-C4-C3	3.00	110.45	104.34
3	A	502	GCF	C3-C2-N7	-2.98	124.49	127.47
2	B	501	PLG	C3-C4-C5	-2.97	115.87	118.72
2	A	501	PLG	C6-N1-C2	2.96	124.66	119.17
3	C	502	GCF	C5-C4-C3	2.89	110.22	104.34
2	B	501	PLG	C6-N1-C2	2.84	124.43	119.17
2	B	501	PLG	OP3-P-OP4	-2.78	99.33	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	GCF	C8-C3-C2	2.69	121.20	117.64
3	A	502	GCF	C13-C10-N11	2.68	125.53	119.65
3	C	502	GCF	C15-C14-C4	2.66	115.25	112.40
3	A	502	GCF	F46-C35-C18	-2.65	107.10	112.93
2	A	501	PLG	OP3-P-OP1	2.61	120.92	110.68
3	A	502	GCF	C15-C14-C4	2.60	115.19	112.40
2	A	501	PLG	OP3-P-OP4	-2.59	99.83	106.73
3	A	503	GCF	C10-C5-C6	-2.54	101.33	104.01
2	A	501	PLG	OXT-C-CA	2.54	121.56	112.74
3	C	502	GCF	C36-C14-C4	2.53	115.11	112.40
2	A	501	PLG	C4-C4A-N	2.51	116.27	111.58
3	C	502	GCF	C13-C10-N11	2.50	125.14	119.65
2	C	501	PLG	OP3-P-OP1	2.46	120.31	110.68
3	A	503	GCF	C15-C14-C4	2.43	115.01	112.40
3	C	502	GCF	C10-C5-C6	-2.43	101.44	104.01
2	B	501	PLG	C4A-C4-C5	2.38	122.36	119.71
3	A	503	GCF	C13-C10-N11	2.34	124.79	119.65
3	C	502	GCF	C14-C4-C3	-2.31	106.61	110.32
3	A	502	GCF	C14-C4-C3	-2.27	106.68	110.32
3	A	503	GCF	C3-C2-N7	-2.21	125.26	127.47
3	A	502	GCF	C36-C14-C4	2.19	114.75	112.40
3	A	502	GCF	C10-C5-C6	-2.16	101.73	104.01
2	B	501	PLG	C4-C4A-N	2.15	115.60	111.58
3	A	502	GCF	C8-C3-C2	2.13	120.46	117.64
2	B	501	PLG	OP4-P-OP1	-2.07	100.67	106.47
2	C	501	PLG	C2A-C2-N1	2.06	121.69	117.67
3	C	502	GCF	C8-C3-C2	2.03	120.33	117.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
3	A	502	GCF	C42-C49-C50-C51
2	C	501	PLG	O-C-CA-N
2	C	501	PLG	OXT-C-CA-N
2	C	501	PLG	C4-C4A-N-CA
3	A	502	GCF	C17-C16-C4-C5
3	A	503	GCF	C17-C16-C4-C5

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Mol	Chain	Res	Type	Atoms
3	C	502	GCF	C17-C16-C4-C5
2	A	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
3	A	503	GCF	C49-C50-C51-O58
3	A	502	GCF	C21-C16-C4-C5
3	A	503	GCF	C21-C16-C4-C5
3	A	503	GCF	C17-C16-C4-C14
3	A	503	GCF	C21-C16-C4-C14
3	A	503	GCF	C49-C50-C51-O61
2	A	501	PLG	C5A-OP4-P-OP3
2	B	501	PLG	C5A-OP4-P-OP2
2	B	501	PLG	C5A-OP4-P-OP3
3	C	502	GCF	C49-C50-C51-O58
3	C	502	GCF	C49-C50-C51-O61

There are no ring outliers.

3 monomers are involved in 3 short contacts:

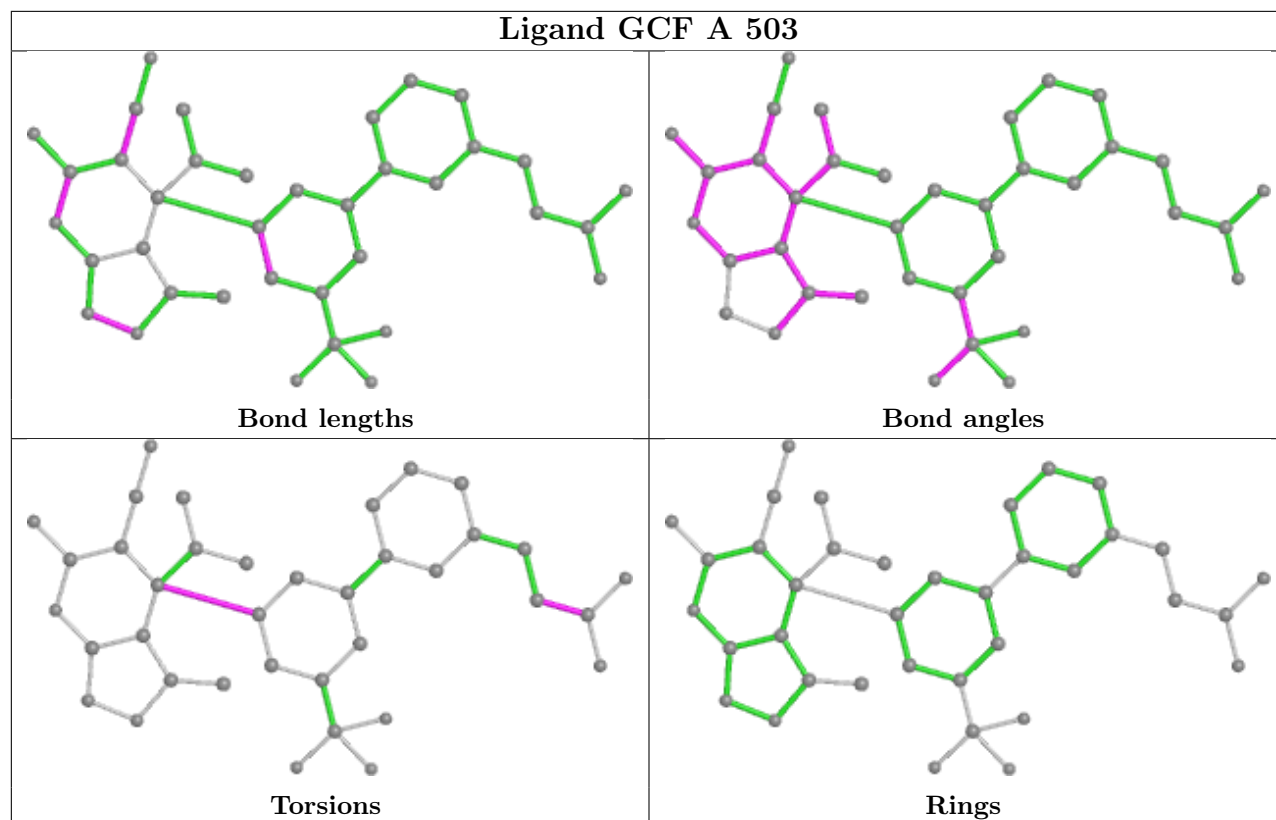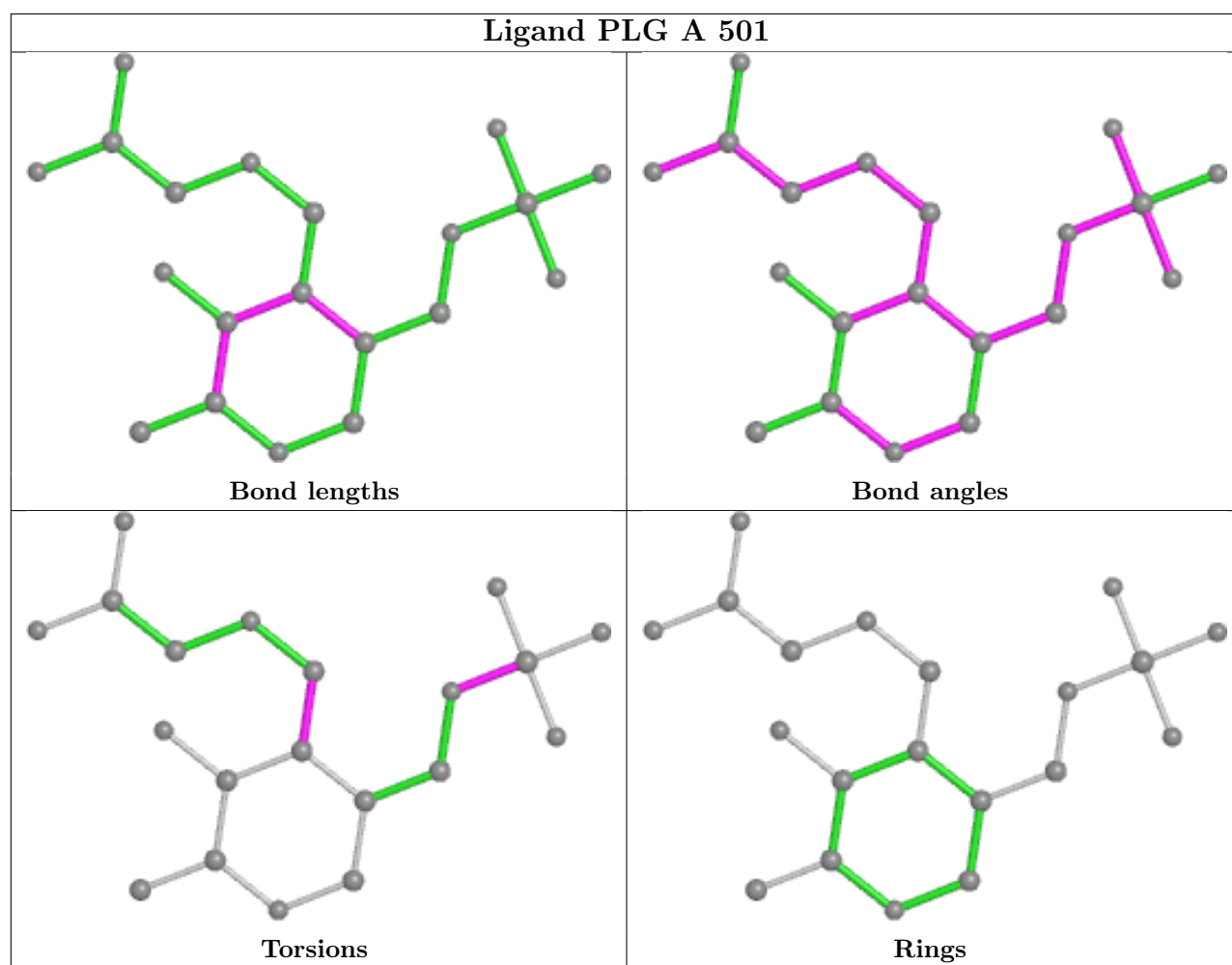| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GCF	1	0
3	C	502	GCF	1	0
3	A	503	GCF	1	0

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 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 PLG B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand PLG C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GCF A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GCF C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GCF A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand PLG A 501

