



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 AM UTC

PDB ID : 4ZDB / pdb_00004zdb
Title : Yeast enoyl-CoA isomerase (ScECI2) complexed with acetoacetyl-CoA
Authors : Onwukwe, G.U.; Koski, M.K.; Wierenga, R.K.
Deposited on : 2015-04-17
Resolution : 2.14 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

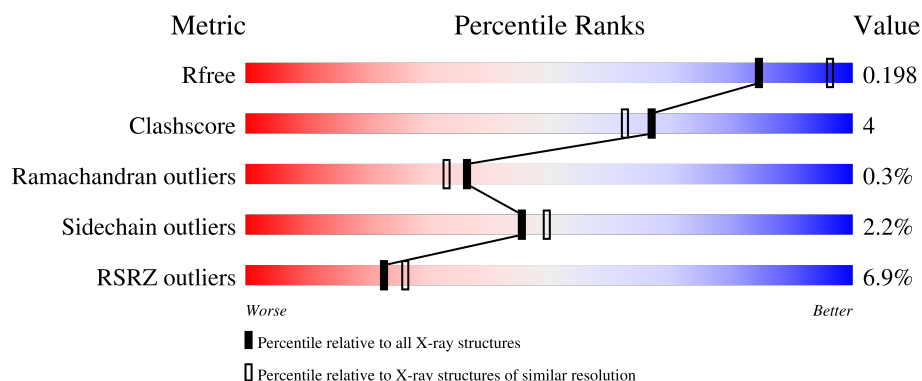
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	300	6% 83% 5% • 11%
1	B	300	5% 81% 5% • 13%
1	C	300	6% 82% 5% 12%

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
4	GOL	A	307	-	-	X	-
4	GOL	B	305	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7002 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 3,2-trans-enoyl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	2	0
			2143	1378	354	400	11			
1	B	261	Total	C	N	O	S	0	2	0
			2092	1352	341	388	11			
1	C	263	Total	C	N	O	S	0	2	0
			2112	1362	349	390	11			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q05871
A	-18	GLY	-	expression tag	UNP Q05871
A	-17	SER	-	expression tag	UNP Q05871
A	-16	SER	-	expression tag	UNP Q05871
A	-15	HIS	-	expression tag	UNP Q05871
A	-14	HIS	-	expression tag	UNP Q05871
A	-13	HIS	-	expression tag	UNP Q05871
A	-12	HIS	-	expression tag	UNP Q05871
A	-11	HIS	-	expression tag	UNP Q05871
A	-10	HIS	-	expression tag	UNP Q05871
A	-9	SER	-	expression tag	UNP Q05871
A	-8	SER	-	expression tag	UNP Q05871
A	-7	GLY	-	expression tag	UNP Q05871
A	-6	LEU	-	expression tag	UNP Q05871
A	-5	VAL	-	expression tag	UNP Q05871
A	-4	PRO	-	expression tag	UNP Q05871
A	-3	ARG	-	expression tag	UNP Q05871
A	-2	GLY	-	expression tag	UNP Q05871
A	-1	SER	-	expression tag	UNP Q05871
A	0	HIS	-	expression tag	UNP Q05871
A	25	ILE	MET	conflict	UNP Q05871
B	-19	MET	-	initiating methionine	UNP Q05871
B	-18	GLY	-	expression tag	UNP Q05871

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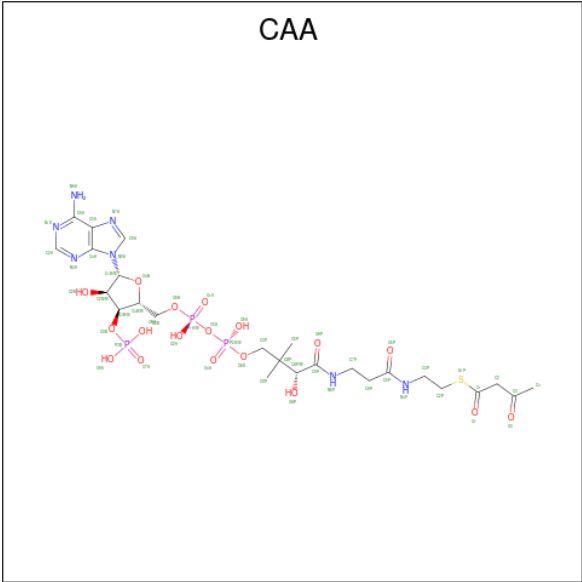
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q05871
B	-16	SER	-	expression tag	UNP Q05871
B	-15	HIS	-	expression tag	UNP Q05871
B	-14	HIS	-	expression tag	UNP Q05871
B	-13	HIS	-	expression tag	UNP Q05871
B	-12	HIS	-	expression tag	UNP Q05871
B	-11	HIS	-	expression tag	UNP Q05871
B	-10	HIS	-	expression tag	UNP Q05871
B	-9	SER	-	expression tag	UNP Q05871
B	-8	SER	-	expression tag	UNP Q05871
B	-7	GLY	-	expression tag	UNP Q05871
B	-6	LEU	-	expression tag	UNP Q05871
B	-5	VAL	-	expression tag	UNP Q05871
B	-4	PRO	-	expression tag	UNP Q05871
B	-3	ARG	-	expression tag	UNP Q05871
B	-2	GLY	-	expression tag	UNP Q05871
B	-1	SER	-	expression tag	UNP Q05871
B	0	HIS	-	expression tag	UNP Q05871
B	25	ILE	MET	conflict	UNP Q05871
C	-19	MET	-	initiating methionine	UNP Q05871
C	-18	GLY	-	expression tag	UNP Q05871
C	-17	SER	-	expression tag	UNP Q05871
C	-16	SER	-	expression tag	UNP Q05871
C	-15	HIS	-	expression tag	UNP Q05871
C	-14	HIS	-	expression tag	UNP Q05871
C	-13	HIS	-	expression tag	UNP Q05871
C	-12	HIS	-	expression tag	UNP Q05871
C	-11	HIS	-	expression tag	UNP Q05871
C	-10	HIS	-	expression tag	UNP Q05871
C	-9	SER	-	expression tag	UNP Q05871
C	-8	SER	-	expression tag	UNP Q05871
C	-7	GLY	-	expression tag	UNP Q05871
C	-6	LEU	-	expression tag	UNP Q05871
C	-5	VAL	-	expression tag	UNP Q05871
C	-4	PRO	-	expression tag	UNP Q05871
C	-3	ARG	-	expression tag	UNP Q05871
C	-2	GLY	-	expression tag	UNP Q05871
C	-1	SER	-	expression tag	UNP Q05871
C	0	HIS	-	expression tag	UNP Q05871
C	25	ILE	MET	conflict	UNP Q05871

