



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:45 AM UTC

PDB ID : 4N5M / pdb_00004n5m
Title : Crystal structure of (R)-3-hydroxybutyryl-CoA dehydrogenase from *Ralstonia eutropha* in complexed with acetoacetyl-CoA
Authors : Kim, J.-E.; Kim, S.; Kim, K.-J.
Deposited on : 2013-10-10
Resolution : 1.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

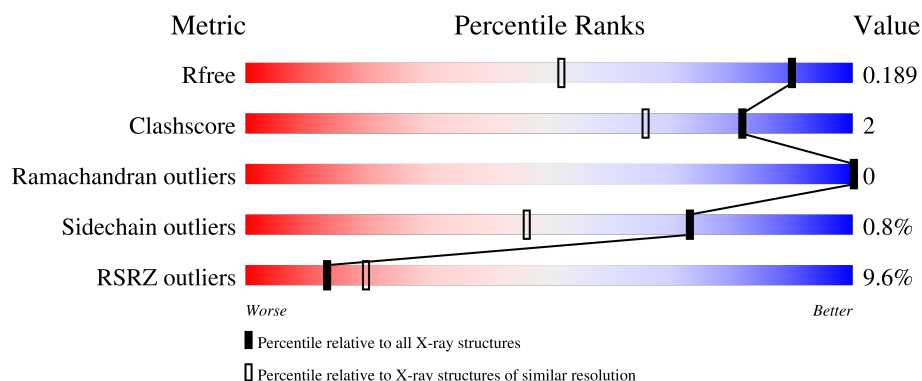
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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 $\leq 5\%$. 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	270	9% 77% 13% 9%
1	B	270	9% 82% 9% 9%

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
3	GOL	A	304	-	-	X	-
3	GOL	B	303	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4397 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 Acetoacetyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1851	1158	326	357	10			
1	B	246	Total	C	N	O	S	0	1	0
			1859	1162	327	360	10			

There are 48 discrepancies between the modelled and reference sequences:

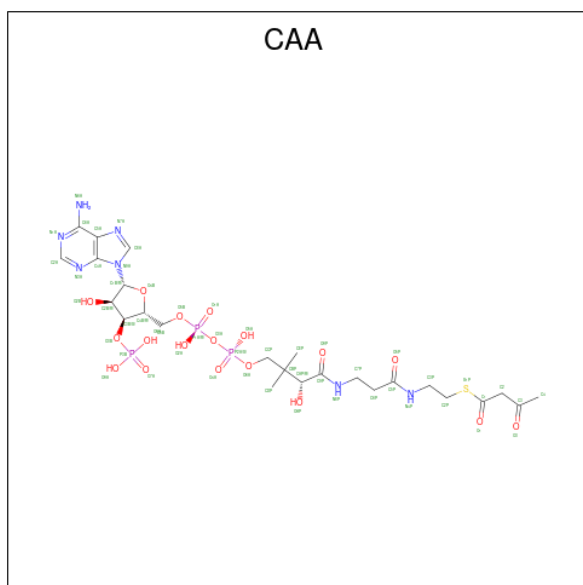
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P14697
A	-22	SER	-	expression tag	UNP P14697
A	-21	TYR	-	expression tag	UNP P14697
A	-20	TYR	-	expression tag	UNP P14697
A	-19	HIS	-	expression tag	UNP P14697
A	-18	HIS	-	expression tag	UNP P14697
A	-17	HIS	-	expression tag	UNP P14697
A	-16	HIS	-	expression tag	UNP P14697
A	-15	HIS	-	expression tag	UNP P14697
A	-14	HIS	-	expression tag	UNP P14697
A	-13	ASP	-	expression tag	UNP P14697
A	-12	TYR	-	expression tag	UNP P14697
A	-11	ASP	-	expression tag	UNP P14697
A	-10	ILE	-	expression tag	UNP P14697
A	-9	PRO	-	expression tag	UNP P14697
A	-8	THR	-	expression tag	UNP P14697
A	-7	GLU	-	expression tag	UNP P14697
A	-6	ASN	-	expression tag	UNP P14697
A	-5	LEU	-	expression tag	UNP P14697
A	-4	TYR	-	expression tag	UNP P14697
A	-3	PHE	-	expression tag	UNP P14697
A	-2	GLN	-	expression tag	UNP P14697
A	-1	GLY	-	expression tag	UNP P14697
A	0	ALA	-	expression tag	UNP P14697
B	-23	MET	-	expression tag	UNP P14697

