



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:00 PM UTC

PDB ID : 3VBP / pdb_00003vbp
Title : Crystal Structure of the D94N mutant of AntD, an N-acyltransferase from Bacillus cereus in complex with dTDP and Coenzyme A
Authors : Kubiak, R.L.; Holden, H.M.
Deposited on : 2012-01-02
Resolution : 2.30 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

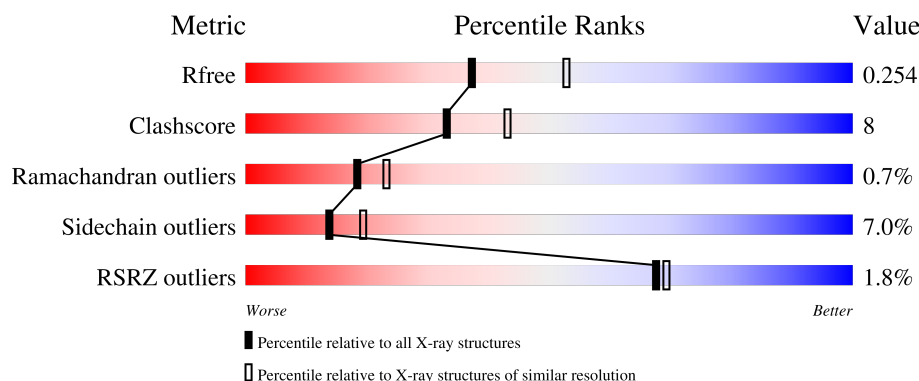
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	205	 67% 20% • 10%
1	C	205	 65% 20% 5% 9%
1	E	205	 70% 18% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4664 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 Galactoside O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	3	0
			1443	934	241	262	6			
1	C	187	Total	C	N	O	S	0	0	0
			1444	932	241	265	6			
1	E	185	Total	C	N	O	S	0	0	0
			1429	925	238	260	6			

There are 54 discrepancies between the modelled and reference sequences:

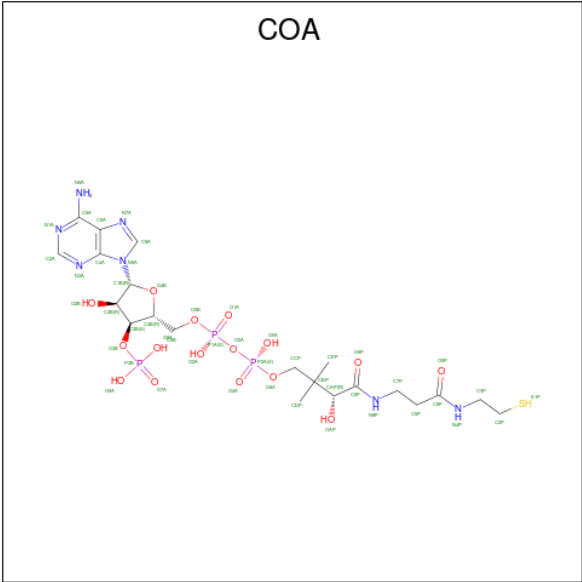
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP D7WGJ0
A	-15	GLY	-	expression tag	UNP D7WGJ0
A	-14	SER	-	expression tag	UNP D7WGJ0
A	-13	HIS	-	expression tag	UNP D7WGJ0
A	-12	HIS	-	expression tag	UNP D7WGJ0
A	-11	HIS	-	expression tag	UNP D7WGJ0
A	-10	HIS	-	expression tag	UNP D7WGJ0
A	-9	HIS	-	expression tag	UNP D7WGJ0
A	-8	HIS	-	expression tag	UNP D7WGJ0
A	-7	GLU	-	expression tag	UNP D7WGJ0
A	-6	ASN	-	expression tag	UNP D7WGJ0
A	-5	LEU	-	expression tag	UNP D7WGJ0
A	-4	TYR	-	expression tag	UNP D7WGJ0
A	-3	PHE	-	expression tag	UNP D7WGJ0
A	-2	GLN	-	expression tag	UNP D7WGJ0
A	-1	GLY	-	expression tag	UNP D7WGJ0
A	0	HIS	-	expression tag	UNP D7WGJ0
A	94	ASN	ASP	engineered mutation	UNP D7WGJ0
C	-16	MET	-	expression tag	UNP D7WGJ0
C	-15	GLY	-	expression tag	UNP D7WGJ0
C	-14	SER	-	expression tag	UNP D7WGJ0
C	-13	HIS	-	expression tag	UNP D7WGJ0
C	-12	HIS	-	expression tag	UNP D7WGJ0

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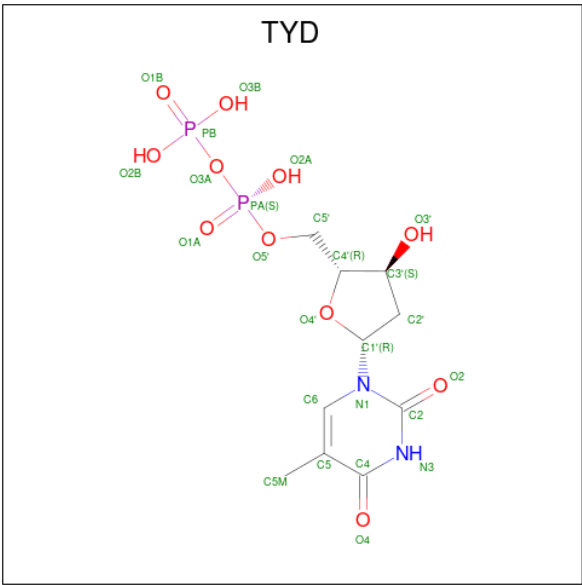
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP D7WGJ0
C	-10	HIS	-	expression tag	UNP D7WGJ0
C	-9	HIS	-	expression tag	UNP D7WGJ0
C	-8	HIS	-	expression tag	UNP D7WGJ0
C	-7	GLU	-	expression tag	UNP D7WGJ0
C	-6	ASN	-	expression tag	UNP D7WGJ0
C	-5	LEU	-	expression tag	UNP D7WGJ0
C	-4	TYR	-	expression tag	UNP D7WGJ0
C	-3	PHE	-	expression tag	UNP D7WGJ0
C	-2	GLN	-	expression tag	UNP D7WGJ0
C	-1	GLY	-	expression tag	UNP D7WGJ0
C	0	HIS	-	expression tag	UNP D7WGJ0
C	94	ASN	ASP	engineered mutation	UNP D7WGJ0
E	-16	MET	-	expression tag	UNP D7WGJ0
E	-15	GLY	-	expression tag	UNP D7WGJ0
E	-14	SER	-	expression tag	UNP D7WGJ0
E	-13	HIS	-	expression tag	UNP D7WGJ0
E	-12	HIS	-	expression tag	UNP D7WGJ0
E	-11	HIS	-	expression tag	UNP D7WGJ0
E	-10	HIS	-	expression tag	UNP D7WGJ0
E	-9	HIS	-	expression tag	UNP D7WGJ0
E	-8	HIS	-	expression tag	UNP D7WGJ0
E	-7	GLU	-	expression tag	UNP D7WGJ0
E	-6	ASN	-	expression tag	UNP D7WGJ0
E	-5	LEU	-	expression tag	UNP D7WGJ0
E	-4	TYR	-	expression tag	UNP D7WGJ0
E	-3	PHE	-	expression tag	UNP D7WGJ0
E	-2	GLN	-	expression tag	UNP D7WGJ0
E	-1	GLY	-	expression tag	UNP D7WGJ0
E	0	HIS	-	expression tag	UNP D7WGJ0
E	94	ASN	ASP	engineered mutation	UNP D7WGJ0

