Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:53 pm BST

PDB ID	:	3QMN
Title	:	Crystal Structure of 4'-Phosphopantetheinyl Transferase AcpS from Vibrio cholerae O1 biovar eltor
Authors	:	Kim, Y.; Halavaty, A.S.; Zhou, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-02-04
Resolution	:	1.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

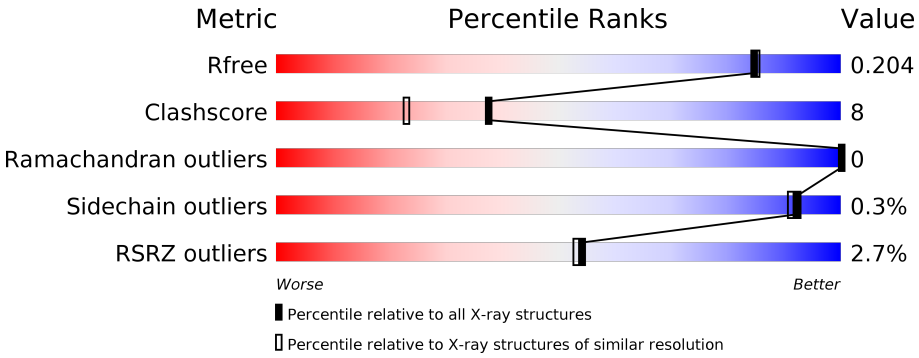
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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% 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	129	5% 88% 10%
1	B	129	6% 90% 8%
1	C	129	2% 84% 13%
1	D	129	2% 83% 15%
1	E	129	5% 87% 12%
1	F	129	3% 82% 16%

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Mol	Chain	Length	Quality of chain
1	G	129	2% 84% 14%
1	H	129	3% 81% 16%
1	I	129	% 84% 13%
1	J	129	% 88% 9%
1	K	129	2% 84% 14%
1	L	129	2% 88% 10%
1	M	129	5% 81% 16%
1	N	129	2% 84% 14%
1	O	129	2% 89% 9%
1	P	129	2% 88% 10%
1	Q	129	% 87% 11%
1	R	129	5% 88% 9%
1	S	129	2% 81% 16%
1	T	129	3% 91% 6%
1	U	129	3% 85% 12%
1	V	129	3% 88% 10%
1	W	129	% 83% 14%
1	X	129	2% 89% 9%

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
5	MPD	M	2572	-	-	X	-
6	ACT	A	2597	-	-	X	-
6	ACT	C	2598	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28565 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 Holo-[acyl-carrier-protein] synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	Se	0	7	0
			1035	644	193	196	2			
1	B	126	Total	C	N	O	Se	0	4	0
			1006	628	186	190	2			
1	C	126	Total	C	N	O	Se	0	7	0
			1033	643	191	197	2			
1	D	126	Total	C	N	O	Se	0	9	0
			1056	657	199	198	2			
1	E	127	Total	C	N	O	Se	0	5	0
			1029	642	191	194	2			
1	F	126	Total	C	N	O	Se	0	6	0
			1022	638	187	195	2			
1	G	126	Total	C	N	O	Se	0	3	0
			995	622	181	190	2			
1	H	126	Total	C	N	O	Se	0	8	0
			1043	651	192	198	2			
1	I	126	Total	C	N	O	Se	0	5	0
			1018	635	187	194	2			
1	J	126	Total	C	N	O	Se	0	3	0
			999	626	185	186	2			
1	K	126	Total	C	N	O	Se	0	6	0
			1020	638	189	191	2			
1	L	126	Total	C	N	O	Se	0	6	0
			1022	637	187	196	2			
1	M	126	Total	C	N	O	Se	0	6	0
			1022	638	188	194	2			
1	N	126	Total	C	N	O	Se	0	6	0
			1024	641	189	192	2			
1	O	127	Total	C	N	O	Se	0	5	0
			1023	637	191	193	2			
1	P	126	Total	C	N	O	Se	0	6	0
			1025	642	189	192	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	126	Total	C	N	O	Se	0	4	0
			1011	631	189	189	2			
1	R	126	Total	C	N	O	Se	0	6	0
			1024	638	190	194	2			
1	S	125	Total	C	N	O	Se	0	11	0
			1062	660	197	203	2			
1	T	126	Total	C	N	O	Se	0	6	0
			1023	638	187	196	2			
1	U	126	Total	C	N	O	Se	0	8	0
			1045	650	191	202	2			
1	V	126	Total	C	N	O	Se	0	4	0
			1009	630	186	191	2			
1	W	125	Total	C	N	O	Se	0	4	0
			1000	625	180	193	2			
1	X	126	Total	C	N	O	Se	0	5	0
			1022	636	191	193	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
A	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
B	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
B	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
C	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
C	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
D	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
D	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
E	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
E	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
E	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
F	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
F	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
F	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
G	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
G	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
G	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
H	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
H	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
I	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
I	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
I	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
J	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
J	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
J	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
K	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
K	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
K	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
L	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
L	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
L	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
M	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
M	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
M	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
N	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
N	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
N	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
O	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
O	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
O	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
P	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
P	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
P	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
Q	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
Q	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
Q	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
R	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
R	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
R	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
S	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
S	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
S	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
T	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
T	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
T	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
U	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
U	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
U	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
V	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
V	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6

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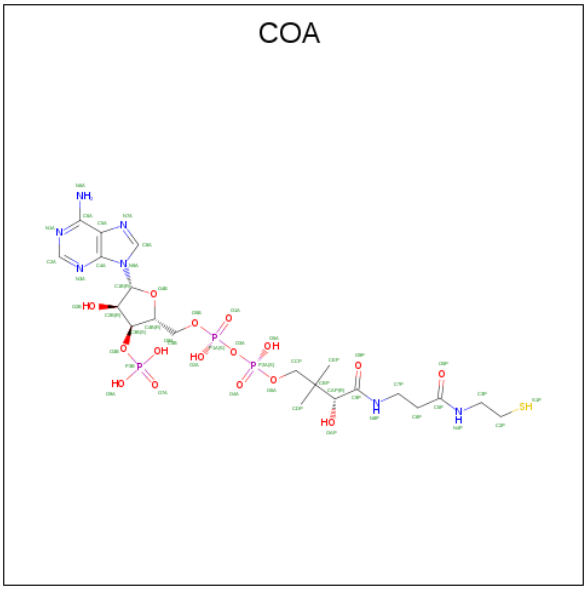
Chain	Residue	Modelled	Actual	Comment	Reference
V	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
W	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
W	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
W	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6
X	-2	SER	-	EXPRESSION TAG	UNP Q9KPB6
X	-1	ASN	-	EXPRESSION TAG	UNP Q9KPB6
X	0	ALA	-	EXPRESSION TAG	UNP Q9KPB6

- 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	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	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		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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		
2	N	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	N	1	Total	C	N	O	P	S	0	1
			48	21	7	16	3	1		
2	O	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	P	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	Q	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	R	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	S	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	T	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	U	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	W	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	W	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	X	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	T	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	2	Total Ca 2 2	0	0
4	K	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	W	2	Total Ca 2 2	0	0
4	N	1	Total Ca 1 1	0	0
4	X	2	Total Ca 2 2	0	0
4	S	2	Total Ca 2 2	0	0
4	J	2	Total Ca 2 2	0	0
4	E	2	Total Ca 2 2	0	0
4	V	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	R	2	Total Ca 2 2	0	0
4	M	2	Total Ca 2 2	0	0

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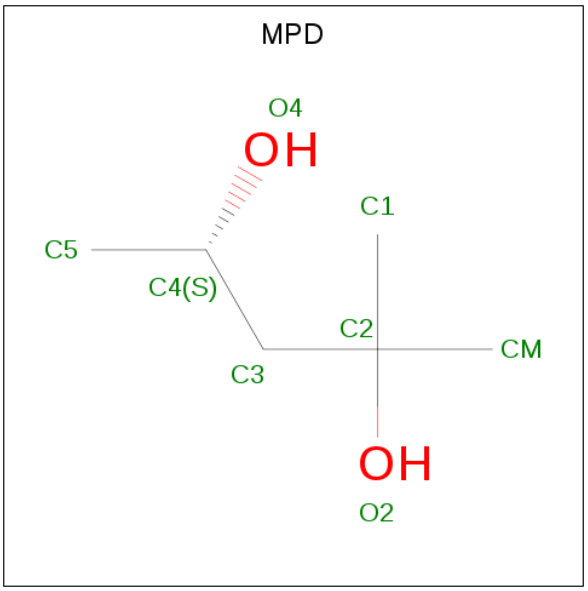
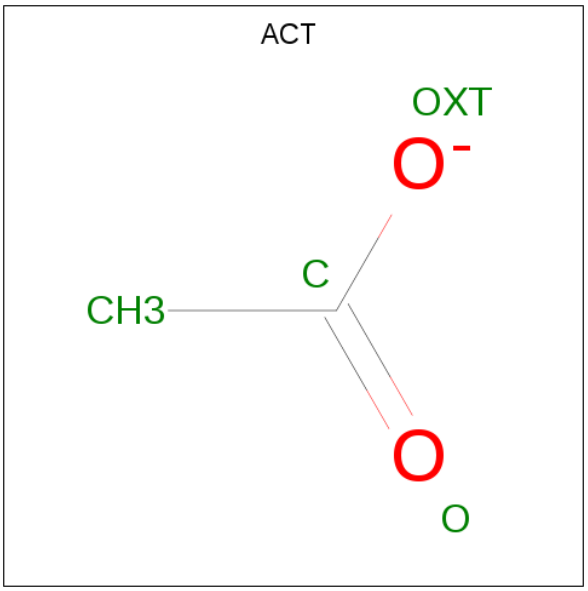
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Ca 2 2	0	0
4	I	2	Total Ca 2 2	0	0
4	U	2	Total Ca 2 2	0	0
4	L	2	Total Ca 2 2	0	0
4	G	2	Total Ca 2 2	0	0
4	Q	2	Total Ca 2 2	0	0
4	H	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	T	2	Total Ca 2 2	0	0
4	O	1	Total Ca 1 1	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



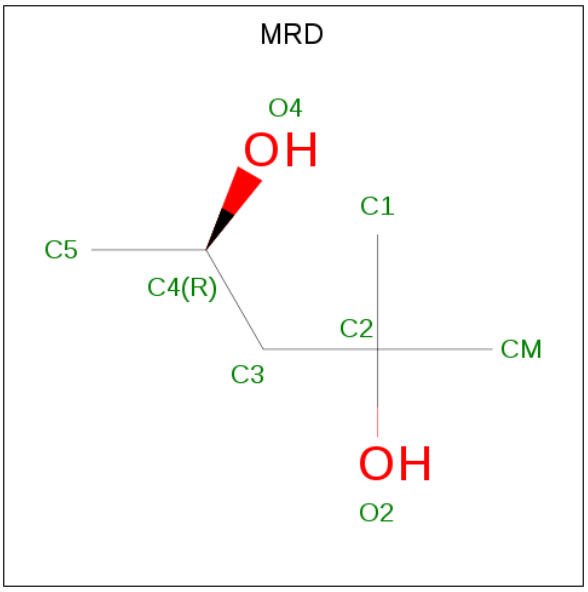
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	H	1	Total C O 8 6 2	0	0
5	I	1	Total C O 8 6 2	0	0
5	M	1	Total C O 8 6 2	0	0
5	O	1	Total C O 8 6 2	0	0
5	P	1	Total C O 8 6 2	0	0
5	Q	1	Total C O 8 6 2	0	0
5	R	1	Total C O 8 6 2	0	0
5	S	1	Total C O 8 6 2	0	0
5	U	1	Total C O 8 6 2	0	0
5	V	1	Total C O 8 6 2	0	0
5	W	1	Total C O 8 6 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



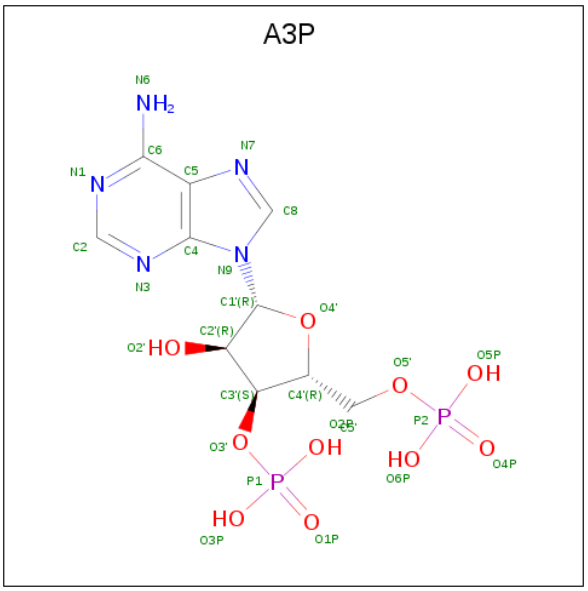
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	R	1	Total C O 4 2 2	0	0
6	T	1	Total C O 4 2 2	0	0
6	W	1	Total C O 4 2 2	0	0

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	6	2		
7	F	1	Total	C	O	0	0
			8	6	2		
7	K	1	Total	C	O	0	0
			8	6	2		
7	L	1	Total	C	O	0	0
			8	6	2		
7	N	1	Total	C	O	0	0
			8	6	2		
7	T	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	O	1	Total	C	N	O	P	0	1
			27	10	5	10	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	115	Total	O	0	8
			119	119		
9	B	80	Total	O	0	2
			81	81		
9	C	123	Total	O	0	7
			126	126		
9	D	121	Total	O	0	5
			124	124		
9	E	97	Total	O	0	5
			100	100		
9	F	104	Total	O	0	6
			107	107		
9	G	78	Total	O	0	5
			81	81		
9	H	84	Total	O	0	5
			87	87		
9	I	102	Total	O	0	3
			105	105		
9	J	130	Total	O	0	11
			137	137		
9	K	113	Total	O	0	7
			116	116		

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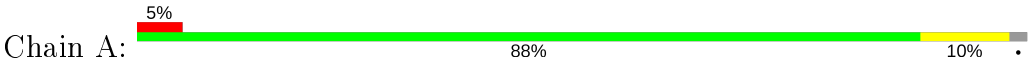
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	134	Total O 137 137	0	4
9	M	103	Total O 105 105	0	4
9	N	127	Total O 132 132	0	11
9	O	101	Total O 105 105	0	6
9	P	106	Total O 110 110	0	6
9	Q	103	Total O 104 104	0	3
9	R	99	Total O 100 100	0	1
9	S	110	Total O 114 114	0	12
9	T	81	Total O 81 81	0	2
9	U	108	Total O 113 113	0	5
9	V	85	Total O 85 85	0	0
9	W	99	Total O 100 100	0	1
9	X	84	Total O 86 86	0	4

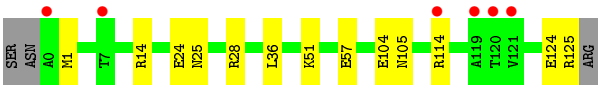
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Holo-[acyl-carrier-protein] synthase

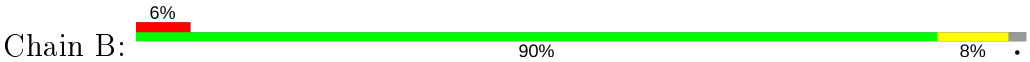
Chain A:

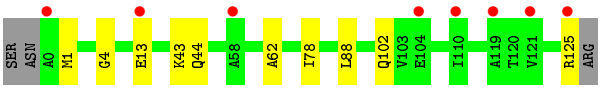




• Molecule 1: Holo-[acyl-carrier-protein] synthase

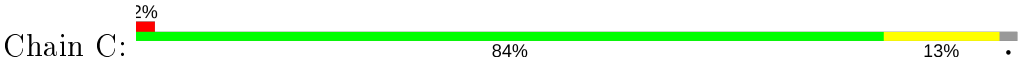
Chain B:

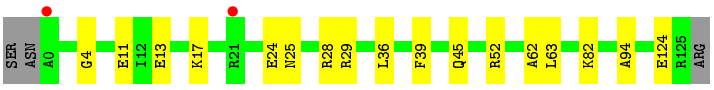




• Molecule 1: Holo-[acyl-carrier-protein] synthase

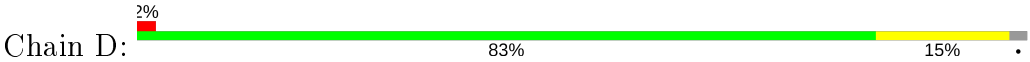
Chain C:

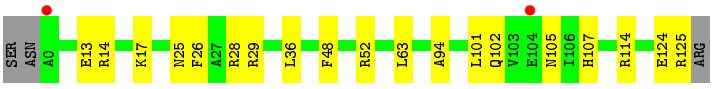




• Molecule 1: Holo-[acyl-carrier-protein] synthase

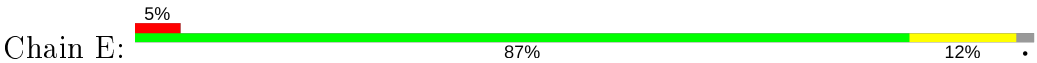
Chain D:

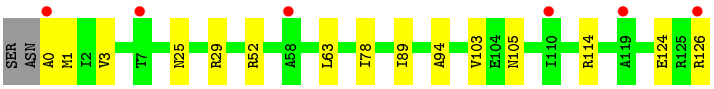




• Molecule 1: Holo-[acyl-carrier-protein] synthase

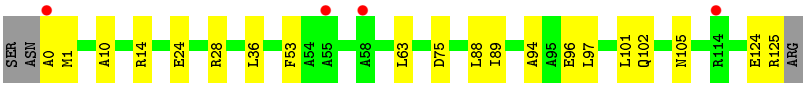
Chain E:





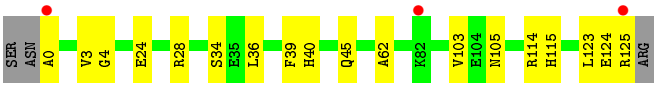
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain F:



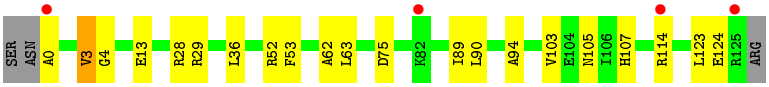
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain G:



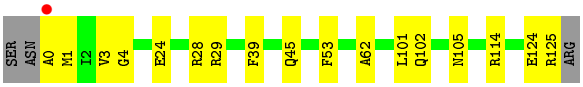
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain H:



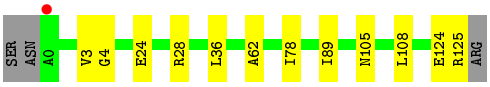
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain I:



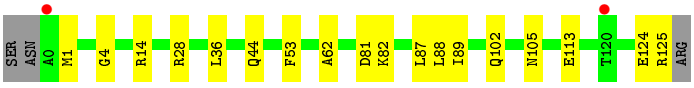
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain J:



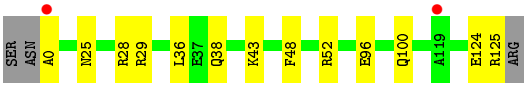
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain K:



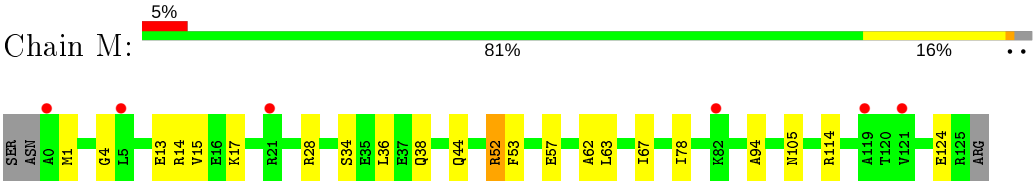
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain L:



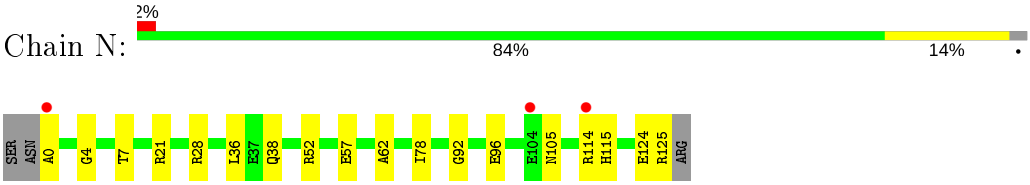
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain M:



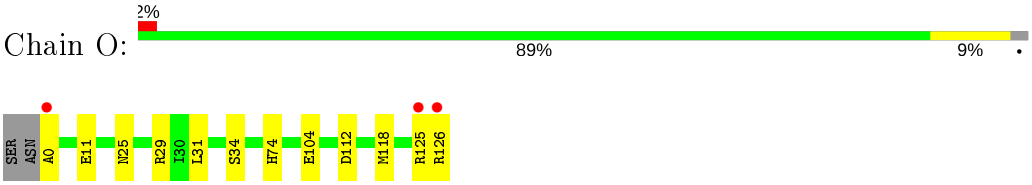
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain N:



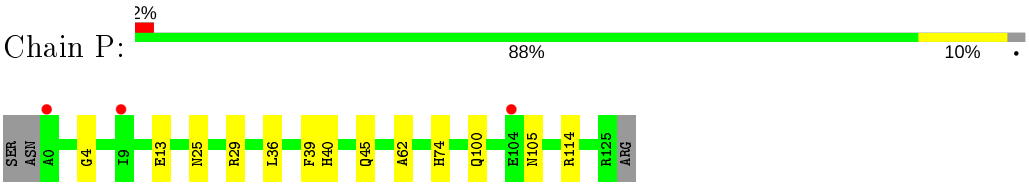
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain O:



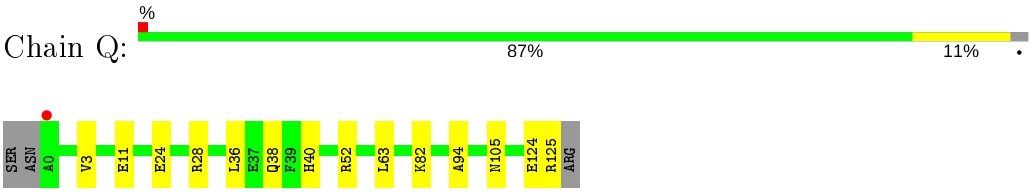
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain P:



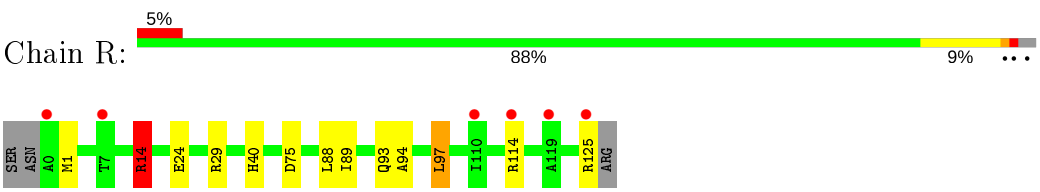
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain Q:



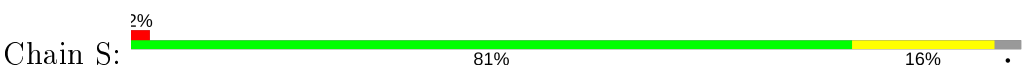
• Molecule 1: Holo-[acyl-carrier-protein] synthase

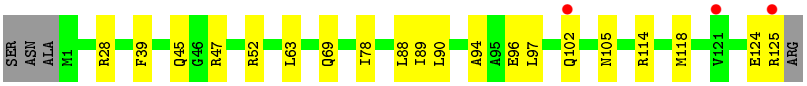
Chain R:



• Molecule 1: Holo-[acyl-carrier-protein] synthase

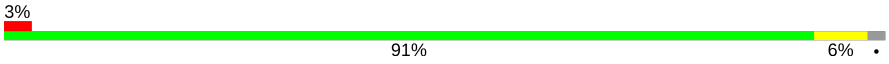
Chain S:

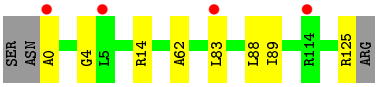




• Molecule 1: Holo-[acyl-carrier-protein] synthase

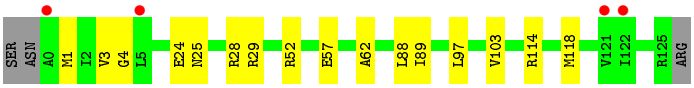
Chain T:





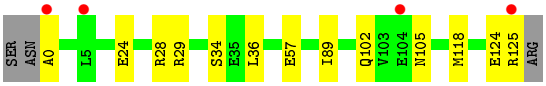
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain U:



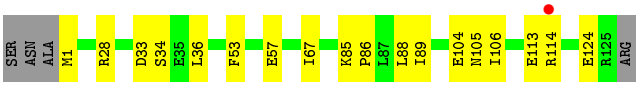
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain V:



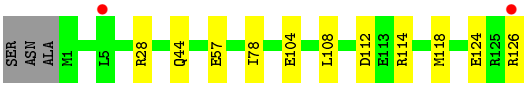
• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain W:



• Molecule 1: Holo-[acyl-carrier-protein] synthase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.55Å 139.04Å 138.32Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	29.89 – 1.85 29.75 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.89-1.85) 99.2 (29.75-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.156 , 0.191 0.171 , 0.204	Depositor DCC
R_{free} test set	15148 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28565	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, A3P, CL, CA, COA, ACT, MRD

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	0.58	0/1045	0.78	0/1397
1	B	0.58	0/1016	0.77	0/1359
1	C	0.64	0/1043	0.81	0/1395
1	D	0.61	0/1066	0.78	0/1425
1	E	0.55	0/1039	0.76	0/1388
1	F	0.56	0/1032	0.79	0/1380
1	G	0.48	0/1005	0.74	0/1346
1	H	0.53	0/1053	0.72	0/1408
1	I	0.55	0/1028	0.76	0/1375
1	J	0.64	0/1009	0.79	0/1350
1	K	0.62	1/1030 (0.1%)	0.78	0/1377
1	L	0.62	0/1032	0.80	0/1381
1	M	0.60	0/1032	0.77	0/1380
1	N	0.63	0/1034	0.79	0/1383
1	O	0.57	0/1034	0.76	0/1382
1	P	0.55	0/1036	0.77	0/1386
1	Q	0.56	0/1021	0.76	0/1365
1	R	0.56	0/1034	0.82	1/1383 (0.1%)
1	S	0.60	0/1073	0.77	0/1436
1	T	0.52	0/1034	0.74	0/1384
1	U	0.61	0/1055	0.78	0/1411
1	V	0.55	0/1019	0.76	0/1363
1	W	0.60	0/1011	0.80	0/1355
1	X	0.59	0/1033	0.76	0/1381
All	All	0.58	1/24814 (0.0%)	0.77	1/33190 (0.0%)

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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	113	GLU	CB-CG	-5.32	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	14	ARG	NE-CZ-NH1	5.83	123.22	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	52[A]	ARG	Sidechain

