



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:54 AM UTC

PDB ID : 7VE0 / pdb_00007ve0
Title : Crystal Structure of Ritonavir bound Plasmepsin II (PMII) from Plasmodium falciparum
Authors : Mishra, V.; Rathore, I.; Bhaumik, P.
Deposited on : 2021-09-07
Resolution : 1.90 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

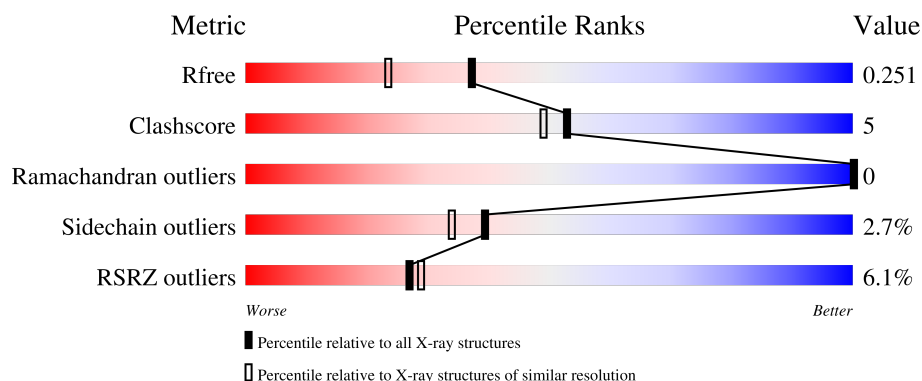
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	331	5% 90% 9% .
1	B	331	7% 87% 11% ..

2 Entry composition [i](#)

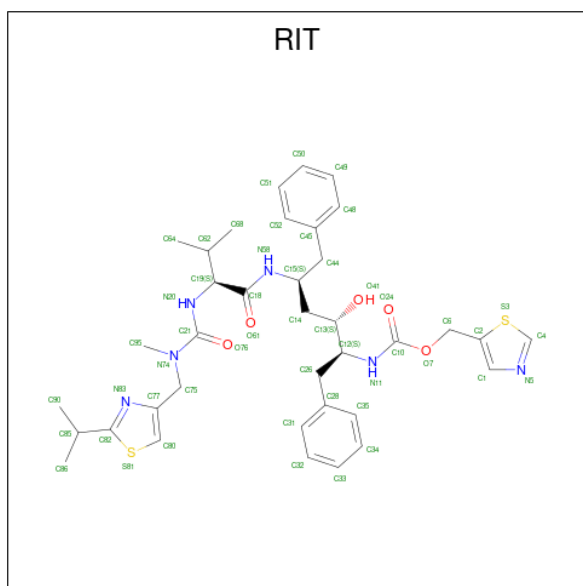
There are 5 unique types of molecules in this entry. The entry contains 6239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasmepsin II.

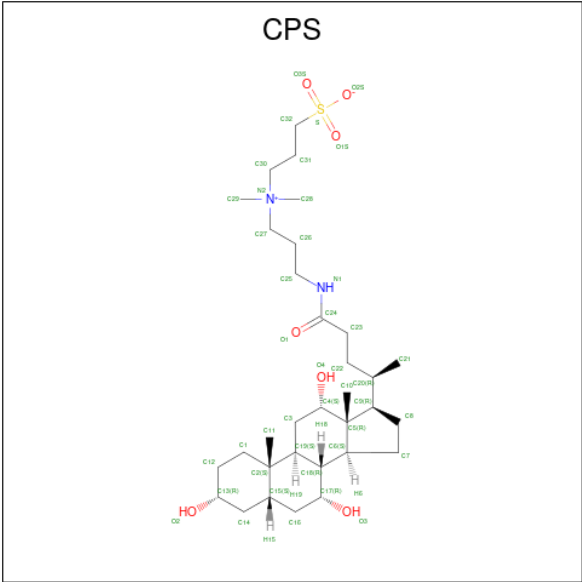
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	6	0
			2645	1713	409	512	11			
1	B	326	Total	C	N	O	S	0	5	0
			2612	1694	401	506	11			

- Molecule 2 is RITONAVIR (CCD ID: RIT) (formula: $C_{37}H_{48}N_6O_5S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
2	B	1	Total	C	N	O	S	0	1
			100	74	12	10	4		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



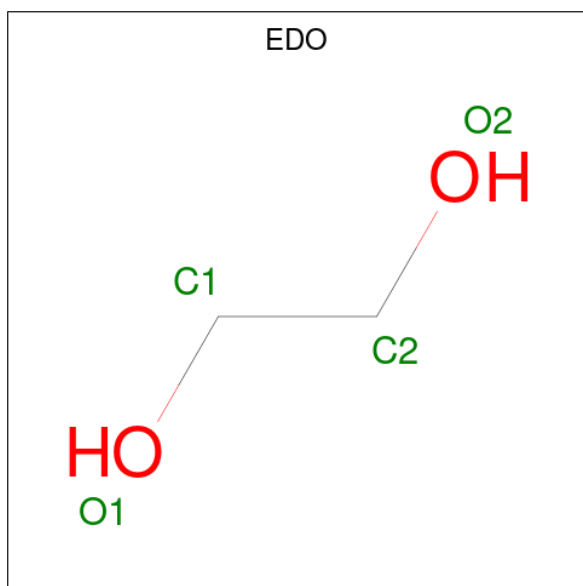
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 42	C 32	N 2	O 7	S 1	0	0
3	A	1	Total 26	C 23	O 3	0			0
3	A	1	Total 29	C 24	N 1	O 4	0		
3	A	1	Total 23	C 20	O 3	0			0
3	A	1	Total 29	C 24	N 1	O 4	0		
3	A	1	Total 42	C 32	N 2	O 7	S 1	0	0
3	A	1	Total 36	C 30	N 2	O 4	0		
3	B	1	Total 29	C 24	N 1	O 4	0		
3	B	1	Total 36	C 30	N 2	O 4	0		
3	B	1	Total 29	C 24	N 1	O 4	0		
3	B	1	Total 30	C 25	N 1	O 4	0		
3	B	1	Total 29	C 24	N 1	O 4	0		
3	B	1	Total 22	C 19	O 3	0			0
3	B	1	Total 27	C 24	O 3	0			0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	25	1	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

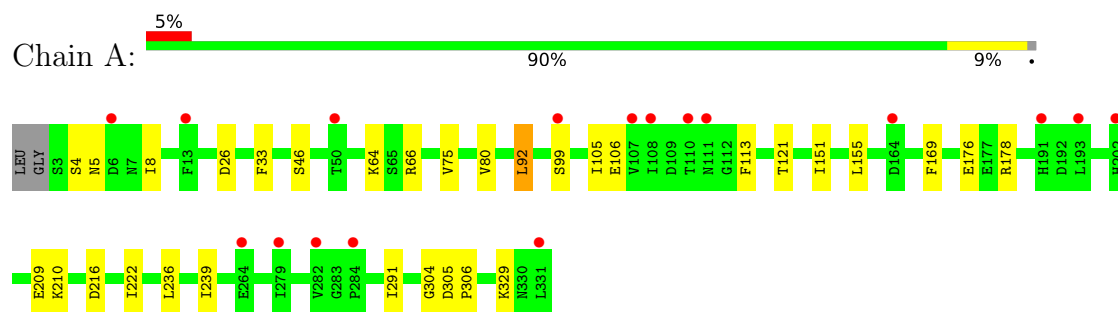
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	161	Total	O	0	0
			161	161		

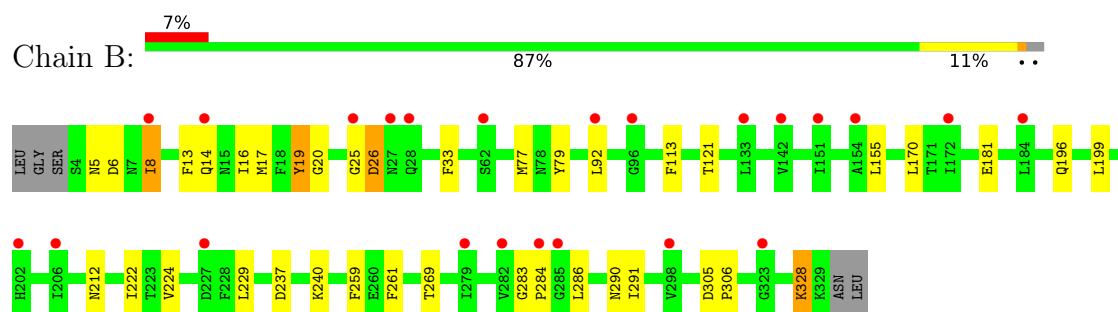
3 Residue-property plots [i](#)

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

• Molecule 1: Plasmepsin II



• Molecule 1: Plasmepsin II



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.29Å 70.41Å 106.67Å 90.00° 133.61° 90.00°	Depositor
Resolution (Å)	39.89 – 1.90 39.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.89-1.90) 96.3 (39.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.261 (Not available) , 0.251	Depositor DCC
R_{free} test set	3067 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.108 for h+2*k,-h-l 0.026 for h,-k,-h-l 0.029 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6239	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CPS, RIT, EDO

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	1.03	2/2720 (0.1%)	1.24	0/3701
1	B	0.98	0/2687	1.25	3/3657 (0.1%)
All	All	1.00	2/5407 (0.0%)	1.25	3/7358 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	C-O	7.20	1.31	1.23
1	A	169	PHE	C-O	5.89	1.31	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	25	GLY	CA-C-O	-6.09	118.26	122.22
1	B	19	TYR	CA-C-N	5.01	125.47	121.61
1	B	19	TYR	C-N-CA	5.01	125.47	121.61

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	PHE	Peptide
1	B	33	PHE	Peptide

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	2645	0	2576	17	0
1	B	2612	0	2543	19	0
2	A	50	0	48	0	0
2	B	100	0	96	9	0
3	A	227	0	314	13	0
3	B	232	0	318	4	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
5	A	204	0	0	0	0
5	B	161	0	0	0	0
All	All	6239	0	5907	59	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 5.

