Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 01:38 am BST

PDB ID	:	2VAT
Title	:	Crystal structure of deacetylcephalosporin C acetyltransferase in complex with coenzyme A
Authors	:	Lejon, S.; Ellis, J.; Valegard, K.
Deposited on	:	2007-09-04
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:

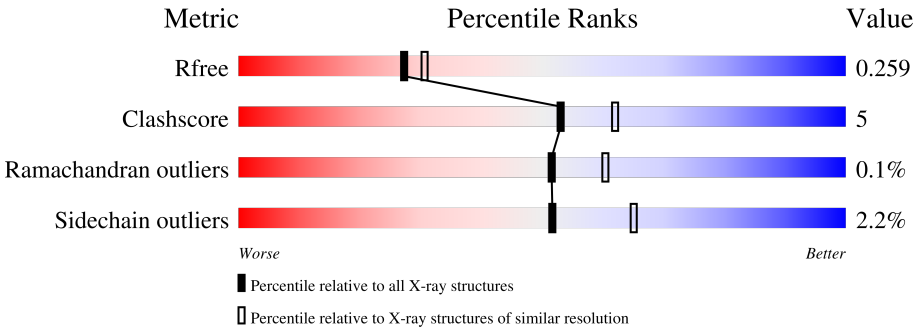
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	444	68% 10% 22%
1	B	444	71% 7% • 22%
1	C	444	69% 7% • 22%
1	D	444	70% 6% • 22%
1	E	444	70% 7% • 22%
1	F	444	68% 9% 23%
1	G	444	68% 8% • 23%

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Mol	Chain	Length	Quality of chain
1	H	444	67% 10% 22%
1	I	444	69% 8% 22%
1	J	444	68% 9% 23%
1	K	444	68% 9% 23%
1	L	444	68% 7% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	H	1384	-	-	X	-
3	ACT	K	1386	-	-	X	-

2 Entry composition (i)

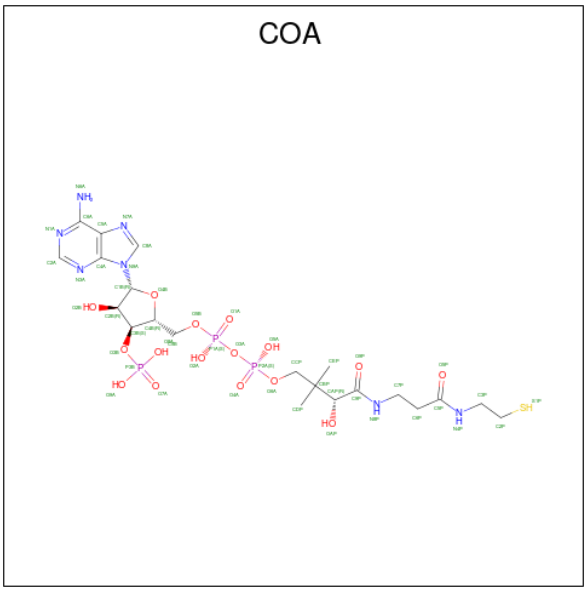
There are 5 unique types of molecules in this entry. The entry contains 35013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE.

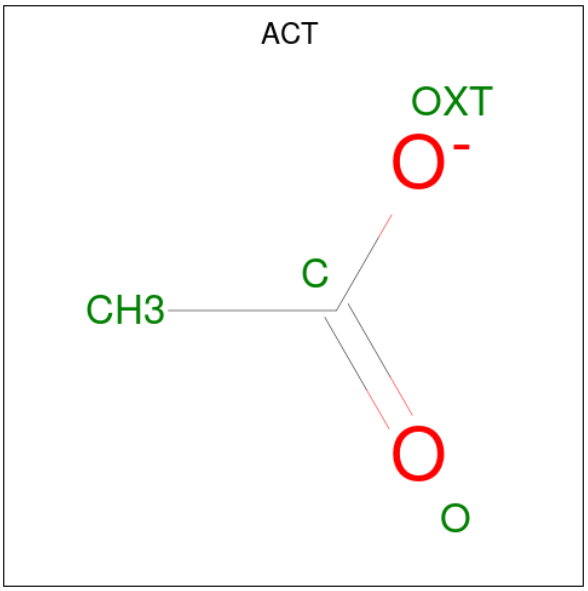
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	4	0
			2744	1731	485	509	19			
1	B	347	Total	C	N	O	S	0	3	0
			2744	1731	488	506	19			
1	C	345	Total	C	N	O	S	0	4	0
			2745	1730	488	508	19			
1	D	345	Total	C	N	O	S	0	4	0
			2748	1732	488	509	19			
1	E	346	Total	C	N	O	S	0	5	0
			2744	1732	487	506	19			
1	F	342	Total	C	N	O	S	0	2	0
			2694	1700	474	501	19			
1	G	342	Total	C	N	O	S	0	6	0
			2733	1724	484	506	19			
1	H	345	Total	C	N	O	S	0	8	0
			2760	1741	492	508	19			
1	I	347	Total	C	N	O	S	0	3	0
			2739	1728	485	507	19			
1	J	344	Total	C	N	O	S	0	4	0
			2724	1719	482	504	19			
1	K	344	Total	C	N	O	S	0	5	0
			2732	1724	485	504	19			
1	L	341	Total	C	N	O	S	0	3	0
			2697	1702	476	500	19			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



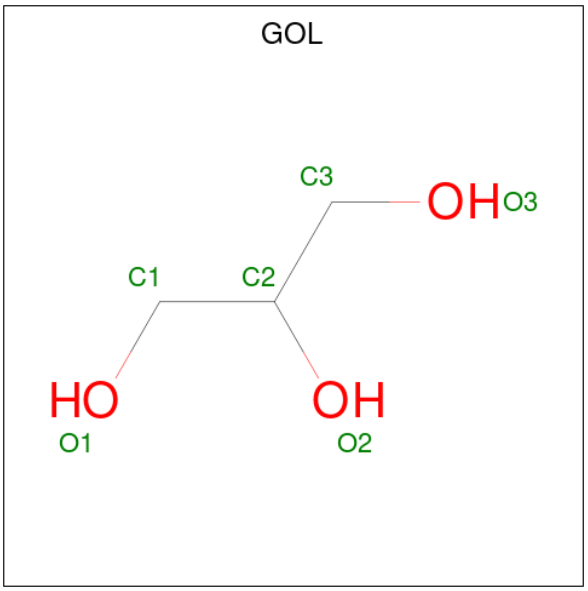
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	165	Total O 165 165	0	0
5	B	171	Total O 171 171	0	0
5	C	137	Total O 137 137	0	0
5	D	123	Total O 123 123	0	0
5	E	165	Total O 165 165	0	0
5	F	102	Total O 102 102	0	0
5	G	140	Total O 140 140	0	0
5	H	144	Total O 144 144	0	0
5	I	164	Total O 164 164	0	0
5	J	80	Total O 80 80	0	0

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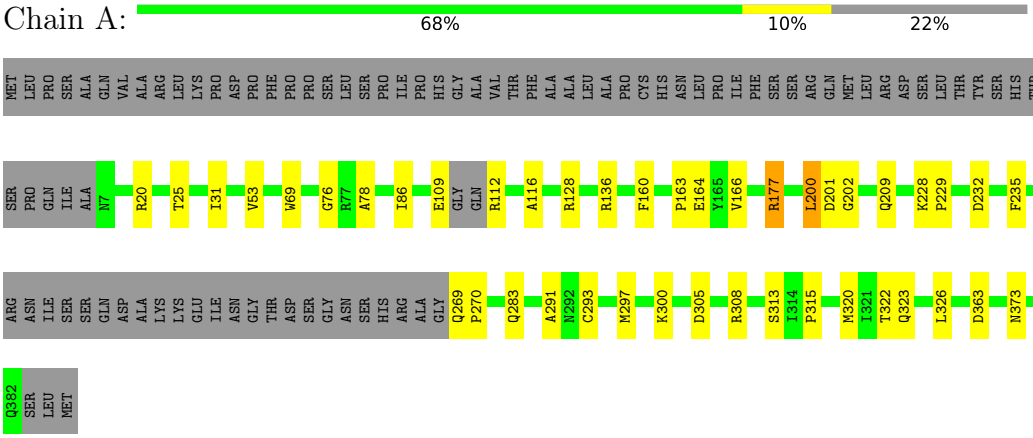
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	78	Total O 78 78	0	0
5	L	104	Total O 104 104	0	0

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. 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. 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.

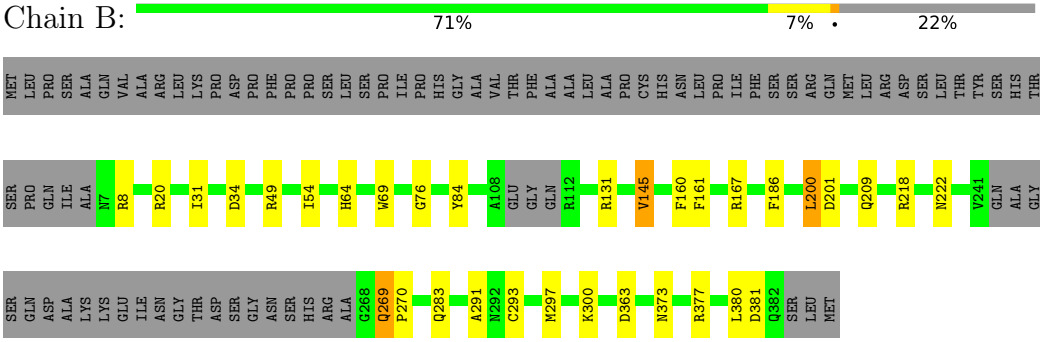
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain A:



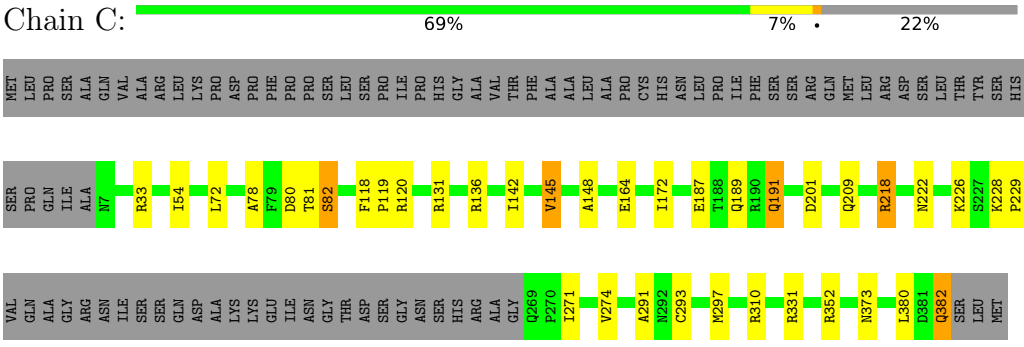
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain B:



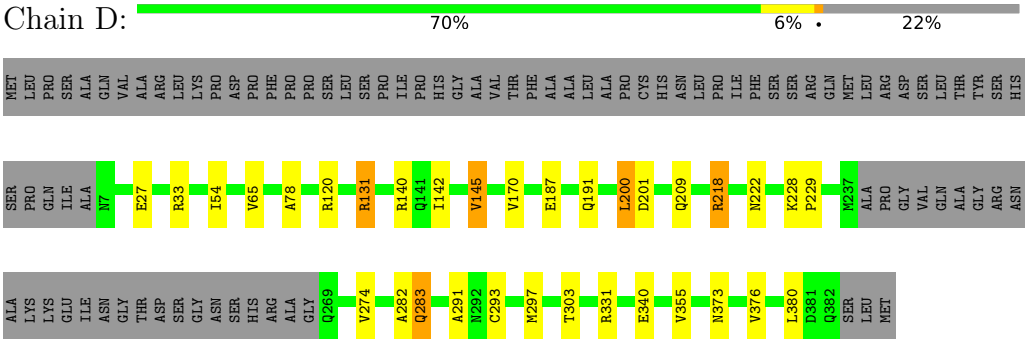
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain C:



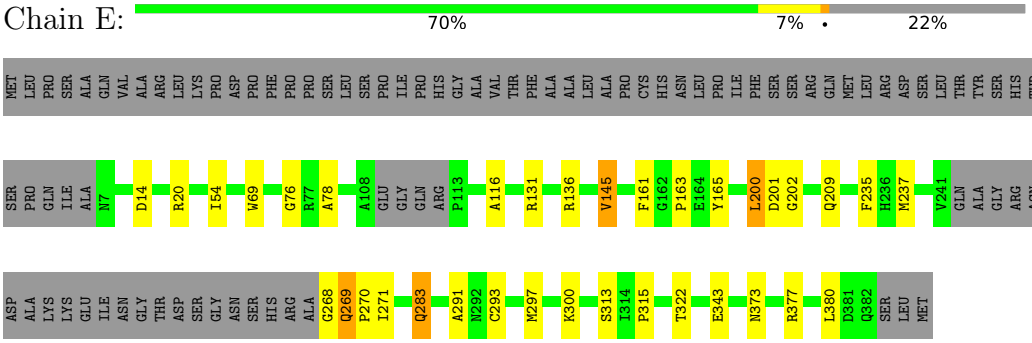
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain D:



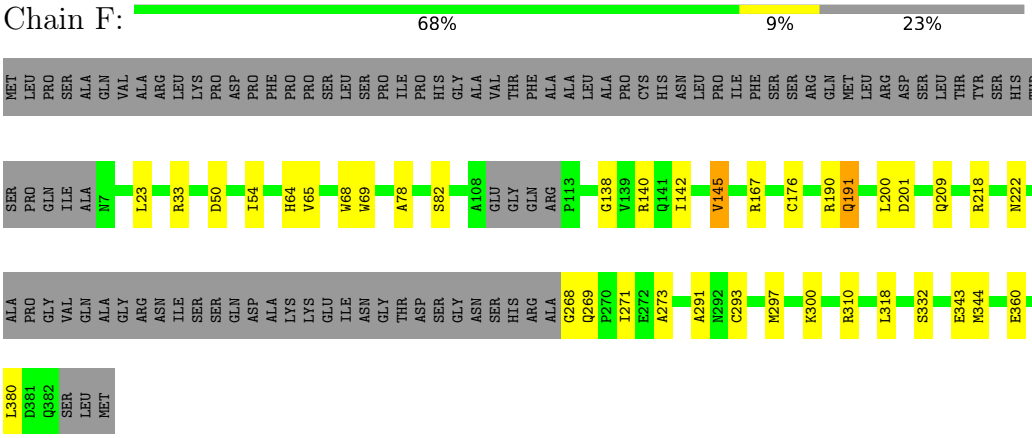
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain E:



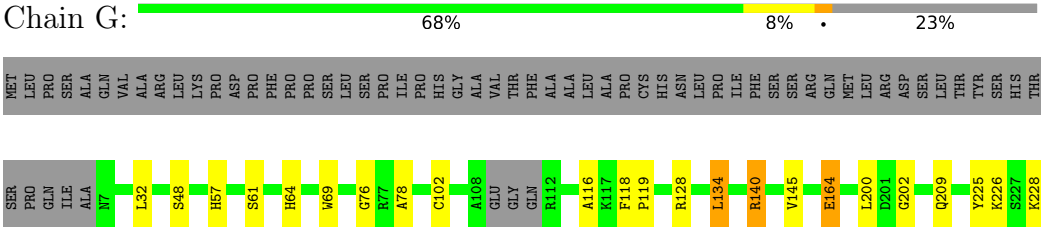
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

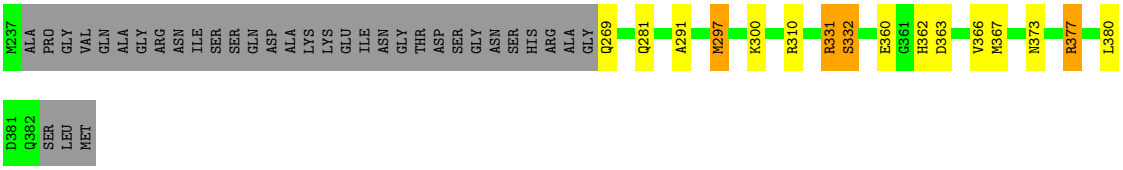
Chain F:



• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

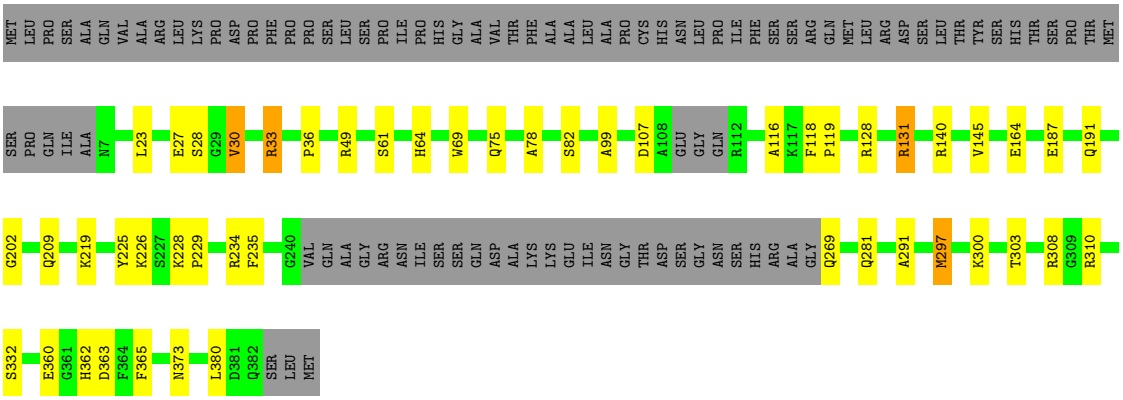
Chain G:





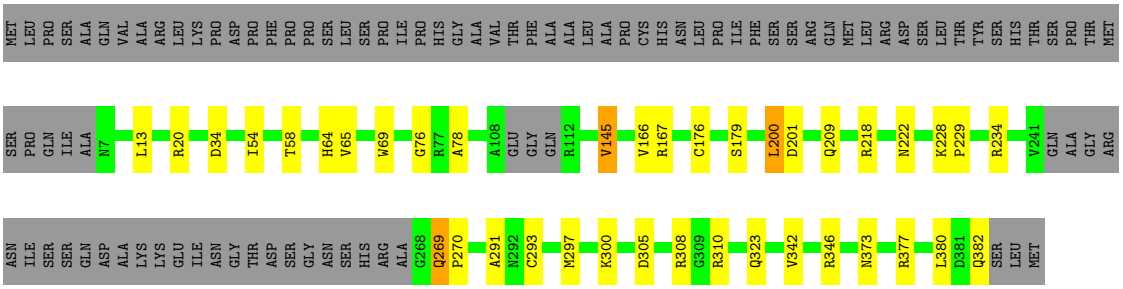
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain H:



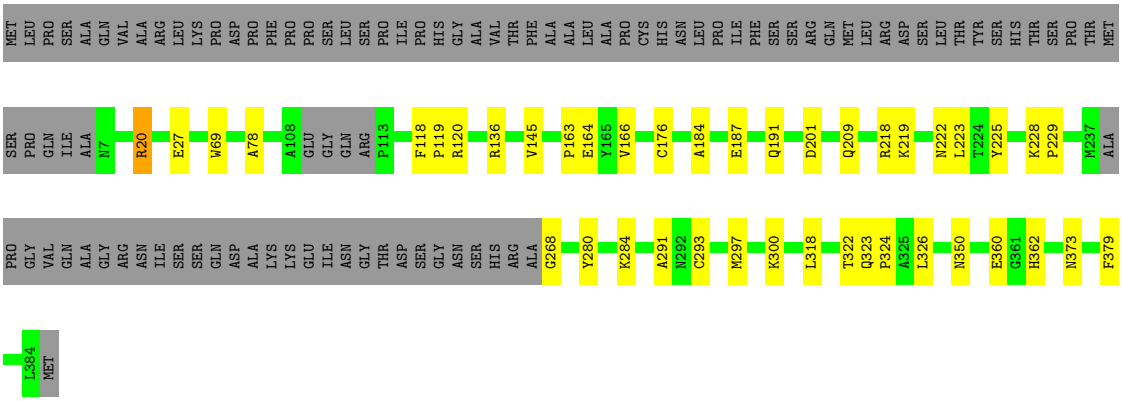
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain I:



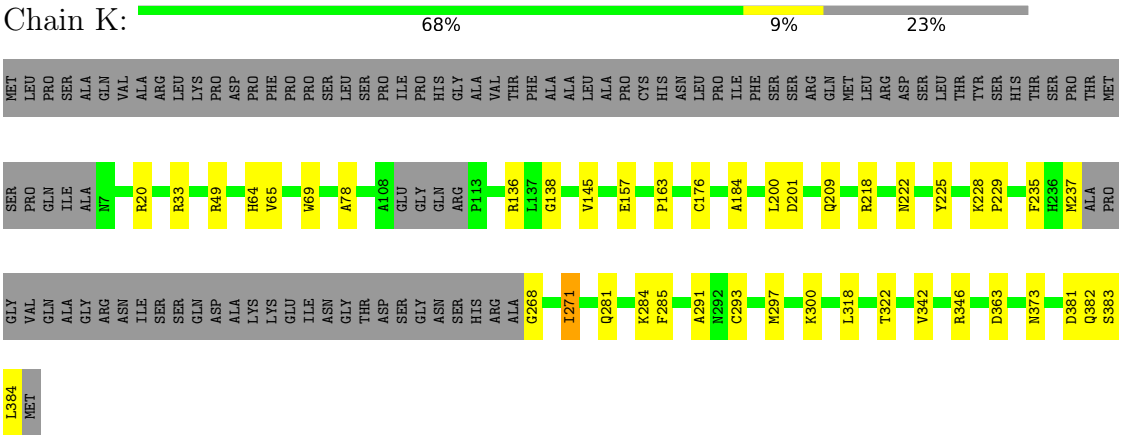
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain J:



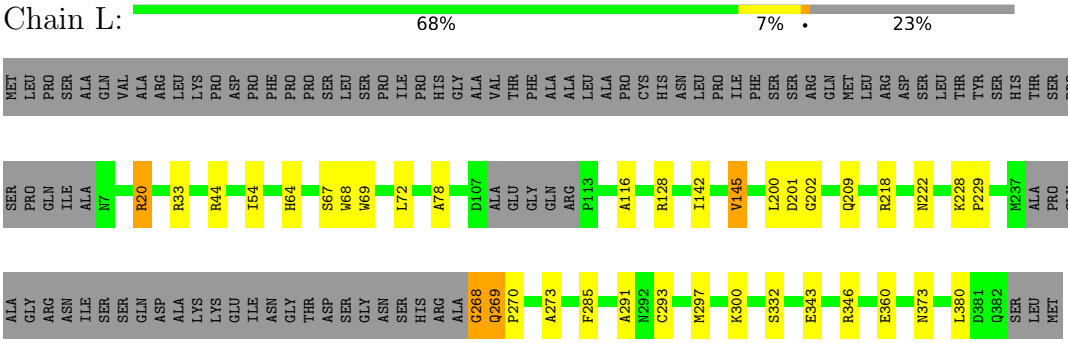
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain K:



• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.96Å 109.28Å 197.00Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	122.17 – 2.20 27.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (122.17-2.20) 98.9 (27.45-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.230 0.263 , 0.259	Depositor DCC
R_{free} test set	10106 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 16.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	35013	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, 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	0.89	3/2816 (0.1%)	0.75	4/3817 (0.1%)
1	B	0.99	10/2816 (0.4%)	0.76	3/3816 (0.1%)
1	C	0.89	6/2820 (0.2%)	0.71	1/3821 (0.0%)
1	D	0.94	5/2826 (0.2%)	0.74	2/3829 (0.1%)
1	E	0.85	1/2822 (0.0%)	0.70	0/3823
1	F	0.89	5/2759 (0.2%)	0.75	6/3739 (0.2%)
1	G	0.87	3/2813 (0.1%)	0.73	3/3811 (0.1%)
1	H	0.84	0/2844	0.73	4/3852 (0.1%)
1	I	0.87	2/2811 (0.1%)	0.73	3/3810 (0.1%)
1	J	0.89	2/2795 (0.1%)	0.72	1/3786 (0.0%)
1	K	0.86	1/2806 (0.0%)	0.69	0/3800
1	L	0.86	1/2765 (0.0%)	0.71	0/3746
All	All	0.89	39/33693 (0.1%)	0.73	27/45650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	PHE	CE1-CZ	-11.74	1.15	1.37
1	B	186	PHE	CG-CD2	-11.20	1.22	1.38
1	D	340	GLU	CD-OE1	-10.64	1.14	1.25
1	D	340	GLU	CD-OE2	-10.50	1.14	1.25
1	B	186	PHE	CE2-CZ	-9.88	1.18	1.37
1	D	27	GLU	CD-OE1	-9.79	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	ARG	CZ-NH1	-9.34	1.21	1.33
1	B	186	PHE	CG-CD1	-9.34	1.24	1.38
1	F	190	ARG	CZ-NH1	-9.25	1.21	1.33
1	J	27	GLU	CD-OE1	-8.68	1.16	1.25
1	B	8	ARG	CZ-NH2	-8.47	1.22	1.33
1	A	326	LEU	CG-CD1	-8.46	1.20	1.51
1	D	27	GLU	CD-OE2	-7.39	1.17	1.25
1	J	27	GLU	CD-OE2	-7.33	1.17	1.25
1	F	190	ARG	CZ-NH2	-7.07	1.23	1.33
1	F	176	CYS	CB-SG	-6.41	1.71	1.82
1	D	200	LEU	CG-CD1	-6.34	1.28	1.51
1	C	189	GLN	CD-NE2	-6.34	1.17	1.32
1	C	191	GLN	CD-NE2	-6.16	1.17	1.32
1	G	102	CYS	CB-SG	-6.13	1.71	1.82
1	B	373	ASN	CG-OD1	-6.06	1.10	1.24
1	G	332	SER	CB-OG	5.87	1.49	1.42
1	C	382	GLN	CD-OE1	-5.79	1.11	1.24
1	A	326	LEU	CG-CD2	-5.71	1.30	1.51
1	E	200	LEU	CG-CD1	-5.67	1.30	1.51
1	C	189	GLN	CD-OE1	-5.64	1.11	1.24
1	I	200	LEU	CG-CD1	-5.64	1.30	1.51
1	B	373	ASN	CG-ND2	-5.62	1.18	1.32
1	A	200	LEU	CG-CD1	-5.54	1.31	1.51
1	G	200	LEU	CG-CD1	-5.53	1.31	1.51
1	I	176	CYS	CB-SG	-5.46	1.73	1.81
1	C	191	GLN	CD-OE1	-5.17	1.12	1.24
1	B	200	LEU	CG-CD2	-5.16	1.32	1.51
1	L	200	LEU	CG-CD2	-5.12	1.32	1.51
1	K	200	LEU	CG-CD1	-5.08	1.33	1.51
1	C	82	SER	CB-OG	-5.05	1.35	1.42
1	F	200	LEU	CG-CD1	-5.05	1.33	1.51
1	B	200	LEU	CG-CD1	-5.04	1.33	1.51
1	F	191	GLN	CD-OE1	-5.00	1.12	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	B	8	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	D	340	GLU	OE1-CD-OE2	-10.00	111.30	123.30
1	D	27	GLU	OE1-CD-OE2	-9.88	111.44	123.30
1	J	27	GLU	OE1-CD-OE2	-9.78	111.56	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	190	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	A	177	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	8	ARG	NH1-CZ-NH2	-8.10	110.49	119.40
1	A	326	LEU	CD1-CG-CD2	-7.87	86.89	110.50
1	F	190	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
1	B	8	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	F	190	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	C	310	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	G	297	MET	CG-SD-CE	6.54	110.66	100.20
1	H	297	MET	CG-SD-CE	6.49	110.58	100.20
1	H	310	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	H	310	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	I	310	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	I	167	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	128[A]	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	G	310	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	H	30	VAL	CG1-CB-CG2	5.47	119.66	110.90
1	F	310	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	134	LEU	CB-CG-CD1	5.35	120.09	111.00
1	I	310	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	F	310	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	167	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	268	GLY	Peptide

5.2 Too-close contacts (i)

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	2744	0	2656	25	0
1	B	2744	0	2663	18	0
1	C	2745	0	2662	30	0
1	D	2748	0	2669	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2744	0	2669	26	0
1	F	2694	0	2599	30	0
1	G	2733	0	2652	27	0
1	H	2760	0	2685	44	0
1	I	2739	0	2655	33	0
1	J	2724	0	2641	33	0
1	K	2732	0	2653	44	0
1	L	2697	0	2607	33	0
2	A	48	0	32	2	0
2	B	48	0	32	2	0
2	C	48	0	32	0	0
2	D	48	0	32	0	0
2	E	48	0	31	1	0
2	F	48	0	32	3	0
2	G	48	0	32	5	0
2	H	48	0	32	6	0
2	I	48	0	32	1	0
2	J	48	0	32	3	0
2	K	48	0	32	4	0
2	L	48	0	32	1	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	1	0
3	H	4	0	3	3	0
3	I	4	0	3	0	0
3	J	4	0	3	0	0
3	K	4	0	3	2	0
3	L	4	0	3	1	0
4	B	6	0	8	0	0
4	I	6	0	8	0	0
5	A	165	0	0	0	0
5	B	171	0	0	6	0
5	C	137	0	0	8	0
5	D	123	0	0	5	0
5	E	165	0	0	3	0
5	F	102	0	0	7	0
5	G	140	0	0	3	0
5	H	144	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	164	0	0	3	0
5	J	80	0	0	3	0
5	K	78	0	0	5	0
5	L	104	0	0	7	0
All	All	35013	0	32246	357	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 5.