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (CCD ID: TYD) (formula: C₁₀H₁₆N₂O₁₁P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P		0	0
			25	10	2	11	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	E	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	C	35	Total	O	0	0
			35	35		
5	E	37	Total	O	0	0
			37	37		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	71.34Å 71.34Å 138.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.74 – 2.30 40.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.74-2.30) 97.7 (40.74-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.259 0.185 , 0.254	Depositor DCC
R_{free} test set	1498 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: TYD, CL, COA

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	0.67	0/1478	1.42	12/1992 (0.6%)
1	C	0.65	0/1470	1.40	10/1981 (0.5%)
1	E	0.63	0/1455	1.42	9/1962 (0.5%)
All	All	0.65	0/4403	1.41	31/5935 (0.5%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ILE	CA-C-N	8.13	128.19	119.90
1	A	106	ILE	C-N-CA	8.13	128.19	119.90
1	C	133	PHE	N-CA-C	7.79	119.08	110.13
1	C	102	MET	N-CA-C	7.18	121.23	109.24
1	C	103	GLY	CA-C-N	6.69	126.83	119.87
1	C	103	GLY	C-N-CA	6.69	126.83	119.87
1	A	126	ILE	CA-C-N	6.63	126.40	120.10
1	A	126	ILE	C-N-CA	6.63	126.40	120.10
1	A	74	GLY	N-CA-C	6.51	119.58	112.29
1	A	113	VAL	N-CA-C	6.22	117.33	108.93
1	E	26	LYS	N-CA-C	-5.97	105.84	113.01
1	A	185	SER	CB-CA-C	5.94	121.99	110.46
1	E	53	LYS	N-CA-C	5.91	117.92	108.41
1	C	49	ILE	N-CA-C	-5.89	99.00	107.78
1	E	152	GLU	CA-CB-CG	5.89	125.87	114.10
1	E	133	PHE	N-CA-C	5.78	116.77	110.13
1	A	175	ILE	CB-CA-C	-5.69	103.75	112.05
1	C	113	VAL	N-CA-C	5.57	115.59	108.12
1	C	62	ILE	CB-CA-C	-5.54	104.22	111.81
1	C	10	LEU	N-CA-C	5.40	116.98	111.14
1	A	102	MET	N-CA-C	5.34	118.15	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	74	GLY	N-CA-C	5.32	118.92	112.48
1	A	142	VAL	N-CA-C	5.28	115.89	109.30
1	A	91	ALA	N-CA-C	-5.27	106.53	113.17
1	A	75	ILE	N-CA-C	-5.23	100.59	108.12
1	C	129	HIS	CB-CA-C	-5.22	104.31	111.73
1	E	102	MET	N-CA-C	5.22	117.95	109.24
1	C	108	ASN	N-CA-C	5.21	118.42	111.75
1	E	126	ILE	CA-C-N	5.12	126.31	120.53
1	E	126	ILE	C-N-CA	5.12	126.31	120.53
1	E	147	MET	CG-SD-CE	-5.04	89.80	100.90

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	1443	0	1503	27	0
1	C	1444	0	1491	27	0
1	E	1429	0	1480	27	0
2	A	48	0	32	1	0
2	C	48	0	32	1	0
2	E	48	0	32	1	0
3	A	25	0	13	1	0
3	C	25	0	13	1	0
3	E	25	0	13	0	0
4	C	1	0	0	0	0
5	A	56	0	0	1	0
5	C	35	0	0	0	0
5	E	37	0	0	0	0
All	All	4664	0	4609	71	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 8.

All (71) 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:102:MET:HE1	1:E:125:ILE:HD13	1.17	1.15
1:A:102:MET:HE1	1:E:125:ILE:CD1	1.91	1.01
1:A:102:MET:CE	1:E:125:ILE:HD13	1.97	0.94
1:C:94:ASN:HD22	1:C:95:ASP:H	1.31	0.79
1:A:98:GLY:O	1:E:175:ILE:HG23	1.85	0.77
1:A:93:ILE:HG22	2:A:189:COA:H22	1.71	0.71
1:E:53:LYS:O	1:E:74:GLY:HA2	1.95	0.67
1:A:15:PHE:HA	1:A:33:PRO:O	1.97	0.65
1:E:175:ILE:HA	1:E:178:LEU:HD12	1.78	0.65
1:A:53:LYS:HB3	1:A:74:GLY:HA2	1.80	0.63
1:E:108:ASN:HA	1:E:111:LYS:HD2	1.82	0.60
1:E:133:PHE:HB3	1:E:134:PRO:CD	2.32	0.60
1:E:93:ILE:HG12	1:E:134:PRO:HG2	1.84	0.59
1:A:160:TYR:HB3	1:A:165:VAL:HB	1.86	0.56
1:A:144:VAL:HG13	1:A:148[A]:SER:OG	2.06	0.55
1:A:121:LYS:HB2	1:A:140:GLU:HA	1.88	0.55
1:A:102:MET:HE1	1:E:125:ILE:CG1	2.36	0.54
1:A:106:ILE:O	1:A:111:LYS:HE2	2.08	0.54
1:E:141:GLY:O	1:E:171:ARG:HD3	2.08	0.54
1:A:121:LYS:NZ	5:A:245:HOH:O	2.27	0.53
1:C:10:LEU:HA	1:C:13:ILE:HD12	1.90	0.53
1:C:160:TYR:HB3	1:C:165:VAL:HB	1.91	0.53
1:A:3:SER:HB2	1:C:31:TYR:OH	2.10	0.52
1:C:184:LYS:O	1:C:187:ASN:HB2	2.09	0.51
1:A:2:ASN:HB3	3:A:301:TYD:H2'1	1.93	0.51
1:A:86:ARG:NH2	1:C:65:TYR:O	2.38	0.50
1:C:7:GLN:O	1:C:11:LYS:HG2	2.12	0.49
1:C:133:PHE:CZ	2:C:189:COA:H61	2.48	0.49
1:A:38:ILE:HG23	1:A:42:VAL:HG21	1.95	0.48
1:A:89:VAL:HG22	1:A:132:ILE:HG13	1.94	0.48
1:E:15:PHE:C	1:E:17:SER:N	2.71	0.48
1:C:161:VAL:O	1:C:165:VAL:HA	2.13	0.48
1:C:86:ARG:HD3	1:E:86:ARG:HG2	1.96	0.48
1:A:181:GLU:HG2	1:C:110:TYR:HE1	1.79	0.47
3:C:301:TYD:H6	3:C:301:TYD:O5'	2.15	0.47
1:E:15:PHE:C	1:E:17:SER:H	2.23	0.46
1:A:40:ASN:O	1:A:41:ASN:HB2	2.14	0.46
1:A:148[A]:SER:HB2	1:A:165:VAL:HG12	1.98	0.46
1:E:160:TYR:HB3	1:E:165:VAL:HB	1.97	0.45
1:C:16:LEU:HB2	1:C:34:GLY:O	2.16	0.45
1:E:18:VAL:O	1:E:18:VAL:HG13	2.16	0.45
1:C:95:ASP:O	1:C:102:MET:HE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:O	1:C:174:LYS:C	2.59	0.45
1:C:126:ILE:HD12	1:C:132:ILE:HD11	1.99	0.45
1:E:42:VAL:HA	1:E:60:SER:O	2.17	0.45
1:A:156:ASP:HB3	1:A:157:TRP:CD1	2.52	0.44
1:E:25:SER:C	1:E:27:LYS:N	2.74	0.44
1:A:106:ILE:HA	1:A:107:PRO:HD2	1.77	0.44
1:E:100:ALA:HB1	1:E:111:LYS:HA	2.00	0.44
1:C:10:LEU:HD22	1:C:18:VAL:HG21	2.00	0.43
1:C:53:LYS:O	1:C:74:GLY:HA2	2.18	0.43
1:A:148[B]:SER:HB3	1:A:165:VAL:HG12	1.98	0.43
1:C:93:ILE:HG12	1:C:134:PRO:HG2	2.01	0.43
1:E:7:GLN:HA	1:E:10:LEU:HD12	2.00	0.43
1:C:3:SER:O	1:C:26:LYS:HG3	2.18	0.43
1:E:25:SER:C	1:E:27:LYS:H	2.26	0.42
1:C:143:ALA:HB3	1:C:159:ILE:HG12	2.00	0.42
1:C:79:ASP:O	1:C:80:PHE:HB2	2.19	0.42
1:C:125:ILE:HD13	1:E:102:MET:HE1	2.00	0.42
1:A:36:ILE:HA	1:A:54:VAL:O	2.20	0.42
1:C:21:ASN:CG	1:C:21:ASN:O	2.63	0.42
1:C:129:HIS:CG	1:E:131:ILE:HD11	2.55	0.42
1:E:23:LEU:O	1:E:43:ARG:HA	2.20	0.42
1:E:133:PHE:HB3	1:E:134:PRO:HD2	2.00	0.42
1:E:93:ILE:HG22	2:E:189:COA:H22	2.00	0.41
1:C:16:LEU:O	1:C:16:LEU:HG	2.20	0.41
1:A:79:ASP:O	1:A:80:PHE:HB2	2.20	0.40
1:A:100:ALA:HB1	1:A:111:LYS:HA	2.03	0.40
1:C:40:ASN:O	1:C:58:SER:HB3	2.21	0.40
1:C:44:ILE:HG12	1:C:62:ILE:HG13	2.03	0.40
1:E:148:SER:HB3	1:E:165:VAL:HG12	2.03	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	186/205 (91%)	175 (94%)	11 (6%)	0	100	100
1	C	185/205 (90%)	168 (91%)	17 (9%)	0	100	100
1	E	183/205 (89%)	165 (90%)	14 (8%)	4 (2%)	5	4
All	All	554/615 (90%)	508 (92%)	42 (8%)	4 (1%)	18	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	156	ASP
1	E	16	LEU
1	E	17	SER
1	E	39	GLY