Bond lengths

Bond angles

Torsions

Rings
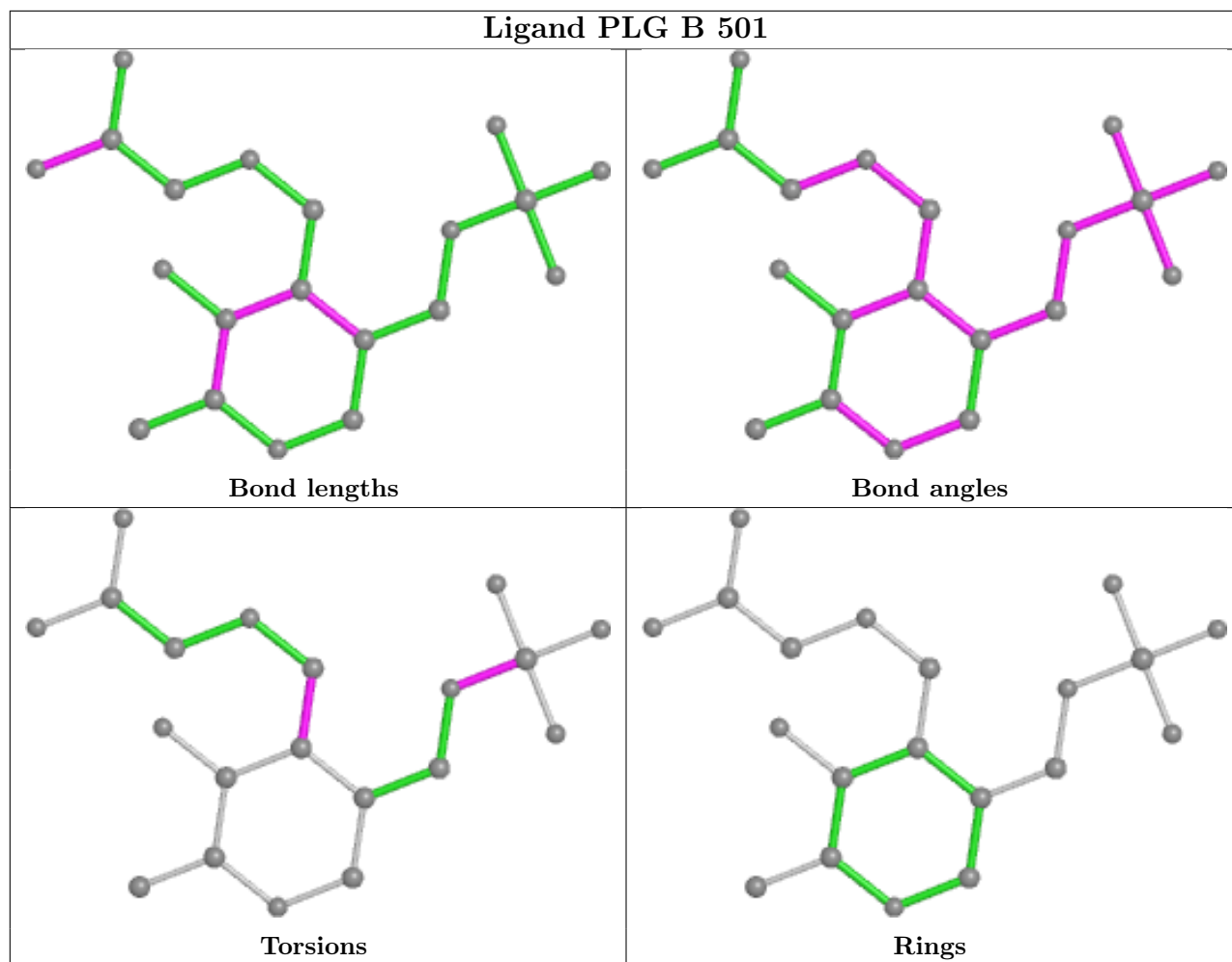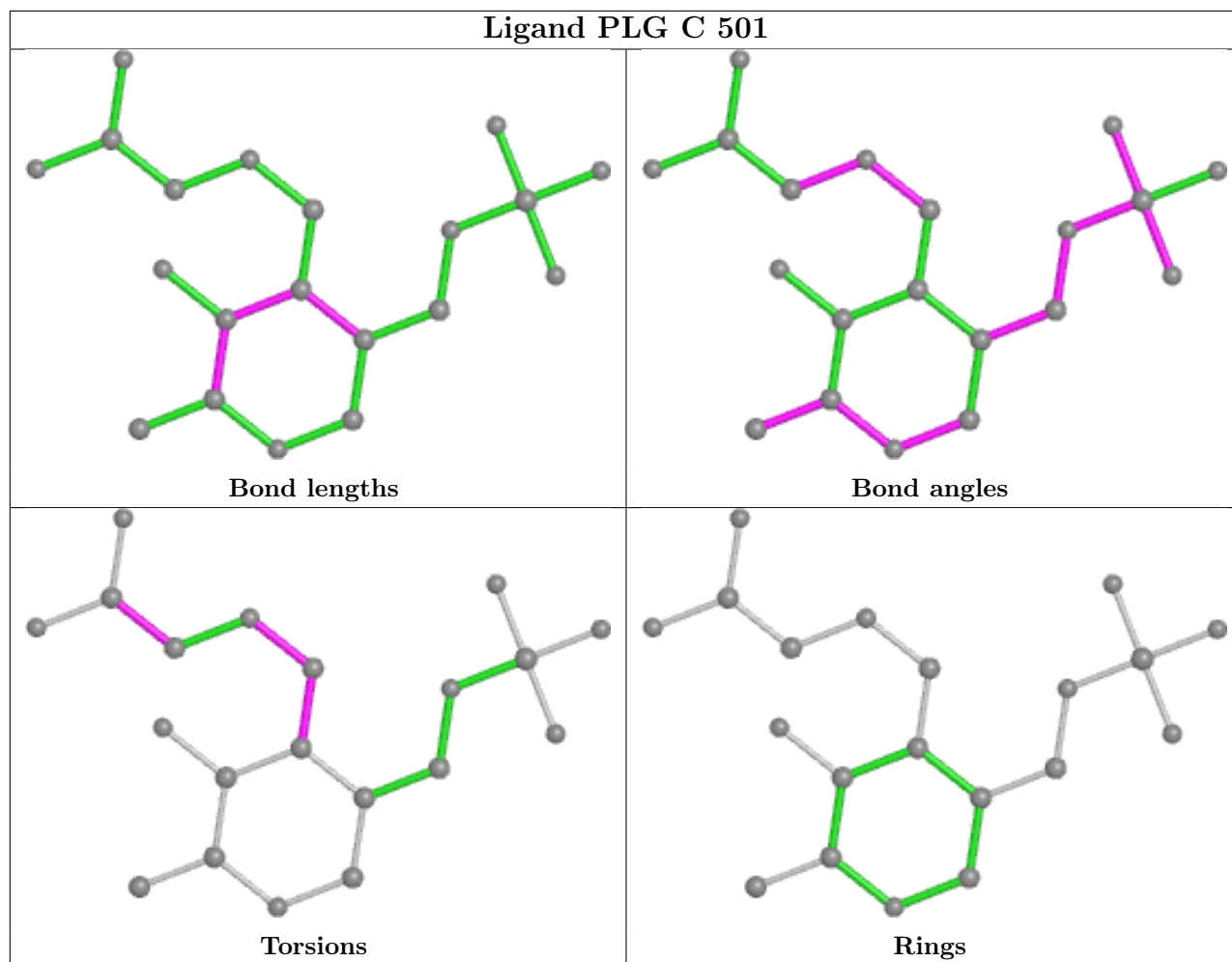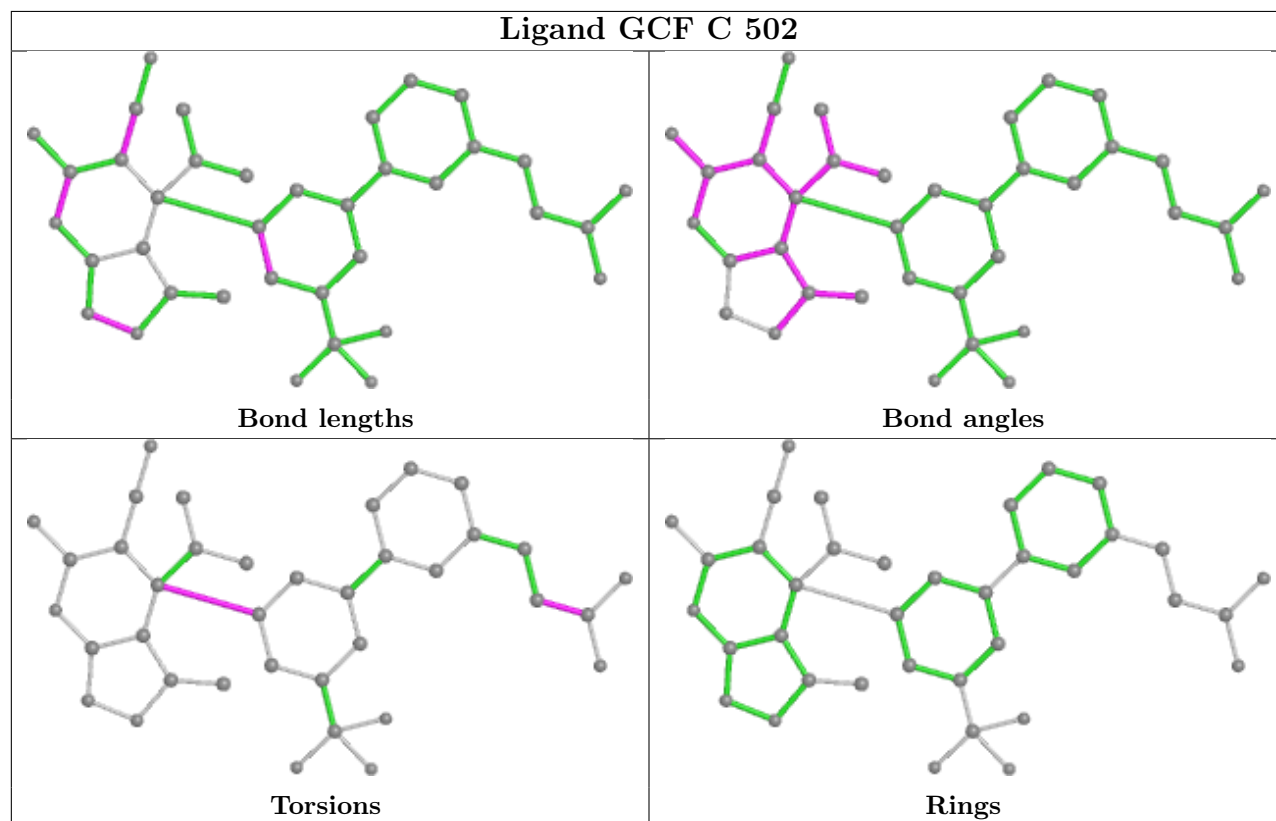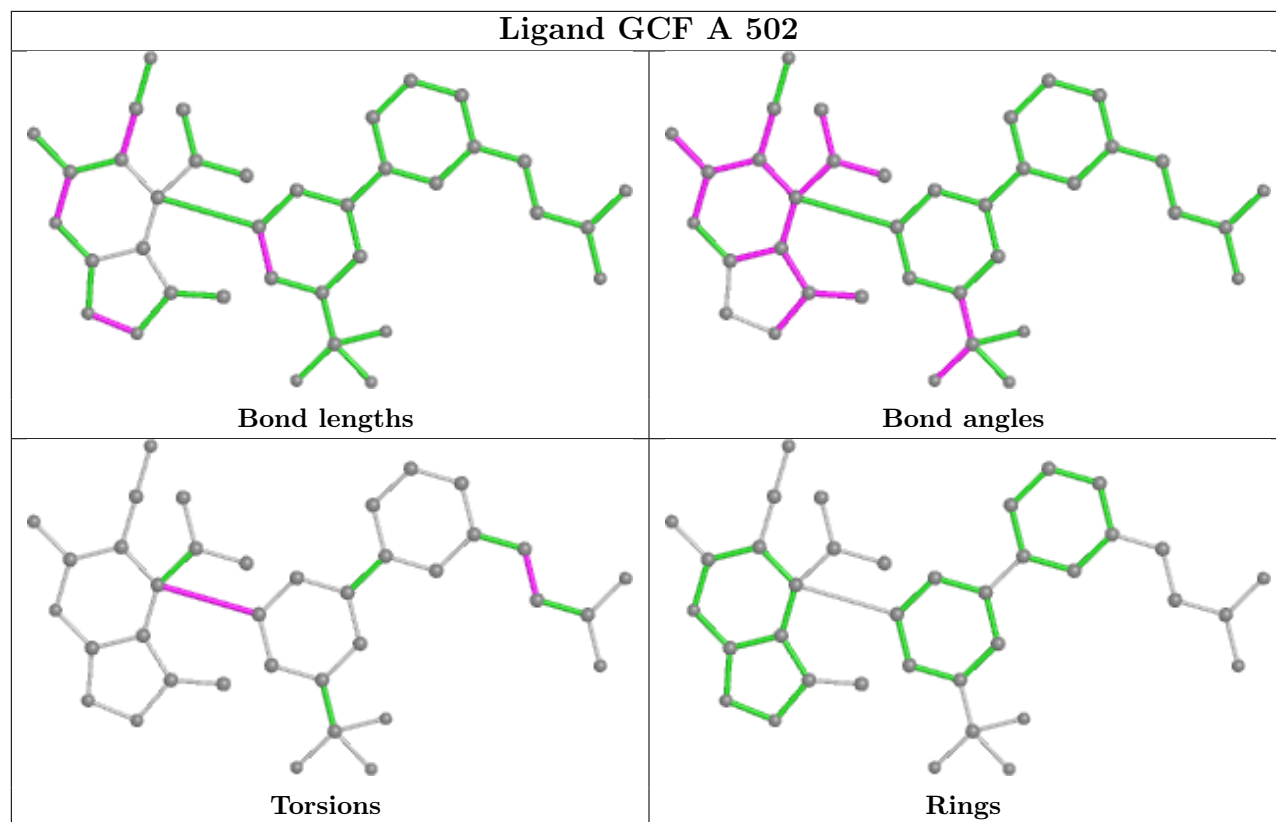
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	442/442 (100%)	0.96	50 (11%)	5	4	14, 28, 45, 63	0
1	B	442/442 (100%)	1.04	56 (12%)	3	3	15, 28, 45, 62	0
1	C	442/442 (100%)	1.02	46 (10%)	6	6	16, 28, 45, 66	0
All	All	1326/1326 (100%)	1.01	152 (11%)	4	4	14, 28, 45, 66	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	VAL	8.7
1	C	364	CYS	8.6
1	B	364	CYS	6.4
1	A	412	LEU	6.4
1	C	138	LYS	6.3
1	B	2	PHE	6.0
1	A	413	VAL	5.9
1	B	365	VAL	5.8
1	B	363	ASP	5.0
1	B	10	ILE	4.9
1	B	442	PRO	4.8
1	A	138	LYS	4.5
1	C	365	VAL	4.5
1	A	366	SER	4.5
1	C	65	GLY	4.3
1	B	198	CYS	4.2
1	A	362	VAL	4.1
1	B	169	MET	4.0
1	C	412	LEU	3.9
1	C	413	VAL	3.8
1	C	257	ILE	3.8
1	C	409	GLY	3.7
1	B	138	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	419	LEU	3.7
