Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 11:27 PM JST

PDB ID	:	5YG0
Title	:	Plasmodium vivax SHMT bound with PLP-glycine and GS657
Authors	:	Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Schwertz, G.; Diederich, F.
Deposited on	:	2017-09-22
Resolution	:	2.33 Å(reported)

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

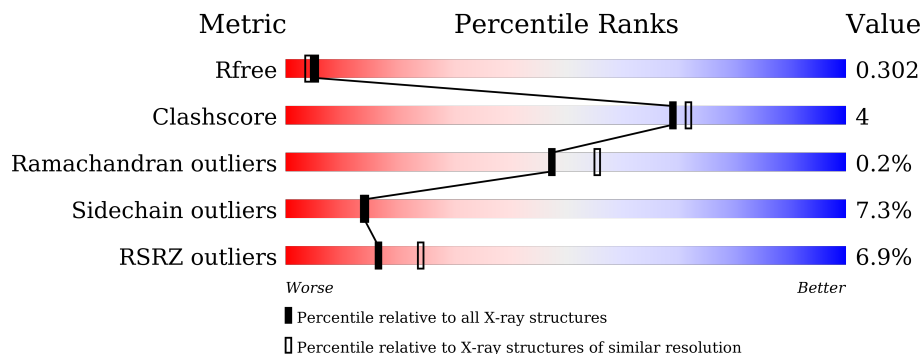|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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:
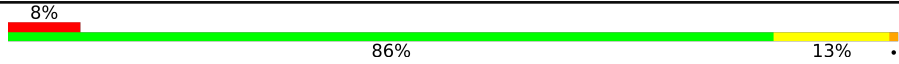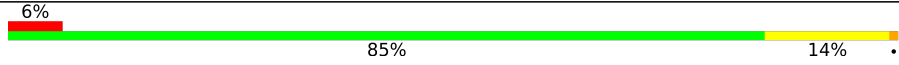*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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		0.302
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		7.3%
RSRZ outliers		6.9%

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	8% / 86% / 13% / ·
1	B	442	6% / 85% / 14% / ·
1	C	442	6% / 85% / 14% / ·

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10777 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.

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: $C_{10}H_{15}N_2O_7P$).

PLG
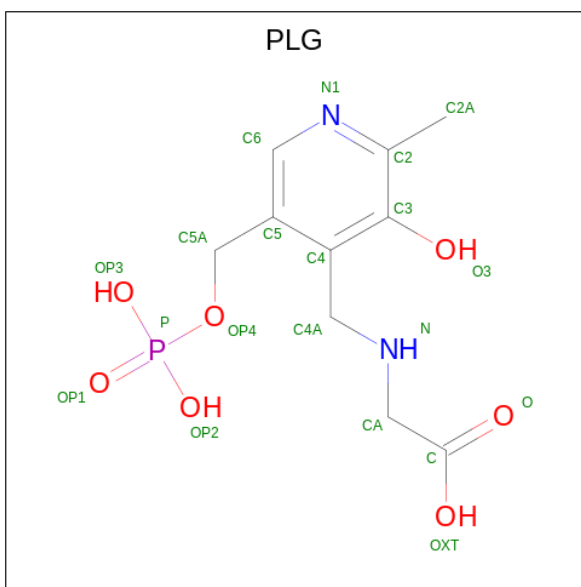
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 2-[1-[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]piperidin-4-yl]ethanoic acid (three-letter code: 8UR) (formula: $C_{25}H_{28}F_3N_5O_3$).
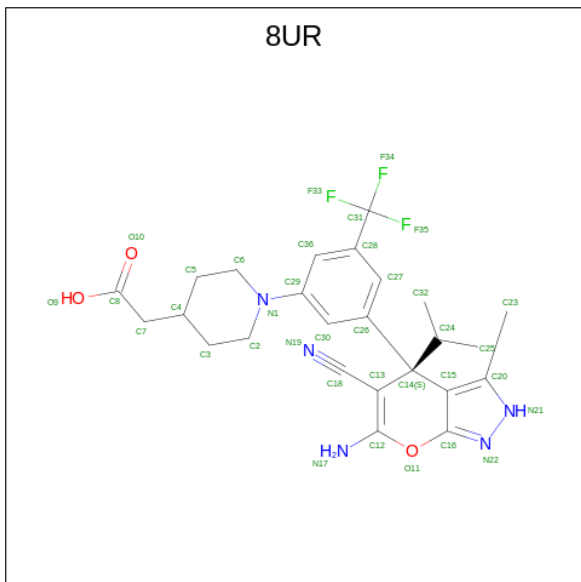
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	25	3	5	3		
3	B	1	Total	C	F	N	O	0	0
			36	25	3	5	3		
3	C	1	Total	C	F	N	O	0	0
			36	25	3	5	3		

- 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	85	Total	O	0	0
			85	85		
5	B	73	Total	O	0	0
			73	73		
5	C	75	Total	O	0	0
			75	75		

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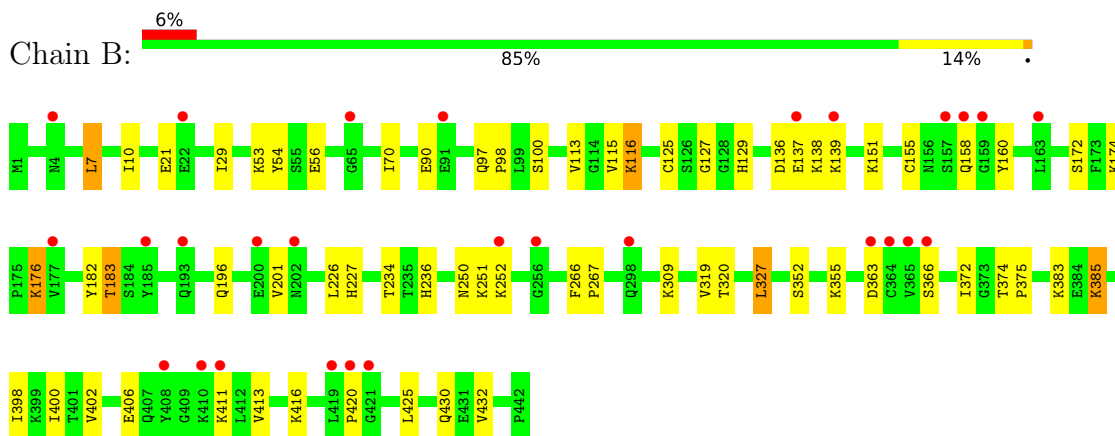 = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
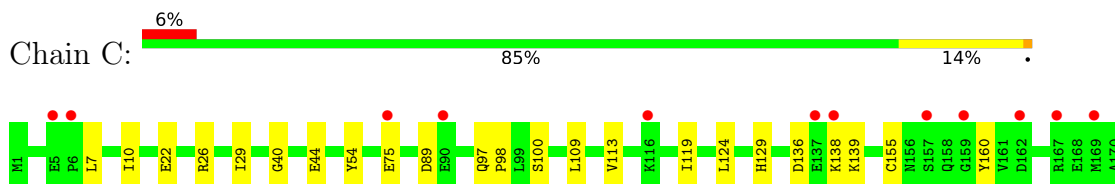
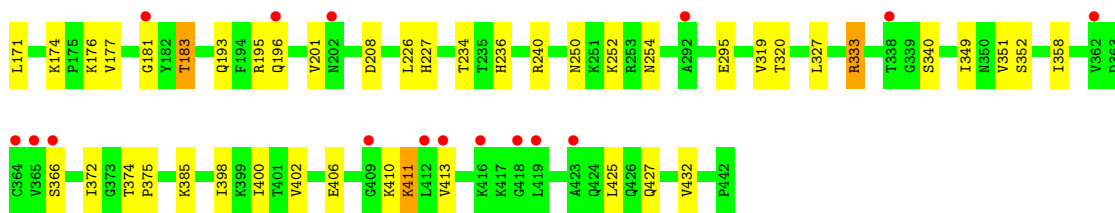• Molecule 1: Serine hydroxymethyltransferase
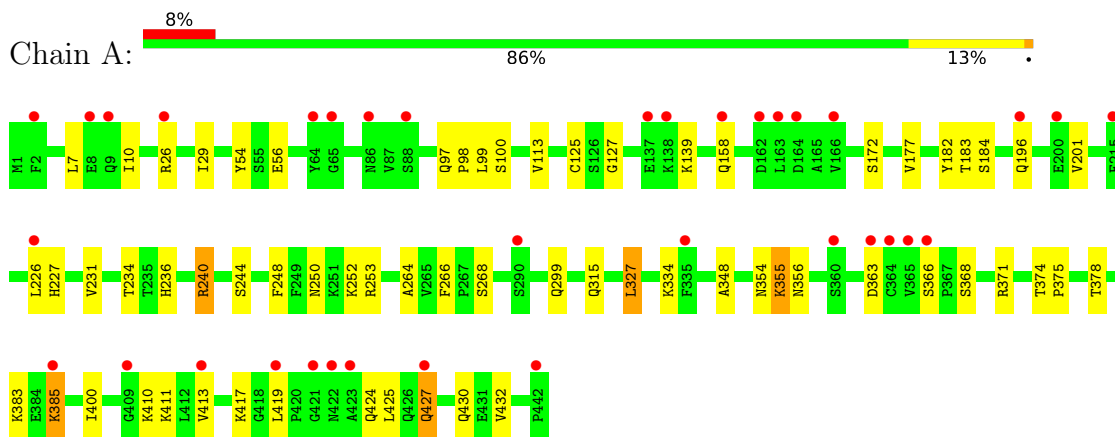
Chain A:

• Molecule 1: Serine hydroxymethyltransferase

Chain B:

• Molecule 1: Serine hydroxymethyltransferase

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.56Å 58.62Å 233.05Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.33 29.09 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.33) 96.3 (29.09-2.33)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.88 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.241 , 0.311 0.241 , 0.302	Depositor DCC
R_{free} test set	5606 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 6.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.022 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.023 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.469 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.468 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10777	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: PLG, 8UR, CL

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	0.57	0/3521	0.73	2/4754 (0.0%)
1	B	0.58	0/3521	0.72	0/4754
1	C	0.57	0/3521	0.71	0/4754
All	All	0.58	0/10563	0.72	2/14262 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	253	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	23	0
1	B	3458	0	3477	25	0
1	C	3458	0	3477	26	0
2	A	20	0	11	0	0
2	B	20	0	11	1	0
2	C	20	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	36	0	0	1	0
3	B	36	0	0	1	0
3	C	36	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	85	0	0	2	0
5	B	73	0	0	1	0
5	C	75	0	0	1	0
All	All	10777	0	10464	77	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 (77) 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:113:VAL:HG12	1:B:176:LYS:HB3	1.73	0.69
1:A:348:ALA:HB2	1:A:419:LEU:HD23	1.77	0.67
1:C:155:CYS:HB2	1:C:160:TYR:O	2.00	0.61
1:C:171:LEU:O	1:C:174:LYS:HE2	2.04	0.57
1:C:113:VAL:HG12	1:C:176:LYS:HB3	1.85	0.57
1:C:319:VAL:HG12	1:C:320:THR:HG23	1.87	0.57
1:B:53:LYS:HG2	1:B:70:ILE:HG13	1.87	0.56
1:C:40:GLY:O	1:C:44:GLU:HG3	2.07	0.55
1:A:234:THR:HB	1:A:236:HIS:CE1	2.43	0.54
1:B:29:ILE:HD12	1:B:432:VAL:HG13	1.89	0.54
1:B:319:VAL:HG12	1:B:320:THR:HG23	1.89	0.53
1:B:234:THR:HB	1:B:236:HIS:CE1	2.44	0.53
3:B:502:8UR:C18	3:B:502:8UR:C27	2.86	0.53
1:C:427:GLN:HE21	1:C:427:GLN:HA	1.74	0.53
1:C:333:ARG:HD3	1:C:358:ILE:HD11	1.90	0.52
3:C:502:8UR:C18	3:C:502:8UR:C27	2.87	0.52
1:A:7:LEU:HA	1:A:10:ILE:HG22	1.91	0.52
1:A:299:GLN:HG3	1:A:378:THR:HG23	1.91	0.51
1:B:56:GLU:HG2	1:B:266:PHE:CZ	2.46	0.51
1:C:234:THR:HB	1:C:236:HIS:CE1	2.46	0.51
1:C:201:VAL:O	1:C:201:VAL:HG12	2.12	0.50
3:A:502:8UR:C27	3:A:502:8UR:C18	2.89	0.50
1:A:29:ILE:HD12	1:A:432:VAL:HG13	1.93	0.50
1:B:327:LEU:C	1:B:327:LEU:HD12	2.34	0.48
1:A:400:ILE:HG21	1:A:425:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LYS:HD3	1:C:201:VAL:HG13	1.96	0.48
1:A:240:ARG:HD3	5:A:677:HOH:O	2.14	0.48
1:A:427:GLN:HE21	1:A:427:GLN:HA	1.78	0.47
1:C:240:ARG:HD3	5:C:673:HOH:O	2.14	0.47
1:B:7:LEU:HA	1:B:10:ILE:HG22	1.96	0.47
1:C:195:ARG:HB2	1:C:227:HIS:HB3	1.97	0.47
1:A:56:GLU:HG2	1:A:266:PHE:CE1	2.51	0.46
1:A:411:LYS:HE2	1:A:411:LYS:HA	1.98	0.46
1:C:374:THR:N	1:C:375:PRO:CD	2.79	0.46
1:A:315:GLN:O	1:A:334:LYS:NZ	2.43	0.45
1:C:427:GLN:HA	1:C:427:GLN:NE2	2.31	0.45
1:B:400:ILE:HG21	1:B:425:LEU:HD21	1.99	0.45
1:C:7:LEU:HA	1:C:10:ILE:HG22	1.98	0.45
1:B:113:VAL:HG12	1:B:176:LYS:HD2	1.99	0.45
1:B:226:LEU:HB2	1:B:227:HIS:CD2	2.52	0.45
1:C:129:HIS:HA	1:C:183:THR:HG21	1.99	0.44
1:B:174:LYS:CD	1:B:201:VAL:CG1	2.95	0.44
1:C:398:ILE:O	1:C:402:VAL:HG23	2.18	0.44
1:B:374:THR:N	1:B:375:PRO:CD	2.81	0.44
1:A:226:LEU:HB2	1:A:227:HIS:CD2	2.53	0.44
1:A:264:ALA:HA	1:A:268:SER:HB2	1.99	0.44
1:C:109:LEU:HD22	1:C:119:ILE:HG21	2.00	0.44
1:C:411:LYS:HA	1:C:411:LYS:CE	2.48	0.44
1:A:327:LEU:HD12	1:A:327:LEU:C	2.38	0.43
1:B:183:THR:HB	2:B:501:PLG:O3	2.19	0.43
1:A:374:THR:N	1:A:375:PRO:CD	2.81	0.43
1:B:383:LYS:CB	1:B:385:LYS:HE3	2.48	0.43
1:B:129:HIS:HA	1:B:183:THR:HG21	2.00	0.43
1:A:97:GLN:N	1:A:98:PRO:CD	2.82	0.43
1:A:99:LEU:HD12	5:A:668:HOH:O	2.18	0.43
1:B:97:GLN:N	1:B:98:PRO:CD	2.82	0.43
1:B:266:PHE:CD1	1:B:267:PRO:HA	2.54	0.42
1:C:226:LEU:HB2	1:C:227:HIS:CD2	2.54	0.42
1:A:354:ASN:ND2	1:A:355:LYS:O	2.51	0.42
1:B:115:VAL:O	1:B:116:LYS:HG2	2.18	0.42
1:A:184:SER:HB3	1:A:371:ARG:HD3	2.02	0.42
1:B:398:ILE:O	1:B:402:VAL:HG23	2.20	0.42
1:C:29:ILE:HD12	1:C:432:VAL:HG13	2.00	0.42
1:C:97:GLN:N	1:C:98:PRO:CD	2.83	0.42
1:A:113:VAL:CG1	1:A:177:VAL:HG23	2.50	0.41
1:A:231:VAL:HB	1:A:248:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HD2	1:B:201:VAL:CG1	2.50	0.41
1:A:383:LYS:HB2	1:A:385:LYS:HE3	2.01	0.41
1:C:113:VAL:CG1	1:C:177:VAL:HG23	2.50	0.41
1:B:155:CYS:HB2	1:B:160:TYR:O	2.20	0.41
1:B:416:LYS:O	1:B:420:PRO:HD3	2.21	0.41
1:A:127:GLY:O	1:A:182:TYR:HB3	2.21	0.41
1:B:251:LYS:HG2	5:B:671:HOH:O	2.20	0.40
1:C:349:ILE:HG13	1:C:351:VAL:HG23	2.03	0.40
1:C:400:ILE:HG21	1:C:425:LEU:HD21	2.02	0.40
1:B:127:GLY:O	1:B:182:TYR:HB3	2.21	0.40
1:C:181:GLY:HA3	1:C:208:ASP:O	2.21	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%)	422 (96%)	17 (4%)	1 (0%)	47	55
1	B	440/442 (100%)	426 (97%)	13 (3%)	1 (0%)	47	55
1	C	440/442 (100%)	423 (96%)	17 (4%)	0	100	100
All	All	1320/1326 (100%)	1271 (96%)	47 (4%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	CYS
1	A	125	CYS

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%)	356 (93%)	25 (7%)	16	18
1	B	381/381 (100%)	351 (92%)	30 (8%)	12	12
1	C	381/381 (100%)	353 (93%)	28 (7%)	14	14
All	All	1143/1143 (100%)	1060 (93%)	83 (7%)	14	14