All (59) 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)
3:A:407:CPS:H10B	3:A:407:CPS:H22A	1.59	0.84
3:A:403:CPS:H21B	3:A:403:CPS:H10B	1.73	0.70
1:B:237:ASP:HA	4:B:410:EDO:H11	1.73	0.70
1:A:5:ASN:HB2	1:A:176:GLU:OE2	2.00	0.61
3:A:407:CPS:H22A	3:A:407:CPS:C10	2.31	0.61
1:A:26:ASP:OD2	1:A:66:ARG:HG2	2.02	0.59
1:A:80:VAL:HG22	3:A:402:CPS:H21A	1.84	0.58
3:A:407:CPS:H10B	3:A:407:CPS:C22	2.31	0.58
3:A:407:CPS:H21	3:A:407:CPS:C24	2.35	0.57
1:B:26:ASP:C	1:B:26:ASP:OD1	2.48	0.55
1:B:13:PHE:CE2	1:B:121[B]:THR:HG21	2.41	0.55
1:A:209:GLU:HG2	1:A:210:LYS:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:OE1	1:A:178:ARG:HD3	2.08	0.53
1:B:14:GLN:HB3	3:B:402:CPS:H23	1.90	0.53
1:A:239:ILE:HG21	3:A:405:CPS:H11B	1.90	0.53
1:B:19:TYR:CE2	1:B:121[B]:THR:HG22	2.44	0.53
3:B:402:CPS:H10B	3:B:402:CPS:H21A	1.92	0.52
2:B:401[A]:RIT:C49	2:B:401[A]:RIT:H953	2.40	0.52
3:A:407:CPS:H28A	3:A:407:CPS:H25	1.92	0.52
1:B:77:MET:HE3	1:B:79:TYR:CZ	2.47	0.49
1:A:5:ASN:HD22	1:A:176:GLU:HG2	1.79	0.48
1:B:8:ILE:HD11	1:B:20:GLY:HA3	1.96	0.48
1:B:8:ILE:HG23	1:B:170:LEU:HB3	1.94	0.48
2:B:401[A]:RIT:N11	2:B:401[A]:RIT:H35	2.28	0.48
2:B:401[B]:RIT:H35	2:B:401[B]:RIT:N11	2.28	0.48
1:A:155:LEU:HD12	1:A:155:LEU:C	2.38	0.47
3:B:404:CPS:H21A	3:B:404:CPS:H10B	1.96	0.47
1:A:222:ILE:O	1:A:291:ILE:HA	2.14	0.47
3:A:407:CPS:H28A	3:A:407:CPS:C25	2.45	0.47
1:B:305:ASP:HB3	1:B:306:PRO:HD3	1.97	0.47
2:B:401[A]:RIT:H35	2:B:401[A]:RIT:C10	2.45	0.46
3:B:402:CPS:H7A	3:B:403:CPS:H3	1.97	0.46
1:A:75:VAL:CG1	1:A:105:ILE:HG23	2.46	0.45
2:B:401[B]:RIT:H35	2:B:401[B]:RIT:C10	2.46	0.45
1:B:16:ILE:HG23	1:B:17:MET:HG2	1.98	0.45
1:B:283:GLY:HA2	1:B:286:LEU:HD12	1.99	0.44
1:A:305:ASP:HB3	1:A:306:PRO:HD3	2.00	0.44
1:B:181:GLU:HG2	1:B:328:LYS:HG2	1.99	0.44
1:A:4:SER:OG	1:A:5:ASN:N	2.49	0.43
3:A:407:CPS:C10	3:A:407:CPS:C22	2.93	0.43
1:B:199:LEU:HD13	1:B:261:PHE:HB3	2.01	0.43
1:A:46:SER:HB2	1:A:106:GLU:HG2	2.00	0.42
1:A:75:VAL:HG11	1:A:105:ILE:HG23	2.01	0.42
3:A:403:CPS:H10B	3:A:403:CPS:C21	2.46	0.42
3:A:403:CPS:C21	3:A:403:CPS:C10	2.98	0.42
1:B:224:VAL:CG2	1:B:229:LEU:HB2	2.49	0.42
2:B:401[A]:RIT:C10	2:B:401[A]:RIT:C35	2.97	0.42
3:A:403:CPS:H21B	3:A:403:CPS:C10	2.46	0.42
1:A:5:ASN:CB	1:A:176:GLU:OE2	2.67	0.42
2:B:401[B]:RIT:C10	2:B:401[B]:RIT:C35	2.98	0.42
1:A:216:ASP:O	1:A:304:GLY:HA2	2.20	0.42
1:B:196:GLN:OE1	1:B:212:ASN:ND2	2.47	0.41
1:B:155:LEU:C	1:B:155:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92[B]:LEU:HD21	1:A:99:SER:HB3	2.03	0.41
1:B:259:PHE:O	1:B:269:THR:HA	2.21	0.41
2:B:401[A]:RIT:N11	2:B:401[A]:RIT:C35	2.84	0.41
2:B:401[B]:RIT:N11	2:B:401[B]:RIT:C35	2.84	0.41
1:B:222:ILE:O	1:B:291:ILE:HA	2.21	0.40
1:B:283:GLY:HA3	1:B:284:PRO:HA	1.95	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	333/331 (101%)	319 (96%)	14 (4%)	0	100	100
1	B	329/331 (99%)	318 (97%)	11 (3%)	0	100	100
All	All	662/662 (100%)	637 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	300/295 (102%)	291 (97%)	9 (3%)	36	30
1	B	296/295 (100%)	287 (97%)	9 (3%)	36	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	596/590 (101%)	578 (97%)	18 (3%)	39 30

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	64	LYS
1	A	92[A]	LEU
1	A	92[B]	LEU
1	A	113	PHE
1	A	121	THR
1	A	236[A]	LEU
1	A	236[B]	LEU
1	A	329	LYS
1	B	5	ASN
1	B	6	ASP
1	B	8	ILE
1	B	26	ASP
1	B	92	LEU
1	B	113	PHE
1	B	240	LYS
1	B	290	ASN
1	B	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	B	28	GLN
1	B	78	ASN
1	B	277	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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	RIT	A	401	-	52,53,53	1.00	2 (3%)	62,71,71	1.49	9 (14%)
4	EDO	A	409	-	3,3,3	0.14	0	2,2,2	0.02	0
3	CPS	B	405	-	33,33,45	0.40	0	52,52,70	0.46	0
3	CPS	B	402	-	32,32,45	0.41	0	51,51,70	0.53	0
3	CPS	A	402	-	45,45,45	0.40	0	70,70,70	0.68	1 (1%)
4	EDO	B	410	-	3,3,3	0.23	0	2,2,2	0.12	0
3	CPS	A	403	-	29,29,45	0.41	0	47,47,70	0.76	2 (4%)
3	CPS	A	404	-	32,32,45	0.45	0	51,51,70	0.53	0
3	CPS	A	408	-	39,39,45	0.43	0	61,61,70	0.53	0
3	CPS	B	407	-	25,25,45	0.52	0	39,41,70	0.60	0
3	CPS	A	406	-	32,32,45	0.43	0	51,51,70	0.46	0
3	CPS	A	407	-	45,45,45	0.40	0	70,70,70	0.97	4 (5%)
3	CPS	B	409	-	33,33,45	0.43	0	52,52,70	0.66	0
3	CPS	B	404	-	32,32,45	0.42	0	51,51,70	0.61	0
2	RIT	B	401[A]	-	52,53,53	1.04	2 (3%)	62,71,71	1.35	8 (12%)
3	CPS	B	408	-	30,30,45	0.44	0	47,48,70	0.51	0
3	CPS	A	405	-	26,26,45	0.48	0	42,43,70	0.54	0
3	CPS	B	406	-	32,32,45	0.44	0	51,51,70	0.56	0
3	CPS	B	403	-	39,39,45	0.40	0	61,61,70	0.53	0
2	RIT	B	401[B]	-	52,53,53	1.04	2 (3%)	62,71,71	1.36	9 (14%)

