



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:16 AM UTC

PDB ID : 2WAT / pdb_00002wat
Title : Structure of the fungal type I FAS PPT domain in complex with CoA
Authors : Johansson, P.; Mulincacci, B.; Koestler, C.; Grninger, M.
Deposited on : 2009-02-15
Resolution : 2.20 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

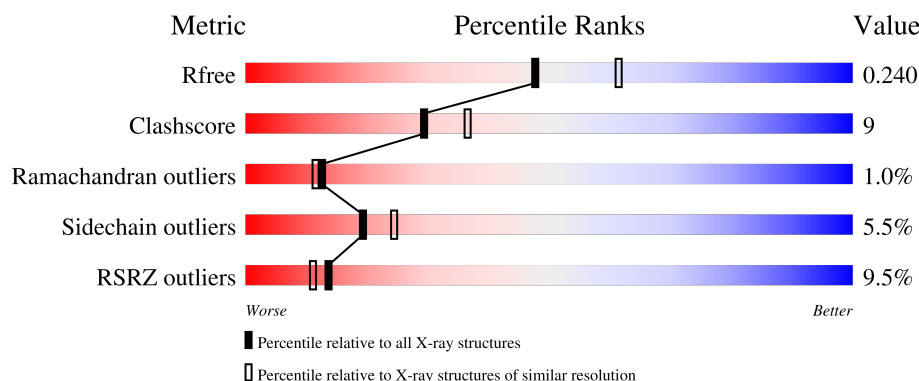
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	122	10% 82% 15% ..
1	B	122	11% 77% 18% ..
1	C	122	8% 83% 11% ...
1	D	122	8% 86% 10% ..
1	E	122	9% 84% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	122	10% 80% 11% • • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6020 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.

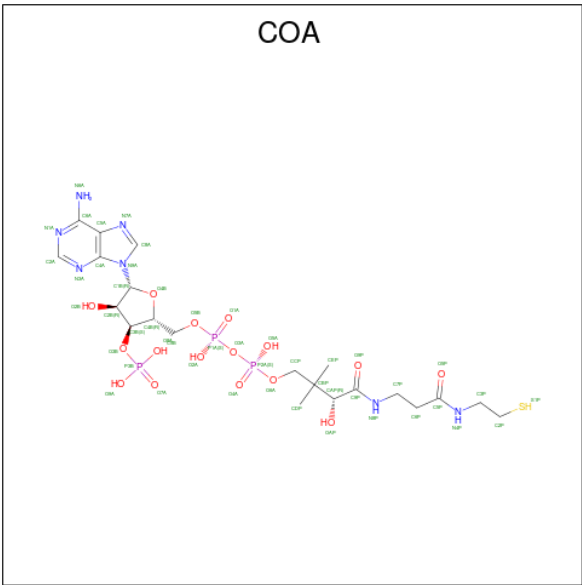
- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			887	553	152	181	1			
1	B	120	Total	C	N	O	S	0	0	0
			881	550	150	180	1			
1	C	120	Total	C	N	O	S	0	0	0
			881	550	150	180	1			
1	D	120	Total	C	N	O	S	0	0	0
			881	550	150	180	1			
1	E	120	Total	C	N	O	S	0	0	0
			881	550	150	180	1			
1	F	115	Total	C	N	O	S	0	0	0
			855	535	145	174	1			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

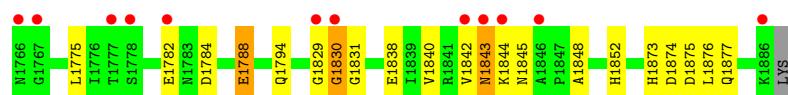
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total 84	O 84	0	0
5	B	113	Total 113	O 113	0	0
5	C	88	Total 88	O 88	0	0
5	D	85	Total 85	O 85	0	0
5	E	80	Total 80	O 80	0	0
5	F	55	Total 55	O 55	0	0

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.

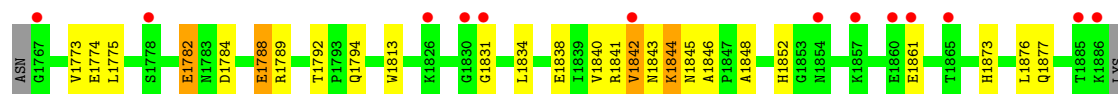
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

Chain A: 



- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

Chain B: 



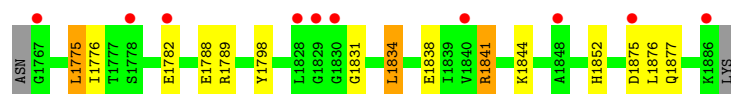
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

Chain C: 



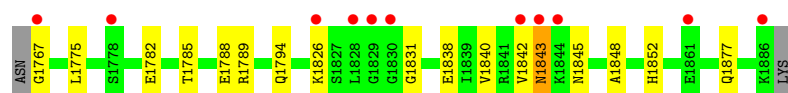
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

Chain D: 

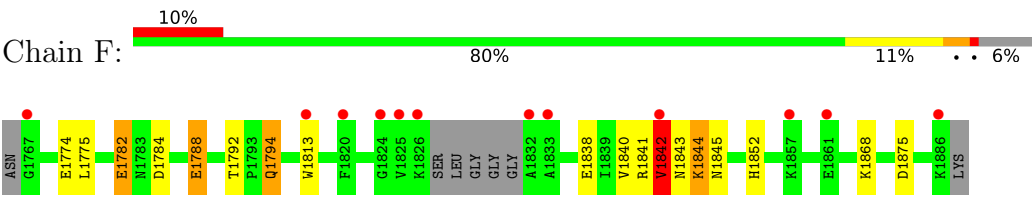


- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

Chain E: 



● Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.59Å 73.76Å 105.69Å 90.00° 130.80° 90.00°	Depositor
Resolution (Å)	80.01 – 2.20 80.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (80.01-2.20) 97.7 (80.01-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.252 0.205 , 0.240	Depositor DCC
R_{free} test set	2105 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6020	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: MG, COA, CL

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	0.41	0/898	0.72	0/1217
1	B	0.43	0/892	0.70	0/1209
1	C	0.40	0/892	0.73	1/1209 (0.1%)
1	D	0.46	0/892	0.74	0/1209
1	E	0.39	0/892	0.70	0/1209
1	F	0.38	0/865	0.72	0/1172
All	All	0.41	0/5331	0.72	1/7225 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1842	VAL	CB-CA-C	-5.56	102.17	111.29

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	887	0	879	18	0
1	B	881	0	878	30	0
1	C	881	0	878	20	0
1	D	881	0	878	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	881	0	878	11	0
1	F	855	0	852	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	B	96	0	64	3	0
3	C	48	0	32	0	0
3	E	96	0	64	2	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	84	0	0	1	1
5	B	113	0	0	8	1
5	C	88	0	0	2	0
5	D	85	0	0	1	0
5	E	80	0	0	2	0
5	F	55	0	0	3	0
All	All	6020	0	5403	94	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 9.