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	54	TYR
1	A	100	SER
1	A	139	LYS
1	A	158	GLN
1	A	172	SER
1	A	183	THR
1	A	196	GLN
1	A	201	VAL
1	A	244	SER
1	A	250	ASN
1	A	252	LYS
1	A	327	LEU
1	A	355	LYS
1	A	356	ASN
1	A	363	ASP
1	A	366	SER
1	A	368	SER
1	A	385	LYS
1	A	410	LYS
1	A	413	VAL
1	A	417	LYS
1	A	424	GLN
1	A	427	GLN
1	A	430	GLN
1	B	7	LEU

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Mol	Chain	Res	Type
1	B	21	GLU
1	B	54	TYR
1	B	90	GLU
1	B	100	SER
1	B	116	LYS
1	B	136	ASP
1	B	137	GLU
1	B	138	LYS
1	B	139	LYS
1	B	151	LYS
1	B	158	GLN
1	B	172	SER
1	B	176	LYS
1	B	183	THR
1	B	196	GLN
1	B	250	ASN
1	B	252	LYS
1	B	309	LYS
1	B	327	LEU
1	B	352	SER
1	B	355	LYS
1	B	363	ASP
1	B	366	SER
1	B	372	ILE
1	B	385	LYS
1	B	406	GLU
1	B	411	LYS
1	B	413	VAL
1	B	430	GLN
1	C	22	GLU
1	C	26	ARG
1	C	54	TYR
1	C	75	GLU
1	C	89	ASP
1	C	100	SER
1	C	124	LEU
1	C	136	ASP
1	C	138	LYS
1	C	139	LYS
1	C	183	THR
1	C	193	GLN
1	C	196	GLN

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	252	LYS
1	C	254	ASN
1	C	295	GLU
1	C	327	LEU
1	C	333	ARG
1	C	340	SER
1	C	352	SER
1	C	366	SER
1	C	372	ILE
1	C	385	LYS
1	C	406	GLU
1	C	410	LYS
1	C	411	LYS
1	C	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	A	424	GLN
1	A	427	GLN
1	B	193	GLN
1	B	227	HIS
1	B	347	ASN
1	C	227	HIS
1	C	424	GLN
1	C	427	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	#$|Z| > 2$
3	8UR	C	502	-	34,39,39	2.40	3 (8%)	46,60,60	2.05	12 (26%)
3	8UR	A	502	-	34,39,39	2.48	2 (5%)	46,60,60	2.17	11 (23%)
2	PLG	A	501	-	20,20,20	2.90	3 (15%)	25,28,28	2.65	7 (28%)
3	8UR	B	502	-	34,39,39	2.35	2 (5%)	46,60,60	2.14	12 (26%)
2	PLG	B	501	-	20,20,20	2.83	3 (15%)	25,28,28	2.54	8 (32%)
2	PLG	C	501	-	20,20,20	2.73	3 (15%)	25,28,28	2.11	5 (20%)

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
3	8UR	C	502	-	-	6/26/58/58	0/4/4/4
3	8UR	A	502	-	-	4/26/58/58	0/4/4/4
2	PLG	A	501	-	-	5/12/12/12	0/1/1/1
3	8UR	B	502	-	-	4/26/58/58	0/4/4/4
2	PLG	B	501	-	-	8/12/12/12	0/1/1/1
2	PLG	C	501	-	-	8/12/12/12	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	8UR	C18-C13	-11.33	1.27	1.42
3	C	502	8UR	C18-C13	-11.27	1.27	1.42
3	B	502	8UR	C18-C13	-10.24	1.28	1.42
2	B	501	PLG	C3-C2	8.43	1.49	1.40
2	A	501	PLG	C3-C2	8.38	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLG	C3-C2	7.95	1.48	1.40
3	B	502	8UR	O11-C12	7.63	1.45	1.36
3	A	502	8UR	O11-C12	7.50	1.45	1.36
2	A	501	PLG	C5-C4	6.82	1.50	1.40
3	C	502	8UR	O11-C12	6.74	1.44	1.36
2	B	501	PLG	C3-C4	6.41	1.49	1.40
2	A	501	PLG	C3-C4	6.27	1.49	1.40
2	C	501	PLG	C3-C4	6.19	1.49	1.40
2	C	501	PLG	C5-C4	6.11	1.49	1.40
2	B	501	PLG	C5-C4	6.08	1.49	1.40
3	C	502	8UR	N22-N21	2.24	1.42	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PLG	C4A-N-CA	9.49	122.48	112.58
2	B	501	PLG	C4A-N-CA	8.71	121.67	112.58
3	B	502	8UR	C2-N1-C6	8.29	129.82	111.52
3	A	502	8UR	C2-N1-C6	7.29	127.61	111.52
3	C	502	8UR	C2-N1-C6	7.22	127.45	111.52
2	C	501	PLG	C4A-N-CA	7.12	120.02	112.58
3	A	502	8UR	O11-C12-N17	6.44	114.84	110.22
3	B	502	8UR	O11-C12-N17	5.87	114.44	110.22
3	C	502	8UR	C3-C4-C7	-4.46	106.34	111.52
2	B	501	PLG	C4A-C4-C3	4.35	124.70	120.04
3	B	502	8UR	C13-C12-N17	-4.34	123.12	127.47
3	A	502	8UR	C13-C12-N17	-4.29	123.18	127.47
3	C	502	8UR	O11-C12-N17	4.22	113.25	110.22
2	A	501	PLG	OP2-P-OP4	-3.90	96.35	106.73
3	C	502	8UR	C25-C24-C14	3.80	116.47	112.40
3	A	502	8UR	C3-C4-C7	-3.75	107.16	111.52
2	C	501	PLG	OP2-P-OP4	-3.48	97.46	106.73
2	A	501	PLG	C3-C4-C5	-3.41	115.44	118.72
2	C	501	PLG	C6-N1-C2	3.30	125.28	119.17
2	A	501	PLG	C4A-C4-C5	3.29	123.37	119.71
2	B	501	PLG	OP3-P-OP2	3.29	120.22	107.64
2	A	501	PLG	OP4-C5A-C5	3.22	115.49	109.35
2	B	501	PLG	OP4-P-OP1	-3.08	97.84	106.47
2	B	501	PLG	C6-N1-C2	3.07	124.84	119.17
3	B	502	8UR	C15-C14-C13	3.00	110.44	104.34
3	C	502	8UR	C36-C29-N1	-2.96	118.15	121.33
3	B	502	8UR	C20-C15-C16	-2.95	100.89	104.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PLG	C6-N1-C2	2.90	124.54	119.17
3	C	502	8UR	C13-C12-N17	-2.87	124.60	127.47
3	C	502	8UR	C23-C20-N21	2.81	125.82	119.65
3	A	502	8UR	C15-C14-C13	2.80	110.04	104.34
3	B	502	8UR	C23-C20-N21	2.80	125.79	119.65
3	A	502	8UR	C20-C15-C16	-2.77	101.08	104.01
2	B	501	PLG	OXT-C-CA	2.70	122.11	112.74
2	C	501	PLG	C4A-C4-C3	2.66	122.89	120.04
2	C	501	PLG	OP4-C5A-C5	2.58	114.27	109.35
3	C	502	8UR	F34-C31-F35	2.58	115.19	105.72
3	A	502	8UR	C32-C24-C14	2.54	115.12	112.40
3	C	502	8UR	C20-C15-C16	-2.54	101.33	104.01
2	B	501	PLG	OP4-C5A-C5	2.48	114.08	109.35
3	A	502	8UR	C36-C29-N1	-2.47	118.68	121.33
3	C	502	8UR	C15-C14-C13	2.46	109.35	104.34
3	A	502	8UR	C23-C20-N21	2.37	124.87	119.65
3	B	502	8UR	C3-C4-C7	-2.37	108.77	111.52
3	B	502	8UR	F34-C31-F35	2.36	114.37	105.72
3	B	502	8UR	C25-C24-C14	2.33	114.90	112.40
2	B	501	PLG	C3-C2-N1	-2.31	117.79	120.77
3	A	502	8UR	C24-C14-C13	-2.27	106.68	110.32
3	A	502	8UR	C25-C24-C14	2.26	114.82	112.40
3	C	502	8UR	C27-C28-C31	2.23	122.60	119.58
2	A	501	PLG	C3-C2-N1	-2.22	117.89	120.77
3	C	502	8UR	C32-C24-C14	2.19	114.75	112.40
3	B	502	8UR	C32-C24-C14	2.17	114.73	112.40
3	B	502	8UR	C26-C14-C13	-2.04	103.72	109.33
3	B	502	8UR	F34-C31-C28	-2.00	108.53	112.93

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C5A-OP4-P-OP1
2	A	501	PLG	C5A-OP4-P-OP2
2	A	501	PLG	C5A-OP4-P-OP3
2	B	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5A-OP4-P-OP2
2	B	501	PLG	C5A-OP4-P-OP3
2	C	501	PLG	C5-C4-C4A-N
2	C	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP2