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	RIT	A	401	-	-	6/53/53/53	0/4/4/4
4	EDO	A	409	-	-	1/1/1/1	-
3	CPS	B	405	-	-	2/11/76/90	0/4/4/4
3	CPS	B	402	-	-	5/9/74/90	0/4/4/4
3	CPS	A	402	-	-	5/25/90/90	0/4/4/4
4	EDO	B	410	-	-	1/1/1/1	-
3	CPS	A	403	-	-	5/6/71/90	0/4/4/4
3	CPS	A	404	-	-	0/9/74/90	0/4/4/4
3	CPS	A	408	-	-	2/17/82/90	0/4/4/4
3	CPS	B	407	-	-	-	0/4/4/4
3	CPS	A	406	-	-	0/9/74/90	0/4/4/4
3	CPS	A	407	-	-	16/25/90/90	0/4/4/4
3	CPS	B	409	-	-	6/11/76/90	0/4/4/4
3	CPS	B	404	-	-	5/9/74/90	0/4/4/4
2	RIT	B	401[A]	-	-	6/53/53/53	0/4/4/4
3	CPS	B	408	-	-	0/7/72/90	0/4/4/4
3	CPS	A	405	-	-	-	0/4/4/4
3	CPS	B	406	-	-	1/9/74/90	0/4/4/4
3	CPS	B	403	-	-	1/17/82/90	0/4/4/4
2	RIT	B	401[B]	-	-	8/53/53/53	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	RIT	O7-C10	5.31	1.45	1.35
2	B	401[A]	RIT	O7-C10	5.26	1.45	1.35
2	A	401	RIT	O7-C10	5.17	1.45	1.35
2	A	401	RIT	C82-N83	2.58	1.36	1.30
2	B	401[B]	RIT	C82-N83	2.54	1.35	1.30
2	B	401[A]	RIT	C82-N83	2.50	1.35	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	RIT	C14-C15-C44	-5.32	106.46	112.44
2	B	401[B]	RIT	C1-C2-S3	4.07	113.17	108.45
2	B	401[A]	RIT	C1-C2-S3	4.06	113.16	108.45
2	B	401[A]	RIT	C14-C15-C44	-4.04	107.90	112.44
2	A	401	RIT	C1-C2-S3	4.03	113.13	108.45
2	B	401[B]	RIT	C14-C15-C44	-3.86	108.10	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	RIT	C6-O7-C10	3.61	119.86	115.67
2	B	401[A]	RIT	O7-C10-N11	3.61	118.17	110.45
2	B	401[B]	RIT	O7-C10-N11	3.57	118.09	110.45
2	A	401	RIT	C95-N74-C75	-3.44	111.82	116.89
2	A	401	RIT	O7-C10-O24	-3.01	118.48	124.26
2	A	401	RIT	O7-C10-N11	2.92	116.70	110.45
3	A	407	CPS	C5-C9-C20	2.91	123.01	119.48
2	B	401[A]	RIT	O7-C10-O24	-2.83	118.83	124.26
2	B	401[B]	RIT	O7-C10-O24	-2.83	118.83	124.26
2	B	401[B]	RIT	C2-C1-N5	-2.79	111.55	116.42
3	A	407	CPS	C8-C9-C5	-2.78	100.85	103.54
2	B	401[B]	RIT	C77-C75-N74	-2.78	107.33	112.66
2	B	401[A]	RIT	C2-C1-N5	-2.78	111.56	116.42
2	A	401	RIT	C2-C1-N5	-2.76	111.59	116.42
3	A	407	CPS	C25-N1-C24	2.74	127.93	122.82
2	A	401	RIT	C6-C2-S3	-2.62	113.82	120.97
3	A	403	CPS	C5-C9-C20	2.61	122.65	119.48
2	B	401[A]	RIT	C6-C2-S3	-2.50	114.14	120.97
2	B	401[B]	RIT	C6-C2-S3	-2.49	114.16	120.97
3	A	402	CPS	C9-C5-C6	-2.49	97.62	100.11
3	A	403	CPS	C8-C9-C5	-2.47	101.14	103.54
3	A	407	CPS	C9-C5-C6	-2.46	97.65	100.11
2	B	401[A]	RIT	C6-O7-C10	2.38	118.44	115.67
2	B	401[B]	RIT	C6-O7-C10	2.36	118.41	115.67
2	B	401[A]	RIT	C80-C77-N83	-2.22	111.67	115.12
2	A	401	RIT	C80-C77-N83	-2.20	111.70	115.12
2	B	401[B]	RIT	C80-C77-N83	-2.20	111.71	115.12

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401[A]	RIT	S81-C82-C85-C90
2	B	401[B]	RIT	S81-C82-C85-C86
3	A	402	CPS	N2-C30-C31-C32
3	A	402	CPS	C30-C31-C32-S
3	A	403	CPS	C21-C20-C22-C23
3	A	407	CPS	C22-C20-C9-C5
3	A	407	CPS	C21-C20-C9-C8
3	A	407	CPS	C26-C27-N2-C30
3	A	407	CPS	C22-C20-C9-C8
2	A	401	RIT	N11-C10-O7-C6

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Mol	Chain	Res	Type	Atoms
3	A	407	CPS	C23-C24-N1-C25
2	A	401	RIT	O24-C10-O7-C6
3	A	402	CPS	C31-C30-N2-C28
3	A	407	CPS	C26-C27-N2-C29
3	A	403	CPS	C22-C20-C9-C8
3	A	407	CPS	O1-C24-N1-C25
3	A	402	CPS	C31-C30-N2-C29
3	A	407	CPS	C26-C27-N2-C28
3	A	403	CPS	C9-C20-C22-C23
3	A	408	CPS	C9-C20-C22-C23
3	B	404	CPS	C21-C20-C9-C5
3	A	408	CPS	C21-C20-C22-C23
3	A	407	CPS	N1-C25-C26-C27
3	A	403	CPS	C21-C20-C9-C8
3	A	407	CPS	C21-C20-C9-C5
3	A	403	CPS	C22-C20-C9-C5
3	A	407	CPS	C31-C32-S-O2S
3	B	404	CPS	C22-C20-C9-C8
3	B	402	CPS	C21-C20-C9-C5
3	B	402	CPS	C22-C20-C9-C8
3	A	402	CPS	C31-C30-N2-C27
2	B	401[A]	RIT	N20-C21-N74-C75
4	B	410	EDO	O1-C1-C2-O2
3	B	404	CPS	C21-C20-C9-C8
3	A	407	CPS	C31-C32-S-O3S
3	A	407	CPS	C31-C32-S-O1S
2	B	401[A]	RIT	C13-C14-C15-N58
2	B	401[B]	RIT	C13-C14-C15-N58
2	B	401[A]	RIT	O76-C21-N74-C75
3	B	402	CPS	C20-C22-C23-C24
3	B	406	CPS	C20-C22-C23-C24
2	A	401	RIT	N74-C75-C77-N83
2	B	401[B]	RIT	N74-C75-C77-C80
2	B	401[B]	RIT	N74-C75-C77-N83
2	A	401	RIT	S81-C82-C85-C90
2	A	401	RIT	N74-C75-C77-C80
3	B	402	CPS	C21-C20-C9-C8
3	A	407	CPS	C25-C26-C27-N2
2	B	401[A]	RIT	N83-C82-C85-C86
2	B	401[B]	RIT	N83-C82-C85-C90
3	B	405	CPS	C23-C24-N1-C25
3	B	409	CPS	C23-C24-N1-C25

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Mol	Chain	Res	Type	Atoms
3	B	404	CPS	C22-C20-C9-C5
3	B	409	CPS	C22-C20-C9-C5
3	B	405	CPS	O1-C24-N1-C25
3	B	409	CPS	O1-C24-N1-C25
3	A	407	CPS	C22-C23-C24-O1
3	B	409	CPS	C22-C20-C9-C8
2	B	401[B]	RIT	N58-C18-C19-N20
3	B	404	CPS	C21-C20-C22-C23
2	B	401[B]	RIT	O61-C18-C19-N20
3	B	409	CPS	C21-C20-C9-C5
4	A	409	EDO	O1-C1-C2-O2
2	A	401	RIT	N83-C82-C85-C86
3	B	409	CPS	C9-C20-C22-C23
3	A	407	CPS	C22-C23-C24-N1
2	B	401[A]	RIT	O41-C13-C14-C15
2	B	401[B]	RIT	O41-C13-C14-C15
3	B	403	CPS	C25-C26-C27-N2
3	B	402	CPS	C22-C20-C9-C5

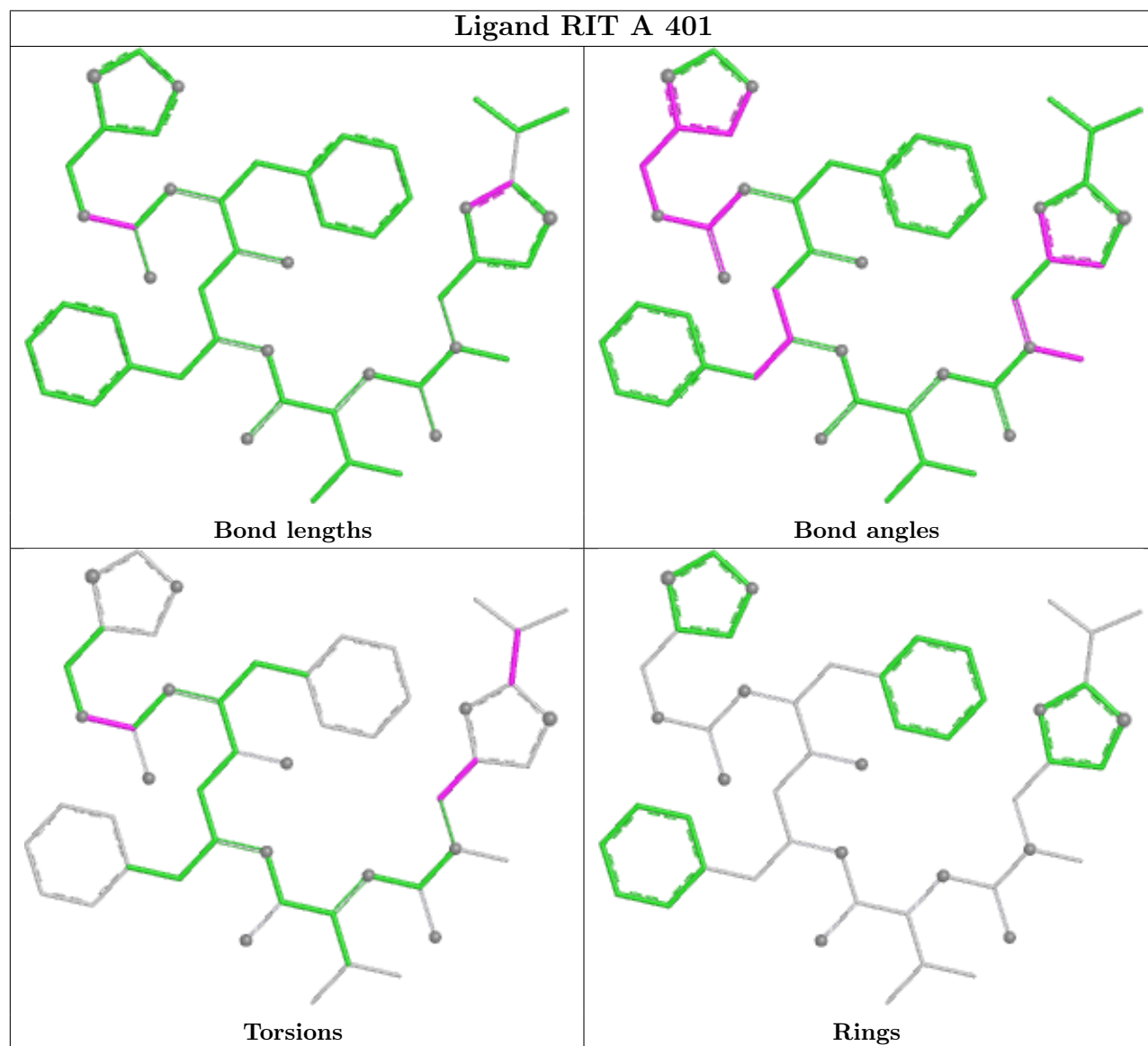
There are no ring outliers.