All (94) 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:B:1773:VAL:CG2	1:B:1877:GLN:HG3	1.97	0.94
1:B:1843:ASN:N	5:B:2065:HOH:O	2.12	0.82
1:B:1773:VAL:HG22	1:B:1877:GLN:HG3	1.62	0.81
1:C:1842:VAL:C	1:C:1844:LYS:H	1.94	0.76
1:C:1794:GLN:HG2	5:C:2050:HOH:O	1.92	0.69
1:A:1877:GLN:HE22	1:B:1877:GLN:HE22	1.41	0.69
1:B:1841:ARG:HD3	5:B:2060:HOH:O	1.91	0.69
1:B:1838:GLU:OE1	1:B:1852:HIS:HE1	1.75	0.69
1:A:1838:GLU:OE1	1:A:1852:HIS:HE1	1.75	0.68
1:C:1842:VAL:HG23	1:C:1843:ASN:N	2.07	0.68
1:E:1826:LYS:HG3	1:F:1843:ASN:HB3	1.76	0.68
1:D:1776:ILE:HG12	1:D:1876:LEU:O	1.94	0.66
1:C:1841:ARG:O	1:C:1842:VAL:HG13	1.97	0.65
1:F:1792:THR:HB	1:F:1794:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1844:LYS:HG3	1:B:1845:ASN:ND2	2.12	0.64
1:E:1838:GLU:OE1	1:E:1852:HIS:HE1	1.82	0.63
3:E:2888:COA:H121	3:E:2888:COA:H51A	1.81	0.62
1:F:1844:LYS:HG3	1:F:1845:ASN:ND2	2.15	0.61
1:E:1789:ARG:NH2	1:E:1831:GLY:O	2.33	0.61
1:B:1794:GLN:H	1:B:1794:GLN:CD	2.09	0.60
1:E:1789:ARG:NH1	5:E:2013:HOH:O	2.28	0.60
1:B:1774:GLU:O	1:B:1877:GLN:HB2	2.01	0.60
1:A:1842:VAL:O	1:A:1845:ASN:HB2	2.02	0.59
1:E:1842:VAL:O	1:E:1845:ASN:HB2	2.03	0.58
1:F:1788:GLU:HB3	5:F:2011:HOH:O	2.03	0.58
1:B:1840:VAL:C	1:B:1841:ARG:HD2	2.29	0.58
1:F:1840:VAL:C	1:F:1841:ARG:HD2	2.29	0.58
1:D:1876:LEU:HB3	1:D:1877:GLN:HG3	1.87	0.56
1:D:1798:TYR:CE1	1:D:1841:ARG:HG3	2.41	0.56
1:C:1789:ARG:NH2	1:C:1831:GLY:O	2.39	0.55
1:B:1840:VAL:HG23	1:B:1848:ALA:HB3	1.88	0.55
1:B:1844:LYS:NZ	5:B:2070:HOH:O	2.38	0.55
1:D:1775:LEU:HD22	5:E:2066:HOH:O	2.06	0.55
1:F:1841:ARG:HD3	5:F:2032:HOH:O	2.06	0.55
1:D:1789:ARG:NH2	1:D:1831:GLY:O	2.41	0.54
1:D:1798:TYR:CZ	1:D:1841:ARG:HG3	2.43	0.54
1:F:1784:ASP:O	1:F:1788:GLU:HB2	2.08	0.54
1:A:1877:GLN:NE2	1:B:1877:GLN:HE22	2.04	0.53
1:B:1789:ARG:NH1	5:B:2019:HOH:O	2.43	0.52
1:A:1840:VAL:HG23	1:A:1848:ALA:HB3	1.92	0.52
1:F:1844:LYS:CG	1:F:1845:ASN:ND2	2.74	0.51
1:A:1875:ASP:OD2	1:F:1875:ASP:OD2	2.28	0.51
1:B:1846:ALA:HB3	5:B:2065:HOH:O	2.11	0.51
1:C:1842:VAL:C	1:C:1844:LYS:N	2.61	0.51
1:B:1844:LYS:CG	1:B:1845:ASN:ND2	2.73	0.50
1:C:1838:GLU:OE1	1:C:1852:HIS:HE1	1.94	0.50
1:B:1789:ARG:NH2	1:B:1831:GLY:O	2.46	0.49
1:D:1877:GLN:HE22	1:E:1877:GLN:NE2	2.11	0.49
3:B:2888:COA:O2B	1:C:1847:PRO:HG3	2.13	0.49
1:F:1841:ARG:HG2	5:F:2035:HOH:O	2.12	0.48
1:A:1842:VAL:O	1:A:1843:ASN:C	2.57	0.48
1:B:1774:GLU:HG3	1:B:1813:TRP:HD1	1.78	0.48
1:D:1838:GLU:OE1	1:D:1852:HIS:HE1	1.97	0.48
1:C:1775:LEU:HD12	1:C:1877:GLN:HG2	1.95	0.48
1:A:1876:LEU:HB3	1:B:1876:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1813:TRP:CH2	1:B:1834:LEU:HD12	2.50	0.47
1:E:1767:GLY:O	1:F:1868:LYS:HE3	2.15	0.47
1:E:1842:VAL:O	1:E:1843:ASN:C	2.57	0.47
1:F:1842:VAL:HB	1:F:1843:ASN:H	1.60	0.46
1:B:1773:VAL:HG23	1:B:1877:GLN:HG3	1.92	0.46
1:B:1792:THR:HB	1:B:1794:GLN:HE22	1.81	0.46
1:F:1838:GLU:OE1	1:F:1852:HIS:HE1	1.98	0.46
1:A:1830:GLY:HA2	1:A:1831:GLY:HA2	1.57	0.46
1:C:1782:GLU:OE1	1:F:1782:GLU:OE1	2.33	0.46
1:E:1785:THR:O	1:E:1789:ARG:HB2	2.15	0.46
1:C:1782:GLU:OE2	1:F:1782:GLU:OE2	2.34	0.45
1:E:1840:VAL:HG23	1:E:1848:ALA:HB3	1.97	0.45
1:B:1782:GLU:HG2	5:B:2039:HOH:O	2.16	0.45
1:B:1834:LEU:HD23	3:B:2888:COA:H22	1.99	0.44
1:D:1789:ARG:HG3	5:D:2038:HOH:O	2.17	0.44
1:A:1844:LYS:HB3	1:C:1826:LYS:HG2	2.00	0.44
3:B:2887:COA:O9P	3:B:2887:COA:H133	2.17	0.44
1:A:1874:ASP:HB2	5:A:2081:HOH:O	2.18	0.44
1:D:1776:ILE:HG12	1:D:1876:LEU:C	2.43	0.43
1:C:1842:VAL:CG2	1:C:1843:ASN:N	2.62	0.43
1:B:1792:THR:HB	1:B:1794:GLN:NE2	2.34	0.43
1:B:1784:ASP:O	1:B:1788:GLU:HB2	2.19	0.43
1:E:1794:GLN:NE2	1:E:1840:VAL:HG12	2.34	0.43
1:C:1886:LYS:NZ	5:C:2082:HOH:O	2.52	0.42
1:B:1846:ALA:N	5:B:2065:HOH:O	2.44	0.42
1:A:1874:ASP:OD2	1:C:1877:GLN:OE1	2.37	0.42
1:C:1842:VAL:HB	1:C:1843:ASN:H	1.42	0.42
1:B:1794:GLN:H	1:B:1794:GLN:NE2	2.18	0.42
1:A:1877:GLN:HE22	1:B:1877:GLN:NE2	2.13	0.41
1:A:1784:ASP:O	1:A:1788:GLU:HB2	2.20	0.41
1:A:1844:LYS:HB2	1:C:1826:LYS:HG3	2.02	0.41
1:B:1861:GLU:HG3	5:B:2085:HOH:O	2.20	0.41
1:A:1842:VAL:O	1:A:1843:ASN:O	2.39	0.41
1:C:1840:VAL:HG23	1:C:1848:ALA:HB3	2.02	0.41
1:D:1834:LEU:CD1	3:E:2887:COA:H62	2.50	0.41
1:A:1829:GLY:O	1:A:1830:GLY:O	2.39	0.41
1:C:1875:ASP:CG	1:D:1875:ASP:OD2	2.64	0.41
1:A:1844:LYS:HB2	1:C:1826:LYS:CG	2.51	0.40
1:F:1774:GLU:HG3	1:F:1813:TRP:HD1	1.86	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)
5:A:2044:HOH:O	5:B:2019:HOH:O[4_454]	2.10	0.10