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



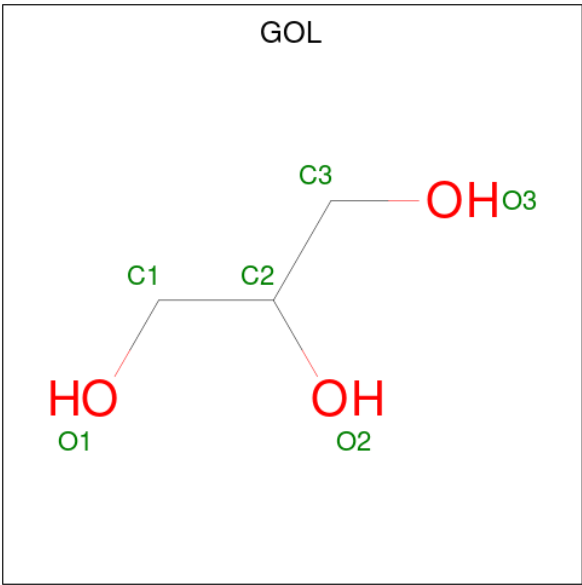
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: C₂₅H₄₀N₇O₁₈P₃S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

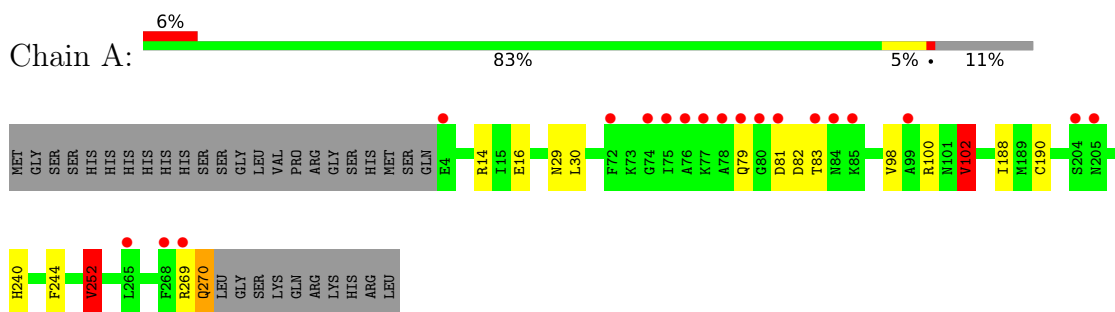
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total 155	O 155	0	0
5	B	123	Total 123	O 123	0	0
5	C	133	Total 133	O 133	0	0

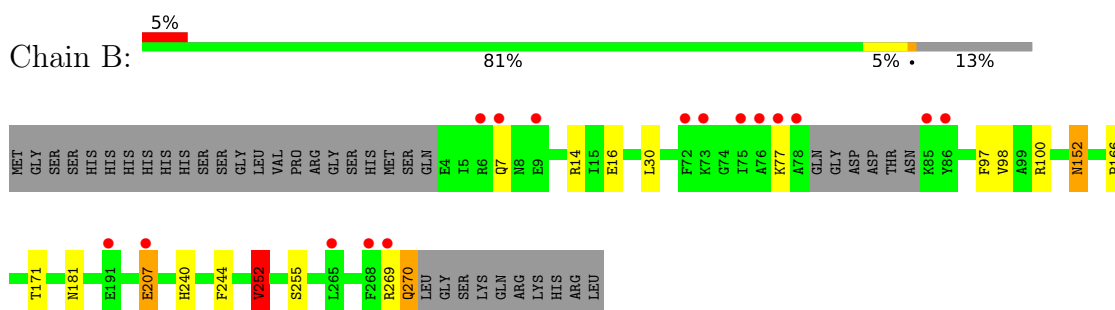
3 Residue-property plots [i](#)

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.

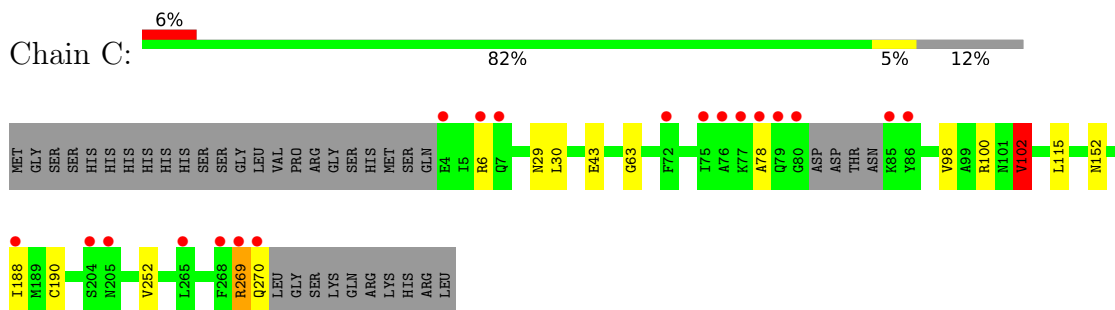
- Molecule 1: 3,2-trans-enoyl-CoA isomerase