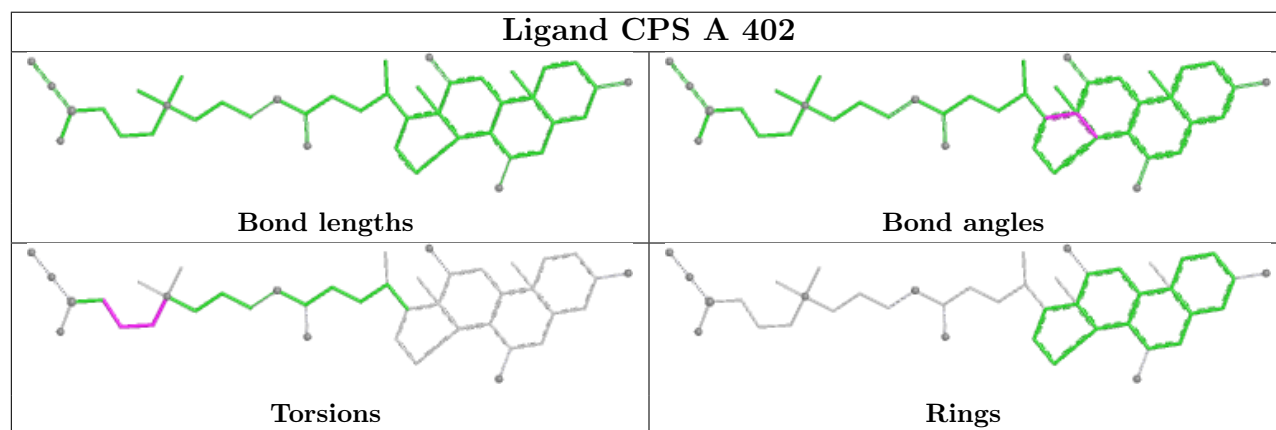
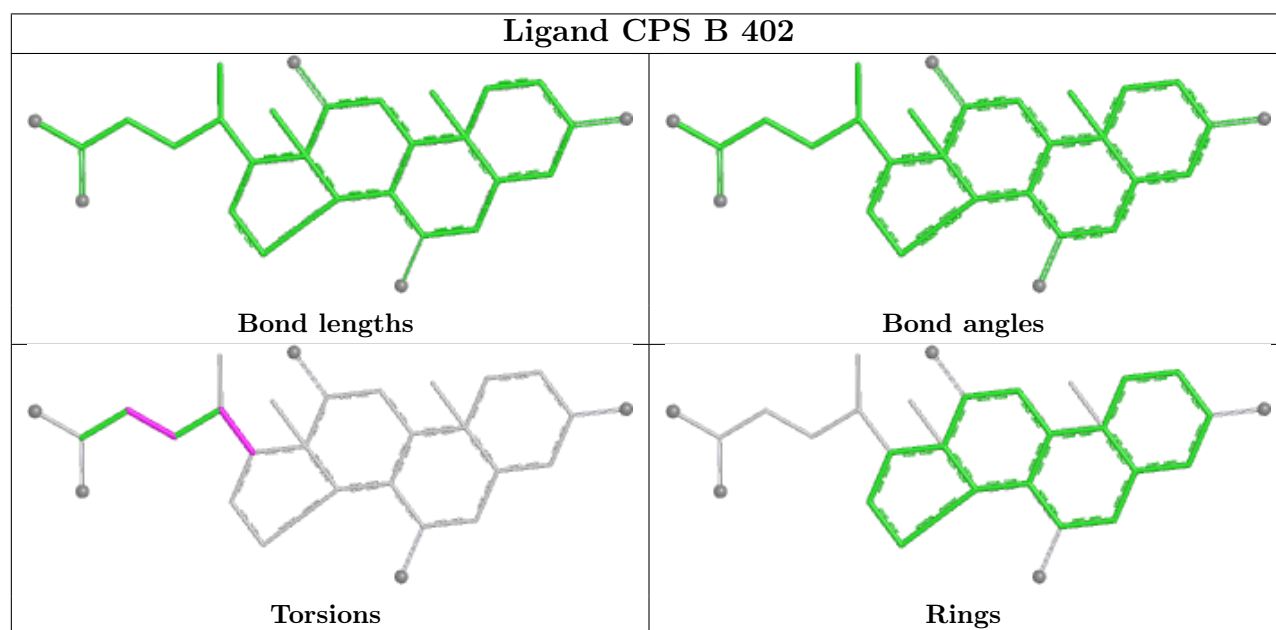
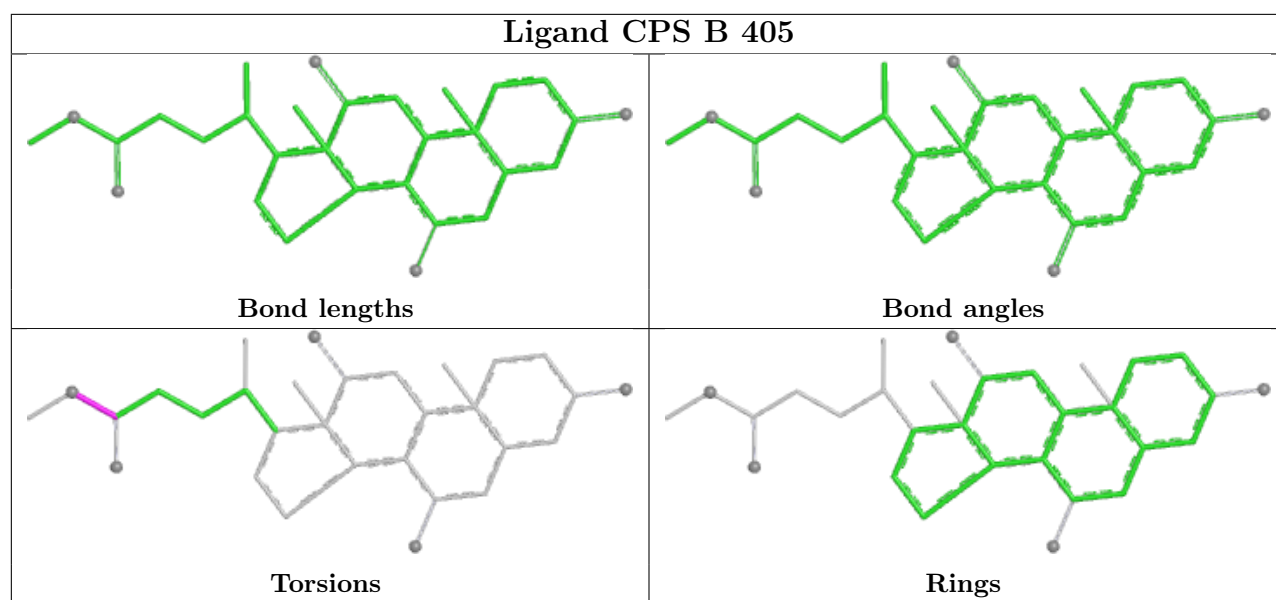
10 monomers are involved in 27 short contacts:

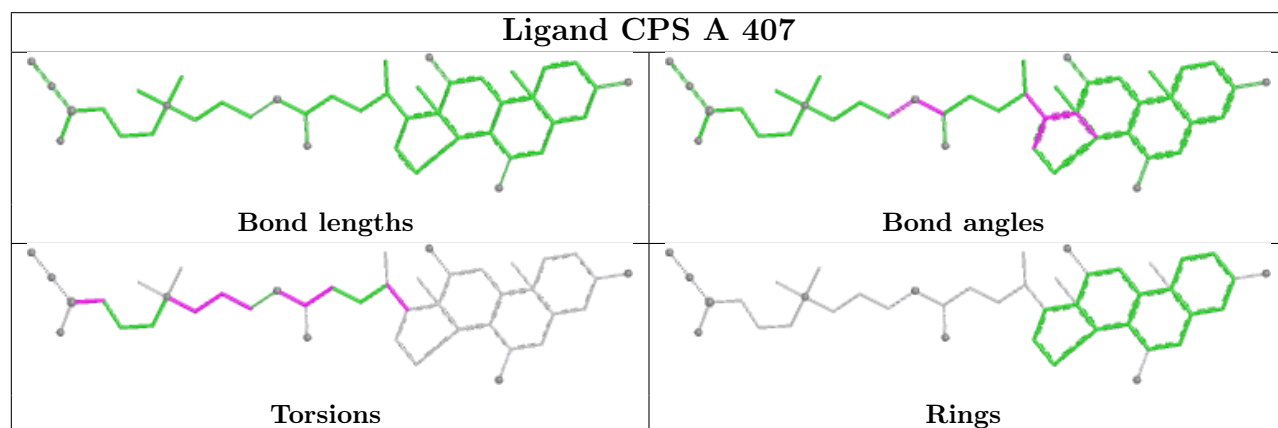
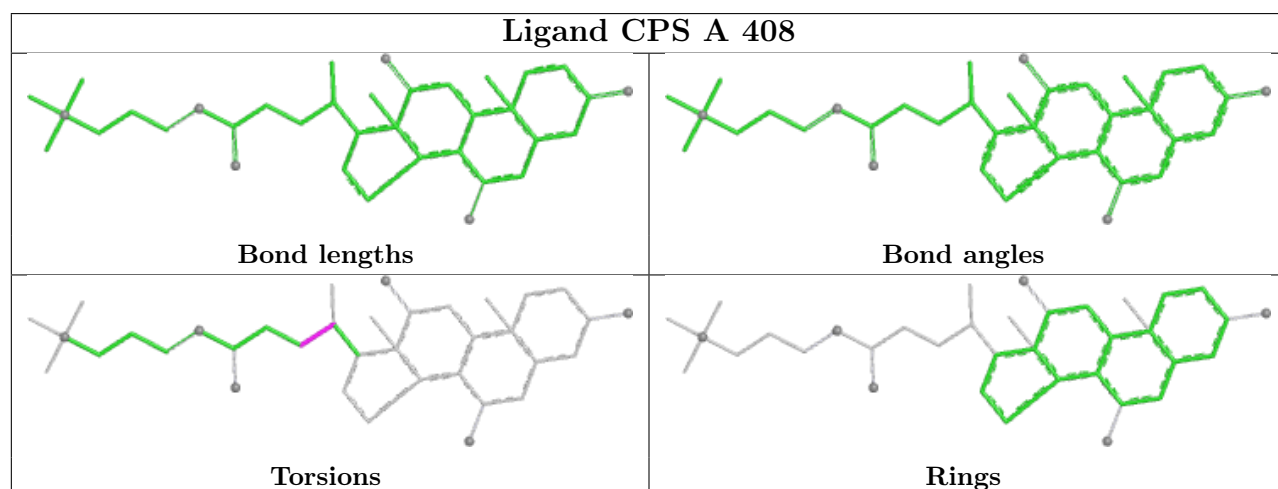
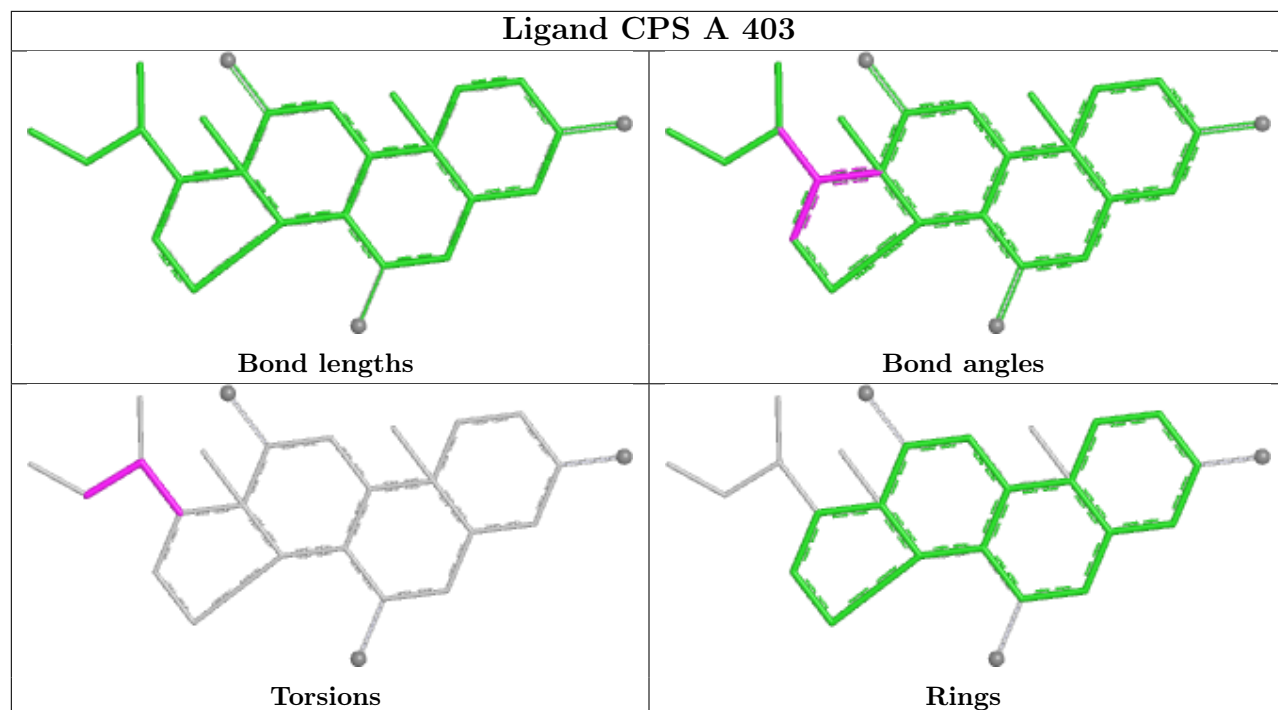
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	CPS	3	0
3	A	402	CPS	1	0
4	B	410	EDO	1	0
3	A	403	CPS	4	0
3	A	407	CPS	7	0
3	B	404	CPS	1	0
2	B	401[A]	RIT	5	0
3	A	405	CPS	1	0
3	B	403	CPS	1	0
2	B	401[B]	RIT	4	0

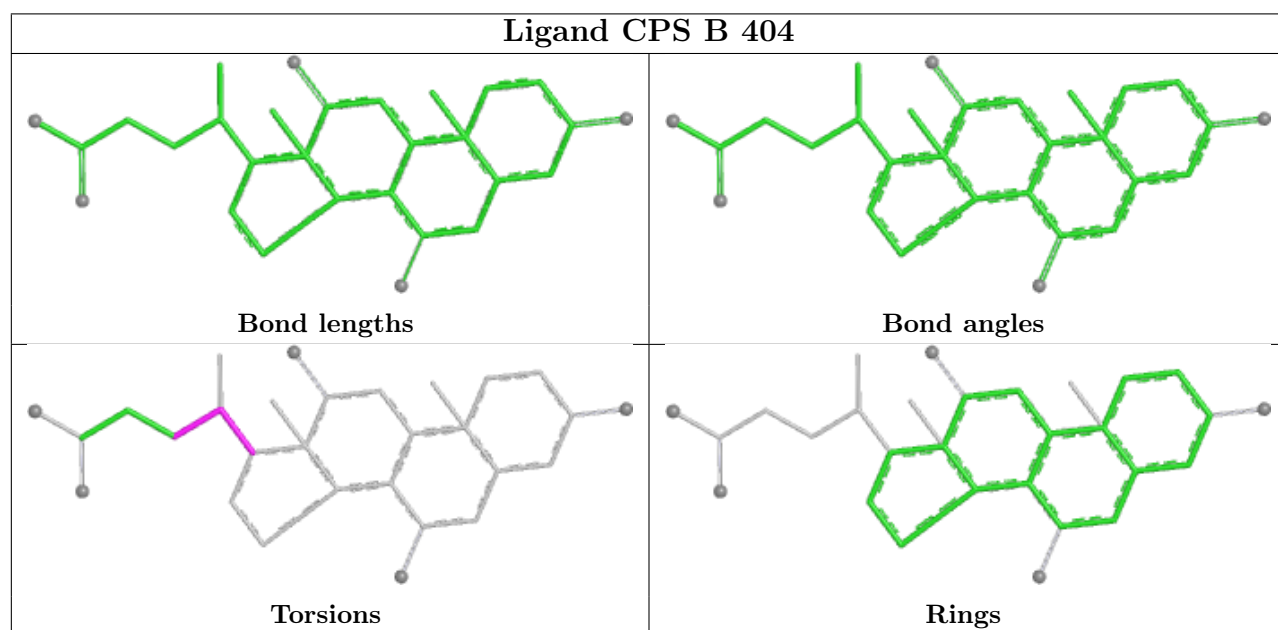
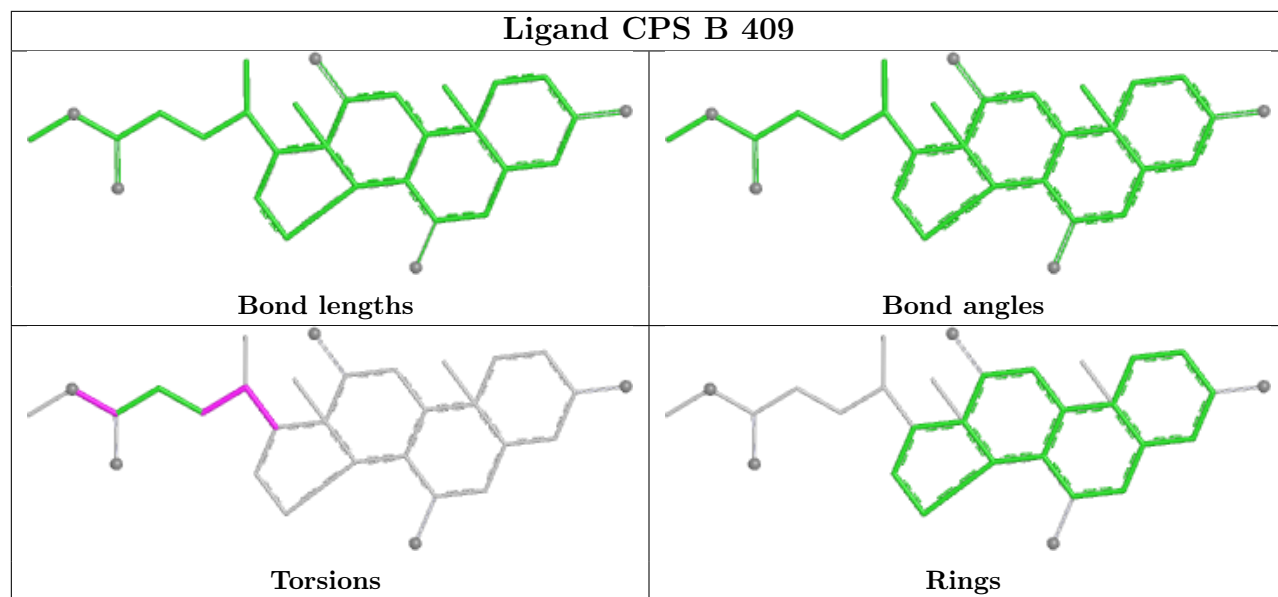
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