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	159/174 (91%)	147 (92%)	12 (8%)	12	17
1	C	158/174 (91%)	143 (90%)	15 (10%)	8	10
1	E	156/174 (90%)	150 (96%)	6 (4%)	29	44
All	All	473/522 (91%)	440 (93%)	33 (7%)	14	19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	12	LYS
1	A	26	LYS
1	A	32	ASN
1	A	53	LYS
1	A	109	GLN
1	A	121	LYS
1	A	125	ILE
1	A	144	VAL

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Mol	Chain	Res	Type
1	A	169	LYS
1	A	175	ILE
1	A	184	LYS
1	C	3	SER
1	C	10	LEU
1	C	12	LYS
1	C	13	ILE
1	C	18	VAL
1	C	32	ASN
1	C	37	SER
1	C	58	SER
1	C	72	GLU
1	C	84	SER
1	C	94	ASN
1	C	109	GLN
1	C	125	ILE
1	C	136	VAL
1	C	186	MET
1	E	12	LYS
1	E	22	VAL
1	E	109	GLN
1	E	138	ILE
1	E	152	GLU
1	E	177	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	99	ASN
1	A	108	ASN
1	C	21	ASN
1	C	32	ASN
1	C	41	ASN
1	C	94	ASN
1	C	109	GLN
1	E	7	GLN
1	E	32	ASN
1	E	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	TYD	E	301	-	25,26,26	1.33	3 (12%)	38,40,40	1.88	10 (26%)
3	TYD	C	301	-	25,26,26	1.39	4 (16%)	38,40,40	1.90	10 (26%)
2	COA	E	189	-	47,50,50	1.03	3 (6%)	69,75,75	1.91	16 (23%)
2	COA	C	189	-	47,50,50	0.99	4 (8%)	69,75,75	2.07	16 (23%)
2	COA	A	189	-	47,50,50	1.00	3 (6%)	69,75,75	1.93	19 (27%)
3	TYD	A	301	-	25,26,26	1.47	3 (12%)	38,40,40	1.80	7 (18%)

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	TYD	E	301	-	-	0/16/28/28	0/2/2/2
3	TYD	C	301	-	-	5/16/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	E	189	-	-	7/48/64/64	0/3/3/3
2	COA	C	189	-	-	6/48/64/64	0/3/3/3
2	COA	A	189	-	-	15/48/64/64	0/3/3/3
3	TYD	A	301	-	-	6/16/28/28	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	189	COA	P1A-O3A	3.99	1.63	1.59
3	C	301	TYD	C6-C5	3.69	1.40	1.34
3	A	301	TYD	PA-O3A	3.68	1.63	1.59
3	A	301	TYD	C6-C5	3.62	1.40	1.34
3	A	301	TYD	C4-C5	-3.35	1.39	1.44
3	E	301	TYD	C6-C5	3.22	1.39	1.34
3	C	301	TYD	C4-C5	-3.11	1.39	1.44
2	C	189	COA	P1A-O3A	3.08	1.62	1.59
3	E	301	TYD	C4-C5	-3.04	1.39	1.44
3	C	301	TYD	PA-O3A	2.87	1.62	1.59
2	E	189	COA	P2A-O3A	2.86	1.62	1.59
2	A	189	COA	P1A-O3A	2.74	1.62	1.59
2	A	189	COA	P2A-O3A	2.72	1.62	1.59
2	C	189	COA	P2A-O3A	2.46	1.62	1.59
2	C	189	COA	C8A-N7A	2.40	1.36	1.31
3	E	301	TYD	PA-O3A	2.28	1.62	1.59
2	E	189	COA	C8A-N7A	2.15	1.35	1.31
2	A	189	COA	C4A-N9A	-2.10	1.33	1.37
3	C	301	TYD	C2-N1	-2.09	1.35	1.38
2	C	189	COA	P3B-O3B	2.06	1.63	1.59

