



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:22 PM UTC

PDB ID : 7BCZ / pdb_00007bcz
Title : Structure of the 4'-phosphopantetheinyl transferase PcpS from *Pseudomonas aeruginosa*
Authors : Carivenc, C.; Mourey, L.; Pedelacq, J.D.
Deposited on : 2020-12-21
Resolution : 2.40 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

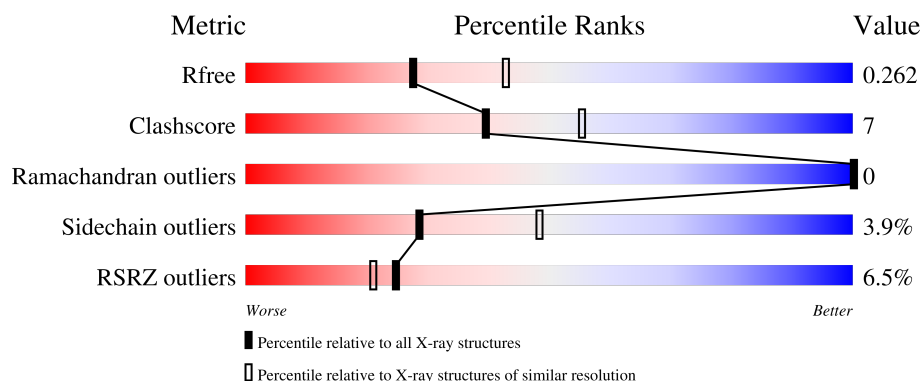
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	245	8% 78% 18% ...
1	B	245	5% 83% 14% ..
1	C	245	5% 78% 18% ..
1	D	245	7% 74% 22% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7843 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.

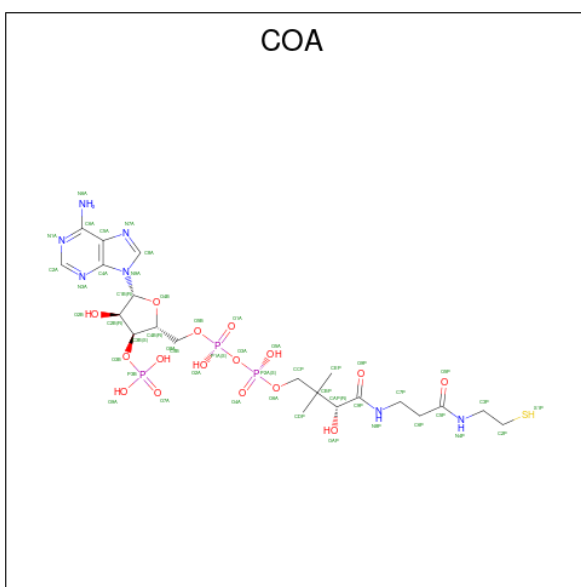
- Molecule 1 is a protein called 4'-phosphopantetheinyl transferase EntD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1889	1204	349	332	4			
1	B	239	Total	C	N	O	S	0	0	0
			1855	1184	337	331	3			
1	C	238	Total	C	N	O	S	0	1	0
			1859	1187	344	325	3			
1	D	242	Total	C	N	O	S	0	0	0
			1885	1202	349	330	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A6N0ZM94
A	-1	SER	-	expression tag	UNP A0A6N0ZM94
A	0	HIS	-	expression tag	UNP A0A6N0ZM94
B	-2	GLY	-	expression tag	UNP A0A6N0ZM94
B	-1	SER	-	expression tag	UNP A0A6N0ZM94
B	0	HIS	-	expression tag	UNP A0A6N0ZM94
C	-2	GLY	-	expression tag	UNP A0A6N0ZM94
C	-1	SER	-	expression tag	UNP A0A6N0ZM94
C	0	HIS	-	expression tag	UNP A0A6N0ZM94
D	-2	GLY	-	expression tag	UNP A0A6N0ZM94
D	-1	SER	-	expression tag	UNP A0A6N0ZM94
D	0	HIS	-	expression tag	UNP A0A6N0ZM94

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

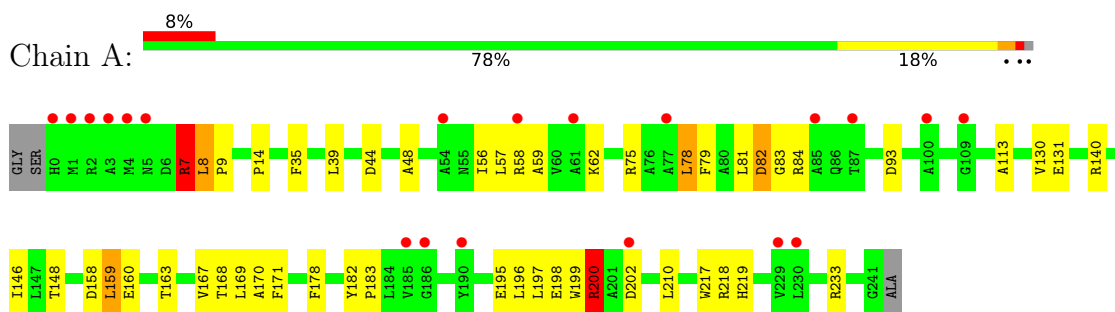
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total 41	O 41	0	0
5	B	48	Total 48	O 48	0	0
5	C	44	Total 44	O 44	0	0
5	D	28	Total 28	O 28	0	0

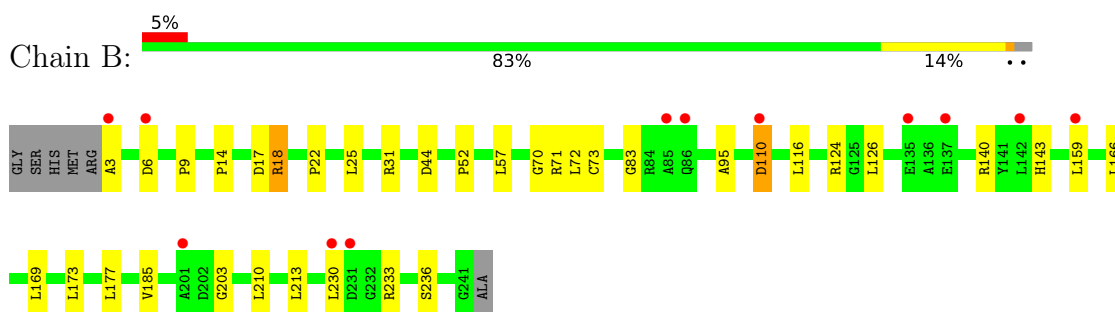
3 Residue-property plots [i](#)

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.

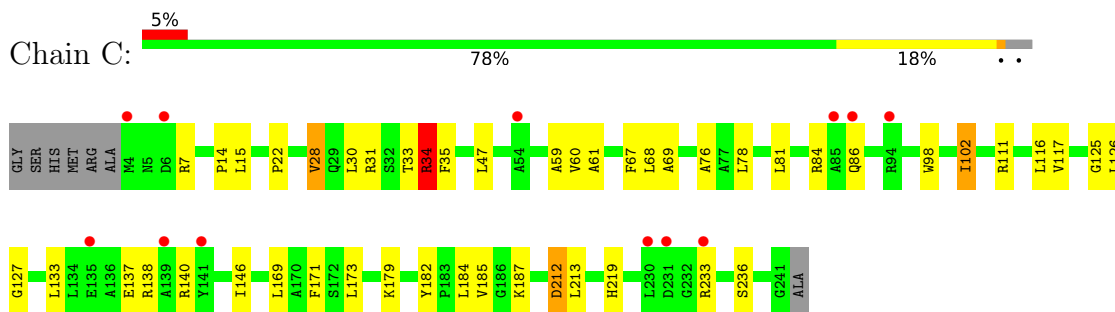
- Molecule 1: 4'-phosphopantetheinyl transferase EntD



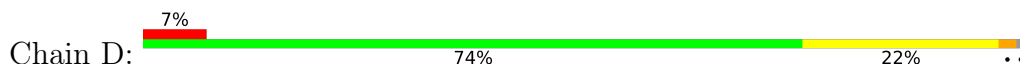
- Molecule 1: 4'-phosphopantetheinyl transferase EntD