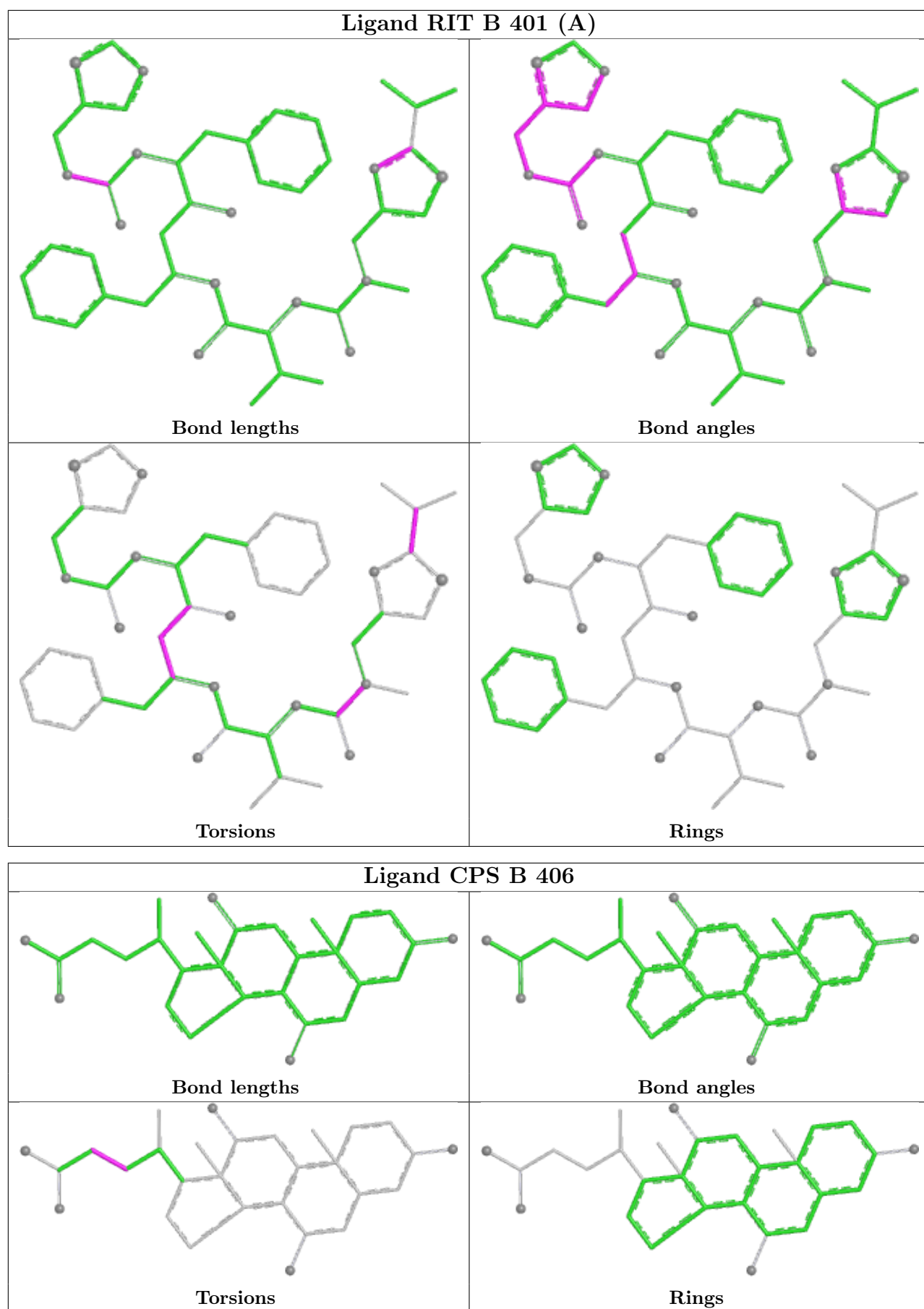
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

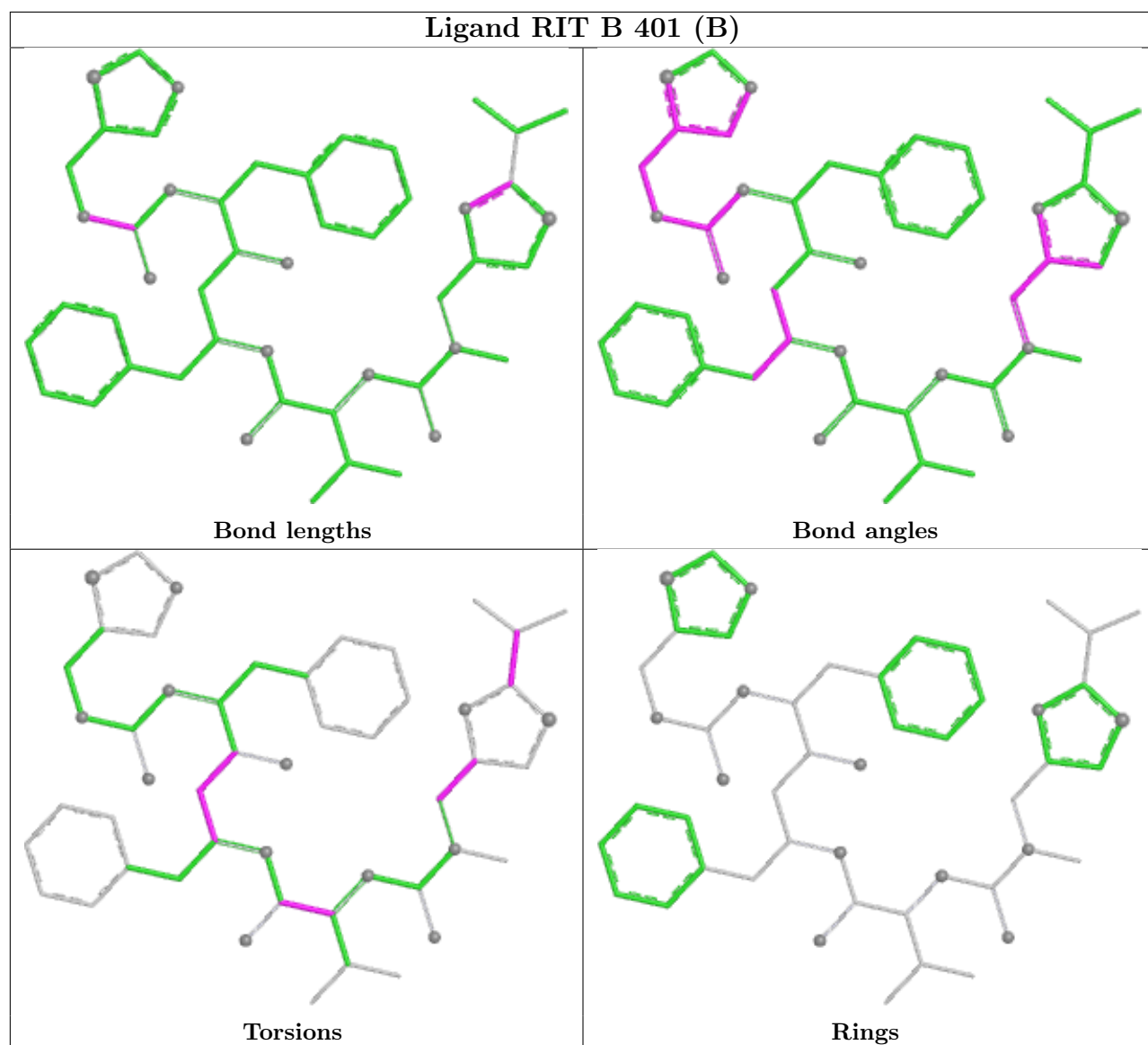
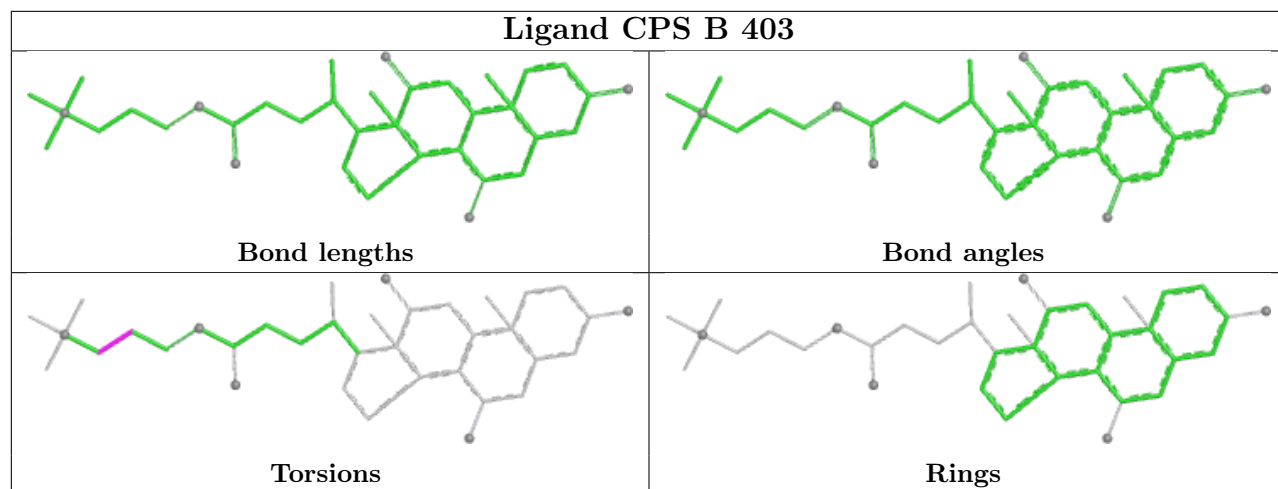












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/331 (99%)	0.67	17 (5%) 33 35	18, 46, 65, 94	6 (1%)
1	B	326/331 (98%)	0.85	23 (7%) 22 23	21, 51, 81, 107	5 (1%)
All	All	655/662 (98%)	0.76	40 (6%) 27 29	18, 48, 76, 107	11 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	LEU	4.8
1	B	298	VAL	4.2
1	A	279	ILE	4.0
1	B	282	VAL	3.5
1	B	279	ILE	3.4
1	A	284	PRO	3.3
1	B	25	GLY	3.2
1	B	284	PRO	2.8
1	A	13	PHE	2.8
1	B	151	ILE	2.8
1	B	27	ASN	2.7
1	B	227	ASP	2.7
1	B	62	SER	2.7
1	B	206	ILE	2.7
1	A	202	HIS	2.6
1	A	111	ASN	2.6
1	A	164	ASP	2.5
1	A	282	VAL	2.4
1	B	285	GLY	2.4
1	B	28	GLN	2.3
1	B	172	ILE	2.3
1	A	264	GLU	2.3
1	B	92	LEU	2.3
1	B	202	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	2.3
1	B	14	GLN	2.3
1	B	184	LEU	2.3
1	B	8	ILE	2.2
1	A	6	ASP	2.2
1	A	193	LEU	2.2
1	B	154	ALA	2.2
1	A	50	THR	2.1
1	B	323	GLY	2.1
1	B	96	GLY	2.1
1	A	99	SER	2.1
1	A	110	THR	2.1
1	A	107	VAL	2.1
1	B	133	LEU	2.1
1	B	142	VAL	2.0
1	A	191	HIS	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(Å ²)	Q<0.9
3	CPS	B	409	30/42	0.65	0.19	66,67,70,72	0
4	EDO	B	410	4/4	0.73	0.22	43,43,43,47	0
4	EDO	A	409	4/4	0.74	0.19	48,49,49,52	0
3	CPS	B	406	29/42	0.80	0.15	56,60,71,73	0
3	CPS	A	408	36/42	0.81	0.17	67,76,80,81	0
3	CPS	A	402	42/42	0.81	0.17	46,50,100,101	0
3	CPS	B	407	22/42	0.81	0.18	61,63,68,71	0