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	189	COA	C3P-N4P-C5P	5.80	133.63	122.82
2	C	189	COA	C5A-C4A-N3A	-5.74	118.82	126.72
2	C	189	COA	C3P-N4P-C5P	5.61	133.26	122.82
3	C	301	TYD	N3-C2-N1	5.59	122.17	114.89
2	E	189	COA	CDP-CBP-CCP	-5.16	99.70	108.22
2	A	189	COA	C3P-N4P-C5P	5.15	132.42	122.82
2	A	189	COA	N9A-C8A-N7A	-5.07	106.74	113.94
3	C	301	TYD	C6-N1-C2	-5.02	116.31	121.30
3	A	301	TYD	N3-C2-N1	4.95	121.33	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	189	COA	C5A-C4A-N3A	-4.92	119.94	126.72
2	C	189	COA	N3A-C2A-N1A	-4.83	121.27	128.58
2	C	189	COA	N9A-C8A-N7A	-4.82	107.09	113.94
3	E	301	TYD	C5M-C5-C4	4.75	123.86	118.78
2	A	189	COA	C4A-N9A-C8A	4.66	110.63	105.74
3	E	301	TYD	N3-C2-N1	4.39	120.61	114.89
2	E	189	COA	N3A-C2A-N1A	-4.36	121.98	128.58
3	A	301	TYD	C4-N3-C2	-4.36	121.62	127.34
2	C	189	COA	C4A-N9A-C8A	4.17	110.11	105.74
3	E	301	TYD	C5M-C5-C6	-4.07	117.34	122.85
2	C	189	COA	N3A-C4A-N9A	3.97	133.91	127.17
2	C	189	COA	C4A-C5A-N7A	-3.95	106.07	110.58
3	A	301	TYD	C5-C4-N3	3.93	118.74	115.32
2	A	189	COA	N3A-C2A-N1A	-3.90	122.68	128.58
2	C	189	COA	C2A-N3A-C4A	3.88	121.31	111.83
2	C	189	COA	C5A-N7A-C8A	3.82	109.46	103.45
2	A	189	COA	C5A-C4A-N3A	-3.76	121.54	126.72
3	C	301	TYD	C4-N3-C2	-3.72	122.46	127.34
2	A	189	COA	C5A-N7A-C8A	3.61	109.12	103.45
2	C	189	COA	CDP-CBP-CCP	-3.60	102.29	108.22
3	A	301	TYD	O4'-C1'-N1	3.59	114.24	107.86
2	A	189	COA	CDP-CBP-CCP	-3.56	102.34	108.22
2	E	189	COA	N9A-C8A-N7A	-3.52	108.94	113.94
2	E	189	COA	C2A-N3A-C4A	3.51	120.39	111.83
2	C	189	COA	O4B-C1B-N9A	-3.29	101.77	108.09
2	A	189	COA	C4A-C5A-N7A	-3.28	106.83	110.58
3	C	301	TYD	O4'-C1'-N1	3.28	113.68	107.86
3	E	301	TYD	C4-N3-C2	-3.27	123.06	127.34
2	E	189	COA	C4A-C5A-N7A	-3.25	106.86	110.58
3	E	301	TYD	O4'-C1'-N1	3.16	113.48	107.86
3	A	301	TYD	C6-N1-C2	-3.16	118.16	121.30
2	E	189	COA	N3A-C4A-N9A	3.11	132.46	127.17
2	E	189	COA	C5A-N7A-C8A	2.96	108.10	103.45
3	E	301	TYD	O2-C2-N3	-2.90	116.14	121.49
3	A	301	TYD	O2-C2-N3	-2.88	116.18	121.49
3	E	301	TYD	C6-N1-C2	-2.87	118.44	121.30
3	C	301	TYD	O4-C4-C5	-2.78	121.73	124.92
2	A	189	COA	N3A-C4A-N9A	2.72	131.80	127.17
2	A	189	COA	C6P-C5P-N4P	-2.68	111.46	116.34
2	E	189	COA	C4A-N9A-C8A	2.64	108.51	105.74
2	C	189	COA	O2A-P1A-O1A	2.62	124.61	112.44
2	E	189	COA	O5A-P2A-O3A	2.57	114.23	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	189	COA	C2A-N3A-C4A	2.57	118.11	111.83
2	E	189	COA	CEP-CBP-CDP	2.50	114.19	109.20
3	C	301	TYD	O2-C2-N3	-2.50	116.88	121.49
3	C	301	TYD	O3B-PB-O2B	2.43	116.91	107.80
2	A	189	COA	O3B-C3B-C2B	-2.39	103.09	111.68
2	C	189	COA	O5A-P2A-O3A	2.37	113.68	107.27
3	C	301	TYD	C5-C4-N3	2.37	117.38	115.32
2	A	189	COA	C4A-N9A-C1B	-2.37	121.09	126.63
3	E	301	TYD	O2A-PA-O3A	2.33	113.57	107.27
2	A	189	COA	O6A-CCP-CBP	2.32	114.28	110.55
3	E	301	TYD	C1'-N1-C2	2.31	122.18	117.66
3	A	301	TYD	O4-C4-C5	-2.29	122.30	124.92
2	A	189	COA	O9A-P3B-O8A	2.27	116.31	107.80
2	E	189	COA	C2P-C3P-N4P	-2.26	107.18	112.31
2	C	189	COA	O3B-P3B-O7A	-2.25	101.30	109.33
3	C	301	TYD	C1'-N1-C2	2.23	122.02	117.66
2	C	189	COA	C7P-C6P-C5P	2.22	116.09	112.39
2	C	189	COA	O5A-P2A-O4A	2.19	122.64	112.44
3	E	301	TYD	C2'-C1'-N1	-2.17	108.38	113.81
2	E	189	COA	C3B-C2B-C1B	2.16	104.65	99.89
2	A	189	COA	O9P-C9P-N8P	-2.15	118.44	122.98
2	A	189	COA	O3B-P3B-O7A	-2.12	101.79	109.33
2	A	189	COA	O9P-C9P-CAP	2.09	126.73	120.89
2	E	189	COA	O3B-C3B-C2B	-2.06	104.29	111.68
2	E	189	COA	O5A-P2A-O6A	-2.05	98.26	107.57
2	A	189	COA	O9A-P3B-O3B	-2.04	97.90	105.85
3	C	301	TYD	C5M-C5-C4	2.03	120.95	118.78

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	189	COA	CCP-O6A-P2A-O4A
2	A	189	COA	OAP-CAP-CBP-CCP
2	A	189	COA	C9P-CAP-CBP-CCP
2	A	189	COA	OAP-CAP-CBP-CDP
2	A	189	COA	C9P-CAP-CBP-CDP
2	A	189	COA	OAP-CAP-CBP-CEP
2	C	189	COA	OAP-CAP-CBP-CCP
2	E	189	COA	OAP-CAP-CBP-CCP
3	A	301	TYD	C5'-O5'-PA-O2A
3	A	301	TYD	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	C	301	TYD	C5'-O5'-PA-O1A
3	C	301	TYD	C5'-O5'-PA-O2A
3	C	301	TYD	C5'-O5'-PA-O3A
3	A	301	TYD	O4'-C4'-C5'-O5'
3	A	301	TYD	C3'-C4'-C5'-O5'
3	C	301	TYD	O4'-C4'-C5'-O5'
2	C	189	COA	OAP-CAP-CBP-CEP
2	E	189	COA	OAP-CAP-CBP-CEP
3	C	301	TYD	C3'-C4'-C5'-O5'
3	A	301	TYD	PB-O3A-PA-O5'
2	A	189	COA	O9P-C9P-CAP-OAP
2	C	189	COA	C9P-CAP-CBP-CCP
2	E	189	COA	CEP-CBP-CCP-O6A
2	E	189	COA	S1P-C2P-C3P-N4P
2	A	189	COA	CCP-O6A-P2A-O3A
2	A	189	COA	CCP-O6A-P2A-O5A
3	A	301	TYD	C5'-O5'-PA-O1A
2	C	189	COA	OAP-CAP-CBP-CDP
2	A	189	COA	C9P-CAP-CBP-CEP
2	A	189	COA	P2A-O3A-P1A-O1A
2	C	189	COA	P1A-O3A-P2A-O5A
2	A	189	COA	CBP-CCP-O6A-P2A
2	E	189	COA	CDP-CBP-CCP-O6A
2	E	189	COA	C3B-O3B-P3B-O7A
2	A	189	COA	N8P-C9P-CAP-OAP
2	C	189	COA	N8P-C9P-CAP-OAP
2	E	189	COA	N8P-C9P-CAP-OAP
2	A	189	COA	S1P-C2P-C3P-N4P
2	A	189	COA	P2A-O3A-P1A-O2A