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	1035	0	1044	17	0
1	B	1006	0	1020	7	0
1	C	1033	0	1039	19	0
1	D	1056	0	1069	22	0
1	E	1029	0	1044	12	0
1	F	1022	0	1032	20	0
1	G	995	0	1004	18	0
1	H	1043	0	1053	19	0
1	I	1018	0	1026	20	0
1	J	999	0	1021	16	0
1	K	1020	0	1041	19	0
1	L	1022	0	1028	12	0
1	M	1022	0	1034	27	0
1	N	1024	0	1044	19	0
1	O	1023	0	1033	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1025	0	1040	12	0
1	Q	1011	0	1028	11	0
1	R	1024	0	1034	18	0
1	S	1062	0	1065	23	0
1	T	1023	0	1025	7	0
1	U	1045	0	1044	23	0
1	V	1009	0	1021	13	0
1	W	1000	0	1004	16	0
1	X	1022	0	1035	14	0
2	A	96	0	64	4	0
2	C	48	0	32	0	0
2	D	48	0	32	2	0
2	E	48	0	32	0	0
2	F	48	0	32	1	0
2	G	48	0	32	0	0
2	H	48	0	32	2	0
2	I	48	0	32	1	0
2	J	48	0	32	0	0
2	K	48	0	32	0	0
2	L	48	0	32	0	0
2	N	96	0	61	8	0
2	O	48	0	32	0	0
2	P	48	0	32	0	0
2	Q	48	0	32	0	0
2	R	48	0	32	0	0
2	S	48	0	32	4	0
2	T	48	0	32	0	0
2	U	48	0	32	0	0
2	W	96	0	64	12	0
2	X	48	0	32	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	P	1	0	0	0	0
3	T	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	2	0	0	0	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0
4	T	2	0	0	0	0
4	U	2	0	0	0	0
4	V	2	0	0	0	0
4	W	2	0	0	0	0
4	X	2	0	0	0	0
5	A	8	0	14	2	0
5	B	8	0	14	1	0
5	C	8	0	14	0	0
5	E	8	0	14	0	0
5	G	8	0	14	0	0
5	H	8	0	14	2	0
5	I	8	0	14	1	0
5	M	8	0	14	6	0
5	O	8	0	14	0	0
5	P	8	0	14	0	0
5	Q	8	0	14	1	0
5	R	8	0	14	0	0
5	S	8	0	14	2	0
5	U	8	0	14	1	0
5	V	8	0	14	0	0
5	W	8	0	14	0	0
6	A	4	0	3	3	0
6	C	4	0	3	3	0
6	E	4	0	3	1	0
6	K	8	0	6	1	0
6	R	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	4	0	3	1	0
6	W	4	0	3	0	0
7	D	8	0	14	4	0
7	F	8	0	14	3	0
7	K	8	0	14	4	0
7	L	8	0	14	0	0
7	N	8	0	14	3	0
7	T	8	0	14	0	0
8	O	27	0	9	1	0
9	A	119	0	0	3	0
9	B	81	0	0	2	0
9	C	126	0	0	9	0
9	D	124	0	0	3	0
9	E	100	0	0	4	0
9	F	107	0	0	4	0
9	G	81	0	0	2	0
9	H	87	0	0	4	0
9	I	105	0	0	3	0
9	J	137	0	0	2	0
9	K	116	0	0	6	0
9	L	137	0	0	3	0
9	M	105	0	0	4	0
9	N	132	0	0	5	0
9	O	105	0	0	2	0
9	P	110	0	0	2	0
9	Q	104	0	0	3	0
9	R	100	0	0	4	0
9	S	114	0	0	10	0
9	T	81	0	0	2	0
9	U	113	0	0	3	0
9	V	85	0	0	5	0
9	W	100	0	0	4	0
9	X	86	0	0	2	0
All	All	28565	0	25934	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (403) 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:F:89:ILE:HD13	9:F:510:HOH:O	1.36	1.25
1:K:87:LEU:HD21	9:K:1004:HOH:O	1.34	1.23
1:M:38[B]:GLN:HG2	9:M:2465[B]:HOH:O	1.41	1.18
1:N:7[B]:THR:CG2	1:O:118:MSE:HE3	1.82	1.10
1:J:28[A]:ARG:HD2	1:J:36:LEU:HD11	1.34	1.08
1:T:89:ILE:HD13	9:T:1853:HOH:O	1.54	1.07
1:F:97:LEU:O	1:F:101:LEU:HD13	1.58	1.00
1:S:47[B]:ARG:HD3	9:S:1756[B]:HOH:O	1.62	0.98
1:U:24[B]:GLU:HG3	1:U:28[B]:ARG:NH2	1.79	0.98
1:D:28[B]:ARG:CG	1:D:28[B]:ARG:HH11	1.79	0.95
1:O:34:SER:HB3	9:O:1406[B]:HOH:O	1.67	0.94
1:J:3:VAL:HG11	1:J:125:ARG:HE	1.35	0.92
1:S:89:ILE:HD13	9:S:1741:HOH:O	1.69	0.91
1:W:57[B]:GLU:OE2	2:W:2105:COA:H142	1.71	0.90
1:H:0:ALA:O	1:I:0:ALA:HB3	1.72	0.90
1:J:28[A]:ARG:HD2	1:J:36:LEU:CD1	2.02	0.90
1:Q:38:GLN:HG3	9:Q:1593:HOH:O	1.73	0.89
1:U:24[B]:GLU:CG	1:U:28[B]:ARG:NH2	2.36	0.89
1:M:57[B]:GLU:OE2	2:N:1221:COA:H143	1.73	0.89
1:D:28[B]:ARG:HH11	1:D:28[B]:ARG:HG3	1.36	0.89
7:N:2565:MRD:C5	7:N:2565:MRD:O2	2.21	0.88
1:M:38[B]:GLN:H	1:M:38[B]:GLN:HE21	1.22	0.88
1:N:7[B]:THR:HG21	1:O:118:MSE:HE3	1.54	0.86
1:M:38[B]:GLN:H	1:M:38[B]:GLN:NE2	1.73	0.86
1:O:0:ALA:HB1	1:O:125:ARG:NH1	1.91	0.86
6:C:2598:ACT:CH3	9:C:2501:HOH:O	2.24	0.85
1:L:28:ARG:HG2	1:L:36:LEU:HD11	1.59	0.84
1:C:24[B]:GLU:O	1:C:28[B]:ARG:HG3	1.77	0.84
1:G:3:VAL:CG1	1:G:125:ARG:HG3	2.08	0.83
1:F:96[B]:GLU:HG3	9:F:534:HOH:O	1.78	0.83
1:K:1:MSE:HB2	1:L:124:GLU:OE2	1.79	0.82
1:G:3:VAL:HG21	1:G:103:VAL:HG22	1.59	0.82
1:F:28[A]:ARG:HG2	1:F:36:LEU:HD11	1.63	0.81
1:J:24:GLU:OE2	1:J:28[A]:ARG:HD3	1.79	0.81
1:N:7[B]:THR:CG2	1:O:118:MSE:CE	2.57	0.81
1:W:57[B]:GLU:OE2	2:W:2105:COA:CEP	2.29	0.81
1:B:1:MSE:HB2	1:C:124:GLU:OE2	1.82	0.80
1:N:38:GLN:HG3	9:N:1268:HOH:O	1.81	0.79
1:C:28[A]:ARG:HG2	1:C:36:LEU:HD11	1.63	0.79
1:X:57[B]:GLU:OE2	2:X:1944:COA:H142	1.81	0.79
1:O:0:ALA:HB1	1:O:125:ARG:HH11	1.47	0.77
1:A:57[B]:GLU:OE2	2:A:129:COA:H142	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1696:COA:H142	1:U:57[B]:GLU:OE2	1.85	0.77
7:D:2573:MRD:H5C3	7:D:2573:MRD:O2	1.85	0.77
1:Q:28[A]:ARG:HG2	1:Q:36:LEU:HD11	1.66	0.76
1:V:34:SER:HB3	9:V:2489:HOH:O	1.84	0.76
1:U:24[B]:GLU:HG2	1:U:28[B]:ARG:HH22	1.51	0.75
1:C:13[B]:GLU:OE2	1:C:17:LYS:NZ	2.20	0.75
1:S:52[A]:ARG:NH2	9:S:1724:HOH:O	2.20	0.74
1:C:24[A]:GLU:OE2	1:C:28[A]:ARG:NE	2.20	0.74
1:D:52[B]:ARG:HD3	9:D:334:HOH:O	1.85	0.74
1:F:0:ALA:N	1:F:125:ARG:O	2.20	0.74
1:N:114:ARG:HD2	1:N:115:HIS:CE1	2.23	0.74
1:D:101:LEU:O	1:D:125:ARG:NH2	2.20	0.73
1:L:52[B]:ARG:HD3	9:L:1057:HOH:O	1.88	0.73
7:N:2565:MRD:H5C3	7:N:2565:MRD:O2	1.87	0.73
5:B:127:MPD:H52	5:B:127:MPD:O2	1.90	0.72
1:A:14:ARG:NH1	5:A:2570:MPD:O2	2.22	0.72
1:H:105[B]:ASN:HB3	1:H:124[B]:GLU:HG3	1.70	0.72
1:M:28:ARG:HG2	1:M:36:LEU:HD11	1.70	0.72
1:M:57[B]:GLU:OE2	2:N:1221:COA:CEP	2.37	0.72
1:V:57[A]:GLU:OE1	2:W:2019:COA:CEP	2.38	0.72
1:G:24:GLU:OE1	1:G:40:HIS:NE2	2.23	0.71
1:G:114:ARG:HD2	1:G:115:HIS:CE1	2.26	0.71
1:N:0:ALA:O	1:N:125:ARG:HD2	1.91	0.71
1:F:24:GLU:O	1:F:28[B]:ARG:HG3	1.91	0.71
1:L:0:ALA:HB1	1:L:125:ARG:O	1.91	0.70
1:E:52[B]:ARG:NH1	9:E:432:HOH:O	2.24	0.70
1:I:28[B]:ARG:NH1	9:I:772:HOH:O	2.25	0.70
2:N:1333[A]:COA:H141	9:N:2227:HOH:O	1.92	0.69
1:C:52[B]:ARG:NH1	9:C:240:HOH:O	2.25	0.69
1:Q:52[B]:ARG:NH2	9:Q:1560:HOH:O	2.25	0.69
1:K:88:LEU:C	1:K:89:ILE:HD12	2.13	0.69
1:H:52[B]:ARG:NH1	9:H:2280:HOH:O	2.25	0.69
1:V:57[A]:GLU:OE1	2:W:2019:COA:H142	1.93	0.69
1:R:24[A]:GLU:OE2	1:R:40:HIS:NE2	2.24	0.69
1:C:29:ARG:NH2	9:C:246:HOH:O	2.26	0.68
1:D:29[B]:ARG:NH1	9:D:2194:HOH:O	2.27	0.68
1:T:14:ARG:HD3	1:U:114:ARG:NH2	2.09	0.68
1:R:88:LEU:C	1:R:89:ILE:HD12	2.13	0.68
1:W:89:ILE:HD13	9:W:2088:HOH:O	1.93	0.68
1:R:89:ILE:N	1:R:89:ILE:HD12	2.08	0.68
1:A:104:GLU:CG	9:A:164:HOH:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:57[B]:GLU:OE2	2:X:1944:COA:CEP	2.42	0.67
1:A:28[A]:ARG:HG2	1:A:36:LEU:HD11	1.77	0.67
1:X:104:GLU:CD	1:X:126:ARG:HB2	2.15	0.67
6:C:2598:ACT:H3	9:C:2501:HOH:O	1.88	0.66
1:S:88:LEU:C	1:S:89:ILE:HD12	2.16	0.66
1:L:48:PHE:O	1:L:52[B]:ARG:HG2	1.95	0.66
1:N:7[B]:THR:HG22	1:O:118:MSE:CE	2.25	0.66
2:W:2105:COA:H121	2:W:2105:COA:HN8	1.60	0.66
1:M:52[B]:ARG:NH2	9:M:1193:HOH:O	2.29	0.65
1:D:13:GLU:OE2	1:D:17:LYS:NZ	2.30	0.65
1:F:96[B]:GLU:CG	9:F:534:HOH:O	2.42	0.65
9:G:580:HOH:O	1:H:114[A]:ARG:HG3	1.96	0.65
6:C:2598:ACT:H2	9:C:2501:HOH:O	1.94	0.65
1:M:14:ARG:NH1	5:M:2572:MPD:O4	2.30	0.64
1:M:38[B]:GLN:N	1:M:38[B]:GLN:NE2	2.45	0.64
1:N:7[B]:THR:HG22	1:O:118:MSE:HE3	1.76	0.64
1:G:28:ARG:HG2	1:G:36:LEU:HD11	1.79	0.64
1:E:0:ALA:N	1:E:126:ARG:O	2.29	0.64
1:G:0:ALA:HB3	1:I:0:ALA:O	1.97	0.64
1:G:105[A]:ASN:HB2	1:G:124[A]:GLU:CG	2.27	0.64
1:K:14:ARG:NH2	7:K:2564:MRD:O4	2.31	0.64
1:P:105:ASN:ND2	1:R:1:MSE:CE	2.61	0.64
1:E:3:VAL:HG21	1:E:103:VAL:HG22	1.80	0.63
1:I:3:VAL:HG11	1:I:101:LEU:HB3	1.80	0.63
1:J:28[A]:ARG:CD	1:J:36:LEU:CD1	2.76	0.63
1:H:89:ILE:HD12	1:H:89:ILE:N	2.12	0.63
7:N:2565:MRD:H5C2	7:N:2565:MRD:O2	1.97	0.63
1:D:28[B]:ARG:HG3	1:D:28[B]:ARG:NH1	2.10	0.62
1:Q:24:GLU:OE1	1:Q:40:HIS:NE2	2.28	0.62
1:M:34:SER:O	1:M:38[B]:GLN:NE2	2.32	0.62
1:G:3:VAL:HG13	1:G:125:ARG:HG3	1.82	0.62
1:U:89:ILE:N	1:U:89:ILE:HD12	2.15	0.62
1:S:105:ASN:HB2	1:S:124[A]:GLU:CG	2.30	0.62
1:G:105[B]:ASN:ND2	1:I:1:MSE:HE3	2.14	0.62
1:W:1:MSE:HB2	1:X:124:GLU:OE2	2.00	0.62
1:A:25:ASN:OD1	1:A:28[B]:ARG:NH2	2.33	0.61
1:F:10:ALA:HB1	7:F:2559:MRD:H5C1	1.82	0.61
1:H:53:PHE:CE2	5:H:631:MPD:H52	2.35	0.61
1:B:44:GLN:HG2	9:B:175:HOH:O	1.99	0.61
1:S:118:MSE:HE1	1:U:118:MSE:HG3	1.82	0.61
1:V:0:ALA:N	1:V:125:ARG:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:67:ILE:HB	2:W:2105:COA:O9P	2.00	0.61
1:V:28:ARG:HG2	1:V:36:LEU:HD11	1.81	0.61
1:P:105:ASN:ND2	1:R:1:MSE:HE3	2.16	0.61
1:U:24[B]:GLU:CG	1:U:28[B]:ARG:HH22	2.06	0.61
1:F:102:GLN:OE1	1:F:125:ARG:NH2	2.34	0.61
1:K:105:ASN:HB2	1:K:124:GLU:HG3	1.83	0.60
9:H:2211:HOH:O	1:I:114[A]:ARG:HG3	2.02	0.60
1:T:88:LEU:C	1:T:89:ILE:HD12	2.22	0.60
1:D:28[B]:ARG:CG	1:D:28[B]:ARG:NH1	2.51	0.60
1:C:25:ASN:O	1:C:29:ARG:HG3	2.02	0.59
1:H:105[B]:ASN:HB3	1:H:124[B]:GLU:CG	2.32	0.59
1:N:28:ARG:HG2	1:N:36:LEU:HD11	1.85	0.59
1:P:13:GLU:HG3	9:P:1427:HOH:O	2.01	0.59
1:K:82[A]:LYS:HG3	9:K:953:HOH:O	2.02	0.59
1:S:96[A]:GLU:HA	1:S:96[A]:GLU:OE2	2.01	0.59
1:J:78:ILE:HD12	1:J:108:LEU:CD2	2.33	0.59
1:U:52:ARG:NH2	9:U:2249:HOH:O	2.31	0.59
1:I:29:ARG:CZ	9:I:760:HOH:O	2.49	0.59
1:A:104:GLU:HG3	9:A:164:HOH:O	2.02	0.59
1:K:89:ILE:HD13	9:K:941:HOH:O	2.02	0.59
1:M:53:PHE:CD2	5:M:2572:MPD:H52	2.38	0.58
1:S:47[B]:ARG:CD	9:S:1756[B]:HOH:O	2.33	0.58
5:M:2572:MPD:O4	5:M:2572:MPD:O2	2.21	0.58
1:N:7[B]:THR:HG21	9:O:1350:HOH:O	2.03	0.58
1:M:63:LEU:HD21	1:M:94:ALA:HA	1.84	0.58
1:S:89:ILE:N	1:S:89:ILE:HD12	2.19	0.58
1:F:88:LEU:C	1:F:89:ILE:HD12	2.23	0.58
1:I:24[B]:GLU:O	1:I:28[B]:ARG:HG3	2.04	0.57
1:B:102:GLN:OE1	1:B:125:ARG:NH2	2.37	0.57
2:W:2105:COA:O1A	1:X:112:ASP:OD1	2.22	0.57
1:D:48:PHE:O	1:D:52[B]:ARG:HG2	2.04	0.57
1:V:118:MSE:HE1	1:X:118:MSE:HG3	1.87	0.57
1:M:52[B]:ARG:CZ	9:M:1193:HOH:O	2.52	0.57
1:R:14:ARG:HH11	1:R:14:ARG:HG2	1.69	0.57
6:E:2594:ACT:H2	9:E:435:HOH:O	2.03	0.57
1:V:57[A]:GLU:OE1	2:W:2019:COA:H143	2.03	0.57
1:U:24[B]:GLU:OE2	1:U:28[B]:ARG:NH1	2.37	0.57
1:D:28[B]:ARG:HH11	1:D:28[B]:ARG:HG2	1.67	0.57
1:J:3:VAL:HG11	1:J:125:ARG:NE	2.14	0.56
1:I:105:ASN:HB2	1:I:124[B]:GLU:HG3	1.86	0.56
1:L:28:ARG:HG2	1:L:36:LEU:CD1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28[A]:ARG:HG2	1:D:36:LEU:HD11	1.86	0.56
1:V:102:GLN:OE1	1:V:125:ARG:NH2	2.39	0.56
1:D:105[A]:ASN:HB2	1:D:124[A]:GLU:HG3	1.87	0.56
1:N:57:GLU:OE2	2:N:1333[A]:COA:H71	2.06	0.56
1:S:28:ARG:HG2	9:S:1754:HOH:O	2.06	0.56
1:C:28[A]:ARG:HG2	1:C:36:LEU:CD1	2.36	0.56
2:D:283:COA:C2P	7:F:2559:MRD:H1C2	2.36	0.56
1:J:24:GLU:HG3	1:J:28[A]:ARG:HG3	1.88	0.56
1:K:105:ASN:HB2	1:K:124:GLU:CG	2.36	0.56
1:M:53:PHE:CE2	5:M:2572:MPD:H52	2.42	0.55
1:T:83:LEU:N	1:T:83:LEU:HD12	2.21	0.55
1:O:0:ALA:CB	1:O:125:ARG:HH11	2.17	0.55
1:Q:11:GLU:OE2	1:R:114[A]:ARG:NH1	2.40	0.55
1:V:34:SER:CB	9:V:2489:HOH:O	2.49	0.55
6:K:629:ACT:H2	9:K:977:HOH:O	2.07	0.55
1:U:24[B]:GLU:HG3	1:U:28[B]:ARG:CZ	2.35	0.55
1:R:14:ARG:HH11	1:R:14:ARG:CG	2.20	0.55
1:X:28:ARG:NH1	9:X:2167:HOH:O	2.38	0.55
1:X:114[B]:ARG:NH1	9:X:2092:HOH:O	2.38	0.55
1:E:63[B]:LEU:HD11	1:E:94:ALA:HB1	1.89	0.54
1:H:3:VAL:HG11	1:H:103:VAL:HG22	1.90	0.54
1:K:81:ASP:HB3	9:K:1004:HOH:O	2.05	0.54
1:C:29:ARG:CZ	9:C:246:HOH:O	2.56	0.54
1:A:105:ASN:HB2	1:A:124:GLU:HG3	1.89	0.54
2:A:127:COA:O4A	6:A:2597:ACT:H3	2.07	0.54
1:A:104:GLU:HG2	9:A:164:HOH:O	2.03	0.54
1:A:57[B]:GLU:OE2	2:A:129:COA:CEP	2.54	0.54
1:M:14:ARG:NH1	5:M:2572:MPD:O2	2.35	0.54
1:W:105:ASN:HB2	1:W:124[A]:GLU:HG3	1.90	0.53
5:U:1698:MPD:O4	5:U:1698:MPD:O2	2.17	0.53
1:D:102:GLN:HB2	1:D:125:ARG:NH2	2.23	0.53
1:P:105:ASN:ND2	1:R:1:MSE:HE1	2.24	0.53
1:F:89:ILE:N	1:F:89:ILE:HD12	2.24	0.53
1:O:25:ASN:O	1:O:29:ARG:HG3	2.09	0.53
7:D:2573:MRD:C5	7:D:2573:MRD:O2	2.56	0.52
1:J:105:ASN:HB2	1:J:124:GLU:HG3	1.89	0.52
1:W:105:ASN:HB2	1:W:124[B]:GLU:HG2	1.91	0.52
2:N:1333[A]:COA:O1A	1:O:112:ASP:OD1	2.27	0.52
1:N:52[B]:ARG:NH1	9:N:1245:HOH:O	2.20	0.52
1:S:63[B]:LEU:HD21	1:S:97:LEU:HD12	1.92	0.52
1:K:88:LEU:O	1:K:89:ILE:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:89:ILE:N	1:T:89:ILE:HD12	2.25	0.52
1:W:53:PHE:CZ	1:W:57[A]:GLU:OE2	2.62	0.52
1:E:89:ILE:HD13	9:E:449:HOH:O	2.09	0.52
2:F:477:COA:H121	2:F:477:COA:O9P	2.10	0.52
1:S:105:ASN:HB2	1:S:124[A]:GLU:HG3	1.92	0.51
2:S:1696:COA:C6P	2:S:1696:COA:O9P	2.58	0.51
1:M:67:ILE:H	2:N:1221:COA:H141	1.75	0.51
1:U:24[B]:GLU:O	1:U:28[B]:ARG:HG2	2.10	0.51
2:A:127:COA:O1A	6:A:2597:ACT:O	2.28	0.51
1:M:114:ARG:NH1	9:M:1206:HOH:O	2.43	0.51
2:W:2019:COA:O9P	2:W:2019:COA:H121	2.11	0.51
2:S:1696:COA:CEP	1:U:57[B]:GLU:OE2	2.58	0.50
2:W:2105:COA:N8P	2:W:2105:COA:H121	2.24	0.50
1:I:29:ARG:NH2	9:I:760:HOH:O	2.43	0.50
1:O:0:ALA:O	1:O:125:ARG:NE	2.45	0.50
1:U:24[B]:GLU:CG	1:U:28[B]:ARG:CZ	2.89	0.50
1:G:4:GLY:HA3	1:G:62:ALA:O	2.11	0.50
1:L:25:ASN:O	1:L:29:ARG:HG3	2.12	0.50
1:C:82:LYS:HG3	9:C:218:HOH:O	2.12	0.50
1:V:24:GLU:OE1	9:V:2018:HOH:O	2.20	0.50
1:A:114[B]:ARG:NH1	1:C:11:GLU:OE1	2.43	0.50
1:A:105:ASN:HB2	1:A:124:GLU:CG	2.42	0.50
1:K:14:ARG:NH2	7:K:2564:MRD:O2	2.45	0.50
1:R:29[B]:ARG:NE	9:R:2230:HOH:O	2.39	0.50
6:T:2568:ACT:H1	9:T:1796:HOH:O	2.12	0.50
1:H:28:ARG:HG2	1:H:36:LEU:HD11	1.94	0.50
1:M:105:ASN:HB2	1:M:124:GLU:HG3	1.93	0.50
2:N:1221:COA:O1A	9:N:1259[B]:HOH:O	2.20	0.49
1:N:21:ARG:NH1	9:N:1299:HOH:O	2.32	0.49
1:S:114[B]:ARG:HG3	9:U:1722:HOH:O	2.12	0.49
1:A:24:GLU:OE1	1:A:28[A]:ARG:NE	2.43	0.49
1:F:53:PHE:CE2	7:F:2559:MRD:H5C2	2.47	0.49
1:P:36[B]:LEU:HG	1:P:40:HIS:CE1	2.47	0.49
1:I:102:GLN:OE1	1:I:125:ARG:NH1	2.46	0.49
1:S:124[A]:GLU:OE2	1:U:1:MSE:HE3	2.12	0.49
1:G:34:SER:HB2	9:G:597:HOH:O	2.11	0.49
1:J:105:ASN:HB2	1:J:124:GLU:CG	2.43	0.49
1:E:25:ASN:O	1:E:29[A]:ARG:HG3	2.12	0.49
1:K:102:GLN:OE1	1:K:125:ARG:NH2	2.46	0.49
1:R:97:LEU:HD21	9:R:1673:HOH:O	2.12	0.49
1:A:14:ARG:NH1	5:A:2570:MPD:O4	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:102[A]:GLN:OE1	1:S:125:ARG:NH1	2.45	0.49
1:S:47[A]:ARG:HD2	9:S:2481[A]:HOH:O	2.12	0.49
1:I:105:ASN:HB2	1:I:124[B]:GLU:CG	2.43	0.48
1:U:25:ASN:O	1:U:29[A]:ARG:HG3	2.13	0.48
1:W:113:GLU:OE2	9:W:2045:HOH:O	2.20	0.48
1:D:14[A]:ARG:HE	7:D:2573:MRD:H5C3	1.78	0.48
1:I:24[B]:GLU:HG3	1:I:28[B]:ARG:HH11	1.77	0.48
1:C:24[A]:GLU:CG	1:C:28[A]:ARG:HE	2.26	0.48
1:N:52[B]:ARG:HE	1:N:78:ILE:HB	1.79	0.48
1:U:24[B]:GLU:HG2	1:U:28[B]:ARG:NH2	2.11	0.48
9:V:1952:HOH:O	1:W:114:ARG:HG3	2.13	0.48
2:D:283:COA:O5A	9:D:2368:HOH:O	2.20	0.48
1:M:15:VAL:CG2	5:M:2572:MPD:H53	2.43	0.48
1:R:125:ARG:NH2	9:R:1682:HOH:O	2.43	0.48
1:R:89:ILE:CD1	1:R:89:ILE:N	2.75	0.48
1:N:52[B]:ARG:NE	1:N:78:ILE:HB	2.29	0.47
1:G:3:VAL:HG23	1:G:123:LEU:HB2	1.95	0.47
1:X:78:ILE:HD12	1:X:108:LEU:CD2	2.44	0.47
1:O:31:LEU:O	1:O:74[A]:HIS:CE1	2.67	0.47
1:X:78:ILE:HD12	1:X:108:LEU:HD21	1.95	0.47
1:D:25:ASN:O	1:D:29[B]:ARG:HG3	2.15	0.47
1:J:28[A]:ARG:CD	1:J:36:LEU:HD13	2.44	0.47
1:K:28:ARG:HG2	1:K:36:LEU:HD11	1.96	0.47
1:M:44[B]:GLN:NE2	3:M:2555:CL:CL	2.78	0.47
1:P:100:GLN:HG2	2:X:1944:COA:H71	1.97	0.47
1:F:1:MSE:HG2	1:F:125:ARG:HD3	1.97	0.47
1:J:28[A]:ARG:CD	1:J:36:LEU:HD11	2.24	0.47
1:K:1:MSE:CB	1:L:124:GLU:OE2	2.60	0.47
1:M:13:GLU:HG2	1:M:17:LYS:HE2	1.97	0.46
1:P:74[B]:HIS:CD2	9:P:1506:HOH:O	2.67	0.46
1:F:24:GLU:HG3	1:F:28[B]:ARG:HG3	1.97	0.46
1:B:1:MSE:CB	1:C:124:GLU:OE2	2.59	0.46
1:D:105[A]:ASN:HB2	1:D:124[A]:GLU:CG	2.46	0.46
1:K:53:PHE:CE2	7:K:2564:MRD:H5C2	2.50	0.46
1:E:105:ASN:HB2	1:E:124:GLU:CG	2.45	0.46
1:D:114:ARG:NH1	1:F:14:ARG:HD3	2.30	0.46
1:G:105[A]:ASN:HB2	1:G:124[A]:GLU:HG3	1.96	0.46
1:H:63[A]:LEU:HD23	1:H:123:LEU:CD1	2.46	0.46
1:P:25:ASN:O	1:P:29[A]:ARG:HG3	2.16	0.46
1:E:105:ASN:HB2	1:E:124:GLU:HG2	1.97	0.46
1:K:14:ARG:HH22	7:K:2564:MRD:HA	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:88:LEU:C	1:U:89:ILE:HD12	2.36	0.46
1:U:97:LEU:HD11	9:U:1937:HOH:O	2.16	0.46
1:E:78:ILE:N	1:E:78:ILE:HD12	2.31	0.46
1:J:89:ILE:HD12	9:J:879:HOH:O	2.16	0.46
1:A:1:MSE:HE3	1:A:125:ARG:HH11	1.81	0.45
1:G:39:PHE:CE1	1:G:45:GLN:HB3	2.51	0.45
1:D:14[B]:ARG:HD2	1:E:114:ARG:NH2	2.31	0.45
1:H:53:PHE:CD2	5:H:631:MPD:H52	2.51	0.45
1:L:43:LYS:NZ	9:L:2452:HOH:O	2.49	0.45
1:P:114:ARG:HH21	1:R:14:ARG:HD2	1.82	0.45
1:T:0:ALA:HB1	1:T:125:ARG:O	2.17	0.45
1:W:104:GLU:HA	1:W:104:GLU:OE1	2.17	0.45
1:A:114[A]:ARG:HG3	9:C:282:HOH:O	2.15	0.45
1:D:26:PHE:HA	1:D:29[B]:ARG:NE	2.31	0.45
1:G:3:VAL:HG11	1:G:125:ARG:HG3	1.94	0.45
1:P:4:GLY:HA3	1:P:62:ALA:O	2.17	0.45
1:H:13[B]:GLU:HG2	9:H:672:HOH:O	2.17	0.45
6:R:2595:ACT:H2	9:R:1631:HOH:O	2.16	0.45
1:S:78:ILE:N	1:S:78:ILE:HD12	2.31	0.45
1:V:105:ASN:HB2	1:V:124:GLU:HG3	1.98	0.45
1:X:104:GLU:OE1	1:X:126:ARG:HB2	2.16	0.45
1:G:105[A]:ASN:OD1	1:I:1:MSE:HE3	2.16	0.45
1:L:96:GLU:O	1:L:100:GLN:HG3	2.17	0.45
1:T:4:GLY:HA3	1:T:62:ALA:O	2.17	0.45
1:K:4:GLY:HA3	1:K:62:ALA:O	2.17	0.44
1:L:0:ALA:CB	1:L:125:ARG:O	2.63	0.44
1:S:39:PHE:CE1	1:S:45:GLN:HB3	2.52	0.44
1:Q:24:GLU:HG2	9:Q:1592:HOH:O	2.16	0.44
5:S:1697:MPD:HM1	5:S:1697:MPD:H52	1.98	0.44
5:Q:2567:MPD:O4	5:Q:2567:MPD:O2	2.32	0.44
2:W:2105:COA:CCP	2:W:2105:COA:HN8	2.27	0.44
2:H:630:COA:O6A	2:H:630:COA:O9P	2.36	0.44
1:S:47[A]:ARG:CD	9:S:2481[A]:HOH:O	2.66	0.44
8:O:2575[B]:A3P:O2'	8:O:2575[B]:A3P:O2P	2.36	0.43
5:S:1697:MPD:H53	9:S:1707:HOH:O	2.19	0.43
1:G:105[B]:ASN:HD22	1:I:1:MSE:HE3	1.80	0.43
1:M:78:ILE:HD12	1:M:78:ILE:N	2.34	0.43
1:S:89:ILE:CD1	1:S:89:ILE:N	2.82	0.43
1:H:75:ASP:HB3	1:H:94:ALA:HB3	2.00	0.43
1:Q:28[B]:ARG:HG2	1:Q:36:LEU:HD11	2.01	0.43
2:W:2019:COA:O9P	2:W:2019:COA:CCP	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:ARG:HB3	1:R:14:ARG:NH1	2.33	0.43
1:W:85:LYS:HG2	1:W:86:PRO:HD2	2.01	0.43
1:C:39:PHE:CE1	1:C:45:GLN:HB3	2.54	0.43
1:J:4:GLY:HA3	1:J:62:ALA:O	2.19	0.43
1:M:44[B]:GLN:HG3	1:M:44[B]:GLN:O	2.18	0.43
1:V:29[B]:ARG:HE	1:V:29[B]:ARG:HB3	1.66	0.43
1:J:78:ILE:HD12	1:J:108:LEU:HD21	2.01	0.43
1:K:44:GLN:HG2	9:K:1000:HOH:O	2.18	0.43
1:P:39:PHE:CE1	1:P:45:GLN:HB3	2.54	0.43
1:B:4:GLY:HA3	1:B:62:ALA:O	2.18	0.42
1:M:67:ILE:HB	2:N:1221:COA:HN8	1.84	0.42
1:Q:105:ASN:HB2	1:Q:124[B]:GLU:CG	2.49	0.42
1:B:78:ILE:CD1	1:B:88:LEU:HD13	2.49	0.42
1:C:52[B]:ARG:CZ	9:C:240:HOH:O	2.64	0.42
1:F:63:LEU:HD11	1:F:94:ALA:HB1	2.01	0.42
1:F:75:ASP:OD1	9:F:555:HOH:O	2.21	0.42
1:H:13[B]:GLU:HG3	9:H:2277:HOH:O	2.19	0.42
1:N:92:GLY:O	1:N:96[A]:GLU:HG2	2.18	0.42
1:Q:63:LEU:HD11	1:Q:94:ALA:HB1	2.00	0.42
9:W:2126:HOH:O	1:X:114[A]:ARG:HG2	2.18	0.42
1:X:44[B]:GLN:O	1:X:44[B]:GLN:HG3	2.19	0.42
1:B:13[A]:GLU:HG3	9:B:142:HOH:O	2.20	0.42
1:E:1:MSE:HB2	1:F:124[A]:GLU:OE1	2.19	0.42
1:H:29:ARG:HD2	2:I:699:COA:S1P	2.59	0.42
1:L:38[B]:GLN:HB2	9:L:1112:HOH:O	2.18	0.42
1:A:51:LYS:NZ	6:A:2597:ACT:OXT	2.39	0.42
1:F:28[A]:ARG:HG2	1:F:36:LEU:CD1	2.44	0.42
1:S:47[A]:ARG:NH2	9:S:2234[A]:HOH:O	2.53	0.42
1:W:33:ASP:HA	1:W:36:LEU:HD12	2.01	0.42
1:D:63:LEU:HD11	1:D:94:ALA:HA	2.00	0.42
1:K:89:ILE:HD12	1:K:89:ILE:N	2.35	0.42
1:M:4:GLY:HA3	1:M:62:ALA:O	2.20	0.42
1:U:3:VAL:HG21	1:U:103:VAL:HG22	2.01	0.42
1:D:105[B]:ASN:ND2	1:D:107:HIS:NE2	2.68	0.42
1:C:63:LEU:HD21	1:C:94:ALA:HA	2.02	0.42
1:M:114:ARG:NH1	1:O:11:GLU:OE1	2.53	0.42
1:Q:3:VAL:CG2	1:Q:125:ARG:HG3	2.50	0.42
1:N:4:GLY:HA3	1:N:62:ALA:O	2.20	0.41
1:W:88:LEU:HD23	1:W:106:ILE:HG21	2.01	0.41
1:N:105:ASN:HB2	1:N:124:GLU:CG	2.50	0.41
1:O:104:GLU:HG3	1:O:126:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:93:GLN:NE2	1:R:97:LEU:CD1	2.83	0.41
1:W:28:ARG:HG2	1:W:36:LEU:HD11	2.02	0.41
1:D:14[A]:ARG:HE	7:D:2573:MRD:C5	2.33	0.41
1:A:1:MSE:HE3	1:A:125:ARG:NH1	2.35	0.41
2:H:630:COA:CCP	2:H:630:COA:O9P	2.68	0.41
1:S:69:GLN:NE2	9:S:1753:HOH:O	2.38	0.41
1:G:3:VAL:HG21	1:G:103:VAL:CG2	2.42	0.41
1:H:105[B]:ASN:OD1	1:H:107:HIS:NE2	2.54	0.41
1:N:96[A]:GLU:HA	1:N:96[A]:GLU:OE1	2.21	0.41
1:U:89:ILE:N	1:U:89:ILE:CD1	2.82	0.41
1:C:4:GLY:HA3	1:C:62:ALA:O	2.20	0.41
1:I:53:PHE:CE2	5:I:2561:MPD:H52	2.55	0.41
1:J:3:VAL:CG1	1:J:125:ARG:HE	2.18	0.41
1:C:24[A]:GLU:OE2	1:C:28[A]:ARG:CZ	2.69	0.41
1:X:57[B]:GLU:OE2	1:X:57[B]:GLU:HA	2.21	0.41
1:H:105[B]:ASN:ND2	1:H:124[B]:GLU:OE2	2.53	0.41
2:S:1696:COA:S1P	1:U:29[B]:ARG:HD3	2.61	0.41
1:S:63[A]:LEU:HD11	1:S:94:ALA:HB1	2.03	0.41
1:W:34:SER:HB3	9:W:2100:HOH:O	2.21	0.41
1:F:105:ASN:HB2	1:F:124[B]:GLU:CG	2.51	0.41
1:H:4:GLY:HA3	1:H:62:ALA:O	2.21	0.41
1:M:28:ARG:HG2	1:M:36:LEU:CD1	2.47	0.41
1:I:24[A]:GLU:HG2	9:J:819:HOH:O	2.20	0.40
1:P:105:ASN:HD21	1:R:1:MSE:HE1	1.85	0.40
1:I:4:GLY:HA3	1:I:62:ALA:O	2.21	0.40
1:E:52[B]:ARG:CZ	9:E:432:HOH:O	2.66	0.40
1:I:0:ALA:HA	1:I:125:ARG:O	2.21	0.40
1:I:39:PHE:CE1	1:I:45:GLN:HB3	2.56	0.40
1:H:89:ILE:CD1	1:H:89:ILE:N	2.82	0.40
1:R:75:ASP:HB3	1:R:94:ALA:HB3	2.03	0.40
1:U:4:GLY:HA3	1:U:62:ALA:O	2.21	0.40
1:Q:105:ASN:HB2	1:Q:124[B]:GLU:HG3	2.04	0.40
1:V:89:ILE:HG13	9:V:1992:HOH:O	2.21	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	131/129 (102%)	127 (97%)	4 (3%)	0	100	100
1	B	128/129 (99%)	126 (98%)	2 (2%)	0	100	100
1	C	131/129 (102%)	127 (97%)	4 (3%)	0	100	100
1	D	133/129 (103%)	130 (98%)	3 (2%)	0	100	100
1	E	130/129 (101%)	128 (98%)	2 (2%)	0	100	100
1	F	130/129 (101%)	127 (98%)	3 (2%)	0	100	100
1	G	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	H	132/129 (102%)	129 (98%)	3 (2%)	0	100	100
1	I	129/129 (100%)	127 (98%)	2 (2%)	0	100	100
1	J	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	K	130/129 (101%)	128 (98%)	2 (2%)	0	100	100
1	L	130/129 (101%)	128 (98%)	2 (2%)	0	100	100
1	M	130/129 (101%)	126 (97%)	4 (3%)	0	100	100
1	N	130/129 (101%)	126 (97%)	4 (3%)	0	100	100
1	O	130/129 (101%)	126 (97%)	4 (3%)	0	100	100
1	P	130/129 (101%)	127 (98%)	3 (2%)	0	100	100
1	Q	128/129 (99%)	125 (98%)	3 (2%)	0	100	100
1	R	130/129 (101%)	127 (98%)	3 (2%)	0	100	100
1	S	134/129 (104%)	130 (97%)	4 (3%)	0	100	100
1	T	130/129 (101%)	127 (98%)	3 (2%)	0	100	100
1	U	132/129 (102%)	130 (98%)	2 (2%)	0	100	100
1	V	128/129 (99%)	126 (98%)	2 (2%)	0	100	100
1	W	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	X	129/129 (100%)	126 (98%)	3 (2%)	0	100	100
All	All	3116/3096 (101%)	3045 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	106/100 (106%)	106 (100%)	0	100	100
1	B	103/100 (103%)	102 (99%)	1 (1%)	76	69
1	C	106/100 (106%)	106 (100%)	0	100	100
1	D	108/100 (108%)	108 (100%)	0	100	100
1	E	105/100 (105%)	105 (100%)	0	100	100
1	F	105/100 (105%)	105 (100%)	0	100	100
1	G	102/100 (102%)	102 (100%)	0	100	100
1	H	107/100 (107%)	105 (98%)	2 (2%)	57	43
1	I	104/100 (104%)	104 (100%)	0	100	100
1	J	102/100 (102%)	102 (100%)	0	100	100
1	K	105/100 (105%)	105 (100%)	0	100	100
1	L	105/100 (105%)	105 (100%)	0	100	100
1	M	105/100 (105%)	104 (99%)	1 (1%)	76	69
1	N	105/100 (105%)	105 (100%)	0	100	100
1	O	105/100 (105%)	105 (100%)	0	100	100
1	P	105/100 (105%)	105 (100%)	0	100	100
1	Q	103/100 (103%)	102 (99%)	1 (1%)	76	69
1	R	105/100 (105%)	103 (98%)	2 (2%)	57	43
1	S	110/100 (110%)	109 (99%)	1 (1%)	78	72
1	T	105/100 (105%)	105 (100%)	0	100	100
1	U	107/100 (107%)	107 (100%)	0	100	100
1	V	103/100 (103%)	103 (100%)	0	100	100
1	W	103/100 (103%)	103 (100%)	0	100	100
1	X	105/100 (105%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2519/2400 (105%)	2511 (100%)	8 (0%)	92 91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	LYS
1	H	3	VAL
1	H	90	LEU
1	M	1	MSE
1	Q	82	LYS
1	R	14	ARG
1	R	97	LEU
1	S	90	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	B	69	GLN
1	C	100	GLN
1	E	102	GLN
1	H	69	GLN
1	I	93	GLN
1	J	102	GLN
1	O	38	GLN
1	O	100	GLN
1	P	69	GLN
1	P	105	ASN
1	Q	93	GLN
1	Q	102	GLN
1	R	100	GLN
1	R	105	ASN
1	S	100	GLN
1	T	44	GLN
1	T	105	ASN
1	T	115	HIS
1	X	69	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 110 ligands modelled in this entry, 55 are monoatomic - leaving 55 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	$\#\|Z\| > 2$
5	MPD	I	2561	-	7,7,7	0.30	0	9,10,10	0.17	0
5	MPD	E	2560	-	7,7,7	0.38	0	9,10,10	0.23	0
2	COA	Q	1515	4	41,50,50	1.12	1 (2%)	52,75,75	1.49	8 (15%)
7	MRD	N	2565	-	7,7,7	0.22	0	9,10,10	0.36	0
5	MPD	Q	2567	-	7,7,7	0.28	0	9,10,10	0.37	0
5	MPD	S	1697	-	7,7,7	0.27	0	9,10,10	0.24	0
2	COA	J	780	4	41,50,50	1.12	2 (4%)	52,75,75	1.43	7 (13%)
5	MPD	P	1425	-	7,7,7	0.27	0	9,10,10	0.25	0
2	COA	W	2105	4	41,50,50	1.05	1 (2%)	52,75,75	1.45	6 (11%)
5	MPD	A	2570	-	7,7,7	0.27	0	9,10,10	0.19	0
8	A3P	O	2575[B]	-	26,29,29	0.94	1 (3%)	31,45,45	1.24	3 (9%)
5	MPD	R	2566	-	7,7,7	0.24	0	9,10,10	0.24	0
7	MRD	L	2562	-	7,7,7	0.35	0	9,10,10	0.28	0
2	COA	X	1944	4	41,50,50	0.99	1 (2%)	52,75,75	1.43	9 (17%)
2	COA	W	2019	4	41,50,50	1.06	1 (2%)	52,75,75	1.43	9 (17%)
6	ACT	K	629	4	1,3,3	1.23	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	COA	A	127	4	41,50,50	1.13	2 (4%)	52,75,75	1.48	11 (21%)
5	MPD	H	631	-	7,7,7	0.23	0	9,10,10	0.29	0
2	COA	N	1221	4	41,50,50	1.05	1 (2%)	52,75,75	1.43	8 (15%)
2	COA	P	1424	4	41,50,50	1.10	1 (2%)	52,75,75	1.40	7 (13%)
6	ACT	K	2563	-	1,3,3	1.68	0	0,3,3	0.00	-
5	MPD	O	1334	-	7,7,7	0.26	0	9,10,10	0.26	0
6	ACT	R	2595	4	1,3,3	2.12	1 (100%)	0,3,3	0.00	-
5	MPD	W	2106	-	7,7,7	0.29	0	9,10,10	0.21	0
2	COA	F	477	4	41,50,50	0.98	1 (2%)	52,75,75	1.36	8 (15%)
7	MRD	K	2564	-	7,7,7	0.30	0	9,10,10	0.49	0
2	COA	H	630	4	41,50,50	1.00	1 (2%)	52,75,75	1.53	9 (17%)
7	MRD	F	2559	-	7,7,7	0.27	0	9,10,10	0.27	0
2	COA	T	1791	4	41,50,50	1.01	2 (4%)	52,75,75	1.31	7 (13%)
6	ACT	A	2597	4	1,3,3	1.80	0	0,3,3	0.00	-
5	MPD	C	2571	-	7,7,7	0.28	0	9,10,10	0.33	0
2	COA	R	1606	4	41,50,50	1.06	1 (2%)	52,75,75	1.52	10 (19%)
2	COA	G	570	4	41,50,50	1.04	1 (2%)	52,75,75	1.40	9 (17%)
6	ACT	C	2598	-	1,3,3	1.91	0	0,3,3	0.00	-
2	COA	I	699	4	41,50,50	1.00	1 (2%)	52,75,75	1.54	12 (23%)
5	MPD	U	1698	-	7,7,7	0.31	0	9,10,10	0.25	0
6	ACT	E	2594	4	1,3,3	1.73	0	0,3,3	0.00	-
7	MRD	T	2569	-	7,7,7	0.29	0	9,10,10	0.16	0
2	COA	C	169	4	41,50,50	1.03	1 (2%)	52,75,75	1.49	10 (19%)
6	ACT	T	2568	4	1,3,3	1.24	0	0,3,3	0.00	-
5	MPD	M	2572	-	7,7,7	0.28	0	9,10,10	0.27	0
2	COA	L	1008	4	41,50,50	1.04	1 (2%)	52,75,75	1.47	10 (19%)
2	COA	E	387	4	41,50,50	1.11	1 (2%)	52,75,75	1.36	7 (13%)
7	MRD	D	2573	-	7,7,7	0.22	0	9,10,10	0.28	0
5	MPD	B	127	-	7,7,7	0.24	0	9,10,10	0.17	0
2	COA	D	283	4	41,50,50	1.05	2 (4%)	52,75,75	1.33	8 (15%)
2	COA	A	129	4	41,50,50	1.13	1 (2%)	52,75,75	1.40	4 (7%)
2	COA	K	900	4	41,50,50	0.90	1 (2%)	52,75,75	1.61	9 (17%)
2	COA	S	1696	4	41,50,50	1.08	1 (2%)	52,75,75	1.45	9 (17%)
2	COA	U	1854	4	41,50,50	1.02	1 (2%)	52,75,75	1.39	8 (15%)
6	ACT	W	2596	4	1,3,3	1.63	0	0,3,3	0.00	-
2	COA	N	1333[A]	-	41,50,50	1.00	1 (2%)	52,75,75	1.51	4 (7%)
2	COA	O	1127	4	41,50,50	1.05	1 (2%)	52,75,75	1.39	9 (17%)
5	MPD	G	571	-	7,7,7	0.24	0	9,10,10	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MPD	V	1945	-	7,7,7	0.23	0	9,10,10	0.24	0