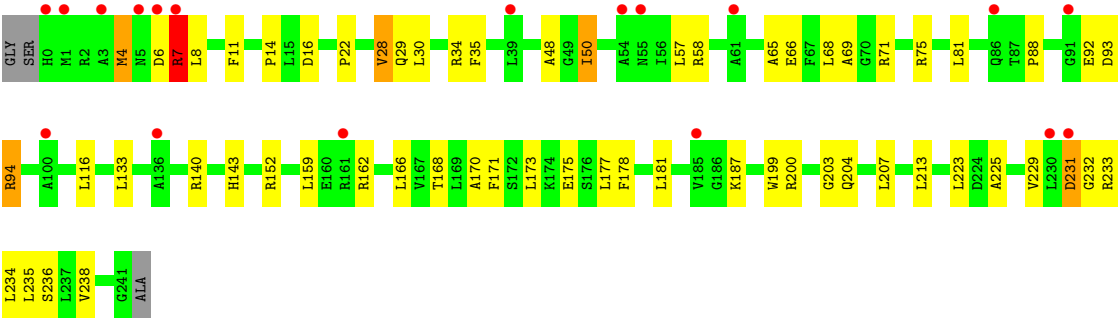


- Molecule 1: 4'-phosphopantetheinyl transferase EntD



- Molecule 1: 4'-phosphopantetheinyl transferase EntD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.36Å 78.87Å 81.12Å 85.62° 84.62° 73.86°	Depositor
Resolution (Å)	42.49 – 2.40 42.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (42.49-2.40) 91.9 (42.49-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.210 , 0.262 0.212 , 0.262	Depositor DCC
R_{free} test set	2010 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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: COA, MG, NA

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	0.82	14/1933 (0.7%)	0.59	0/2626
1	B	0.66	6/1898 (0.3%)	0.52	1/2582 (0.0%)
1	C	0.98	19/1902 (1.0%)	0.61	4/2585 (0.2%)
1	D	0.96	14/1929 (0.7%)	0.60	2/2621 (0.1%)
All	All	0.86	53/7662 (0.7%)	0.58	7/10414 (0.1%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	LEU	C-O	-10.79	1.09	1.24
1	D	28	VAL	C-O	-8.59	1.15	1.24
1	C	68	LEU	C-O	-8.19	1.14	1.24
1	C	125	GLY	C-O	-8.05	1.15	1.24
1	C	182	TYR	C-O	-8.04	1.16	1.24
1	C	185	VAL	C-O	-7.47	1.16	1.24
1	C	212	ASP	CA-C	-7.11	1.43	1.52
1	D	235	LEU	C-O	-7.10	1.15	1.24
1	A	169	LEU	C-O	-6.93	1.16	1.24
1	C	34	ARG	C-O	-6.85	1.15	1.24
1	C	126	LEU	C-O	-6.83	1.15	1.23
1	D	16	ASP	C-O	-6.82	1.15	1.24
1	D	229	VAL	C-O	-6.55	1.17	1.24
1	C	59	ALA	C-O	-6.54	1.15	1.23
1	D	170	ALA	C-O	-6.53	1.16	1.24
1	B	73	CYS	C-O	-6.53	1.16	1.24
1	C	213	LEU	CA-C	-6.50	1.44	1.52
1	D	66	GLU	C-O	-6.47	1.16	1.24
1	A	198	GLU	C-O	-6.37	1.16	1.23
1	D	69	ALA	C-O	-6.36	1.16	1.24
1	D	29	GLN	C-O	-6.27	1.16	1.24
1	B	72	LEU	C-O	-6.23	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	THR	C-O	-6.22	1.16	1.24
1	C	67	PHE	C-O	-6.21	1.17	1.24
1	B	70	GLY	C-O	-6.20	1.16	1.23
1	D	236	SER	C-O	-6.15	1.16	1.23
1	A	196	LEU	C-O	-6.14	1.16	1.24
1	A	167	VAL	C-O	-6.08	1.17	1.24
1	C	69	ALA	C-O	-6.01	1.17	1.24
1	C	212	ASP	C-O	-5.96	1.16	1.24
1	C	137	GLU	C-O	-5.87	1.16	1.24
1	D	234	LEU	C-O	-5.81	1.17	1.23
1	B	83	GLY	C-O	-5.81	1.16	1.24
1	B	71	ARG	C-O	-5.74	1.17	1.24
1	C	127	GLY	C-O	-5.71	1.16	1.23
1	A	81	LEU	C-O	-5.69	1.17	1.24
1	C	33	THR	C-O	-5.66	1.17	1.23
1	A	195	GLU	C-O	-5.64	1.16	1.23
1	A	168	THR	C-O	-5.57	1.17	1.24
1	C	60	VAL	C-O	-5.53	1.17	1.24
1	C	35	PHE	C-O	-5.39	1.17	1.23
1	A	170	ALA	C-O	-5.39	1.17	1.24
1	A	7	ARG	C-O	-5.37	1.17	1.23
1	C	184	LEU	C-O	-5.32	1.17	1.24
1	D	8	LEU	C-O	-5.22	1.17	1.24
1	A	200	ARG	C-O	-5.20	1.17	1.23
1	A	59	ALA	C-O	-5.20	1.16	1.23
1	A	217	TRP	CA-C	-5.15	1.47	1.53
1	A	82	ASP	C-O	-5.14	1.17	1.23
1	A	8	LEU	C-O	-5.12	1.17	1.24
1	D	4	MET	C-O	-5.06	1.17	1.24
1	B	17	ASP	C-O	-5.05	1.17	1.24
1	D	65	ALA	C-O	-5.04	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	ARG	N-CA-C	9.53	123.50	110.35
1	B	83	GLY	N-CA-C	6.72	124.65	115.30
1	D	81	LEU	N-CA-C	6.01	117.63	111.14
1	C	213	LEU	CA-C-O	-5.24	113.18	119.15
1	C	67	PHE	N-CA-C	5.18	117.33	111.11
1	C	61	ALA	N-CA-C	5.08	117.47	111.33
1	C	185	VAL	N-CA-C	5.04	119.31	113.42

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	1889	0	1900	32	0
1	B	1855	0	1852	16	0
1	C	1859	0	1869	19	1
1	D	1885	0	1895	43	1
2	A	48	0	32	1	0
2	B	48	0	32	1	0
2	C	48	0	32	1	0
2	D	48	0	32	1	0
3	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	41	0	0	2	0
5	B	48	0	0	1	0
5	C	44	0	0	3	0
5	D	28	0	0	1	0
All	All	7843	0	7644	102	1

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 7.