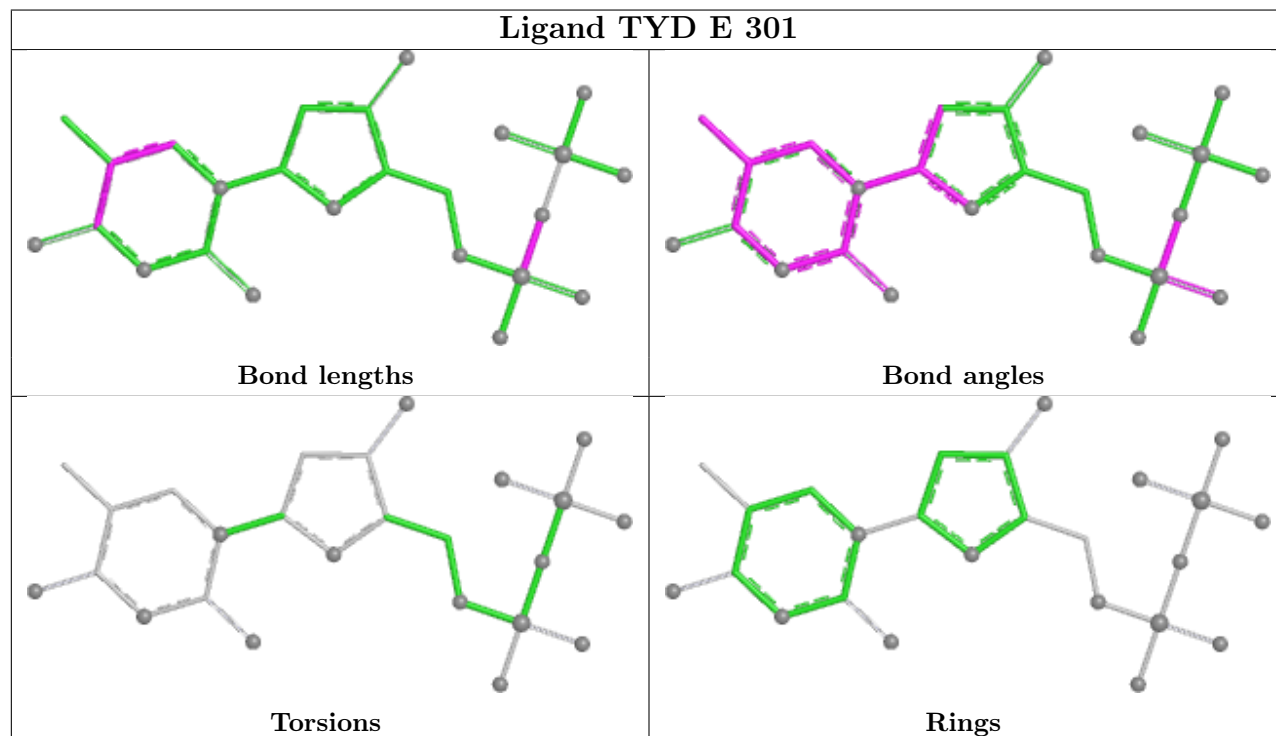
There are no ring outliers.

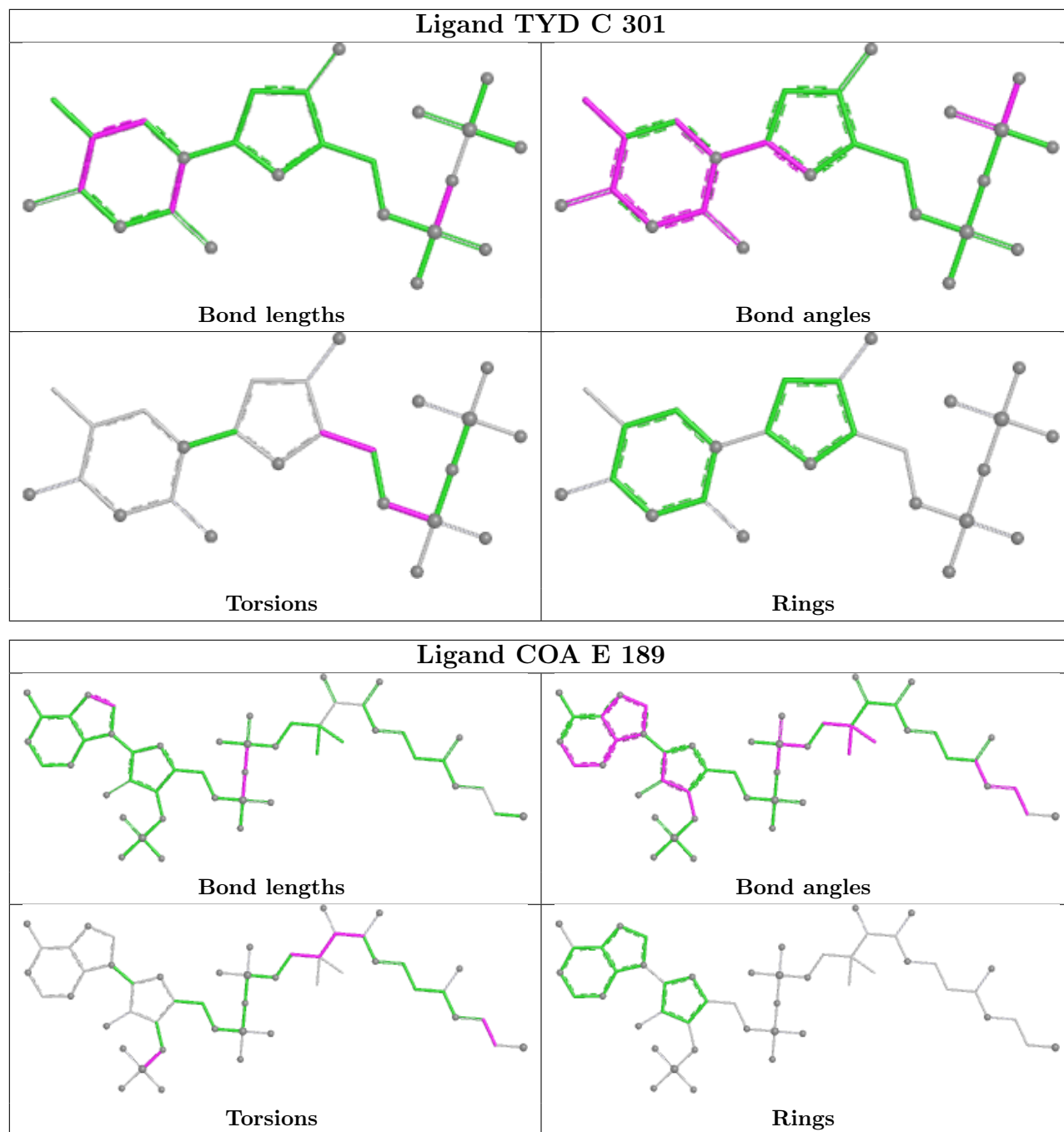
5 monomers are involved in 5 short contacts:

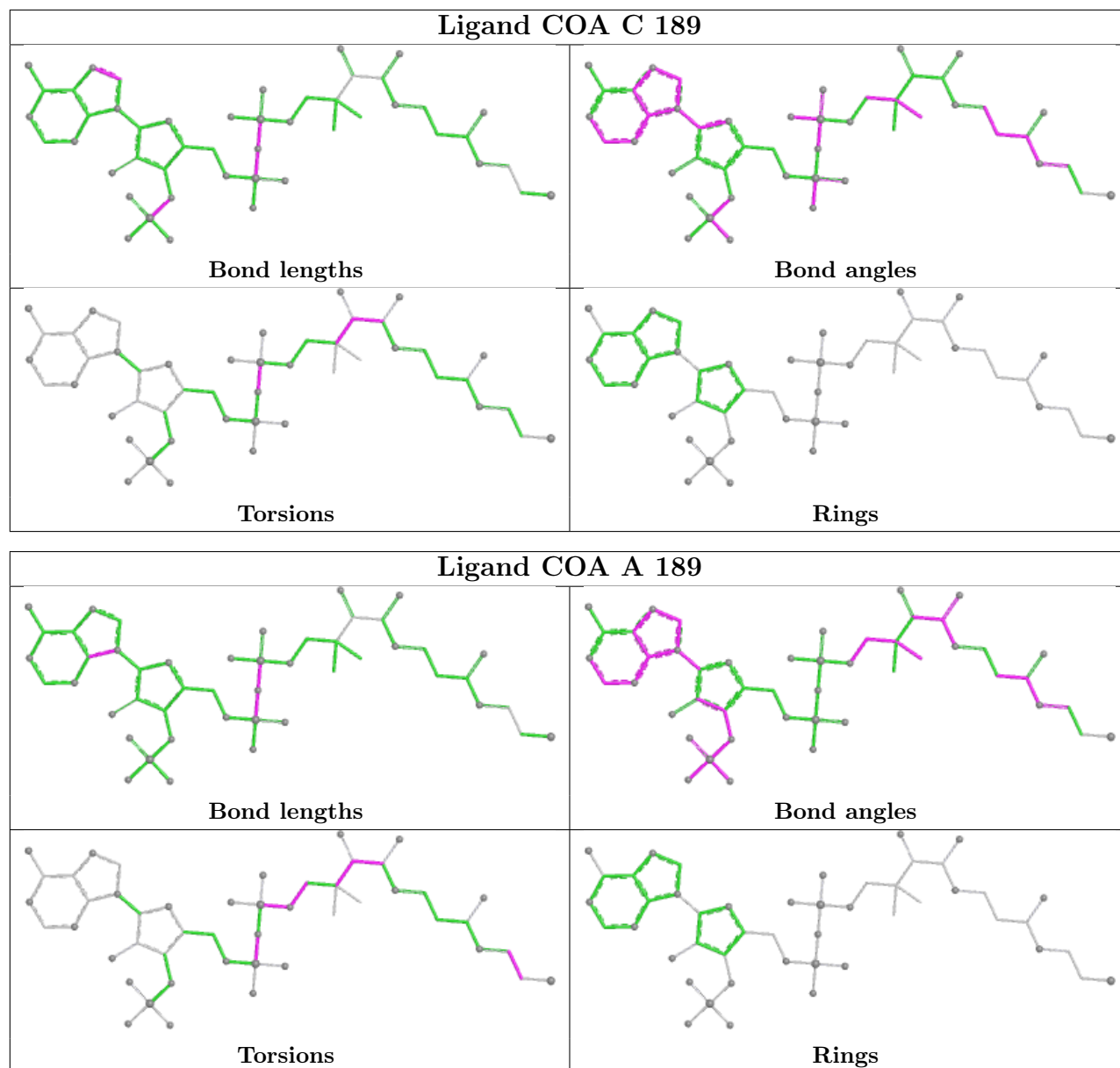
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	TYD	1	0
2	E	189	COA	1	0
2	C	189	COA	1	0
2	A	189	COA	1	0
3	A	301	TYD	1	0

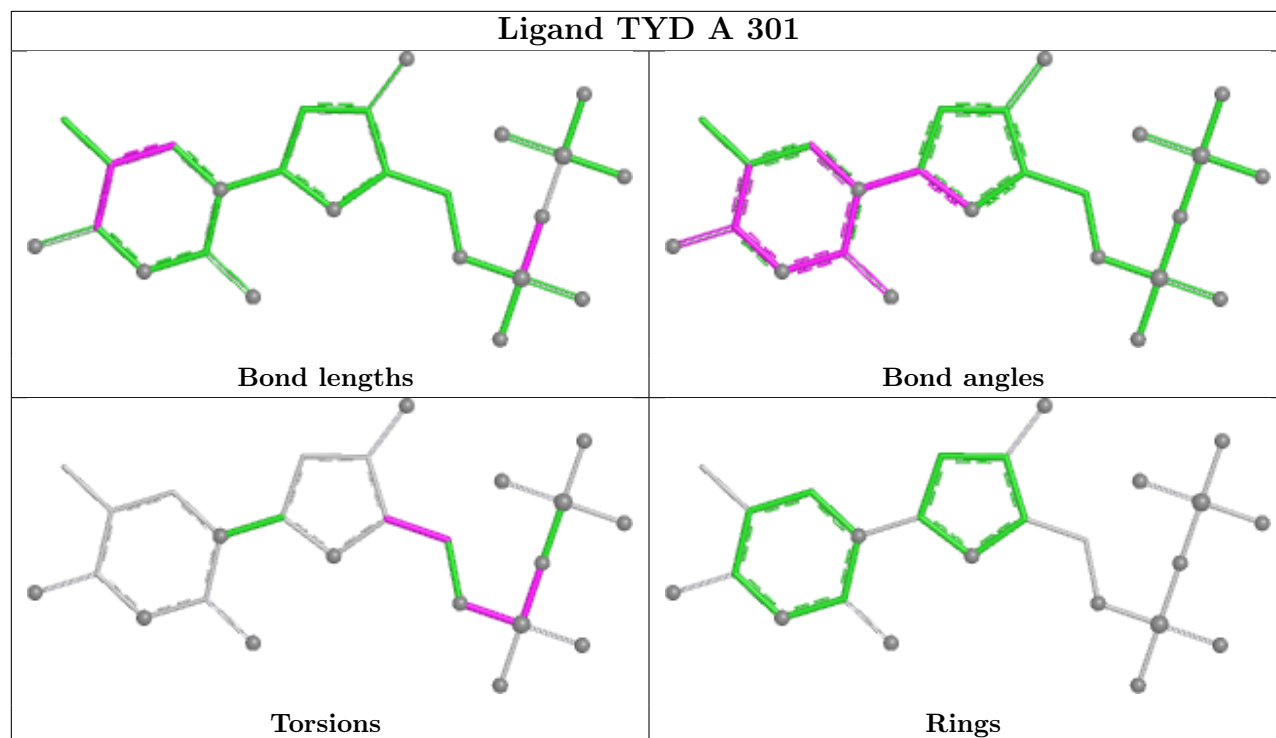
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	185/205 (90%)	-0.25	3 (1%) 70 72	12, 28, 59, 81	3 (1%)
1	C	187/205 (91%)	-0.06	4 (2%) 63 65	14, 33, 65, 95	0
1	E	185/205 (90%)	-0.09	3 (1%) 70 72	15, 34, 63, 78	0
All	All	557/615 (90%)	-0.13	10 (1%) 67 69	12, 32, 64, 95	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	188	SER	3.0
1	A	186	MET	2.7
1	A	105	THR	2.2
1	C	10	LEU	2.2
1	E	11	LYS	2.2
1	A	7	GLN	2.1
1	E	186	MET	2.1
1	E	105	THR	2.1
1	C	11	LYS	2.0
1	C	2	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