All (357) 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:K:218[A]:ARG:NE	1:K:222[A]:ASN:HD21	1.04	1.42
1:K:218[A]:ARG:NE	1:K:222[A]:ASN:ND2	1.78	1.29
1:J:218:ARG:CZ	1:J:222[A]:ASN:OD1	1.98	1.11
1:H:363[A]:ASP:OD1	2:H:1383:COA:C6P	1.99	1.11
1:E:14:ASP:OD1	5:E:2005:HOH:O	1.72	1.08
1:K:218[A]:ARG:CZ	1:K:222[A]:ASN:ND2	2.20	1.04
1:H:363[A]:ASP:OD1	2:H:1383:COA:H61	1.60	1.01
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:HH11	1.29	0.98
1:H:363[A]:ASP:OD1	2:H:1383:COA:H62	1.62	0.98
1:J:218:ARG:NH2	1:J:222[A]:ASN:OD1	1.98	0.95
1:E:269:GLN:H	1:E:270:PRO:HD2	1.31	0.94
1:K:218[A]:ARG:HE	1:K:222[A]:ASN:HD21	1.08	0.94
1:C:120[B]:ARG:HD3	5:C:2107:HOH:O	1.66	0.93
1:H:131[A]:ARG:HG3	1:H:131[A]:ARG:HH11	1.35	0.90
1:D:331:ARG:NH1	1:I:382:GLN:HE21	1.69	0.89
1:J:360:GLU:O	5:J:2076:HOH:O	1.89	0.88
1:C:120[B]:ARG:HH21	1:C:120[B]:ARG:HG3	1.37	0.87
1:K:218[A]:ARG:CD	1:K:222[A]:ASN:HD21	1.89	0.85
1:L:20:ARG:HH11	1:L:20:ARG:HG3	1.39	0.85
1:K:218[A]:ARG:CD	1:K:222[A]:ASN:ND2	2.40	0.84
1:L:269:GLN:H	1:L:270:PRO:HD2	1.39	0.84
1:K:78:ALA:H	1:K:373:ASN:HD21	1.26	0.84
1:D:120[B]:ARG:HD3	5:D:2098:HOH:O	1.79	0.82
1:J:218:ARG:NE	1:J:222[A]:ASN:HD21	1.78	0.80
1:D:65:VAL:HG22	5:D:2030:HOH:O	1.80	0.79
1:D:120[B]:ARG:HH11	1:D:120[B]:ARG:CG	1.95	0.79
1:H:131[A]:ARG:HH11	1:H:131[A]:ARG:CG	1.95	0.79
1:J:78:ALA:H	1:J:373:ASN:HD21	1.31	0.79
2:B:1383:COA:O9A	5:B:2170:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:332:SER:OG	1:H:360:GLU:O	2.01	0.78
1:G:331:ARG:HG3	1:G:331:ARG:HH11	1.49	0.78
1:E:269:GLN:H	1:E:270:PRO:CD	1.98	0.77
1:D:331:ARG:NH1	1:I:382:GLN:NE2	2.33	0.76
1:H:308[B]:ARG:HH21	1:H:308[B]:ARG:HG3	1.51	0.76
1:H:303:THR:OG1	5:H:2117:HOH:O	1.67	0.75
1:K:218[A]:ARG:CZ	1:K:222[A]:ASN:HD21	1.86	0.74
1:C:164:GLU:HB3	5:C:2066:HOH:O	1.87	0.74
1:I:78:ALA:H	1:I:373:ASN:HD21	1.35	0.73
1:F:332:SER:OG	1:F:360:GLU:O	2.05	0.73
2:H:1383:COA:O9P	2:H:1383:COA:H131	1.87	0.72
1:A:78:ALA:H	1:A:373:ASN:ND2	1.87	0.72
1:A:209:GLN:HE22	1:A:291:ALA:H	1.37	0.72
1:F:64:HIS:HD2	5:F:2003:HOH:O	1.73	0.72
1:D:209:GLN:HE22	1:D:291:ALA:H	1.39	0.71
1:E:209:GLN:HE22	1:E:291:ALA:H	1.38	0.71
1:I:209:GLN:HE22	1:I:291:ALA:H	1.38	0.71
1:E:78:ALA:H	1:E:373:ASN:HD21	1.38	0.71
1:G:281:GLN:HE22	2:G:1383:COA:H52A	1.54	0.71
1:A:78:ALA:H	1:A:373:ASN:HD21	1.36	0.71
1:F:68:TRP:CZ2	5:F:2018:HOH:O	2.42	0.71
1:C:120[B]:ARG:HH21	1:C:120[B]:ARG:CG	2.04	0.70
1:K:218[B]:ARG:NH2	1:K:281:GLN:O	2.25	0.70
1:L:343:GLU:HG3	5:L:2092:HOH:O	1.91	0.70
1:H:64:HIS:HD2	5:H:2003:HOH:O	1.75	0.69
1:K:297:MET:O	1:K:300:LYS:HB2	1.92	0.69
1:K:363:ASP:OD1	2:K:1385:COA:H62	1.93	0.69
1:L:332:SER:OG	1:L:360:GLU:O	2.06	0.69
1:K:78:ALA:H	1:K:373:ASN:ND2	1.90	0.68
1:I:78:ALA:H	1:I:373:ASN:ND2	1.90	0.68
1:C:209:GLN:HE22	1:C:291:ALA:H	1.41	0.68
1:H:128[A]:ARG:HE	3:H:1384:ACT:H1	1.59	0.67
1:E:78:ALA:H	1:E:373:ASN:ND2	1.91	0.67
1:B:209:GLN:HE22	1:B:291:ALA:H	1.42	0.67
1:D:331:ARG:HH12	1:I:382:GLN:HE21	1.42	0.67
1:G:209:GLN:HE22	1:G:291:ALA:H	1.42	0.67
1:J:78:ALA:H	1:J:373:ASN:ND2	1.92	0.66
1:L:68:TRP:CZ2	5:L:2021:HOH:O	2.47	0.66
1:D:33:ARG:HD2	5:D:2037:HOH:O	1.96	0.66
1:F:50:ASP:HB3	1:F:140[A]:ARG:NH1	2.10	0.66
1:G:64:HIS:HD2	5:G:2005:HOH:O	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:GLU:HB3	5:J:2029:HOH:O	1.95	0.66
1:D:293:CYS:O	1:D:297:MET:HG3	1.96	0.66
1:I:293:CYS:O	1:I:297:MET:HG3	1.96	0.66
1:H:209:GLN:HE22	1:H:291:ALA:H	1.44	0.65
1:D:218:ARG:CZ	1:D:222:ASN:HB2	2.26	0.65
1:F:343:GLU:HG3	5:F:2090:HOH:O	1.97	0.65
1:K:268:GLY:N	2:K:1385:COA:H62A	1.94	0.65
1:J:209:GLN:HE22	1:J:291:ALA:H	1.45	0.65
1:K:64:HIS:HD2	5:K:2003:HOH:O	1.80	0.65
1:D:228:LYS:HB3	1:D:229:PRO:HD3	1.79	0.65
1:A:109:GLU:HA	1:A:109:GLU:OE1	1.97	0.64
1:F:209:GLN:HE22	1:F:291:ALA:H	1.46	0.64
1:J:218:ARG:NE	1:J:222[A]:ASN:ND2	2.44	0.64
1:K:381:ASP:HB3	5:K:2076:HOH:O	1.97	0.64
1:K:209:GLN:HE22	1:K:291:ALA:H	1.44	0.64
1:B:293:CYS:O	1:B:297:MET:HG3	1.98	0.63
1:J:293:CYS:O	1:J:297:MET:HG3	1.98	0.63
1:L:209:GLN:HE22	1:L:291:ALA:H	1.46	0.63
1:B:269:GLN:H	1:B:270:PRO:HD2	1.64	0.63
1:D:120[B]:ARG:CG	1:D:120[B]:ARG:NH1	2.58	0.63
1:C:120[B]:ARG:CD	5:C:2107:HOH:O	2.37	0.63
1:D:78:ALA:H	1:D:373:ASN:HD21	1.46	0.63
1:F:78:ALA:H	1:F:373:ASN:HD21	1.45	0.63
1:E:237:MET:HG3	1:E:271:ILE:HD12	1.81	0.63
1:L:78:ALA:H	1:L:373:ASN:HD21	1.46	0.63
1:C:293:CYS:O	1:C:297:MET:HG3	1.98	0.62
1:K:218[A]:ARG:HD2	1:K:222[A]:ASN:OD1	1.99	0.62
1:F:293:CYS:O	1:F:297:MET:HG3	1.99	0.62
1:J:218:ARG:CZ	1:J:222[A]:ASN:CG	2.68	0.62
1:J:297:MET:O	1:J:300:LYS:HB2	1.99	0.62
1:G:331:ARG:HG3	1:G:331:ARG:NH1	2.15	0.61
1:C:81:THR:OG1	1:F:138:GLY:HA2	2.00	0.61
1:H:33[A]:ARG:NH2	1:H:107:ASP:OD2	2.24	0.61
1:L:20:ARG:HH11	1:L:20:ARG:CG	2.12	0.61
1:L:20:ARG:HG3	1:L:20:ARG:NH1	2.14	0.61
1:L:68:TRP:NE1	5:L:2021:HOH:O	2.33	0.61
1:L:269:GLN:H	1:L:270:PRO:CD	2.12	0.61
1:I:64:HIS:HD2	5:I:2004:HOH:O	1.82	0.61
1:H:281:GLN:HE22	2:H:1383:COA:H52A	1.66	0.61
1:J:218:ARG:NE	1:J:222[A]:ASN:OD1	2.34	0.61
1:J:218:ARG:HE	1:J:222[A]:ASN:HD21	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218[B]:ARG:HG3	1:K:285:PHE:CG	2.37	0.60
1:L:293:CYS:O	1:L:297:MET:HG3	2.01	0.60
1:K:218[A]:ARG:HD2	1:K:222[A]:ASN:CG	2.22	0.59
1:B:84:TYR:HE1	1:B:377[B]:ARG:HH22	1.50	0.59
1:B:76:GLY:O	1:B:377[A]:ARG:HD3	2.03	0.59
1:D:78:ALA:H	1:D:373:ASN:ND2	1.99	0.59
1:G:78:ALA:H	1:G:373:ASN:HD21	1.48	0.59
1:H:131[A]:ARG:HG3	1:H:131[A]:ARG:NH1	2.10	0.59
1:E:237:MET:CG	1:E:271:ILE:HD12	2.33	0.59
1:K:218[A]:ARG:CD	1:K:222[A]:ASN:CG	2.71	0.59
1:F:50:ASP:HB3	1:F:140[A]:ARG:HH12	1.68	0.58
1:E:237:MET:HG3	1:E:271:ILE:CD1	2.34	0.57
1:F:78:ALA:H	1:F:373:ASN:ND2	2.02	0.57
1:C:331:ARG:NH2	5:C:2114:HOH:O	2.38	0.57
1:G:226:LYS:NZ	1:G:363[B]:ASP:OD1	2.24	0.56
1:K:293:CYS:O	1:K:297:MET:HG3	2.04	0.56
1:H:27:GLU:OE1	1:H:308[A]:ARG:NH2	2.35	0.56
1:A:25:THR:HG21	3:B:1385:ACT:H3	1.86	0.56
1:F:268:GLY:O	1:F:273:ALA:HB3	2.05	0.56
1:G:78:ALA:H	1:G:373:ASN:ND2	2.03	0.56
1:H:75:GLN:HG3	1:H:82:SER:OG	2.05	0.56
1:L:64:HIS:HD2	5:L:2003:HOH:O	1.89	0.56
1:G:332:SER:OG	1:G:360:GLU:O	2.13	0.56
1:G:363[A]:ASP:OD1	2:G:1383:COA:H61	2.05	0.56
1:H:308[B]:ARG:HH21	1:H:308[B]:ARG:CG	2.17	0.56
1:L:78:ALA:H	1:L:373:ASN:ND2	2.03	0.56
1:C:228:LYS:HB3	1:C:229:PRO:HD3	1.87	0.56
1:C:78:ALA:H	1:C:373:ASN:HD21	1.53	0.56
1:J:280:TYR:OH	2:J:1385:COA:O7A	2.17	0.56
1:K:235:PHE:CE2	1:K:268:GLY:O	2.60	0.55
1:H:226:LYS:NZ	1:H:363[B]:ASP:OD1	2.27	0.55
1:K:281:GLN:HB2	5:K:2043:HOH:O	2.06	0.55
1:G:116:ALA:HB2	1:G:202:GLY:HA3	1.88	0.55
1:I:346:ARG:CZ	1:K:346[B]:ARG:HG3	2.37	0.55
1:L:297:MET:O	1:L:300:LYS:HB2	2.06	0.55
1:C:120[A]:ARG:NH1	5:C:2054:HOH:O	2.40	0.54
1:G:76:GLY:O	1:G:377:ARG:NH1	2.40	0.54
1:L:68:TRP:CE2	5:L:2021:HOH:O	2.61	0.54
1:C:33:ARG:HD2	5:C:2047:HOH:O	2.07	0.54
1:G:164[B]:GLU:HB2	5:G:2071:HOH:O	2.06	0.54
1:I:218:ARG:CZ	1:I:222:ASN:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:MET:O	1:G:300:LYS:HB2	2.07	0.54
1:E:131[A]:ARG:HD3	1:E:161:PHE:CE1	2.43	0.54
1:F:297:MET:O	1:F:300:LYS:HB2	2.07	0.53
1:H:116:ALA:HB2	1:H:202:GLY:HA3	1.89	0.53
1:H:27:GLU:CD	1:H:308[A]:ARG:HH12	2.11	0.53
1:K:20:ARG:O	1:K:136[A]:ARG:NH2	2.41	0.53
1:B:20:ARG:HD3	1:B:34:ASP:OD1	2.09	0.53
1:K:163:PRO:HG3	1:K:322:THR:CG2	2.39	0.53
1:B:377[B]:ARG:NH1	1:B:381:ASP:OD1	2.40	0.53
1:A:293:CYS:O	1:A:297:MET:HG3	2.09	0.53
1:D:283:GLN:HB3	5:D:2088:HOH:O	2.09	0.53
1:K:218[B]:ARG:CZ	1:K:285:PHE:HB2	2.38	0.53
1:E:343:GLU:HG3	5:E:2150:HOH:O	2.08	0.52
1:F:68:TRP:HZ2	5:F:2018:HOH:O	1.88	0.52
1:E:283:GLN:HB3	5:E:2117:HOH:O	2.08	0.52
1:C:78:ALA:H	1:C:373:ASN:ND2	2.07	0.52
1:H:28:SER:OG	1:H:30:VAL:HG13	2.08	0.52
1:G:48:SER:O	1:G:140[A]:ARG:NE	2.43	0.52
1:F:218:ARG:HD2	1:F:218:ARG:O	2.10	0.52
1:G:128[A]:ARG:HE	3:G:1384:ACT:H1	1.75	0.52
1:G:281:GLN:NE2	2:G:1383:COA:H52A	2.23	0.52
1:I:20:ARG:HD3	1:I:34:ASP:OD1	2.09	0.52
1:H:61:SER:CB	5:H:2035:HOH:O	2.59	0.51
1:F:218:ARG:CZ	1:F:222:ASN:HB2	2.41	0.51
1:C:120[B]:ARG:CG	1:C:120[B]:ARG:NH2	2.67	0.51
1:H:128[A]:ARG:HE	3:H:1384:ACT:CH3	2.23	0.51
1:K:163:PRO:HG3	1:K:322:THR:HG22	1.92	0.51
1:J:268:GLY:N	2:J:1385:COA:H62A	2.09	0.51
1:L:20:ARG:CG	1:L:20:ARG:NH1	2.69	0.51
1:J:163:PRO:HG3	1:J:322:THR:CG2	2.41	0.51
1:H:61:SER:HB2	5:H:2035:HOH:O	2.10	0.51
1:B:269:GLN:H	1:B:270:PRO:CD	2.23	0.50
1:B:297:MET:O	1:B:300:LYS:HB2	2.10	0.50
1:C:72:LEU:HA	1:C:373:ASN:HD22	1.77	0.50
1:C:191:GLN:HE21	1:J:219:LYS:NZ	2.10	0.50
1:F:23:LEU:HD23	1:F:33:ARG:HG2	1.94	0.50
1:H:128[A]:ARG:NE	3:H:1384:ACT:H1	2.27	0.50
1:C:218:ARG:CZ	1:C:222:ASN:HB2	2.42	0.50
1:E:131[A]:ARG:HD2	1:E:165:TYR:CE2	2.46	0.50
1:J:120:ARG:HD3	5:J:2019:HOH:O	2.11	0.50
1:H:78:ALA:H	1:H:373:ASN:HD21	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:ALA:HB2	1:L:202:GLY:HA3	1.94	0.49
1:F:54:ILE:HB	1:F:145:VAL:HB	1.94	0.49
1:I:65:VAL:HA	5:I:2036:HOH:O	2.11	0.49
1:E:76:GLY:O	1:E:377:ARG:HD3	2.12	0.49
1:L:54:ILE:HB	1:L:145:VAL:HB	1.94	0.49
1:K:157:GLU:O	3:K:1386:ACT:OXT	2.30	0.49
1:H:164[B]:GLU:HB2	5:H:2075:HOH:O	2.11	0.49
1:K:65:VAL:HG22	5:K:2012:HOH:O	2.12	0.49
1:F:228:LYS:HB3	1:F:229:PRO:HD3	1.95	0.48
1:H:78:ALA:H	1:H:373:ASN:ND2	2.11	0.48
1:G:228:LYS:HB3	1:G:229:PRO:HD3	1.96	0.48
1:G:366:VAL:HG21	2:G:1383:COA:H71	1.95	0.48
1:J:163:PRO:HG3	1:J:322:THR:HG22	1.94	0.48
1:L:218[A]:ARG:CZ	1:L:222[A]:ASN:HB2	2.43	0.48
1:D:331:ARG:HH11	1:I:382:GLN:NE2	2.07	0.48
1:I:228:LYS:HB3	1:I:229:PRO:HD3	1.95	0.48
1:I:346:ARG:NH2	1:K:346[A]:ARG:CD	2.76	0.48
1:G:331:ARG:HH11	1:G:331:ARG:CG	2.22	0.48
1:H:23:LEU:HD23	1:H:33[B]:ARG:HB3	1.95	0.48
1:I:297:MET:O	1:I:300:LYS:HB2	2.13	0.48
1:L:128[A]:ARG:HE	3:L:1384:ACT:H2	1.79	0.48
1:I:76:GLY:O	1:I:377:ARG:HD3	2.14	0.48
1:F:191:GLN:HE21	1:H:219:LYS:NZ	2.11	0.47
1:I:342:VAL:O	1:I:346:ARG:HG3	2.14	0.47
1:L:228:LYS:HB3	1:L:229:PRO:HD3	1.96	0.47
1:D:218:ARG:HG2	1:D:282:ALA:HA	1.95	0.47
1:L:218[A]:ARG:NH2	1:L:222[A]:ASN:HB2	2.30	0.47
1:A:160:PHE:HB3	1:B:31:ILE:HD12	1.96	0.47
1:A:235:PHE:HA	1:A:269:GLN:O	2.15	0.47
1:B:218:ARG:CZ	1:B:222:ASN:HB2	2.45	0.47
1:H:228:LYS:HB3	1:H:229:PRO:HD3	1.97	0.47
1:F:54:ILE:CD1	1:F:142:ILE:HD13	2.45	0.47
1:H:297:MET:O	1:H:300:LYS:HB2	2.15	0.47
1:I:13:LEU:HB2	1:L:44:ARG:NH2	2.30	0.47
1:I:305:ASP:O	1:I:308:ARG:HG2	2.15	0.47
1:E:20:ARG:O	1:E:136:ARG:NH1	2.48	0.47
1:F:54:ILE:HD11	1:F:142:ILE:HD13	1.97	0.46
1:A:76:GLY:O	1:A:377:ARG:HD3	2.16	0.46
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:NH1	2.09	0.46
1:B:131[A]:ARG:HD3	1:B:161:PHE:CZ	2.51	0.46
1:C:54:ILE:HB	1:C:145:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:O	1:A:323:GLN:HG2	2.15	0.46
1:I:65:VAL:HG22	5:I:2036:HOH:O	2.14	0.46
1:I:269:GLN:H	1:I:270:PRO:CD	2.28	0.46
3:K:1386:ACT:H3	5:K:2055:HOH:O	2.15	0.46
1:B:64:HIS:HD2	5:B:2004:HOH:O	1.99	0.46
2:F:1383:COA:H131	2:F:1383:COA:H72	1.98	0.46
1:A:363:ASP:OD1	2:A:1383:COA:H62	2.15	0.45
1:F:363:ASP:OD1	2:F:1383:COA:C7P	2.63	0.45
1:E:54:ILE:HB	1:E:145:VAL:HB	1.98	0.45
1:L:33:ARG:HD3	5:L:2028:HOH:O	2.16	0.45
1:B:167:ARG:HD2	5:B:2079:HOH:O	2.17	0.45
1:H:49:ARG:HH21	1:H:49:ARG:HG3	1.81	0.45
1:B:54:ILE:HB	1:B:145:VAL:HB	1.99	0.45
1:L:72:LEU:HA	1:L:373:ASN:HD22	1.82	0.45
1:G:57:HIS:HB2	1:G:61:SER:OG	2.16	0.45
1:F:218:ARG:NH2	1:F:222:ASN:HB2	2.32	0.45
1:A:297:MET:O	1:A:300:LYS:HB2	2.17	0.45
1:G:234:ARG:O	1:G:269:GLN:HA	2.16	0.45
1:F:68:TRP:CE2	5:F:2018:HOH:O	2.65	0.45
1:A:20:ARG:O	1:A:136:ARG:NH1	2.50	0.45
1:H:234:ARG:O	1:H:269:GLN:HA	2.16	0.45
1:I:346:ARG:HH22	1:K:346[A]:ARG:HG2	1.82	0.44
1:C:226:LYS:HD3	5:C:2132:HOH:O	2.18	0.44
1:D:303:THR:CG2	5:D:2098:HOH:O	2.66	0.44
1:H:365:PHE:HZ	2:H:1383:COA:H32	1.83	0.44
1:J:326:LEU:HD22	1:J:379:PHE:HB2	1.98	0.44
1:H:36:PRO:HD2	1:H:99:ALA:HB2	1.99	0.44
1:L:68:TRP:HZ2	5:L:2021:HOH:O	1.93	0.44
1:I:346:ARG:NH2	1:K:346[A]:ARG:HG2	2.33	0.44
1:K:342:VAL:O	1:K:346[A]:ARG:HG3	2.18	0.44
1:D:331:ARG:HH11	1:I:382:GLN:HE21	1.58	0.44
1:E:297:MET:O	1:E:300:LYS:HB2	2.17	0.44
1:C:80:ASP:OD1	1:C:82:SER:HB2	2.18	0.44
1:D:187:GLU:O	1:D:191:GLN:HG3	2.18	0.44
1:F:68:TRP:NE1	5:F:2018:HOH:O	2.51	0.44
1:H:235:PHE:HA	1:H:269:GLN:O	2.18	0.44
1:K:225:TYR:CD2	2:K:1385:COA:H61	2.52	0.44
1:L:268:GLY:HA2	1:L:273:ALA:CB	2.48	0.44
1:D:274:VAL:HG11	1:K:184:ALA:HA	1.98	0.43
1:A:228:LYS:HB3	1:A:229:PRO:HD3	2.00	0.43
1:J:187:GLU:O	1:J:191:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:MET:HE3	5:B:2012:HOH:O	2.18	0.43
2:L:1383:COA:H131	2:L:1383:COA:H71	1.99	0.43
1:C:54:ILE:CD1	1:C:142:ILE:HD13	2.49	0.43
1:F:363:ASP:OD1	2:F:1383:COA:H71	2.19	0.43
1:D:54:ILE:CD1	1:D:142:ILE:HD13	2.49	0.43
1:D:355:VAL:HB	1:I:382:GLN:HG2	2.00	0.43
1:I:346:ARG:HD2	1:K:346[B]:ARG:NH1	2.34	0.43
1:J:166:VAL:O	1:J:323:GLN:HG2	2.18	0.43
1:A:320:MET:CE	5:B:2012:HOH:O	2.67	0.43
1:A:163:PRO:HG3	1:A:322:THR:CG2	2.49	0.43
1:A:305:ASP:O	1:A:308:ARG:HG2	2.18	0.43
1:D:170:VAL:HG11	1:D:376:VAL:HG22	1.99	0.43
1:K:218[A]:ARG:CD	1:K:222[A]:ASN:OD1	2.53	0.43
1:I:234:ARG:O	1:I:269:GLN:HB3	2.18	0.42
1:E:268:GLY:N	2:E:1383:COA:H62A	2.17	0.42
1:G:367:MET:SD	2:G:1383:COA:H132	2.59	0.42
1:G:225:TYR:HA	1:G:362:HIS:HB3	2.00	0.42
1:E:163:PRO:HG3	1:E:322:THR:CG2	2.48	0.42
1:F:318:LEU:HD13	1:F:344:MET:HA	2.01	0.42
1:C:218:ARG:O	1:C:218:ARG:HG3	2.10	0.42
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.91	0.42
1:I:166:VAL:O	1:I:323:GLN:HG2	2.20	0.42
1:J:228:LYS:HB3	1:J:229:PRO:HD3	2.02	0.42
1:A:269:GLN:N	1:A:270:PRO:HD2	2.35	0.42
1:A:313:SER:HB2	1:A:315:PRO:HD2	2.02	0.42
1:I:54:ILE:HB	1:I:145:VAL:HB	2.02	0.42
1:K:228:LYS:HB3	1:K:229:PRO:HD3	2.02	0.42
2:A:1383:COA:H71	2:A:1383:COA:H10	1.90	0.42
1:C:148:ALA:HA	1:C:172:ILE:O	2.20	0.42
1:E:116:ALA:HB2	1:E:202:GLY:HA3	2.01	0.42
1:E:209:GLN:HE21	1:E:209:GLN:HB3	1.66	0.42
1:A:53:VAL:HB	1:A:86:ILE:HD13	2.02	0.41
1:A:232:ASP:OD1	1:I:179:SER:HB2	2.20	0.41
1:J:225:TYR:HA	1:J:362:HIS:HB3	2.02	0.41
1:L:218[B]:ARG:HB2	1:L:285:PHE:CD1	2.55	0.41
1:D:54:ILE:HB	1:D:145:VAL:HB	2.02	0.41
1:F:54:ILE:HD11	1:F:142:ILE:CD1	2.50	0.41
1:J:218:ARG:NE	1:J:222[A]:ASN:CG	2.72	0.41
1:K:382:GLN:HB3	1:K:384:LEU:CD2	2.51	0.41
1:C:187:GLU:O	1:C:191:GLN:HG3	2.20	0.41
1:E:235:PHE:HA	1:E:269:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:THR:HB	2:I:1383:COA:H31	2.02	0.41
1:K:176:CYS:SG	1:K:318:LEU:HD21	2.60	0.41
1:A:31:ILE:HD12	1:B:160:PHE:HB3	2.03	0.41
1:C:54:ILE:HD11	1:C:142:ILE:HD13	2.03	0.41
1:E:237:MET:HG2	1:E:271:ILE:HD12	2.03	0.41
1:H:27:GLU:OE1	1:H:308[A]:ARG:NH1	2.53	0.41
1:J:324:PRO:HA	1:J:350:ASN:O	2.21	0.41
1:E:293:CYS:O	1:E:297:MET:HG3	2.21	0.41
1:J:20:ARG:O	1:J:136[A]:ARG:NH1	2.53	0.41
1:C:274:VAL:HG11	1:J:184:ALA:HA	2.01	0.41
1:D:131:ARG:O	1:D:131:ARG:HG3	2.19	0.41
1:G:164[A]:GLU:HB3	5:G:2071:HOH:O	2.19	0.41
1:K:284:LYS:NZ	2:K:1385:COA:O9A	2.48	0.41
1:A:109:GLU:CD	1:A:112:ARG:N	2.74	0.41
1:E:163:PRO:HG3	1:E:322:THR:HG22	2.02	0.41
1:G:32:LEU:HD21	1:G:119:PRO:HG2	2.02	0.41
1:H:118:PHE:HA	1:H:119:PRO:HD3	1.91	0.41
1:I:13:LEU:HB2	1:L:44:ARG:HH21	1.86	0.41
1:J:118:PHE:HA	1:J:119:PRO:HD3	1.90	0.41
1:J:176:CYS:SG	1:J:318:LEU:HD21	2.60	0.41
1:J:223:LEU:HD23	1:J:223:LEU:HA	1.93	0.41
1:J:284:LYS:NZ	2:J:1385:COA:O9A	2.46	0.41
1:C:352:ARG:NH1	5:C:2126:HOH:O	2.48	0.41
1:D:54:ILE:HD11	1:D:142:ILE:HD13	2.02	0.41
1:E:313:SER:HB2	1:E:315:PRO:HD2	2.04	0.40
1:K:237:MET:HG3	1:K:271:ILE:HD12	2.03	0.40
1:B:49:ARG:NH2	5:B:2033:HOH:O	2.52	0.40
1:B:363:ASP:OD1	2:B:1383:COA:H72	2.21	0.40
1:H:225:TYR:HA	1:H:362:HIS:HB3	2.03	0.40
1:A:116:ALA:HB2	1:A:202:GLY:HA3	2.03	0.40
1:F:65:VAL:HG22	5:F:2018:HOH:O	2.21	0.40
1:G:118:PHE:HA	1:G:119:PRO:HD3	1.94	0.40
1:H:187:GLU:O	1:H:191:GLN:HG3	2.22	0.40
1:K:49:ARG:HD2	1:K:138:GLY:O	2.21	0.40
1:L:54:ILE:HD11	1:L:142:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/444 (77%)	332 (97%)	11 (3%)	0	100	100
1	B	343/444 (77%)	332 (97%)	10 (3%)	1 (0%)	41	46
1	C	344/444 (78%)	334 (97%)	10 (3%)	0	100	100
1	D	345/444 (78%)	335 (97%)	10 (3%)	0	100	100
1	E	344/444 (78%)	333 (97%)	10 (3%)	1 (0%)	41	46
1	F	336/444 (76%)	325 (97%)	11 (3%)	0	100	100
1	G	341/444 (77%)	332 (97%)	9 (3%)	0	100	100
1	H	345/444 (78%)	334 (97%)	11 (3%)	0	100	100
1	I	343/444 (77%)	333 (97%)	9 (3%)	1 (0%)	41	46
1	J	340/444 (77%)	327 (96%)	13 (4%)	0	100	100
1	K	341/444 (77%)	328 (96%)	13 (4%)	0	100	100
1	L	336/444 (76%)	327 (97%)	8 (2%)	1 (0%)	41	46
All	All	4101/5328 (77%)	3972 (97%)	125 (3%)	4 (0%)	51	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	GLN
1	E	269	GLN
1	I	269	GLN
1	L	269	GLN

