W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 12:30 PM EDT

PDB ID	:	3H0S
Title	:	Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 7
Authors	:	Vajdos, F.
Deposited on	:	2009-04-10
Resolution	:	2.43 Å(reported)

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

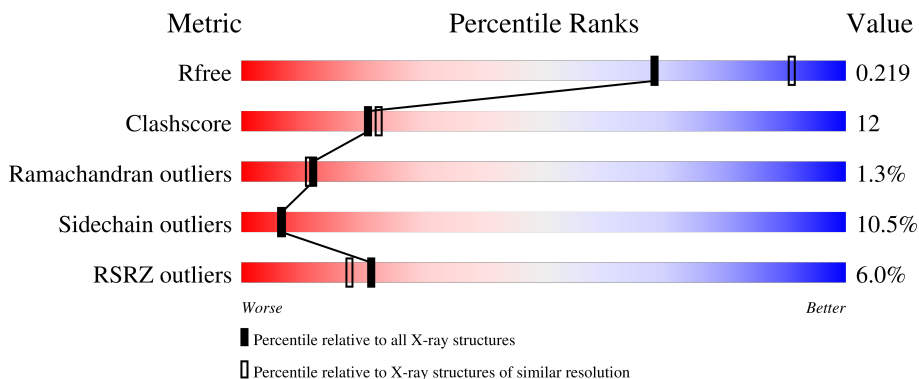|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.43 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		0.219
Clashscore		12
Ramachandran outliers		1.3%
Sidechain outliers		10.5%
RSRZ outliers		6.0%

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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	769	4% — 65% / 20% / 5% · 10%
1	B	769	6% — 62% / 21% / · · 12%
1	C	769	6% — 65% / 17% / 5% · 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	3	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18770 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	1	0
			5538	3525	957	1037	19			
1	B	677	Total	C	N	O	S	0	0	0
			5395	3439	928	1009	19			
1	C	668	Total	C	N	O	S	0	0	0
			5324	3391	916	998	19			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
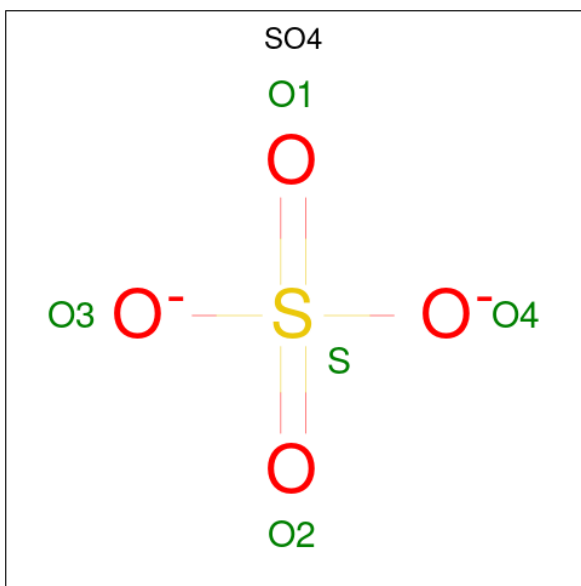
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1'-(1H-indazol-7-ylcarbonyl)-6-methylspiro[chromene-2,4'-piperidin]-4(3H)-one (three-letter code: B38) (formula: $C_{22}H_{21}N_3O_3$).
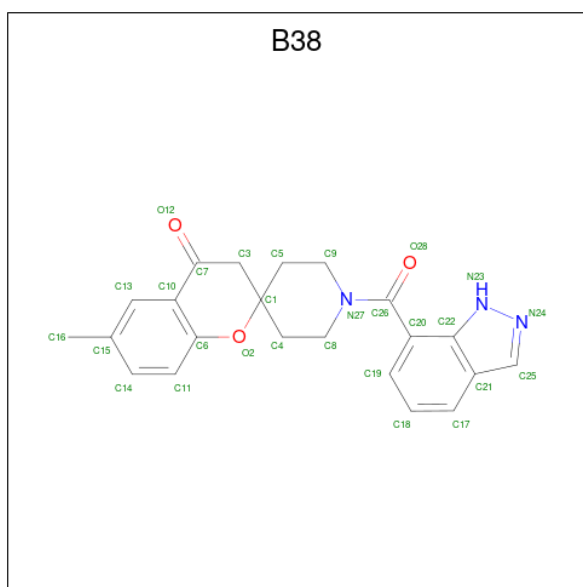
B38