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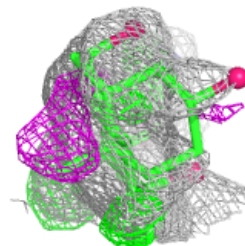
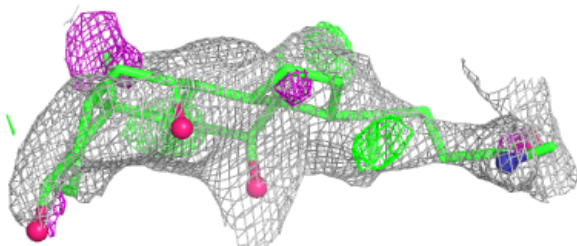
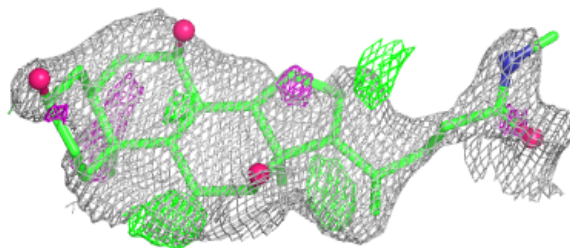
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CPS	B	404	29/42	0.82	0.13	60,61,68,69	0
3	CPS	A	407	42/42	0.83	0.18	70,77,112,112	0
3	CPS	A	404	29/42	0.83	0.15	68,70,75,75	0
3	CPS	B	408	27/42	0.84	0.14	61,63,64,66	0
3	CPS	B	402	29/42	0.84	0.13	59,61,64,64	0
3	CPS	A	403	26/42	0.85	0.13	49,52,57,58	0
3	CPS	A	405	23/42	0.86	0.15	69,71,72,73	0
3	CPS	B	405	30/42	0.87	0.12	47,49,52,54	0
3	CPS	A	406	29/42	0.88	0.12	41,42,45,47	0
2	RIT	B	401[B]	50/50	0.90	0.12	36,41,51,53	50
2	RIT	A	401	50/50	0.90	0.12	35,44,57,60	0
2	RIT	B	401[A]	50/50	0.90	0.12	38,43,53,55	50
3	CPS	B	403	36/42	0.90	0.11	50,52,55,56	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.

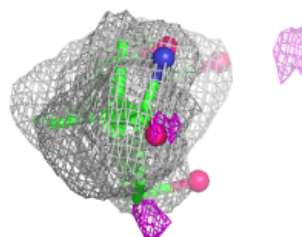
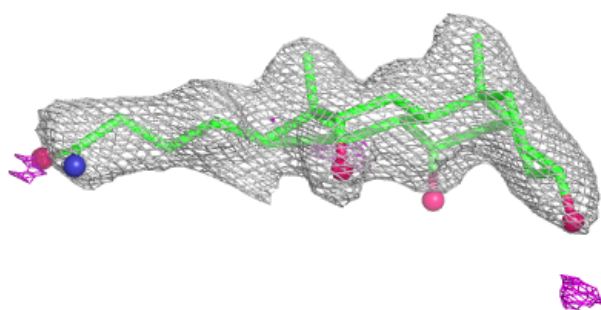
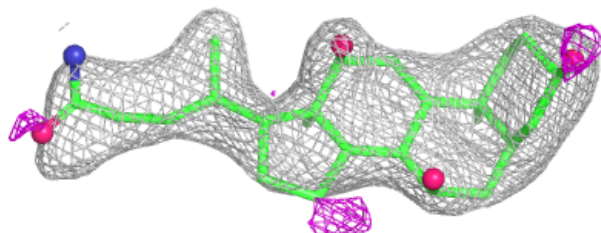
Electron density around CPS B 409:

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

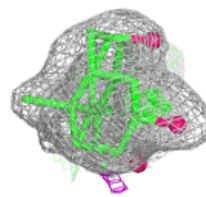
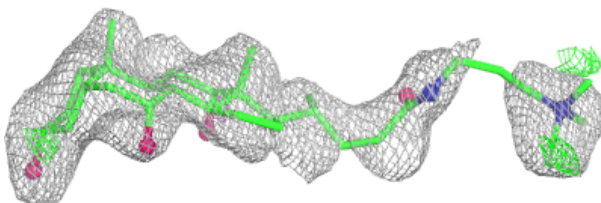
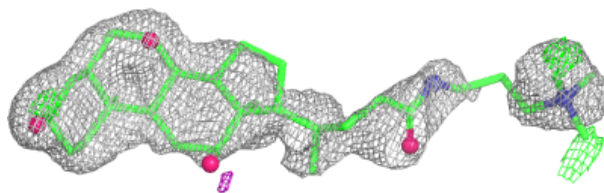


Electron density around CPS B 406:

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

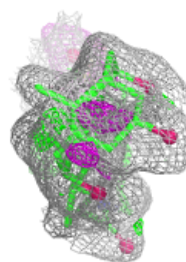
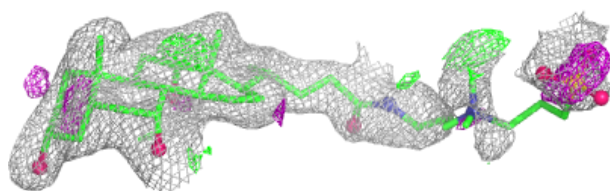
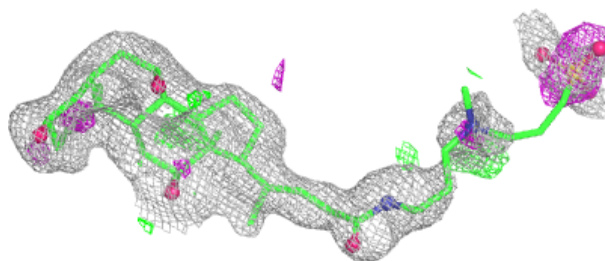
**Electron density around CPS A 408:**

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

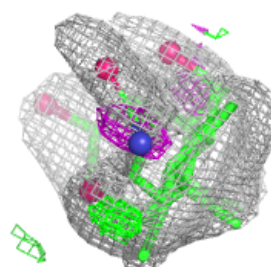
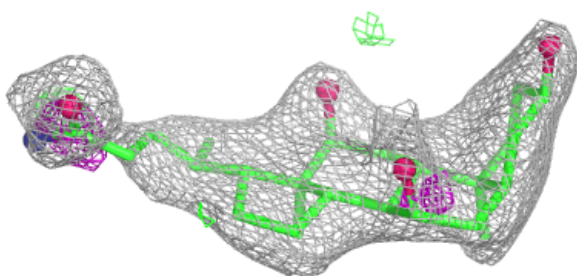
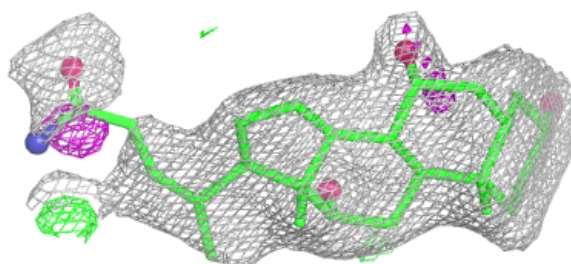


Electron density around CPS A 402:

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

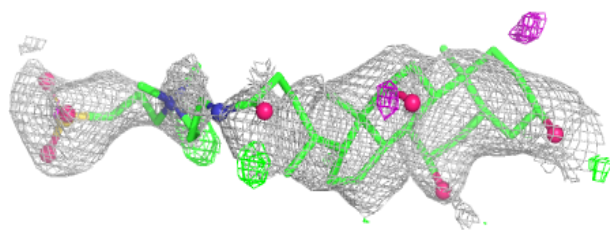
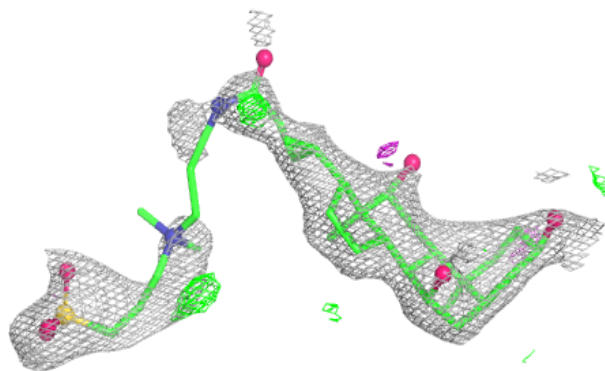
**Electron density around CPS B 404:**