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	293/372 (79%)	286 (98%)	7 (2%)	49	62
1	B	292/372 (78%)	286 (98%)	6 (2%)	53	67
1	C	293/372 (79%)	286 (98%)	7 (2%)	49	62
1	D	294/372 (79%)	286 (97%)	8 (3%)	44	57
1	E	293/372 (79%)	287 (98%)	6 (2%)	55	69
1	F	287/372 (77%)	280 (98%)	7 (2%)	49	62
1	G	293/372 (79%)	283 (97%)	10 (3%)	37	47
1	H	295/372 (79%)	286 (97%)	9 (3%)	40	51
1	I	292/372 (78%)	287 (98%)	5 (2%)	60	74
1	J	291/372 (78%)	287 (99%)	4 (1%)	67	80
1	K	292/372 (78%)	286 (98%)	6 (2%)	53	67
1	L	288/372 (77%)	281 (98%)	7 (2%)	49	62
All	All	3503/4464 (78%)	3421 (98%)	82 (2%)	52	63

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	TRP
1	A	164	GLU
1	A	177	ARG
1	A	200	LEU
1	A	201	ASP
1	A	283	GLN
1	A	380	LEU
1	B	69	TRP
1	B	145	VAL
1	B	200	LEU
1	B	201	ASP
1	B	283	GLN
1	B	380	LEU
1	C	131	ARG
1	C	145	VAL
1	C	201	ASP
1	C	218	ARG
1	C	271	ILE
1	C	380	LEU
1	C	382	GLN

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Mol	Chain	Res	Type
1	D	131	ARG
1	D	140	ARG
1	D	145	VAL
1	D	200	LEU
1	D	201	ASP
1	D	218	ARG
1	D	283	GLN
1	D	380	LEU
1	E	69	TRP
1	E	145	VAL
1	E	200	LEU
1	E	201	ASP
1	E	283	GLN
1	E	380	LEU
1	F	69	TRP
1	F	82	SER
1	F	145	VAL
1	F	201	ASP
1	F	269	GLN
1	F	271	ILE
1	F	380	LEU
1	G	69	TRP
1	G	134	LEU
1	G	140[A]	ARG
1	G	140[B]	ARG
1	G	145	VAL
1	G	164[A]	GLU
1	G	164[B]	GLU
1	G	331	ARG
1	G	377	ARG
1	G	380	LEU
1	H	33[A]	ARG
1	H	33[B]	ARG
1	H	69	TRP
1	H	131[A]	ARG
1	H	131[B]	ARG
1	H	140[A]	ARG
1	H	140[B]	ARG
1	H	145	VAL
1	H	380	LEU
1	I	69	TRP
1	I	145	VAL

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Mol	Chain	Res	Type
1	I	200	LEU
1	I	201	ASP
1	I	380	LEU
1	J	20	ARG
1	J	69	TRP
1	J	145	VAL
1	J	201	ASP
1	K	33	ARG
1	K	69	TRP
1	K	145	VAL
1	K	201	ASP
1	K	271	ILE
1	K	383	SER
1	L	20	ARG
1	L	67	SER
1	L	69	TRP
1	L	145	VAL
1	L	201	ASP
1	L	346	ARG
1	L	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	373	ASN
1	B	64	HIS
1	B	75	GLN
1	B	209	GLN
1	B	269	GLN
1	C	189	GLN
1	C	191	GLN
1	C	209	GLN
1	C	373	ASN
1	D	209	GLN
1	D	269	GLN
1	D	373	ASN
1	E	209	GLN
1	E	373	ASN
1	F	64	HIS
1	F	191	GLN
1	F	209	GLN

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Mol	Chain	Res	Type
1	F	269	GLN
1	F	373	ASN
1	G	64	HIS
1	G	209	GLN
1	G	269	GLN
1	G	281	GLN
1	G	373	ASN
1	H	64	HIS
1	H	209	GLN
1	H	281	GLN
1	H	373	ASN
1	I	209	GLN
1	I	373	ASN
1	I	382	GLN
1	J	64	HIS
1	J	209	GLN
1	J	373	ASN
1	K	64	HIS
1	K	209	GLN
1	K	373	ASN
1	L	64	HIS
1	L	209	GLN
1	L	373	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	A	1383	-	41,50,50	2.13	15 (36%)	52,75,75	1.43	7 (13%)
3	ACT	D	1384	-	3,3,3	0.74	0	3,3,3	1.09	0
3	ACT	G	1384	-	3,3,3	0.95	0	3,3,3	0.37	0
2	COA	B	1383	-	41,50,50	1.73	4 (9%)	52,75,75	1.28	3 (5%)
2	COA	D	1383	-	41,50,50	1.85	4 (9%)	52,75,75	1.18	3 (5%)
2	COA	K	1385	-	41,50,50	1.80	4 (9%)	52,75,75	1.22	2 (3%)
2	COA	I	1383	-	41,50,50	1.73	4 (9%)	52,75,75	1.27	4 (7%)
3	ACT	E	1384	-	3,3,3	0.80	0	3,3,3	0.99	0
3	ACT	F	1384	-	3,3,3	0.71	0	3,3,3	0.99	0
2	COA	C	1383	-	41,50,50	1.84	4 (9%)	52,75,75	1.25	4 (7%)
3	ACT	B	1385	-	3,3,3	0.66	0	3,3,3	1.19	0
2	COA	H	1383	-	41,50,50	2.02	10 (24%)	52,75,75	1.77	8 (15%)
4	GOL	B	1384	-	5,5,5	0.36	0	5,5,5	0.36	0
2	COA	F	1383	-	41,50,50	1.87	3 (7%)	52,75,75	1.22	3 (5%)
3	ACT	J	1386	-	3,3,3	0.77	0	3,3,3	1.09	0
4	GOL	I	1384	-	5,5,5	0.39	0	5,5,5	0.20	0
3	ACT	I	1385	-	3,3,3	0.78	0	3,3,3	0.67	0
2	COA	L	1383	-	41,50,50	1.82	3 (7%)	52,75,75	1.26	2 (3%)
3	ACT	H	1384	-	3,3,3	0.91	0	3,3,3	0.36	0
2	COA	G	1383	-	41,50,50	1.80	3 (7%)	52,75,75	1.20	3 (5%)
3	ACT	A	1384	-	3,3,3	0.73	0	3,3,3	1.03	0
3	ACT	K	1386	-	3,3,3	0.85	0	3,3,3	0.61	0
3	ACT	L	1384	-	3,3,3	0.69	0	3,3,3	0.94	0
2	COA	E	1383	-	41,50,50	2.08	12 (29%)	52,75,75	1.49	9 (17%)
3	ACT	C	1384	-	3,3,3	0.77	0	3,3,3	0.91	0
2	COA	J	1385	-	41,50,50	1.79	4 (9%)	52,75,75	1.14	2 (3%)

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	A	1383	-	-	13/44/64/64	0/3/3/3
2	COA	H	1383	-	-	20/44/64/64	0/3/3/3
2	COA	B	1383	-	-	18/44/64/64	0/3/3/3
4	GOL	B	1384	-	-	1/4/4/4	-
2	COA	E	1383	-	-	11/44/64/64	0/3/3/3
2	COA	F	1383	-	-	18/44/64/64	0/3/3/3
2	COA	D	1383	-	-	7/44/64/64	0/3/3/3
2	COA	L	1383	-	-	8/44/64/64	0/3/3/3
2	COA	J	1385	-	-	13/44/64/64	0/3/3/3
2	COA	K	1385	-	-	14/44/64/64	0/3/3/3
2	COA	G	1383	-	-	14/44/64/64	0/3/3/3
2	COA	I	1383	-	-	15/44/64/64	0/3/3/3
4	GOL	I	1384	-	-	2/4/4/4	-
2	COA	C	1383	-	-	10/44/64/64	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1383	COA	O9P-C9P	9.84	1.42	1.23
2	C	1383	COA	O9P-C9P	9.63	1.42	1.23
2	L	1383	COA	O9P-C9P	9.55	1.42	1.23
2	G	1383	COA	O9P-C9P	9.49	1.42	1.23
2	K	1385	COA	O9P-C9P	9.45	1.42	1.23
2	D	1383	COA	O9P-C9P	9.44	1.42	1.23
2	J	1385	COA	O9P-C9P	9.15	1.41	1.23
2	I	1383	COA	O9P-C9P	9.04	1.41	1.23
2	B	1383	COA	O9P-C9P	8.79	1.40	1.23
2	H	1383	COA	O9P-C9P	8.70	1.40	1.23
2	A	1383	COA	O9P-C9P	8.04	1.39	1.23
2	E	1383	COA	O9P-C9P	7.99	1.39	1.23
2	D	1383	COA	C2A-N3A	4.79	1.39	1.32
2	C	1383	COA	C2A-N3A	4.58	1.39	1.32
2	F	1383	COA	C2A-N3A	4.44	1.39	1.32
2	L	1383	COA	C2A-N3A	4.28	1.39	1.32
2	J	1385	COA	C2A-N3A	4.28	1.39	1.32
2	G	1383	COA	C2A-N3A	4.27	1.39	1.32
2	K	1385	COA	C2A-N3A	4.15	1.38	1.32
2	I	1383	COA	C2A-N3A	3.89	1.38	1.32
2	B	1383	COA	C2A-N3A	3.76	1.38	1.32
2	E	1383	COA	P3B-O8A	-3.56	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1383	COA	P1A-O2A	-3.24	1.40	1.55
2	E	1383	COA	P1A-O2A	-3.23	1.40	1.55
2	A	1383	COA	P3B-O8A	-3.07	1.43	1.54
2	A	1383	COA	O4B-C1B	-2.99	1.36	1.41
2	G	1383	COA	C2A-N1A	2.91	1.39	1.33
2	A	1383	COA	P3B-O9A	-2.89	1.43	1.54
2	F	1383	COA	C2A-N1A	2.87	1.39	1.33
2	J	1385	COA	C2A-N1A	2.85	1.39	1.33
2	H	1383	COA	C8A-N7A	-2.76	1.29	1.34
2	C	1383	COA	C2A-N1A	2.75	1.39	1.33
2	L	1383	COA	C2A-N1A	2.73	1.39	1.33
2	K	1385	COA	O4B-C1B	2.69	1.44	1.41
2	H	1383	COA	P3B-O9A	-2.65	1.44	1.54
2	D	1383	COA	C2A-N1A	2.65	1.38	1.33
2	E	1383	COA	O2B-C2B	-2.64	1.36	1.43
2	E	1383	COA	P3B-O9A	-2.62	1.44	1.54
2	D	1383	COA	O4B-C1B	2.62	1.44	1.41
2	A	1383	COA	P2A-O4A	-2.62	1.41	1.50
2	H	1383	COA	P3B-O8A	-2.61	1.44	1.54
2	E	1383	COA	P1A-O1A	-2.58	1.41	1.50
2	B	1383	COA	P3B-O3B	2.57	1.64	1.59
2	B	1383	COA	C2A-N1A	2.48	1.38	1.33
2	E	1383	COA	P2A-O4A	-2.44	1.42	1.50
2	H	1383	COA	C2A-N3A	2.41	1.36	1.32
2	H	1383	COA	C5A-C4A	-2.40	1.34	1.40
2	H	1383	COA	O2B-C2B	-2.39	1.37	1.43
2	A	1383	COA	C5A-N7A	-2.37	1.31	1.39
2	A	1383	COA	C4A-N3A	-2.35	1.32	1.35
2	A	1383	COA	C5A-C4A	-2.35	1.34	1.40
2	E	1383	COA	C5A-N7A	-2.33	1.31	1.39
2	I	1383	COA	P3B-O3B	2.30	1.63	1.59
2	A	1383	COA	P1A-O1A	-2.30	1.42	1.50
2	C	1383	COA	O4B-C1B	2.29	1.44	1.41
2	K	1385	COA	C2A-N1A	2.26	1.38	1.33
2	I	1383	COA	C2A-N1A	2.22	1.38	1.33
2	H	1383	COA	C5A-N7A	-2.20	1.31	1.39
2	A	1383	COA	C9P-N8P	-2.20	1.28	1.33
2	E	1383	COA	P2A-O5A	-2.16	1.45	1.55
2	H	1383	COA	P1A-O2A	-2.15	1.45	1.55
2	A	1383	COA	P2A-O5A	-2.15	1.45	1.55
2	E	1383	COA	C4A-N3A	-2.15	1.32	1.35
2	E	1383	COA	O4B-C4B	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1385	COA	O4B-C1B	2.09	1.44	1.41
2	A	1383	COA	C8A-N7A	-2.08	1.31	1.34
2	H	1383	COA	O4B-C4B	-2.05	1.40	1.45
2	A	1383	COA	O2B-C2B	-2.04	1.38	1.43
2	E	1383	COA	C5A-C4A	-2.01	1.35	1.40
2	A	1383	COA	C6A-N6A	-2.01	1.26	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1383	COA	N3A-C2A-N1A	-6.41	118.66	128.68
2	K	1385	COA	N3A-C2A-N1A	-6.19	119.00	128.68
2	I	1383	COA	N3A-C2A-N1A	-6.04	119.24	128.68
2	F	1383	COA	N3A-C2A-N1A	-5.91	119.44	128.68
2	B	1383	COA	N3A-C2A-N1A	-5.87	119.50	128.68
2	C	1383	COA	N3A-C2A-N1A	-5.84	119.56	128.68
2	H	1383	COA	CDP-CBP-CCP	5.82	117.73	108.23
2	D	1383	COA	N3A-C2A-N1A	-5.76	119.67	128.68
2	J	1385	COA	N3A-C2A-N1A	-5.73	119.72	128.68
2	G	1383	COA	N3A-C2A-N1A	-5.59	119.94	128.68
2	A	1383	COA	N3A-C2A-N1A	-5.58	119.96	128.68
2	H	1383	COA	O6A-CCP-CBP	5.05	118.66	110.55
2	H	1383	COA	N3A-C2A-N1A	-4.93	120.98	128.68
2	E	1383	COA	N3A-C2A-N1A	-4.75	121.25	128.68
2	E	1383	COA	O6A-CCP-CBP	3.36	115.94	110.55
2	B	1383	COA	P2A-O3A-P1A	-3.20	121.84	132.83
2	I	1383	COA	P2A-O3A-P1A	-3.16	121.98	132.83
2	E	1383	COA	C3P-N4P-C5P	-3.12	117.05	122.84
2	E	1383	COA	C4A-C5A-N7A	-3.11	106.16	109.40
2	H	1383	COA	C7P-N8P-C9P	3.04	128.01	122.59
2	C	1383	COA	C7P-C6P-C5P	-2.99	107.39	112.36
2	H	1383	COA	CDP-CBP-CAP	-2.77	104.02	108.82
2	K	1385	COA	P2A-O3A-P1A	-2.77	123.34	132.83
2	A	1383	COA	CDP-CBP-CAP	2.72	113.55	108.82
2	H	1383	COA	O4B-C1B-C2B	-2.70	102.98	106.93
2	I	1383	COA	C3P-N4P-C5P	-2.66	117.89	122.84
2	E	1383	COA	C7P-C6P-C5P	-2.60	108.03	112.36
2	A	1383	COA	C5B-C4B-C3B	-2.59	105.83	114.40
2	A	1383	COA	O6A-CCP-CBP	2.57	114.67	110.55
2	B	1383	COA	C7P-C6P-C5P	-2.52	108.15	112.36
2	F	1383	COA	P2A-O3A-P1A	-2.47	124.34	132.83
2	H	1383	COA	OAP-CAP-CBP	-2.46	104.45	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1383	COA	P2A-O3A-P1A	-2.45	124.42	132.83
2	C	1383	COA	P2A-O3A-P1A	-2.45	124.43	132.83
2	E	1383	COA	CAP-C9P-N8P	2.43	121.42	116.58
2	F	1383	COA	CEP-CBP-CAP	2.37	112.93	108.82
2	E	1383	COA	C1B-N9A-C4A	-2.37	122.48	126.64
2	G	1383	COA	P2A-O3A-P1A	-2.36	124.72	132.83
2	D	1383	COA	P2A-O3A-P1A	-2.34	124.80	132.83
2	D	1383	COA	C7P-C6P-C5P	-2.33	108.48	112.36
2	H	1383	COA	C4A-C5A-N7A	-2.29	107.01	109.40
2	A	1383	COA	CDP-CBP-CCP	2.29	111.97	108.23
2	J	1385	COA	P2A-O3A-P1A	-2.21	125.25	132.83
2	E	1383	COA	O9A-P3B-O3B	2.15	115.64	105.99
2	I	1383	COA	C7P-C6P-C5P	-2.15	108.78	112.36
2	A	1383	COA	C4A-C5A-N7A	-2.12	107.19	109.40
2	C	1383	COA	O3B-C3B-C4B	-2.09	102.54	110.08
2	E	1383	COA	C7P-N8P-C9P	2.06	126.27	122.59
2	G	1383	COA	C4A-C5A-N7A	-2.03	107.28	109.40
2	A	1383	COA	C6P-C5P-N4P	2.01	119.81	116.42