- Molecule 1: 3,2-trans-enoyl-CoA isomerase



- Molecule 1: 3,2-trans-enoyl-CoA isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.94Å 116.94Å 218.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.10 – 2.14 103.10 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.5 (103.10-2.14) 99.5 (103.10-2.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.165 , 0.190 0.175 , 0.198	Depositor DCC
R_{free} test set	4184 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: SO4, CAA, GOL, CME

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	1.05	1/2181 (0.0%)	0.95	5/2945 (0.2%)
1	B	0.90	0/2132	0.86	1/2878 (0.0%)
1	C	0.96	0/2149	0.90	2/2899 (0.1%)
All	All	0.97	1/6462 (0.0%)	0.91	8/8722 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLN	C-O	-22.47	0.78	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	GLN	CA-C-O	-11.39	101.44	120.80
1	C	102	VAL	CB-CA-C	-9.60	98.97	112.22
1	A	102	VAL	CB-CA-C	-9.27	97.25	112.26
1	C	102	VAL	N-CA-CB	7.61	121.99	110.58
1	B	252	VAL	N-CA-CB	-6.43	100.94	110.58
1	A	81	ASP	N-CA-C	6.31	119.10	111.40
1	A	252	VAL	N-CA-CB	-6.17	101.32	110.58
1	A	102	VAL	N-CA-CB	6.12	121.85	110.77

There are no chirality outliers.

There are no planarity outliers.

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	2143	0	2135	16	0
1	B	2092	0	2095	11	0
1	C	2112	0	2113	10	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
3	A	54	0	36	2	0
3	B	54	0	36	1	0
3	C	54	0	36	2	0
4	A	18	0	24	6	0
4	B	12	0	16	5	0
4	C	12	0	16	2	0
5	A	155	0	0	9	0
5	B	123	0	0	6	0
5	C	133	0	0	2	0
All	All	7002	0	6507	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (48) 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:270:GLN:O	1:A:270:GLN:CA	1.87	1.22
1:A:270:GLN:O	1:A:270:GLN:C	0.78	1.03
1:A:188:ILE:HD12	5:A:486:HOH:O	1.74	0.87
4:A:307:GOL:H31	5:A:433:HOH:O	1.86	0.76
1:C:63:GLY:N	2:C:302:SO4:O4	2.21	0.74
1:B:98:VAL:HG13	1:B:252:VAL:HG13	1.69	0.72
1:A:98:VAL:HG13	1:A:252:VAL:HG13	1.70	0.72
1:C:29[A]:ASN:OD1	3:C:303:CAA:H1B	1.97	0.65
1:A:270:GLN:O	1:A:270:GLN:HA	1.93	0.64
1:C:269:ARG:O	1:C:269:ARG:HG2	1.99	0.63
1:C:30:LEU:HD12	3:C:303:CAA:H8A	1.83	0.60
1:B:244:PHE:CE2	4:B:305:GOL:H32	2.37	0.59
1:B:30:LEU:HD12	3:B:303:CAA:H8A	1.86	0.58
4:B:305:GOL:H2	5:B:416:HOH:O	2.04	0.57
1:C:269:ARG:O	1:C:270:GLN:C	2.47	0.57
1:B:207:GLU:HG2	5:B:481:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:O	1:A:269:ARG:HG2	2.05	0.56
4:A:307:GOL:H2	5:A:483:HOH:O	2.06	0.55
4:C:305:GOL:H32	5:C:407:HOH:O	2.08	0.54
4:A:307:GOL:H12	5:A:415:HOH:O	2.08	0.54
1:A:29[B]:ASN:OD1	3:A:305:CAA:H1B	2.07	0.53
1:B:166:PRO:HB3	1:B:171[A]:THR:HG22	1.93	0.51
1:C:6[B]:ARG:HH22	1:C:43:GLU:CD	2.19	0.50
4:A:307:GOL:C1	5:A:415:HOH:O	2.60	0.50
1:C:269:ARG:O	1:C:269:ARG:CG	2.62	0.48
1:A:240:HIS:HD2	5:A:529:HOH:O	1.97	0.48
1:A:244:PHE:CE2	4:A:307:GOL:H32	2.49	0.48
1:A:82:ASP:N	1:A:83:THR:HA	2.28	0.48
1:C:98:VAL:O	1:C:102:VAL:HG22	2.14	0.47
1:A:98:VAL:O	1:A:102:VAL:HG22	2.15	0.47
1:B:240:HIS:HE1	5:B:507:HOH:O	1.98	0.47
4:B:305:GOL:H11	5:B:403:HOH:O	2.14	0.47
4:B:305:GOL:H31	5:B:421:HOH:O	2.15	0.47
1:C:102:VAL:HG13	1:C:252:VAL:HG21	1.97	0.46
1:B:270:GLN:NE2	1:B:270:GLN:HA	2.31	0.45
1:A:240:HIS:HE1	5:A:532:HOH:O	2.00	0.44
1:B:152:ASN:OD1	1:B:181:ASN:ND2	2.50	0.44
4:C:305:GOL:C3	5:C:407:HOH:O	2.66	0.44
1:A:269:ARG:O	1:A:269:ARG:CG	2.65	0.44
1:B:77:LYS:HD3	1:B:77:LYS:HA	1.88	0.43
1:C:6[B]:ARG:HE	1:C:6[B]:ARG:HB3	1.23	0.43
1:A:30:LEU:HD12	3:A:305:CAA:H8A	2.00	0.43
1:B:97:PHE:CE2	1:B:255:SER:OG	2.62	0.43
1:B:14:ARG:NE	1:B:16:GLU:OE2	2.39	0.43
1:A:14:ARG:NE	1:A:16:GLU:OE2	2.35	0.42
4:A:307:GOL:C3	5:A:433:HOH:O	2.59	0.41
4:B:305:GOL:C1	5:B:403:HOH:O	2.68	0.41
1:A:79:GLN:HG3	5:A:465:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/300 (89%)	255 (96%)	11 (4%)	0	100	100
1	B	258/300 (86%)	249 (96%)	8 (3%)	1 (0%)	30	26
1	C	260/300 (87%)	252 (97%)	7 (3%)	1 (0%)	30	26
All	All	784/900 (87%)	756 (96%)	26 (3%)	2 (0%)	36	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	ARG
1	C	78	ALA