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	119/122 (98%)	114 (96%)	3 (2%)	2 (2%)	7	5
1	B	118/122 (97%)	115 (98%)	2 (2%)	1 (1%)	16	16
1	C	118/122 (97%)	114 (97%)	2 (2%)	2 (2%)	7	5
1	D	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
1	E	118/122 (97%)	115 (98%)	2 (2%)	1 (1%)	16	16
1	F	111/122 (91%)	107 (96%)	3 (3%)	1 (1%)	14	14
All	All	702/732 (96%)	681 (97%)	14 (2%)	7 (1%)	12	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1830	GLY
1	A	1843	ASN
1	C	1842	VAL
1	E	1843	ASN
1	C	1843	ASN
1	B	1842	VAL
1	F	1842	VAL

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/97 (98%)	90 (95%)	5 (5%)	20	26
1	B	95/97 (98%)	89 (94%)	6 (6%)	16	19
1	C	95/97 (98%)	90 (95%)	5 (5%)	20	26
1	D	95/97 (98%)	89 (94%)	6 (6%)	16	19
1	E	95/97 (98%)	92 (97%)	3 (3%)	34	47
1	F	93/97 (96%)	87 (94%)	6 (6%)	15	18
All	All	568/582 (98%)	537 (94%)	31 (6%)	19	24

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1775	LEU
1	A	1782	GLU
1	A	1788	GLU
1	A	1794	GLN
1	A	1873	HIS
1	B	1775	LEU
1	B	1782	GLU
1	B	1788	GLU
1	B	1842	VAL
1	B	1844	LYS
1	B	1873	HIS
1	C	1775	LEU
1	C	1782	GLU
1	C	1841	ARG
1	C	1842	VAL
1	C	1876	LEU
1	D	1775	LEU
1	D	1782	GLU
1	D	1788	GLU
1	D	1834	LEU
1	D	1841	ARG
1	D	1844	LYS
1	E	1775	LEU
1	E	1782	GLU
1	E	1788	GLU
1	F	1775	LEU
1	F	1782	GLU
1	F	1788	GLU