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1383	COA	C3B-O3B-P3B-O8A
2	A	1383	COA	OAP-CAP-CBP-CCP
2	A	1383	COA	C9P-CAP-CBP-CCP
2	A	1383	COA	C9P-CAP-CBP-CDP
2	A	1383	COA	OAP-CAP-CBP-CEP
2	A	1383	COA	C9P-CAP-CBP-CEP
2	A	1383	COA	CAP-C9P-N8P-C7P
2	A	1383	COA	C6P-C5P-N4P-C3P
2	A	1383	COA	O5P-C5P-N4P-C3P
2	A	1383	COA	S1P-C2P-C3P-N4P
2	B	1383	COA	C3B-O3B-P3B-O7A
2	B	1383	COA	C5B-O5B-P1A-O1A
2	B	1383	COA	OAP-CAP-CBP-CCP
2	B	1383	COA	OAP-CAP-CBP-CEP
2	B	1383	COA	CAP-C9P-N8P-C7P
2	B	1383	COA	O9P-C9P-N8P-C7P
2	B	1383	COA	S1P-C2P-C3P-N4P
2	C	1383	COA	C6P-C5P-N4P-C3P
2	C	1383	COA	O5P-C5P-N4P-C3P

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Mol	Chain	Res	Type	Atoms
2	C	1383	COA	S1P-C2P-C3P-N4P
2	D	1383	COA	C3B-O3B-P3B-O7A
2	D	1383	COA	CAP-C9P-N8P-C7P
2	D	1383	COA	C5P-C6P-C7P-N8P
2	D	1383	COA	C6P-C5P-N4P-C3P
2	D	1383	COA	S1P-C2P-C3P-N4P
2	E	1383	COA	C3B-O3B-P3B-O8A
2	E	1383	COA	C5B-O5B-P1A-O1A
2	E	1383	COA	OAP-CAP-CBP-CCP
2	E	1383	COA	C9P-CAP-CBP-CCP
2	E	1383	COA	OAP-CAP-CBP-CEP
2	E	1383	COA	C9P-CAP-CBP-CEP
2	E	1383	COA	CAP-C9P-N8P-C7P
2	E	1383	COA	O9P-C9P-N8P-C7P
2	E	1383	COA	S1P-C2P-C3P-N4P
2	F	1383	COA	C5B-O5B-P1A-O1A
2	F	1383	COA	OAP-CAP-CBP-CCP
2	F	1383	COA	C9P-CAP-CBP-CCP
2	F	1383	COA	OAP-CAP-CBP-CDP
2	F	1383	COA	OAP-CAP-CBP-CEP
2	F	1383	COA	C9P-CAP-CBP-CEP
2	F	1383	COA	CAP-C9P-N8P-C7P
2	F	1383	COA	O9P-C9P-N8P-C7P
2	F	1383	COA	S1P-C2P-C3P-N4P
2	G	1383	COA	CCP-O6A-P2A-O3A
2	G	1383	COA	CCP-O6A-P2A-O5A
2	G	1383	COA	CDP-CBP-CCP-O6A
2	G	1383	COA	CEP-CBP-CCP-O6A
2	G	1383	COA	CAP-CBP-CCP-O6A
2	G	1383	COA	CAP-C9P-N8P-C7P
2	G	1383	COA	C5P-C6P-C7P-N8P
2	G	1383	COA	C6P-C5P-N4P-C3P
2	H	1383	COA	C5B-O5B-P1A-O3A
2	H	1383	COA	CCP-O6A-P2A-O3A
2	H	1383	COA	CAP-CBP-CCP-O6A
2	H	1383	COA	C9P-CAP-CBP-CCP
2	H	1383	COA	C9P-CAP-CBP-CDP
2	H	1383	COA	C9P-CAP-CBP-CEP
2	H	1383	COA	O9P-C9P-CAP-OAP
2	H	1383	COA	N8P-C9P-CAP-OAP
2	I	1383	COA	C5B-O5B-P1A-O1A
2	I	1383	COA	OAP-CAP-CBP-CCP

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Mol	Chain	Res	Type	Atoms
2	I	1383	COA	OAP-CAP-CBP-CEP
2	I	1383	COA	CAP-C9P-N8P-C7P
2	I	1383	COA	O9P-C9P-N8P-C7P
2	I	1383	COA	S1P-C2P-C3P-N4P
2	J	1385	COA	C3B-C4B-C5B-O5B
2	J	1385	COA	O4B-C4B-C5B-O5B
2	J	1385	COA	C5B-O5B-P1A-O1A
2	J	1385	COA	C5B-O5B-P1A-O2A
2	J	1385	COA	C5B-O5B-P1A-O3A
2	J	1385	COA	S1P-C2P-C3P-N4P
2	K	1385	COA	C3B-O3B-P3B-O7A
2	K	1385	COA	C3B-C4B-C5B-O5B
2	K	1385	COA	O4B-C4B-C5B-O5B
2	K	1385	COA	C5B-O5B-P1A-O2A
2	K	1385	COA	C5B-O5B-P1A-O3A
2	K	1385	COA	C5P-C6P-C7P-N8P
2	K	1385	COA	C6P-C5P-N4P-C3P
2	K	1385	COA	O5P-C5P-N4P-C3P
2	L	1383	COA	C5B-O5B-P1A-O1A
2	L	1383	COA	CAP-C9P-N8P-C7P
2	L	1383	COA	C5P-C6P-C7P-N8P
2	L	1383	COA	C6P-C5P-N4P-C3P
2	L	1383	COA	O5P-C5P-N4P-C3P
4	I	1384	GOL	O1-C1-C2-C3
2	D	1383	COA	O5P-C5P-N4P-C3P
2	G	1383	COA	O5P-C5P-N4P-C3P
2	D	1383	COA	O9P-C9P-N8P-C7P
2	L	1383	COA	O9P-C9P-N8P-C7P
2	A	1383	COA	O9P-C9P-N8P-C7P
2	F	1383	COA	O5P-C5P-N4P-C3P
2	F	1383	COA	C6P-C5P-N4P-C3P
2	I	1383	COA	C6P-C5P-N4P-C3P
2	I	1383	COA	O5P-C5P-N4P-C3P
2	G	1383	COA	O9P-C9P-N8P-C7P
2	H	1383	COA	CEP-CBP-CCP-O6A
2	B	1383	COA	C6P-C5P-N4P-C3P
2	I	1383	COA	C3B-C4B-C5B-O5B
2	B	1383	COA	O5P-C5P-N4P-C3P
2	B	1383	COA	C5P-C6P-C7P-N8P
2	B	1383	COA	C3B-C4B-C5B-O5B
2	H	1383	COA	C3B-C4B-C5B-O5B
2	J	1385	COA	O5P-C5P-C6P-C7P

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Mol	Chain	Res	Type	Atoms
2	F	1383	COA	O9P-C9P-CAP-OAP
2	B	1383	COA	CDP-CBP-CCP-O6A
2	B	1383	COA	CEP-CBP-CCP-O6A
2	A	1383	COA	OAP-CAP-CBP-CDP
2	B	1383	COA	OAP-CAP-CBP-CDP
2	E	1383	COA	OAP-CAP-CBP-CDP
2	I	1383	COA	OAP-CAP-CBP-CDP
2	H	1383	COA	O9P-C9P-CAP-CBP
2	H	1383	COA	N8P-C9P-CAP-CBP
4	I	1384	GOL	O1-C1-C2-O2
2	B	1383	COA	O4B-C4B-C5B-O5B
2	I	1383	COA	O4B-C4B-C5B-O5B
2	C	1383	COA	C3B-O3B-P3B-O7A
2	G	1383	COA	C3B-O3B-P3B-O7A
2	H	1383	COA	CDP-CBP-CCP-O6A
2	F	1383	COA	C9P-CAP-CBP-CDP
2	K	1385	COA	O9P-C9P-N8P-C7P
2	B	1383	COA	C3B-O3B-P3B-O8A
2	C	1383	COA	C3B-O3B-P3B-O8A
2	G	1383	COA	C3B-O3B-P3B-O8A
2	I	1383	COA	C3B-O3B-P3B-O8A
2	I	1383	COA	C5B-O5B-P1A-O3A
2	J	1385	COA	C3B-O3B-P3B-O9A
2	J	1385	COA	CCP-O6A-P2A-O3A
2	L	1383	COA	P1A-O3A-P2A-O4A
2	K	1385	COA	CAP-C9P-N8P-C7P
2	G	1383	COA	CCP-O6A-P2A-O4A
2	H	1383	COA	C5B-O5B-P1A-O2A
2	H	1383	COA	CCP-O6A-P2A-O5A
2	K	1385	COA	C5B-O5B-P1A-O1A
2	C	1383	COA	O9P-C9P-N8P-C7P
2	J	1385	COA	O9P-C9P-CAP-OAP
2	F	1383	COA	C3B-C4B-C5B-O5B
2	F	1383	COA	O4B-C4B-C5B-O5B
2	H	1383	COA	O4B-C4B-C5B-O5B
2	J	1385	COA	N4P-C5P-C6P-C7P
2	C	1383	COA	CAP-C9P-N8P-C7P
2	C	1383	COA	C5P-C6P-C7P-N8P
2	I	1383	COA	C5P-C6P-C7P-N8P
2	J	1385	COA	C5P-C6P-C7P-N8P
2	I	1383	COA	CDP-CBP-CCP-O6A
2	K	1385	COA	CDP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	K	1385	COA	CEP-CBP-CCP-O6A
2	F	1383	COA	N8P-C9P-CAP-OAP
2	F	1383	COA	C2P-C3P-N4P-C5P
2	L	1383	COA	C2P-C3P-N4P-C5P
2	B	1383	COA	C9P-CAP-CBP-CEP
2	E	1383	COA	C9P-CAP-CBP-CDP
2	F	1383	COA	C3B-O3B-P3B-O8A
2	H	1383	COA	OAP-CAP-CBP-CDP
2	H	1383	COA	OAP-CAP-CBP-CEP
2	K	1385	COA	C3B-O3B-P3B-O9A
2	G	1383	COA	CBP-CCP-O6A-P2A
2	H	1383	COA	CBP-CCP-O6A-P2A
2	A	1383	COA	C5B-O5B-P1A-O1A
2	C	1383	COA	C5B-O5B-P1A-O1A
2	H	1383	COA	C5B-O5B-P1A-O1A
2	J	1385	COA	CCP-O6A-P2A-O4A
4	B	1384	GOL	O1-C1-C2-O2
2	C	1383	COA	O5P-C5P-C6P-C7P
2	B	1383	COA	C9P-CAP-CBP-CCP

There are no ring outliers.

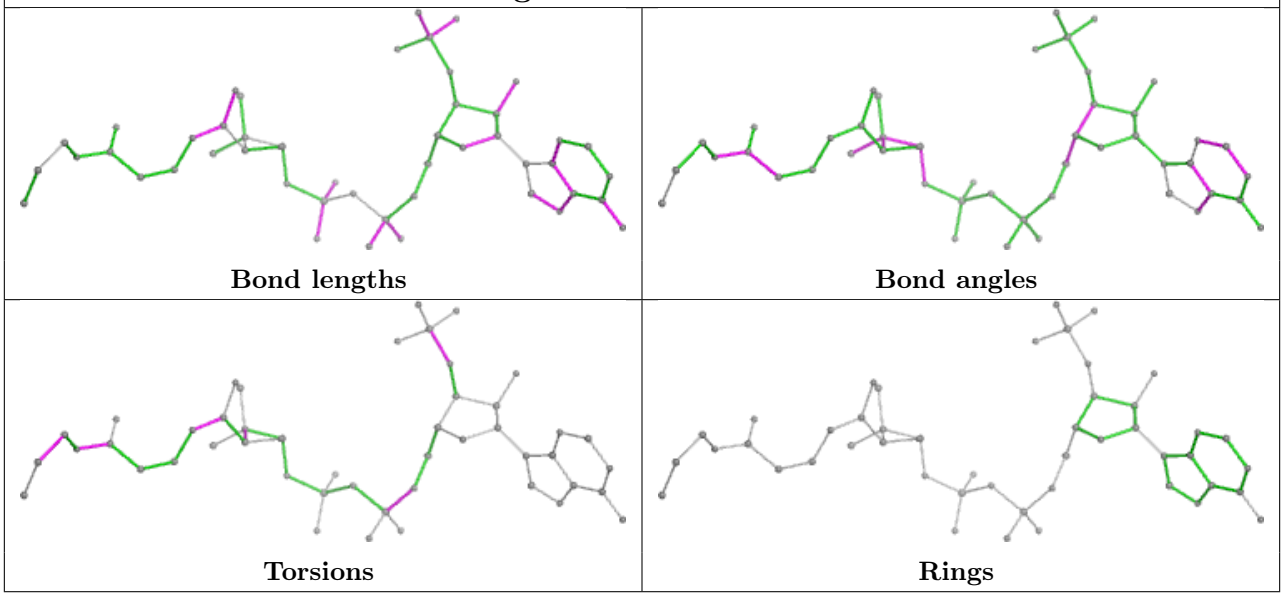
15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1383	COA	2	0
3	G	1384	ACT	1	0
2	B	1383	COA	2	0
2	K	1385	COA	4	0
2	I	1383	COA	1	0
3	B	1385	ACT	1	0
2	H	1383	COA	6	0
2	F	1383	COA	3	0
2	L	1383	COA	1	0
3	H	1384	ACT	3	0
2	G	1383	COA	5	0
3	K	1386	ACT	2	0
3	L	1384	ACT	1	0
2	E	1383	COA	1	0
2	J	1385	COA	3	0

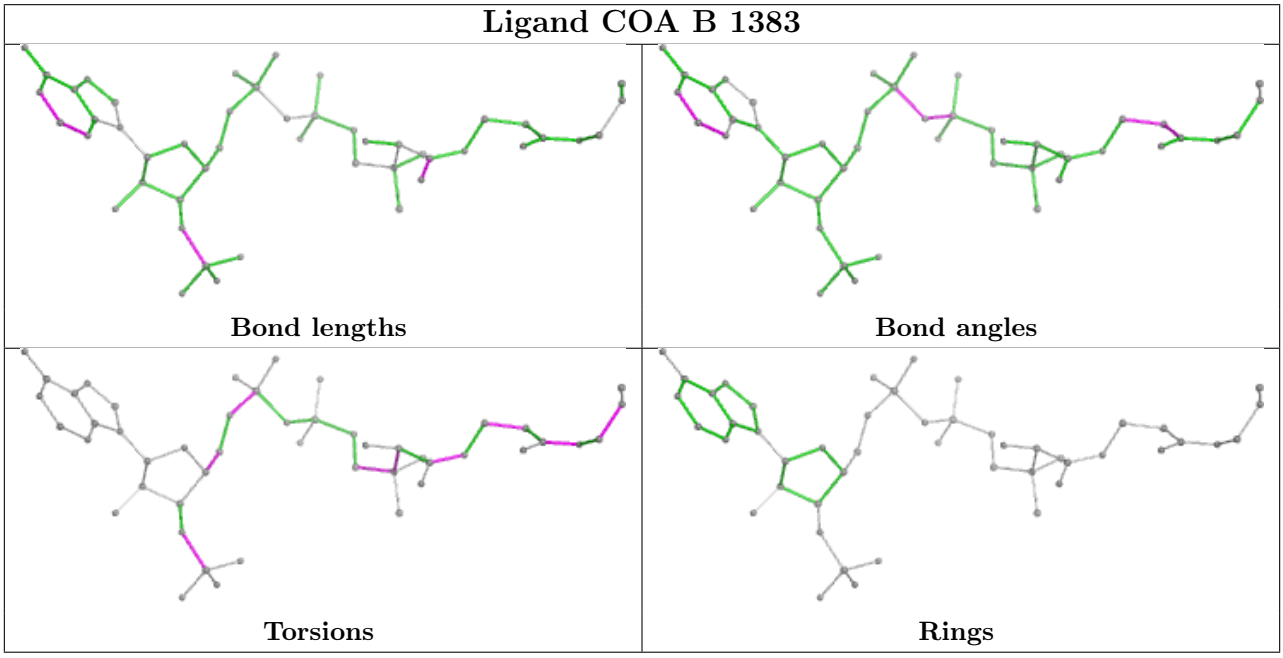
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