All (102) 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:D:4:MET:HA	1:D:7:ARG:HH22	1.31	0.94
1:D:7:ARG:NE	1:D:7:ARG:HA	1.95	0.82
1:D:7:ARG:HA	1:D:7:ARG:HE	1.45	0.81
1:C:34:ARG:NH2	1:D:34:ARG:HD3	1.99	0.78
1:A:210:LEU:O	1:A:219:HIS:ND1	2.20	0.74
1:A:159:LEU:HD13	1:A:159:LEU:O	1.88	0.72
1:D:28:VAL:HG22	1:D:116:LEU:HD22	1.71	0.72
1:D:177:LEU:HD23	1:D:181:LEU:HD23	1.72	0.72
1:C:179:LYS:HE2	2:C:301:COA:H122	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:MET:HA	1:D:7:ARG:NH2	2.06	0.69
1:A:160:GLU:HA	1:A:160:GLU:OE1	1.97	0.64
1:A:62:LYS:NZ	5:A:402:HOH:O	2.28	0.63
1:C:84:ARG:HG3	1:C:86:GLN:HG3	1.81	0.63
1:C:34:ARG:HH21	1:D:34:ARG:HD3	1.64	0.62
1:D:200:ARG:HH21	1:D:204:GLN:CB	2.13	0.62
1:D:28:VAL:CG2	1:D:116:LEU:HD22	2.30	0.61
1:B:185:VAL:HG11	1:B:213:LEU:HB3	1.83	0.61
1:B:110:ASP:OD1	1:B:110:ASP:N	2.34	0.60
1:A:210:LEU:C	1:A:219:HIS:HD1	2.09	0.60
1:D:177:LEU:HD12	1:D:207:LEU:HD22	1.85	0.59
1:C:187:LYS:NZ	5:C:407:HOH:O	2.35	0.58
1:B:230:LEU:O	1:B:233:ARG:HG2	2.04	0.58
1:C:14:PRO:HB2	1:D:14:PRO:HB2	1.86	0.57
1:D:231:ASP:N	1:D:231:ASP:OD1	2.35	0.57
1:A:131:GLU:HG3	1:A:171:PHE:HD1	1.70	0.57
1:A:14:PRO:HB2	1:B:14:PRO:HB2	1.88	0.56
1:B:173:LEU:HD23	1:B:236:SER:HB2	1.88	0.56
1:C:212:ASP:OD1	1:C:219:HIS:N	2.28	0.54
1:D:71:ARG:HD2	1:D:88:PRO:HD2	1.90	0.54
1:D:50:ILE:HD11	1:D:68:LEU:HD13	1.90	0.53
1:D:178:PHE:HB2	2:D:301:COA:H21	1.90	0.53
1:A:178:PHE:HB2	2:A:301:COA:H21	1.91	0.53
1:C:28:VAL:HG13	1:C:116:LEU:HD11	1.90	0.52
1:D:22:PRO:HG3	1:D:203:GLY:HA3	1.90	0.52
1:A:200:ARG:HG3	1:A:202:ASP:OD1	2.08	0.52
1:B:140:ARG:O	1:B:143:HIS:ND1	2.41	0.52
1:D:30:LEU:HD12	1:D:116:LEU:HG	1.91	0.51
1:A:78:LEU:O	1:A:78:LEU:HD13	2.09	0.51
1:C:78:LEU:HG	1:C:117:VAL:HG11	1.93	0.51
1:D:50:ILE:CD1	1:D:68:LEU:HD13	2.41	0.50
1:A:58:ARG:O	1:D:93:ASP:HB3	2.11	0.50
1:B:95:ALA:HB2	2:B:301:COA:C6A	2.42	0.50
1:D:48:ALA:O	1:D:75:ARG:NH2	2.38	0.50
1:A:171:PHE:CZ	1:D:58:ARG:HD2	2.46	0.50
1:A:158:ASP:OD2	1:A:199:TRP:HZ2	1.95	0.49
1:C:173:LEU:HD23	1:C:236:SER:HB2	1.93	0.49
1:A:7:ARG:HE	1:B:18:ARG:HD3	1.78	0.48
1:A:39:LEU:HD22	1:B:230:LEU:HG	1.95	0.48
1:B:3:ALA:HB3	1:B:6:ASP:HB2	1.96	0.47
1:D:7:ARG:NE	1:D:7:ARG:CA	2.71	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD12	1:D:232:GLY:HA2	1.97	0.46
1:A:82:ASP:OD2	1:A:84:ARG:NH2	2.47	0.46
1:A:7:ARG:HA	1:A:7:ARG:HD2	1.69	0.46
1:A:48:ALA:O	1:A:75:ARG:NH2	2.38	0.46
1:D:200:ARG:NH2	1:D:204:GLN:HG3	2.30	0.45
1:D:162:ARG:CZ	1:D:199:TRP:HH2	2.29	0.45
1:A:79:PHE:O	1:A:83:GLY:HA2	2.17	0.45
1:A:210:LEU:C	1:A:219:HIS:ND1	2.72	0.45
1:C:146:ILE:HG12	1:C:171:PHE:HD2	1.82	0.45
1:B:52:PRO:HG2	1:B:57:LEU:HD13	1.99	0.44
1:C:15:LEU:HD13	1:C:76:ALA:HB2	1.99	0.44
1:A:130:VAL:HG21	1:A:233:ARG:HD3	1.99	0.44
1:C:30:LEU:O	1:C:31:ARG:NH1	2.40	0.44
1:A:93:ASP:O	5:A:401:HOH:O	2.21	0.44
1:D:199:TRP:O	1:D:199:TRP:CG	2.70	0.43
1:C:111:ARG:HB2	1:C:233[B]:ARG:HH22	1.83	0.43
1:D:4:MET:CA	1:D:7:ARG:HH22	2.17	0.43
1:A:82:ASP:CG	1:A:84:ARG:HE	2.27	0.43
1:A:131:GLU:HG3	1:A:171:PHE:CD1	2.51	0.43
1:A:182:TYR:HB3	1:A:183:PRO:HD3	2.01	0.43
1:D:231:ASP:OD2	1:D:233:ARG:NH1	2.46	0.43
1:B:9:PRO:HB3	1:B:44:ASP:CG	2.44	0.42
1:A:78:LEU:HD12	1:A:84:ARG:HB2	2.00	0.42
1:B:22:PRO:HG2	1:B:203:GLY:HA3	2.00	0.42
1:D:171:PHE:O	1:D:175:GLU:HG3	2.19	0.42
1:D:231:ASP:CG	1:D:233:ARG:HH22	2.28	0.42
1:D:187:LYS:HD3	1:D:213:LEU:HA	2.01	0.42
1:C:98:TRP:HB3	1:C:102:ILE:HG22	2.02	0.42
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.88	0.42
1:D:181:LEU:HD21	1:D:223:LEU:CD1	2.50	0.42
1:A:140:ARG:HG3	1:A:163:THR:HG21	2.02	0.41
1:B:116:LEU:HG	1:B:126:LEU:HD13	2.02	0.41
1:C:7:ARG:HE	1:C:47:LEU:HD12	1.84	0.41
1:C:133:LEU:O	5:C:401:HOH:O	2.22	0.41
1:A:35:PHE:HE2	1:A:113:ALA:HB2	1.86	0.41
1:D:231:ASP:HB2	1:D:232:GLY:H	1.68	0.41
1:A:56:ILE:O	1:A:56:ILE:HG22	2.20	0.41
1:C:22:PRO:HB3	5:C:437:HOH:O	2.20	0.41
1:D:143:HIS:CD2	1:D:152:ARG:HD2	2.56	0.41
1:D:173:LEU:HB3	1:D:207:LEU:HD21	2.03	0.41
1:D:11:PHE:O	1:D:35:PHE:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:OD2	1:A:199:TRP:CZ2	2.74	0.41
1:B:31:ARG:HD3	1:B:31:ARG:HA	1.88	0.41
1:B:124:ARG:NH1	5:B:416:HOH:O	2.53	0.41
1:D:94:ARG:NH2	5:D:407:HOH:O	2.54	0.41
1:D:225:ALA:HB2	1:D:238:VAL:HG22	2.03	0.40
1:D:92:GLU:C	1:D:94:ARG:H	2.29	0.40
1:D:140:ARG:O	1:D:143:HIS:ND1	2.40	0.40
1:A:146:ILE:HG12	1:A:171:PHE:HD2	1.85	0.40
1:A:9:PRO:HB3	1:A:44:ASP:CG	2.46	0.40
1:D:200:ARG:HH21	1:D:204:GLN:HB2	1.84	0.40
1:C:15:LEU:H	1:C:15:LEU:HG	1.76	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ARG:NH1	1:D:6:ASP:OD1[1_455]	2.16	0.04

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	240/245 (98%)	231 (96%)	9 (4%)	0	100	100
1	B	237/245 (97%)	230 (97%)	7 (3%)	0	100	100
1	C	237/245 (97%)	232 (98%)	5 (2%)	0	100	100
1	D	240/245 (98%)	226 (94%)	14 (6%)	0	100	100
All	All	954/980 (97%)	919 (96%)	35 (4%)	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	187/189 (99%)	178 (95%)	9 (5%)	23	40
1	B	183/189 (97%)	175 (96%)	8 (4%)	25	43
1	C	183/189 (97%)	177 (97%)	6 (3%)	33	55
1	D	186/189 (98%)	180 (97%)	6 (3%)	34	56
All	All	739/756 (98%)	710 (96%)	29 (4%)	28	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LEU
1	A	57	LEU
1	A	78	LEU
1	A	148	THR
1	A	159	LEU
1	A	197	LEU
1	A	200	ARG
1	A	218	ARG
1	B	18	ARG
1	B	25	LEU
1	B	110	ASP
1	B	159	LEU
1	B	166	LEU
1	B	169	LEU
1	B	177	LEU
1	B	210	LEU
1	C	28	VAL
1	C	34	ARG
1	C	81	LEU
1	C	102	ILE
1	C	140	ARG
1	C	169	LEU
1	D	7	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	50	ILE
1	D	57	LEU
1	D	94	ARG
1	D	166	LEU
1	D	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	219	HIS
1	C	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	COA	C	301	3	47,50,50	2.79	11 (23%)	69,75,75	1.61	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	A	301	-	47,50,50	2.96	11 (23%)	69,75,75	1.58	15 (21%)
2	COA	B	301	-	47,50,50	2.73	9 (19%)	69,75,75	1.58	13 (18%)
2	COA	D	301	-	47,50,50	2.73	12 (25%)	69,75,75	1.60	10 (14%)