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Mol	Chain	Res	Type
1	F	1794	GLN
1	F	1842	VAL
1	F	1844	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1794	GLN
1	A	1802	GLN
1	A	1852	HIS
1	B	1794	GLN
1	B	1802	GLN
1	B	1806	GLN
1	B	1845	ASN
1	B	1852	HIS
1	B	1877	GLN
1	C	1802	GLN
1	C	1806	GLN
1	C	1845	ASN
1	C	1852	HIS
1	C	1877	GLN
1	D	1802	GLN
1	D	1806	GLN
1	D	1877	GLN
1	E	1802	GLN
1	E	1852	HIS
1	F	1794	GLN
1	F	1806	GLN
1	F	1845	ASN
1	F	1852	HIS
1	F	1877	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	COA	E	2887	4	47,50,50	1.68	6 (12%)	69,75,75	1.56	10 (14%)
3	COA	B	2888	-	47,50,50	1.67	4 (8%)	69,75,75	1.57	11 (15%)
3	COA	C	2887	-	47,50,50	1.66	5 (10%)	69,75,75	1.66	14 (20%)
3	COA	E	2888	-	47,50,50	1.68	7 (14%)	69,75,75	1.54	12 (17%)
3	COA	B	2887	-	47,50,50	1.65	5 (10%)	69,75,75	1.53	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
3	COA	E	2887	4	-	10/48/64/64	0/3/3/3
3	COA	B	2888	-	-	10/48/64/64	0/3/3/3
3	COA	C	2887	-	-	11/48/64/64	0/3/3/3
3	COA	E	2888	-	-	8/48/64/64	0/3/3/3
3	COA	B	2887	-	-	10/48/64/64	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2887	COA	O9P-C9P	9.36	1.41	1.23
3	B	2887	COA	O9P-C9P	9.26	1.41	1.23
3	B	2888	COA	O9P-C9P	9.17	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2888	COA	O9P-C9P	9.14	1.40	1.23
3	C	2887	COA	O9P-C9P	9.03	1.40	1.23
3	E	2888	COA	C2A-N1A	2.83	1.39	1.33
3	C	2887	COA	P2A-O3A	2.75	1.62	1.59
3	B	2888	COA	C2A-N1A	2.73	1.38	1.33
3	E	2888	COA	C2A-N3A	2.55	1.38	1.33
3	B	2887	COA	C2A-N3A	2.54	1.38	1.33
3	B	2888	COA	C2A-N3A	2.51	1.38	1.33
3	E	2887	COA	P2A-O3A	2.50	1.62	1.59
3	E	2887	COA	P1A-O3A	2.45	1.62	1.59
3	E	2888	COA	P2A-O3A	2.37	1.62	1.59
3	C	2887	COA	C2A-N1A	2.37	1.38	1.33
3	E	2887	COA	C2A-N1A	2.32	1.38	1.33
3	C	2887	COA	C2A-N3A	2.27	1.38	1.33
3	B	2887	COA	C2A-N1A	2.26	1.38	1.33
3	C	2887	COA	P1A-O3A	2.26	1.61	1.59
3	E	2887	COA	C2A-N3A	2.26	1.38	1.33
3	E	2887	COA	C8A-N7A	2.25	1.36	1.31
3	B	2887	COA	C8A-N7A	2.17	1.35	1.31
3	B	2888	COA	C8A-N7A	2.15	1.35	1.31
3	E	2888	COA	P1A-O3A	2.13	1.61	1.59
3	E	2888	COA	C8A-N7A	2.10	1.35	1.31
3	B	2887	COA	C5A-N7A	-2.08	1.35	1.39
3	E	2888	COA	C5A-N7A	-2.02	1.35	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2887	COA	N3A-C2A-N1A	-5.67	119.99	128.58
3	B	2887	COA	N3A-C2A-N1A	-5.60	120.10	128.58
3	B	2888	COA	N3A-C2A-N1A	-5.37	120.45	128.58
3	C	2887	COA	N3A-C2A-N1A	-5.36	120.46	128.58
3	E	2888	COA	N3A-C2A-N1A	-5.34	120.50	128.58
3	B	2887	COA	C5A-C4A-N3A	-4.71	120.23	126.72
3	E	2887	COA	C5A-C4A-N3A	-4.59	120.39	126.72
3	C	2887	COA	C5A-C4A-N3A	-4.52	120.49	126.72
3	E	2888	COA	C5A-C4A-N3A	-4.42	120.64	126.72
3	B	2888	COA	C5A-C4A-N3A	-4.21	120.91	126.72
3	C	2887	COA	N9A-C8A-N7A	-4.01	108.25	113.94
3	B	2887	COA	N9A-C8A-N7A	-4.00	108.25	113.94
3	B	2888	COA	N9A-C8A-N7A	-3.98	108.29	113.94
3	E	2887	COA	N9A-C8A-N7A	-3.80	108.54	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2888	COA	N9A-C8A-N7A	-3.73	108.65	113.94
3	E	2887	COA	C2A-N3A-C4A	3.48	120.32	111.83
3	B	2888	COA	O2A-P1A-O3A	3.47	116.67	107.27
3	B	2887	COA	C5A-N7A-C8A	3.46	108.89	103.45
3	B	2887	COA	C2A-N3A-C4A	3.43	120.22	111.83
3	E	2887	COA	C5A-N7A-C8A	3.42	108.82	103.45
3	C	2887	COA	C5A-N7A-C8A	3.41	108.81	103.45
3	C	2887	COA	C2A-N3A-C4A	3.37	120.07	111.83
3	E	2888	COA	C5A-N7A-C8A	3.31	108.65	103.45
3	B	2887	COA	N3A-C4A-N9A	3.27	132.72	127.17
3	B	2888	COA	C5A-N7A-C8A	3.24	108.54	103.45
3	E	2888	COA	C2A-N3A-C4A	3.16	119.56	111.83
3	B	2888	COA	C2A-N3A-C4A	3.14	119.50	111.83
3	C	2887	COA	N3A-C4A-N9A	3.10	132.45	127.17
3	C	2887	COA	C7P-N8P-C9P	-3.09	116.99	122.55
3	E	2888	COA	N3A-C4A-N9A	3.04	132.34	127.17
3	B	2888	COA	C3B-C2B-C1B	3.01	106.50	99.89
3	E	2887	COA	O2A-P1A-O3A	2.97	115.31	107.27
3	E	2888	COA	O6A-CCP-CBP	-2.89	105.90	110.55
3	B	2888	COA	N3A-C4A-N9A	2.88	132.07	127.17
3	C	2887	COA	O2A-P1A-O3A	2.87	115.04	107.27
3	E	2888	COA	C3B-C2B-C1B	2.84	106.13	99.89
3	E	2887	COA	N3A-C4A-N9A	2.84	131.99	127.17
3	E	2887	COA	C4A-C5A-N7A	-2.61	107.60	110.58
3	C	2887	COA	O6A-CCP-CBP	-2.58	106.39	110.55
3	E	2887	COA	C3B-C2B-C1B	2.56	105.52	99.89
3	B	2887	COA	C3B-C2B-C1B	2.48	105.34	99.89
3	C	2887	COA	C3B-C2B-C1B	2.48	105.34	99.89
3	E	2888	COA	C6A-C5A-C4A	2.39	120.44	117.18
3	C	2887	COA	CAP-C9P-N8P	2.38	121.00	116.48
3	C	2887	COA	C4A-C5A-N7A	-2.30	107.95	110.58
3	B	2887	COA	C4A-C5A-N7A	-2.27	107.99	110.58
3	E	2888	COA	C2B-C1B-N9A	-2.20	107.83	113.30
3	B	2888	COA	O6A-CCP-CBP	-2.18	107.04	110.55
3	E	2888	COA	C4A-C5A-N7A	-2.18	108.09	110.58
3	C	2887	COA	O5B-C5B-C4B	-2.16	101.66	108.99
3	B	2888	COA	C7P-N8P-C9P	-2.14	118.69	122.55
3	B	2887	COA	C6A-C5A-C4A	2.09	120.03	117.18
3	C	2887	COA	C4A-N9A-C8A	2.08	107.93	105.74
3	E	2888	COA	O5B-C5B-C4B	-2.06	101.97	108.99
3	B	2887	COA	C2B-C1B-N9A	-2.05	108.20	113.30
3	B	2888	COA	C4A-N9A-C8A	2.00	107.84	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2887	COA	C7P-N8P-C9P	-2.00	118.95	122.55

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2887	COA	CAP-C9P-N8P-C7P
3	B	2887	COA	S1P-C2P-C3P-N4P
3	B	2888	COA	CCP-O6A-P2A-O3A
3	B	2888	COA	S1P-C2P-C3P-N4P
3	C	2887	COA	CCP-O6A-P2A-O3A
3	C	2887	COA	CCP-O6A-P2A-O5A
3	C	2887	COA	S1P-C2P-C3P-N4P
3	E	2887	COA	CCP-O6A-P2A-O3A
3	E	2887	COA	CCP-O6A-P2A-O5A
3	E	2887	COA	S1P-C2P-C3P-N4P
3	E	2888	COA	C5B-O5B-P1A-O1A
3	E	2888	COA	S1P-C2P-C3P-N4P
3	B	2887	COA	O9P-C9P-N8P-C7P
3	B	2887	COA	C2B-C3B-O3B-P3B
3	B	2888	COA	C2B-C3B-O3B-P3B
3	C	2887	COA	C2B-C3B-O3B-P3B
3	E	2887	COA	C2B-C3B-O3B-P3B
3	E	2888	COA	C2B-C3B-O3B-P3B
3	E	2888	COA	C4B-C3B-O3B-P3B
3	B	2887	COA	C4B-C3B-O3B-P3B
3	B	2888	COA	C4B-C3B-O3B-P3B
3	C	2887	COA	C4B-C3B-O3B-P3B
3	E	2887	COA	C4B-C3B-O3B-P3B
3	B	2887	COA	N8P-C9P-CAP-CBP
3	B	2887	COA	P2A-O3A-P1A-O5B
3	E	2888	COA	C3B-C4B-C5B-O5B
3	B	2888	COA	P2A-O3A-P1A-O1A
3	C	2887	COA	P2A-O3A-P1A-O1A
3	E	2887	COA	P2A-O3A-P1A-O1A
3	E	2888	COA	P2A-O3A-P1A-O1A
3	B	2888	COA	CEP-CBP-CCP-O6A
3	B	2887	COA	C3B-O3B-P3B-O7A
3	E	2888	COA	C3B-O3B-P3B-O7A
3	B	2888	COA	CAP-CBP-CCP-O6A
3	B	2887	COA	CCP-O6A-P2A-O4A
3	C	2887	COA	C5B-O5B-P1A-O1A