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	SER	-	expression tag	UNP P14697
B	-21	TYR	-	expression tag	UNP P14697
B	-20	TYR	-	expression tag	UNP P14697
B	-19	HIS	-	expression tag	UNP P14697
B	-18	HIS	-	expression tag	UNP P14697
B	-17	HIS	-	expression tag	UNP P14697
B	-16	HIS	-	expression tag	UNP P14697
B	-15	HIS	-	expression tag	UNP P14697
B	-14	HIS	-	expression tag	UNP P14697
B	-13	ASP	-	expression tag	UNP P14697
B	-12	TYR	-	expression tag	UNP P14697
B	-11	ASP	-	expression tag	UNP P14697
B	-10	ILE	-	expression tag	UNP P14697
B	-9	PRO	-	expression tag	UNP P14697
B	-8	THR	-	expression tag	UNP P14697
B	-7	GLU	-	expression tag	UNP P14697
B	-6	ASN	-	expression tag	UNP P14697
B	-5	LEU	-	expression tag	UNP P14697
B	-4	TYR	-	expression tag	UNP P14697
B	-3	PHE	-	expression tag	UNP P14697
B	-2	GLN	-	expression tag	UNP P14697
B	-1	GLY	-	expression tag	UNP P14697
B	0	ALA	-	expression tag	UNP P14697

- Molecule 2 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			54	25	7	18	3	1	0
2	B	1	Total	C	N	O	P	S	
			54	25	7	18	3	1	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			6	3	3	0	0
3	A	1	Total	C	O		
			6	3	3	0	0
3	A	1	Total	C	O		
			6	3	3	0	0
3	B	1	Total	C	O		
			6	3	3	0	0
3	B	1	Total	C	O		
			6	3	3	0	0
3	B	1	Total	C	O		
			6	3	3	0	0

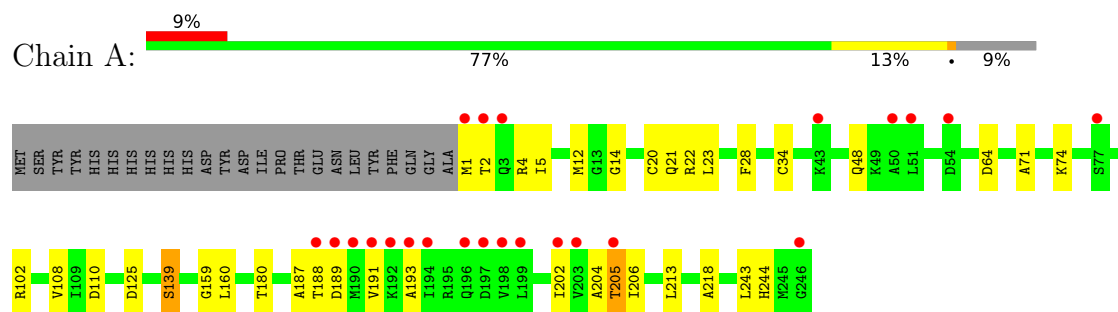
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O		
			275	275	0	0
4	B	268	Total	O		
			268	268	0	0

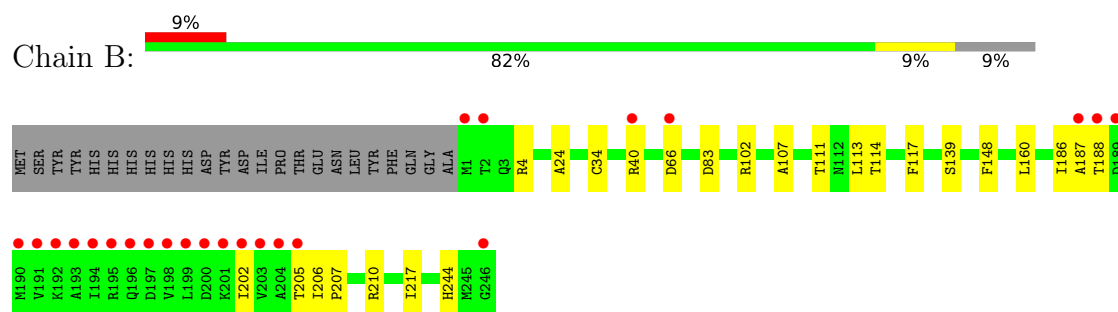
3 Residue-property plots [i](#)