1	C	201	VAL	3.7
1	A	363	ASP	3.6
1	B	9	GLN	3.6
1	B	6	PRO	3.6
1	A	6	PRO	3.5
1	A	125	CYS	3.5
1	A	361	ASP	3.5
1	A	419	LEU	3.4
1	A	141	VAL	3.3
1	C	410	LYS	3.3
1	C	125	CYS	3.2
1	B	90	GLU	3.2
1	B	259	GLN	3.2
1	B	28	THR	3.2
1	A	291	PRO	3.1
1	C	10	ILE	3.1
1	B	201	VAL	3.1
1	B	413	VAL	3.1
1	B	177	VAL	3.0
1	A	1	MET	3.0
1	A	165	ALA	3.0
1	A	228	ALA	3.0
1	A	164	ASP	3.0
1	B	410	LYS	3.0
1	B	331	ASP	2.9
1	C	4	ASN	2.9
1	A	435	TRP	2.9
1	C	408	TYR	2.9
1	C	88	SER	2.9
1	B	436	ALA	2.9
1	A	415	PHE	2.9
1	A	317	ASP	2.8
1	C	417	LYS	2.8
1	B	412	LEU	2.8
1	A	202	ASN	2.8
1	A	5	GLU	2.8
1	B	167	ARG	2.8
1	A	64	TYR	2.8
1	C	389	PHE	2.7
1	B	191	TYR	2.7
1	B	193	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	434	THR	2.7
1	B	137	GLU	2.7
1	B	23	LYS	2.7
1	B	8	GLU	2.7
1	A	68	ASP	2.6
1	C	418	GLY	2.6
1	B	27	GLU	2.6
1	C	7	LEU	2.6
1	B	16	ASP	2.6
1	C	438	ALA	2.6
1	B	392	ASP	2.6
1	B	155	CYS	2.6
1	B	335	PHE	2.6
1	A	203	ALA	2.6
1	B	217	ALA	2.6