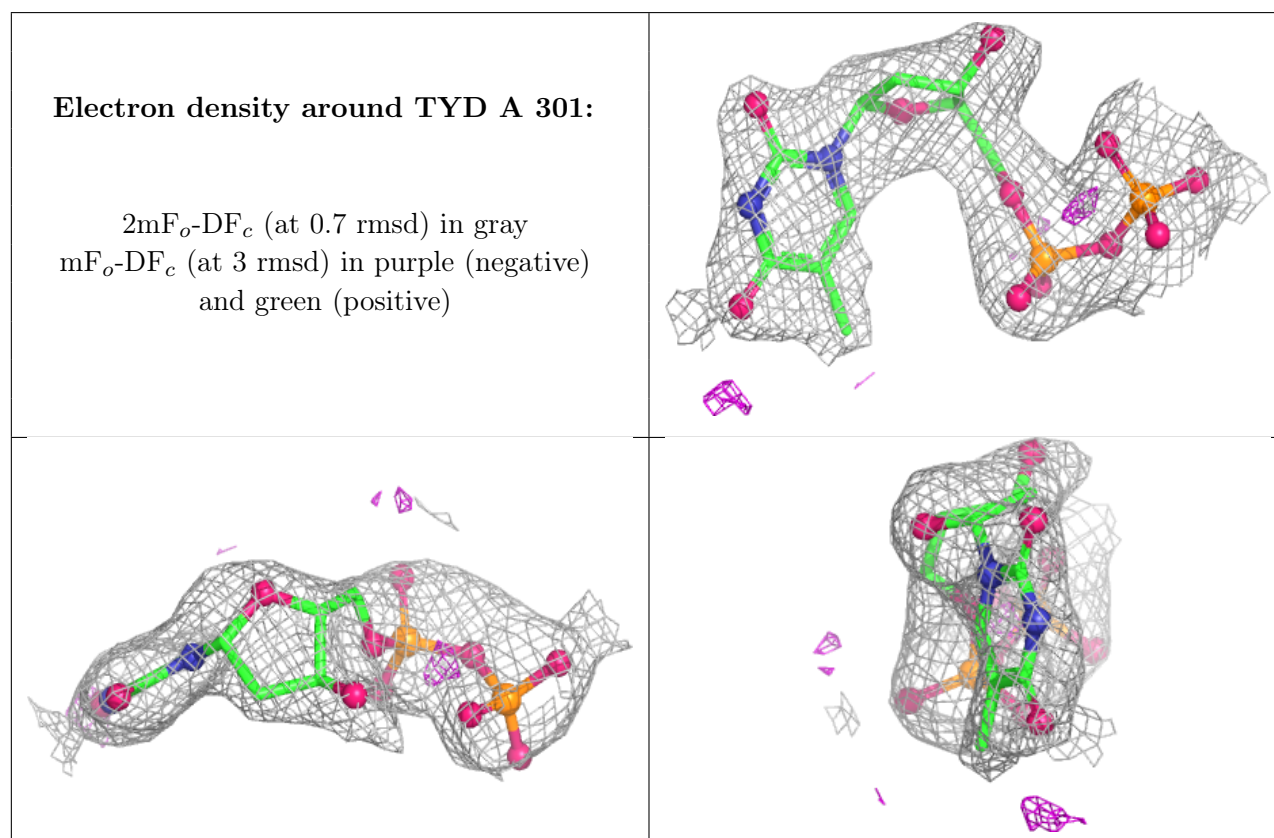
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

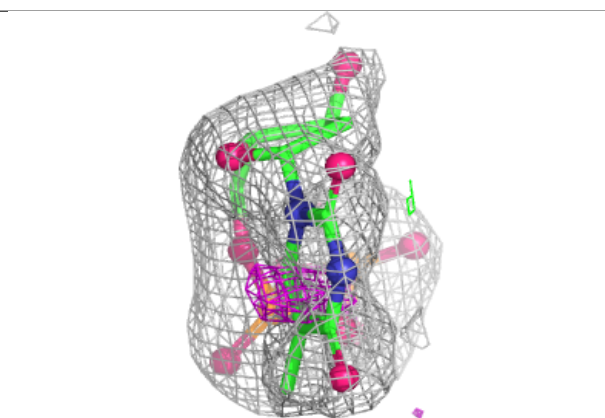
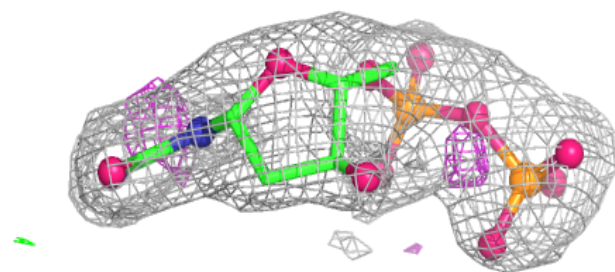
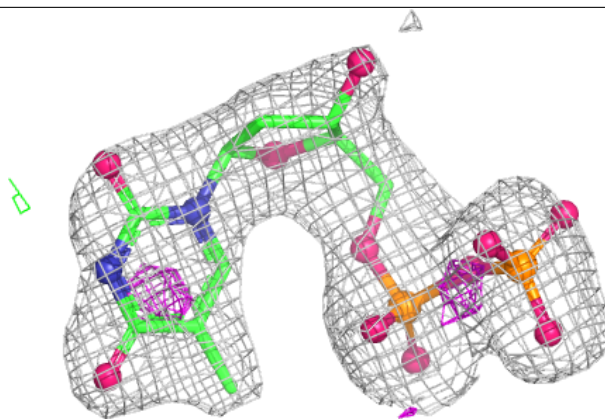
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYD	A	301	25/25	0.85	0.12	62,69,92,93	0
3	TYD	C	301	25/25	0.86	0.12	61,68,82,85	0
3	TYD	E	301	25/25	0.90	0.10	54,65,81,82	0
2	COA	A	189	48/48	0.94	0.07	22,35,52,54	0
2	COA	E	189	48/48	0.95	0.07	20,40,52,56	0
2	COA	C	189	48/48	0.95	0.07	18,31,50,54	0
4	CL	C	190	1/1	0.98	0.05	27,27,27,27	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.