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: Acetoacetyl-CoA reductase



• Molecule 1: Acetoacetyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.57Å 139.57Å 70.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.39 – 1.34 23.39 – 1.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (23.39-1.34) 99.3 (23.39-1.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 1.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.188 0.170 , 0.189	Depositor DCC
R_{free} test set	7752 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4397	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.73	19/1880 (1.0%)	1.51	12/2540 (0.5%)
1	B	1.67	14/1888 (0.7%)	1.49	8/2551 (0.3%)
All	All	1.70	33/3768 (0.9%)	1.50	20/5091 (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	1
1	B	0	1
All	All	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	PRO	N-CD	9.30	1.60	1.47
1	B	206	ILE	C-O	-8.91	1.13	1.24
1	B	187	ALA	CA-C	8.79	1.63	1.53
1	B	187	ALA	C-O	-7.73	1.15	1.23
1	B	206	ILE	C-N	-7.53	1.22	1.33
1	A	34	CYS	CA-C	7.20	1.61	1.52
1	A	180	THR	N-CA	-6.88	1.37	1.46
1	B	188	THR	N-CA	6.73	1.54	1.45
1	A	187	ALA	C-O	-6.71	1.16	1.23
1	A	110	ASP	CG-OD2	-6.68	1.12	1.25
1	A	71	ALA	C-O	6.68	1.31	1.24
1	A	191	VAL	C-O	6.50	1.31	1.24
1	A	12	MET	SD-CE	-6.46	1.63	1.79
1	A	64	ASP	C-O	6.40	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	ASP	CG-OD2	-6.23	1.13	1.25
1	A	205	THR	CB-CG2	-6.08	1.32	1.52
1	B	24	ALA	N-CA	6.01	1.53	1.46
1	A	139	SER	CA-C	5.95	1.60	1.52
1	A	206	ILE	C-O	-5.86	1.16	1.24
1	B	111	THR	CB-CG2	-5.74	1.33	1.52
1	A	188	THR	N-CA	5.56	1.52	1.45
1	A	218	ALA	C-O	-5.50	1.17	1.24
1	A	28	PHE	CA-CB	5.47	1.62	1.53
1	A	14	GLY	C-O	5.40	1.31	1.23
1	A	188	THR	CA-C	5.37	1.59	1.52
1	B	148	PHE	CA-CB	5.29	1.62	1.53
1	B	4	ARG	C-O	-5.23	1.17	1.23
1	A	193	ALA	N-CA	5.18	1.53	1.46
1	B	210	ARG	CA-CB	-5.17	1.45	1.53
1	A	108	VAL	CA-CB	-5.17	1.47	1.54
1	A	204	ALA	C-O	-5.11	1.17	1.24
1	B	117	PHE	CA-C	5.07	1.59	1.52
1	B	217	ILE	C-O	5.02	1.30	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ILE	CA-C-O	21.30	131.05	119.12
1	B	207	PRO	CA-N-CD	-8.68	99.85	112.00
1	A	4	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	A	125	ASP	CA-C-O	-6.55	113.47	120.42
1	A	74	LYS	N-CA-C	-6.24	104.41	111.14
1	B	186	ILE	O-C-N	6.02	129.28	123.14
1	A	5	ILE	O-C-N	6.01	129.71	123.03
1	A	191	VAL	N-CA-C	5.49	116.14	110.82
1	A	213	LEU	O-C-N	-5.39	115.03	121.39
1	A	22	ARG	O-C-N	-5.35	116.06	122.15
1	B	187	ALA	CA-C-O	-5.33	115.91	122.36
1	A	189	ASP	N-CA-C	5.29	117.05	111.28
1	B	114	THR	CB-CA-C	5.18	121.14	110.31
1	A	159	GLY	O-C-N	5.16	127.15	122.19
1	A	23	LEU	O-C-N	5.09	127.52	122.12
1	B	66	ASP	N-CA-C	5.06	116.79	111.28
1	B	113	LEU	CB-CA-C	5.05	119.64	111.26
1	B	107	ALA	N-CA-C	-5.04	105.67	111.07
1	A	20	CYS	O-C-N	5.01	127.23	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	B	102	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1851	0	1848	6	0
1	B	1859	0	1851	7	0
2	A	54	0	36	1	0
2	B	54	0	36	0	0
3	A	18	0	24	5	0
3	B	18	0	21	1	0
4	A	275	0	0	7	0
4	B	268	0	0	1	0
All	All	4397	0	3816	19	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 2.