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	234/261 (90%)	231 (99%)	3 (1%)	61	67
1	B	229/261 (88%)	223 (97%)	6 (3%)	40	42
1	C	230/261 (88%)	224 (97%)	6 (3%)	40	42
All	All	693/783 (88%)	678 (98%)	15 (2%)	45	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	102	VAL
1	A	252	VAL
1	B	7	GLN
1	B	100	ARG
1	B	152	ASN
1	B	207	GLU

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Mol	Chain	Res	Type
1	B	252	VAL
1	B	270	GLN
1	C	100	ARG
1	C	102	VAL
1	C	115	LEU
1	C	152	ASN
1	C	188	ILE
1	C	269	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	240	HIS
1	A	270	GLN
1	B	240	HIS
1	C	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	B	190	1	8,9,10	0.82	0	6,9,11	1.30	0
1	CME	C	190	1	8,9,10	0.97	0	6,9,11	1.46	1 (16%)
1	CME	A	190	1	8,9,10	1.12	0	6,9,11	2.00	1 (16%)

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
1	CME	B	190	1	-	2/5/8/10	-
1	CME	C	190	1	-	3/5/8/10	-
1	CME	A	190	1	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	CME	CB-CA-C	3.41	120.05	110.80
1	C	190	CME	CB-SG-SD	2.23	109.62	103.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	190	CME	CE-SD-SG-CB
1	A	190	CME	SD-CE-CZ-OH
1	B	190	CME	CE-SD-SG-CB
1	B	190	CME	SD-CE-CZ-OH
1	C	190	CME	CE-SD-SG-CB
1	C	190	CME	SD-CE-CZ-OH
1	A	190	CME	CZ-CE-SD-SG
1	C	190	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
4	GOL	A	306	-	5,5,5	0.54	0	5,5,5	0.55	0
2	SO4	A	304	-	4,4,4	0.56	0	6,6,6	0.16	0
4	GOL	B	304	-	5,5,5	0.56	0	5,5,5	0.48	0
4	GOL	A	308	-	5,5,5	0.40	0	5,5,5	1.29	0
2	SO4	C	301	-	4,4,4	0.47	0	6,6,6	0.44	0
2	SO4	C	302	-	4,4,4	0.57	0	6,6,6	0.89	0
2	SO4	A	302	-	4,4,4	0.60	0	6,6,6	0.37	0
2	SO4	B	302	-	4,4,4	0.47	0	6,6,6	0.48	0
3	CAA	A	305	-	53,56,56	1.41	6 (11%)	77,83,83	2.75	20 (25%)
4	GOL	A	307	-	5,5,5	0.73	0	5,5,5	1.03	0
4	GOL	C	305	-	5,5,5	0.77	0	5,5,5	1.01	0
2	SO4	B	301	-	4,4,4	0.49	0	6,6,6	0.44	0
3	CAA	C	303	-	53,56,56	1.33	5 (9%)	77,83,83	2.15	19 (24%)
4	GOL	B	305	-	5,5,5	0.61	0	5,5,5	0.89	0
2	SO4	A	301	-	4,4,4	0.44	0	6,6,6	0.95	0
4	GOL	C	304	-	5,5,5	0.43	0	5,5,5	0.84	0
2	SO4	A	303	-	4,4,4	0.51	0	6,6,6	0.82	0
3	CAA	B	303	-	53,56,56	1.50	7 (13%)	77,83,83	1.87	16 (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
4	GOL	A	306	-	-	2/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-
4	GOL	A	308	-	-	2/4/4/4	-
3	CAA	A	305	-	-	16/55/71/71	0/3/3/3
4	GOL	A	307	-	-	2/4/4/4	-
4	GOL	C	305	-	-	2/4/4/4	-
3	CAA	C	303	-	-	20/55/71/71	0/3/3/3
4	GOL	B	305	-	-	1/4/4/4	-
4	GOL	C	304	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAA	B	303	-	-	9/55/71/71	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	CAA	C5A-C4A	4.96	1.47	1.39
3	B	303	CAA	P2A-O3A	4.80	1.64	1.59
3	B	303	CAA	C5A-C4A	4.74	1.47	1.39
3	A	305	CAA	C5A-C4A	4.64	1.47	1.39
3	B	303	CAA	P1A-O3A	4.30	1.64	1.59
3	A	305	CAA	P2A-O3A	4.24	1.64	1.59
3	A	305	CAA	P1A-O3A	3.92	1.63	1.59
3	C	303	CAA	C1-S1P	-3.86	1.67	1.76
3	B	303	CAA	C1-S1P	-3.57	1.67	1.76
3	C	303	CAA	C5A-C6A	3.08	1.49	1.41
3	A	305	CAA	C5A-N7A	-2.94	1.33	1.39
3	C	303	CAA	P1A-O3A	2.72	1.62	1.59
3	C	303	CAA	P2A-O3A	2.61	1.62	1.59
3	A	305	CAA	C5A-C6A	2.60	1.48	1.41
3	B	303	CAA	C5A-C6A	2.54	1.48	1.41
3	B	303	CAA	C5A-N7A	-2.48	1.34	1.39
3	A	305	CAA	C1-S1P	-2.35	1.70	1.76
3	B	303	CAA	C8A-N9A	-2.05	1.34	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	CAA	C2-C1-S1P	15.13	132.85	113.63
3	C	303	CAA	C2-C1-S1P	8.38	124.28	113.63
3	A	305	CAA	O1-C1-C2	-8.22	109.70	123.40
3	C	303	CAA	C5A-C4A-N3A	-6.10	118.32	126.72