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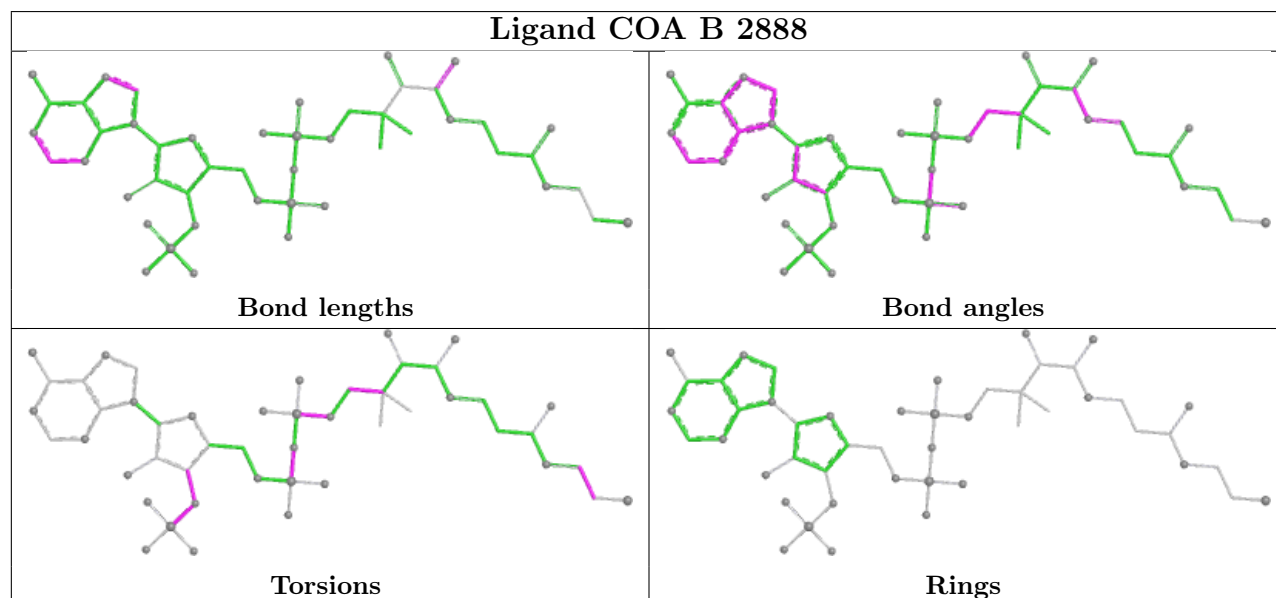
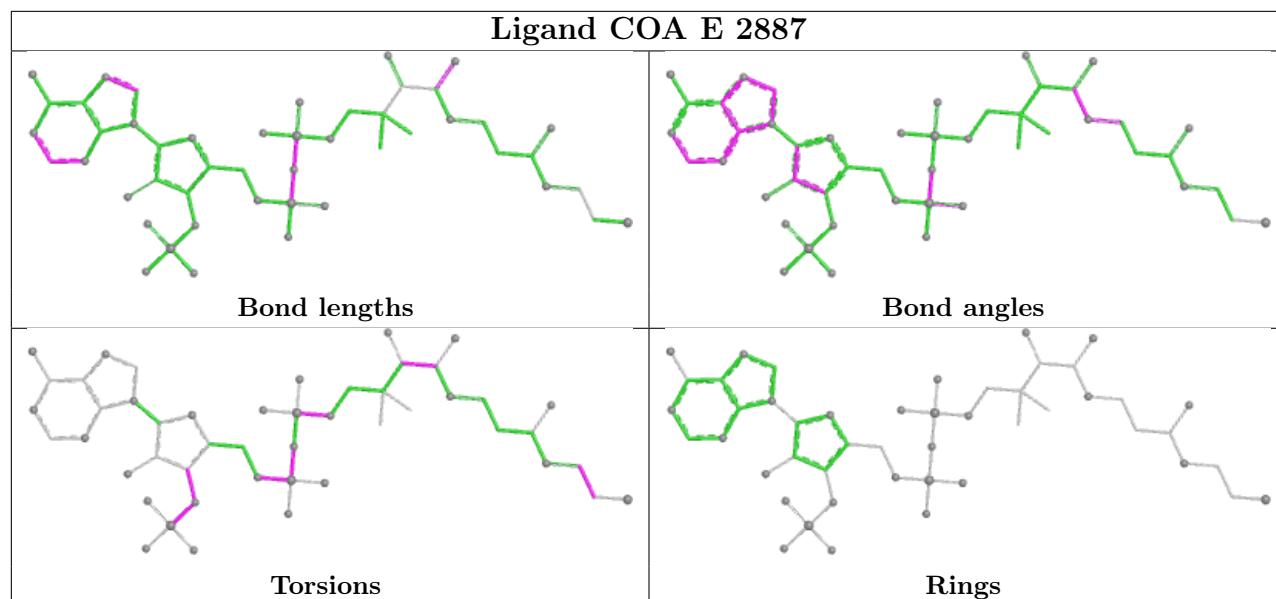
Mol	Chain	Res	Type	Atoms
3	E	2887	COA	C5B-O5B-P1A-O1A
3	C	2887	COA	P2A-O3A-P1A-O2A
3	C	2887	COA	C3B-O3B-P3B-O7A
3	E	2887	COA	C3B-O3B-P3B-O7A
3	B	2887	COA	O9P-C9P-CAP-CBP
3	B	2888	COA	C3B-O3B-P3B-O9A
3	C	2887	COA	C3B-O3B-P3B-O8A
3	B	2888	COA	CDP-CBP-CCP-O6A
3	C	2887	COA	N8P-C9P-CAP-OAP
3	E	2887	COA	N8P-C9P-CAP-OAP
3	E	2888	COA	N8P-C9P-CAP-OAP
3	B	2888	COA	P2A-O3A-P1A-O2A
3	E	2887	COA	P2A-O3A-P1A-O2A