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Mol	Chain	Res	Type	Atoms
2	C	501	PLG	C5A-OP4-P-OP3
3	A	502	8UR	C3-C4-C7-C8
3	A	502	8UR	C5-C4-C7-C8
3	B	502	8UR	C3-C4-C7-C8
3	B	502	8UR	C5-C4-C7-C8
3	C	502	8UR	C3-C4-C7-C8
3	C	502	8UR	C5-C4-C7-C8
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C4-C4A-N-CA
2	C	501	PLG	C4-C4A-N-CA
2	C	501	PLG	O-C-CA-N
2	C	501	PLG	OXT-C-CA-N
2	A	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C5A-OP4-P-OP1
2	B	501	PLG	OXT-C-CA-N
3	C	502	8UR	C15-C14-C26-C27
3	C	502	8UR	C4-C7-C8-O9
3	C	502	8UR	C4-C7-C8-O10
2	B	501	PLG	O-C-CA-N
2	B	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
3	A	502	8UR	C15-C14-C26-C27
3	A	502	8UR	C15-C14-C26-C30
3	B	502	8UR	C15-C14-C26-C27
3	B	502	8UR	C15-C14-C26-C30
3	C	502	8UR	C15-C14-C26-C30

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	8UR	1	0
3	A	502	8UR	1	0
3	B	502	8UR	1	0
2	B	501	PLG	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
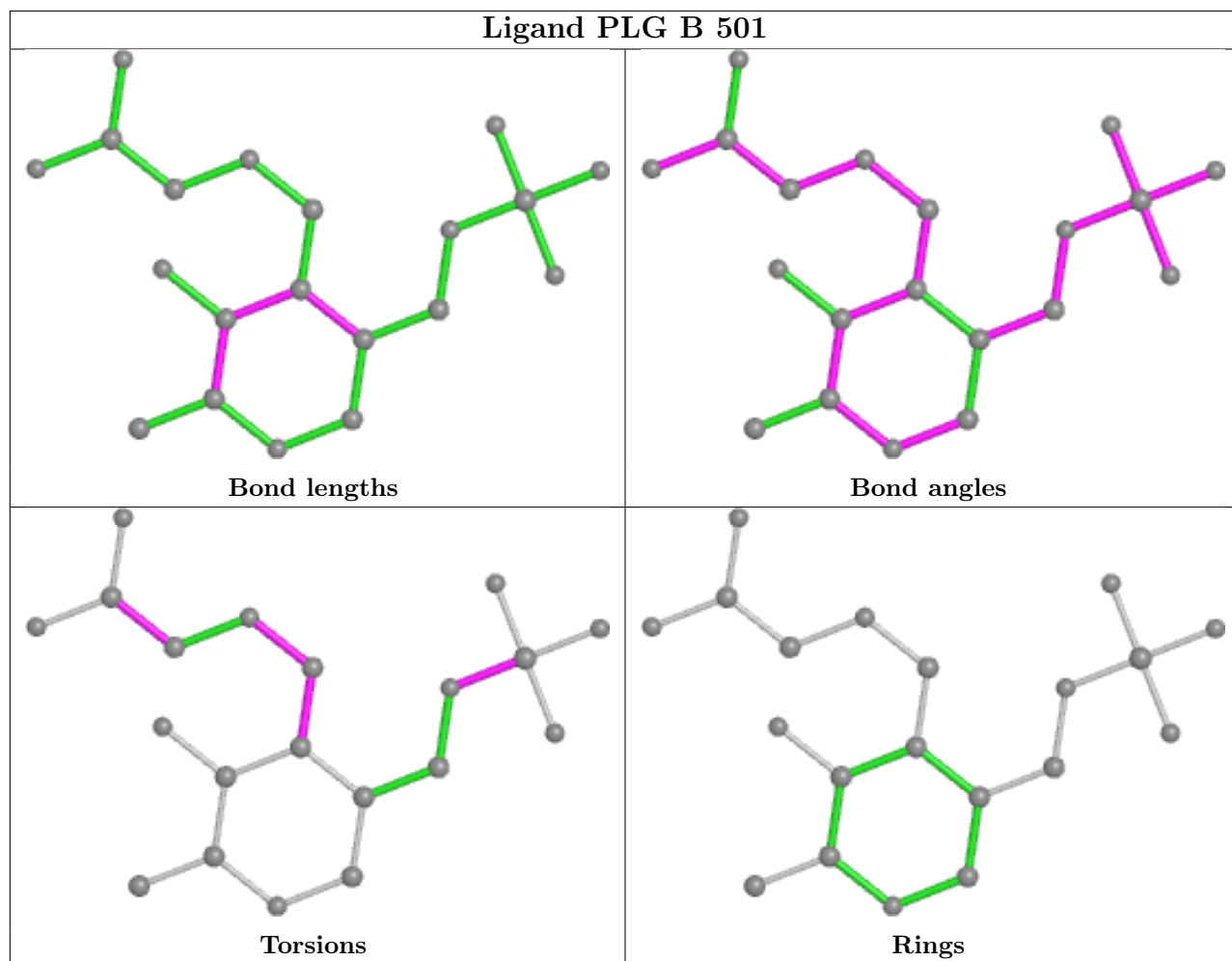
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 8UR C 502

Bond lengths | Bond angles

Torsions | Rings

Ligand 8UR A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand PLG A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 8UR B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand PLG B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand PLG C 501