All (19) 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:21:GLN:HE21	1:A:48:GLN:HE22	1.18	0.92
3:A:304:GOL:H31	4:A:434:HOH:O	1.84	0.76
3:A:304:GOL:H2	4:A:539:HOH:O	1.93	0.69
1:A:205:THR:HG22	1:A:243:LEU:CD1	2.27	0.64
1:A:160:LEU:HD23	1:A:160:LEU:C	2.26	0.60
3:A:304:GOL:C1	4:A:539:HOH:O	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:O	1:A:205:THR:HB	2.02	0.60
3:A:304:GOL:C2	4:A:539:HOH:O	2.49	0.60
1:B:244:HIS:HD2	4:B:424:HOH:O	1.84	0.60
1:B:205:THR:O	1:B:205:THR:HG22	2.05	0.56
1:B:160:LEU:C	1:B:160:LEU:HD23	2.34	0.52
1:A:139:SER:HB2	1:A:160:LEU:HD22	1.91	0.52
1:A:244:HIS:HD2	4:A:430:HOH:O	1.92	0.52
1:B:139:SER:HB2	1:B:160:LEU:HD22	1.94	0.50
2:A:301:CAA:H4'2	4:A:497:HOH:O	2.15	0.47
1:B:34:CYS:O	3:B:303:GOL:H12	2.18	0.44
3:A:304:GOL:C3	4:A:434:HOH:O	2.53	0.44
1:B:202:ILE:O	1:B:205:THR:HB	2.19	0.43
1:B:205:THR:O	1:B:205:THR:CG2	2.70	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	244/270 (90%)	238 (98%)	6 (2%)	0	100	100
1	B	245/270 (91%)	239 (98%)	6 (2%)	0	100	100
All	All	489/540 (91%)	477 (98%)	12 (2%)	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	195/217 (90%)	193 (99%)	2 (1%)	68	37
1	B	196/217 (90%)	195 (100%)	1 (0%)	81	61
All	All	391/434 (90%)	388 (99%)	3 (1%)	73	46

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	B	40	ARG

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	48	GLN
1	A	169	GLN
1	A	244	HIS
1	B	244	HIS

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 ⓘ

8 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	GOL	A	304	-	5,5,5	1.14	1 (20%)	5,5,5	1.30	1 (20%)
3	GOL	B	302	-	5,5,5	0.81	0	5,5,5	0.65	0
3	GOL	B	304	-	5,5,5	1.92	2 (40%)	5,5,5	1.86	2 (40%)
3	GOL	B	303	-	5,5,5	2.72	3 (60%)	5,5,5	2.42	3 (60%)
2	CAA	B	301	-	53,56,56	1.59	10 (18%)	77,83,83	1.90	16 (20%)
3	GOL	A	303	-	5,5,5	0.42	0	5,5,5	0.62	0
2	CAA	A	301	-	53,56,56	1.85	9 (16%)	77,83,83	2.64	21 (27%)
3	GOL	A	302	-	5,5,5	1.84	1 (20%)	5,5,5	1.53	2 (40%)