1	A	434	THR	2.5
1	C	198	CYS	2.5
1	B	415	PHE	2.5
1	C	23	LYS	2.5
1	A	29	ILE	2.5
1	C	333	ARG	2.5
1	C	8	GLU	2.5
1	C	296	TYR	2.5
1	A	409	GLY	2.5
1	A	2	PHE	2.5
1	A	60	LYS	2.5
1	B	176	LYS	2.5
1	A	408	TYR	2.5
1	B	65	GLY	2.5
1	C	431	GLU	2.4
1	B	411	LYS	2.4
1	A	66	GLY	2.4
1	A	169	MET	2.4
1	A	402	VAL	2.4
1	A	430	GLN	2.4
1	A	166	VAL	2.4
1	C	60	LYS	2.4
1	B	160	TYR	2.4
1	B	219	ASN	2.4
1	A	116	LYS	2.4
1	C	399	LYS	2.4
1	C	77	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	189	ILE	2.3
1	B	426	GLN	2.3
1	C	116	LYS	2.3
1	C	419	LEU	2.3
1	B	206	PHE	2.3
1	C	193	GLN	2.3
1	A	22	GLU	2.3
1	C	363	ASP	2.3
1	C	225	PHE	2.3
1	A	244	SER	2.3
1	B	332	LEU	2.3
1	B	256	GLY	2.3
1	B	5	GLU	2.3
1	A	57	GLY	2.2
1	C	64	TYR	2.2
1	C	169	MET	2.2
1	C	402	VAL	2.2
1	B	89	ASP	2.2
1	C	249	PHE	2.2
1	C	434	THR	2.2
1	B	139	LYS	2.2
1	B	414	ASP	2.2
1	B	174	LYS	2.2
1	A	37	LEU	2.2
1	A	9	GLN	2.2
1	A	433	VAL	2.1
1	C	203	ALA	2.1
1	C	366	SER	2.1
1	A	8	GLU	2.1
1	A	348	ALA	2.1
