



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:55 PM EDT

PDB ID : 4N5M
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.

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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

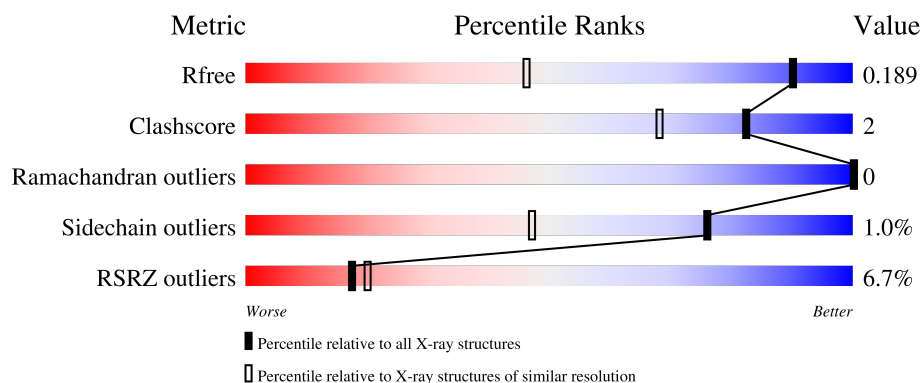
1 Overall quality at a glance

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}	130704	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (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	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	270	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div></div> <div>9%</div> </div> </div>

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 [i](#)

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:

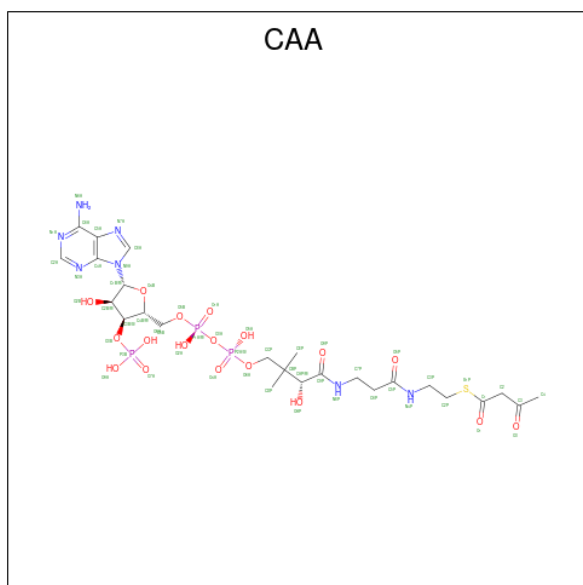
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P14697
A	-22	SER	-	expression tag	UNP P14697
A	-21	TYR	-	expression tag	UNP P14697
A	-20	TYR	-	expression tag	UNP P14697
A	-19	HIS	-	expression tag	UNP P14697
A	-18	HIS	-	expression tag	UNP P14697
A	-17	HIS	-	expression tag	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 (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

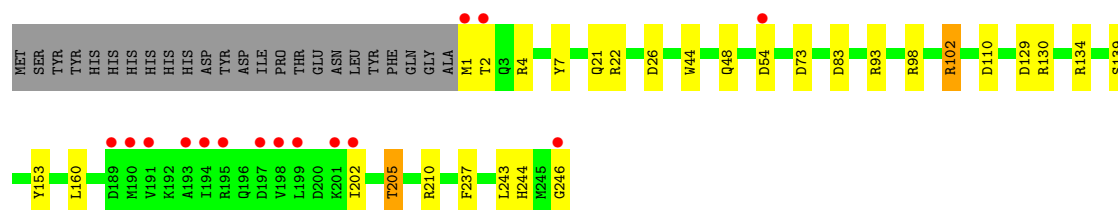
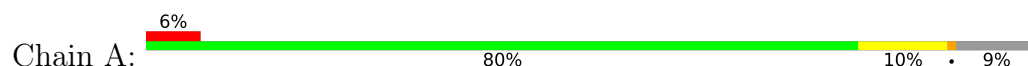
- Molecule 4 is water.