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	1
			39	30	5	4		
3	C	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	861	Total	O	0	0
			861	861		
4	B	762	Total	O	0	0
			762	762		
4	C	780	Total	O	0	0
			780	780		

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: Acetyl-CoA carboxylase

• Molecule 1: Acetyl-CoA carboxylase

• Molecule 1: Acetyl-CoA carboxylase

Chain C:

L2191 E2192 SER PHE ALA GLN ASP LEU ALA LYS LYS ILE ARG ASP SER HIS ASP ASN ALA ILE ASP GLY LEU SER GLU VAL ILE LYS MET LEU SER THR ASP ASP LYS GLU LYS LEU LEU LYS THR LEU LYS LEU GLU HIS HIS HIS HIS HIS HIS

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.72Å 121.68Å 145.99Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	40.70 – 2.43 40.70 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.70-2.43) 98.5 (40.70-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.160 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	15829 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18770	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, B38

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	1.18	20/5668 (0.4%)	1.10	34/7676 (0.4%)
1	B	1.15	14/5516 (0.3%)	1.09	34/7475 (0.5%)
1	C	1.13	13/5441 (0.2%)	1.07	31/7369 (0.4%)
All	All	1.16	47/16625 (0.3%)	1.09	99/22520 (0.4%)

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	2
1	B	0	2
1	C	0	2
All	All	0	6

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1554	GLU	CG-CD	11.50	1.69	1.51
1	C	1575	GLU	CD-OE2	9.50	1.36	1.25
1	A	2117	GLU	CD-OE1	9.17	1.35	1.25
1	B	1575	GLU	CD-OE2	8.64	1.35	1.25
1	A	1805	GLU	CG-CD	8.26	1.64	1.51

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1717	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	B	1745	ARG	NE-CZ-NH2	-16.24	112.18	120.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1717	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	B	1745	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	A	1745	ARG	NE-CZ-NH2	-14.02	113.29	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1786	ASN	Mainchain
1	A	2081	GLU	Peptide
1	B	1745	ARG	Sidechain
1	B	1997	GLY	Peptide
1	C	2044	MET	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	5538	0	5469	137	0
1	B	5395	0	5339	144	0
1	C	5324	0	5264	125	0
2	A	5	0	0	0	0
2	C	10	0	0	2	0
3	A	28	0	21	1	0
3	B	39	0	10	2	0
3	C	28	0	21	1	0
4	A	861	0	0	58	9
4	B	762	0	0	60	0
4	C	780	0	0	60	4
All	All	18770	0	16124	396	9

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 12.

The worst 5 of 396 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:A:1625:SER:HB2	4:A:974:HOH:O	1.37	1.23
1:B:1534:ASP:N	4:B:2475:HOH:O	1.75	1.17
1:A:1556:GLU:HG2	4:A:2327:HOH:O	1.52	1.07
1:B:1960:GLN:HG3	4:B:605:HOH:O	1.54	1.05
1:C:1555:ARG:N	4:C:2372:HOH:O	1.87	1.05

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:HOH:O	4:A:2568:HOH:O[2_555]	1.72	0.48
4:A:307:HOH:O	4:A:2586:HOH:O[2_555]	1.88	0.32
4:A:1181:HOH:O	4:C:126:HOH:O[4_555]	2.04	0.16
4:A:81:HOH:O	4:A:2477:HOH:O[2_555]	2.05	0.15
4:A:1181:HOH:O	4:C:2445:HOH:O[4_555]	2.05	0.15

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	690/769 (90%)	645 (94%)	38 (6%)	7 (1%)	15	16
1	B	673/769 (88%)	622 (92%)	42 (6%)	9 (1%)	12	11
1	C	664/769 (86%)	620 (93%)	34 (5%)	10 (2%)	10	9
All	All	2027/2307 (88%)	1887 (93%)	114 (6%)	26 (1%)	12	11

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	1673	ASN
1	A	1683	ASN
1	B	1481	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1650	ASP