1	C	173	PHE	2.1
1	B	435	TRP	2.1
1	C	430	GLN	2.1
1	B	181	GLY	2.1
1	C	155	CYS	2.1
1	C	436	ALA	2.1
1	B	166	VAL	2.1
1	A	224	PRO	2.1
1	C	353	LEU	2.0
1	B	172	SER	2.0
1	A	167	ARG	2.0
1	A	347	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	178	ILE	2.0
1	A	256	GLY	2.0
1	B	395	ALA	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 monosaccharides 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	CL	C	503	1/1	0.73	0.25	17,17,17,17	1
4	CL	A	504	1/1	0.79	0.17	25,25,25,25	0
3	GCF	A	503	37/37	0.81	0.19	21,24,41,44	0
3	GCF	C	502	37/37	0.82	0.21	23,26,42,44	0
2	PLG	B	501	20/20	0.84	0.22	17,19,22,22	0
3	GCF	A	502	37/37	0.84	0.19	22,25,43,46	0
2	PLG	C	501	20/20	0.90	0.19	17,19,20,22	0
2	PLG	A	501	20/20	0.92	0.17	16,18,20,20	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.
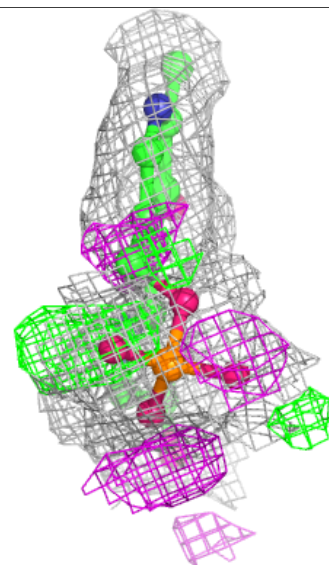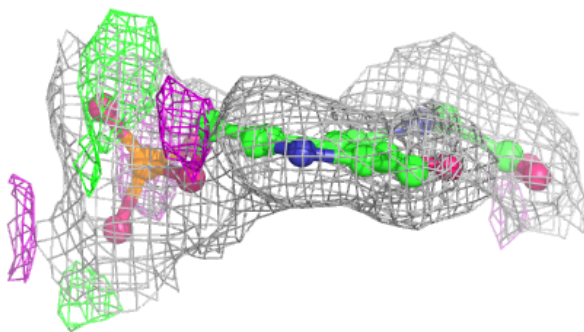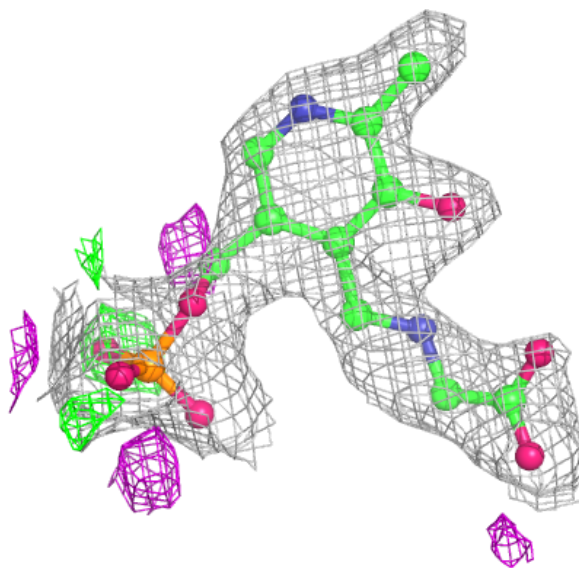
Electron density around GCF A 503:

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

Electron density around GCF C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
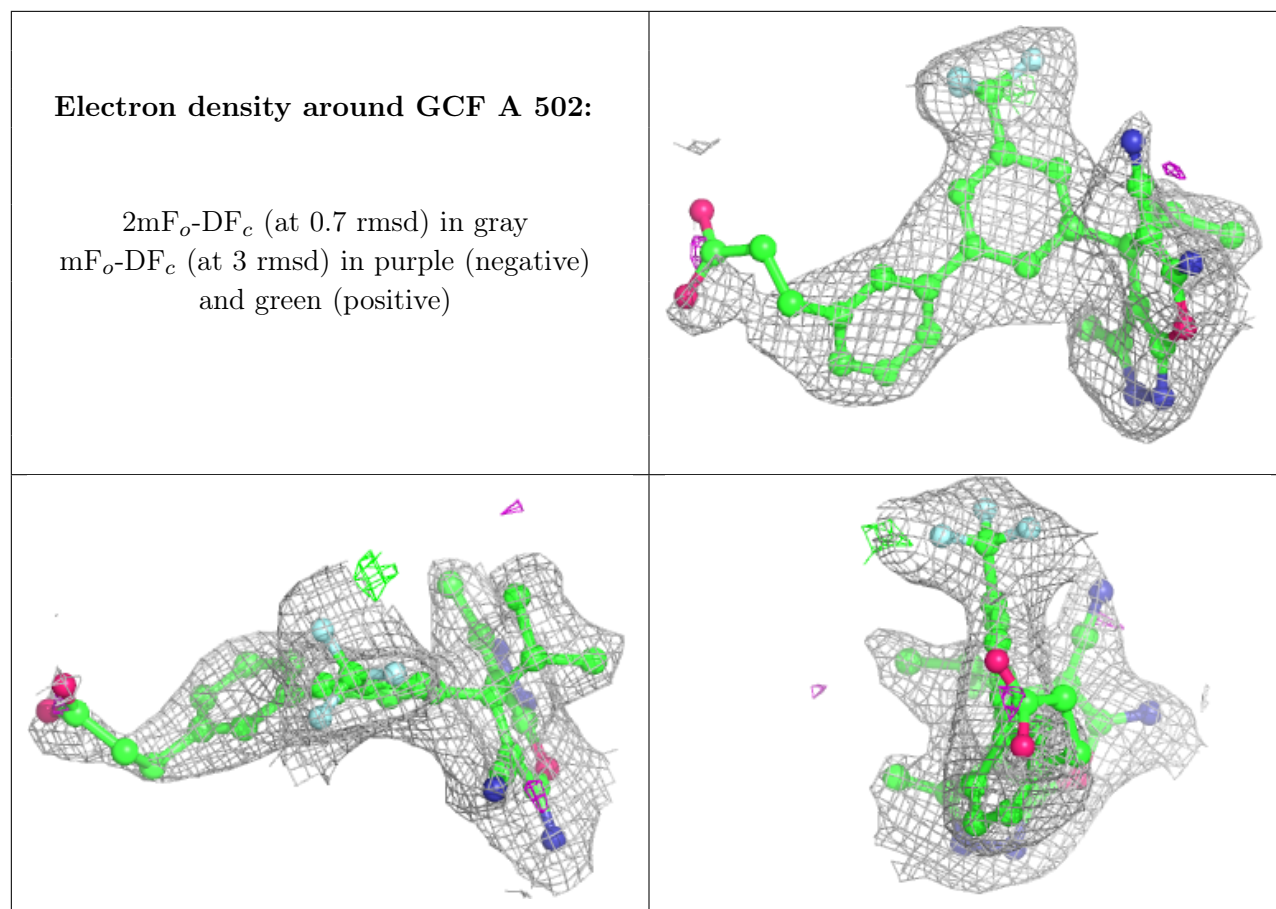and green (positive)
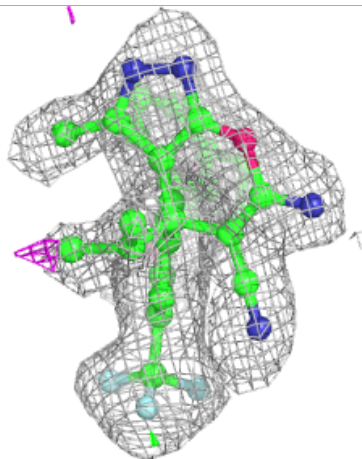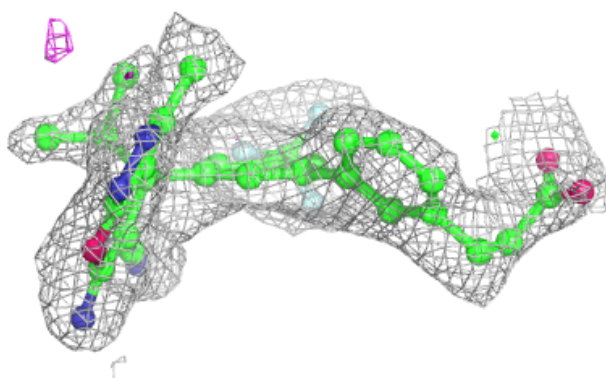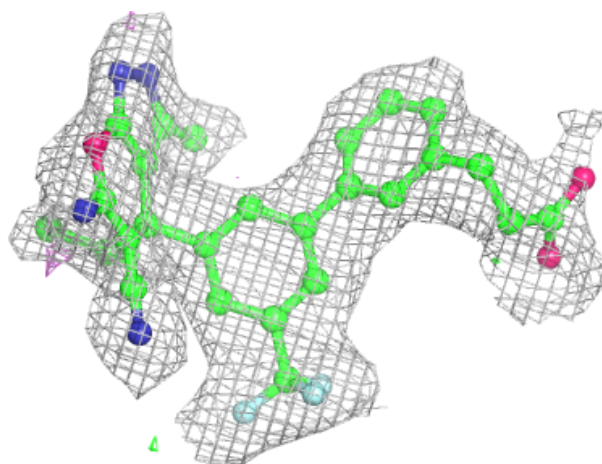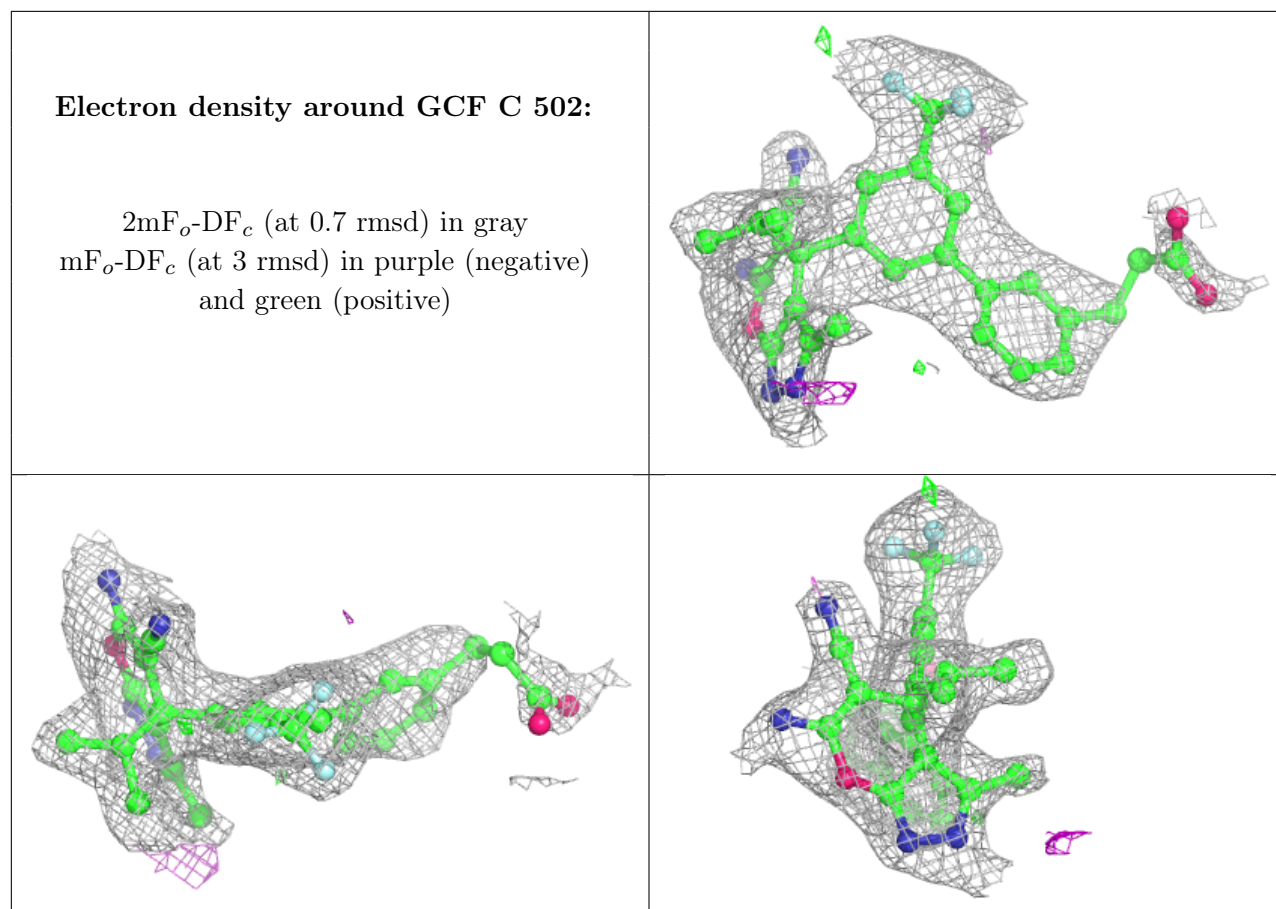
Electron density around PLG B 501:

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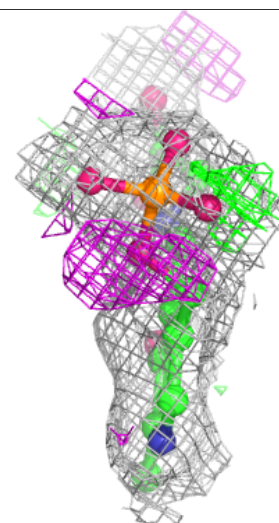mF_o-DF_c (at 3 rmsd) in purple (negative)
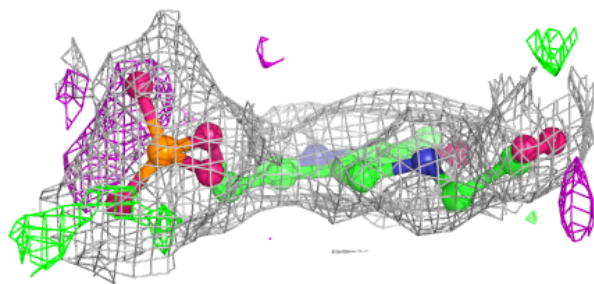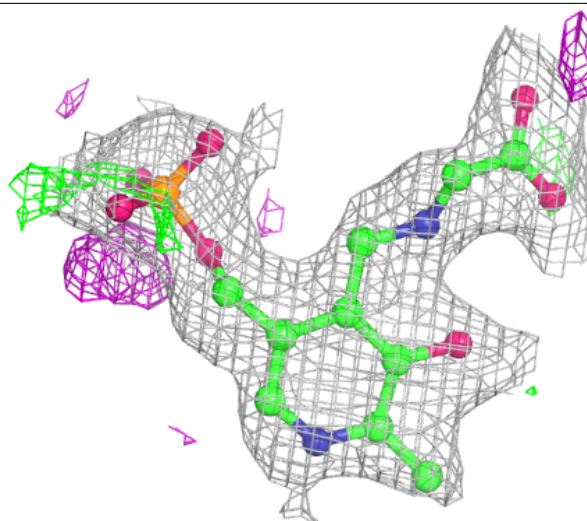and green (positive)

Electron density around GCF A 502:

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

Electron density around PLG C 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
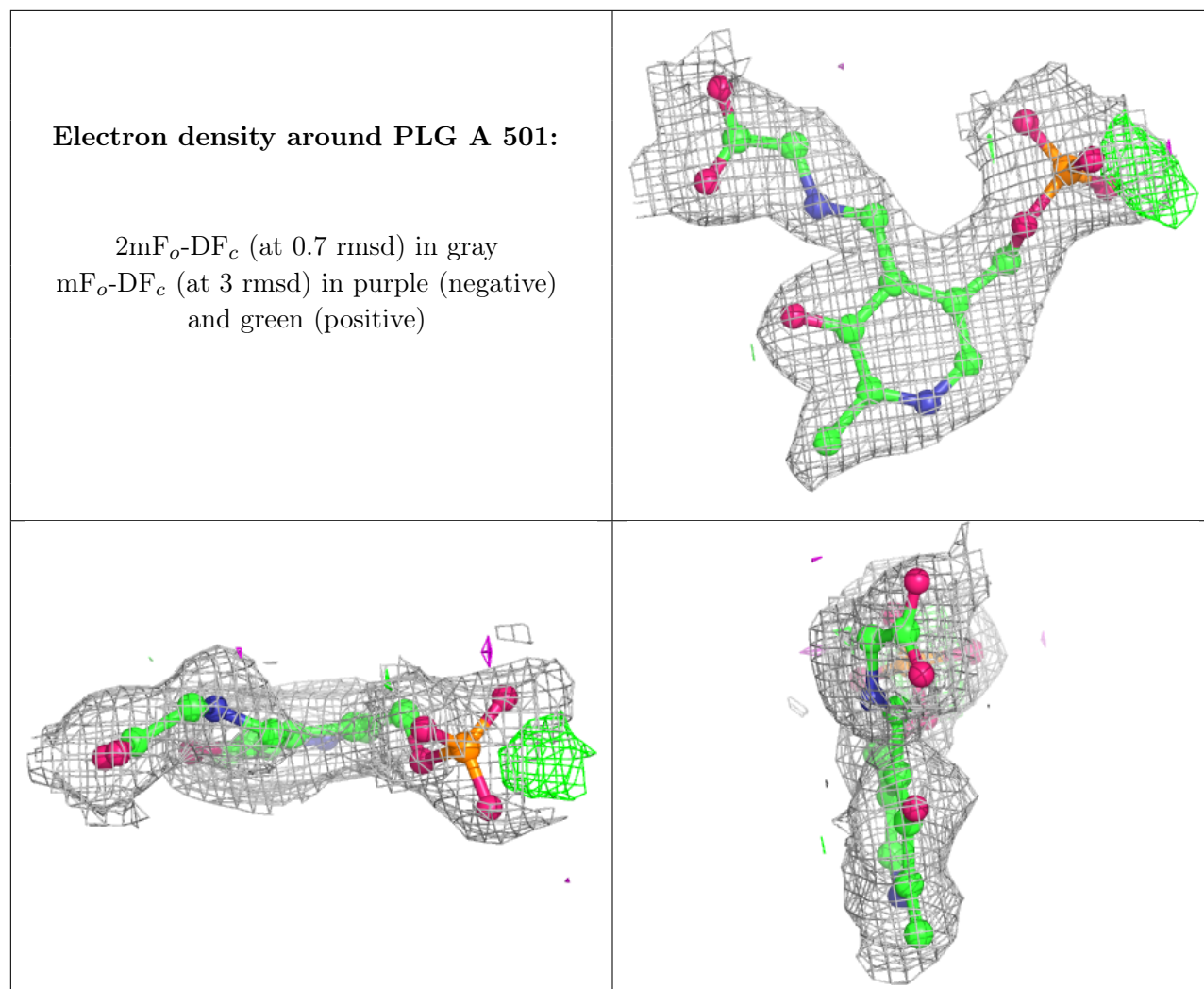mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PLG A 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.