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

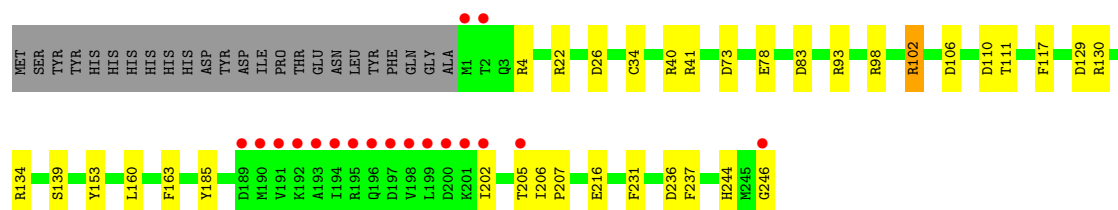
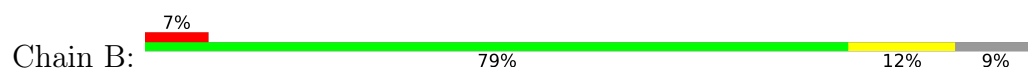
3 Residue-property plots [i](#)

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 23.38 – 1.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (23.39-1.34) 99.4 (23.38-1.34)	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 (5.02%)	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 , 44.5	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	0.97	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	1.33	7/1880 (0.4%)	1.35	19/2540 (0.7%)
1	B	1.29	11/1888 (0.6%)	1.36	25/2551 (1.0%)
All	All	1.31	18/3768 (0.5%)	1.36	44/5091 (0.9%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	PRO	N-CD	9.23	1.60	1.47
1	A	153	TYR	CE2-CZ	-7.18	1.29	1.38
1	B	78	GLU	CD-OE2	6.22	1.32	1.25
1	B	206	ILE	C-N	-6.18	1.22	1.34
1	A	44	TRP	CZ3-CH2	6.02	1.49	1.40
1	A	205	THR	CB-CG2	-6.02	1.32	1.52
1	B	111	THR	CB-CG2	-5.68	1.33	1.52
1	A	110	ASP	CG-OD2	-5.52	1.12	1.25
1	B	246	GLY	CA-C	5.45	1.60	1.51
1	A	153	TYR	CZ-OH	5.38	1.47	1.37
1	B	206	ILE	C-O	-5.37	1.13	1.23
1	A	153	TYR	CG-CD1	-5.24	1.32	1.39
1	B	153	TYR	CE2-CZ	-5.16	1.31	1.38
1	B	83	ASP	CG-OD2	-5.15	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	GLU	CD-OE1	5.15	1.31	1.25
1	B	246	GLY	C-O	5.11	1.31	1.23
1	B	102	ARG	CZ-NH2	5.08	1.39	1.33
1	A	246	GLY	C-O	5.02	1.31	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	A	98	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	4	ARG	NE-CZ-NH2	10.59	125.60	120.30
1	A	130	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	B	130	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	134	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	93	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	B	207	PRO	CA-N-CD	-8.32	99.85	111.50
1	B	4	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	4	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	B	93	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	4	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	210	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	106	ASP	CB-CG-OD1	7.55	125.09	118.30
1	B	129	ASP	CB-CG-OD1	7.43	124.99	118.30
1	B	102	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	73	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	236	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	B	41	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	83	ASP	CB-CG-OD1	-6.77	112.20	118.30
1	B	73	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	A	237	PHE	CB-CG-CD1	6.70	125.49	120.80
1	B	98	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	110	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	26	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	22	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	93	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	134	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	185	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	129	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	83	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	102	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	129	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	26	ASP	CB-CG-OD1	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	PHE	CB-CG-CD1	5.57	124.70	120.80
1	A	130	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	83	ASP	OD1-CG-OD2	5.46	133.67	123.30
1	A	7	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	22	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	206	ILE	CA-C-O	5.21	131.05	120.10
1	B	237	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	B	231	PHE	CG-CD2-CE2	-5.08	115.21	120.80
1	B	130	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	163	PHE	CB-CG-CD2	5.02	124.31	120.80

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
3:A:304:GOL:C1	4:A:539:HOH:O	2.50	0.60
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:A:160:LEU:HD23	1:A:160:LEU:C	2.26	0.55
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
1:B:160:LEU:C	1:B:160:LEU:HD23	2.34	0.48
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 ⓘ

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%)	192 (98%)	3 (2%)	65	32
1	B	196/217 (90%)	195 (100%)	1 (0%)	88	71
All	All	391/434 (90%)	387 (99%)	4 (1%)	76	47