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	COA	C	301	3	-	11/48/64/64	0/3/3/3
2	COA	A	301	-	-	12/48/64/64	0/3/3/3
2	COA	B	301	-	-	9/48/64/64	0/3/3/3
2	COA	D	301	-	-	14/48/64/64	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	COA	P3B-O3B	14.65	1.85	1.59
2	A	301	COA	P3B-O3B	14.19	1.84	1.59
2	C	301	COA	P3B-O3B	13.53	1.83	1.59
2	D	301	COA	P3B-O3B	12.33	1.81	1.59
2	A	301	COA	P1A-O3A	10.75	1.71	1.59
2	D	301	COA	P1A-O3A	10.06	1.70	1.59
2	C	301	COA	P1A-O3A	8.96	1.69	1.59
2	B	301	COA	P1A-O3A	7.58	1.67	1.59
2	B	301	COA	P2A-O6A	3.94	1.74	1.59
2	C	301	COA	P2A-O6A	3.92	1.74	1.59
2	D	301	COA	P2A-O6A	3.55	1.73	1.59
2	A	301	COA	P2A-O6A	3.48	1.73	1.59
2	C	301	COA	C5A-C4A	3.45	1.45	1.39
2	C	301	COA	C2A-N1A	3.36	1.39	1.33
2	C	301	COA	C4A-N3A	3.00	1.40	1.34
2	A	301	COA	C9P-N8P	3.00	1.40	1.33
2	D	301	COA	C9P-N8P	2.98	1.40	1.33
2	D	301	COA	O3B-C3B	-2.96	1.34	1.44
2	C	301	COA	O3B-C3B	-2.86	1.34	1.44
2	A	301	COA	C2A-N1A	2.85	1.39	1.33
2	D	301	COA	C5A-C4A	2.71	1.43	1.39
2	D	301	COA	C5P-N4P	2.66	1.39	1.33
2	A	301	COA	C5P-N4P	2.63	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	COA	C5A-C4A	2.60	1.43	1.39
2	B	301	COA	C2B-C3B	2.51	1.58	1.53
2	A	301	COA	C5A-C4A	2.47	1.43	1.39
2	D	301	COA	C2A-N1A	2.37	1.38	1.33
2	A	301	COA	O3B-C3B	-2.37	1.36	1.44
2	A	301	COA	C4A-N3A	2.35	1.38	1.34
2	B	301	COA	O3B-C3B	-2.31	1.36	1.44
2	C	301	COA	C9P-N8P	2.28	1.39	1.33
2	D	301	COA	O6A-CCP	-2.28	1.36	1.43
2	D	301	COA	C4A-N3A	2.23	1.38	1.34
2	B	301	COA	C2A-N1A	2.23	1.37	1.33
2	C	301	COA	C2B-C3B	2.21	1.57	1.53
2	B	301	COA	C9P-N8P	2.20	1.38	1.33
2	A	301	COA	C2B-C3B	2.19	1.57	1.53
2	B	301	COA	O4B-C4B	-2.16	1.40	1.45
2	C	301	COA	C5P-N4P	2.14	1.38	1.33
2	D	301	COA	P2A-O3A	2.07	1.61	1.59
2	D	301	COA	C2B-C3B	2.07	1.57	1.53
2	A	301	COA	O4B-C4B	-2.03	1.40	1.45
2	C	301	COA	O6A-CCP	-2.02	1.37	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	COA	P3B-O3B-C3B	-5.12	109.76	123.43
2	C	301	COA	P3B-O3B-C3B	-4.71	110.86	123.43
2	B	301	COA	P3B-O3B-C3B	-4.67	110.97	123.43
2	D	301	COA	O3B-P3B-O7A	-4.31	93.98	109.33
2	A	301	COA	P3B-O3B-C3B	-4.28	112.01	123.43
2	A	301	COA	O3B-P3B-O7A	-3.92	95.35	109.33
2	A	301	COA	O3A-P1A-O1A	-3.65	99.74	110.70
2	C	301	COA	O3B-P3B-O7A	-3.64	96.34	109.33
2	B	301	COA	O3B-P3B-O7A	-3.50	96.86	109.33
2	B	301	COA	C7P-C6P-C5P	-3.34	106.83	112.39
2	C	301	COA	O3A-P1A-O1A	-3.31	100.75	110.70
2	C	301	COA	C7P-C6P-C5P	-3.26	106.96	112.39
2	D	301	COA	O3A-P1A-O1A	-3.25	100.94	110.70
2	C	301	COA	P1A-O5B-C5B	-3.08	103.72	121.35
2	C	301	COA	O9A-P3B-O8A	3.06	119.27	107.80
2	B	301	COA	P1A-O5B-C5B	-2.99	104.21	121.35
2	D	301	COA	P2A-O6A-CCP	-2.99	104.83	121.12
2	D	301	COA	C7P-C6P-C5P	-2.99	107.42	112.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	COA	O3A-P1A-O1A	-2.92	101.91	110.70
2	B	301	COA	O9A-P3B-O8A	2.91	118.70	107.80
2	D	301	COA	O9A-P3B-O8A	2.90	118.67	107.80
2	A	301	COA	P1A-O5B-C5B	-2.87	104.88	121.35
2	D	301	COA	P1A-O5B-C5B	-2.87	104.88	121.35
2	A	301	COA	P2A-O6A-CCP	-2.83	105.70	121.12
2	C	301	COA	P2A-O6A-CCP	-2.75	106.13	121.12
2	A	301	COA	O9A-P3B-O8A	2.67	117.81	107.80
2	B	301	COA	P2A-O6A-CCP	-2.66	106.62	121.12
2	A	301	COA	N3A-C4A-N9A	2.61	131.61	127.17
2	A	301	COA	C7P-C6P-C5P	-2.53	108.18	112.39
2	A	301	COA	C2A-N1A-C6A	-2.49	114.64	118.73
2	B	301	COA	C3P-N4P-C5P	-2.46	118.24	122.82
2	D	301	COA	N3A-C4A-N9A	2.44	131.31	127.17
2	B	301	COA	C7P-N8P-C9P	-2.43	118.18	122.55
2	C	301	COA	C3P-N4P-C5P	-2.41	118.33	122.82
2	C	301	COA	C7P-N8P-C9P	-2.39	118.25	122.55
2	B	301	COA	N3A-C4A-N9A	2.34	131.14	127.17
2	A	301	COA	O6A-CCP-CBP	-2.32	106.81	110.55
2	A	301	COA	O6A-P2A-O4A	-2.31	99.78	108.94
2	A	301	COA	C5A-C4A-N3A	-2.25	123.62	126.72
2	A	301	COA	C2P-C3P-N4P	-2.24	107.22	112.31
2	D	301	COA	C2A-N1A-C6A	-2.24	115.06	118.73
2	B	301	COA	C2A-N1A-C6A	-2.19	115.13	118.73
2	C	301	COA	C2P-C3P-N4P	-2.19	107.34	112.31
2	C	301	COA	O5A-P2A-O3A	2.13	113.04	107.27
2	D	301	COA	O5A-P2A-O3A	2.13	113.02	107.27
2	B	301	COA	C2P-C3P-N4P	-2.12	107.50	112.31
2	C	301	COA	O6A-CCP-CBP	-2.11	107.15	110.55
2	B	301	COA	C2B-C1B-N9A	-2.08	108.14	113.30
2	C	301	COA	N3A-C4A-N9A	2.08	130.70	127.17
2	A	301	COA	O2A-P1A-O3A	2.06	112.83	107.27
2	A	301	COA	O5A-P2A-O3A	2.01	112.70	107.27

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	COA	CDP-CBP-CCP-O6A
2	A	301	COA	CEP-CBP-CCP-O6A
2	A	301	COA	CAP-CBP-CCP-O6A
2	B	301	COA	P1A-O3A-P2A-O6A

Continued on next page...