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	589/658 (90%)	536 (91%)	53 (9%)	9	10
1	B	574/658 (87%)	508 (88%)	66 (12%)	5	5
1	C	566/658 (86%)	504 (89%)	62 (11%)	6	5
All	All	1729/1974 (88%)	1548 (90%)	181 (10%)	7	6

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2152	ILE
1	C	1769	GLU
1	C	1508	VAL
1	C	1571	VAL
1	C	1852	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1748	GLN
1	C	1911	ASN
1	B	1941	ASN
1	C	1815	ASN
1	C	2011	GLN

5.3.3 RNA (i)

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 ⓘ

7 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	$\#|Z| > 2$
3	B38	B	102[B]	-	32,32,32	2.64	13 (40%)	32,48,48	1.51	5 (15%)
2	SO4	A	2	-	4,4,4	0.28	0	6,6,6	0.84	0
2	SO4	C	3	-	4,4,4	0.13	0	6,6,6	0.47	0
3	B38	B	102[A]	-	32,32,32	2.67	13 (40%)	32,48,48	1.56	5 (15%)
3	B38	A	101	-	32,32,32	2.54	13 (40%)	32,48,48	1.25	3 (9%)
3	B38	C	100	-	32,32,32	2.58	11 (34%)	32,48,48	1.39	4 (12%)
2	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B38	B	102[B]	-	-	4/8/34/34	0/5/5/5
3	B38	C	100	-	-	0/8/34/34	0/5/5/5
3	B38	B	102[A]	-	-	0/8/34/34	0/5/5/5
3	B38	A	101	-	-	0/8/34/34	0/5/5/5

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	102[A]	B38	C13-C15	6.86	1.50	1.39
3	B	102[B]	B38	C13-C15	6.86	1.50	1.39
3	C	100	B38	C13-C15	6.80	1.50	1.39
3	C	100	B38	C14-C11	6.67	1.50	1.38
3	A	101	B38	C14-C11	6.43	1.50	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	100	B38	C3-C7-C10	-3.60	111.51	116.49
3	B	102[A]	B38	O2-C1-C3	-3.33	105.53	109.64
3	B	102[B]	B38	O2-C1-C3	-3.33	105.53	109.64
3	B	102[A]	B38	C6-C10-C7	-3.32	117.94	119.85
3	B	102[B]	B38	C6-C10-C7	-3.32	117.94	119.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	102[B]	B38	C20-C26-N27-C9
3	B	102[B]	B38	O28-C26-N27-C9
3	B	102[B]	B38	C20-C26-N27-C8
3	B	102[B]	B38	O28-C26-N27-C8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	102[B]	B38	2	0
2	C	3	SO4	2	0
3	A	101	B38	1	0
3	C	100	B38	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 B38 B 102 (B)	
Bond lengths	Bond angles
Torsions	Rings