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	54	ASP
1	B	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	87	ASN
1	A	122	GLN
1	A	196	GLN
1	A	244	HIS
1	B	87	ASN
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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	CAA	B	301	-	47,56,56	1.24	7 (14%)	60,83,83	1.81	11 (18%)
2	CAA	A	301	-	47,56,56	1.68	8 (17%)	60,83,83	2.68	15 (25%)
3	GOL	B	304	-	5,5,5	1.89	2 (40%)	5,5,5	1.73	2 (40%)
3	GOL	A	303	-	5,5,5	0.41	0	5,5,5	0.59	0
3	GOL	B	303	-	5,5,5	2.62	3 (60%)	5,5,5	2.30	3 (60%)
3	GOL	B	302	-	5,5,5	0.79	0	5,5,5	0.61	0
3	GOL	A	302	-	5,5,5	1.82	1 (20%)	5,5,5	1.45	1 (20%)
3	GOL	A	304	-	5,5,5	1.07	1 (20%)	5,5,5	1.25	1 (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
2	CAA	B	301	-	-	9/50/71/71	0/3/3/3
2	CAA	A	301	-	-	4/50/71/71	0/3/3/3
3	GOL	B	304	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	B	303	-	-	2/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	A	304	-	-	3/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CAA	O1-C1	-6.80	1.09	1.21
3	B	303	GOL	O2-C2	-4.34	1.30	1.43
3	A	302	GOL	O1-C1	3.84	1.58	1.42
2	B	301	CAA	O1-C1	-3.81	1.14	1.21
2	A	301	CAA	O5P-C5P	3.64	1.30	1.23
3	B	304	GOL	O1-C1	-3.28	1.28	1.42
3	B	303	GOL	C1-C2	-3.07	1.39	1.51
2	A	301	CAA	O3-C3	2.99	1.33	1.21
2	A	301	CAA	C5A-C4A	2.79	1.48	1.40
2	B	301	CAA	OAP-CAP	2.73	1.47	1.42
2	A	301	CAA	C8A-N7A	2.61	1.39	1.34
2	B	301	CAA	C5A-C4A	2.59	1.47	1.40
2	B	301	CAA	O4B-C1B	2.45	1.44	1.41
3	B	304	GOL	O2-C2	2.23	1.50	1.43
2	B	301	CAA	P3B-O3B	2.23	1.63	1.59
3	B	303	GOL	O3-C3	2.19	1.51	1.42
2	B	301	CAA	C2A-N3A	2.13	1.35	1.32
2	B	301	CAA	C2A-N1A	2.11	1.37	1.33
2	A	301	CAA	O9P-C9P	2.10	1.27	1.23
2	A	301	CAA	C2A-N3A	2.05	1.35	1.32
2	A	301	CAA	C3P-N4P	2.05	1.50	1.46
3	A	304	GOL	C1-C2	2.00	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CAA	C2-C1-S1P	11.65	128.20	113.69
2	A	301	CAA	O1-C1-S1P	-11.12	108.17	122.61
2	B	301	CAA	C2-C1-S1P	7.13	122.58	113.69
2	A	301	CAA	C7P-C6P-C5P	-4.62	104.67	112.36
2	B	301	CAA	C7P-C6P-C5P	-4.10	105.52	112.36
2	A	301	CAA	O6A-CCP-CBP	-4.09	103.98	110.55
2	B	301	CAA	N3A-C2A-N1A	-3.76	122.80	128.68
2	A	301	CAA	N3A-C2A-N1A	-3.44	123.31	128.68
2	A	301	CAA	O3-C3-C4	3.40	130.03	121.40
2	B	301	CAA	N6A-C6A-N1A	3.27	125.36	118.57
3	B	303	GOL	C3-C2-C1	3.08	123.67	111.70
2	B	301	CAA	CEP-CBP-CCP	-3.05	103.26	108.23
2	A	301	CAA	C2P-S1P-C1	3.03	111.31	101.87
3	B	304	GOL	C3-C2-C1	-2.98	100.14	111.70
2	B	301	CAA	O1-C1-S1P	-2.90	118.85	122.61
2	B	301	CAA	O1-C1-C2	-2.77	118.55	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CAA	O6A-CCP-CBP	-2.76	106.11	110.55
2	A	301	CAA	O2A-P1A-O1A	2.65	125.32	112.24
2	B	301	CAA	O5A-P2A-O4A	2.64	125.28	112.24
2	A	301	CAA	CDP-CBP-CCP	2.64	112.53	108.23
2	A	301	CAA	O5P-C5P-C6P	-2.62	117.22	122.02
3	B	303	GOL	O2-C2-C1	2.57	120.46	109.12
2	A	301	CAA	O5A-P2A-O4A	2.52	124.71	112.24
2	A	301	CAA	P2A-O3A-P1A	-2.48	124.33	132.83
3	B	303	GOL	O1-C1-C2	2.43	121.83	110.20
3	A	302	GOL	O1-C1-C2	2.38	121.63	110.20
2	B	301	CAA	C1B-N9A-C4A	-2.38	122.46	126.64
2	A	301	CAA	C4-C3-C2	-2.26	110.06	117.89
2	A	301	CAA	C3P-N4P-C5P	-2.23	118.70	122.84
3	A	304	GOL	O3-C3-C2	2.21	120.81	110.20
3	B	304	GOL	O1-C1-C2	-2.19	99.71	110.20
2	B	301	CAA	C5A-C6A-N6A	-2.10	117.16	120.35
2	A	301	CAA	N6A-C6A-N1A	2.08	122.88	118.57