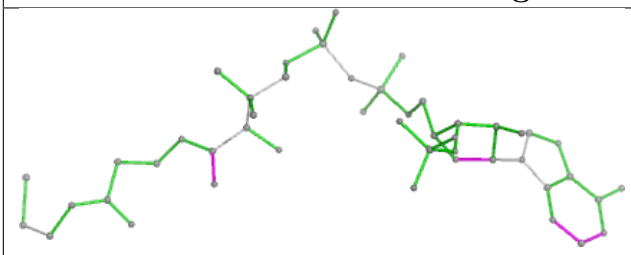
Ligand COA A 1383



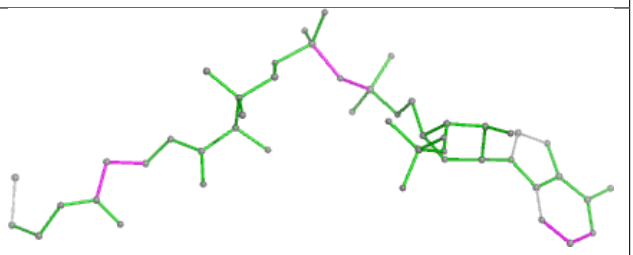
Ligand COA B 1383



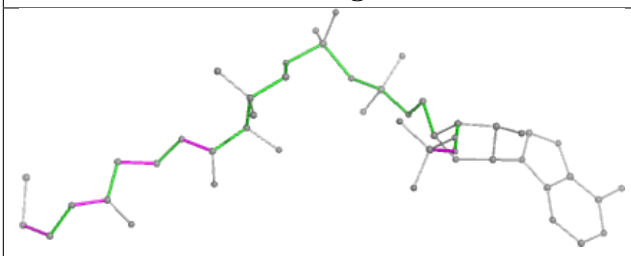
Ligand COA D 1383



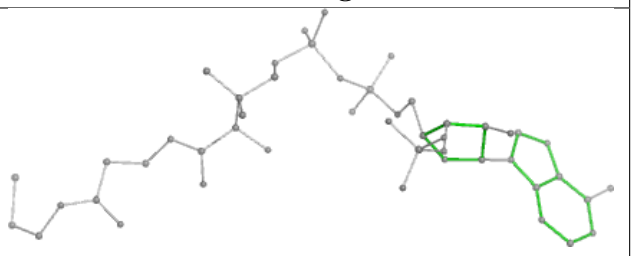
Bond lengths



Bond angles

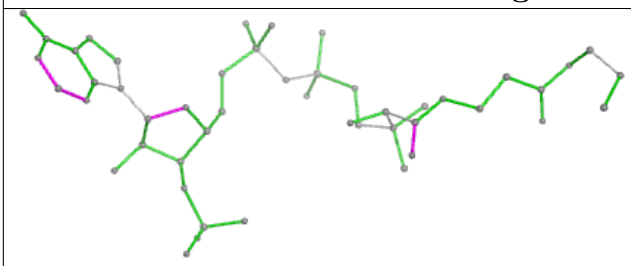


Torsions

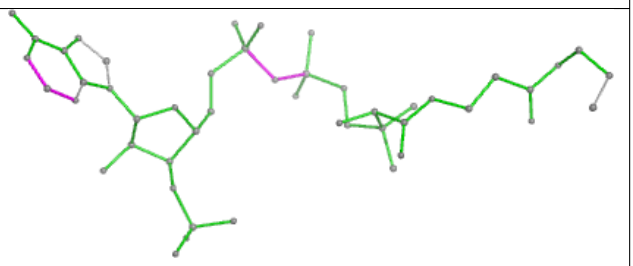


Rings

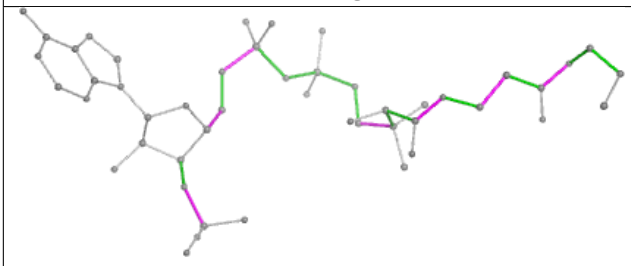
Ligand COA K 1385



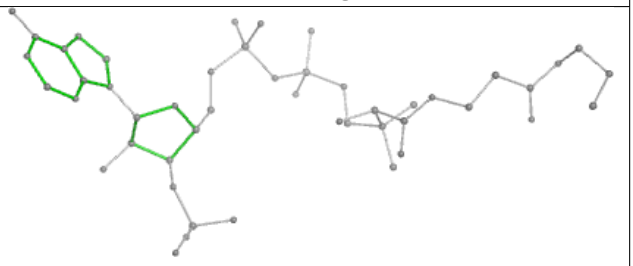
Bond lengths



Bond angles

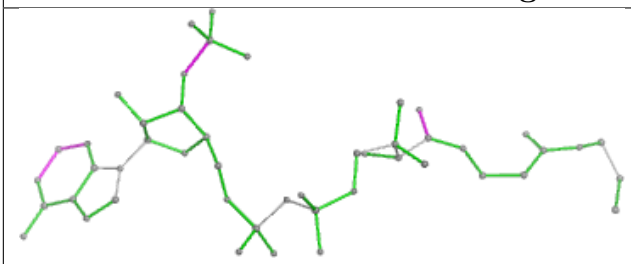


Torsions

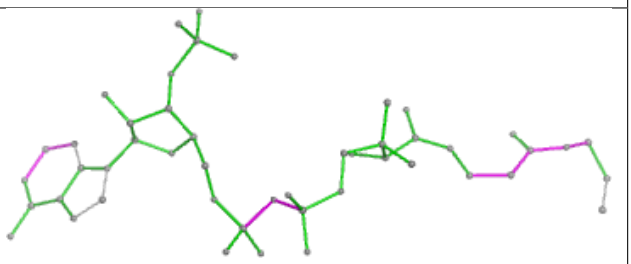


Rings

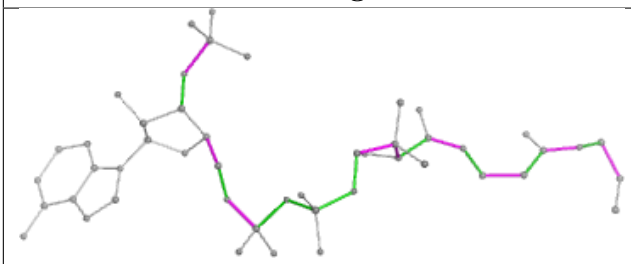
Ligand COA I 1383



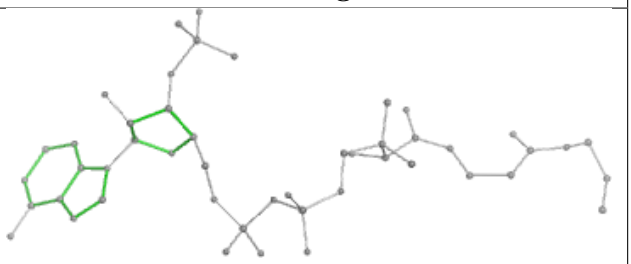
Bond lengths



Bond angles

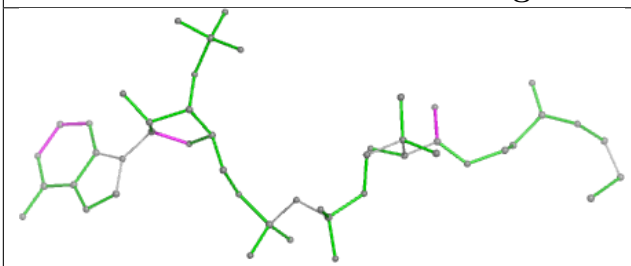


Torsions

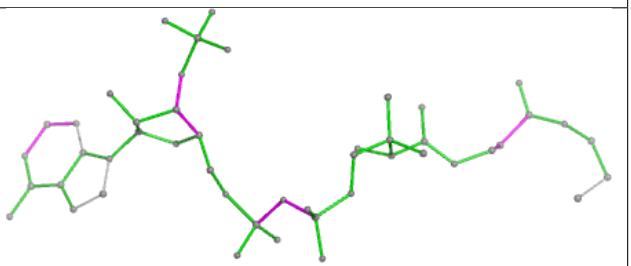


Rings

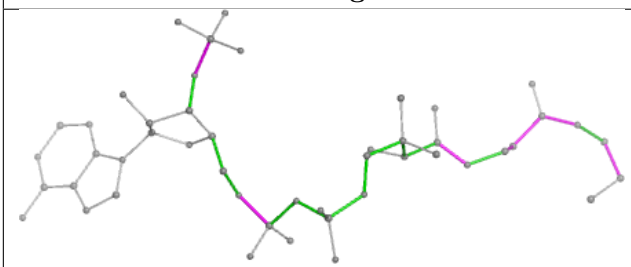
Ligand COA C 1383



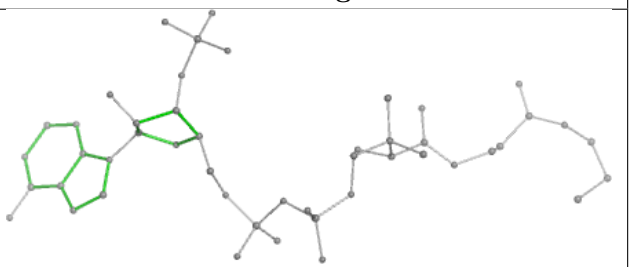
Bond lengths



Bond angles

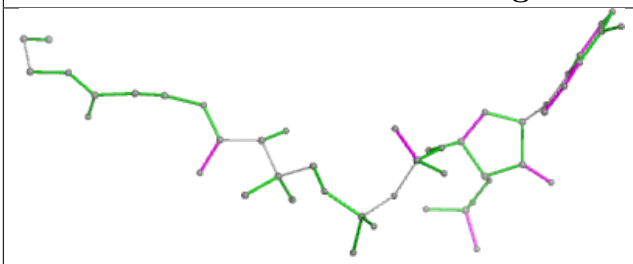


Torsions

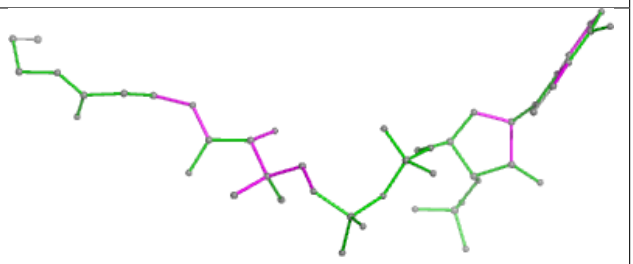


Rings

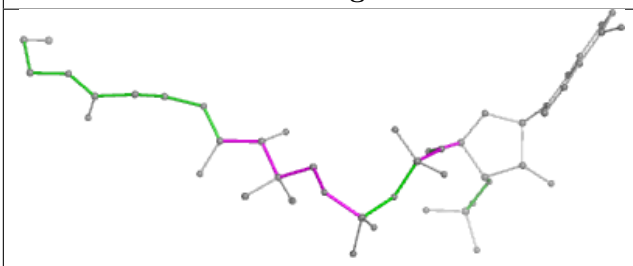
Ligand COA H 1383



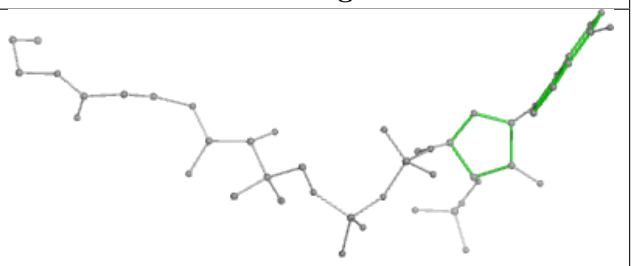
Bond lengths



Bond angles

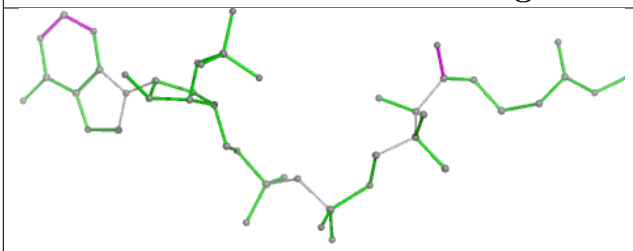


Torsions

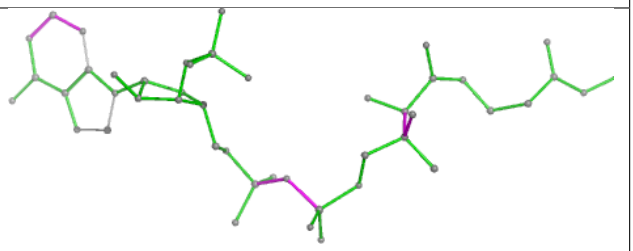


Rings

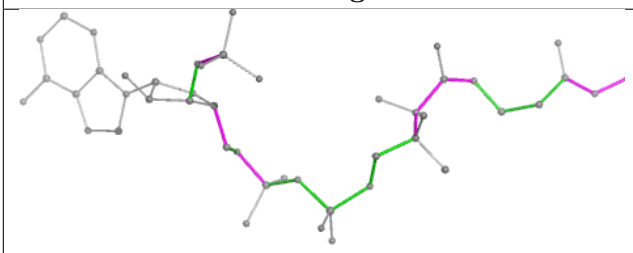
Ligand COA F 1383



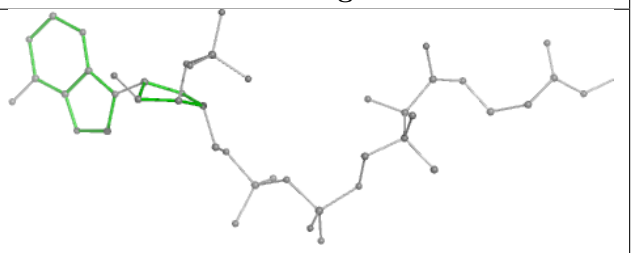
Bond lengths



Bond angles

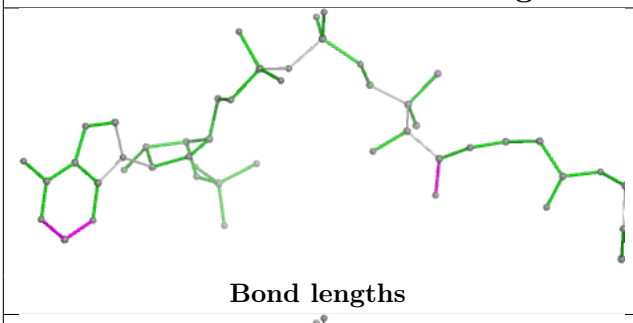


Torsions



Rings

Ligand COA L 1383



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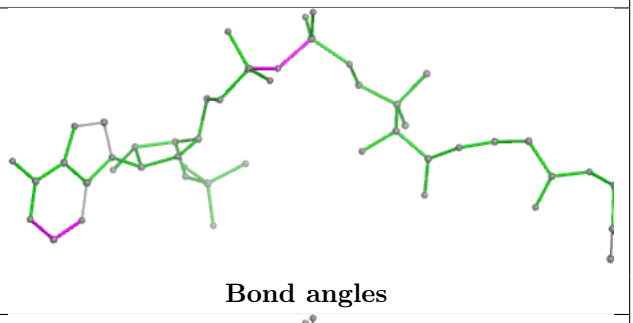
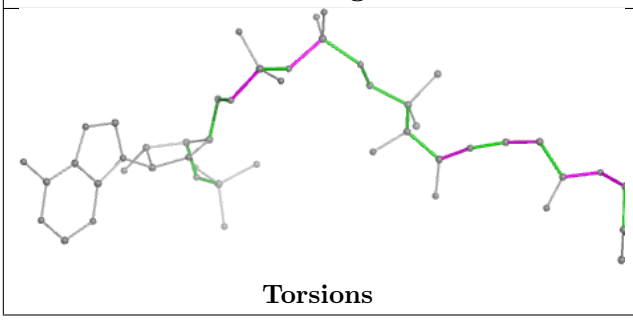
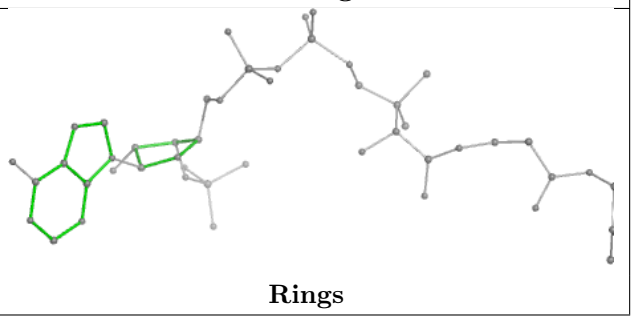