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
5	MPD	I	2561	-	-	0/5/5/5	-
5	MPD	E	2560	-	-	0/5/5/5	-
2	COA	Q	1515	4	-	6/44/64/64	0/3/3/3
7	MRD	N	2565	-	-	3/5/5/5	-
5	MPD	Q	2567	-	-	1/5/5/5	-
5	MPD	S	1697	-	-	2/5/5/5	-
2	COA	J	780	4	-	5/44/64/64	0/3/3/3
5	MPD	P	1425	-	-	0/5/5/5	-
2	COA	W	2105	4	-	8/44/64/64	0/3/3/3
5	MPD	A	2570	-	-	0/5/5/5	-
8	A3P	O	2575[B]	-	-	8/11/31/31	0/3/3/3
7	MRD	L	2562	-	-	0/5/5/5	-
2	COA	X	1944	4	-	6/44/64/64	0/3/3/3
5	MPD	H	631	-	-	1/5/5/5	-
2	COA	A	127	4	-	7/44/64/64	0/3/3/3
2	COA	W	2019	4	-	12/44/64/64	0/3/3/3
2	COA	N	1221	4	-	8/44/64/64	0/3/3/3
2	COA	P	1424	4	-	15/44/64/64	0/3/3/3
5	MPD	W	2106	-	-	2/5/5/5	-
2	COA	F	477	4	-	9/44/64/64	0/3/3/3
7	MRD	K	2564	-	-	2/5/5/5	-
2	COA	H	630	4	-	12/44/64/64	0/3/3/3
7	MRD	F	2559	-	-	0/5/5/5	-
2	COA	T	1791	4	-	4/44/64/64	0/3/3/3
2	COA	L	1008	4	-	3/44/64/64	0/3/3/3
5	MPD	C	2571	-	-	0/5/5/5	-
2	COA	R	1606	4	-	5/44/64/64	0/3/3/3
2	COA	G	570	4	-	5/44/64/64	0/3/3/3
5	MPD	R	2566	-	-	0/5/5/5	-
2	COA	I	699	4	-	6/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	U	1698	-	-	2/5/5/5	-
7	MRD	T	2569	-	-	0/5/5/5	-
2	COA	C	169	4	-	7/44/64/64	0/3/3/3
5	MPD	O	1334	-	-	1/5/5/5	-
5	MPD	M	2572	-	-	3/5/5/5	-
5	MPD	V	1945	-	-	0/5/5/5	-
2	COA	E	387	4	-	8/44/64/64	0/3/3/3
7	MRD	D	2573	-	-	1/5/5/5	-
5	MPD	B	127	-	-	2/5/5/5	-
2	COA	D	283	4	-	4/44/64/64	0/3/3/3
2	COA	A	129	4	-	10/44/64/64	0/3/3/3
2	COA	K	900	4	-	3/44/64/64	0/3/3/3
2	COA	S	1696	4	-	13/44/64/64	0/3/3/3
2	COA	U	1854	4	-	7/44/64/64	0/3/3/3
2	COA	N	1333[A]	-	-	17/44/64/64	0/3/3/3
2	COA	O	1127	4	-	8/44/64/64	0/3/3/3
5	MPD	G	571	-	-	0/5/5/5	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1515	COA	O9P-C9P	5.36	1.34	1.23
2	A	129	COA	O9P-C9P	5.35	1.34	1.23
2	E	387	COA	O9P-C9P	5.21	1.33	1.23
2	P	1424	COA	O9P-C9P	5.18	1.33	1.23
2	N	1333[A]	COA	O9P-C9P	5.13	1.33	1.23
2	N	1221	COA	O9P-C9P	5.13	1.33	1.23
2	G	570	COA	O9P-C9P	5.08	1.33	1.23
2	S	1696	COA	O9P-C9P	5.07	1.33	1.23
2	T	1791	COA	O9P-C9P	5.07	1.33	1.23
2	A	127	COA	O9P-C9P	5.05	1.33	1.23
2	I	699	COA	O9P-C9P	5.03	1.33	1.23
2	W	2019	COA	O9P-C9P	4.99	1.33	1.23
2	X	1944	COA	O9P-C9P	4.98	1.33	1.23
2	W	2105	COA	O9P-C9P	4.97	1.33	1.23
2	O	1127	COA	O9P-C9P	4.95	1.33	1.23
2	H	630	COA	O9P-C9P	4.92	1.33	1.23
2	R	1606	COA	O9P-C9P	4.89	1.33	1.23
2	C	169	COA	O9P-C9P	4.87	1.33	1.23
2	J	780	COA	O9P-C9P	4.86	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1008	COA	O9P-C9P	4.80	1.32	1.23
2	F	477	COA	O9P-C9P	4.76	1.32	1.23
2	U	1854	COA	O9P-C9P	4.71	1.32	1.23
2	D	283	COA	O9P-C9P	4.60	1.32	1.23
2	K	900	COA	O9P-C9P	3.68	1.30	1.23
2	J	780	COA	C2A-N3A	2.70	1.36	1.32
2	D	283	COA	P3B-O3B	2.56	1.64	1.59
8	O	2575[B]	A3P	C5-C4	2.37	1.47	1.40
2	T	1791	COA	C2A-N3A	2.18	1.35	1.32
6	R	2595	ACT	CH3-C	2.12	1.51	1.48
2	A	127	COA	P3B-O3B	2.02	1.63	1.59