There are no chirality outliers.

All (20) torsion outliers are listed below:

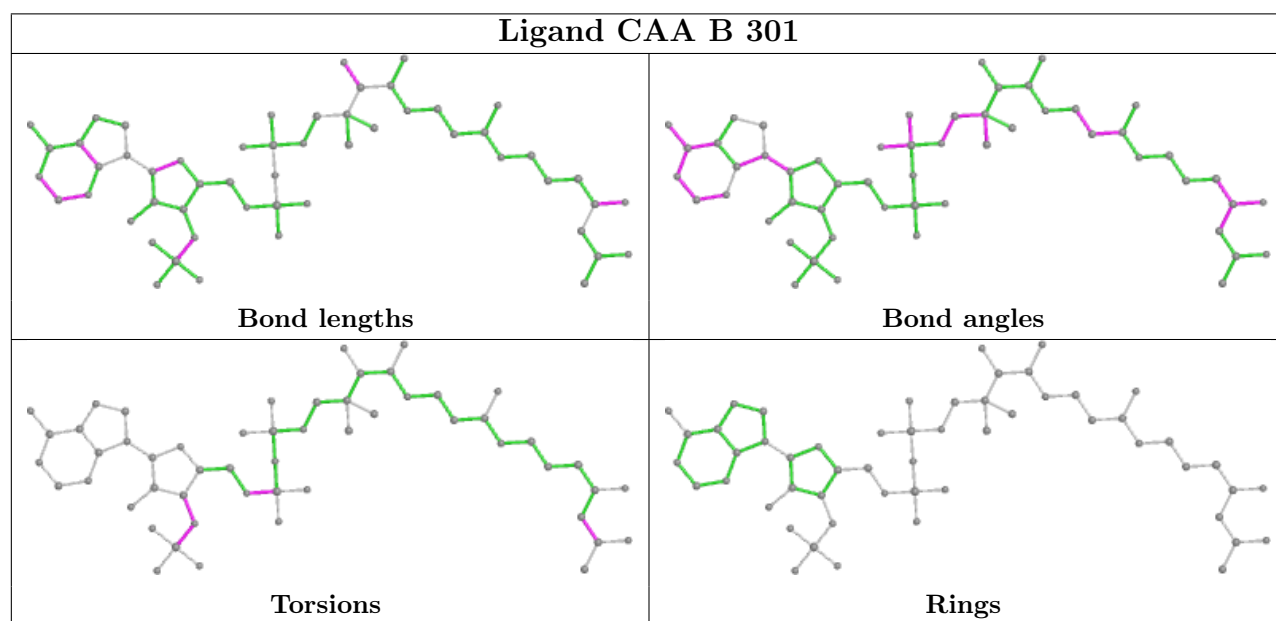
Mol	Chain	Res	Type	Atoms
2	B	301	CAA	C5B-O5B-P1A-O3A
3	B	303	GOL	C1-C2-C3-O3
2	B	301	CAA	C4B-C3B-O3B-P3B
3	A	302	GOL	O1-C1-C2-C3
3	A	304	GOL	O2-C2-C3-O3
3	B	303	GOL	O1-C1-C2-O2
2	A	301	CAA	C5B-O5B-P1A-O3A
3	A	304	GOL	C1-C2-C3-O3
2	B	301	CAA	C5B-O5B-P1A-O1A
2	B	301	CAA	C5B-O5B-P1A-O2A
3	A	302	GOL	O1-C1-C2-O2
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	O1-C1-C2-O2
2	B	301	CAA	C3B-O3B-P3B-O8A
2	B	301	CAA	C3B-O3B-P3B-O9A
2	A	301	CAA	C5B-O5B-P1A-O1A