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	GOL	A	304	-	-	3/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	B	304	-	-	0/4/4/4	-
3	GOL	B	303	-	-	2/4/4/4	-
2	CAA	B	301	-	-	7/55/71/71	0/3/3/3
3	GOL	A	303	-	-	1/4/4/4	-
2	CAA	A	301	-	-	5/55/71/71	0/3/3/3
3	GOL	A	302	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CAA	O1-C1	-7.10	1.09	1.21
2	A	301	CAA	C5A-C4A	5.18	1.48	1.39
2	B	301	CAA	C5A-C4A	4.87	1.47	1.39
3	B	303	GOL	O2-C2	-4.45	1.30	1.43
2	B	301	CAA	P1A-O3A	4.28	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CAA	C8A-N7A	3.99	1.39	1.31
2	B	301	CAA	O1-C1	-3.98	1.14	1.21
3	A	302	GOL	O1-C1	3.86	1.58	1.42
2	A	301	CAA	O5P-C5P	3.74	1.30	1.23
2	B	301	CAA	P2A-O3A	3.50	1.63	1.59
3	B	303	GOL	C1-C2	-3.33	1.39	1.51
3	B	304	GOL	O1-C1	-3.30	1.28	1.42
2	A	301	CAA	O3-C3	3.13	1.33	1.21
2	A	301	CAA	P1A-O3A	2.97	1.62	1.59
2	A	301	CAA	C5A-C6A	2.87	1.49	1.41
2	B	301	CAA	OAP-CAP	2.84	1.47	1.42
2	B	301	CAA	C5A-C6A	2.69	1.48	1.41
2	B	301	CAA	C8A-N7A	2.64	1.36	1.31
3	B	304	GOL	O2-C2	2.30	1.50	1.43
2	B	301	CAA	P3B-O3B	2.28	1.63	1.59
3	B	303	GOL	O3-C3	2.20	1.51	1.42
2	B	301	CAA	C2A-N1A	2.19	1.37	1.33
2	A	301	CAA	O9P-C9P	2.17	1.27	1.23
3	A	304	GOL	C1-C2	2.14	1.59	1.51
2	A	301	CAA	C3P-N4P	2.08	1.50	1.46
2	B	301	CAA	C4A-N9A	-2.04	1.33	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CAA	C2-C1-S1P	11.47	128.20	113.63
2	A	301	CAA	O1-C1-S1P	-11.41	108.17	122.68
2	B	301	CAA	C2-C1-S1P	7.04	122.58	113.63
2	A	301	CAA	C5A-C4A-N3A	-5.91	118.57	126.72
2	A	301	CAA	N3A-C4A-N9A	4.80	135.33	127.17
2	A	301	CAA	C7P-C6P-C5P	-4.64	104.67	112.39
2	B	301	CAA	C7P-C6P-C5P	-4.12	105.52	112.39
2	B	301	CAA	N3A-C4A-N9A	4.10	134.14	127.17
2	B	301	CAA	C5A-C4A-N3A	-4.09	121.09	126.72
2	A	301	CAA	O6A-CCP-CBP	-4.09	103.98	110.55
2	A	301	CAA	C2A-N3A-C4A	4.00	121.61	111.83
2	B	301	CAA	N3A-C2A-N1A	-3.82	122.80	128.58
2	B	301	CAA	C4A-N9A-C8A	3.82	109.75	105.74
2	A	301	CAA	N3A-C2A-N1A	-3.49	123.31	128.58
2	B	301	CAA	C2A-N3A-C4A	3.45	120.26	111.83
2	A	301	CAA	O3-C3-C4	3.41	130.03	121.48
3	B	303	GOL	C3-C2-C1	3.24	123.67	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CAA	C2P-S1P-C1	3.20	111.31	101.84
3	B	304	GOL	C3-C2-C1	-3.18	100.14	111.80
2	B	301	CAA	N6A-C6A-N1A	3.13	125.36	118.38
2	A	301	CAA	C4A-N9A-C8A	3.09	108.98	105.74
2	B	301	CAA	O1-C1-S1P	-3.02	118.85	122.68
2	B	301	CAA	CEP-CBP-CCP	-3.01	103.26	108.22
2	B	301	CAA	O1-C1-C2	-2.92	118.55	123.40
2	A	301	CAA	O2A-P1A-O1A	2.77	125.32	112.44
2	B	301	CAA	O5A-P2A-O4A	2.76	125.28	112.44
2	B	301	CAA	O6A-CCP-CBP	-2.76	106.11	110.55
3	B	303	GOL	O2-C2-C1	2.73	120.46	109.18
2	A	301	CAA	O5P-C5P-C6P	-2.65	117.22	122.02
2	B	301	CAA	O2A-P1A-O3A	2.64	114.40	107.27
2	A	301	CAA	O5A-P2A-O4A	2.64	124.71	112.44
2	A	301	CAA	CDP-CBP-CCP	2.61	112.53	108.22
3	B	303	GOL	O1-C1-C2	2.54	121.83	110.38
3	A	302	GOL	O1-C1-C2	2.50	121.63	110.38
2	B	301	CAA	C5A-C6A-N6A	-2.48	117.16	123.29
2	A	301	CAA	C4A-C5A-N7A	-2.40	107.84	110.58
3	B	304	GOL	O1-C1-C2	-2.37	99.71	110.38
3	A	304	GOL	O3-C3-C2	2.32	120.81	110.38
2	A	301	CAA	C5A-C6A-N6A	-2.24	117.75	123.29
2	A	301	CAA	C4-C3-C2	-2.23	110.06	117.78
2	A	301	CAA	C3P-N4P-C5P	-2.21	118.70	122.82
2	A	301	CAA	N9A-C8A-N7A	-2.09	110.97	113.94
2	B	301	CAA	N9A-C8A-N7A	-2.08	110.98	113.94
3	A	302	GOL	O2-C2-C1	2.03	117.58	109.18
2	A	301	CAA	N6A-C6A-N1A	2.02	122.88	118.38

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	GOL	C1-C2-C3-O3
2	B	301	CAA	C4B-C3B-O3B-P3B
3	A	302	GOL	O1-C1-C2-C3
3	A	304	GOL	O2-C2-C3-O3
3	B	303	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-O2
2	A	301	CAA	C5B-O5B-P1A-O1A
2	A	301	CAA	C5B-O5B-P1A-O3A
2	B	301	CAA	C5B-O5B-P1A-O1A