Bond lengths

Bond angles

Torsions

Rings
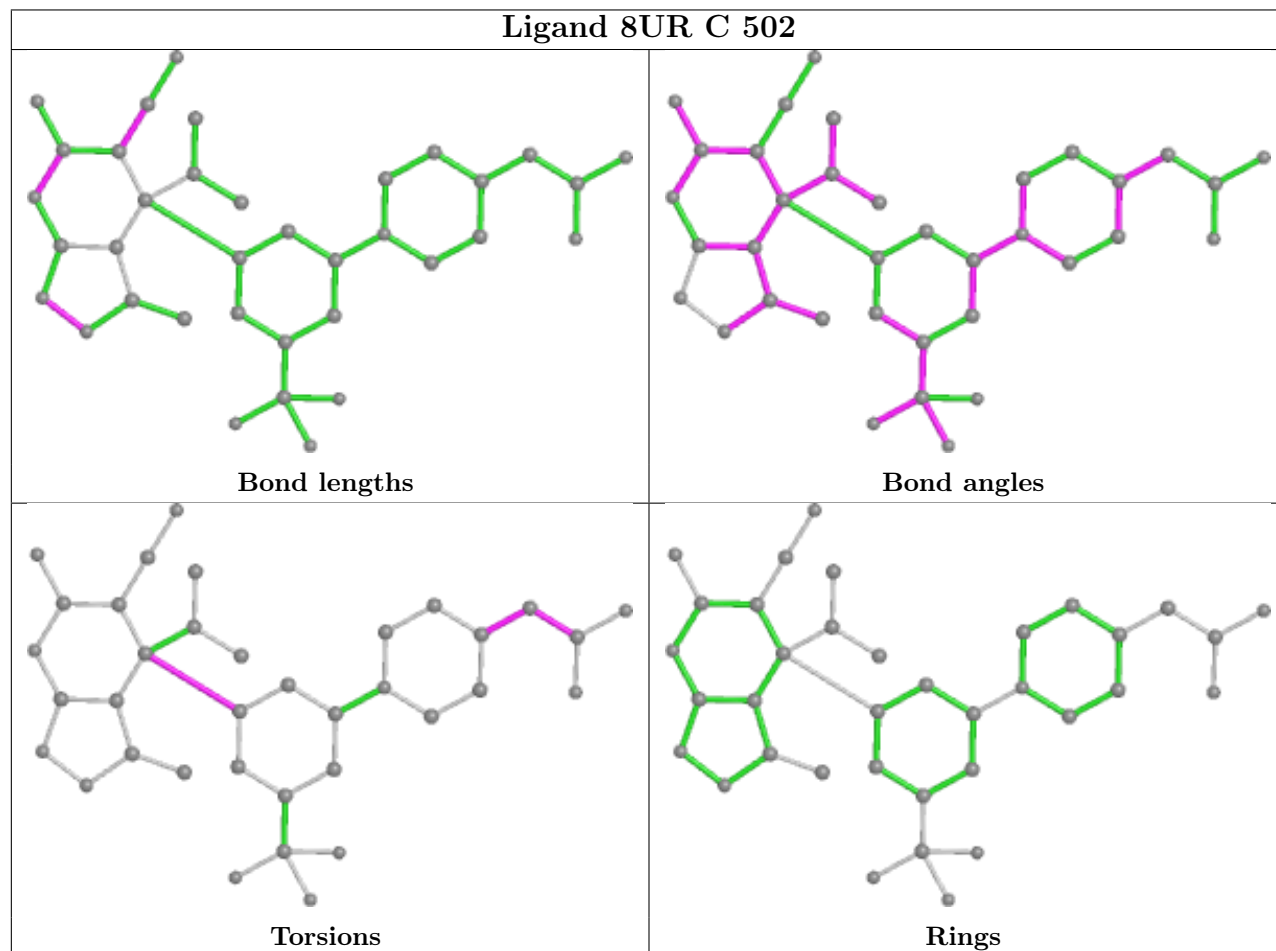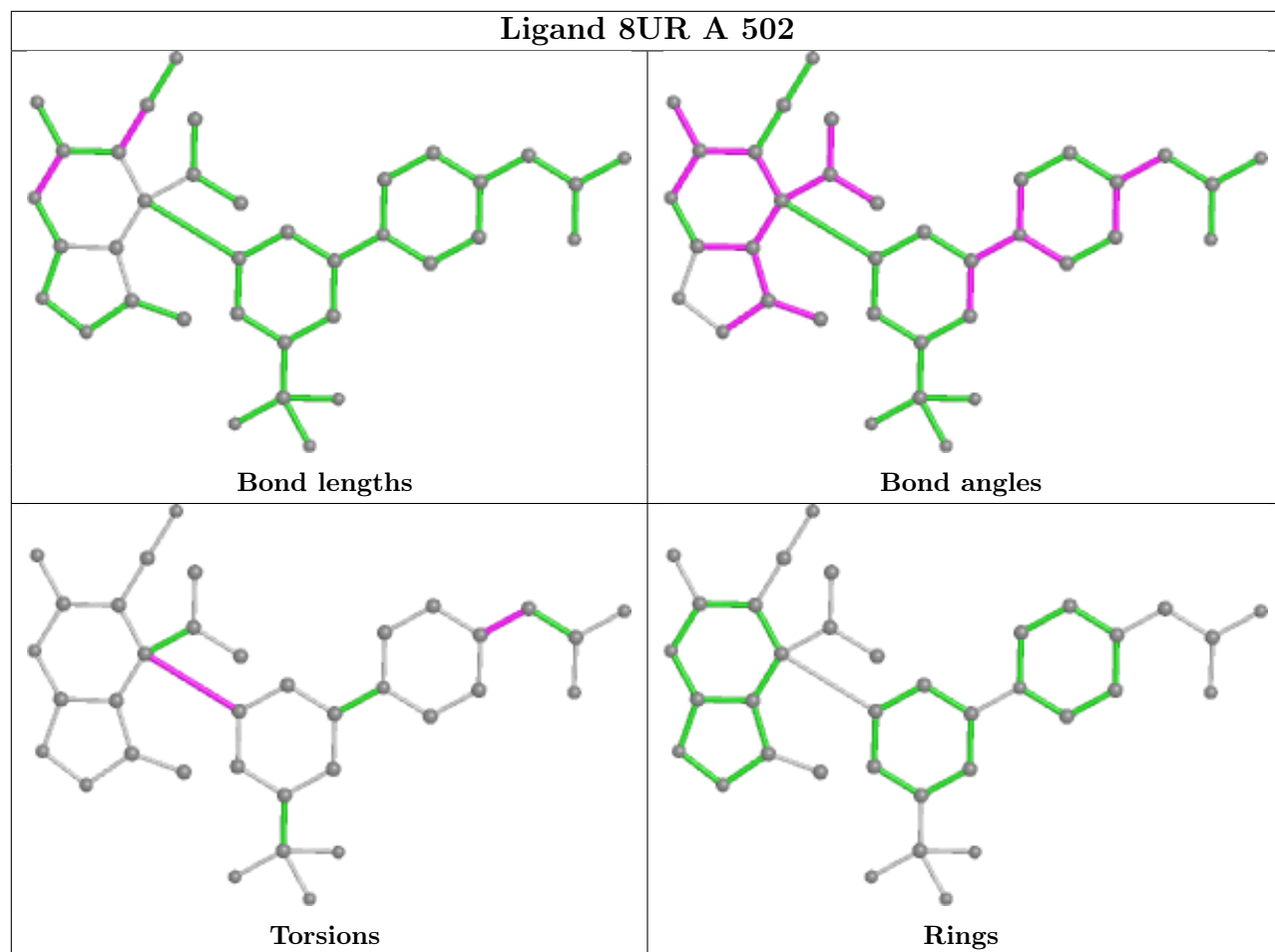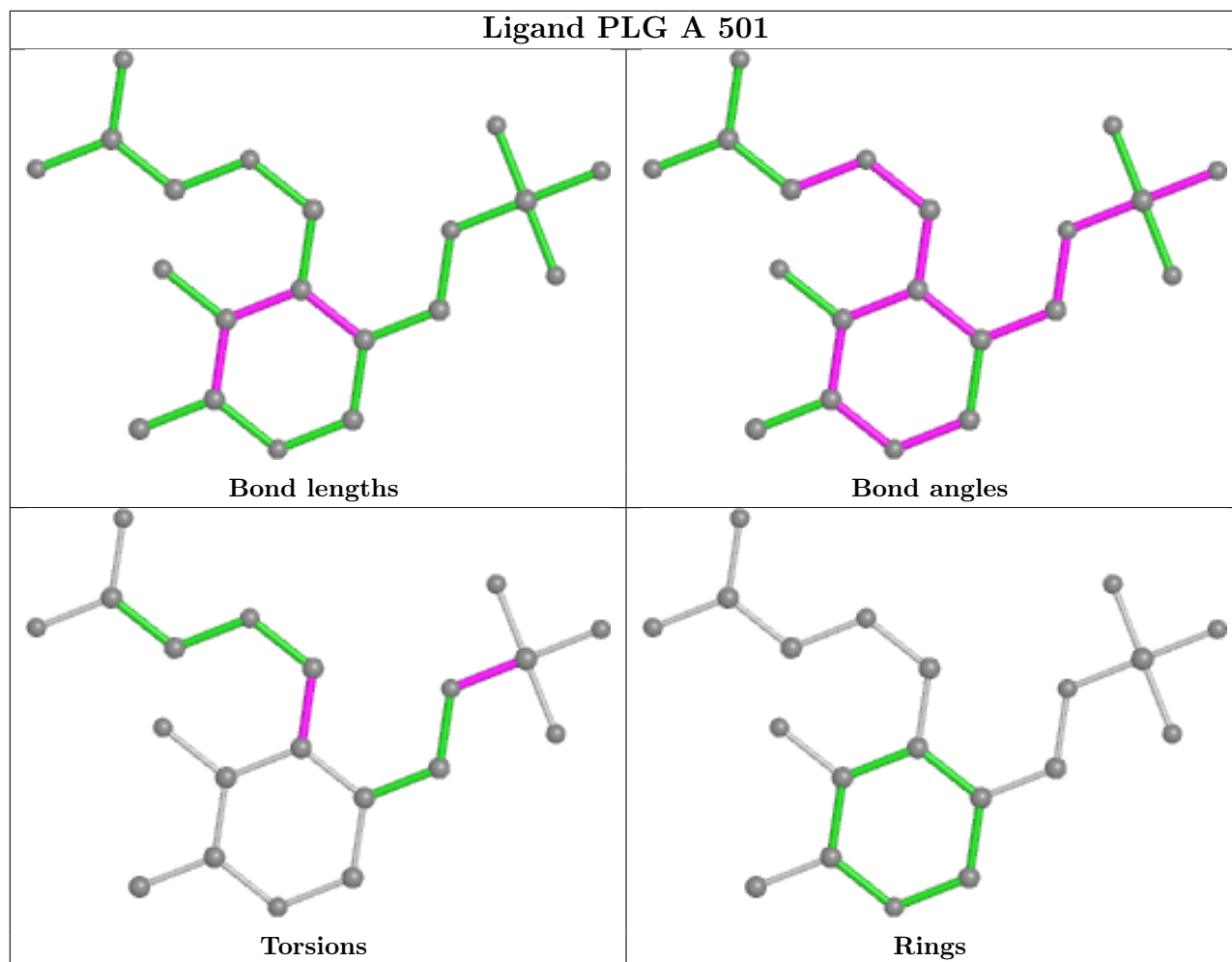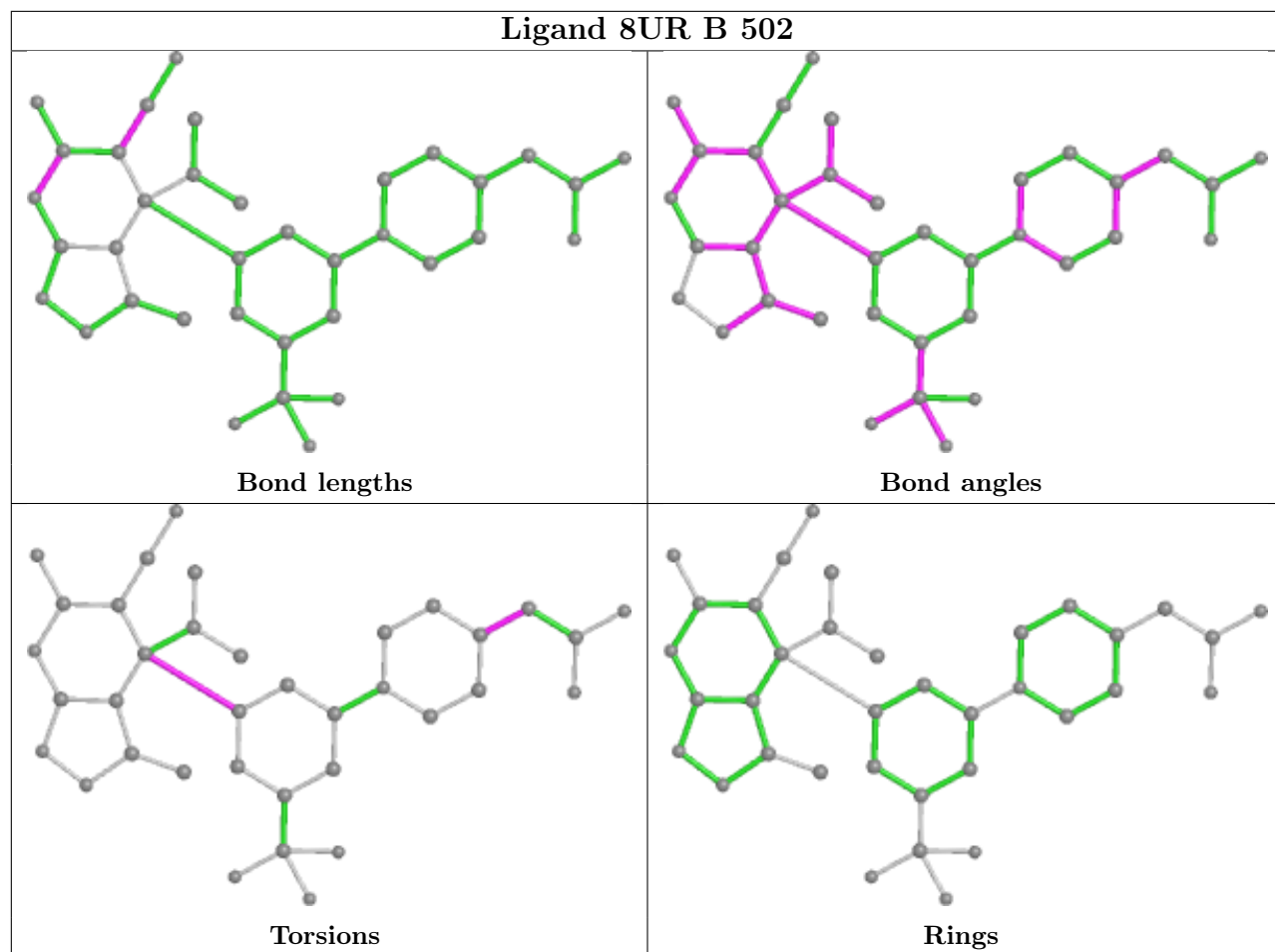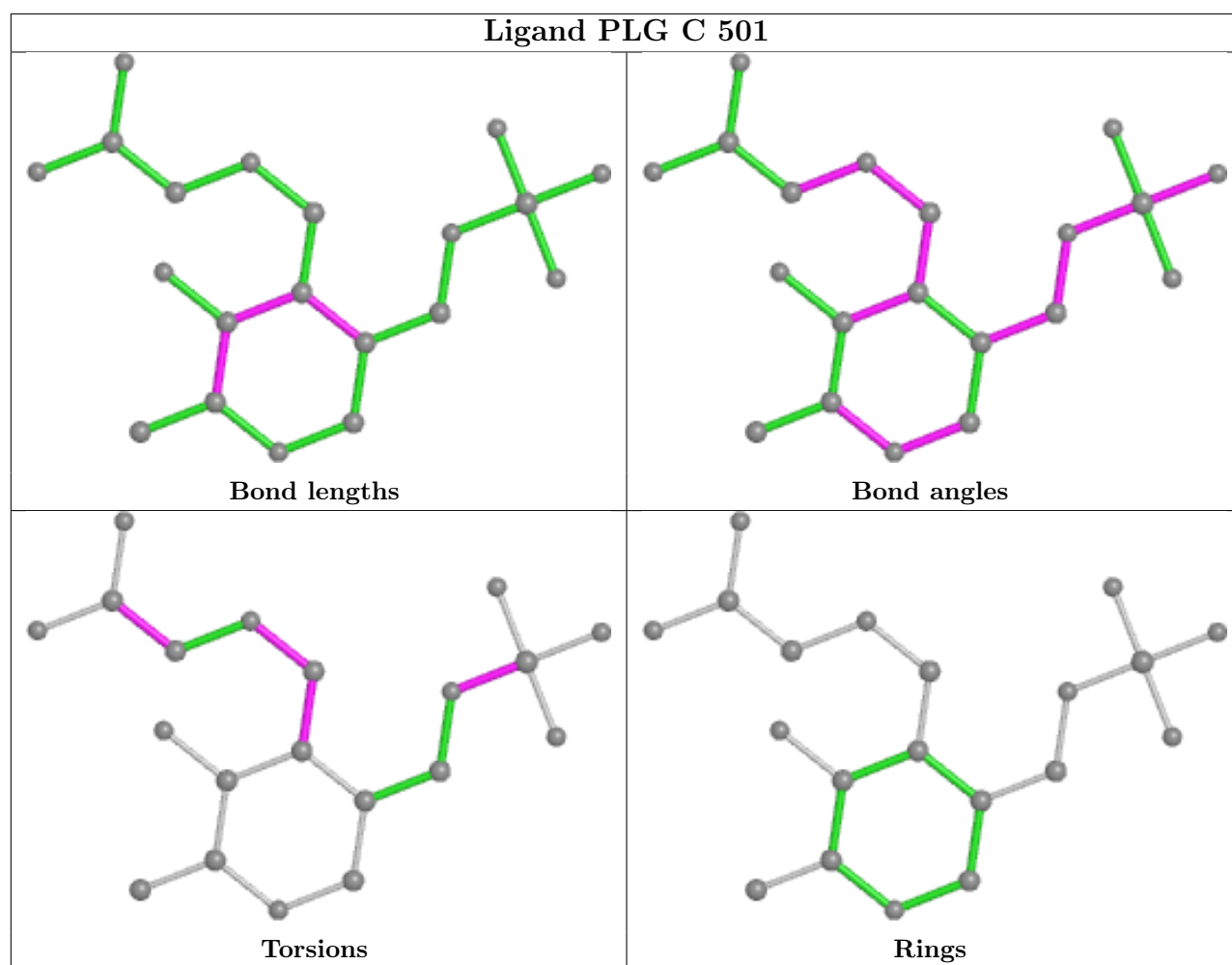
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	442/442 (100%)	0.67	35 (7%)	12	19	14, 29, 54, 98	0
1	B	442/442 (100%)	0.70	28 (6%)	20	28	15, 30, 55, 95	0
1	C	442/442 (100%)	0.70	28 (6%)	20	28	15, 30, 56, 96	0
All	All	1326/1326 (100%)	0.69	91 (6%)	16	24	14, 30, 55, 98	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	VAL	6.9
1	A	364	CYS	6.8
1	C	364	CYS	5.8
1	A	442	PRO	5.2
1	B	365	VAL	5.1
1	B	159	GLY	4.9
1	B	137	GLU	4.5
1	C	365	VAL	4.2
1	C	416	LYS	4.1
1	C	138	LYS	4.0
1	B	364	CYS	3.8
1	C	418	GLY	3.6
1	A	163	LEU	3.6
1	C	137	GLU	3.5
1	A	88	SER	3.4
1	C	366	SER	3.4
1	C	157	SER	3.4
1	B	419	LEU	3.2
1	B	163	LEU	3.2
1	C	412	LEU	3.2
1	A	138	LYS	3.1
1	C	419	LEU	3.0
1	A	65	GLY	3.0