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	1333[A]	COA	C7P-N8P-C9P	5.95	133.19	122.59
2	R	1606	COA	N3A-C2A-N1A	-5.09	120.72	128.68
2	W	2105	COA	N3A-C2A-N1A	-5.09	120.72	128.68
2	J	780	COA	N3A-C2A-N1A	-5.05	120.79	128.68
2	A	129	COA	C7P-N8P-C9P	5.02	131.54	122.59
2	U	1854	COA	N3A-C2A-N1A	-4.99	120.88	128.68
2	K	900	COA	N3A-C2A-N1A	-4.98	120.89	128.68
2	I	699	COA	N3A-C2A-N1A	-4.98	120.90	128.68
2	N	1221	COA	N3A-C2A-N1A	-4.94	120.96	128.68
2	C	169	COA	N3A-C2A-N1A	-4.90	121.02	128.68
2	H	630	COA	N3A-C2A-N1A	-4.85	121.10	128.68
2	S	1696	COA	N3A-C2A-N1A	-4.72	121.31	128.68
2	A	127	COA	N3A-C2A-N1A	-4.63	121.44	128.68
2	Q	1515	COA	N3A-C2A-N1A	-4.63	121.44	128.68
2	F	477	COA	N3A-C2A-N1A	-4.52	121.61	128.68
2	H	630	COA	C6P-C7P-N8P	-4.51	102.80	111.90
2	W	2019	COA	N3A-C2A-N1A	-4.47	121.69	128.68
2	T	1791	COA	N3A-C2A-N1A	-4.45	121.72	128.68
2	E	387	COA	N3A-C2A-N1A	-4.36	121.86	128.68
2	G	570	COA	N3A-C2A-N1A	-4.35	121.88	128.68
2	A	129	COA	N3A-C2A-N1A	-4.33	121.91	128.68
2	N	1333[A]	COA	N3A-C2A-N1A	-4.32	121.92	128.68
2	O	1127	COA	N3A-C2A-N1A	-4.30	121.96	128.68
2	S	1696	COA	C7P-N8P-C9P	4.28	130.22	122.59
2	X	1944	COA	N3A-C2A-N1A	-4.24	122.04	128.68
2	P	1424	COA	N3A-C2A-N1A	-4.20	122.11	128.68
2	K	900	COA	C2P-C3P-N4P	-4.11	102.90	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	1515	COA	C7P-N8P-C9P	4.11	129.93	122.59
2	W	2105	COA	CAP-C9P-N8P	4.03	124.61	116.58
2	L	1008	COA	N3A-C2A-N1A	-3.97	122.48	128.68
2	W	2019	COA	C3P-N4P-C5P	3.96	130.19	122.84
2	C	169	COA	C7P-N8P-C9P	3.74	129.25	122.59
2	D	283	COA	N3A-C2A-N1A	-3.71	122.89	128.68
2	X	1944	COA	C7P-N8P-C9P	3.59	128.98	122.59
2	Q	1515	COA	C6P-C7P-N8P	-3.51	104.82	111.90
2	D	283	COA	C7P-N8P-C9P	3.50	128.84	122.59
2	L	1008	COA	O5A-P2A-O4A	3.44	129.23	112.24
2	P	1424	COA	C7P-N8P-C9P	3.37	128.59	122.59
2	O	1127	COA	C6P-C7P-N8P	-3.36	105.10	111.90
2	R	1606	COA	C6P-C7P-N8P	-3.32	105.19	111.90
8	O	2575[B]	A3P	N3-C2-N1	-3.32	123.50	128.68
2	N	1221	COA	C6P-C7P-N8P	-3.29	105.25	111.90
2	K	900	COA	CEP-CBP-CAP	3.26	114.47	108.82
2	N	1221	COA	C3P-N4P-C5P	3.22	128.81	122.84
2	T	1791	COA	C2P-C3P-N4P	-3.20	104.98	112.31
2	C	169	COA	C3P-N4P-C5P	3.20	128.77	122.84
2	E	387	COA	C3P-N4P-C5P	3.18	128.74	122.84
2	H	630	COA	C3P-N4P-C5P	3.08	128.56	122.84
2	K	900	COA	CDP-CBP-CAP	-3.06	103.52	108.82
2	J	780	COA	O5A-P2A-O4A	3.04	127.25	112.24
2	N	1333[A]	COA	C2P-C3P-N4P	-2.98	105.50	112.31
2	X	1944	COA	C3P-N4P-C5P	2.97	128.34	122.84
2	F	477	COA	C2P-C3P-N4P	-2.96	105.54	112.31
2	C	169	COA	O5A-P2A-O4A	2.90	126.56	112.24
2	W	2019	COA	C7P-N8P-C9P	2.89	127.75	122.59
2	O	1127	COA	C2P-C3P-N4P	-2.87	105.74	112.31
2	L	1008	COA	C7P-N8P-C9P	2.85	127.68	122.59
2	R	1606	COA	O5A-P2A-O4A	2.85	126.34	112.24
2	A	127	COA	O9P-C9P-N8P	-2.83	116.91	122.99
2	S	1696	COA	C3P-N4P-C5P	2.81	128.06	122.84
2	X	1944	COA	C2P-C3P-N4P	-2.80	105.90	112.31
2	I	699	COA	C3P-N4P-C5P	2.80	128.04	122.84
2	R	1606	COA	C3P-N4P-C5P	2.78	128.00	122.84
2	G	570	COA	O2A-P1A-O1A	2.77	125.93	112.24
2	Q	1515	COA	O5A-P2A-O4A	2.76	125.90	112.24
2	A	127	COA	C4A-C5A-N7A	-2.76	106.53	109.40
2	K	900	COA	C7P-N8P-C9P	2.72	127.45	122.59
2	W	2105	COA	OAP-CAP-CBP	-2.71	103.88	110.25
2	W	2105	COA	C3P-N4P-C5P	2.70	127.86	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	1515	COA	O2A-P1A-O1A	2.70	125.59	112.24
2	U	1854	COA	O5A-P2A-O4A	2.69	125.55	112.24
2	U	1854	COA	C6P-C7P-N8P	-2.69	106.47	111.90
2	H	630	COA	O6A-CCP-CBP	2.67	114.83	110.55
2	C	169	COA	C2P-C3P-N4P	-2.66	106.22	112.31
2	S	1696	COA	C2P-C3P-N4P	-2.65	106.26	112.31
2	J	780	COA	C3P-N4P-C5P	2.65	127.75	122.84
2	I	699	COA	C2P-C3P-N4P	-2.63	106.30	112.31
2	K	900	COA	CDP-CBP-CCP	2.61	112.50	108.23
2	P	1424	COA	C3P-N4P-C5P	2.61	127.69	122.84
2	U	1854	COA	C3P-N4P-C5P	2.60	127.67	122.84
2	A	129	COA	C3P-N4P-C5P	2.60	127.66	122.84
2	I	699	COA	O5A-P2A-O4A	2.59	125.04	112.24
2	W	2019	COA	O5A-P2A-O4A	2.58	125.01	112.24
2	X	1944	COA	O5A-P2A-O4A	2.58	124.98	112.24
2	G	570	COA	C6P-C7P-N8P	-2.57	106.70	111.90
2	U	1854	COA	C7P-N8P-C9P	2.56	127.16	122.59
2	P	1424	COA	C2P-C3P-N4P	-2.56	106.46	112.31
2	Q	1515	COA	C3P-N4P-C5P	2.56	127.58	122.84
2	L	1008	COA	O2A-P1A-O1A	2.55	124.85	112.24
2	J	780	COA	C6P-C7P-N8P	-2.54	106.77	111.90
2	F	477	COA	O3B-P3B-O7A	-2.53	99.61	109.39
2	I	699	COA	C2B-C3B-C4B	-2.52	98.75	103.22
2	S	1696	COA	O5A-P2A-O4A	2.52	124.69	112.24
2	F	477	COA	C7P-N8P-C9P	2.51	127.07	122.59
2	T	1791	COA	C3P-N4P-C5P	2.51	127.50	122.84
2	R	1606	COA	C3B-C2B-C1B	2.51	105.45	99.89
2	O	1127	COA	C3P-N4P-C5P	2.50	127.48	122.84
2	E	387	COA	C7P-N8P-C9P	2.50	127.05	122.59
2	U	1854	COA	C2P-C3P-N4P	-2.48	106.64	112.31
2	A	127	COA	C2P-C3P-N4P	-2.48	106.64	112.31
8	O	2575[B]	A3P	C4-C5-N7	-2.47	106.82	109.40
2	R	1606	COA	C2P-C3P-N4P	-2.46	106.69	112.31
2	L	1008	COA	C2B-C3B-C4B	-2.46	98.87	103.22
2	W	2019	COA	C6P-C7P-N8P	-2.45	106.94	111.90
2	F	477	COA	C3P-N4P-C5P	2.45	127.38	122.84
2	A	127	COA	C7P-C6P-C5P	-2.44	108.30	112.36
2	R	1606	COA	C2B-C3B-C4B	-2.43	98.92	103.22
2	A	127	COA	O5A-P2A-O4A	2.42	124.19	112.24
2	X	1944	COA	C7P-C6P-C5P	-2.41	108.35	112.36
2	D	283	COA	C3P-N4P-C5P	2.40	127.29	122.84
2	A	127	COA	CAP-C9P-N8P	2.38	121.32	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	570	COA	C7P-N8P-C9P	2.37	126.81	122.59
2	I	699	COA	O2A-P1A-O1A	2.37	123.95	112.24
2	A	127	COA	C2B-C3B-C4B	-2.36	99.04	103.22
2	X	1944	COA	C4A-C5A-N7A	-2.36	106.94	109.40
2	C	169	COA	C6P-C7P-N8P	-2.35	107.16	111.90
2	L	1008	COA	O3B-P3B-O7A	-2.33	100.40	109.39
2	J	780	COA	O2A-P1A-O1A	2.33	123.75	112.24
2	I	699	COA	C6P-C7P-N8P	-2.32	107.21	111.90
2	G	570	COA	O5A-P2A-O4A	2.31	123.67	112.24
2	N	1221	COA	C2P-C3P-N4P	-2.31	107.03	112.31
2	L	1008	COA	C2P-C3P-N4P	-2.28	107.09	112.31
2	W	2105	COA	O9P-C9P-N8P	-2.28	118.09	122.99
2	H	630	COA	O5A-P2A-O4A	2.27	123.44	112.24
2	I	699	COA	CEP-CBP-CCP	-2.27	104.54	108.23
8	O	2575[B]	A3P	C3'-C2'-C1'	2.26	104.89	99.89
2	G	570	COA	C3P-N4P-C5P	2.25	127.01	122.84
2	R	1606	COA	O2A-P1A-O1A	2.25	123.34	112.24
2	Q	1515	COA	C2B-C3B-C4B	-2.24	99.25	103.22
2	P	1424	COA	C6P-C7P-N8P	-2.24	107.37	111.90
2	K	900	COA	C2B-C3B-C4B	-2.24	99.26	103.22
2	L	1008	COA	C7P-C6P-C5P	-2.23	108.64	112.36
2	P	1424	COA	O5A-P2A-O4A	2.23	123.25	112.24
2	N	1221	COA	C7P-N8P-C9P	2.22	126.55	122.59
2	C	169	COA	C3B-C2B-C1B	2.22	104.81	99.89
2	A	127	COA	C6P-C7P-N8P	-2.22	107.41	111.90
2	W	2019	COA	O2A-P1A-O1A	2.22	123.21	112.24
2	W	2105	COA	O3B-P3B-O7A	-2.21	100.84	109.39
2	O	1127	COA	C4A-C5A-N7A	-2.20	107.10	109.40
2	X	1944	COA	C2B-C3B-C4B	-2.20	99.32	103.22
2	X	1944	COA	O2A-P1A-O1A	2.19	123.09	112.24
2	G	570	COA	C2P-C3P-N4P	-2.19	107.30	112.31
2	N	1221	COA	C1B-N9A-C4A	-2.19	122.79	126.64
2	D	283	COA	O5A-P2A-O4A	2.19	123.05	112.24
2	O	1127	COA	C7P-N8P-C9P	2.19	126.49	122.59
2	W	2019	COA	C3B-C2B-C1B	2.18	104.73	99.89
2	T	1791	COA	C7P-C6P-C5P	-2.18	108.72	112.36
2	D	283	COA	C3B-C2B-C1B	2.17	104.70	99.89
2	F	477	COA	CAP-C9P-N8P	2.17	120.90	116.58
2	I	699	COA	O6A-CCP-CBP	2.16	114.03	110.55
2	T	1791	COA	C1B-N9A-C4A	-2.16	122.84	126.64
2	F	477	COA	C6P-C7P-N8P	-2.16	107.54	111.90
2	J	780	COA	CAP-C9P-N8P	2.16	120.88	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	630	COA	O2A-P1A-O1A	2.16	122.91	112.24
2	T	1791	COA	C4A-C5A-N7A	-2.15	107.16	109.40
2	S	1696	COA	C4A-C5A-N7A	-2.15	107.16	109.40
2	C	169	COA	C4A-C5A-N7A	-2.14	107.16	109.40
2	I	699	COA	C1B-N9A-C4A	-2.14	122.89	126.64
2	R	1606	COA	O9P-C9P-N8P	-2.14	118.41	122.99
2	N	1221	COA	O9P-C9P-N8P	-2.13	118.42	122.99
2	O	1127	COA	O5B-C5B-C4B	-2.13	101.67	108.99
2	K	900	COA	P2A-O3A-P1A	-2.13	125.53	132.83
2	C	169	COA	C2B-C3B-C4B	-2.12	99.46	103.22
2	A	127	COA	CEP-CBP-CAP	2.12	112.50	108.82
2	D	283	COA	C2P-C3P-N4P	-2.12	107.46	112.31
2	E	387	COA	O5A-P2A-O4A	2.12	122.71	112.24
2	Q	1515	COA	C3B-C2B-C1B	2.12	104.58	99.89
2	W	2019	COA	O5B-C5B-C4B	-2.11	101.72	108.99
2	I	699	COA	C7P-N8P-C9P	2.11	126.34	122.59
2	S	1696	COA	O2A-P1A-O1A	2.10	122.61	112.24
2	G	570	COA	O5B-C5B-C4B	-2.09	101.78	108.99
2	N	1333[A]	COA	CDP-CBP-CAP	2.09	112.45	108.82
2	W	2019	COA	C2B-C3B-C4B	-2.09	99.52	103.22
2	E	387	COA	CAP-C9P-N8P	2.09	120.74	116.58
2	S	1696	COA	C1B-N9A-C4A	-2.09	122.97	126.64
2	A	127	COA	C3P-N4P-C5P	2.09	126.71	122.84
2	H	630	COA	C2P-C3P-N4P	-2.09	107.54	112.31
2	D	283	COA	O2A-P1A-O1A	2.08	122.53	112.24
2	E	387	COA	O6A-CCP-CBP	2.08	113.89	110.55
2	L	1008	COA	C3P-N4P-C5P	2.08	126.69	122.84
2	H	630	COA	C2B-C3B-C4B	-2.07	99.55	103.22
2	N	1221	COA	CAP-C9P-N8P	2.07	120.70	116.58
2	L	1008	COA	O8A-P3B-O7A	2.07	118.79	110.68
2	I	699	COA	O9P-C9P-N8P	-2.07	118.55	122.99
2	F	477	COA	O5A-P2A-O4A	2.07	122.46	112.24
2	A	129	COA	C2B-C3B-C4B	-2.07	99.56	103.22
2	O	1127	COA	C2B-C3B-C4B	-2.06	99.56	103.22
2	O	1127	COA	C3B-C2B-C1B	2.06	104.44	99.89
2	G	570	COA	O6A-CCP-CBP	2.05	113.85	110.55
2	T	1791	COA	O9A-P3B-O8A	2.05	115.45	107.64
2	U	1854	COA	C2B-C3B-C4B	-2.04	99.60	103.22
2	D	283	COA	C4A-C5A-N7A	-2.04	107.27	109.40
2	J	780	COA	C2P-C3P-N4P	-2.04	107.65	112.31
2	R	1606	COA	CAP-C9P-N8P	2.04	120.63	116.58
2	K	900	COA	C3B-C2B-C1B	2.04	104.40	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	1854	COA	C1B-N9A-C4A	-2.03	123.07	126.64
2	E	387	COA	C2P-C3P-N4P	-2.02	107.68	112.31
2	S	1696	COA	P2A-O3A-P1A	-2.02	125.89	132.83
2	H	630	COA	C7P-N8P-C9P	2.01	126.18	122.59
2	C	169	COA	O2A-P1A-O1A	2.01	122.17	112.24
2	P	1424	COA	C2B-C3B-C4B	-2.00	99.67	103.22

There are no chirality outliers.

All (216) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	127	COA	C3B-O3B-P3B-O9A
2	A	127	COA	S1P-C2P-C3P-N4P
8	O	2575[B]	A3P	C3'-O3'-P1-O2P
8	O	2575[B]	A3P	C5'-O5'-P2-O4P
8	O	2575[B]	A3P	C5'-O5'-P2-O5P
8	O	2575[B]	A3P	C5'-O5'-P2-O6P
2	H	630	COA	C2P-C3P-N4P-C5P
2	T	1791	COA	C3B-O3B-P3B-O9A
2	C	169	COA	C3B-O3B-P3B-O9A
2	F	477	COA	C3B-O3B-P3B-O9A
2	F	477	COA	CCP-O6A-P2A-O4A
2	F	477	COA	S1P-C2P-C3P-N4P
2	O	1127	COA	CCP-O6A-P2A-O4A
2	O	1127	COA	S1P-C2P-C3P-N4P
2	R	1606	COA	S1P-C2P-C3P-N4P
2	E	387	COA	C2B-C3B-O3B-P3B
2	E	387	COA	C3B-O3B-P3B-O9A
2	E	387	COA	S1P-C2P-C3P-N4P
2	U	1854	COA	C3B-O3B-P3B-O9A
5	S	1697	MPD	C2-C3-C4-O4
2	J	780	COA	C2B-C3B-O3B-P3B
2	J	780	COA	C3B-O3B-P3B-O9A
2	J	780	COA	S1P-C2P-C3P-N4P
2	W	2019	COA	C3B-O3B-P3B-O9A
2	W	2019	COA	O9P-C9P-CAP-CBP
2	W	2019	COA	N8P-C9P-CAP-CBP
2	W	2019	COA	N8P-C9P-CAP-OAP
2	W	2019	COA	C5P-C6P-C7P-N8P
2	W	2019	COA	C2P-C3P-N4P-C5P
2	P	1424	COA	OAP-CAP-CBP-CCP
2	P	1424	COA	OAP-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
2	P	1424	COA	C9P-CAP-CBP-CDP
2	P	1424	COA	OAP-CAP-CBP-CEP
2	P	1424	COA	C9P-CAP-CBP-CEP
2	P	1424	COA	O9P-C9P-CAP-CBP
2	P	1424	COA	N8P-C9P-CAP-CBP
2	P	1424	COA	O9P-C9P-CAP-OAP
2	P	1424	COA	N8P-C9P-CAP-OAP
2	P	1424	COA	S1P-C2P-C3P-N4P
2	I	699	COA	S1P-C2P-C3P-N4P
2	N	1333[A]	COA	CCP-O6A-P2A-O3A
2	N	1333[A]	COA	CCP-O6A-P2A-O4A
2	N	1333[A]	COA	CCP-O6A-P2A-O5A
2	N	1333[A]	COA	CEP-CBP-CCP-O6A
2	N	1333[A]	COA	CAP-CBP-CCP-O6A
2	N	1333[A]	COA	C2P-C3P-N4P-C5P
2	N	1333[A]	COA	S1P-C2P-C3P-N4P
2	Q	1515	COA	S1P-C2P-C3P-N4P
7	N	2565	MRD	C2-C3-C4-C5
2	W	2105	COA	C3B-O3B-P3B-O9A
2	W	2105	COA	O9P-C9P-CAP-CBP
2	W	2105	COA	N8P-C9P-CAP-CBP
2	W	2105	COA	C2P-C3P-N4P-C5P
2	W	2105	COA	S1P-C2P-C3P-N4P
2	K	900	COA	C3B-O3B-P3B-O9A
2	N	1221	COA	C3B-O3B-P3B-O9A
2	N	1221	COA	CCP-O6A-P2A-O4A
2	N	1221	COA	S1P-C2P-C3P-N4P
2	G	570	COA	S1P-C2P-C3P-N4P
2	S	1696	COA	C3B-O3B-P3B-O9A
2	S	1696	COA	C5B-O5B-P1A-O1A
2	S	1696	COA	O9P-C9P-CAP-CBP
2	S	1696	COA	N8P-C9P-CAP-CBP
2	S	1696	COA	N8P-C9P-CAP-OAP
2	S	1696	COA	S1P-C2P-C3P-N4P
2	D	283	COA	C2B-C3B-O3B-P3B
2	D	283	COA	C3B-O3B-P3B-O9A
2	A	129	COA	O9P-C9P-CAP-CBP
2	A	129	COA	N8P-C9P-CAP-CBP
2	A	129	COA	N8P-C9P-CAP-OAP
2	A	129	COA	C5P-C6P-C7P-N8P
2	N	1333[A]	COA	C6P-C7P-N8P-C9P
2	S	1696	COA	C6P-C7P-N8P-C9P

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Mol	Chain	Res	Type	Atoms
8	O	2575[B]	A3P	C2'-C3'-O3'-P1
2	T	1791	COA	C2B-C3B-O3B-P3B
2	C	169	COA	C2B-C3B-O3B-P3B
2	F	477	COA	C2B-C3B-O3B-P3B
2	U	1854	COA	C2B-C3B-O3B-P3B
2	W	2019	COA	C2B-C3B-O3B-P3B
2	P	1424	COA	C2B-C3B-O3B-P3B
2	I	699	COA	C2B-C3B-O3B-P3B
2	N	1333[A]	COA	C2B-C3B-O3B-P3B
2	W	2105	COA	C2B-C3B-O3B-P3B
2	K	900	COA	C2B-C3B-O3B-P3B
2	N	1221	COA	C2B-C3B-O3B-P3B
2	G	570	COA	C2B-C3B-O3B-P3B
2	S	1696	COA	C2B-C3B-O3B-P3B
2	A	129	COA	C2B-C3B-O3B-P3B
2	C	169	COA	C6P-C7P-N8P-C9P
2	A	127	COA	C2B-C3B-O3B-P3B
2	X	1944	COA	C2B-C3B-O3B-P3B
2	H	630	COA	C2B-C3B-O3B-P3B
2	L	1008	COA	C2B-C3B-O3B-P3B
2	O	1127	COA	C2B-C3B-O3B-P3B
2	R	1606	COA	C2B-C3B-O3B-P3B
2	Q	1515	COA	C2B-C3B-O3B-P3B
2	N	1333[A]	COA	CDP-CBP-CCP-O6A
2	A	129	COA	C6P-C7P-N8P-C9P
2	A	127	COA	C4B-C3B-O3B-P3B
2	X	1944	COA	C4B-C3B-O3B-P3B
2	H	630	COA	C4B-C3B-O3B-P3B
2	L	1008	COA	C4B-C3B-O3B-P3B
2	O	1127	COA	C4B-C3B-O3B-P3B
2	R	1606	COA	C4B-C3B-O3B-P3B
2	W	2019	COA	C4B-C3B-O3B-P3B
2	N	1333[A]	COA	C4B-C3B-O3B-P3B
2	Q	1515	COA	C4B-C3B-O3B-P3B
2	G	570	COA	C4B-C3B-O3B-P3B
8	O	2575[B]	A3P	O4'-C4'-C5'-O5'
8	O	2575[B]	A3P	C3'-C4'-C5'-O5'
2	F	477	COA	C4B-C3B-O3B-P3B
2	A	129	COA	C4B-C3B-O3B-P3B
2	F	477	COA	C6P-C7P-N8P-C9P
2	W	2019	COA	O9P-C9P-CAP-OAP
2	N	1333[A]	COA	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	S	1696	COA	O9P-C9P-CAP-OAP
2	A	129	COA	O9P-C9P-CAP-OAP
8	O	2575[B]	A3P	C4'-C3'-O3'-P1
2	T	1791	COA	C4B-C3B-O3B-P3B
2	C	169	COA	C4B-C3B-O3B-P3B
2	E	387	COA	C4B-C3B-O3B-P3B
2	U	1854	COA	C4B-C3B-O3B-P3B
2	J	780	COA	C4B-C3B-O3B-P3B
2	P	1424	COA	C4B-C3B-O3B-P3B
2	I	699	COA	C4B-C3B-O3B-P3B
2	W	2105	COA	C4B-C3B-O3B-P3B
2	K	900	COA	C4B-C3B-O3B-P3B
2	N	1221	COA	C4B-C3B-O3B-P3B
2	D	283	COA	C4B-C3B-O3B-P3B
2	H	630	COA	N8P-C9P-CAP-CBP
2	C	169	COA	N8P-C9P-CAP-CBP
2	H	630	COA	S1P-C2P-C3P-N4P
2	C	169	COA	S1P-C2P-C3P-N4P
2	F	477	COA	P1A-O3A-P2A-O6A
5	M	2572	MPD	O2-C2-C3-C4
7	K	2564	MRD	O2-C2-C3-C4
2	E	387	COA	C6P-C7P-N8P-C9P
2	W	2105	COA	N8P-C9P-CAP-OAP
2	H	630	COA	C5P-C6P-C7P-N8P
2	A	127	COA	C5B-O5B-P1A-O3A
2	X	1944	COA	C3B-O3B-P3B-O8A
2	X	1944	COA	C3B-O3B-P3B-O9A
2	L	1008	COA	C3B-O3B-P3B-O9A
2	O	1127	COA	C3B-O3B-P3B-O9A
2	R	1606	COA	C3B-O3B-P3B-O8A
2	R	1606	COA	C3B-O3B-P3B-O9A
2	P	1424	COA	C3B-O3B-P3B-O9A
2	I	699	COA	C3B-O3B-P3B-O9A
2	Q	1515	COA	C3B-O3B-P3B-O9A
2	N	1221	COA	CCP-O6A-P2A-O3A
2	G	570	COA	C3B-O3B-P3B-O9A
2	S	1696	COA	C5B-O5B-P1A-O3A
2	A	129	COA	C3B-O3B-P3B-O9A
2	A	127	COA	P1A-O3A-P2A-O4A
7	D	2573	MRD	C2-C3-C4-C5
2	F	477	COA	CCP-O6A-P2A-O5A
2	O	1127	COA	CCP-O6A-P2A-O5A

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Mol	Chain	Res	Type	Atoms
2	N	1221	COA	CCP-O6A-P2A-O5A
2	P	1424	COA	C9P-CAP-CBP-CCP
2	H	630	COA	CAP-CBP-CCP-O6A
5	W	2106	MPD	C1-C2-C3-C4
5	M	2572	MPD	C1-C2-C3-C4
5	M	2572	MPD	CM-C2-C3-C4
2	E	387	COA	CAP-CBP-CCP-O6A
2	U	1854	COA	CAP-CBP-CCP-O6A
5	U	1698	MPD	CM-C2-C3-C4
7	N	2565	MRD	CM-C2-C3-C4
7	K	2564	MRD	CM-C2-C3-C4
2	E	387	COA	CDP-CBP-CCP-O6A
2	S	1696	COA	C4B-C3B-O3B-P3B
2	X	1944	COA	OAP-CAP-CBP-CEP
2	N	1333[A]	COA	C5P-C6P-C7P-N8P
2	C	169	COA	O9P-C9P-CAP-CBP
2	N	1333[A]	COA	O9P-C9P-CAP-CBP
2	W	2019	COA	O5P-C5P-C6P-C7P
2	H	630	COA	CDP-CBP-CCP-O6A
2	U	1854	COA	CDP-CBP-CCP-O6A
2	U	1854	COA	N8P-C9P-CAP-CBP
2	N	1333[A]	COA	N8P-C9P-CAP-CBP
2	S	1696	COA	C3B-C4B-C5B-O5B
5	H	631	MPD	O2-C2-C3-C4
5	W	2106	MPD	O2-C2-C3-C4
5	O	1334	MPD	O2-C2-C3-C4
5	B	127	MPD	O2-C2-C3-C4
2	N	1333[A]	COA	N8P-C9P-CAP-OAP
2	H	630	COA	CEP-CBP-CCP-O6A
2	E	387	COA	CEP-CBP-CCP-O6A
2	X	1944	COA	OAP-CAP-CBP-CDP
2	H	630	COA	C3B-O3B-P3B-O8A
2	H	630	COA	OAP-CAP-CBP-CEP
2	F	477	COA	CCP-O6A-P2A-O3A
2	O	1127	COA	C3B-O3B-P3B-O8A
2	O	1127	COA	CCP-O6A-P2A-O3A
2	P	1424	COA	C3B-O3B-P3B-O8A
2	I	699	COA	C3B-O3B-P3B-O8A
2	N	1333[A]	COA	C3B-O3B-P3B-O8A
2	G	570	COA	C3B-O3B-P3B-O8A
2	A	129	COA	C3B-O3B-P3B-O8A
2	A	127	COA	P1A-O3A-P2A-O5A

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Mol	Chain	Res	Type	Atoms
2	Q	1515	COA	P2A-O3A-P1A-O2A
2	N	1221	COA	P1A-O3A-P2A-O4A
2	S	1696	COA	P1A-O3A-P2A-O4A
5	B	127	MPD	C2-C3-C4-C5
5	S	1697	MPD	C2-C3-C4-C5
2	J	780	COA	C6P-C7P-N8P-C9P
2	T	1791	COA	C5B-O5B-P1A-O1A
2	W	2019	COA	CDP-CBP-CCP-O6A
2	I	699	COA	CDP-CBP-CCP-O6A
2	Q	1515	COA	CDP-CBP-CCP-O6A
2	H	630	COA	O9P-C9P-CAP-CBP
2	U	1854	COA	O9P-C9P-CAP-CBP
2	D	283	COA	C6P-C7P-N8P-C9P
5	Q	2567	MPD	C2-C3-C4-O4
5	U	1698	MPD	C2-C3-C4-O4
7	N	2565	MRD	C2-C3-C4-O4
2	W	2019	COA	N4P-C5P-C6P-C7P

There are no ring outliers.