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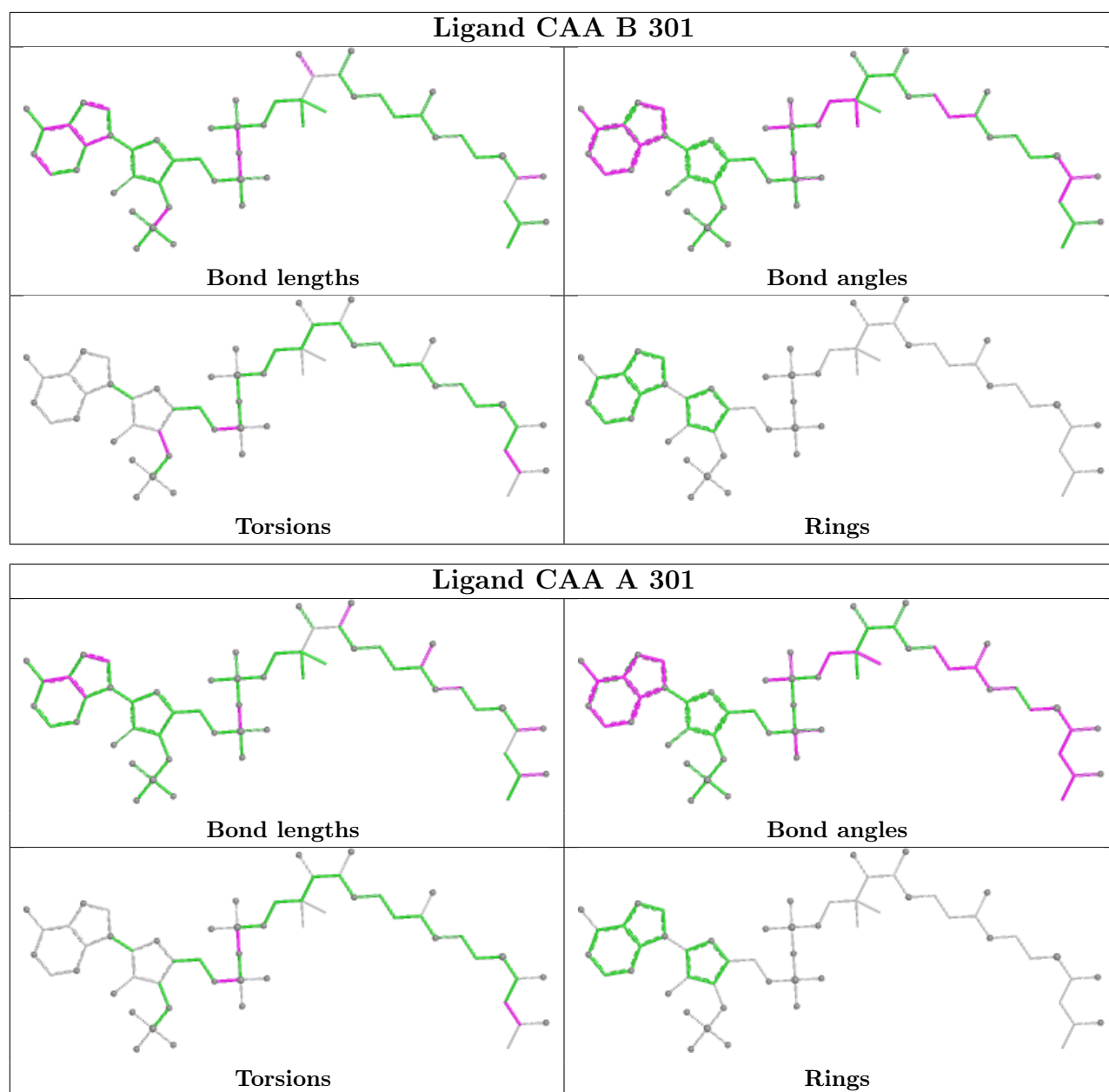
Mol	Chain	Res	Type	Atoms
2	B	301	CAA	C5B-O5B-P1A-O2A
2	B	301	CAA	C5B-O5B-P1A-O3A
2	B	301	CAA	C2B-C3B-O3B-P3B
2	A	301	CAA	C1-C2-C3-O3
2	A	301	CAA	C1-C2-C3-C4
2	B	301	CAA	C1-C2-C3-O3
2	B	301	CAA	C1-C2-C3-C4
3	A	304	GOL	C1-C2-C3-O3
3	A	304	GOL	O1-C1-C2-O2
3	A	303	GOL	C1-C2-C3-O3
2	A	301	CAA	P1A-O3A-P2A-O5A