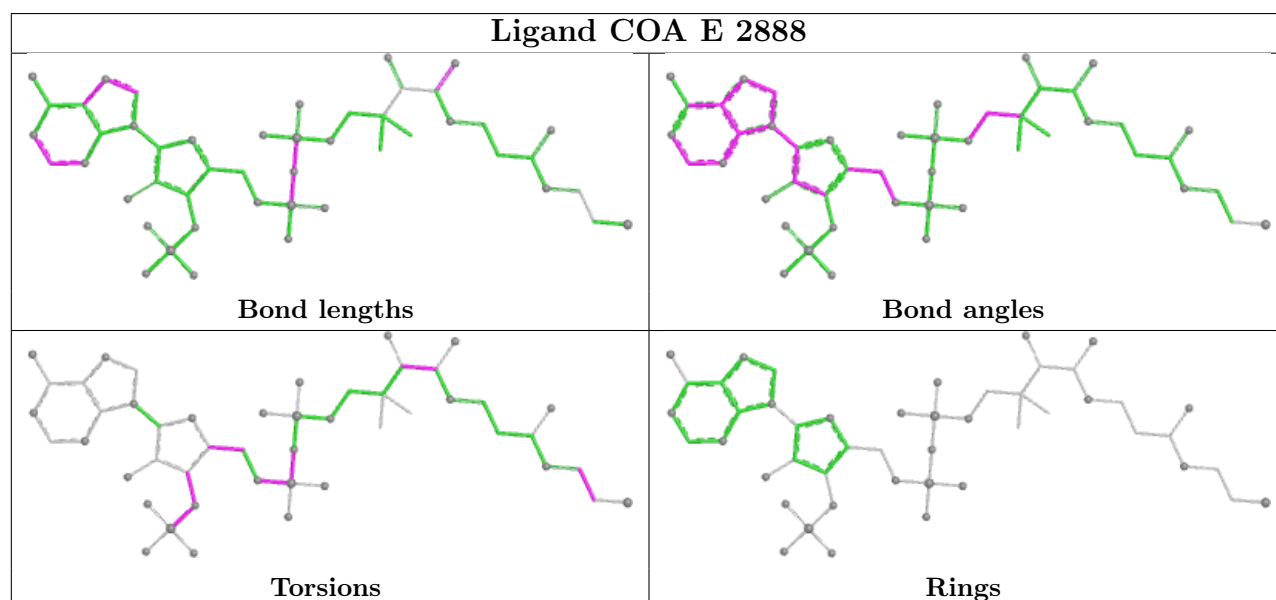
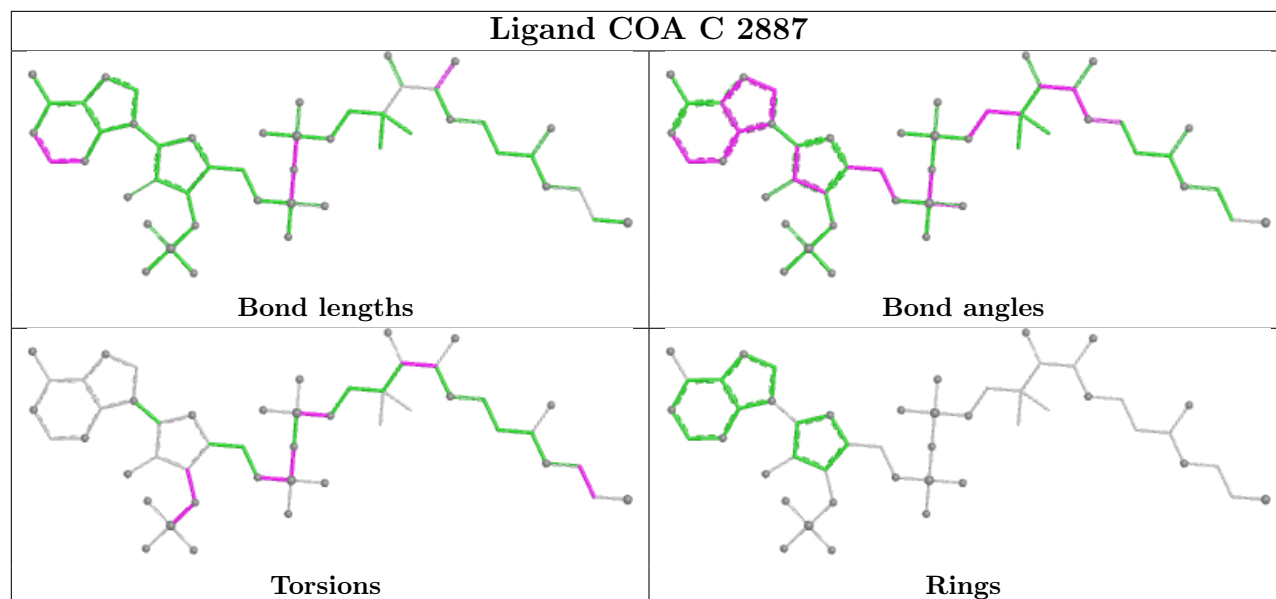
There are no ring outliers.

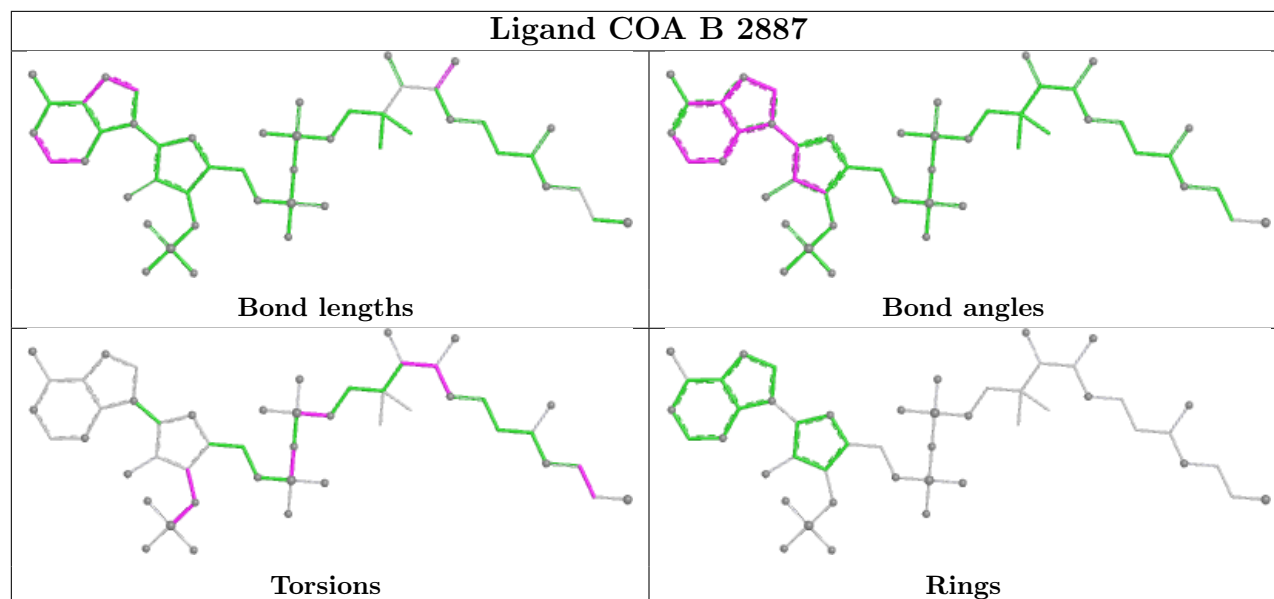
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2887	COA	1	0
3	B	2888	COA	2	0
3	E	2888	COA	1	0
3	B	2887	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	121/122 (99%)	0.42	12 (9%) 13 10	14, 26, 55, 68	0
1	B	120/122 (98%)	0.42	13 (10%) 11 8	14, 26, 45, 61	0
1	C	120/122 (98%)	0.36	10 (8%) 17 15	14, 25, 47, 62	0
1	D	120/122 (98%)	0.42	10 (8%) 17 15	14, 26, 49, 63	0
1	E	120/122 (98%)	0.52	11 (9%) 14 12	16, 29, 53, 66	0
1	F	115/122 (94%)	0.67	12 (10%) 11 9	16, 28, 50, 66	0
All	All	716/732 (97%)	0.47	68 (9%) 14 11	14, 27, 50, 68	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1842	VAL	5.2
1	D	1767	GLY	4.8
1	E	1842	VAL	4.6
1	A	1842	VAL	4.5
1	F	1833	ALA	3.9
1	E	1830	GLY	3.9
1	F	1767	GLY	3.9
1	F	1842	VAL	3.9
1	A	1843	ASN	3.7
1	A	1830	GLY	3.6
1	A	1844	LYS	3.4
1	E	1829	GLY	3.3
1	B	1842	VAL	3.3
1	E	1767	GLY	3.2
1	C	1767	GLY	3.2
1	D	1828	LEU	3.2
1	F	1832	ALA	3.1
1	B	1886	LYS	3.1
1	F	1826	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1778	SER	3.0
1	D	1829	GLY	3.0
1	D	1848	ALA	3.0
1	E	1886	LYS	3.0
1	F	1825	VAL	2.9
1	F	1824	GLY	2.9
1	E	1828	LEU	2.8
1	D	1830	GLY	2.8
1	C	1861	GLU	2.8
1	D	1886	LYS	2.8
1	B	1826	LYS	2.8
1	F	1813	TRP	2.7
1	A	1778	SER	2.7
1	B	1857	LYS	2.7
1	E	1843	ASN	2.7
1	B	1767	GLY	2.7
1	D	1778	SER	2.7
1	A	1886	LYS	2.6
1	B	1861	GLU	2.6
1	A	1829	GLY	2.6
1	A	1766	ASN	2.5
1	C	1828	LEU	2.5
1	E	1778	SER	2.5
1	B	1865	THR	2.4
1	C	1826	LYS	2.4
1	F	1820	PHE	2.4
1	F	1857	LYS	2.4
1	A	1777	THR	2.4
1	E	1826	LYS	2.3
1	C	1779	ILE	2.3
1	A	1767	GLY	2.3
1	D	1782	GLU	2.3
1	D	1840	VAL	2.3
1	B	1830	GLY	2.3
1	E	1861	GLU	2.3
1	A	1846	ALA	2.2
1	B	1885	THR	2.2
1	C	1863	GLY	2.2
1	C	1886	LYS	2.2
1	B	1860	GLU	2.2
1	B	1778	SER	2.2
1	A	1782	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1844	LYS	2.1
1	F	1861	GLU	2.1
1	F	1886	LYS	2.1
1	B	1831	GLY	2.1
1	D	1875	ASP	2.1
1	C	1777	THR	2.0
1	B	1854	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.