Bond angles

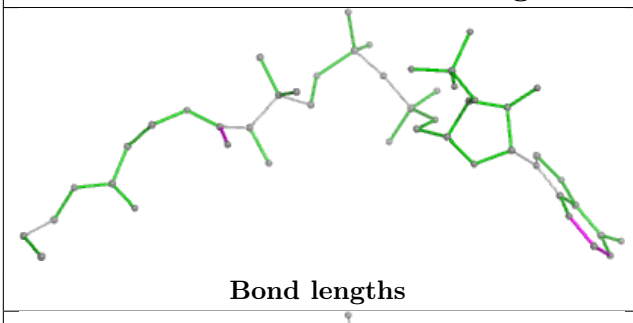


Torsions

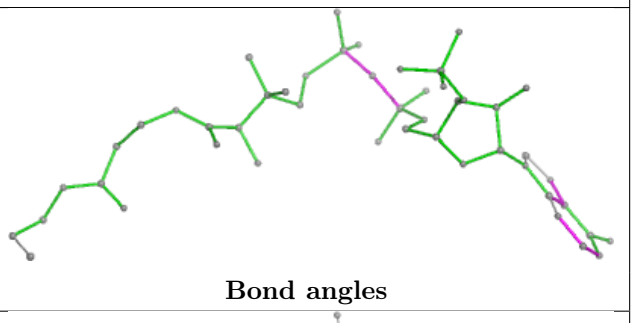


Rings

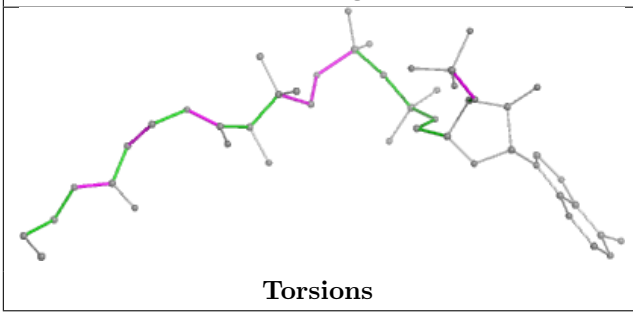
Ligand COA G 1383



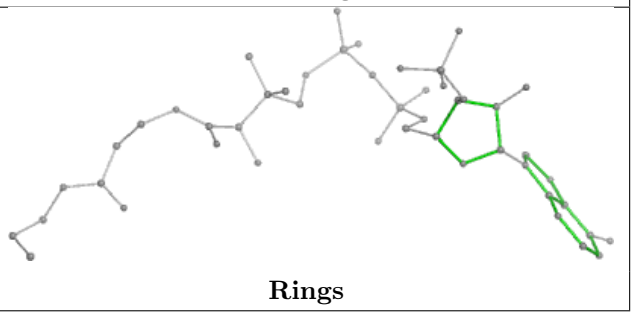
Bond lengths



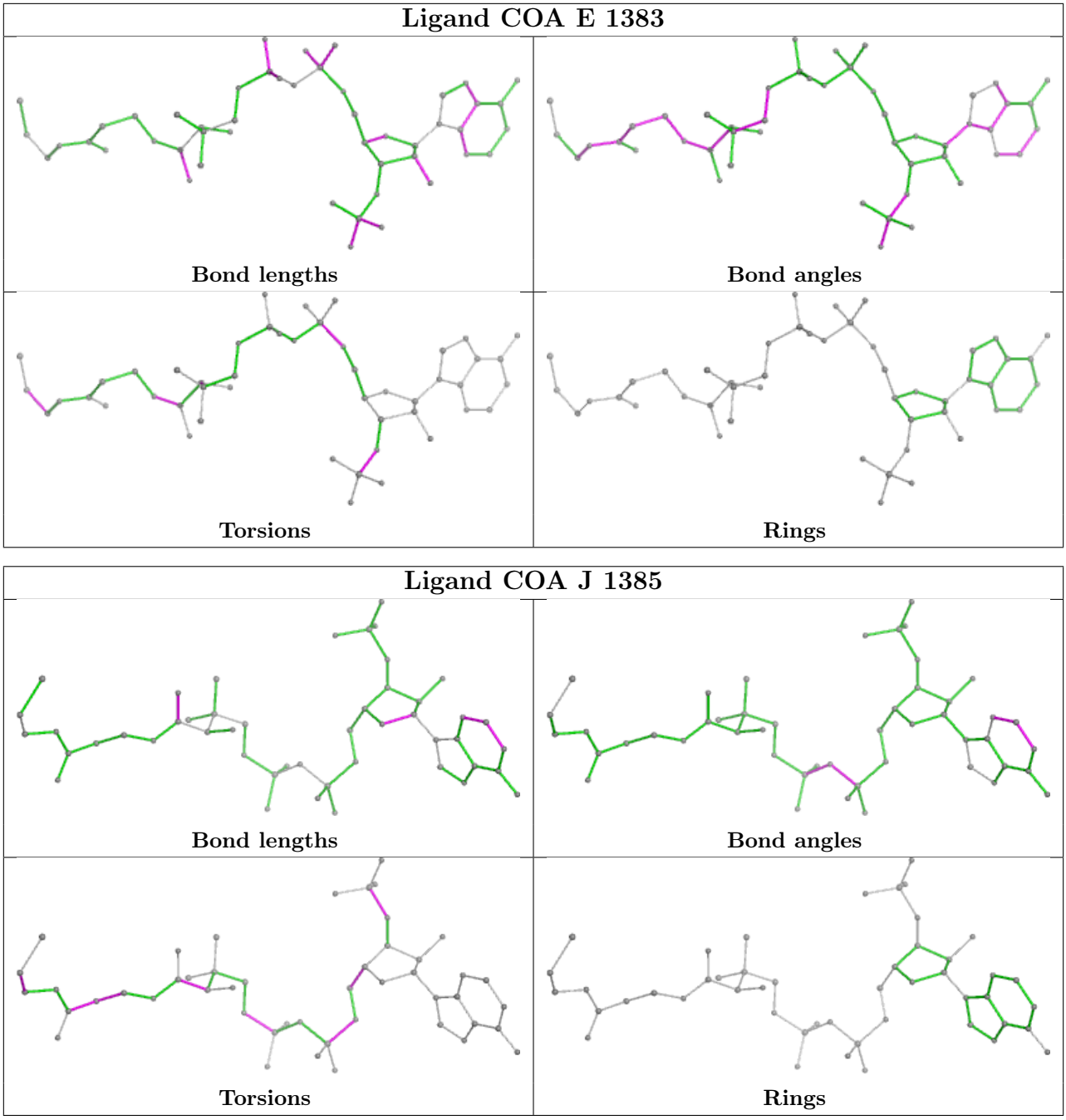
Bond angles



Torsions



Rings



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

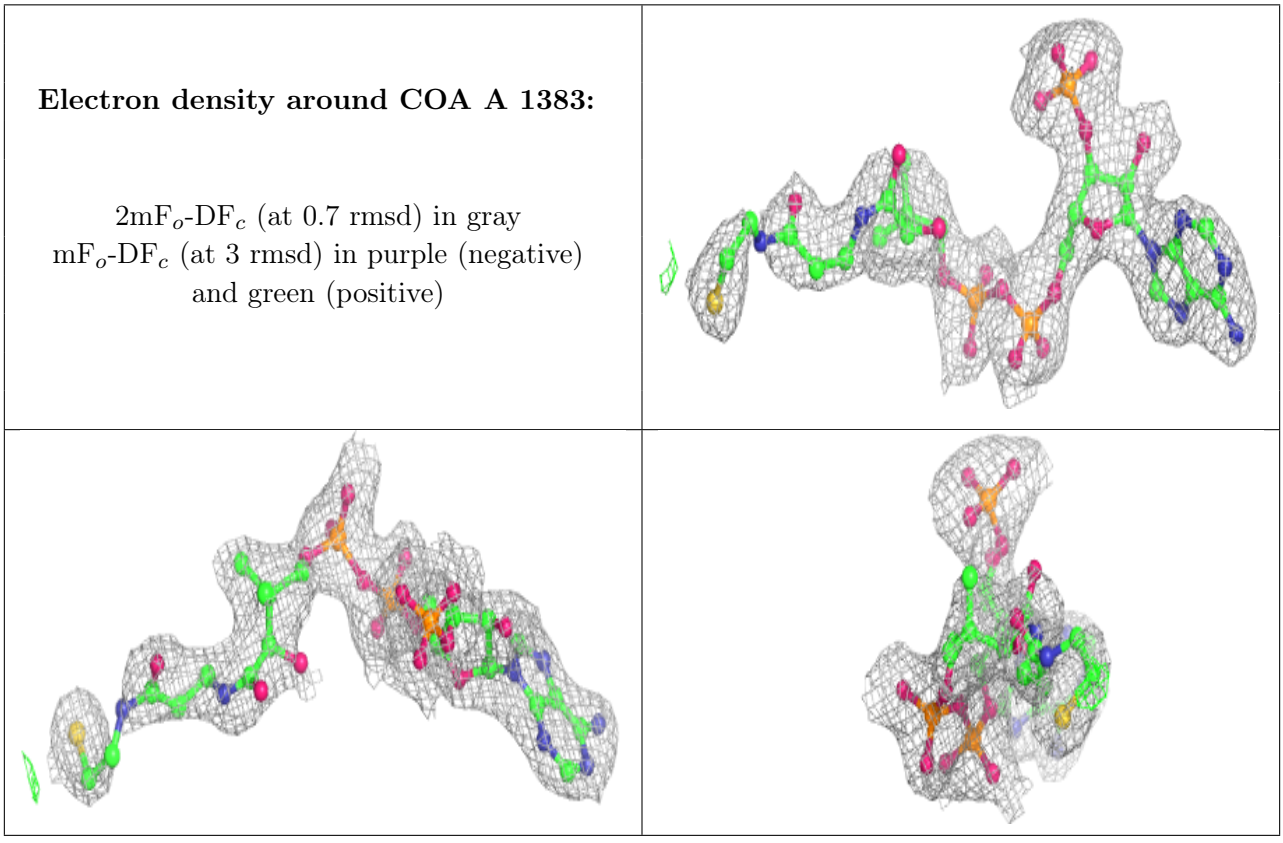
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

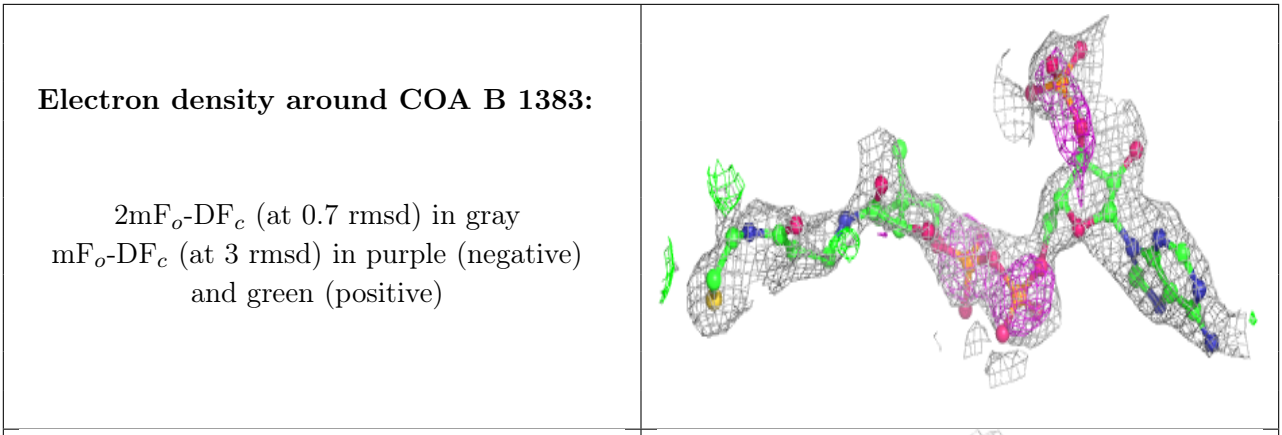
Electron density around COA A 1383:

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



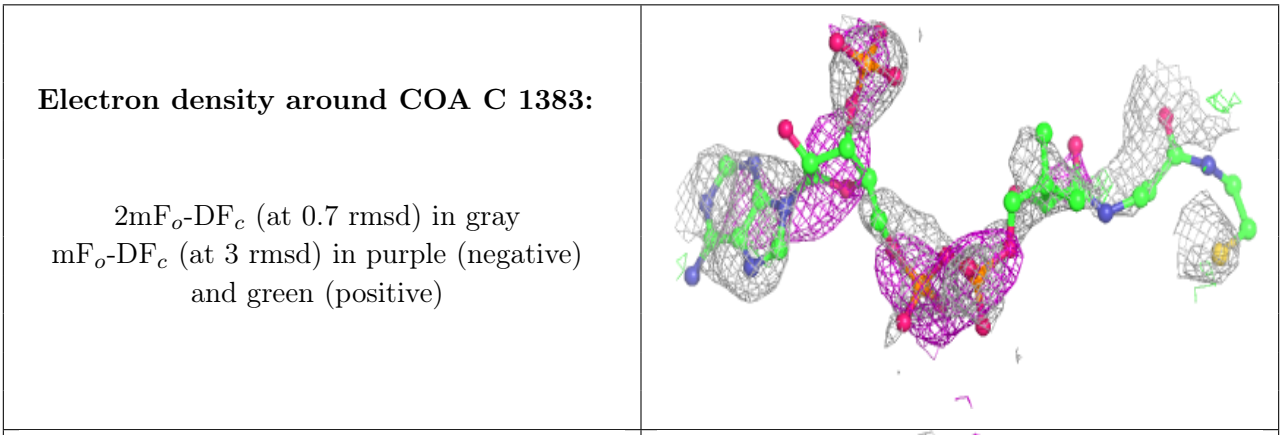
Electron density around COA B 1383:

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



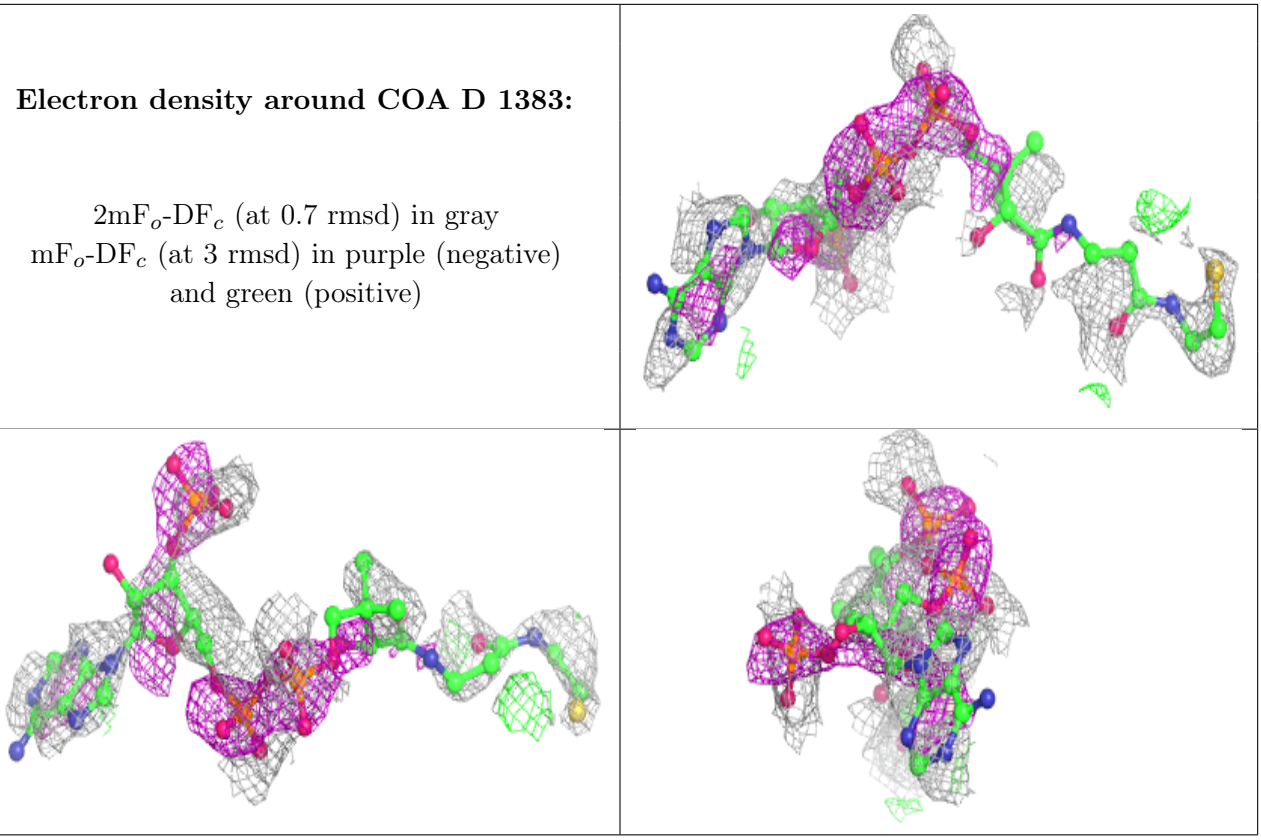
Electron density around COA C 1383:

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



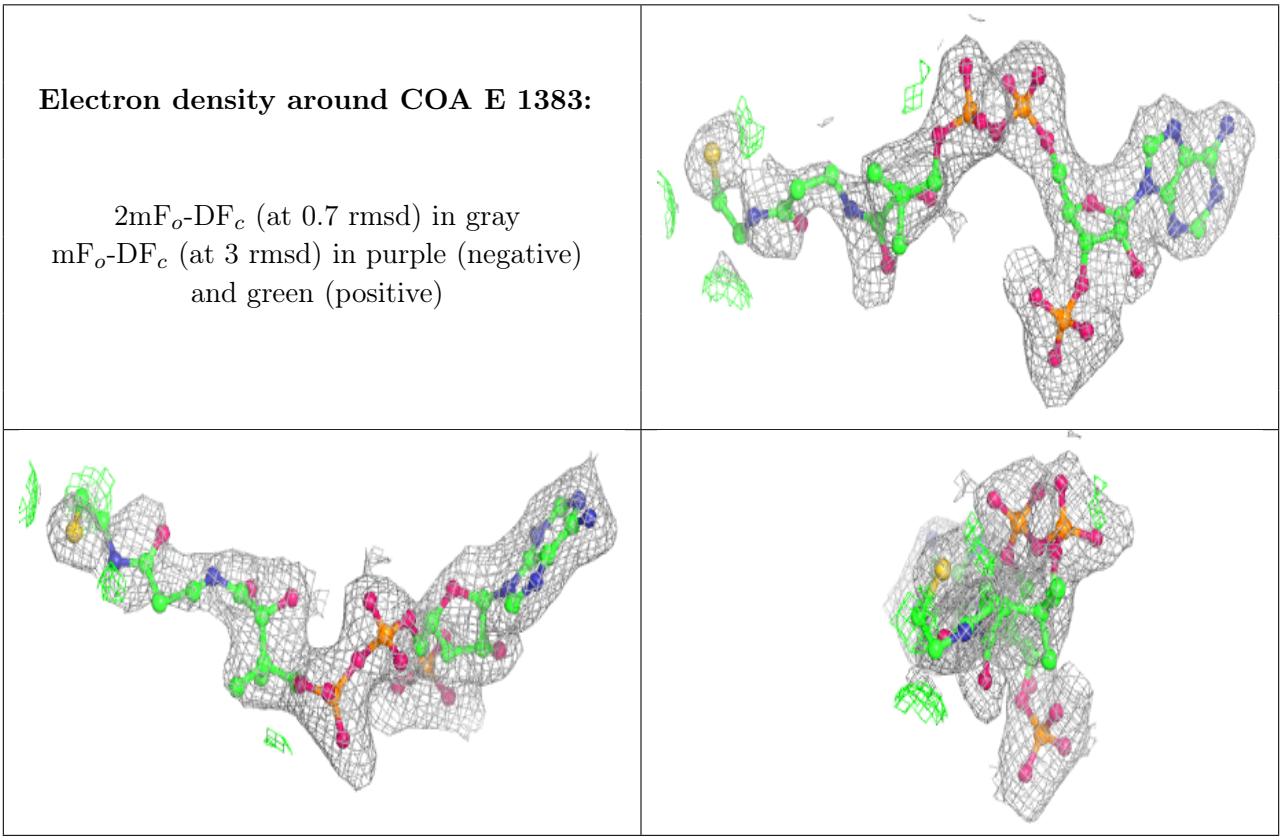
Electron density around COA D 1383:

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



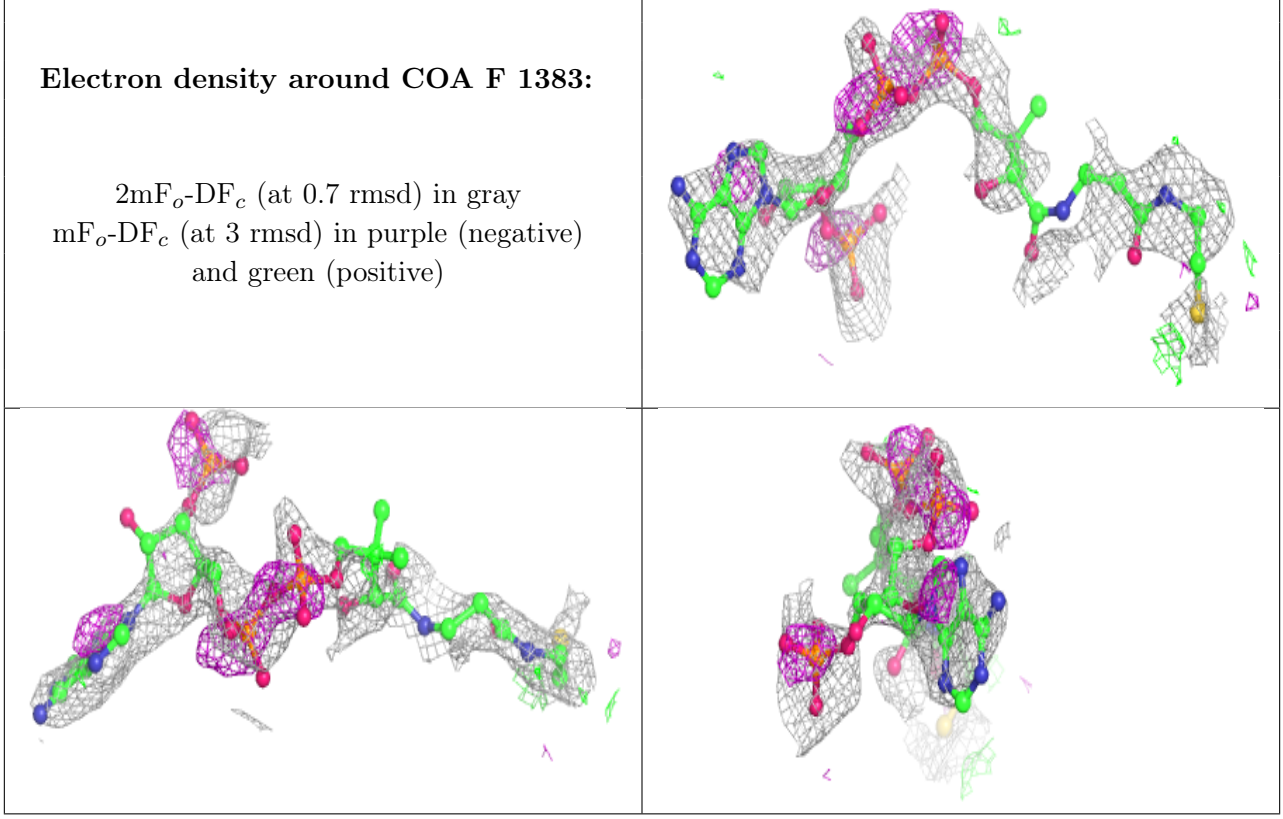
Electron density around COA E 1383:

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



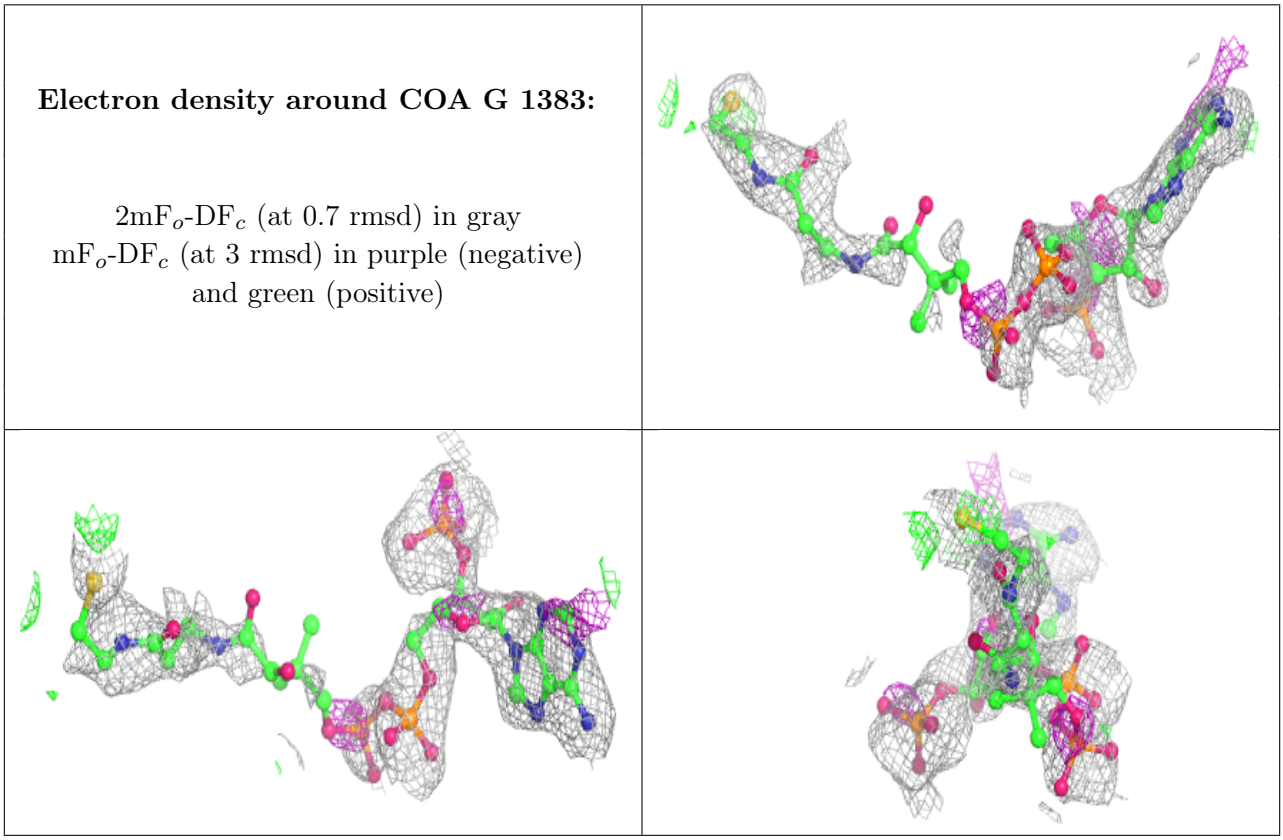
Electron density around COA F 1383:

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



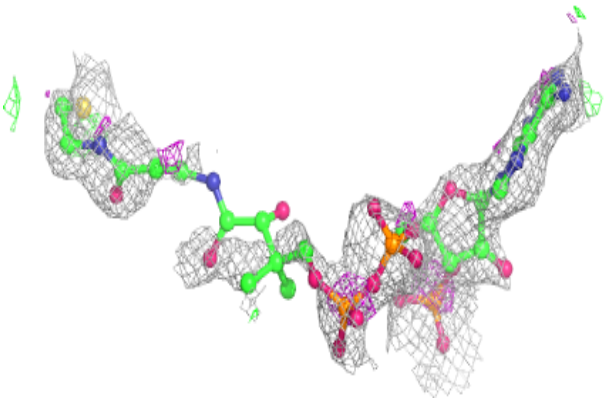
Electron density around COA G 1383:

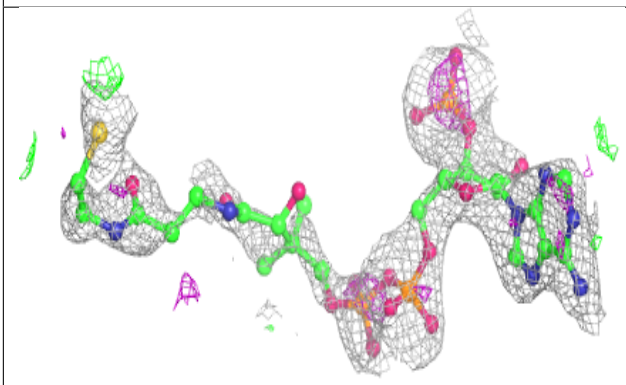
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA H 1383:

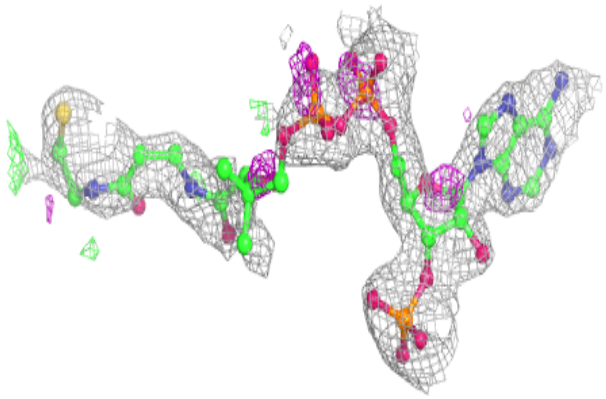
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

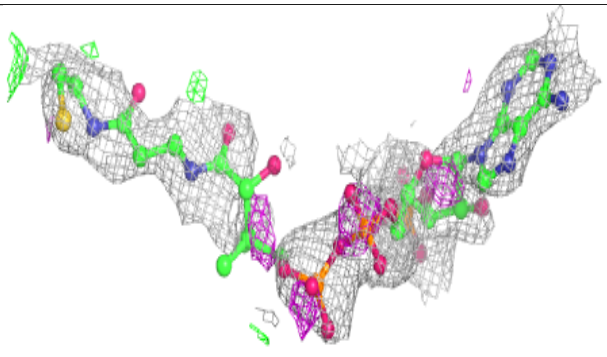


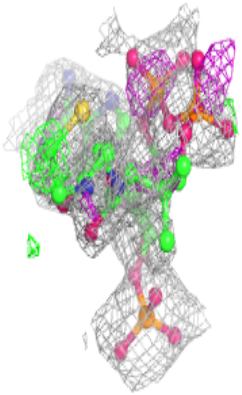


Electron density around COA I 1383:

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

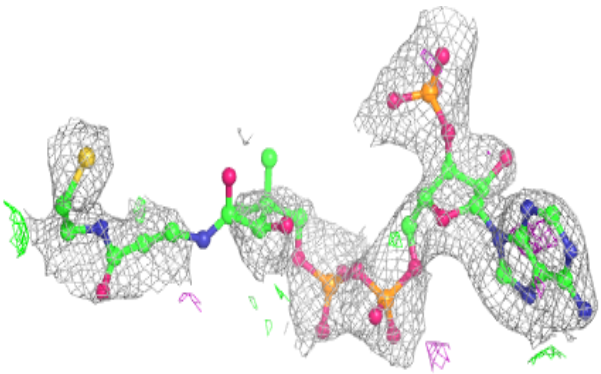


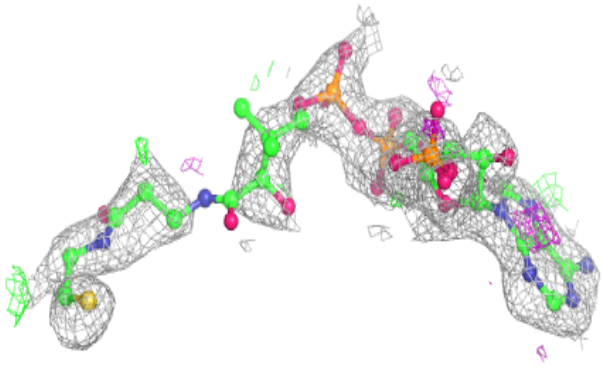


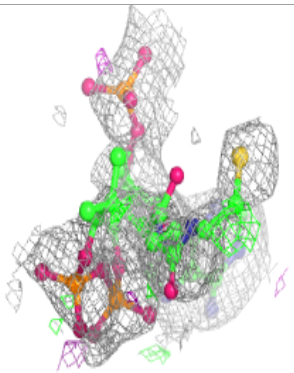


Electron density around COA J 1385:

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

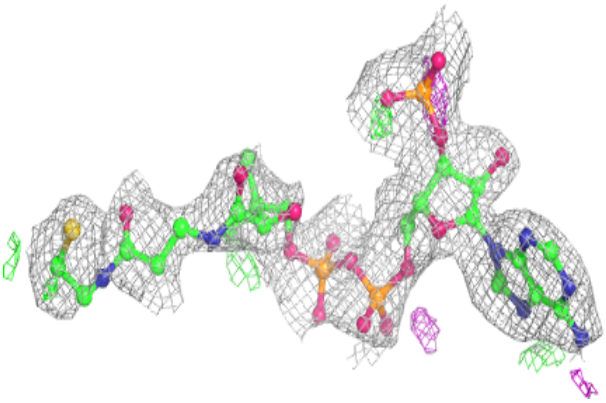


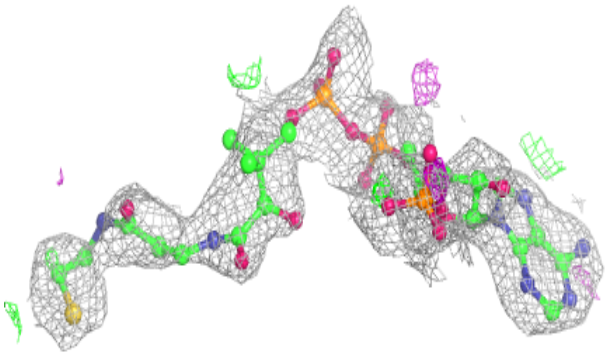


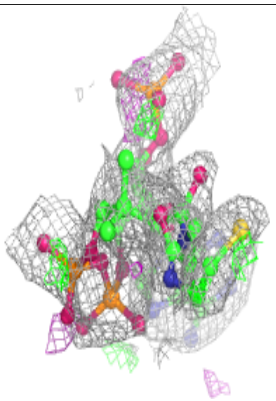


Electron density around COA K 1385:

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

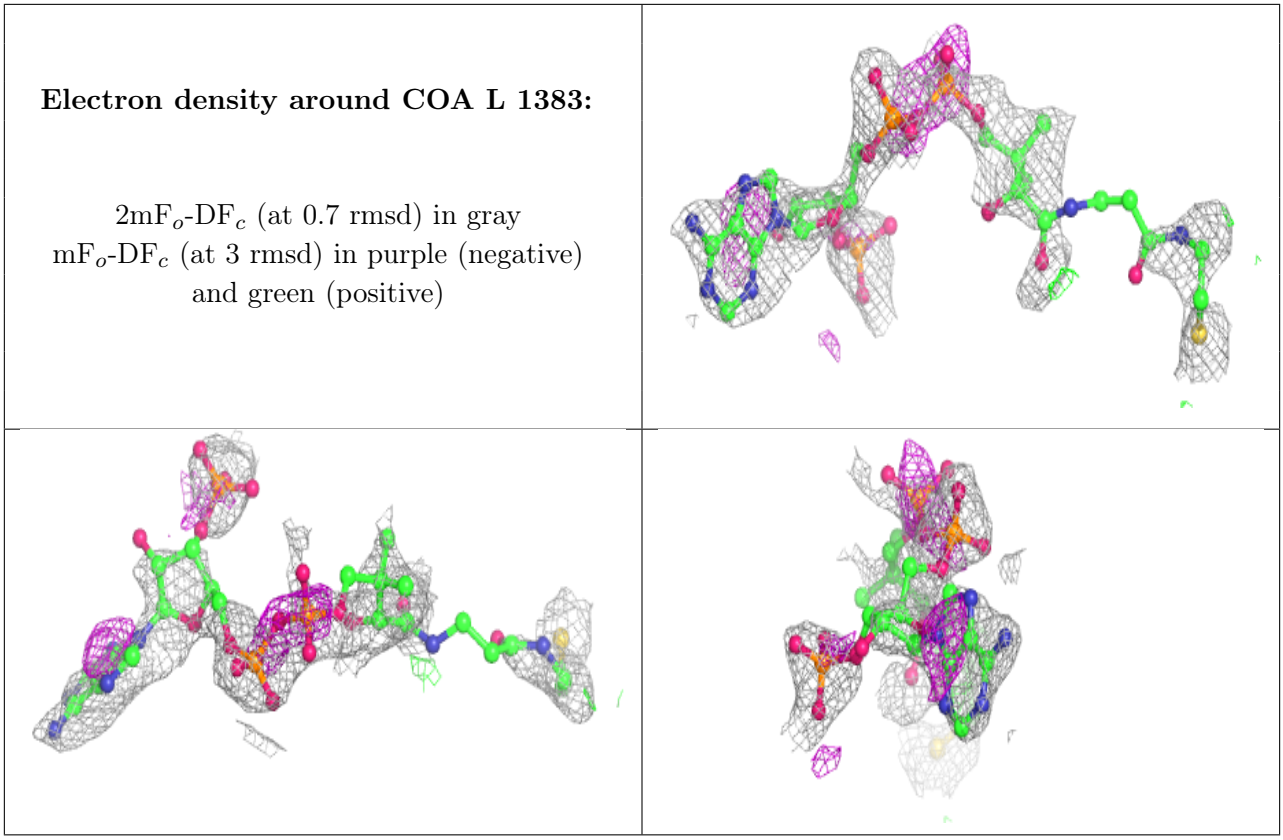






Electron density around COA L 1383:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.