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	GOL	5	0
3	B	303	GOL	1	0
2	A	301	CAA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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	246/270 (91%)	0.18	23 (9%) 14 21	9, 13, 37, 117	0
1	B	246/270 (91%)	0.09	24 (9%) 13 19	8, 12, 35, 56	1 (0%)
All	All	492/540 (91%)	0.13	47 (9%) 13 20	8, 13, 37, 117	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	7.9
1	B	193	ALA	7.1
1	B	191	VAL	6.6
1	A	246	GLY	6.3
1	B	194	ILE	6.1
1	A	193	ALA	5.7
1	A	1	MET	5.6
1	B	246	GLY	5.3
1	B	199	LEU	5.1
1	A	191	VAL	4.9
1	B	190	MET	4.9
1	B	202	ILE	4.9
1	B	198	VAL	4.8
1	A	190	MET	4.7
1	A	202	ILE	4.5
1	B	203	VAL	4.2
1	B	205	THR	4.0
1	B	192	LYS	4.0
1	B	2	THR	3.6
1	B	201	LYS	3.6
1	A	199	LEU	3.5
1	B	189	ASP	3.4
1	B	197	ASP	3.3
1	B	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	THR	3.0
1	A	198	VAL	3.0
1	A	189	ASP	2.9
1	B	204	ALA	2.9
1	B	196	GLN	2.7
1	A	51	LEU	2.7
1	A	43	LYS	2.6
1	A	3	GLN	2.5
1	B	200	ASP	2.5
1	A	50	ALA	2.5
1	A	203	VAL	2.5
1	B	188	THR	2.4
1	B	195	ARG	2.3
1	B	187	ALA	2.2
1	A	194	ILE	2.2
1	A	188	THR	2.2
1	A	54	ASP	2.2
1	A	192	LYS	2.2
1	A	197	ASP	2.2
1	A	77	SER	2.2
1	B	66	ASP	2.1
1	B	40	ARG	2.1
1	A	196	GLN	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](#)

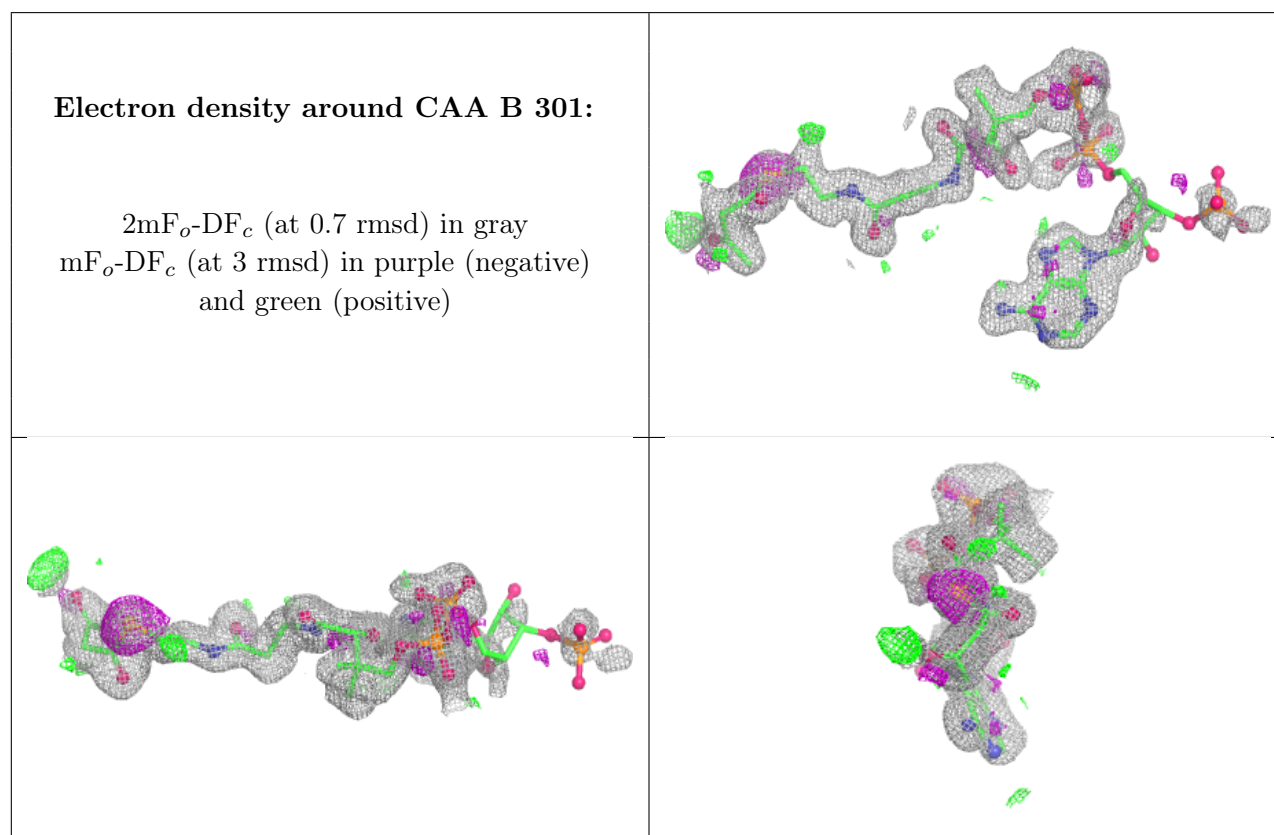
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