Ligand B38 B 102 (A)	
Bond lengths	Bond angles
Torsions	Rings

Ligand B38 A 101

Bond lengths

Bond angles

Torsions

Rings

Ligand B38 C 100

Bond lengths

Bond angles

Torsions

Rings
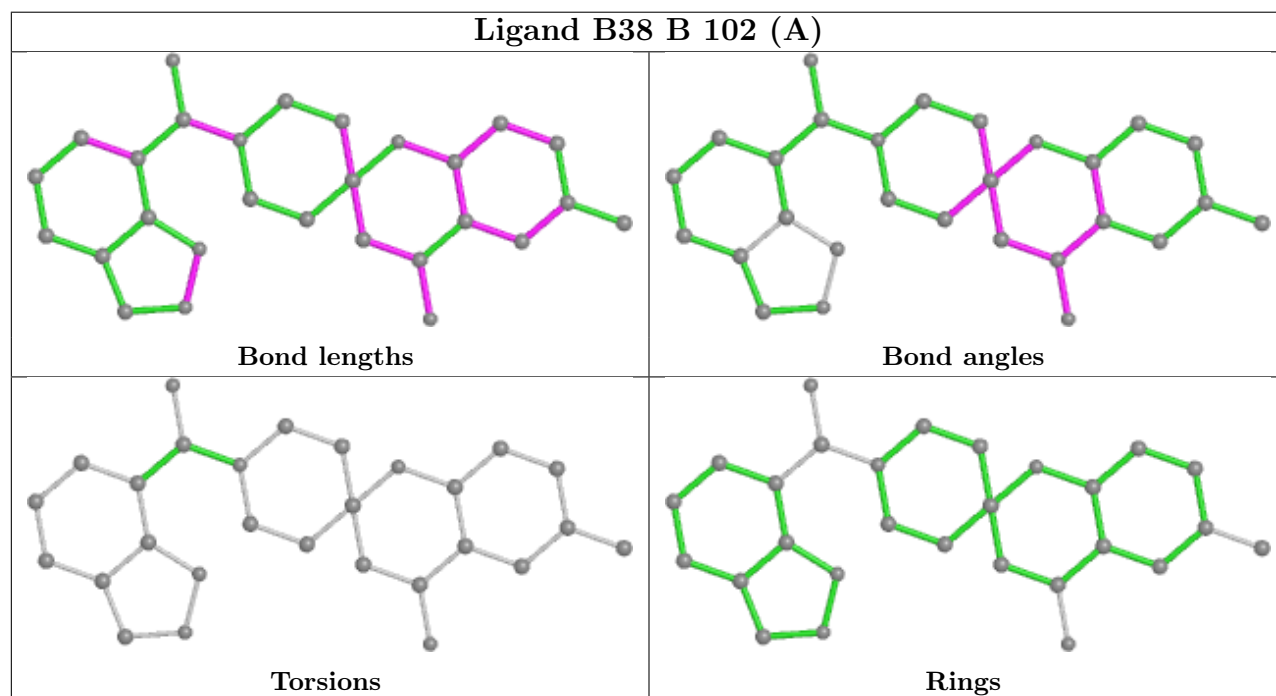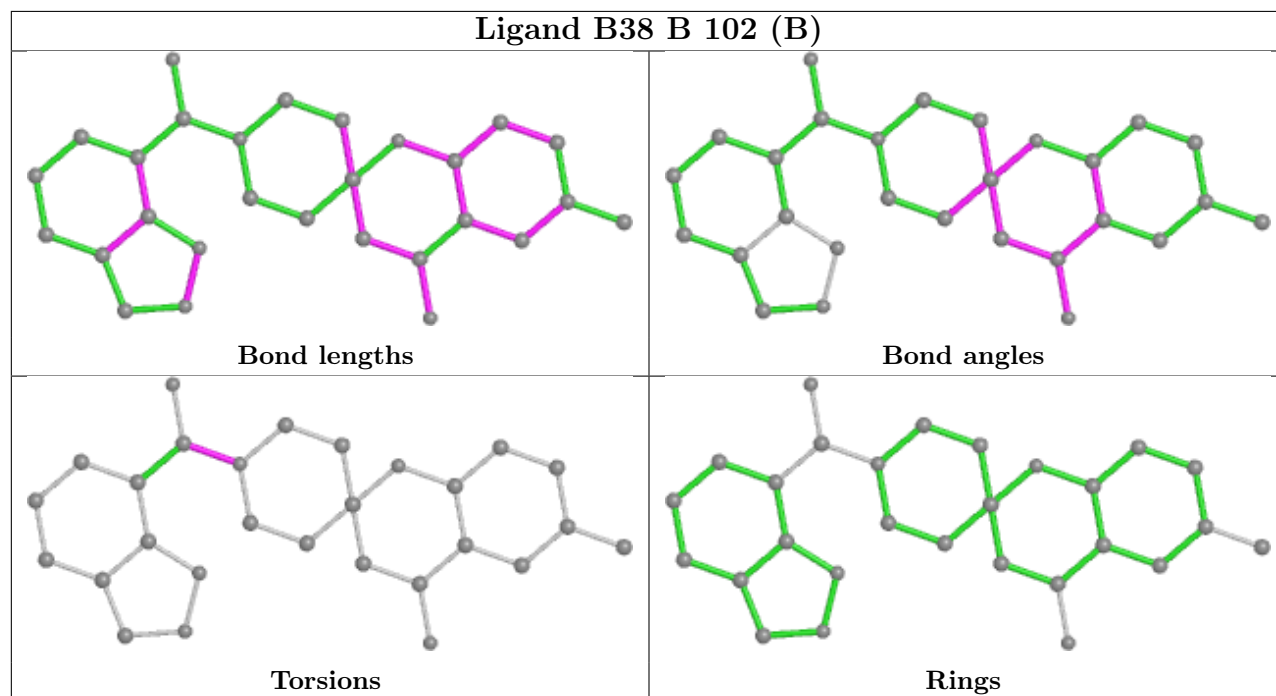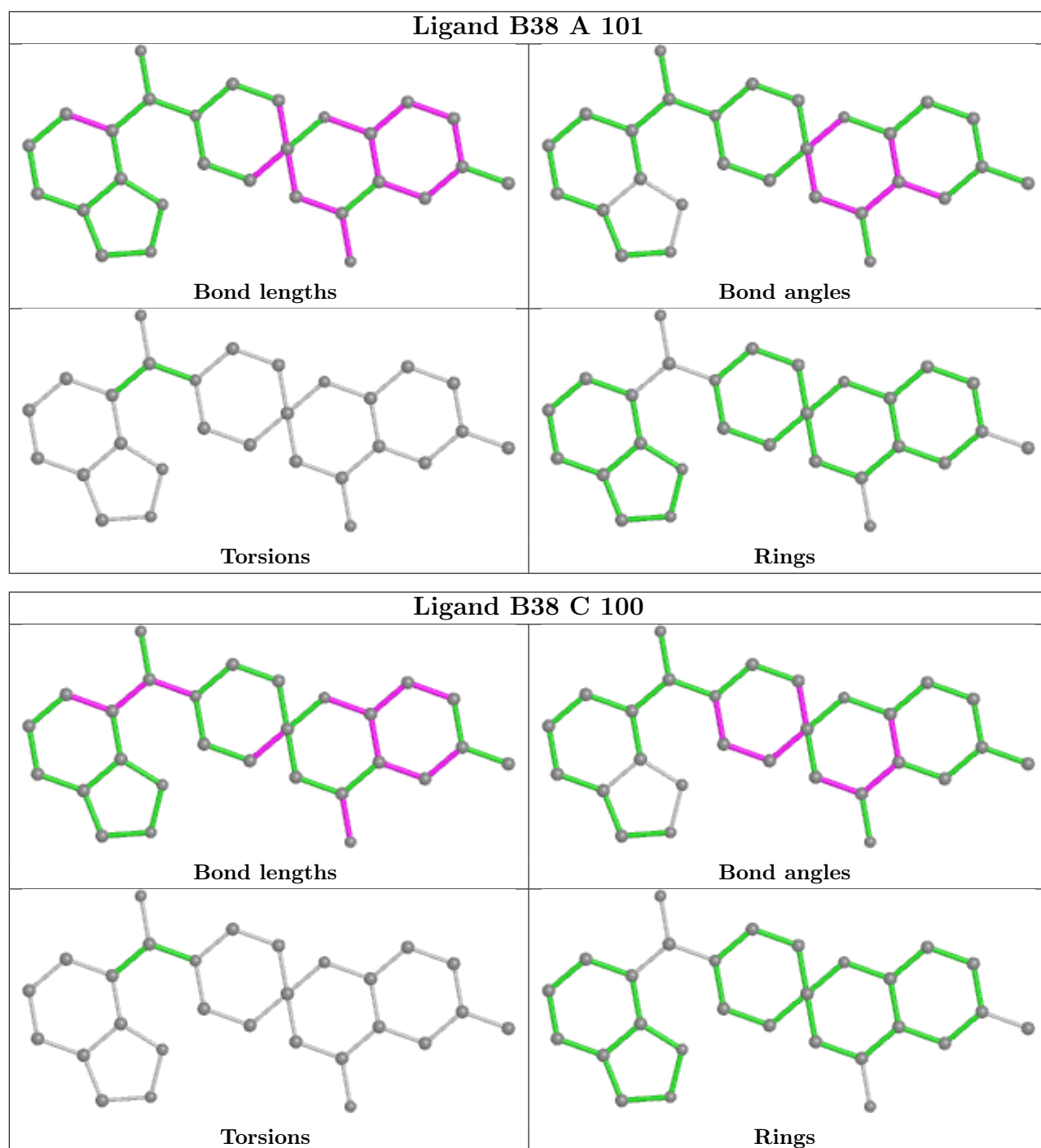
5.7 Other polymers ⓘ