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

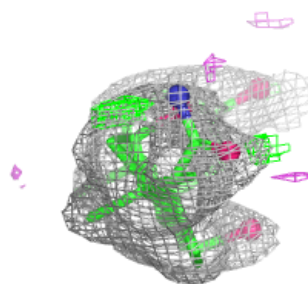
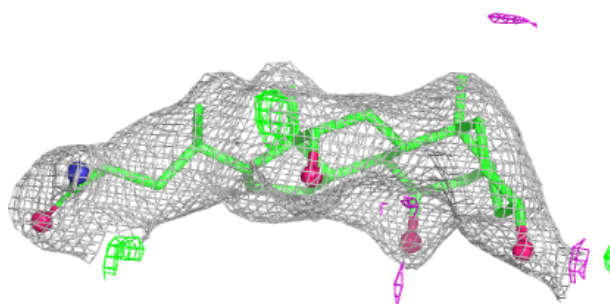
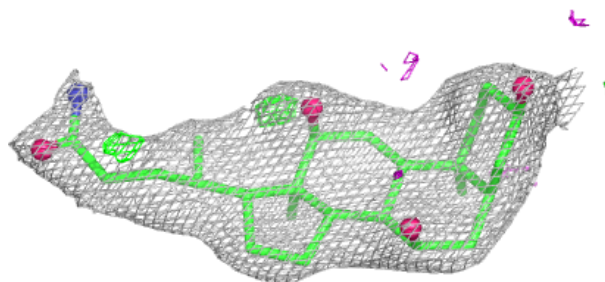


Electron density around CPS A 407:

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

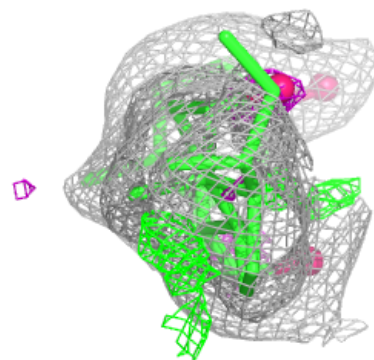
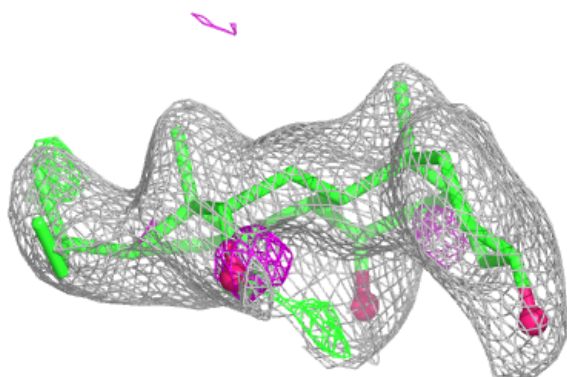
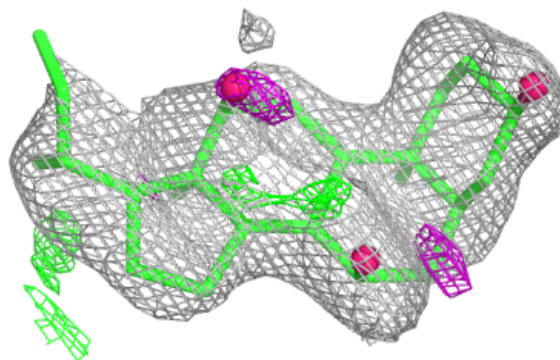
**Electron density around CPS B 402:**

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

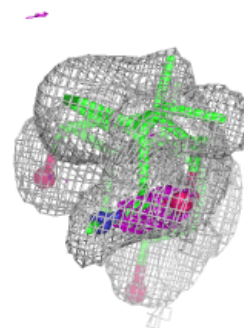
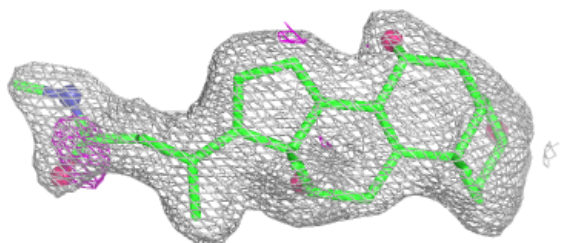
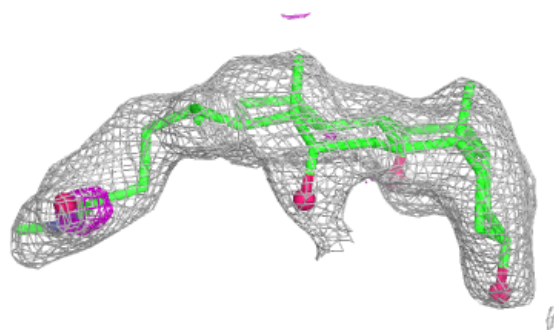


Electron density around CPS A 403:

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

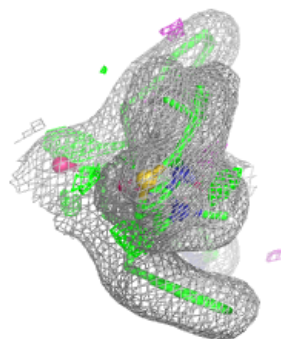
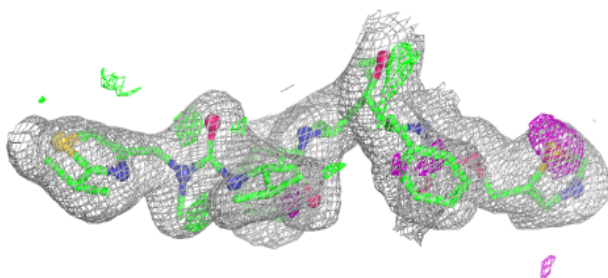
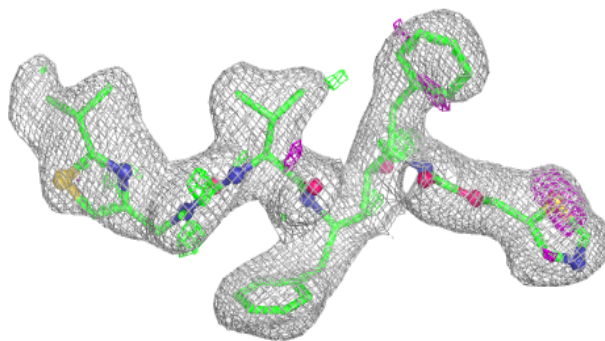
**Electron density around CPS B 405:**

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

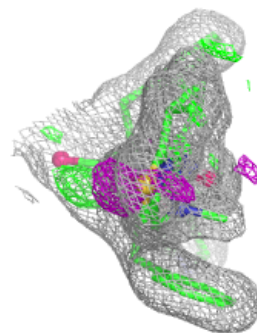
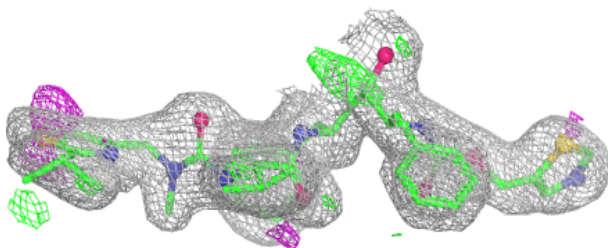
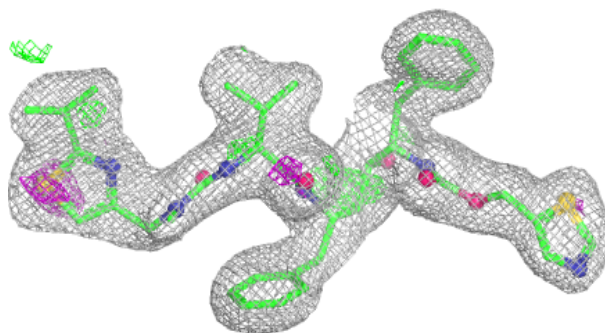


Electron density around RIT B 401 (B):

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

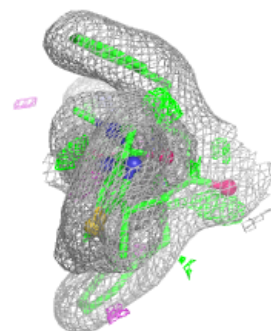
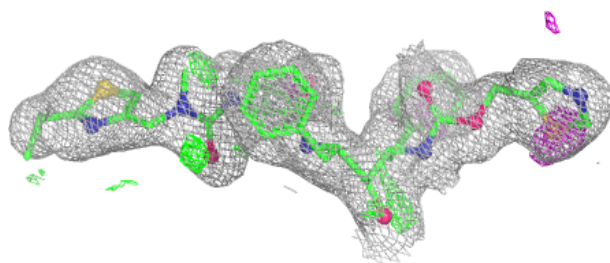
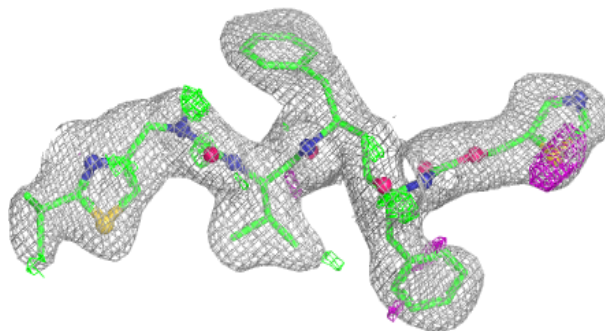
**Electron density around RIT A 401:**

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

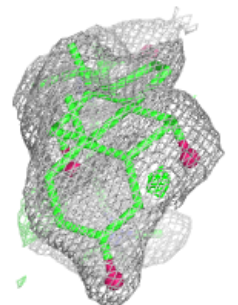
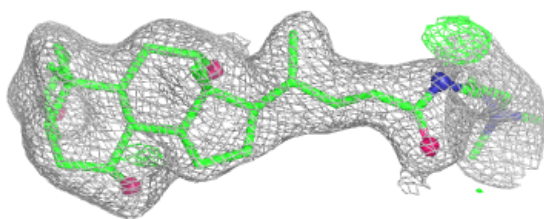
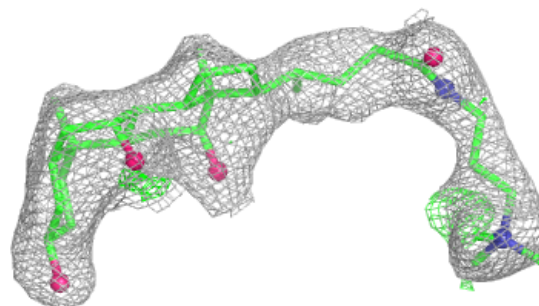


Electron density around RIT B 401 (A):

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

**Electron density around CPS B 403:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.