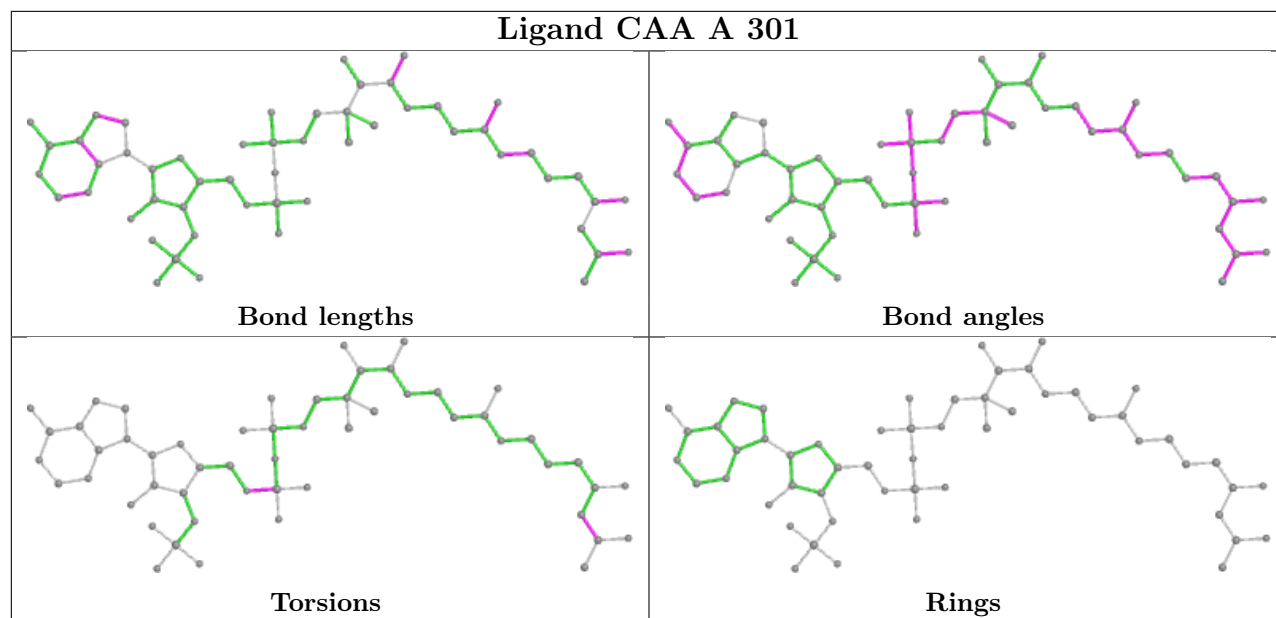
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CAA	1	0
3	B	303	GOL	1	0
3	A	304	GOL	5	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%)	-0.08	15 (6%) 21 23	9, 13, 37, 117	0
1	B	246/270 (91%)	-0.06	18 (7%) 15 17	8, 12, 35, 56	0
All	All	492/540 (91%)	-0.07	33 (6%) 17 20	8, 13, 37, 117	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	12.9
1	A	1	MET	12.2
1	B	193	ALA	8.3
1	B	194	ILE	6.1
1	B	199	LEU	6.0
1	A	193	ALA	5.8
1	A	246	GLY	4.8
1	B	198	VAL	4.7
1	B	197	ASP	4.6
1	B	191	VAL	4.5
1	B	246	GLY	4.4
1	B	190	MET	4.3
1	B	2	THR	4.2
1	B	202	ILE	3.9
1	B	189	ASP	3.7
1	B	201	LYS	3.6
1	A	190	MET	3.5
1	A	199	LEU	3.4
1	A	197	ASP	3.2
1	B	1	MET	3.2
1	A	191	VAL	3.2
1	B	196	GLN	3.2
1	A	202	ILE	3.0
1	A	198	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	195	ARG	2.8
1	B	195	ARG	2.7
1	A	194	ILE	2.5
1	B	200	ASP	2.5
1	A	189	ASP	2.4
1	A	54	ASP	2.4
1	B	192	LYS	2.3
1	A	201	LYS	2.1
1	B	205	THR	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