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	693/769 (90%)	-0.16	31 (4%)	33	30	30, 45, 98, 125	0
1	B	677/769 (88%)	-0.00	43 (6%)	19	16	29, 49, 101, 125	0
1	C	668/769 (86%)	-0.07	49 (7%)	15	11	29, 48, 109, 131	0
All	All	2038/2307 (88%)	-0.08	123 (6%)	21	18	29, 47, 102, 131	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2194	PHE	7.4
1	B	2082	LEU	6.3
1	C	1644	ASN	5.8
1	B	2086	TYR	5.7
1	C	2143	VAL	5.3

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

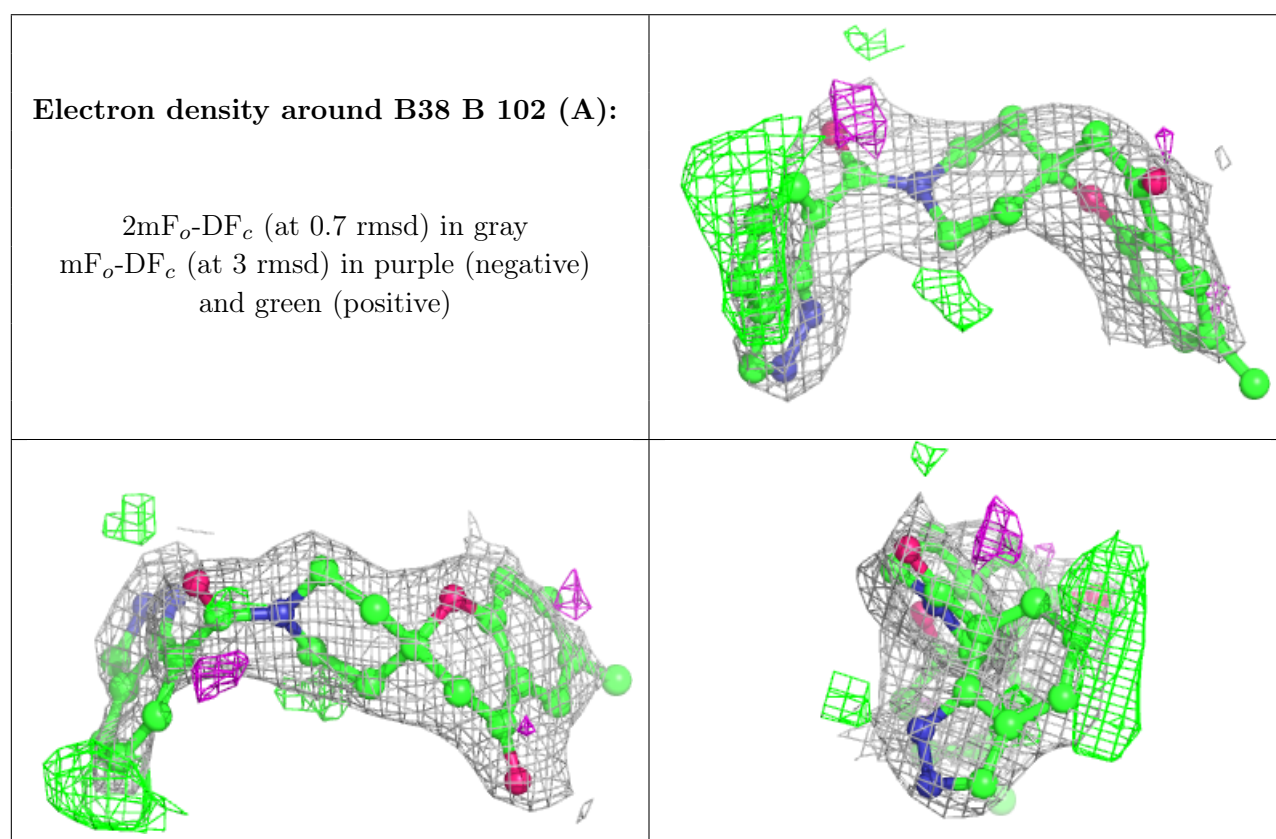There are no non-standard protein/DNA/RNA residues in this entry.