3	C	303	CAA	O1-C1-S1P	-6.00	115.05	122.68
3	B	303	CAA	C2-C1-S1P	5.91	121.13	113.63
3	A	305	CAA	C5A-C4A-N3A	-5.71	118.85	126.72
3	B	303	CAA	C5A-C4A-N3A	-5.45	119.22	126.72
3	A	305	CAA	N3A-C4A-N9A	5.25	136.10	127.17
3	C	303	CAA	N3A-C4A-N9A	5.19	136.00	127.17
3	B	303	CAA	N3A-C4A-N9A	5.13	135.89	127.17
3	A	305	CAA	C3-C2-C1	4.50	131.61	113.95
3	B	303	CAA	O4B-C1B-N9A	4.47	116.67	108.09
3	A	305	CAA	O1-C1-S1P	-4.32	117.19	122.68
3	B	303	CAA	O1-C1-S1P	-4.30	117.22	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	CAA	C2P-C3P-N4P	4.27	121.33	112.41
3	C	303	CAA	O4B-C1B-N9A	4.19	116.14	108.09
3	C	303	CAA	C2A-N3A-C4A	4.17	122.01	111.83
3	B	303	CAA	N3A-C2A-N1A	-3.97	122.57	128.58
3	C	303	CAA	N3A-C2A-N1A	-3.92	122.64	128.58
3	B	303	CAA	C4A-N9A-C8A	3.72	109.65	105.74
3	A	305	CAA	N3A-C2A-N1A	-3.70	122.97	128.58
3	B	303	CAA	C2A-N3A-C4A	3.67	120.79	111.83
3	A	305	CAA	C2A-N3A-C4A	3.66	120.77	111.83
3	C	303	CAA	C4A-C5A-N7A	-3.46	106.63	110.58
3	A	305	CAA	O4B-C1B-N9A	3.33	114.49	108.09
3	B	303	CAA	C4A-C5A-N7A	-3.07	107.07	110.58
3	A	305	CAA	C4A-N9A-C8A	2.96	108.85	105.74
3	A	305	CAA	C4A-C5A-N7A	-2.82	107.35	110.58
3	C	303	CAA	C4A-N9A-C8A	2.81	108.69	105.74
3	B	303	CAA	C5A-N7A-C8A	2.72	107.73	103.45
3	C	303	CAA	CDP-CBP-CCP	2.70	112.68	108.22
3	C	303	CAA	O5P-C5P-C6P	-2.70	117.13	122.02
3	B	303	CAA	C2A-N1A-C6A	2.69	123.15	118.73
3	A	305	CAA	C2A-N1A-C6A	2.61	123.02	118.73
3	C	303	CAA	C5A-N7A-C8A	2.61	107.55	103.45
3	A	305	CAA	N6A-C6A-N1A	2.60	124.17	118.38
3	A	305	CAA	C5A-N7A-C8A	2.58	107.50	103.45
3	C	303	CAA	C6P-C5P-N4P	2.56	121.01	116.34
3	B	303	CAA	N6A-C6A-N1A	2.55	124.05	118.38
3	A	305	CAA	C7P-C6P-C5P	2.46	116.48	112.39
3	C	303	CAA	C2B-C1B-N9A	-2.42	107.30	113.30
3	B	303	CAA	O2A-P1A-O1A	2.35	123.36	112.44
3	B	303	CAA	N9A-C8A-N7A	-2.31	110.66	113.94
3	A	305	CAA	C4-C3-C2	-2.25	110.00	117.78
3	C	303	CAA	C6A-C5A-N7A	2.21	136.35	132.09
3	A	305	CAA	O2A-P1A-O1A	2.21	122.73	112.44
3	C	303	CAA	CAP-C9P-N8P	2.17	120.59	116.48
3	B	303	CAA	O9A-P3B-O8A	2.14	115.83	107.80
3	C	303	CAA	C2A-N1A-C6A	2.12	122.22	118.73
3	A	305	CAA	C2B-C1B-N9A	-2.09	108.11	113.30
3	B	303	CAA	O3B-P3B-O7A	-2.09	101.89	109.33
3	A	305	CAA	O3-C3-C2	2.08	128.98	120.91
3	C	303	CAA	C2P-S1P-C1	2.04	107.86	101.84
3	C	303	CAA	C7P-N8P-C9P	2.03	126.19	122.55

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	CAA	C5B-O5B-P1A-O3A
3	A	305	CAA	OAP-CAP-CBP-CCP
3	A	305	CAA	C9P-CAP-CBP-CCP
3	A	305	CAA	OAP-CAP-CBP-CDP
3	A	305	CAA	C9P-CAP-CBP-CDP
3	A	305	CAA	OAP-CAP-CBP-CEP
3	A	305	CAA	C9P-CAP-CBP-CEP
3	A	305	CAA	C5P-C6P-C7P-N8P
3	A	305	CAA	S1P-C2P-C3P-N4P
3	A	305	CAA	C1-C2-C3-O3
3	B	303	CAA	C5B-O5B-P1A-O1A
3	B	303	CAA	O1-C1-S1P-C2P
3	B	303	CAA	C2-C1-S1P-C2P
3	B	303	CAA	C1-C2-C3-C4
3	C	303	CAA	C5B-O5B-P1A-O2A
3	C	303	CAA	CDP-CBP-CCP-O6A
3	C	303	CAA	CEP-CBP-CCP-O6A
3	C	303	CAA	CAP-CBP-CCP-O6A
3	C	303	CAA	O9P-C9P-CAP-OAP
3	C	303	CAA	N8P-C9P-CAP-OAP
3	C	303	CAA	CAP-C9P-N8P-C7P
3	C	303	CAA	C2P-C3P-N4P-C5P
3	C	303	CAA	S1P-C2P-C3P-N4P
3	C	303	CAA	C3P-C2P-S1P-C1
3	C	303	CAA	O1-C1-S1P-C2P
3	C	303	CAA	C2-C1-S1P-C2P
3	C	303	CAA	C1-C2-C3-O3
3	C	303	CAA	C1-C2-C3-C4
4	A	307	GOL	O1-C1-C2-C3
3	C	303	CAA	O9P-C9P-N8P-C7P
4	A	308	GOL	C1-C2-C3-O3
4	B	304	GOL	C1-C2-C3-O3
3	C	303	CAA	O5P-C5P-C6P-C7P
3	B	303	CAA	C5P-C6P-C7P-N8P
4	A	308	GOL	O2-C2-C3-O3
3	C	303	CAA	N4P-C5P-C6P-C7P
3	B	303	CAA	C1-C2-C3-O3
4	B	304	GOL	O2-C2-C3-O3
3	C	303	CAA	N8P-C9P-CAP-CBP
4	A	306	GOL	O2-C2-C3-O3
4	C	305	GOL	O1-C1-C2-O2
4	C	305	GOL	O1-C1-C2-C3