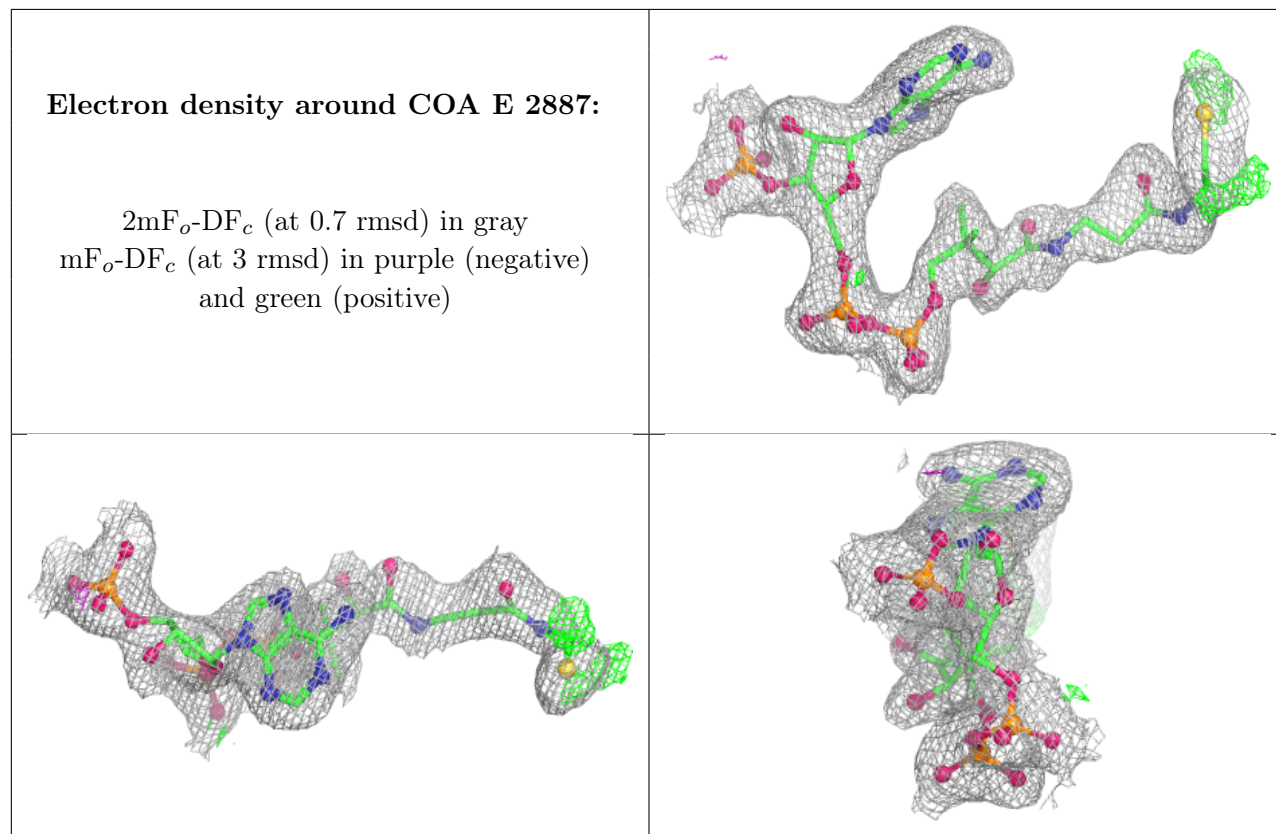
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	MG	B	2889	1/1	0.82	0.17	44,44,44,44	0
2	CL	E	2890	1/1	0.90	0.25	48,48,48,48	0
4	MG	E	2889	1/1	0.90	0.25	60,60,60,60	0
4	MG	B	2890	1/1	0.92	0.10	43,43,43,43	0
2	CL	A	2887	1/1	0.93	0.11	45,45,45,45	0
4	MG	D	2887	1/1	0.94	0.16	36,36,36,36	0
3	COA	E	2887	48/48	0.94	0.09	24,34,50,53	0
3	COA	E	2888	48/48	0.95	0.09	18,31,51,56	0
3	COA	C	2887	48/48	0.96	0.08	10,23,39,52	0
3	COA	B	2887	48/48	0.97	0.07	14,24,39,43	0
3	COA	B	2888	48/48	0.97	0.07	9,20,35,54	0
2	CL	B	2891	1/1	0.97	0.07	55,55,55,55	0
2	CL	D	2889	1/1	0.98	0.17	34,34,34,34	1
4	MG	C	2888	1/1	0.98	0.08	25,25,25,25	0