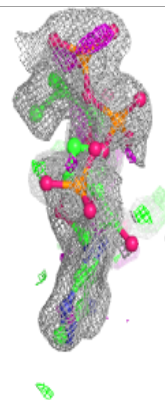
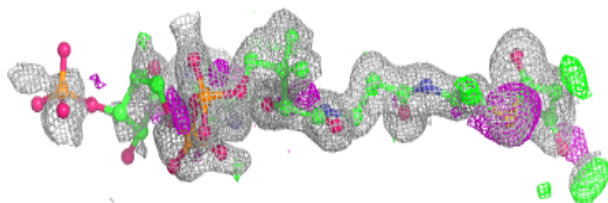
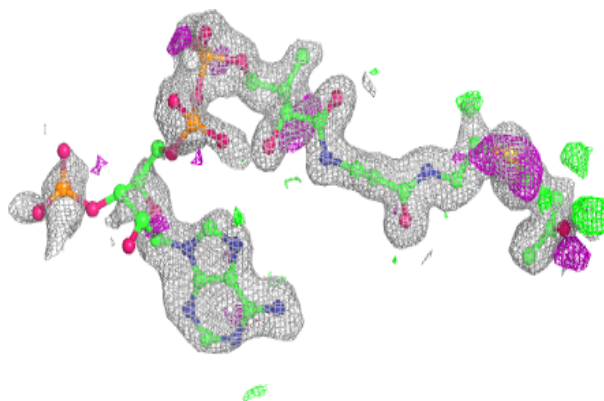
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	304	6/6	0.74	0.18	25,28,34,35	0
3	GOL	A	302	6/6	0.83	0.12	23,26,30,37	0
2	CAA	B	301	54/54	0.86	0.20	23,42,126,131	0
3	GOL	B	302	6/6	0.88	0.14	25,27,27,33	0
2	CAA	A	301	54/54	0.88	0.18	16,38,135,142	0
3	GOL	A	304	6/6	0.92	0.15	21,25,36,43	0
3	GOL	B	303	6/6	0.96	0.06	12,13,20,21	0
3	GOL	A	303	6/6	0.96	0.10	23,31,33,44	0

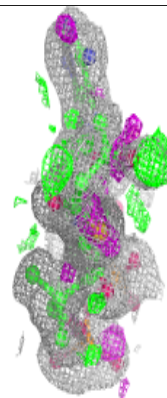
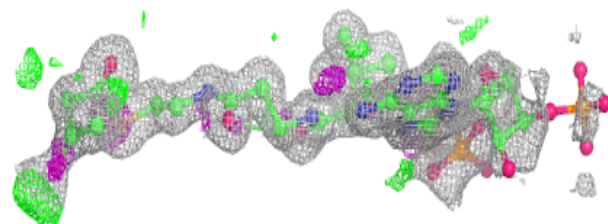
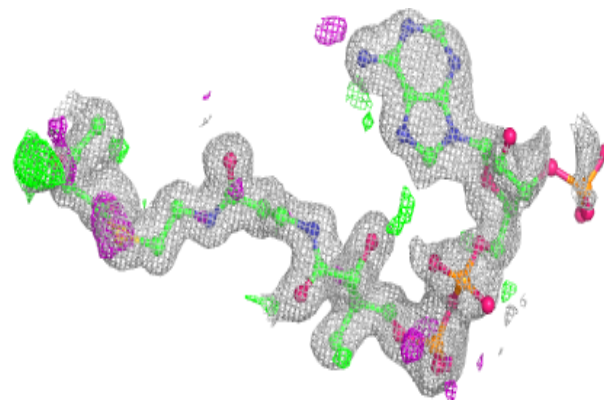
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CAA B 301:

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

**Electron density around CAA A 301:**

$2mF_o-DF_c$ (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.