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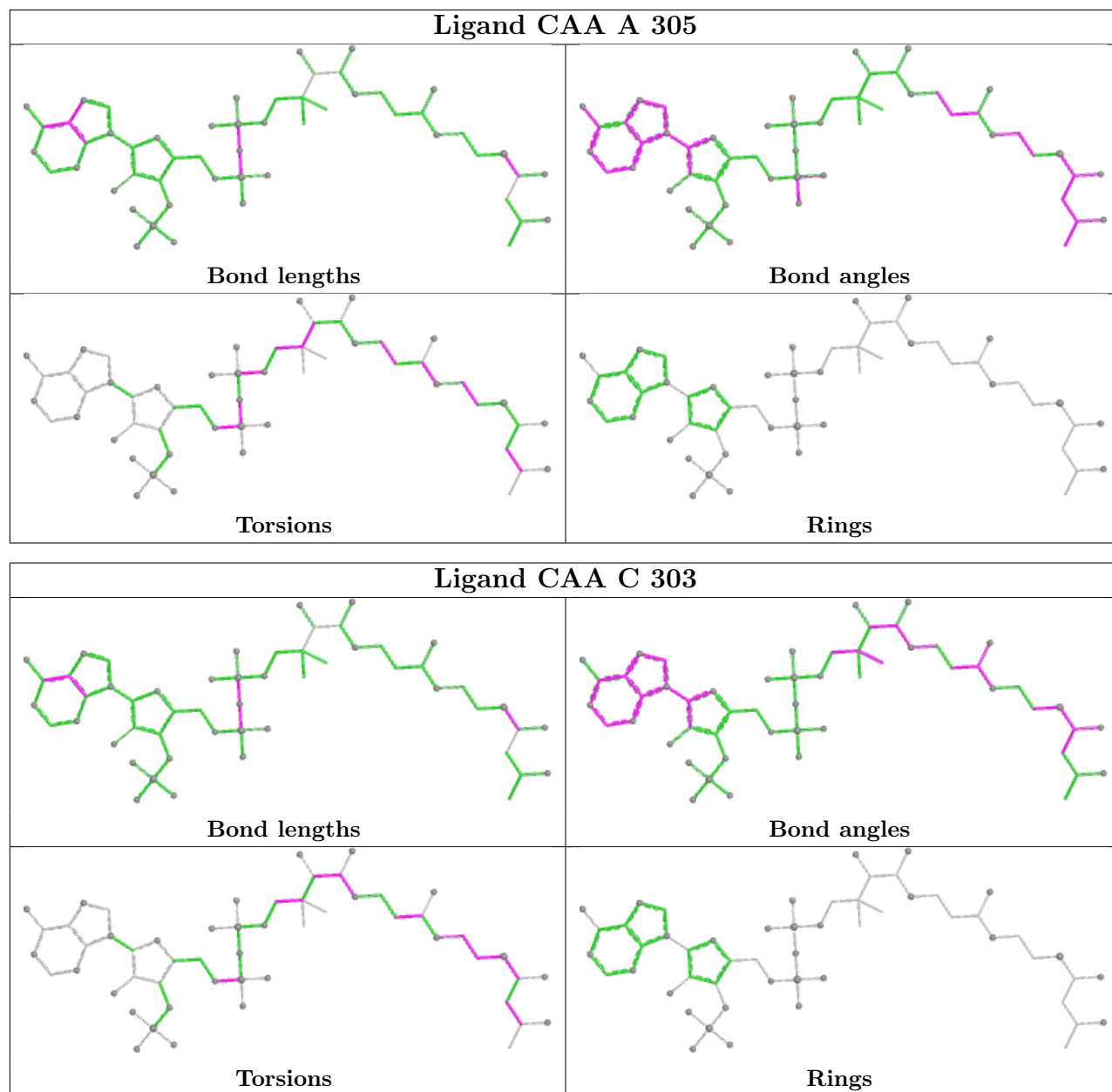
Mol	Chain	Res	Type	Atoms
3	B	303	CAA	O1-C1-C2-C3
3	A	305	CAA	C6P-C5P-N4P-C3P
3	A	305	CAA	C5B-O5B-P1A-O1A
3	A	305	CAA	CCP-O6A-P2A-O4A
3	C	303	CAA	C5B-O5B-P1A-O3A
3	C	303	CAA	O9P-C9P-CAP-CBP
4	B	305	GOL	O1-C1-C2-C3
4	A	307	GOL	O1-C1-C2-O2
3	B	303	CAA	O5P-C5P-C6P-C7P
4	A	306	GOL	C1-C2-C3-O3
4	C	304	GOL	O2-C2-C3-O3
3	B	303	CAA	C3B-O3B-P3B-O8A
3	A	305	CAA	CEP-CBP-CCP-O6A
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3	A	305	CAA	P2A-O3A-P1A-O2A