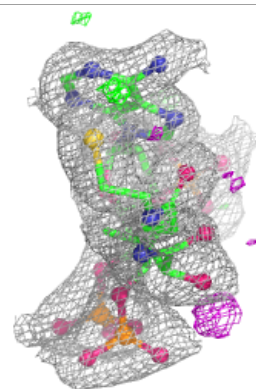
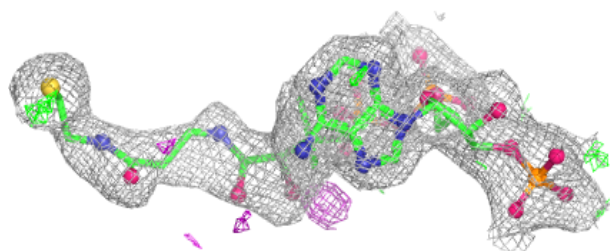
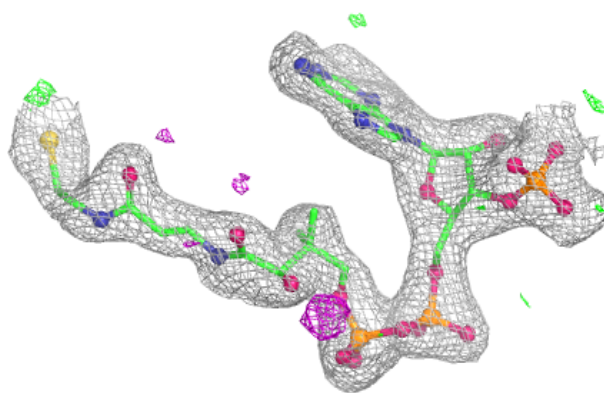
The following is a graphical depiction of the model fit to experimental electron density of all

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.

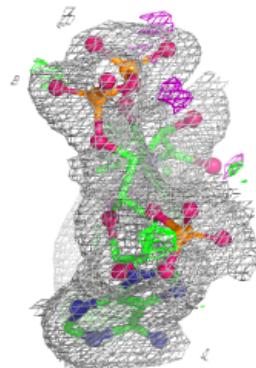
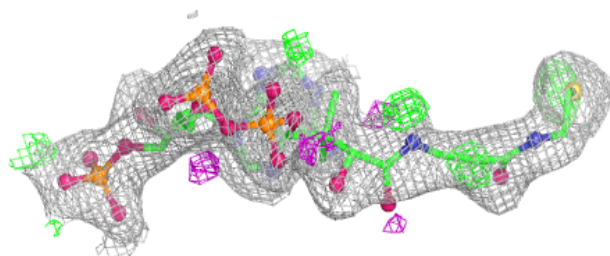
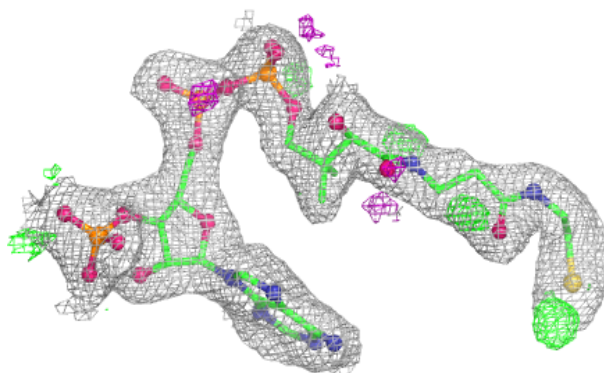


Electron density around COA E 2888:

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

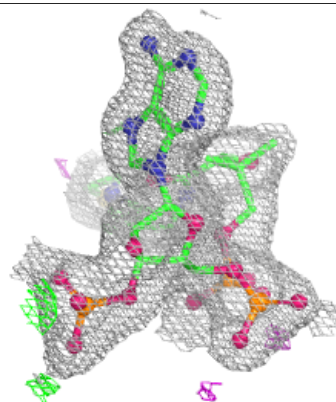
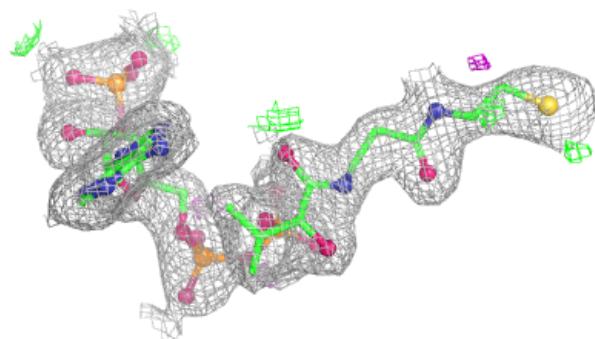
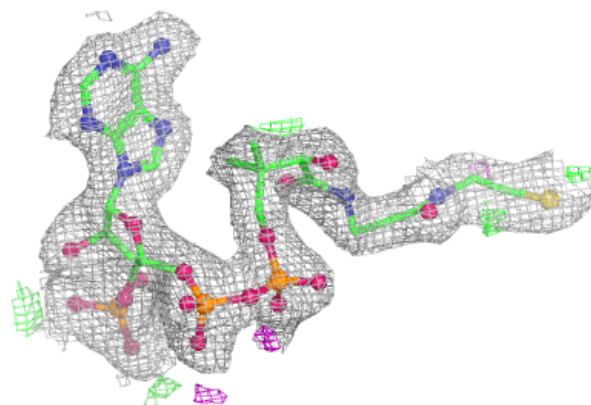
**Electron density around COA C 2887:**

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

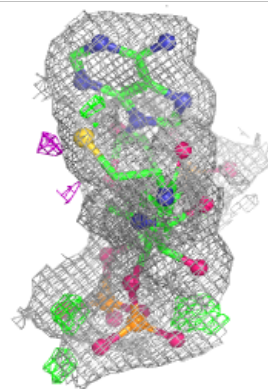
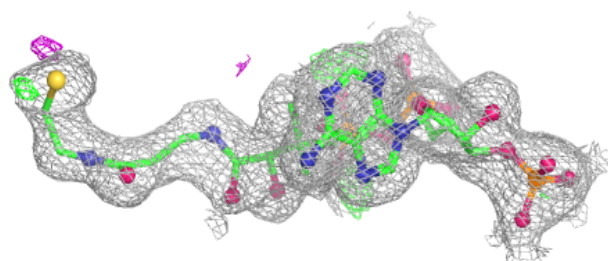
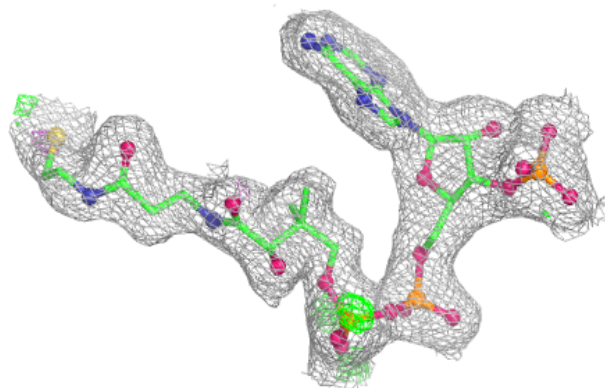


Electron density around COA B 2887:

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

**Electron density around COA B 2888:**

$2mF_o-DF_c$ (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.