Continued from previous page...

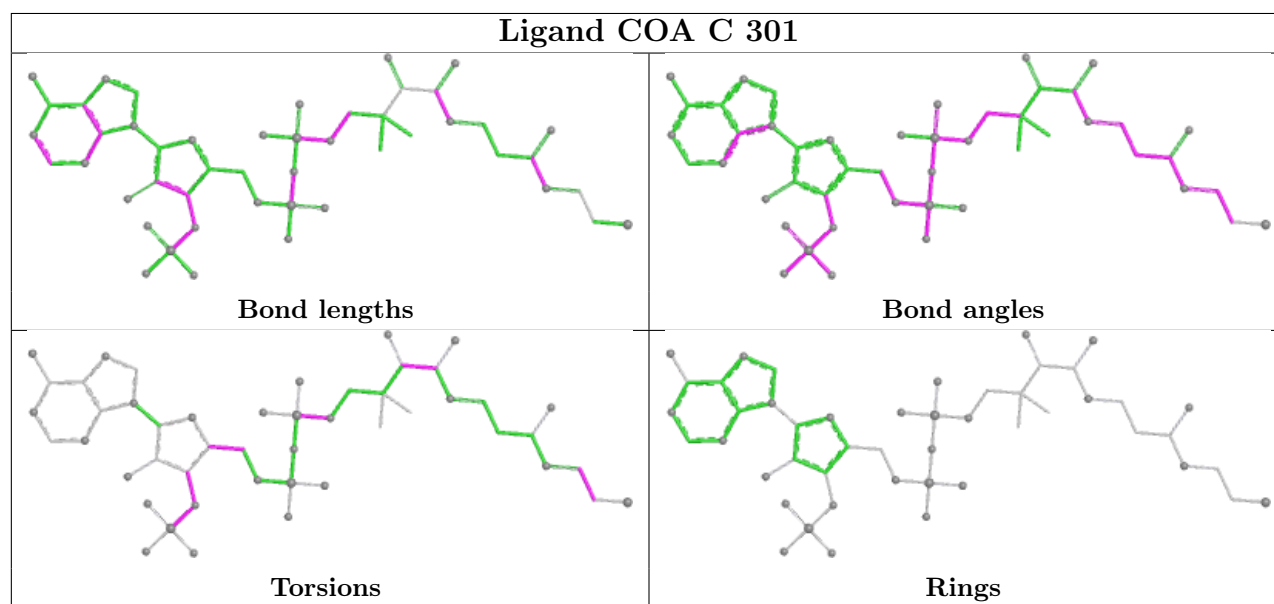
Mol	Chain	Res	Type	Atoms
2	B	301	COA	CDP-CBP-CCP-O6A
2	B	301	COA	CEP-CBP-CCP-O6A
2	C	301	COA	CCP-O6A-P2A-O3A
2	C	301	COA	CCP-O6A-P2A-O4A
2	C	301	COA	CCP-O6A-P2A-O5A
2	D	301	COA	CDP-CBP-CCP-O6A
2	D	301	COA	CEP-CBP-CCP-O6A
2	D	301	COA	OAP-CAP-CBP-CCP
2	D	301	COA	C9P-CAP-CBP-CCP
2	D	301	COA	OAP-CAP-CBP-CDP
2	D	301	COA	C9P-CAP-CBP-CDP
2	D	301	COA	OAP-CAP-CBP-CEP
2	D	301	COA	C9P-CAP-CBP-CEP
2	C	301	COA	C2B-C3B-O3B-P3B
2	D	301	COA	C2B-C3B-O3B-P3B
2	D	301	COA	C4B-C3B-O3B-P3B
2	C	301	COA	C4B-C3B-O3B-P3B
2	D	301	COA	P1A-O3A-P2A-O6A
2	A	301	COA	C5P-C6P-C7P-N8P
2	B	301	COA	C4B-C3B-O3B-P3B
2	A	301	COA	P2A-O3A-P1A-O1A
2	C	301	COA	O9P-C9P-CAP-OAP
2	C	301	COA	C3B-C4B-C5B-O5B
2	A	301	COA	C3B-O3B-P3B-O7A
2	B	301	COA	CAP-CBP-CCP-O6A
2	C	301	COA	S1P-C2P-C3P-N4P
2	D	301	COA	CAP-CBP-CCP-O6A
2	A	301	COA	C4B-C3B-O3B-P3B
2	A	301	COA	P2A-O3A-P1A-O2A
2	B	301	COA	C2B-C3B-O3B-P3B
2	B	301	COA	C2P-C3P-N4P-C5P
2	B	301	COA	C3B-O3B-P3B-O7A
2	D	301	COA	C3B-O3B-P3B-O7A
2	C	301	COA	O4B-C4B-C5B-O5B
2	A	301	COA	C2B-C3B-O3B-P3B
2	A	301	COA	OAP-CAP-CBP-CDP
2	C	301	COA	C3B-O3B-P3B-O7A
2	A	301	COA	N8P-C9P-CAP-OAP
2	B	301	COA	N8P-C9P-CAP-OAP
2	C	301	COA	N8P-C9P-CAP-OAP
2	D	301	COA	N8P-C9P-CAP-OAP
2	A	301	COA	P1A-O3A-P2A-O5A