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
3	B38	B	102[A]	28/28	0.85	0.26	83,88,91,92	11
3	B38	B	102[B]	28/28	0.85	0.26	83,90,91,92	11
3	B38	C	100	28/28	0.88	0.17	67,78,82,83	0
3	B38	A	101	28/28	0.90	0.16	71,80,90,91	0
2	SO4	A	2	5/5	0.96	0.28	85,86,88,91	0
2	SO4	C	3	5/5	0.96	0.38	120,120,121,122	0
2	SO4	C	1	5/5	0.98	0.20	81,82,83,84	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.
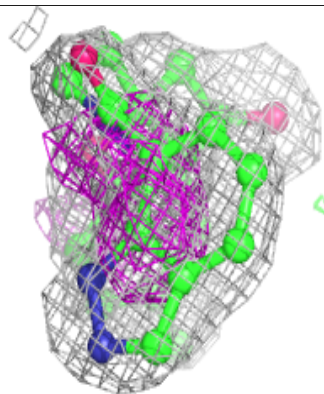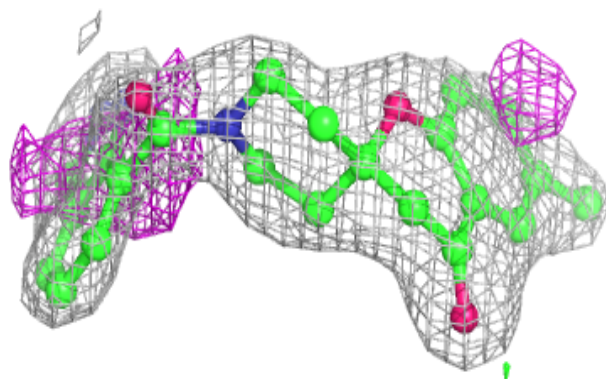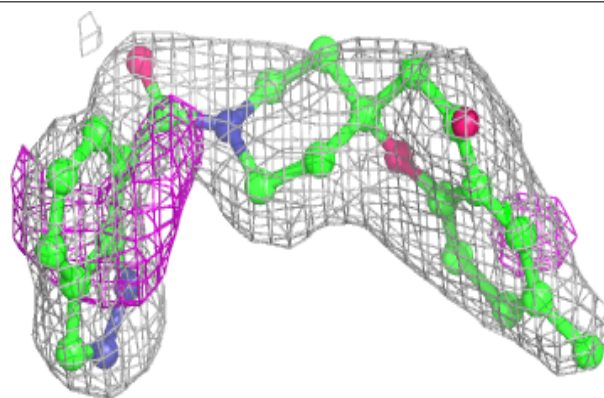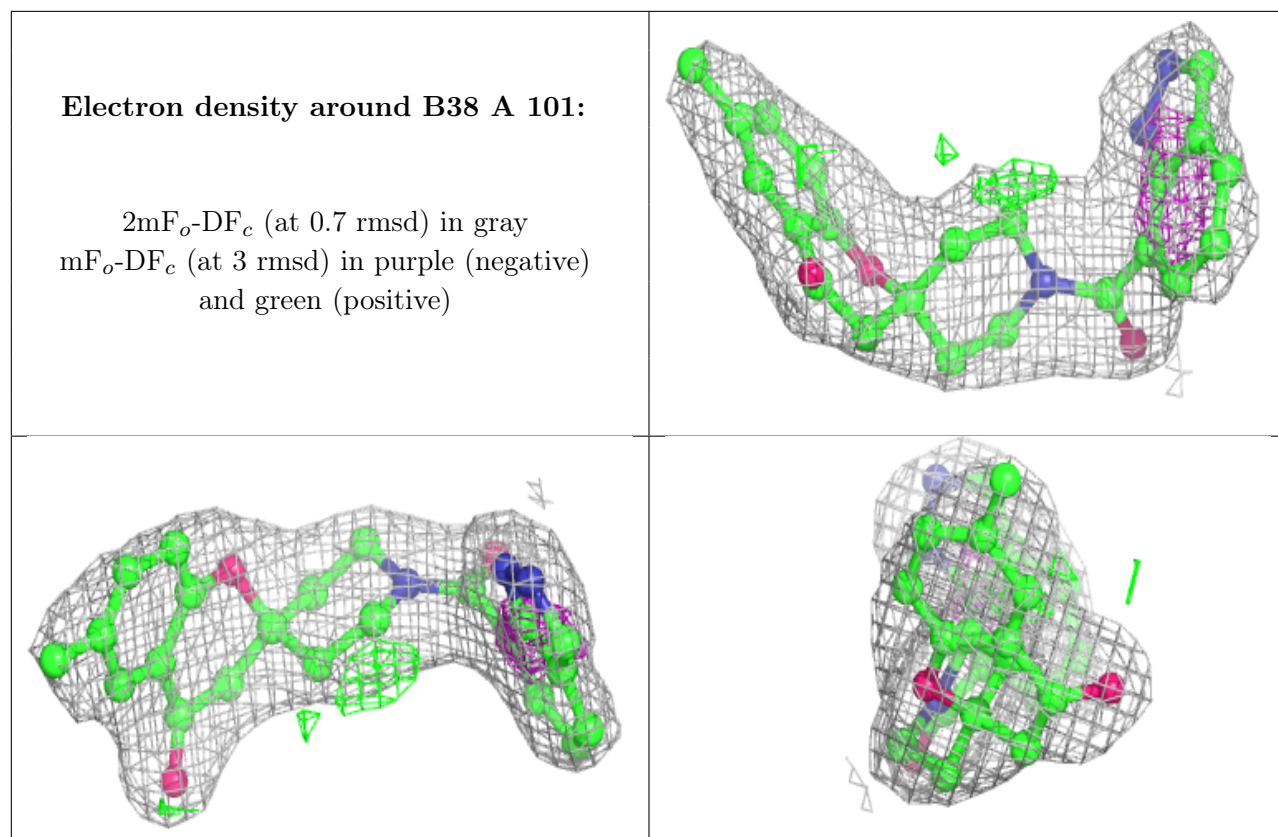