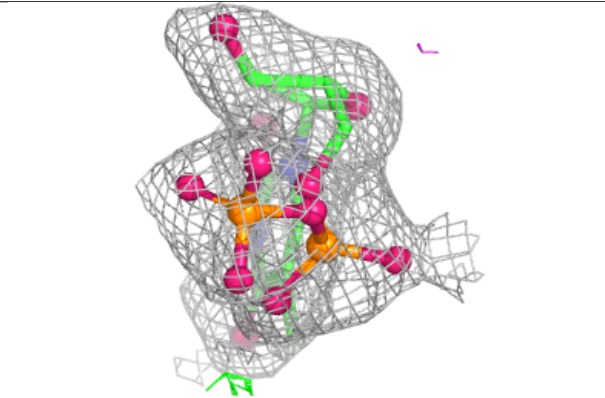
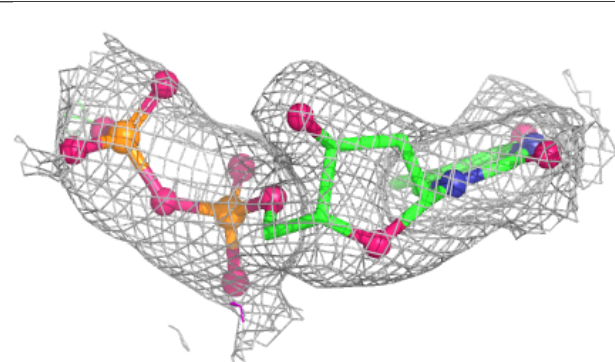
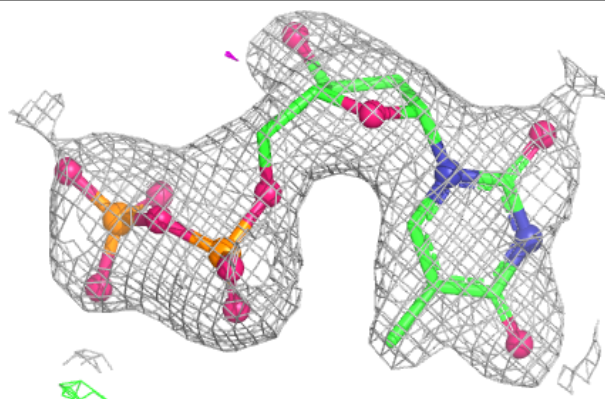


Electron density around TYD C 301:

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

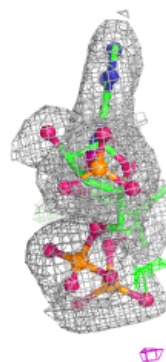
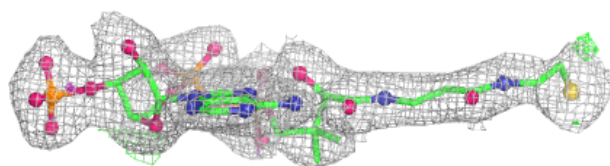
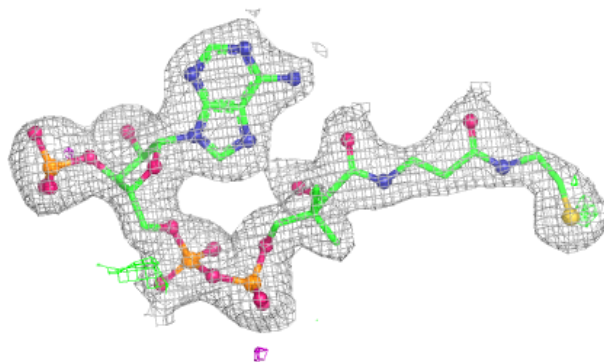
**Electron density around TYD E 301:**

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

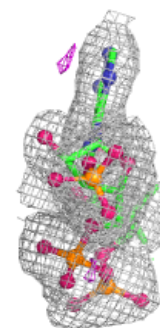
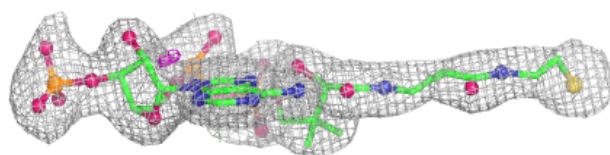
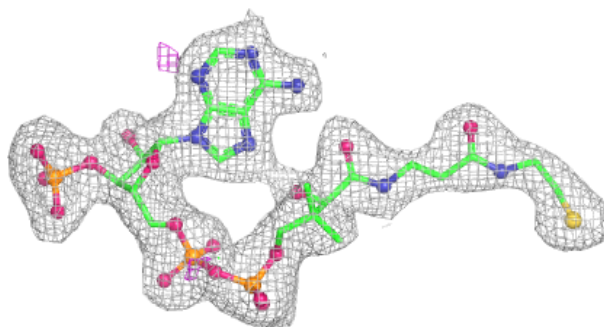


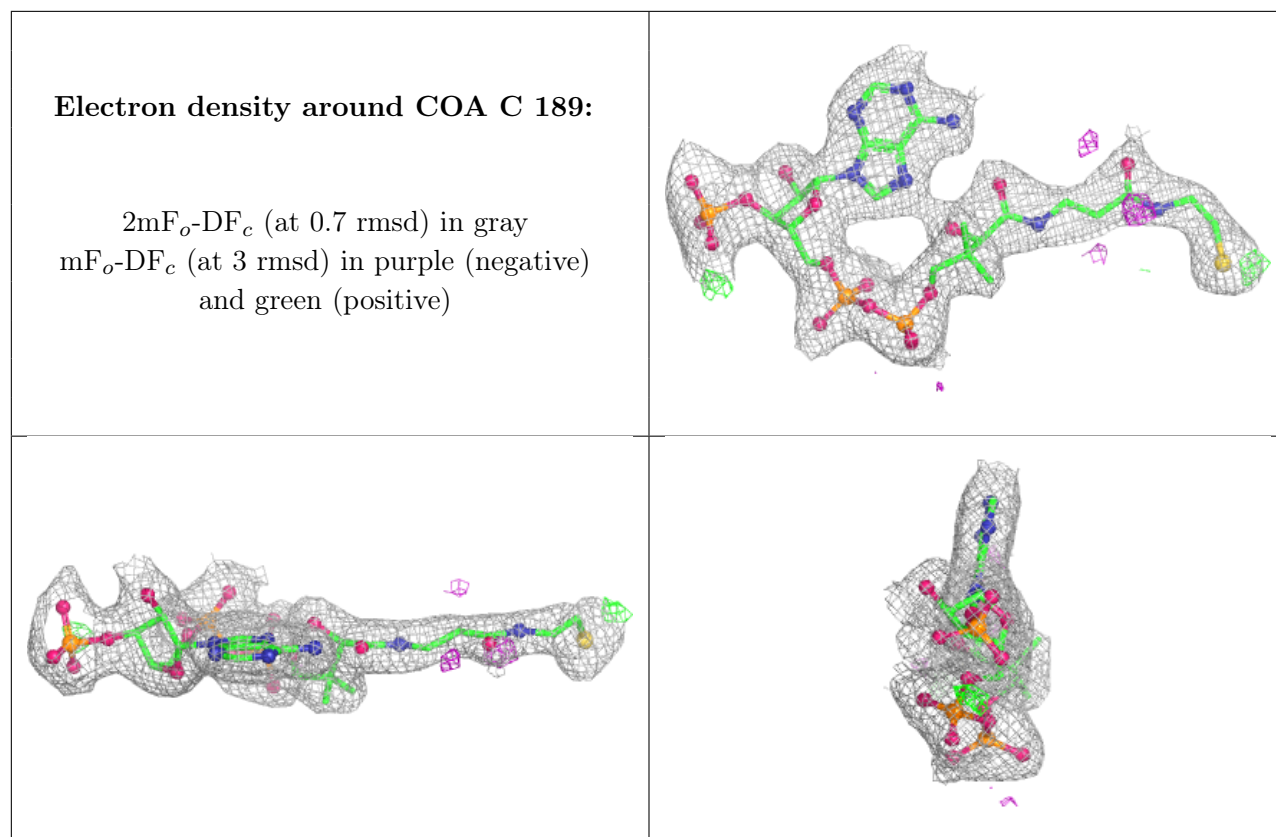
Electron density around COA A 189:

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

**Electron density around COA E 189:**

$2mF_o-DF_c$ (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.