31 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2561	MPD	1	0
7	N	2565	MRD	3	0
5	Q	2567	MPD	1	0
5	S	1697	MPD	2	0
2	W	2105	COA	7	0
5	A	2570	MPD	2	0
8	O	2575[B]	A3P	1	0
2	X	1944	COA	3	0
2	W	2019	COA	5	0
6	K	629	ACT	1	0
2	A	127	COA	2	0
5	H	631	MPD	2	0
2	N	1221	COA	5	0
6	R	2595	ACT	1	0
2	F	477	COA	1	0
7	K	2564	MRD	4	0
2	H	630	COA	2	0
7	F	2559	MRD	3	0
6	A	2597	ACT	3	0
6	C	2598	ACT	3	0

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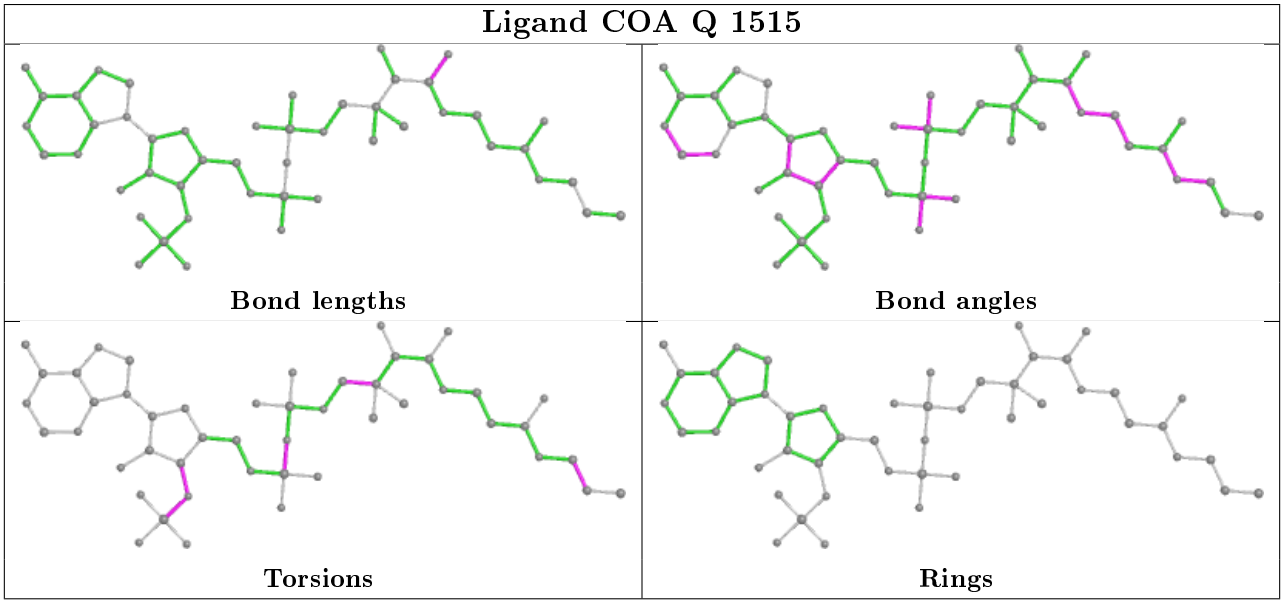
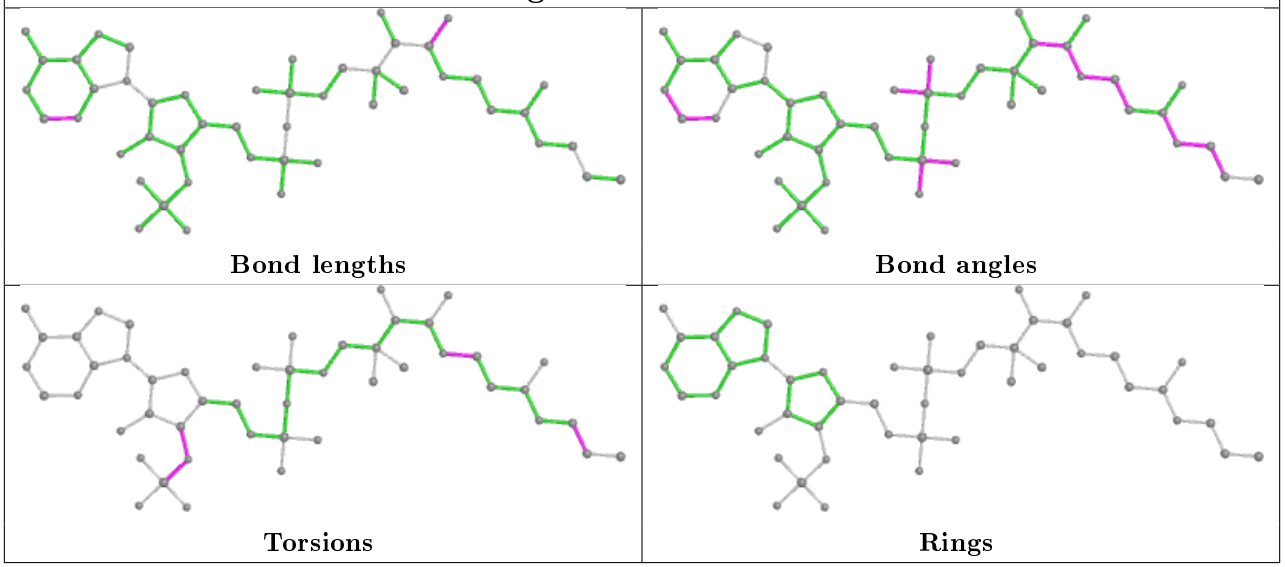
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	699	COA	1	0
5	U	1698	MPD	1	0
6	E	2594	ACT	1	0
6	T	2568	ACT	1	0
5	M	2572	MPD	6	0
7	D	2573	MRD	4	0
5	B	127	MPD	1	0
2	D	283	COA	2	0
2	A	129	COA	2	0
2	S	1696	COA	4	0
2	N	1333[A]	COA	3	0

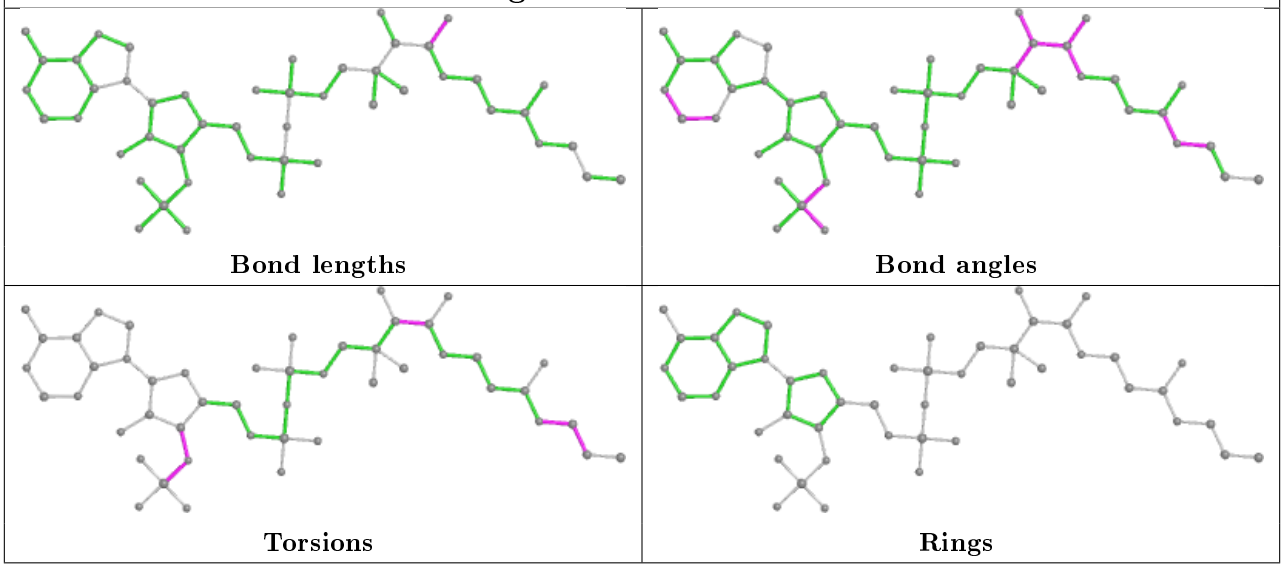
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



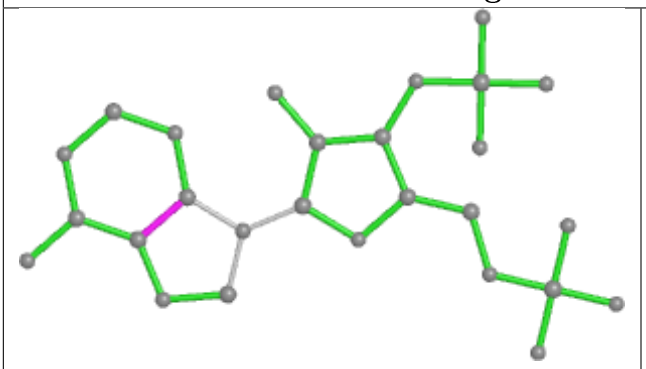
Ligand COA J 780



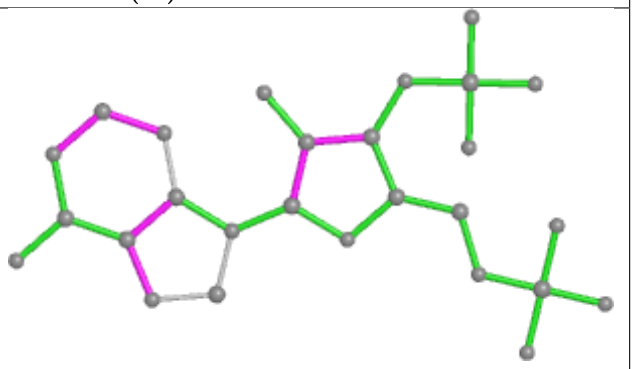
Ligand COA W 2105



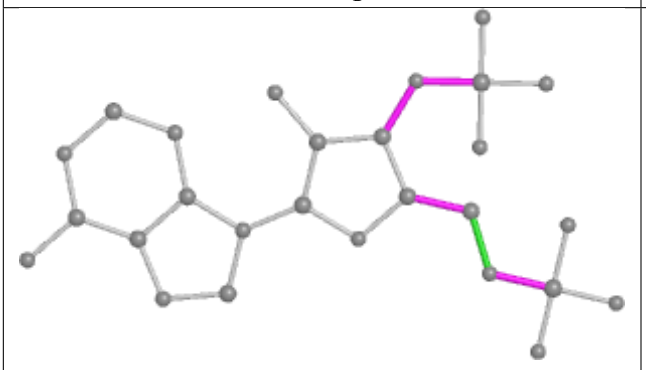
Ligand A3P O 2575 (B)