Electron density around B38 B 102 (A):

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

Electron density around B38 B 102 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
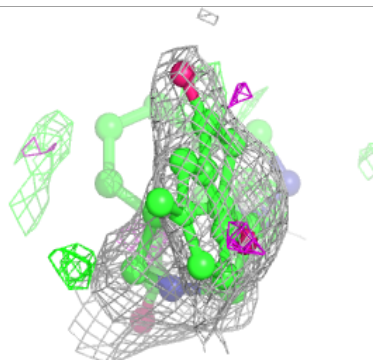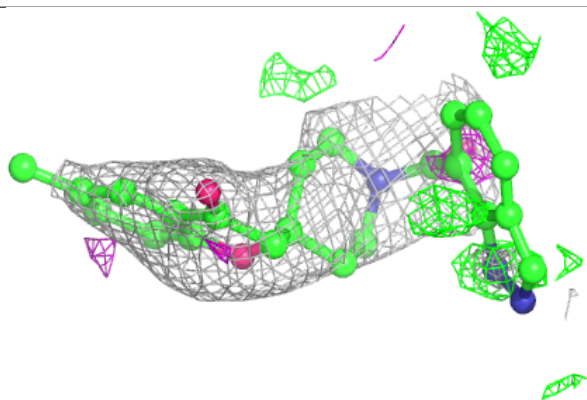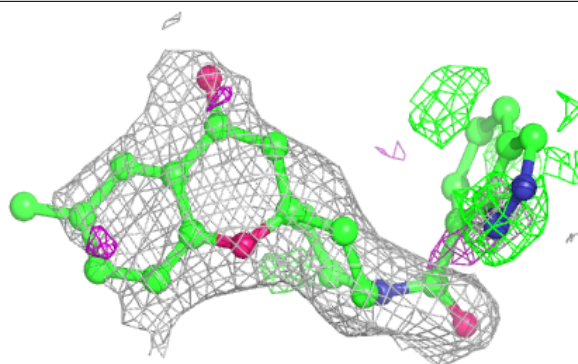
Electron density around B38 C 100:

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

Electron density around B38 A 101:

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.