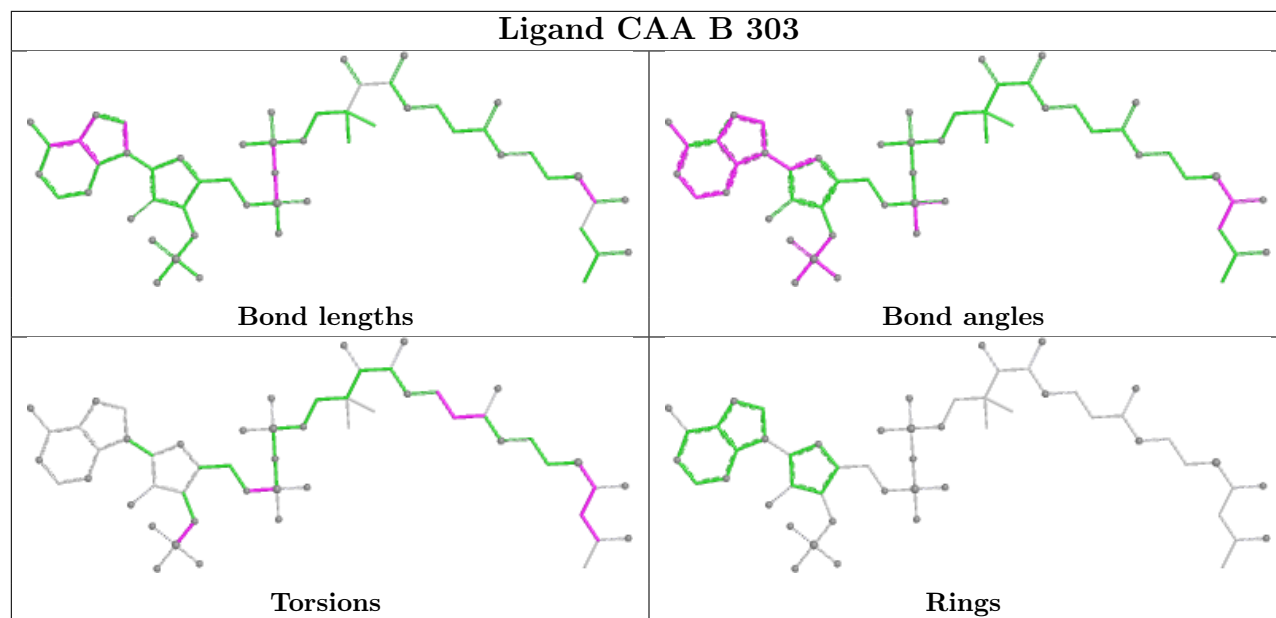
There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	SO4	1	0
3	A	305	CAA	2	0
4	A	307	GOL	6	0
4	C	305	GOL	2	0
3	C	303	CAA	2	0
4	B	305	GOL	5	0
3	B	303	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	266/300 (88%)	0.04	19 (7%) 22 25	20, 31, 79, 134	2 (0%)
1	B	260/300 (86%)	0.38	16 (6%) 26 30	18, 41, 74, 104	2 (0%)
1	C	262/300 (87%)	0.07	19 (7%) 21 24	23, 33, 71, 109	2 (0%)
All	All	788/900 (87%)	0.16	54 (6%) 23 26	18, 34, 74, 134	6 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	PHE	6.3
1	A	78	ALA	5.3
1	B	78	ALA	5.2
1	C	80	GLY	5.1
1	A	72	PHE	5.1
1	C	72	PHE	4.3
1	C	75	ILE	4.3
1	C	78	ALA	4.2
1	A	84	ASN	4.0
1	A	83	THR	4.0
1	B	76	ALA	3.7
1	A	75	ILE	3.5
1	B	85	LYS	3.3
1	A	85	LYS	3.2
1	B	265	LEU	3.1
1	B	6	ARG	3.1
1	C	268	PHE	3.0
1	A	76	ALA	3.0
1	A	81	ASP	3.0
1	C	79	GLN	2.9
1	B	191	GLU	2.8
1	C	86	TYR	2.8
1	A	268	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	77	LYS	2.7
1	B	77	LYS	2.7
1	C	76	ALA	2.7
1	C	7	GLN	2.6
1	B	269	ARG	2.6
1	A	269	ARG	2.6
1	B	75	ILE	2.5
1	C	77	LYS	2.5
1	C	85	LYS	2.5
1	C	204	SER	2.5
1	C	270	GLN	2.5
1	C	205	ASN	2.5
1	C	269	ARG	2.4
1	B	86	TYR	2.4
1	A	99	ALA	2.4
1	A	205	ASN	2.4
1	A	204	SER	2.3
1	C	265	LEU	2.3
1	B	268	PHE	2.3
1	B	7	GLN	2.3
1	A	79	GLN	2.2
1	C	188	ILE	2.2
1	A	4	GLU	2.2
1	C	4	GLU	2.2
1	A	74	GLY	2.1
1	A	80	GLY	2.1
1	B	9	GLU	2.1
1	B	207	GLU	2.1
1	B	73	LYS	2.1
1	A	265	LEU	2.1
1	C	6[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	A	190	10/11	0.86	0.16	32,42,59,60	0
1	CME	B	190	10/11	0.88	0.16	37,52,71,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	C	190	10/11	0.88	0.15	33,46,67,75	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