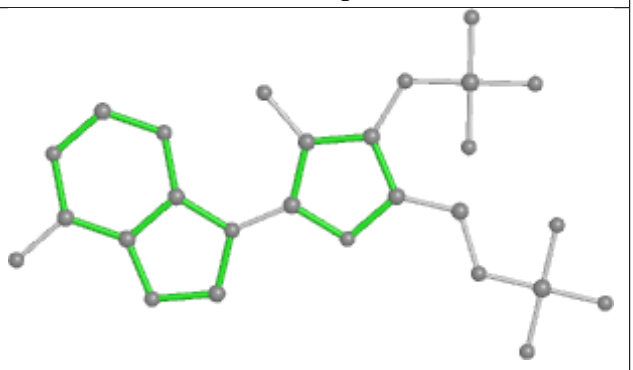
Bond lengths



Bond angles

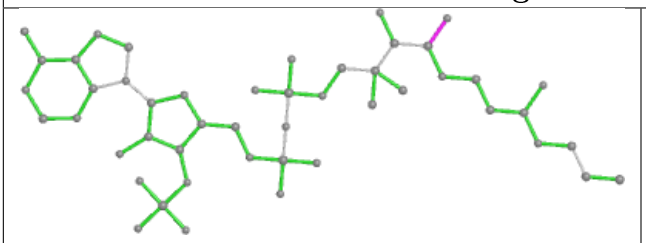


Torsions

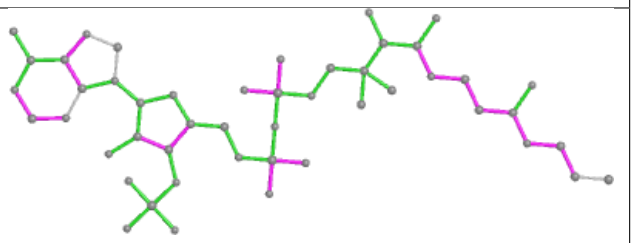


Rings

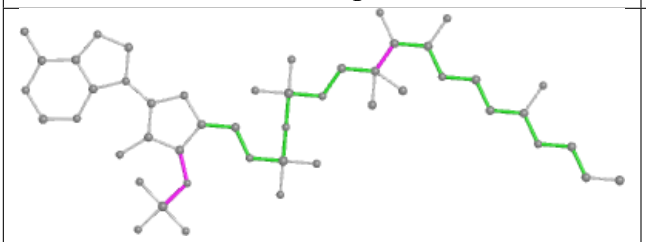
Ligand COA X 1944



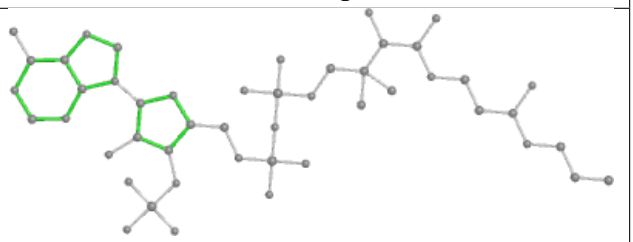
Bond lengths



Bond angles

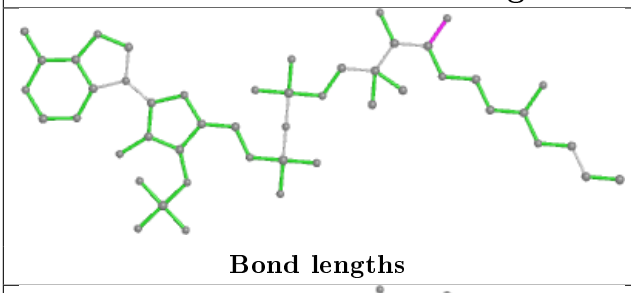


Torsions

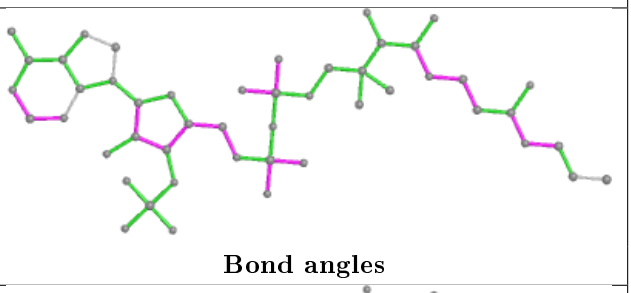


Rings

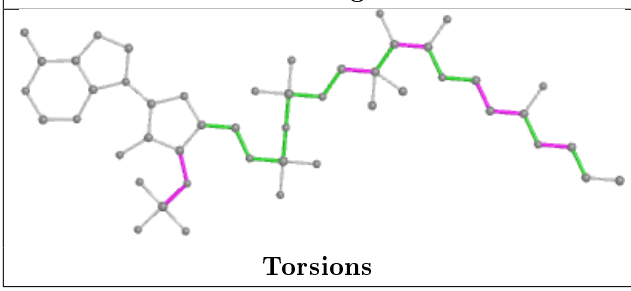
Ligand COA W 2019



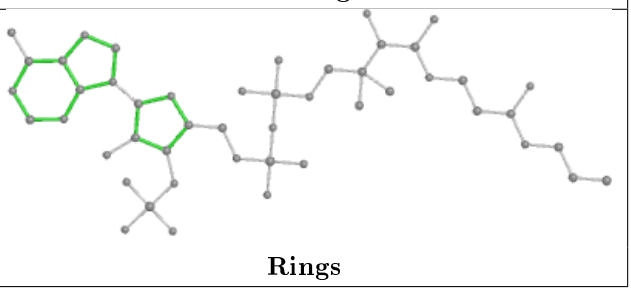
Bond lengths



Bond angles

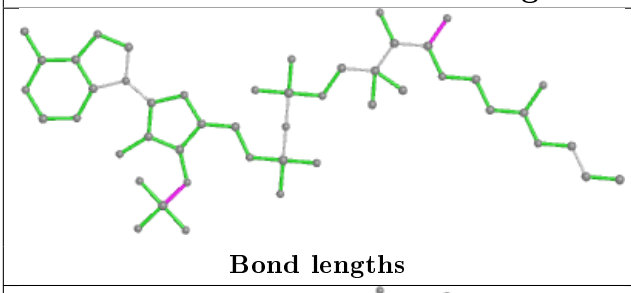


Torsions

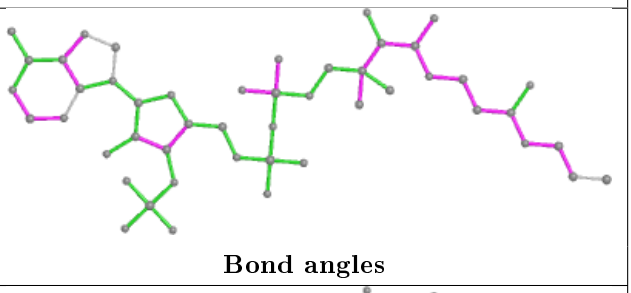


Rings

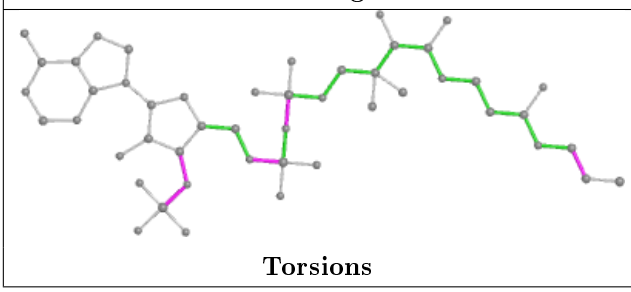
Ligand COA A 127



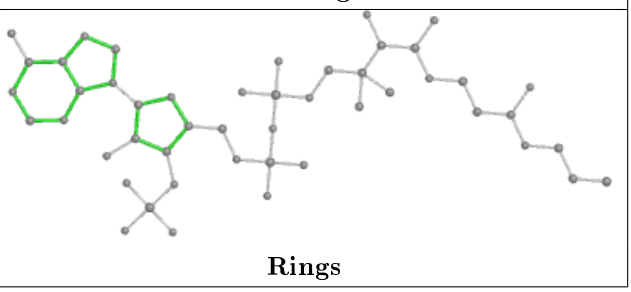
Bond lengths



Bond angles

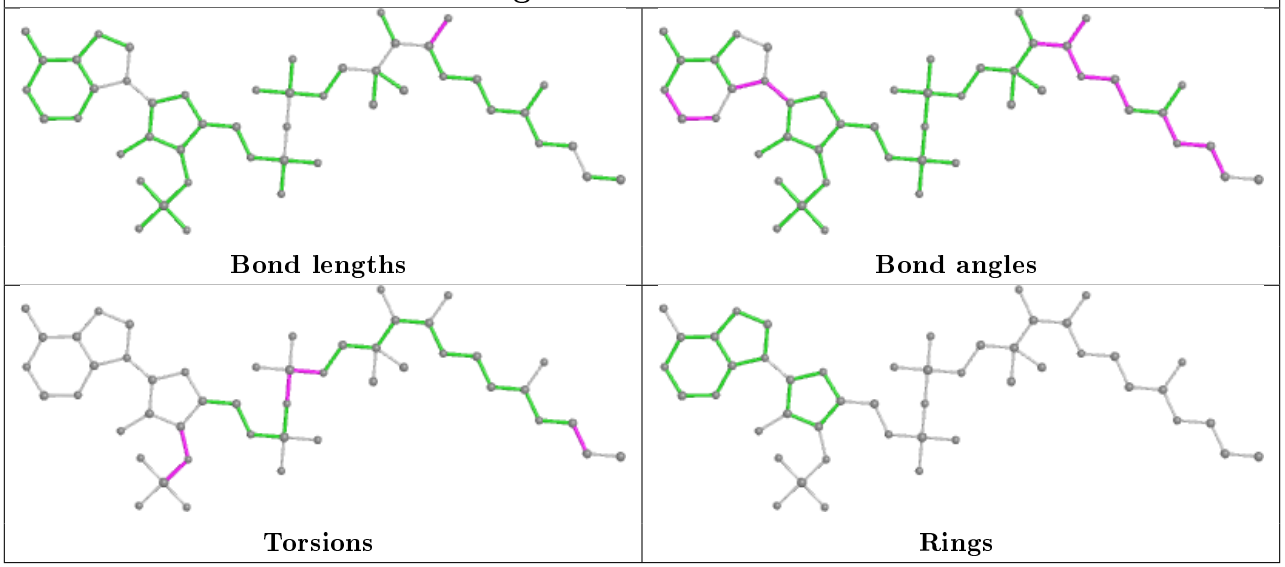


Torsions



Rings

Ligand COA N 1221



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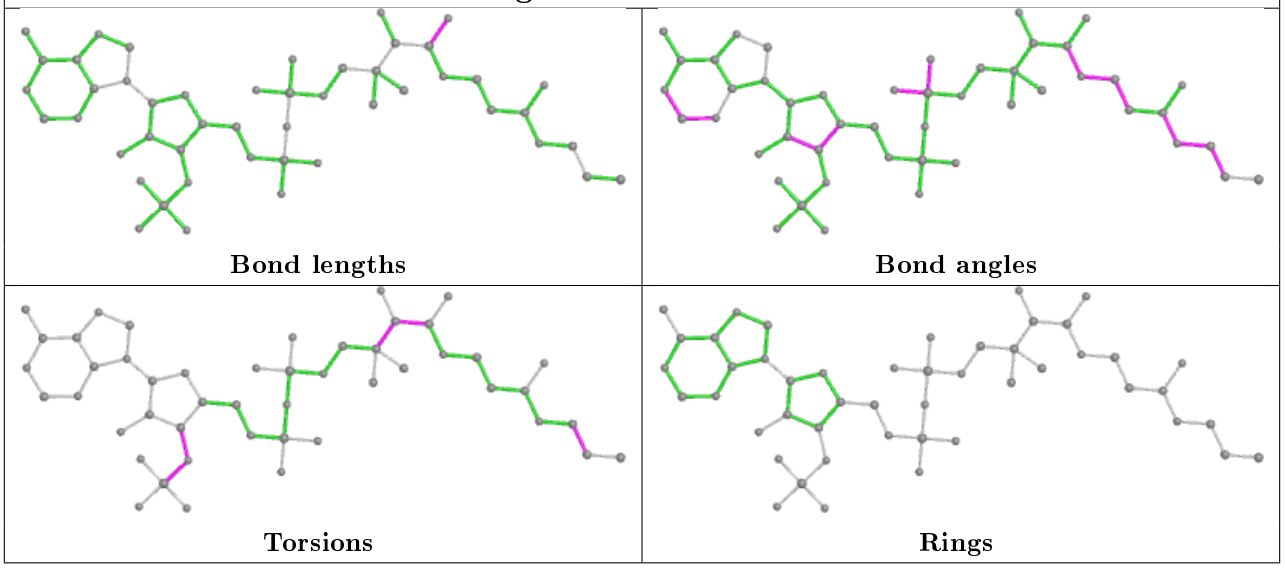
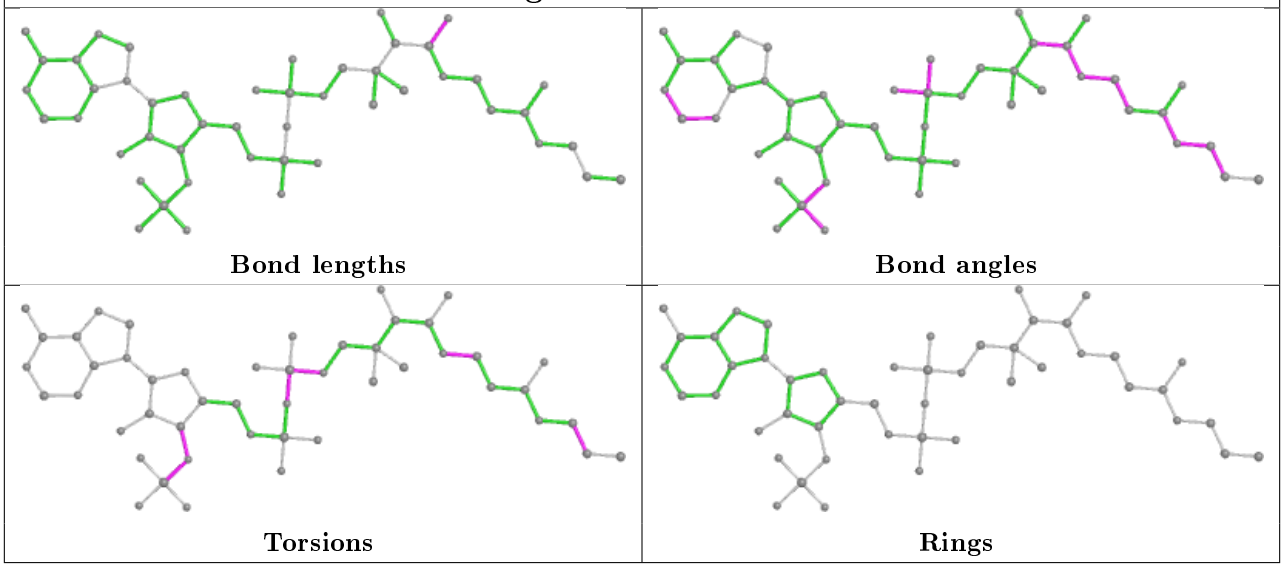
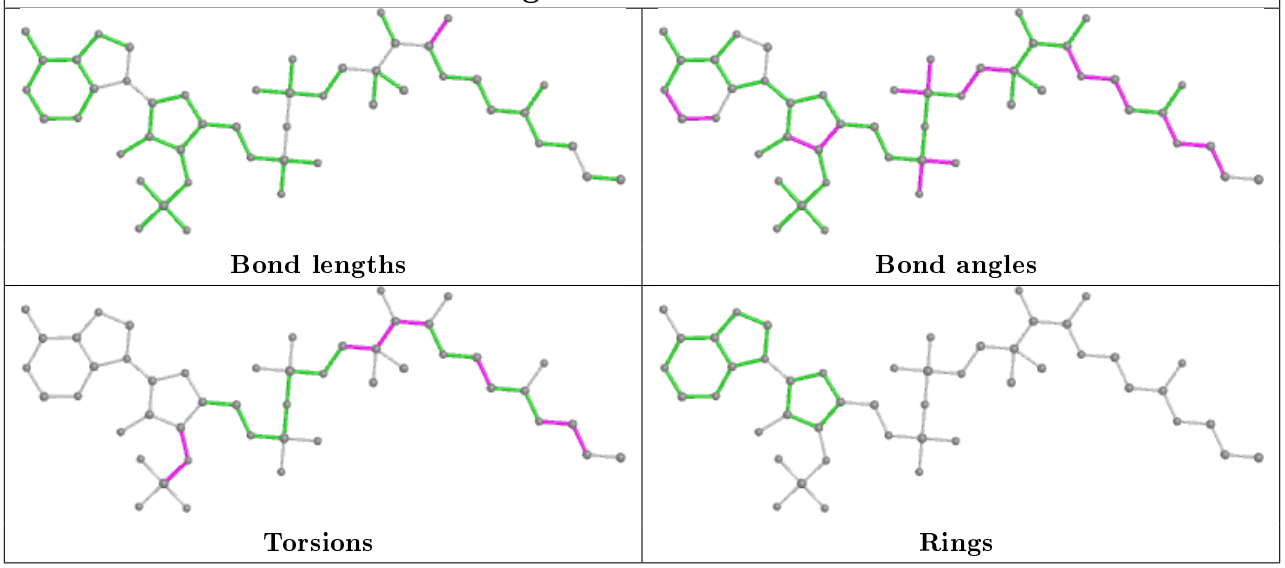