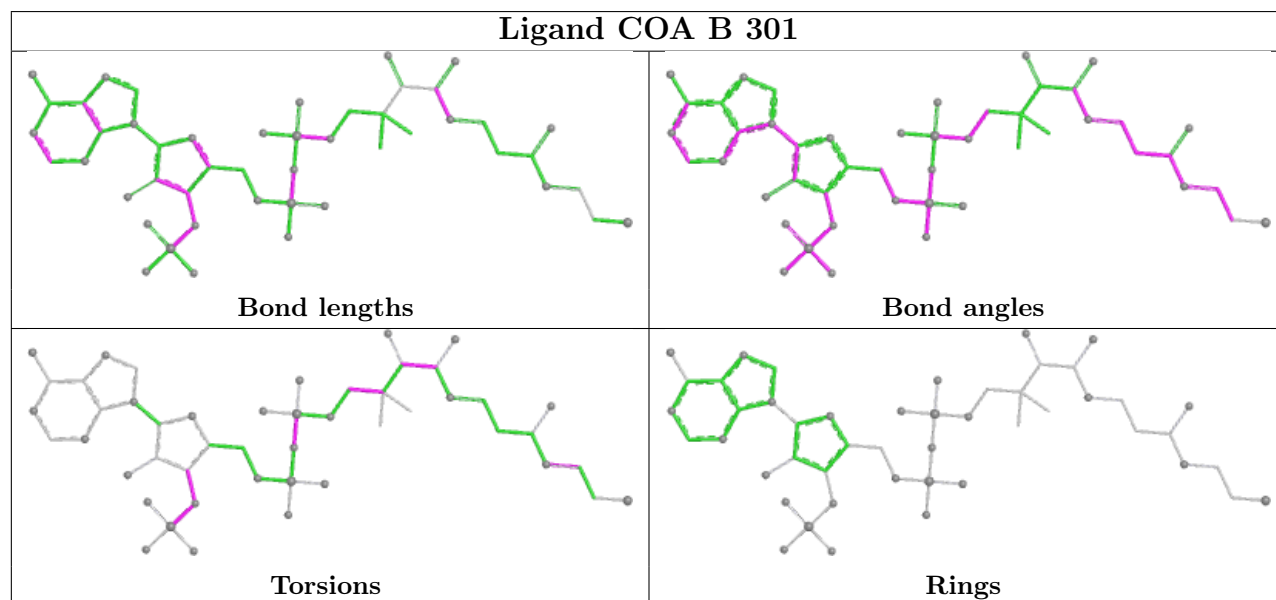
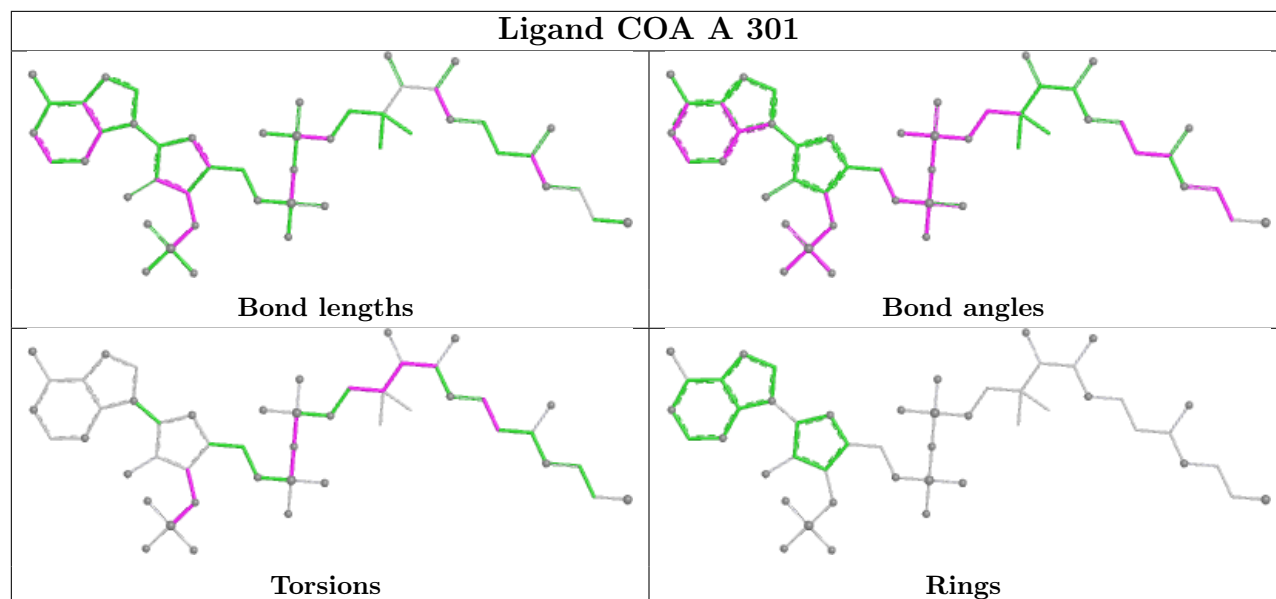
There are no ring outliers.

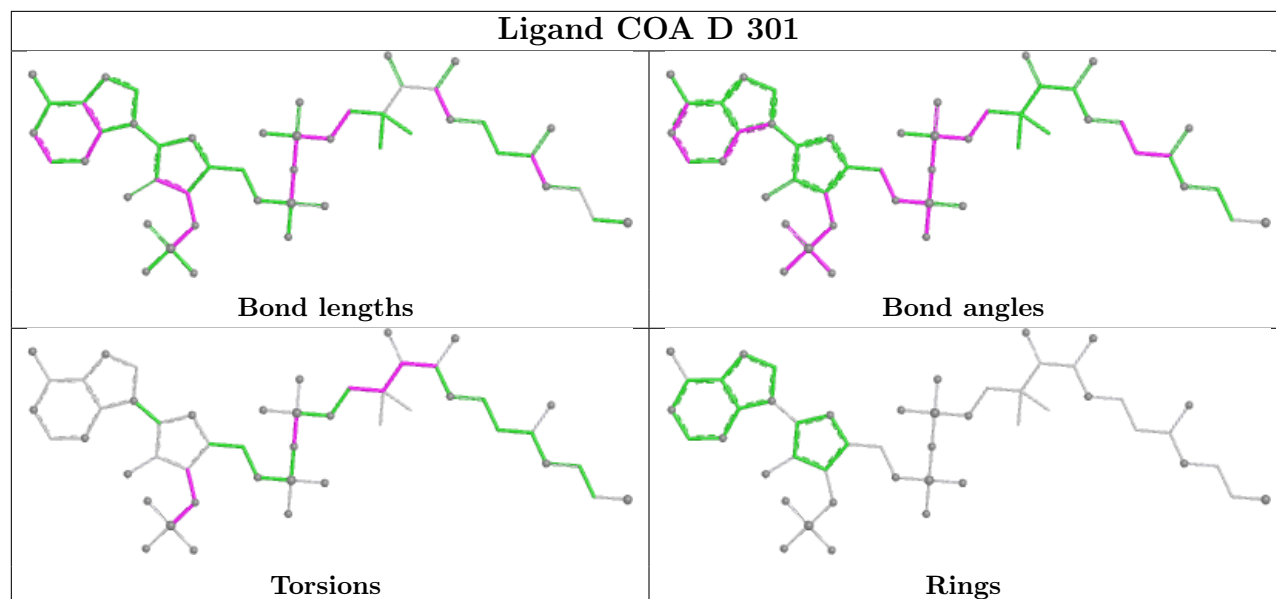
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	COA	1	0
2	A	301	COA	1	0
2	B	301	COA	1	0
2	D	301	COA	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	242/245 (98%)	0.68	20 (8%) 17 14	23, 48, 74, 87	0
1	B	239/245 (97%)	0.54	12 (5%) 34 30	22, 42, 70, 86	0
1	C	238/245 (97%)	0.53	12 (5%) 34 30	23, 42, 69, 81	1 (0%)
1	D	242/245 (98%)	0.73	18 (7%) 20 17	28, 48, 78, 94	0
All	All	961/980 (98%)	0.62	62 (6%) 25 21	22, 45, 74, 94	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	4.3
1	D	55	ASN	4.1
1	B	230	LEU	3.8
1	C	141	TYR	3.7
1	B	3	ALA	3.7
1	C	230	LEU	3.5
1	B	110	ASP	3.5
1	C	4	MET	3.3
1	A	0	HIS	3.3
1	D	54	ALA	3.2
1	B	85	ALA	3.1
1	C	233[A]	ARG	3.1
1	D	231	ASP	3.1
1	A	1	MET	3.0
1	A	4	MET	3.0
1	B	231	ASP	3.0
1	D	136	ALA	3.0
1	A	109	GLY	3.0
1	A	185	VAL	2.9
1	A	230	LEU	2.9
1	B	6	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	87	THR	2.8
1	A	54	ALA	2.7
1	A	58	ARG	2.7
1	C	231	ASP	2.7
1	A	186	GLY	2.7
1	C	139	ALA	2.7
1	D	0	HIS	2.7
1	A	2	ARG	2.6
1	A	190	TYR	2.6
1	A	202	ASP	2.6
1	D	91	GLY	2.5
1	B	142	LEU	2.4
1	D	3	ALA	2.4
1	C	6	ASP	2.4
1	D	86	GLN	2.3
1	B	135	GLU	2.3
1	D	61	ALA	2.3
1	D	100	ALA	2.3
1	A	229	VAL	2.3
1	A	100	ALA	2.2
1	C	85	ALA	2.2
1	D	161	ARG	2.2
1	A	5	ASN	2.2
1	A	85	ALA	2.2
1	D	5	ASN	2.2
1	D	1	MET	2.2
1	B	86	GLN	2.1
1	D	7	ARG	2.1
1	D	39	LEU	2.1
1	B	137	GLU	2.1
1	C	86	GLN	2.1
1	A	77	ALA	2.1
1	C	94	ARG	2.1
1	D	185	VAL	2.1
1	B	201	ALA	2.1
1	C	54	ALA	2.1
1	C	135	GLU	2.1
1	A	61	ALA	2.0
1	B	159	LEU	2.0
1	D	230	LEU	2.0
1	D	6	ASP	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](#)