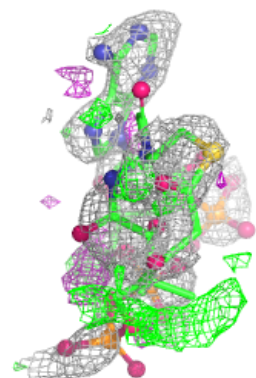
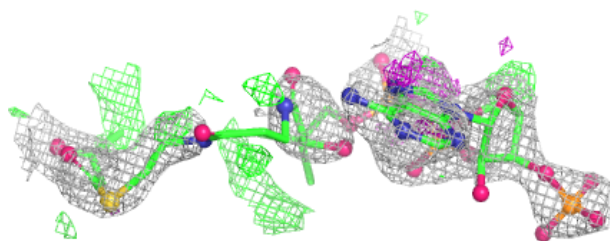
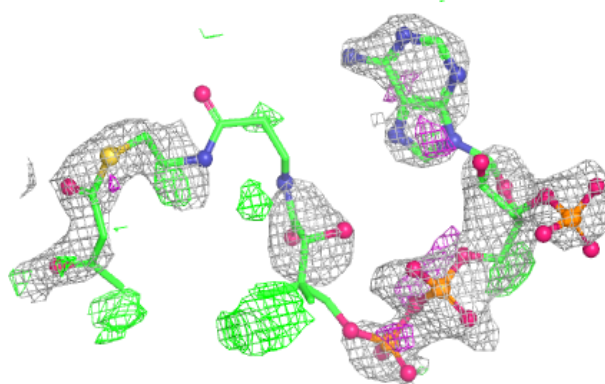
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAA	C	303	54/54	0.73	0.24	67,90,117,133	54
3	CAA	B	303	54/54	0.74	0.24	70,92,108,111	54
3	CAA	A	305	54/54	0.76	0.21	57,78,98,113	54
2	SO4	B	302	5/5	0.78	0.15	70,72,80,100	0
4	GOL	A	308	6/6	0.83	0.14	46,49,53,56	0
2	SO4	C	301	5/5	0.84	0.11	81,85,103,107	0
2	SO4	B	301	5/5	0.85	0.11	72,72,79,82	0
2	SO4	C	302	5/5	0.85	0.17	40,40,44,46	5
4	GOL	C	304	6/6	0.85	0.21	49,56,58,63	0
2	SO4	A	303	5/5	0.86	0.19	35,43,46,48	5
2	SO4	A	304	5/5	0.87	0.19	54,55,56,62	5
2	SO4	A	301	5/5	0.88	0.11	63,67,73,81	0
4	GOL	B	304	6/6	0.88	0.19	50,57,58,73	0
4	GOL	A	306	6/6	0.88	0.17	48,50,54,55	0
4	GOL	A	307	6/6	0.92	0.17	43,59,60,61	0
2	SO4	A	302	5/5	0.92	0.13	86,91,107,108	0
4	GOL	C	305	6/6	0.92	0.15	37,51,56,59	0
4	GOL	B	305	6/6	0.93	0.14	40,53,60,61	0

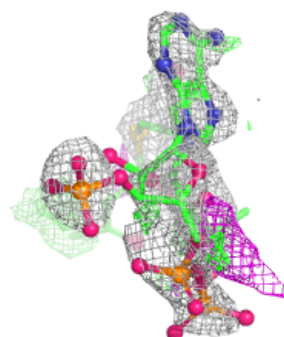
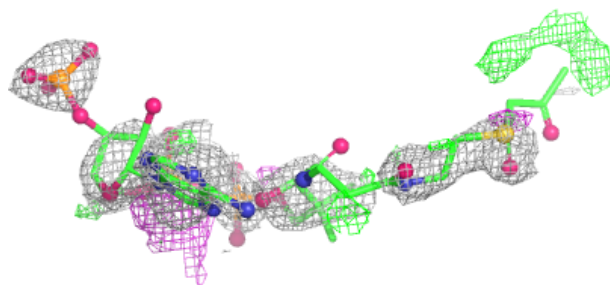
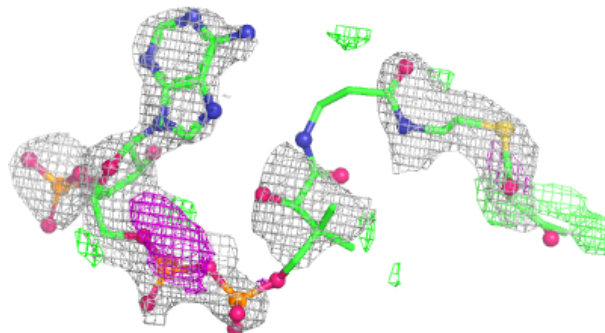
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAA C 303:

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

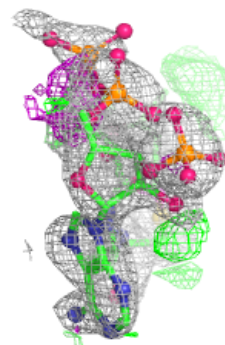
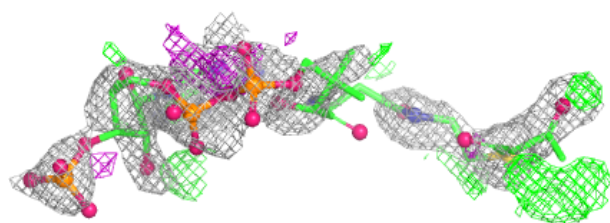
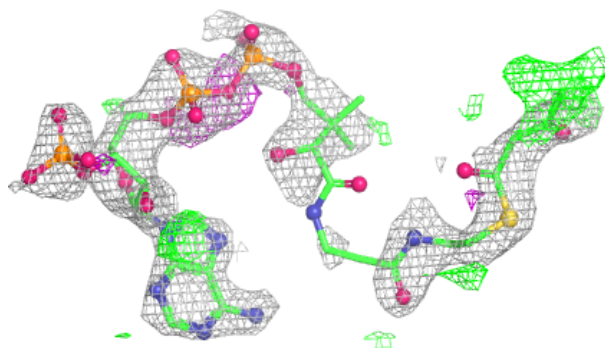
**Electron density around CAA B 303:**

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



Electron density around CAA A 305:

$2mF_o - DF_c$ (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.