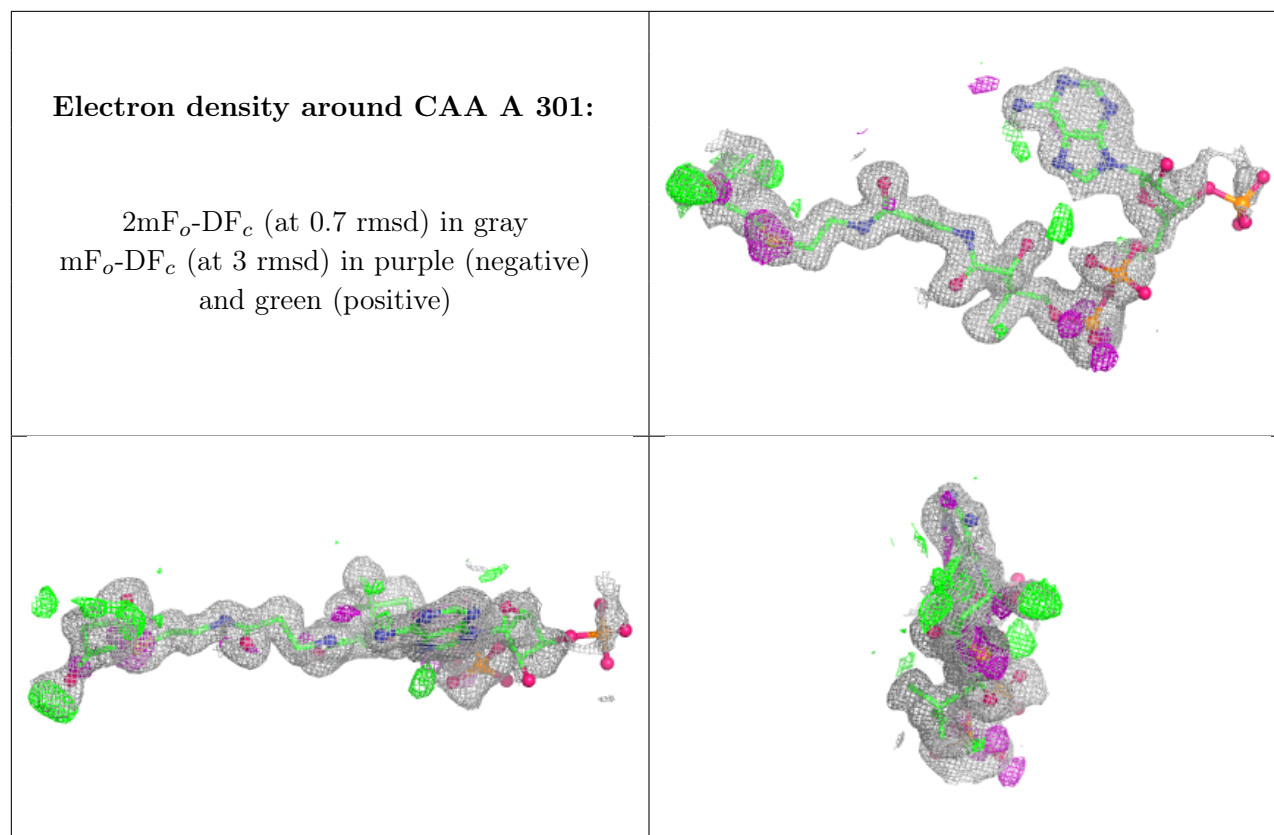
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	304	6/6	0.77	0.15	25,28,34,35	0
3	GOL	A	304	6/6	0.88	0.12	21,25,36,43	0
2	CAA	B	301	54/54	0.89	0.15	23,42,126,131	0
3	GOL	A	302	6/6	0.89	0.12	23,26,30,37	0
3	GOL	B	302	6/6	0.92	0.10	25,27,27,33	0
2	CAA	A	301	54/54	0.92	0.14	16,38,135,142	0
3	GOL	A	303	6/6	0.94	0.10	23,31,33,44	0
3	GOL	B	303	6/6	0.96	0.06	12,13,20,21	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.