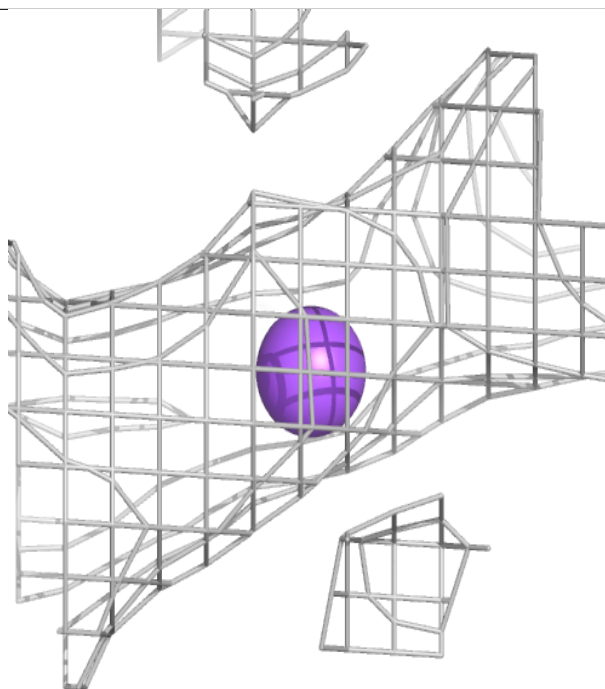
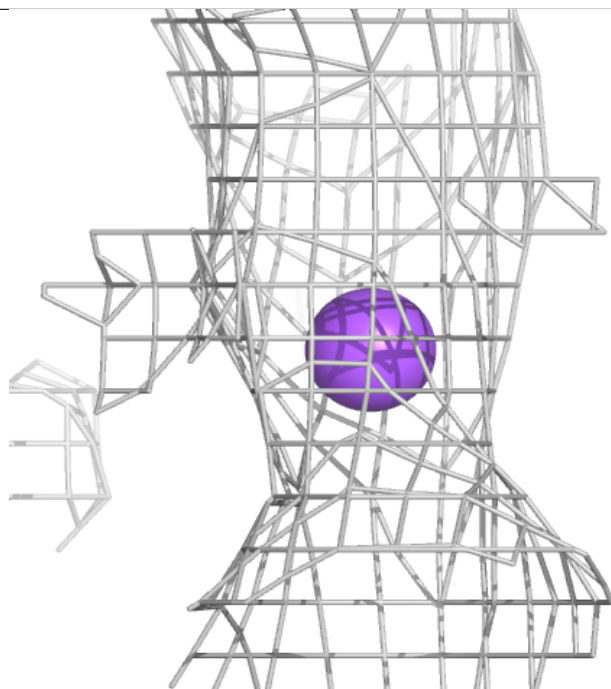
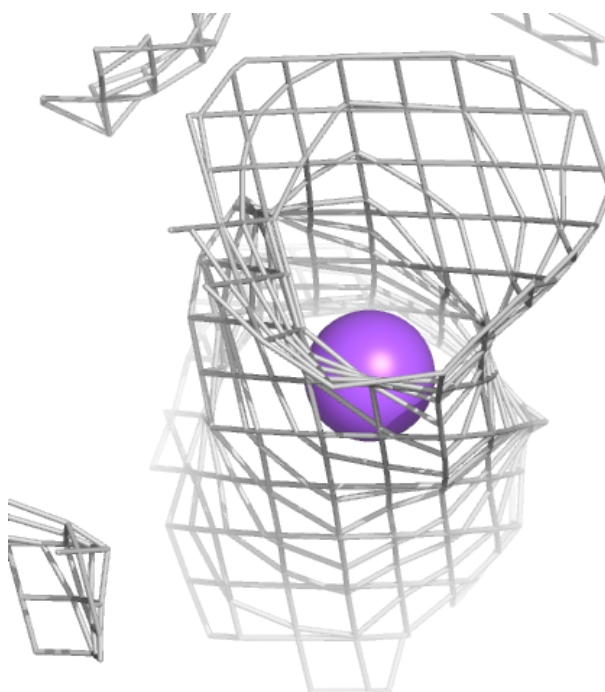
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	302	1/1	0.89	0.11	66,66,66,66	0
2	COA	A	301	48/48	0.92	0.10	31,42,54,55	0
3	MG	C	302	1/1	0.93	0.06	39,39,39,39	0
2	COA	D	301	48/48	0.93	0.10	28,46,62,63	0
2	COA	C	301	48/48	0.94	0.09	27,38,44,47	0
2	COA	B	301	48/48	0.95	0.09	19,36,47,50	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.

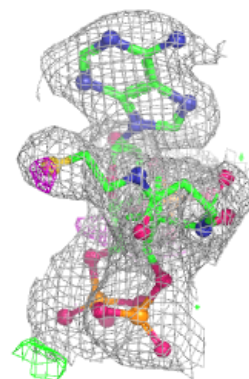
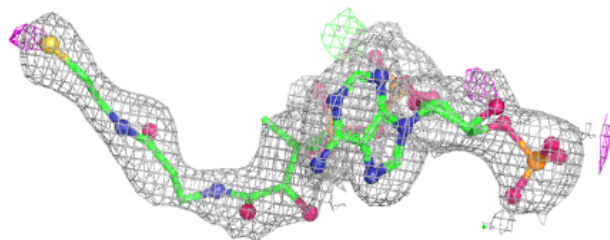
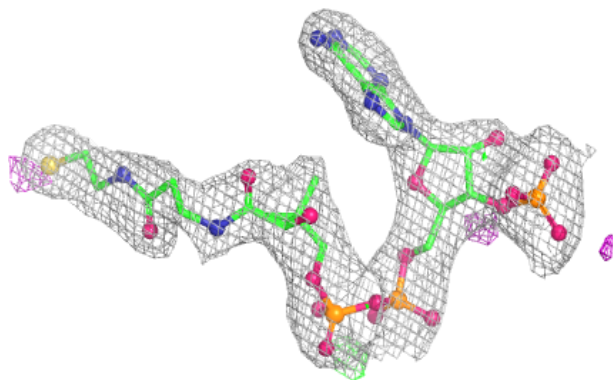
Electron density around NA D 302:

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



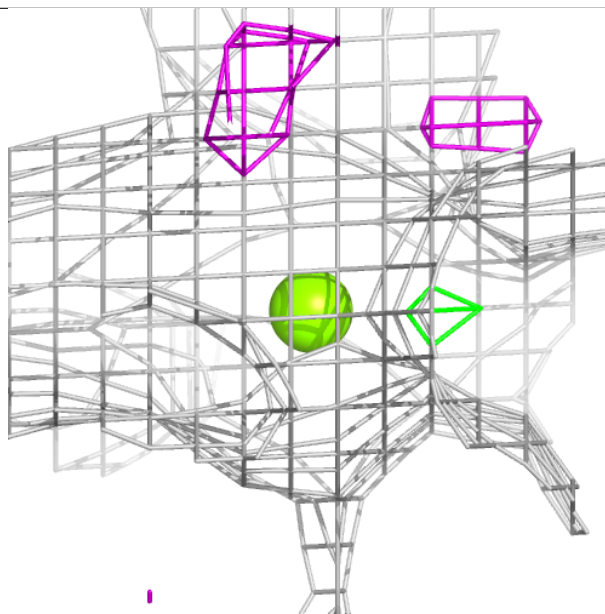
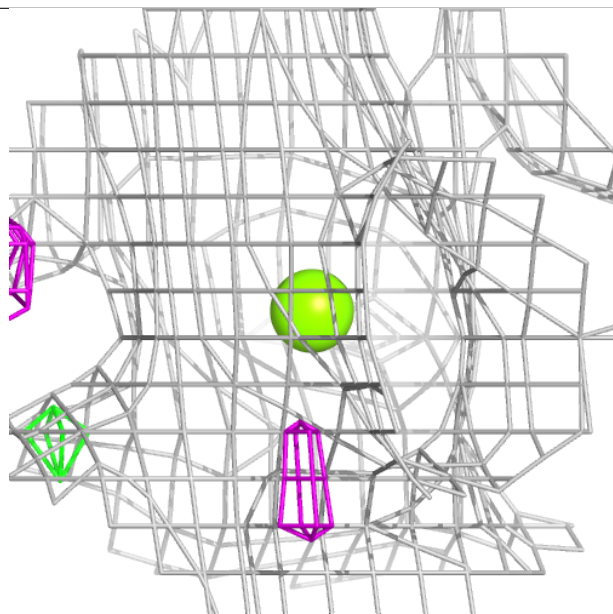
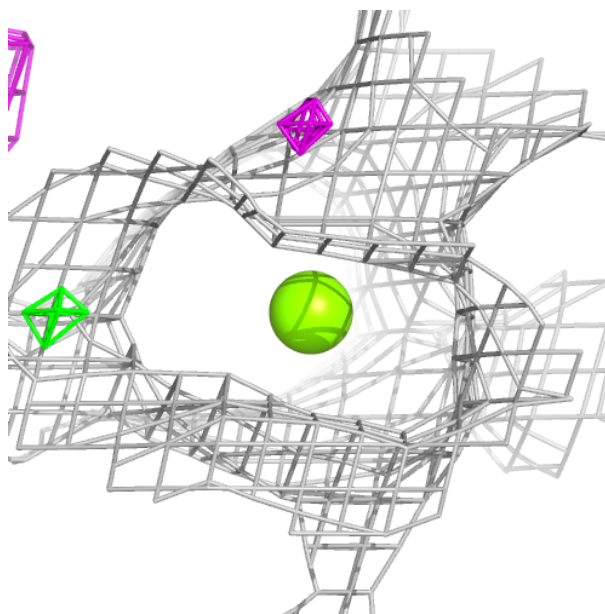
Electron density around COA A 301:

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



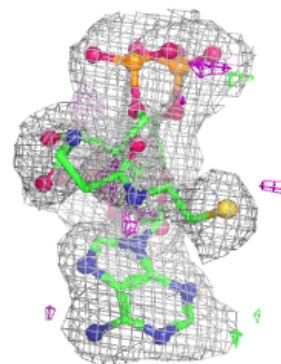
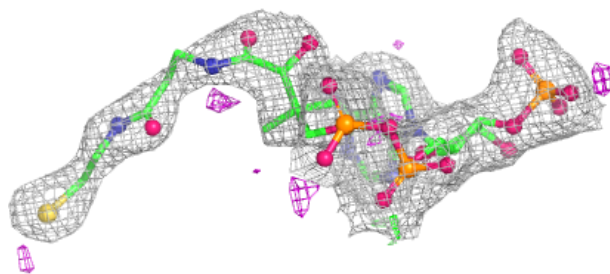
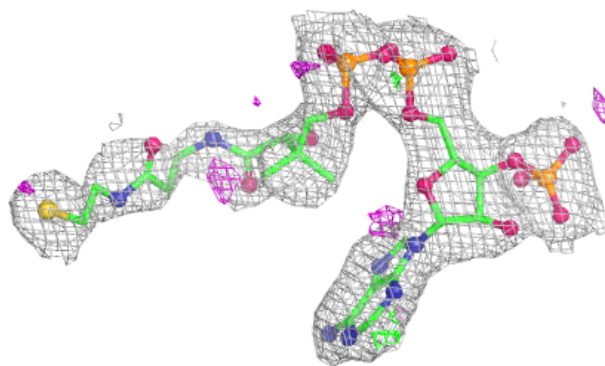
Electron density around MG C 302:

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

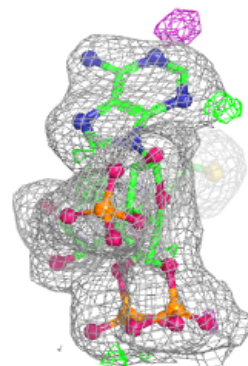
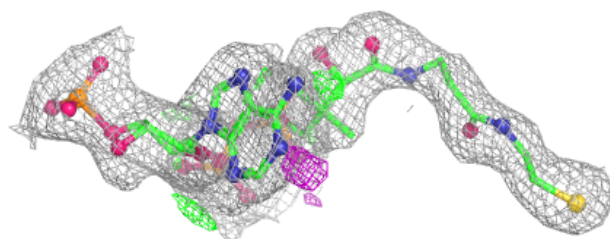
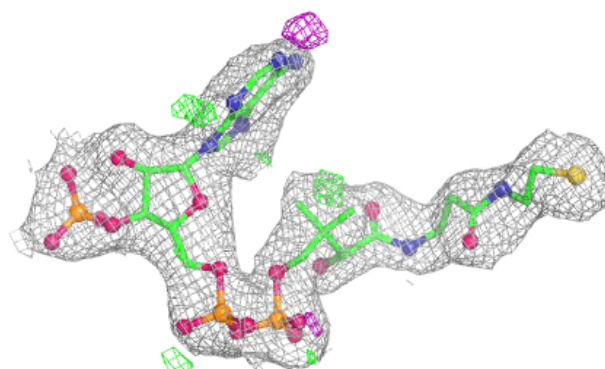


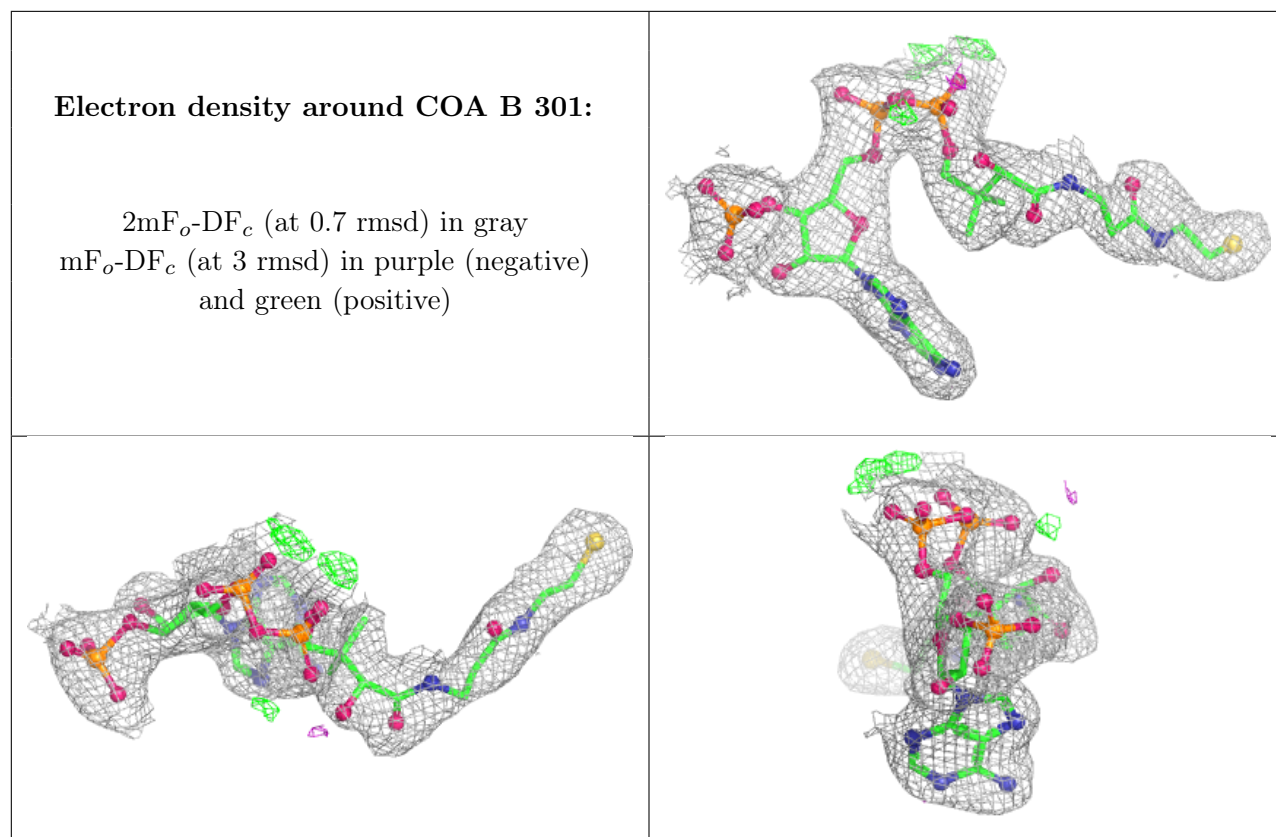
Electron density around COA D 301:

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

**Electron density around COA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.