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Full wwPDB X-ray Structure Validation Report 5YG0

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Mol	Chain	Res	Type	RSRZ
1	A	409	GLY	3.0
1	B	420	PRO	3.0
1	A	196	GLN	3.0
1	A	64	TYR	2.9
1	B	65	GLY	2.9
1	A	2	PHE	2.9
1	B	158	GLN	2.9
1	C	409	GLY	2.9
1	A	8	GLU	2.9
1	A	423	ALA	2.8
1	A	366	SER	2.7
1	A	162	ASP	2.7
1	A	226	LEU	2.7
1	B	200	GLU	2.6
1	B	421	GLY	2.6
1	C	423	ALA	2.6
1	A	363	ASP	2.6
1	B	366	SER	2.6
1	A	137	GLU	2.6
1	B	363	ASP	2.6
1	B	157	SER	2.5
1	B	202	ASN	2.5
1	A	290	SER	2.5
1	C	202	ASN	2.5
1	C	90	GLU	2.5
1	C	181	GLY	2.5
1	B	410	LYS	2.4
1	A	200	GLU	2.4
1	B	411	LYS	2.4
1	B	91	GLU	2.4
1	B	185	TYR	2.4
1	A	158	GLN	2.3
1	A	427	GLN	2.3
1	C	338	THR	2.3
1	B	22	GLU	2.3
1	C	5	GLU	2.3
1	A	335	PHE	2.3
1	A	86	ASN	2.3
1	A	215	PHE	2.3
1	C	413	VAL	2.3
1	B	4	ASN	2.2
1	A	166	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	164	ASP	2.2
1	A	26	ARG	2.2
1	B	256	GLY	2.2
1	C	196	GLN	2.2
1	B	177	VAL	2.2
1	C	169	MET	2.2
1	A	413	VAL	2.2
1	A	421	GLY	2.2
1	A	419	LEU	2.2
1	C	162	ASP	2.1
1	B	139	LYS	2.1
1	A	385	LYS	2.1
1	B	252	LYS	2.1
1	A	360	SER	2.1
1	C	167	ARG	2.1
1	C	292	ALA	2.1
1	B	298	GLN	2.1
1	A	422	ASN	2.1
1	C	6	PRO	2.1
1	C	362	VAL	2.1
1	C	75	GLU	2.1
1	B	408	TYR	2.1
1	B	193	GLN	2.0
1	C	116	LYS	2.0
1	A	9	GLN	2.0
1	C	159	GLY	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	8UR	A	502	36/36	0.85	0.20	27,31,50,52	0
3	8UR	C	502	36/36	0.86	0.21	25,29,50,52	0
3	8UR	B	502	36/36	0.87	0.21	27,31,52,54	0
4	CL	C	503	1/1	0.89	0.12	32,32,32,32	1
4	CL	A	503	1/1	0.92	0.10	29,29,29,29	0
2	PLG	C	501	20/20	0.93	0.14	18,21,22,23	0
2	PLG	B	501	20/20	0.93	0.15	17,21,22,22	0
2	PLG	A	501	20/20	0.94	0.15	20,23,25,26	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 8UR A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
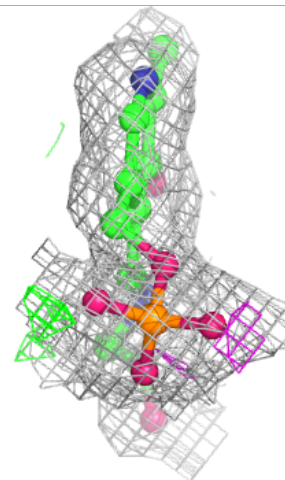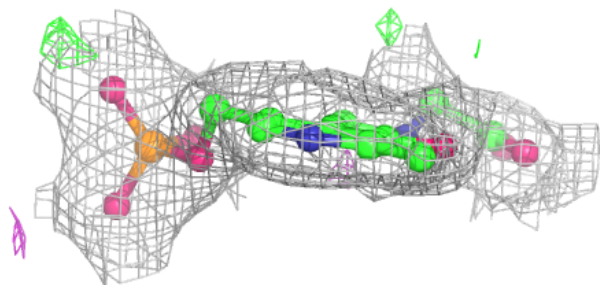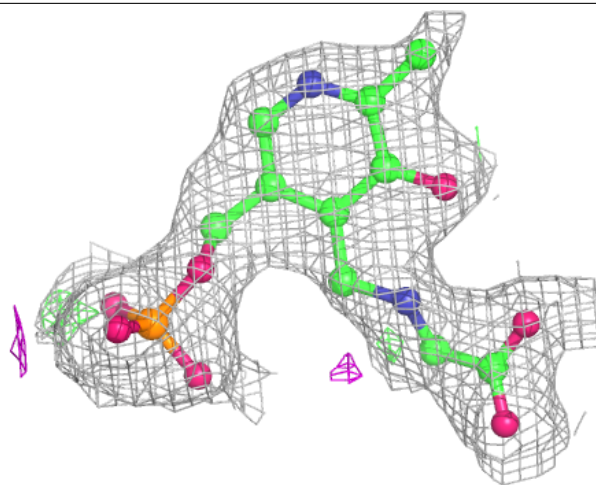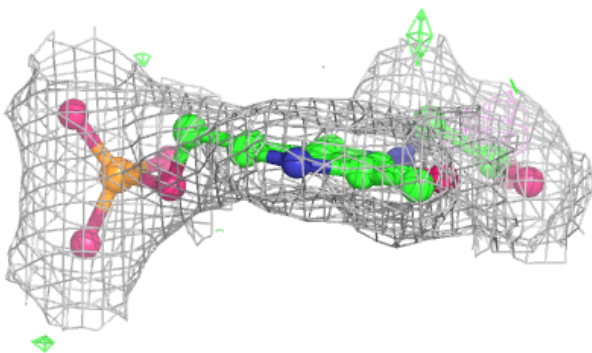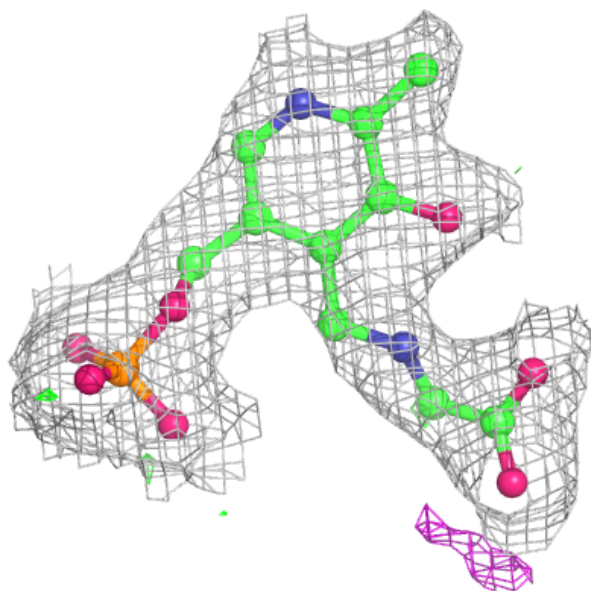$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
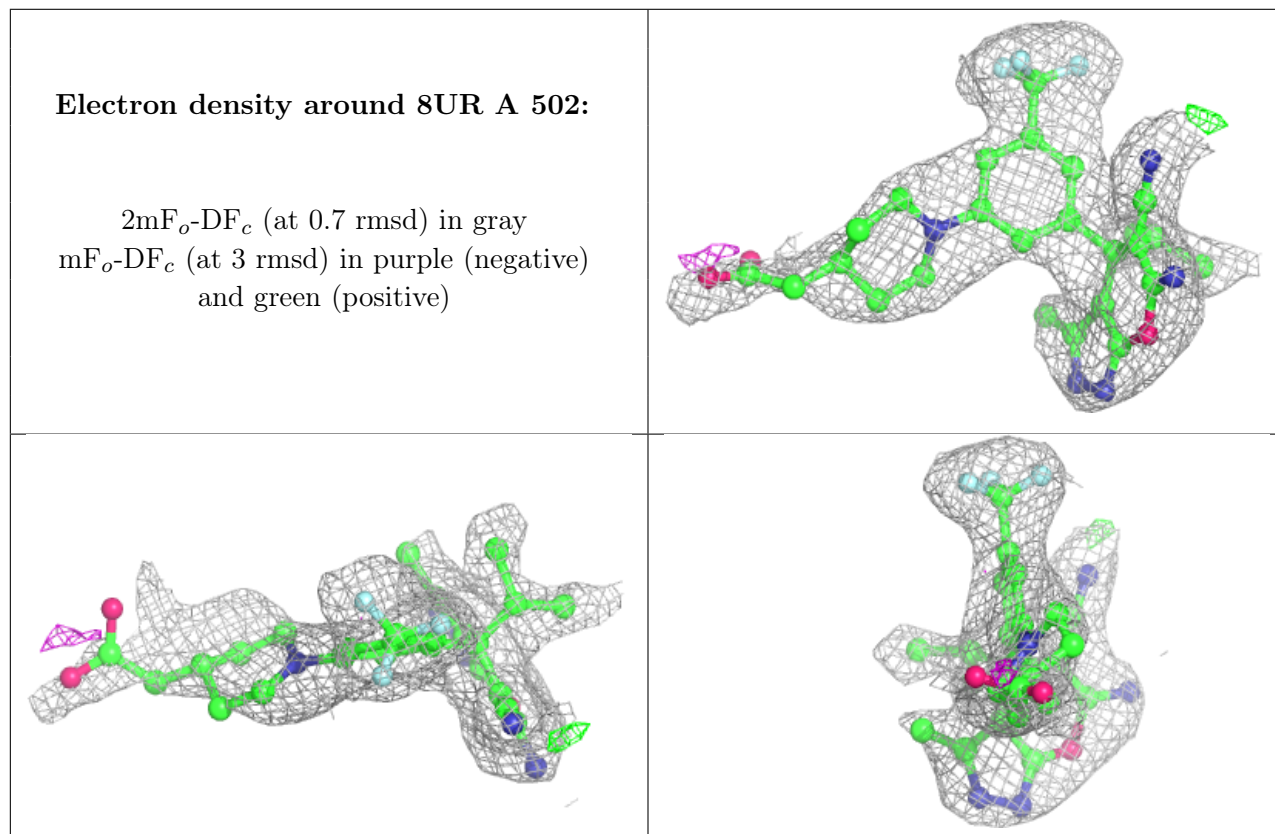
Electron density around 8UR C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
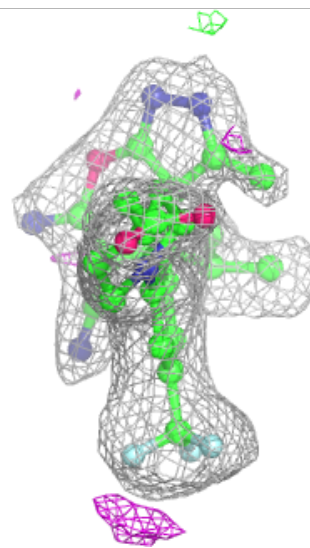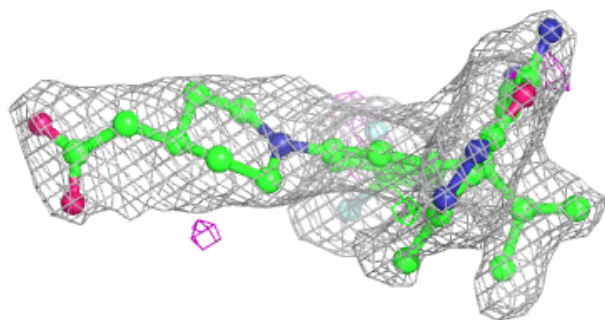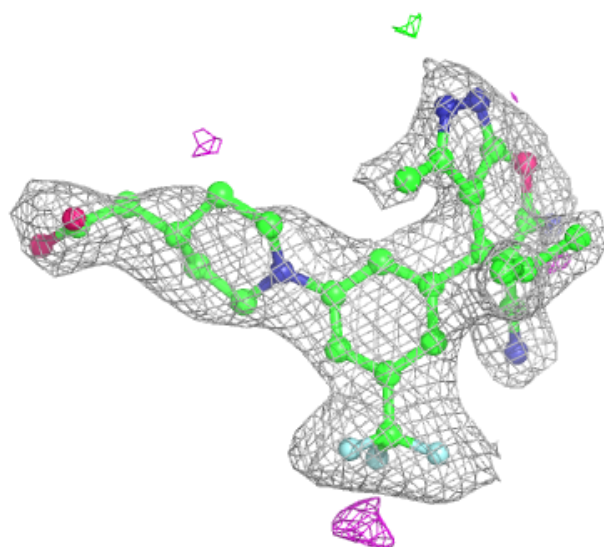
Electron density around 8UR B 502:

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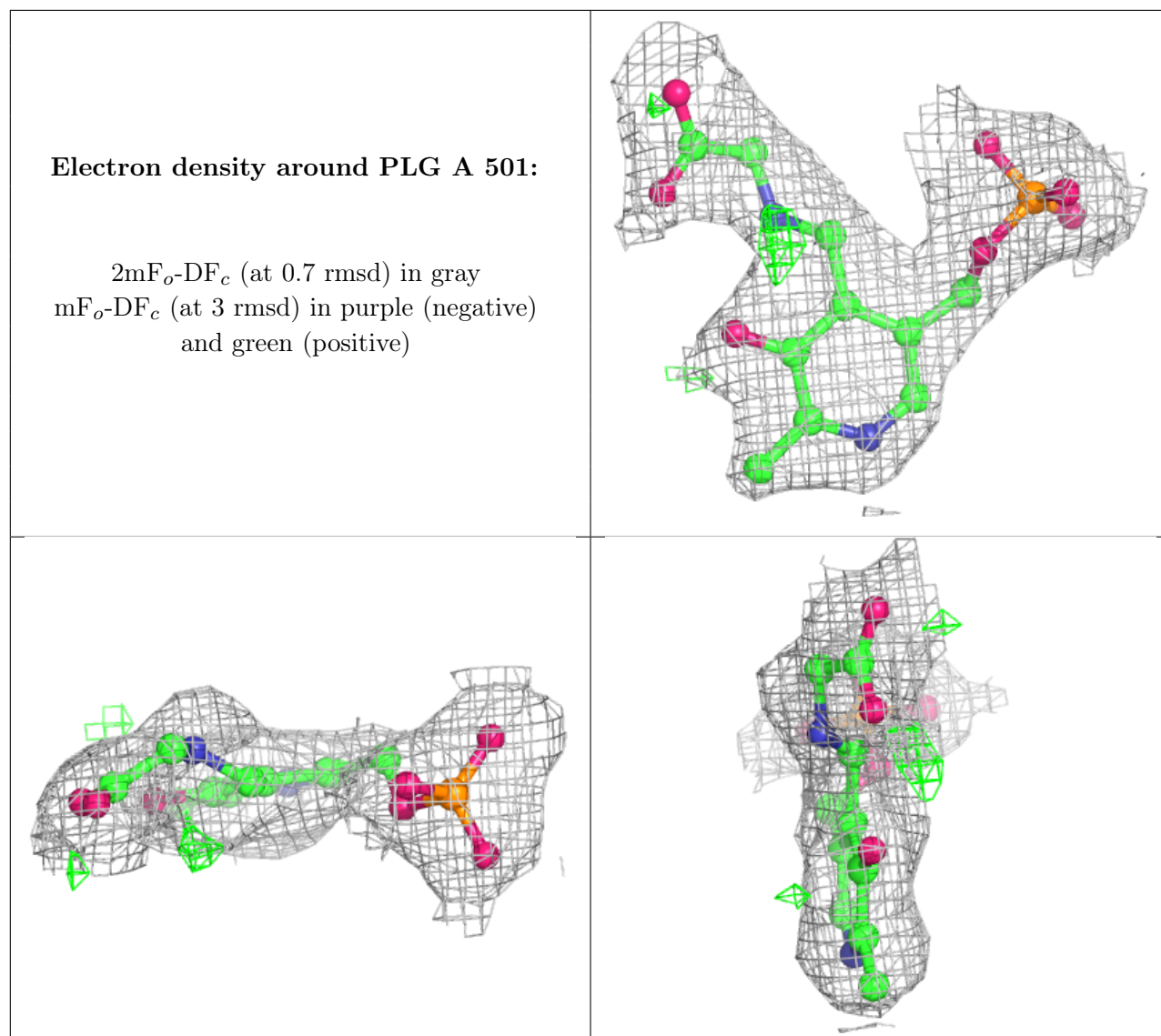and green (positive)
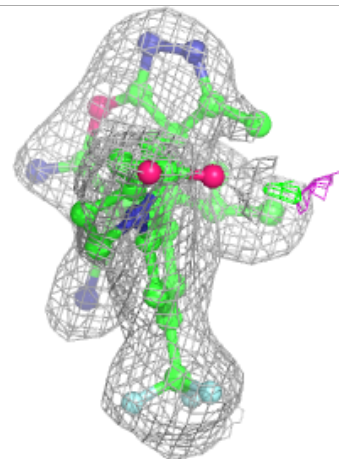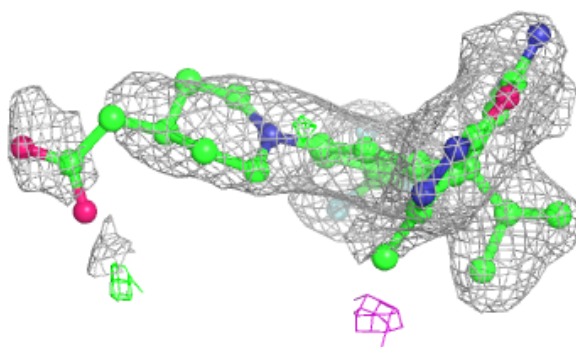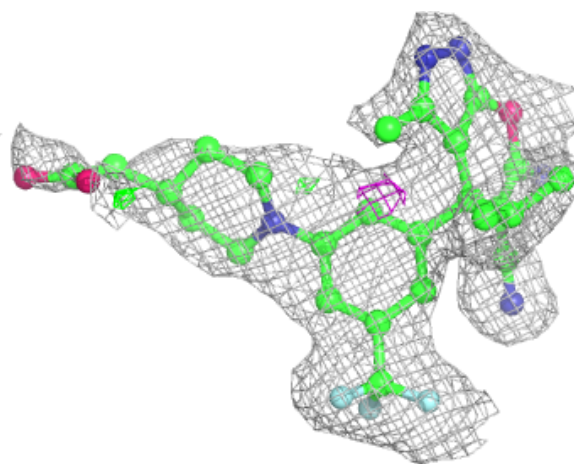
Electron density around PLG C 501:

$2mF_o$-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 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 PLG A 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.