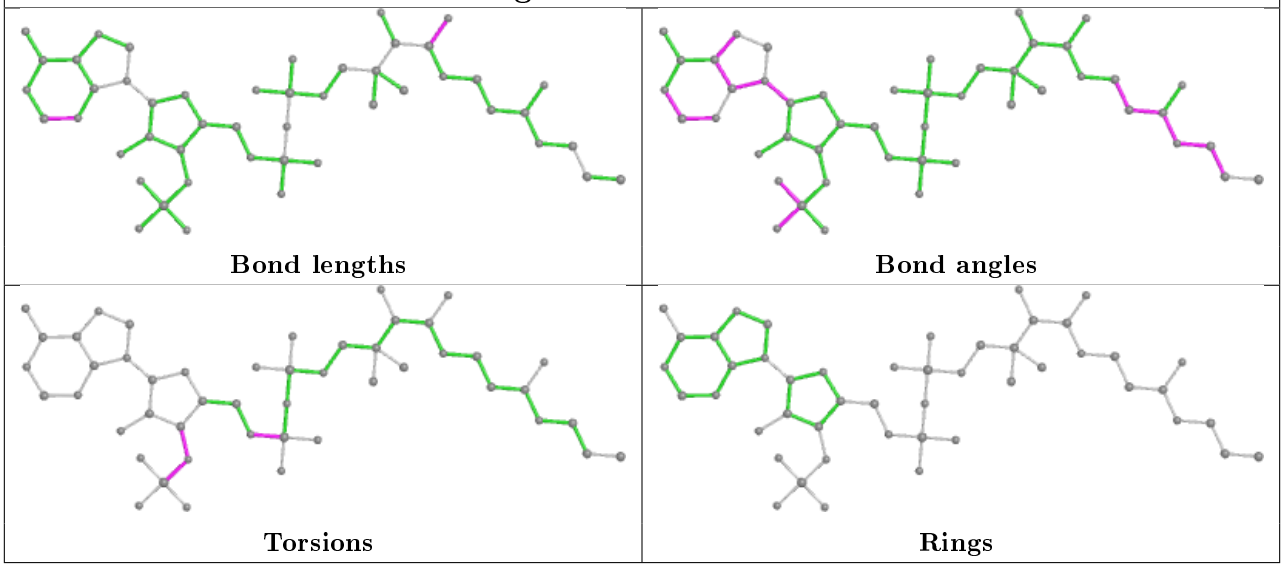
Ligand COA F 477



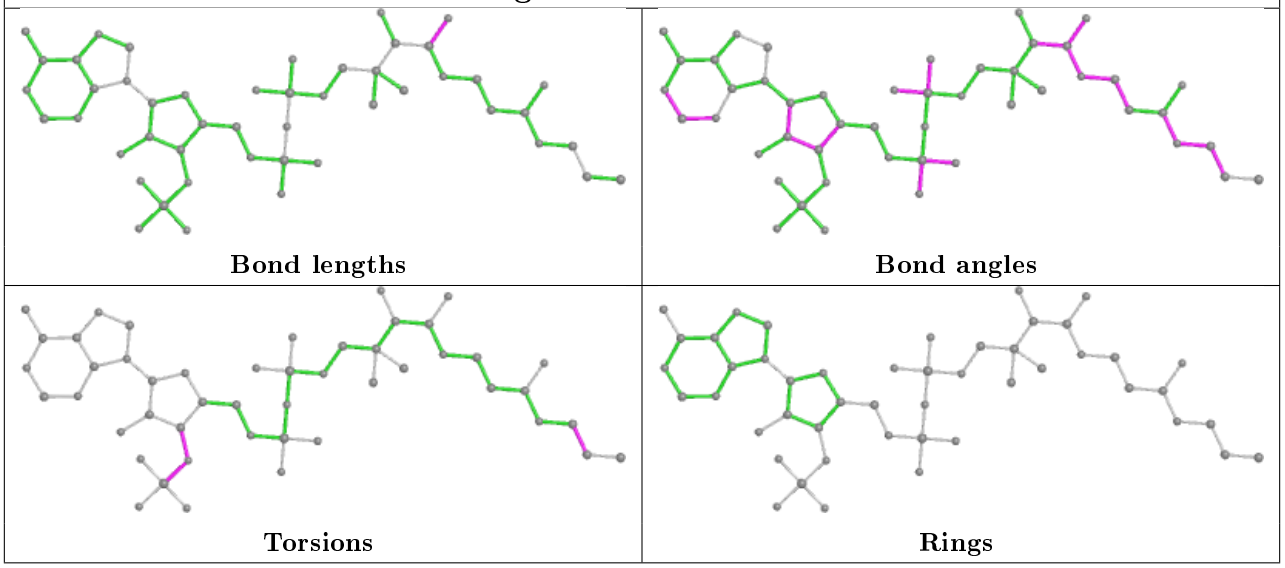
Ligand COA H 630



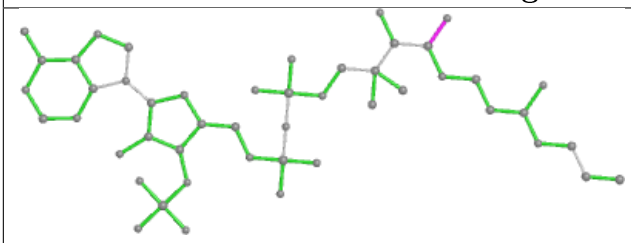
Ligand COA T 1791



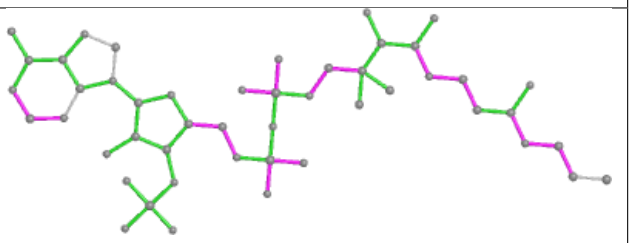
Ligand COA R 1606



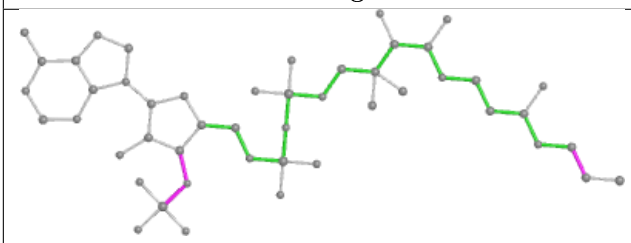
Ligand COA G 570



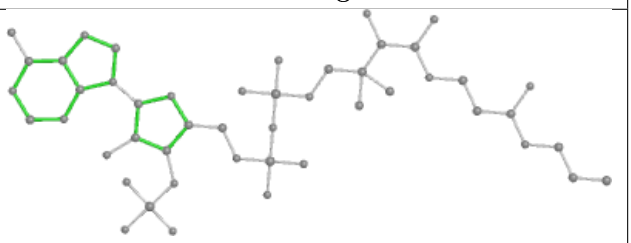
Bond lengths



Bond angles

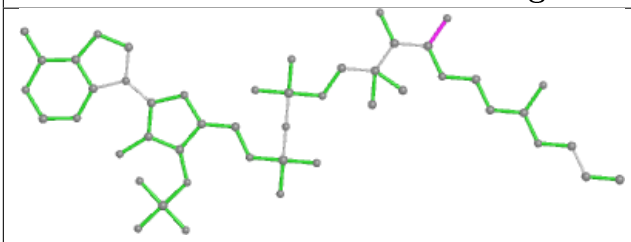


Torsions

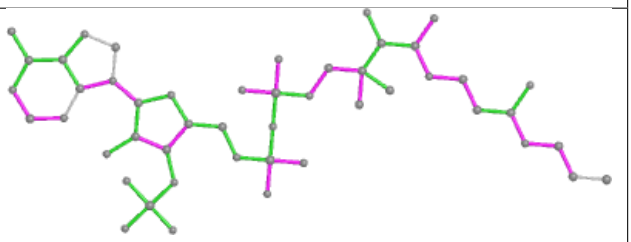


Rings

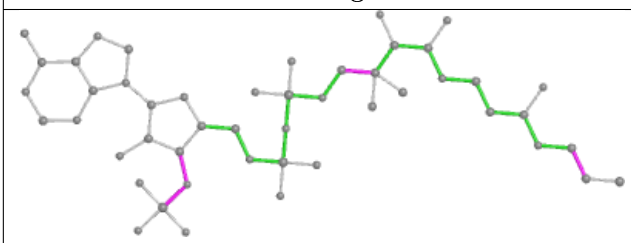
Ligand COA I 699



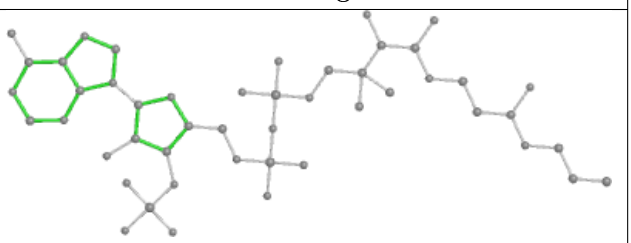
Bond lengths



Bond angles

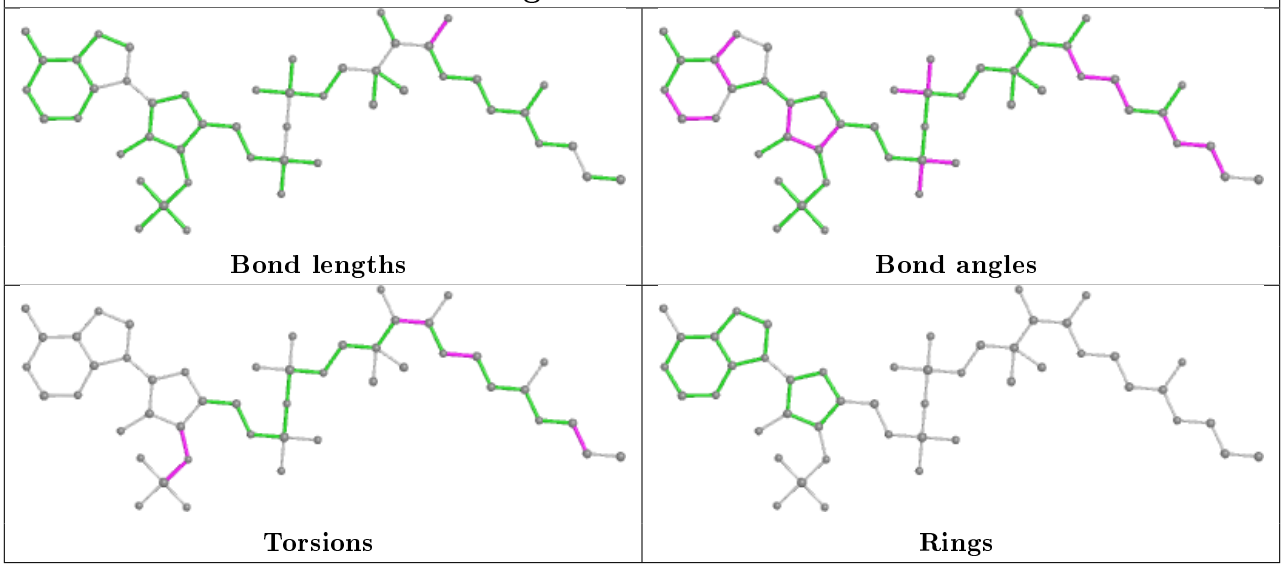


Torsions

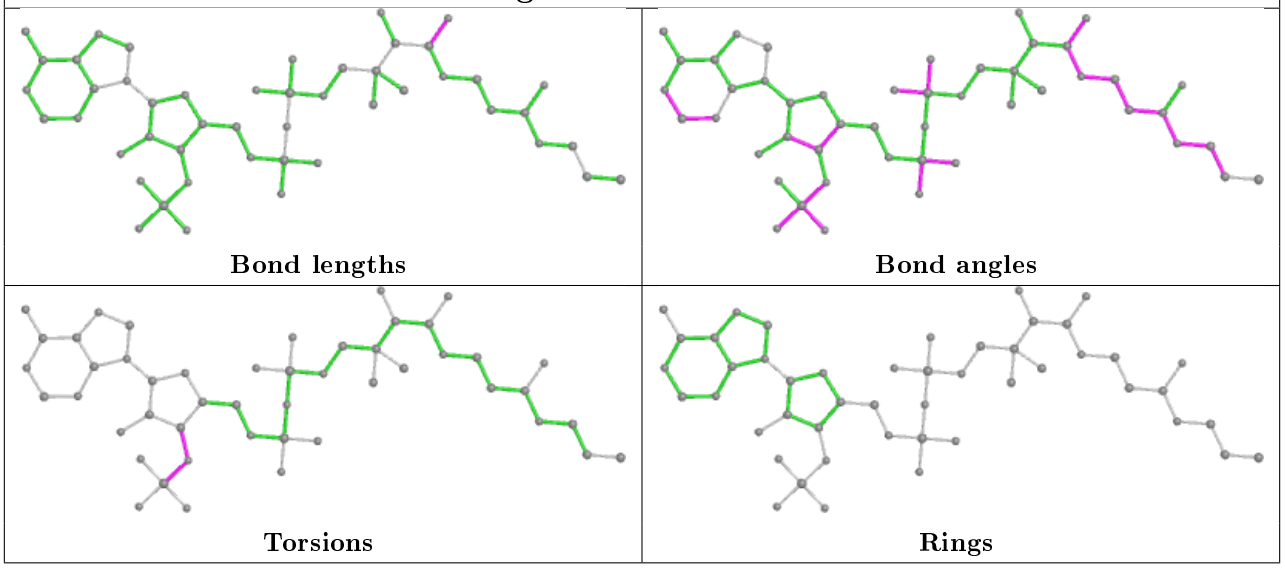


Rings

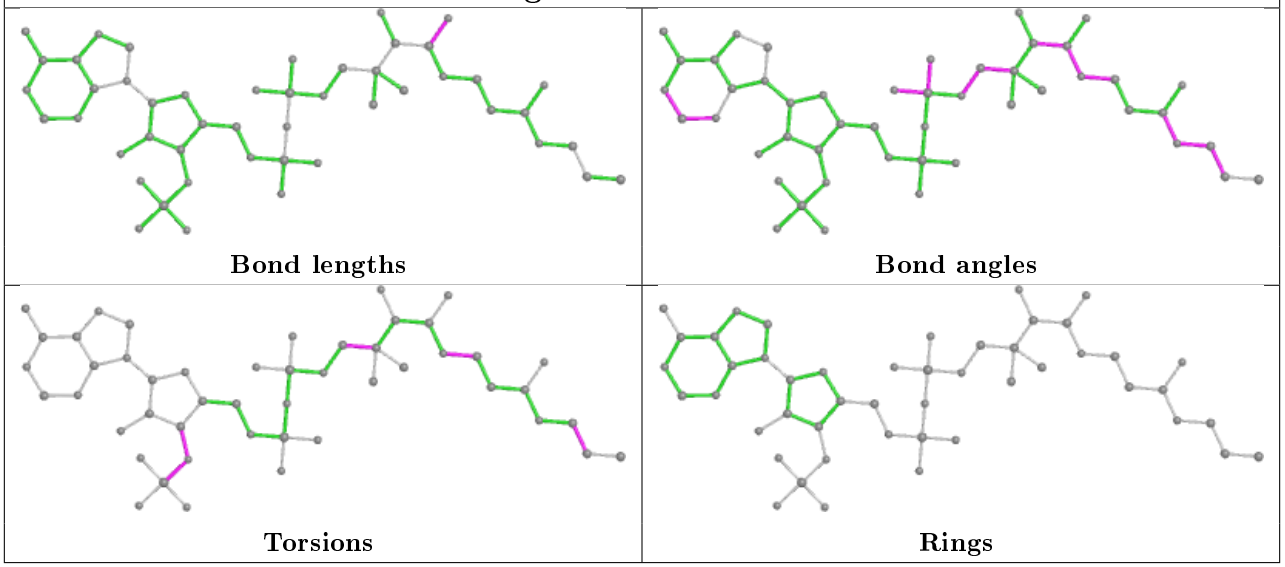
Ligand COA C 169



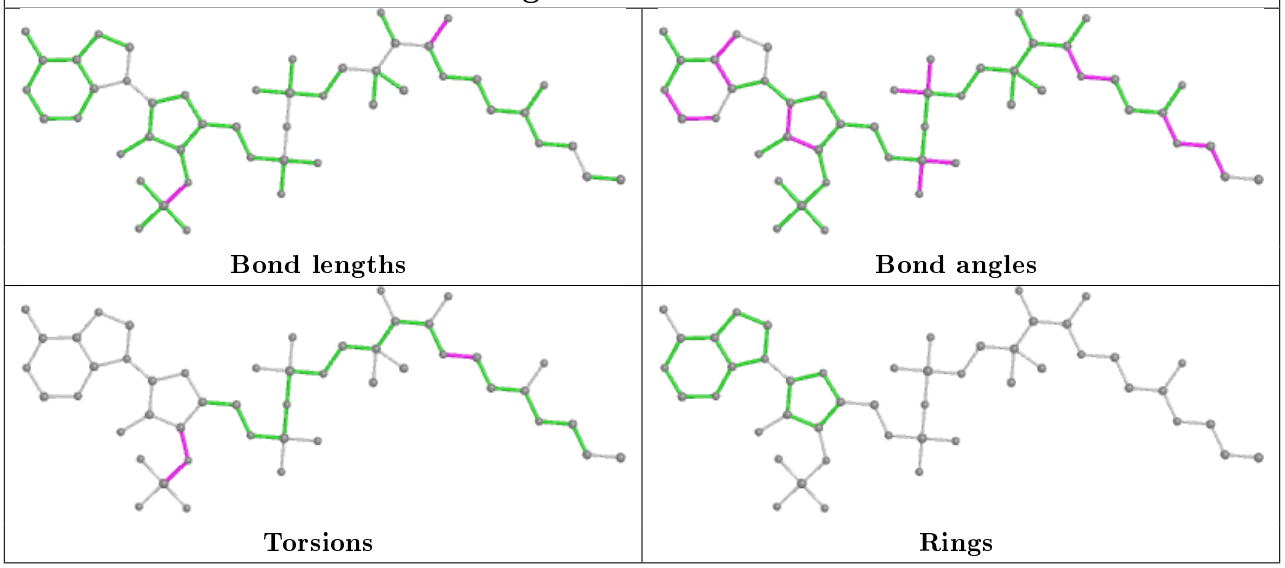
Ligand COA L 1008



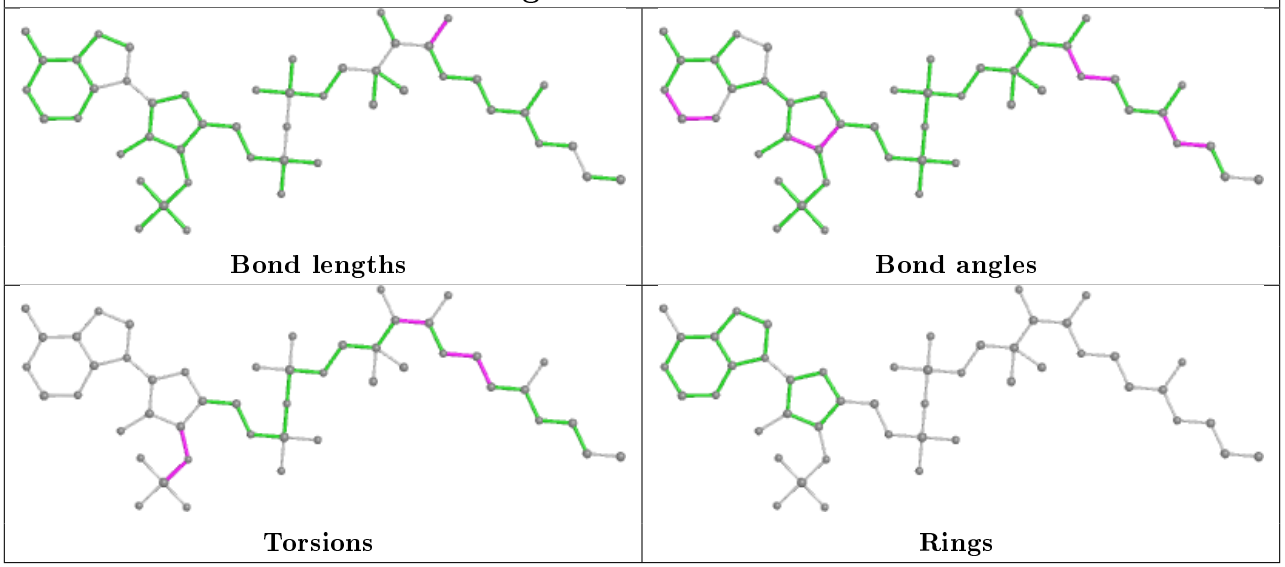
Ligand COA E 387



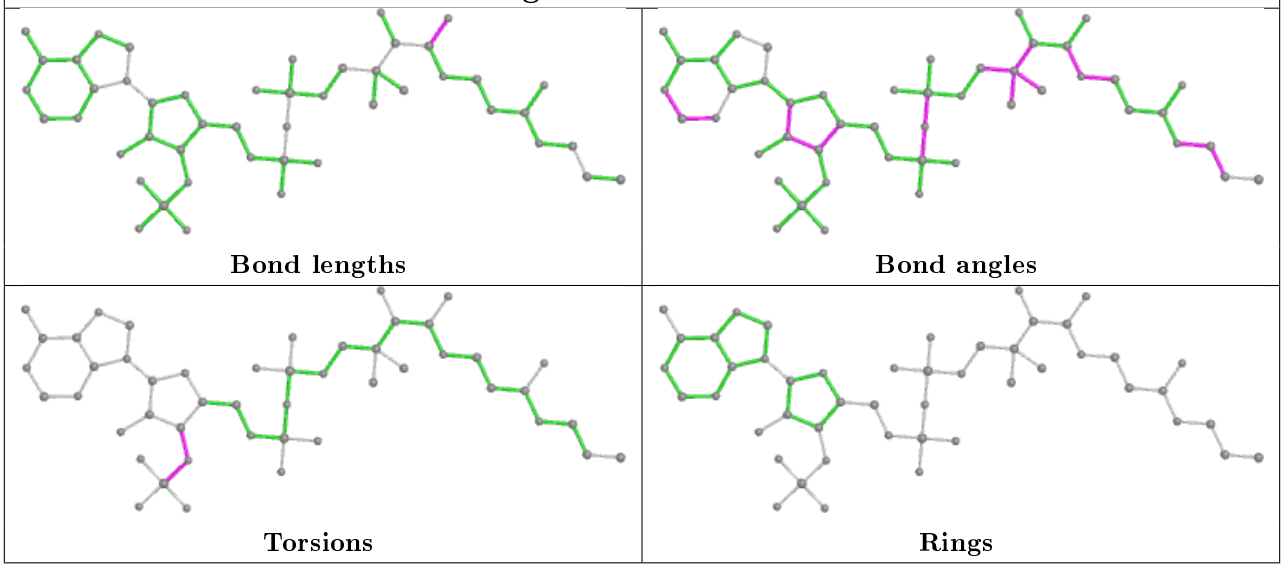
Ligand COA D 283



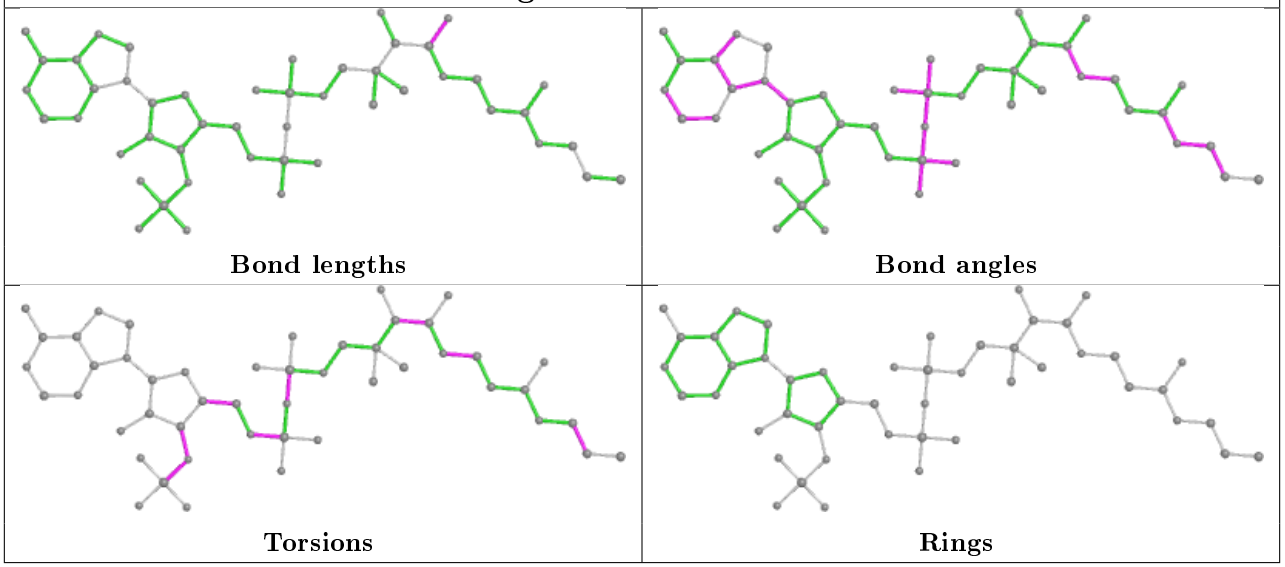
Ligand COA A 129



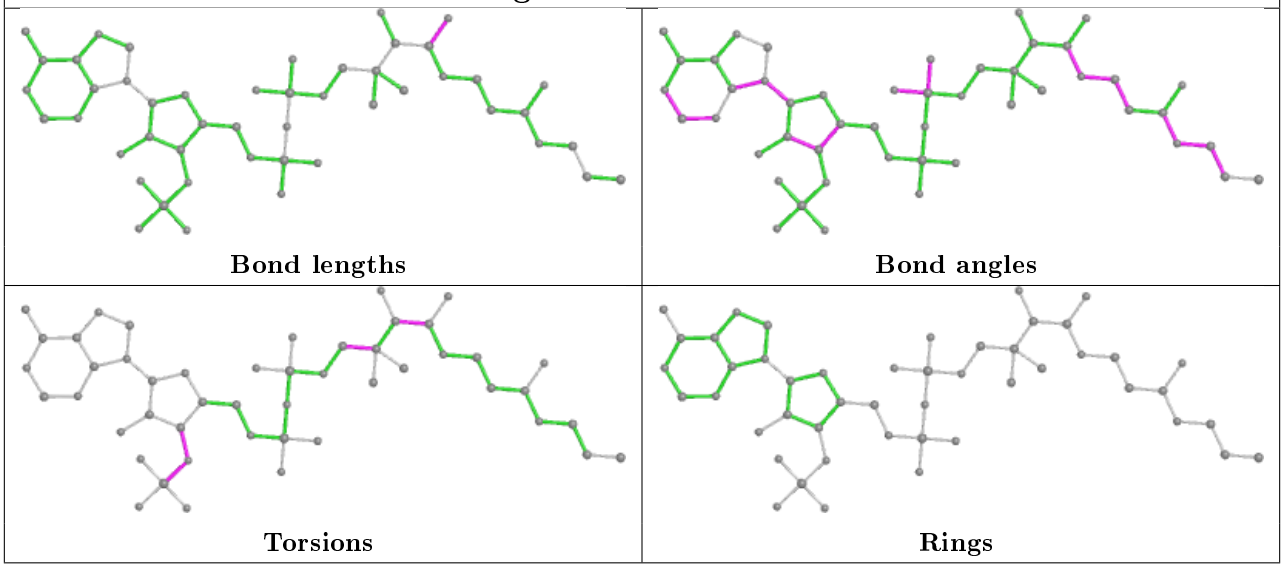
Ligand COA K 900

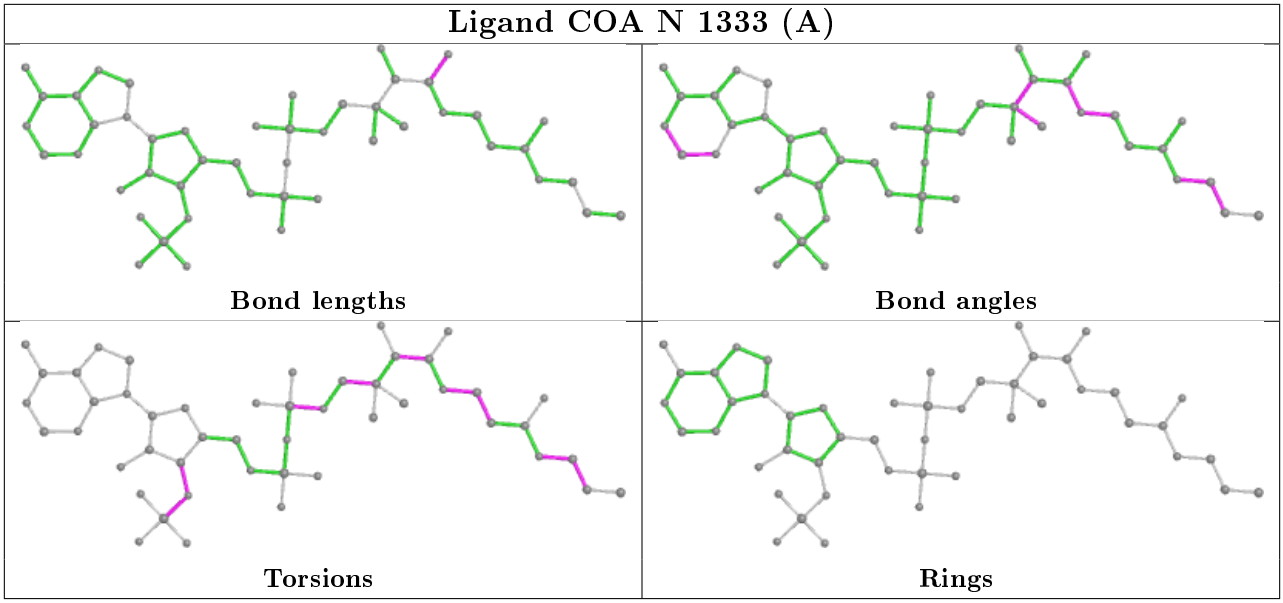


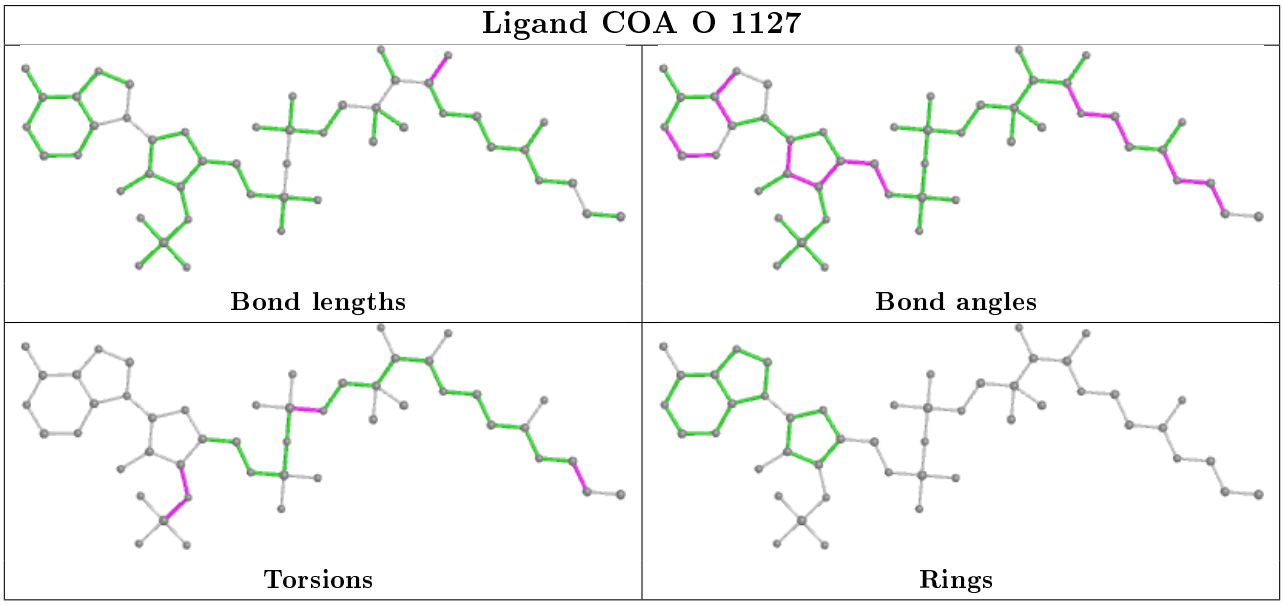
Ligand COA S 1696



Ligand COA U 1854







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, 95^{th} 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	124/129 (96%)	0.14	6 (4%)	30	29	15, 25, 37, 43	0
1	B	124/129 (96%)	0.17	8 (6%)	18	18	16, 26, 41, 47	0
1	C	124/129 (96%)	0.03	2 (1%)	72	72	12, 21, 36, 45	0
1	D	124/129 (96%)	-0.06	2 (1%)	72	72	15, 22, 35, 44	0
1	E	125/129 (96%)	0.18	6 (4%)	30	29	16, 24, 38, 56	0
1	F	124/129 (96%)	0.14	4 (3%)	47	45	16, 24, 37, 46	0
1	G	124/129 (96%)	0.26	3 (2%)	59	57	20, 34, 52, 59	0
1	H	124/129 (96%)	0.02	4 (3%)	47	45	19, 30, 47, 54	0
1	I	124/129 (96%)	-0.03	1 (0%)	86	86	18, 26, 39, 49	0
1	J	124/129 (96%)	-0.02	1 (0%)	86	86	13, 21, 35, 44	0
1	K	124/129 (96%)	0.09	2 (1%)	72	72	14, 23, 37, 46	0
1	L	124/129 (96%)	-0.06	2 (1%)	72	72	13, 21, 34, 46	0
1	M	124/129 (96%)	0.24	6 (4%)	30	29	15, 24, 37, 44	0
1	N	124/129 (96%)	0.01	3 (2%)	59	57	13, 21, 34, 45	0
1	O	125/129 (96%)	0.09	3 (2%)	59	57	16, 26, 42, 59	0
1	P	124/129 (96%)	0.05	3 (2%)	59	57	18, 27, 39, 49	0
1	Q	124/129 (96%)	-0.06	1 (0%)	86	86	17, 26, 37, 47	0
1	R	124/129 (96%)	0.03	6 (4%)	30	29	17, 26, 40, 48	0
1	S	123/129 (95%)	0.11	3 (2%)	59	57	17, 25, 39, 46	0
1	T	124/129 (96%)	0.19	4 (3%)	47	45	18, 30, 46, 52	0
1	U	124/129 (96%)	0.11	4 (3%)	47	45	14, 23, 37, 52	0
1	V	124/129 (96%)	0.11	4 (3%)	47	45	18, 28, 42, 50	0
1	W	123/129 (95%)	0.00	1 (0%)	86	86	17, 25, 39, 43	0
1	X	124/129 (96%)	0.07	2 (1%)	72	72	16, 26, 40, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	2976/3096 (96%)	0.08	81 (2%) 54 53	12, 25, 41, 63	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	0	ALA	7.9
1	X	126	ARG	7.0
1	E	126	ARG	7.0
1	J	0	ALA	6.4
1	O	126	ARG	5.9
1	C	0	ALA	4.9
1	G	0	ALA	4.6
1	K	0	ALA	4.5
1	B	0	ALA	4.4
1	A	0	ALA	4.2
1	U	0	ALA	4.2
1	P	0	ALA	4.1
1	F	0	ALA	4.0
1	Q	0	ALA	3.7
1	T	0	ALA	3.6
1	E	0	ALA	3.5
1	I	0	ALA	3.5
1	O	0	ALA	3.3
1	H	0	ALA	3.2
1	N	0	ALA	3.2
1	D	0	ALA	3.1
1	H	82[A]	LYS	3.0
1	M	0	ALA	3.0
1	L	0	ALA	3.0
1	B	125	ARG	3.0
1	R	0	ALA	2.9
1	H	125	ARG	2.8
1	T	83	LEU	2.7
1	E	7	THR	2.7
1	A	114[A]	ARG	2.6
1	F	55	ALA	2.6
1	X	5	LEU	2.6
1	A	7	THR	2.6
1	R	119	ALA	2.6
1	M	82[A]	LYS	2.6
1	S	102[A]	GLN	2.5
1	U	122	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	2.5
1	T	114[A]	ARG	2.5
1	C	21	ARG	2.4
1	G	82	LYS	2.4
1	M	5	LEU	2.4
1	K	120	THR	2.4
1	B	110	ILE	2.4
1	O	125	ARG	2.3
1	W	114	ARG	2.3
1	B	119	ALA	2.3
1	A	120	THR	2.3
1	B	104	GLU	2.3
1	S	121	VAL	2.3
1	R	110	ILE	2.3
1	E	119	ALA	2.3
1	T	5	LEU	2.3
1	A	121	VAL	2.3
1	U	5	LEU	2.2
1	M	21	ARG	2.2
1	V	104	GLU	2.2
1	V	125	ARG	2.2
1	B	58	ALA	2.2
1	R	114[A]	ARG	2.2
1	N	114	ARG	2.2
1	B	13[A]	GLU	2.2
1	B	121	VAL	2.2
1	F	114	ARG	2.1
1	R	7	THR	2.1
1	M	119	ALA	2.1
1	S	125	ARG	2.1
1	M	121	VAL	2.1
1	P	104	GLU	2.1
1	E	110	ILE	2.1
1	D	104	GLU	2.1
1	E	58	ALA	2.0
1	L	119	ALA	2.0
1	H	114[A]	ARG	2.0
1	N	104	GLU	2.0
1	G	125	ARG	2.0
1	R	125	ARG	2.0
1	U	121	VAL	2.0
1	F	58	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	9	ILE	2.0
1	V	5	LEU	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MPD	S	1697	8/8	0.67	0.28	65,66,68,68	0
6	ACT	R	2595	4/4	0.78	0.17	39,39,39,40	4
7	MRD	L	2562	8/8	0.80	0.16	43,45,46,47	0
6	ACT	K	2563	4/4	0.80	0.20	47,48,48,49	0
7	MRD	F	2559	8/8	0.80	0.26	73,73,74,74	0
6	ACT	C	2598	4/4	0.81	0.20	47,48,48,48	0
7	MRD	K	2564	8/8	0.81	0.25	57,59,59,59	0
6	ACT	W	2596	4/4	0.82	0.23	50,50,50,50	0
5	MPD	V	1945	8/8	0.86	0.21	53,54,54,54	0
6	ACT	A	2597	4/4	0.87	0.19	35,36,37,38	0
5	MPD	M	2572	8/8	0.89	0.22	63,63,64,64	0
5	MPD	W	2106	8/8	0.90	0.17	47,48,49,49	0
5	MPD	G	571	8/8	0.90	0.18	46,47,50,51	0
5	MPD	Q	2567	8/8	0.90	0.15	47,49,50,51	0
7	MRD	T	2569	8/8	0.90	0.16	46,48,49,49	0
5	MPD	U	1698	8/8	0.91	0.17	45,45,47,48	0
5	MPD	C	2571	8/8	0.91	0.16	52,53,54,54	0
4	CA	X	2550	1/1	0.91	0.08	50,50,50,50	1
5	MPD	A	2570	8/8	0.91	0.15	45,46,47,47	0
4	CA	M	2530	1/1	0.91	0.09	41,41,41,41	1
5	MPD	R	2566	8/8	0.91	0.12	46,48,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	E	2594	4/4	0.92	0.11	50,50,50,50	0
5	MPD	O	1334	8/8	0.92	0.10	55,56,57,58	0
5	MPD	E	2560	8/8	0.92	0.12	45,46,47,47	0
5	MPD	H	631	8/8	0.92	0.14	55,57,57,57	0
6	ACT	T	2568	4/4	0.92	0.13	54,55,55,55	0
6	ACT	K	629	4/4	0.93	0.11	45,46,46,46	0
5	MPD	I	2561	8/8	0.93	0.14	48,50,51,52	0
4	CA	N	2532	1/1	0.93	0.10	43,43,43,43	1
5	MPD	P	1425	8/8	0.93	0.13	49,49,51,51	0
5	MPD	B	127	8/8	0.93	0.11	51,52,54,54	0
4	CA	E	2554	1/1	0.93	0.14	44,44,44,44	1
7	MRD	D	2573	8/8	0.93	0.16	51,51,52,53	0
4	CA	X	2556	1/1	0.94	0.09	35,35,35,35	1
2	COA	N	1333[A]	48/48	0.94	0.15	24,44,68,69	48
4	CA	V	2557	1/1	0.94	0.10	47,47,47,47	0
2	COA	E	387	48/48	0.94	0.13	19,28,64,70	0
2	COA	W	2105	48/48	0.94	0.12	20,34,67,72	0
3	CL	L	2543	1/1	0.94	0.08	43,43,43,43	0
4	CA	U	2546	1/1	0.94	0.09	27,27,27,27	1
4	CA	Q	2535	1/1	0.94	0.08	35,35,35,35	1
4	CA	A	2514	1/1	0.94	0.10	36,36,36,36	1
2	COA	H	630	48/48	0.95	0.12	30,35,71,74	0
4	CA	W	2548	1/1	0.95	0.10	38,38,38,38	1
2	COA	I	699	48/48	0.95	0.12	22,30,66,69	0
2	COA	G	570	48/48	0.95	0.12	25,33,68,74	0
7	MRD	N	2565	8/8	0.95	0.10	45,46,47,48	0
4	CA	T	2545	1/1	0.95	0.06	29,29,29,29	1
2	COA	A	129	48/48	0.95	0.12	23,33,70,75	0
2	COA	F	477	48/48	0.96	0.11	20,30,57,65	0
2	COA	O	1127	48/48	0.96	0.11	21,29,65,71	0
2	COA	Q	1515	48/48	0.96	0.10	23,32,70,75	0
2	COA	X	1944	48/48	0.96	0.11	24,32,58,65	0
2	COA	C	169	48/48	0.96	0.12	18,26,68,73	0
4	CA	I	2525	1/1	0.96	0.07	31,31,31,31	1
2	COA	U	1854	48/48	0.96	0.11	21,29,67,72	0
2	COA	N	1221	48/48	0.96	0.11	18,28,68,72	0
2	COA	R	1606	48/48	0.96	0.12	21,29,65,70	0
3	CL	C	2558	1/1	0.96	0.05	41,41,41,41	0
2	COA	T	1791	48/48	0.96	0.09	23,28,45,55	0
2	COA	W	2019	48/48	0.96	0.11	22,32,72,75	0
2	COA	P	1424	48/48	0.96	0.12	22,29,69,75	0
4	CA	I	2521	1/1	0.97	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	A3P	O	2575[B]	27/27	0.97	0.11	5,9,22,23	27
4	CA	A	2552	1/1	0.97	0.12	35,35,35,35	1
2	COA	L	1008	48/48	0.97	0.10	17,26,48,59	0
2	COA	J	780	48/48	0.97	0.10	17,26,54,65	0
4	CA	G	2520	1/1	0.97	0.04	44,44,44,44	0
4	CA	P	2534	1/1	0.97	0.07	42,42,42,42	0
4	CA	W	2549	1/1	0.97	0.07	35,35,35,35	1
4	CA	D	2540	1/1	0.97	0.04	30,30,30,30	1
4	CA	R	2512	1/1	0.97	0.07	36,36,36,36	1
4	CA	G	2523	1/1	0.97	0.05	42,42,42,42	1
4	CA	C	2553	1/1	0.97	0.06	32,32,32,32	1
2	COA	A	127	48/48	0.97	0.09	17,25,40,54	0
4	CA	P	1426	1/1	0.97	0.05	36,36,36,36	1
2	COA	S	1696	48/48	0.97	0.10	21,29,66,72	0
2	COA	D	283	48/48	0.97	0.11	18,28,53,65	0
4	CA	F	2518	1/1	0.97	0.08	54,54,54,54	0
3	CL	G	2574	1/1	0.98	0.07	51,51,51,51	0
4	CA	L	2528	1/1	0.98	0.05	31,31,31,31	1
4	CA	O	2531	1/1	0.98	0.04	34,34,34,34	1
4	CA	F	2516	1/1	0.98	0.06	34,34,34,34	1
2	COA	K	900	48/48	0.98	0.09	16,20,39,48	0
4	CA	E	2519	1/1	0.98	0.06	26,26,26,26	1
4	CA	H	2522	1/1	0.98	0.04	48,48,48,48	0
3	CL	E	2591	1/1	0.98	0.05	42,42,42,42	0
4	CA	C	2513	1/1	0.98	0.07	23,23,23,23	1
4	CA	U	2537	1/1	0.98	0.12	34,34,34,34	1
4	CA	J	2542	1/1	0.98	0.06	29,29,29,29	1
3	CL	A	128	1/1	0.98	0.13	48,48,48,48	0
4	CA	V	2547	1/1	0.98	0.09	37,37,37,37	1
4	CA	D	2517	1/1	0.98	0.07	27,27,27,27	1
3	CL	M	2555	1/1	0.98	0.07	48,48,48,48	0
3	CL	T	2592	1/1	0.98	0.10	51,51,51,51	0
4	CA	R	1607	1/1	0.98	0.05	34,34,34,34	1
4	CA	L	2526	1/1	0.98	0.04	26,26,26,26	1
4	CA	S	2538	1/1	0.98	0.12	36,36,36,36	1
4	CA	B	2515	1/1	0.99	0.06	29,29,29,29	1
4	CA	K	569	1/1	0.99	0.09	20,20,20,20	1
3	CL	J	2541	1/1	0.99	0.05	43,43,43,43	0
3	CL	P	2544	1/1	0.99	0.04	49,49,49,49	0
4	CA	S	2539	1/1	0.99	0.05	26,26,26,26	1
4	CA	T	1792	1/1	0.99	0.05	26,26,26,26	1
4	CA	M	2533	1/1	0.99	0.06	28,28,28,28	1

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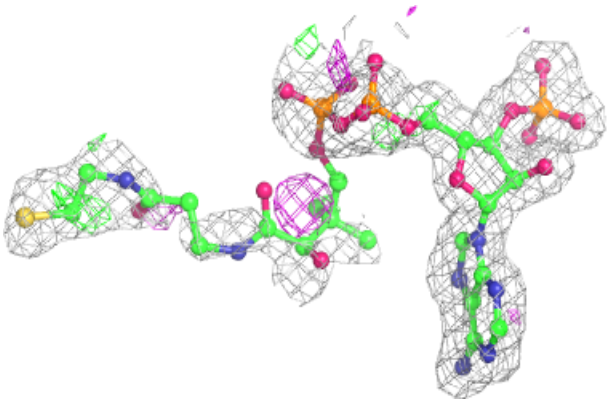
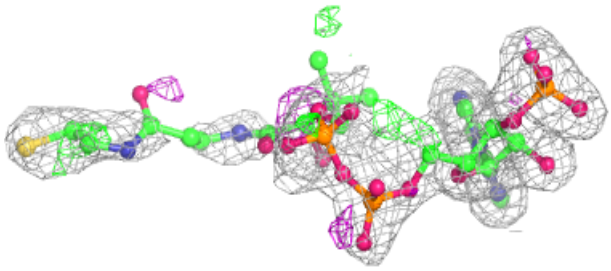
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	2551	1/1	0.99	0.09	38,38,38,38	1
4	CA	H	2524	1/1	0.99	0.06	36,36,36,36	1
4	CA	J	2527	1/1	0.99	0.07	21,21,21,21	1
4	CA	Q	2536	1/1	0.99	0.06	28,28,28,28	1
4	CA	K	2529	1/1	1.00	0.04	31,31,31,31	1

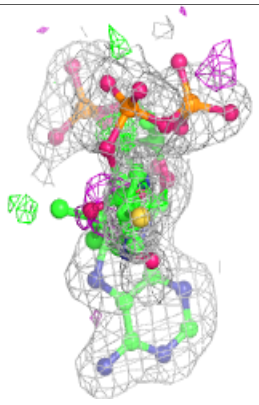
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA N 1333 (A):

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

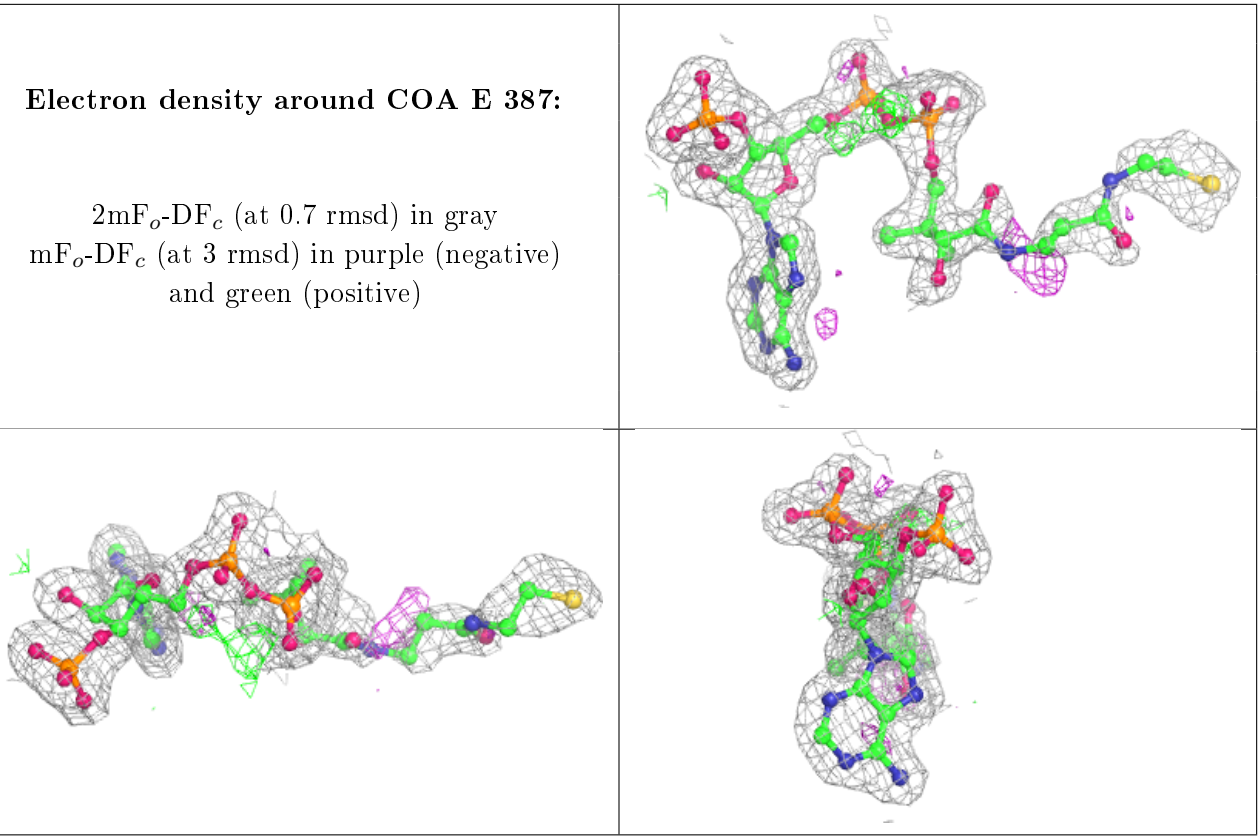






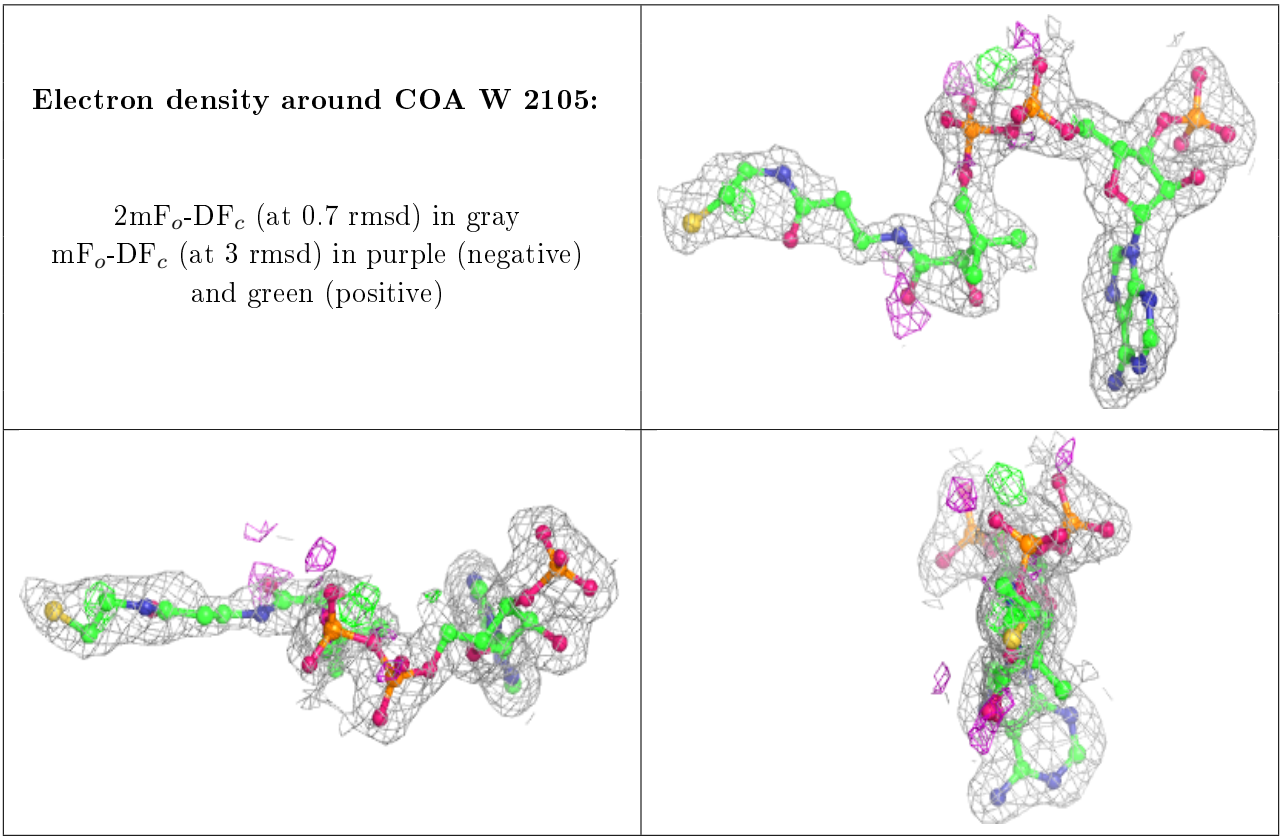
Electron density around COA E 387:

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



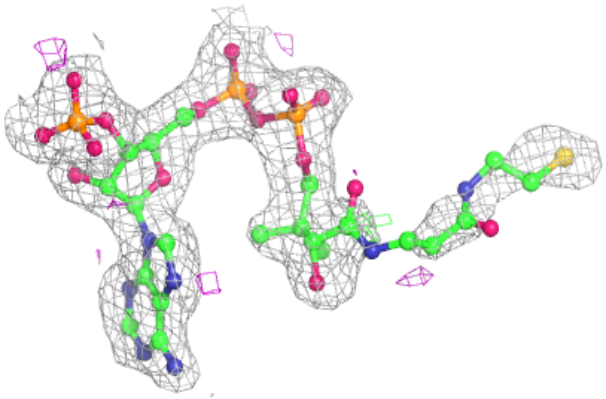
Electron density around COA W 2105:

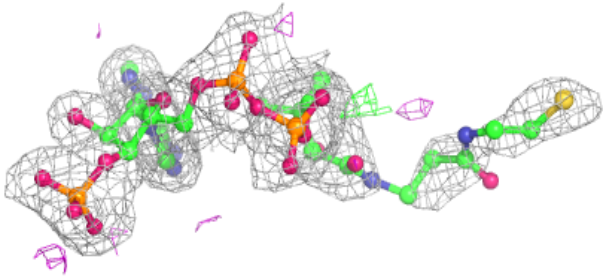
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

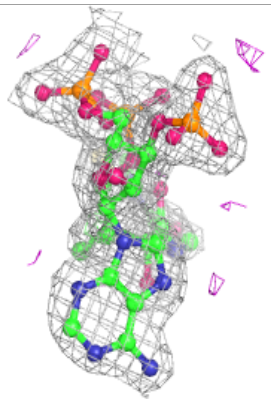


Electron density around COA H 630:

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

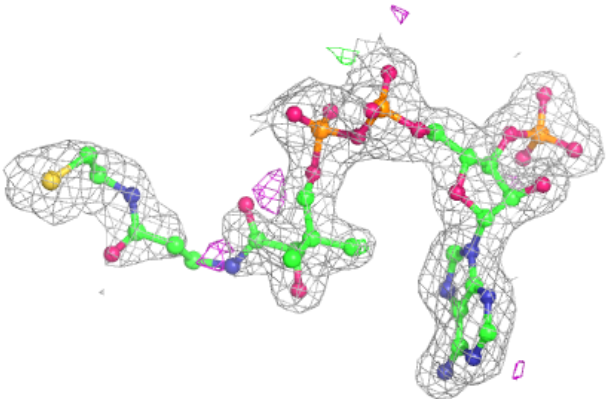


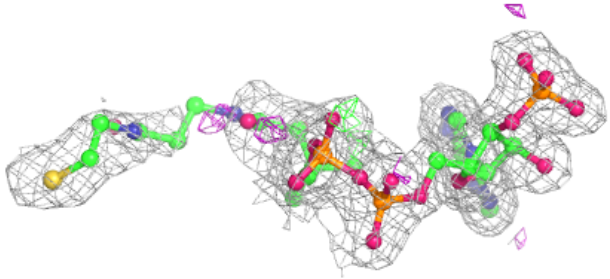


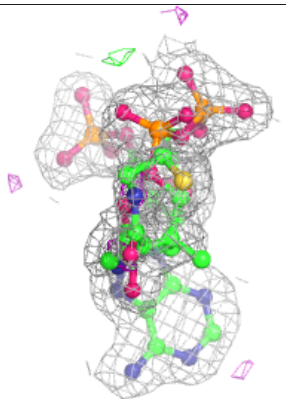


Electron density around COA I 699:

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

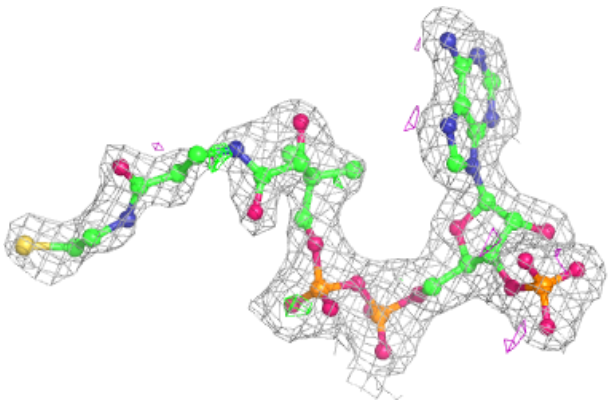


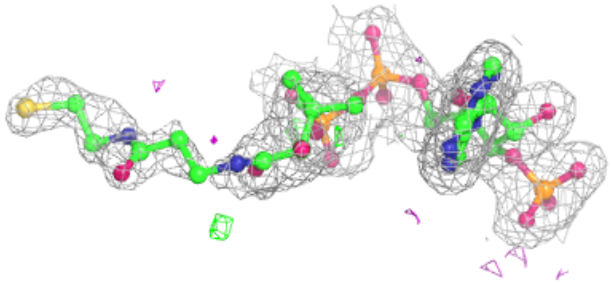


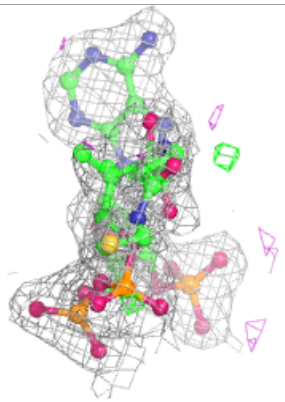


Electron density around COA G 570:

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

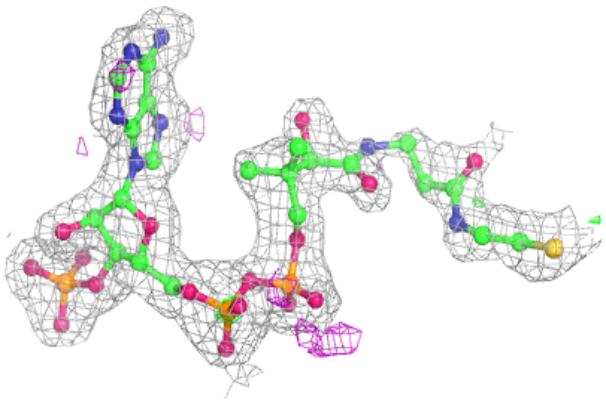


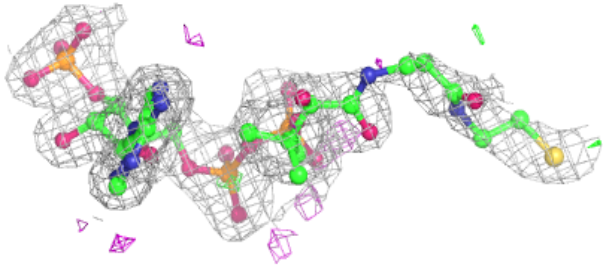


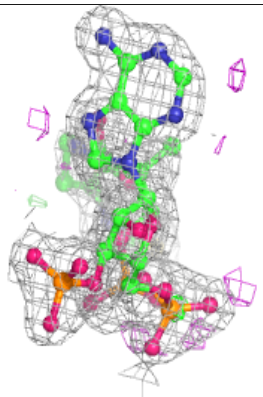


Electron density around COA A 129:

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

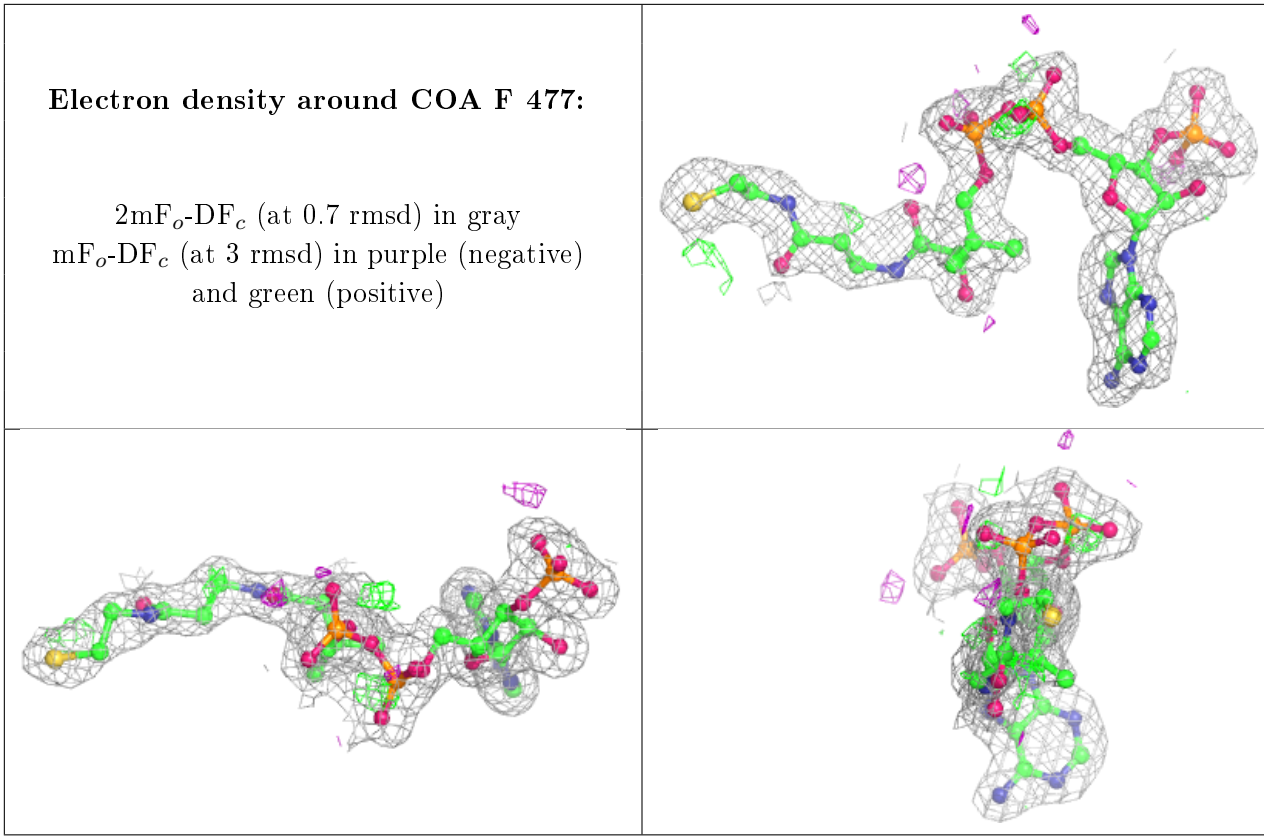






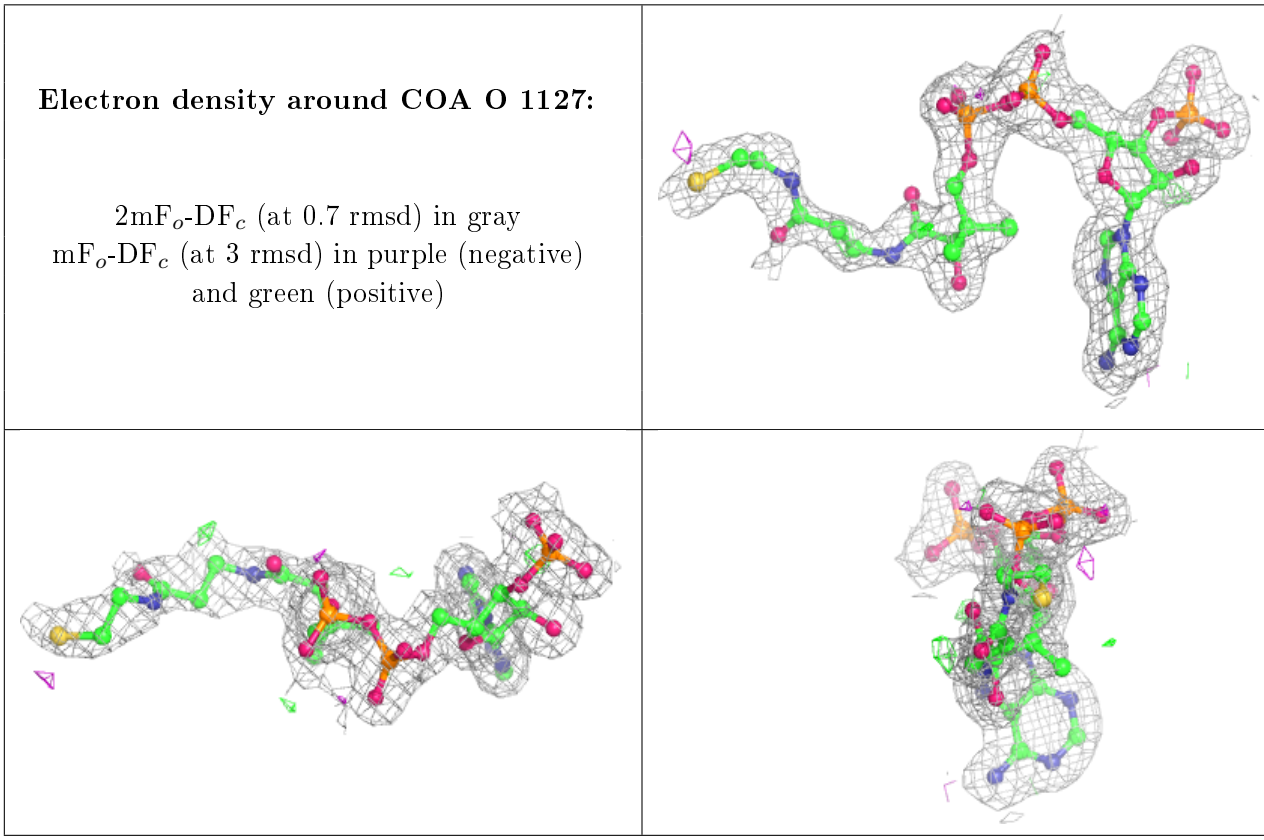
Electron density around COA F 477:

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



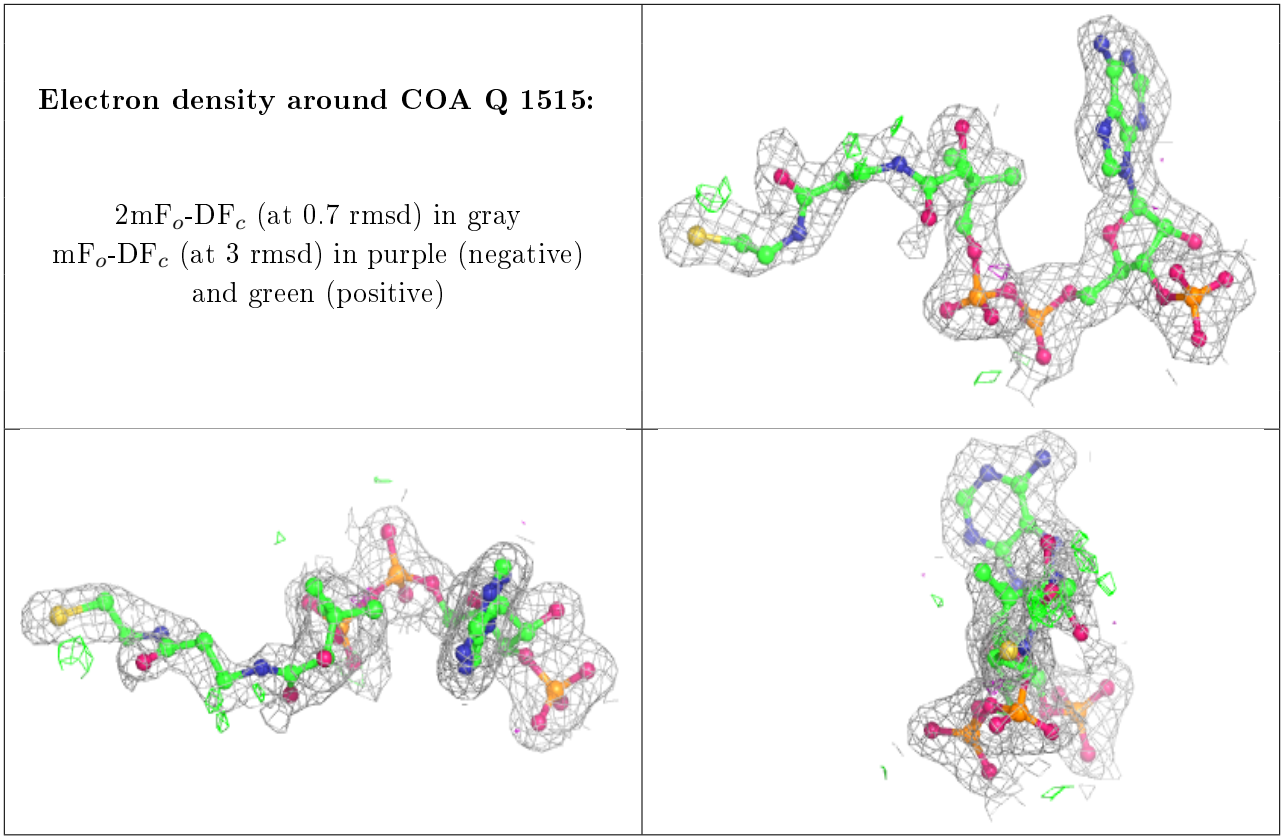
Electron density around COA O 1127:

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



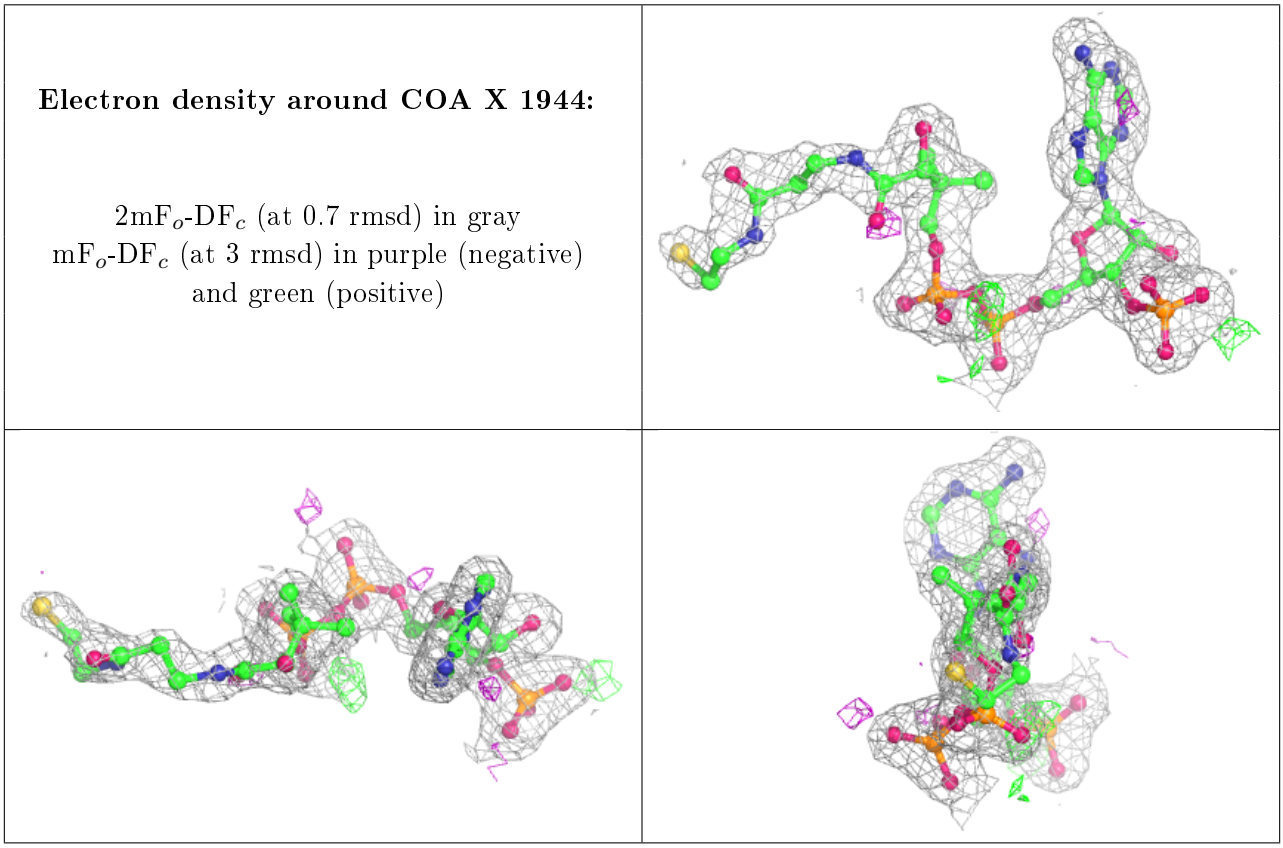
Electron density around COA Q 1515:

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



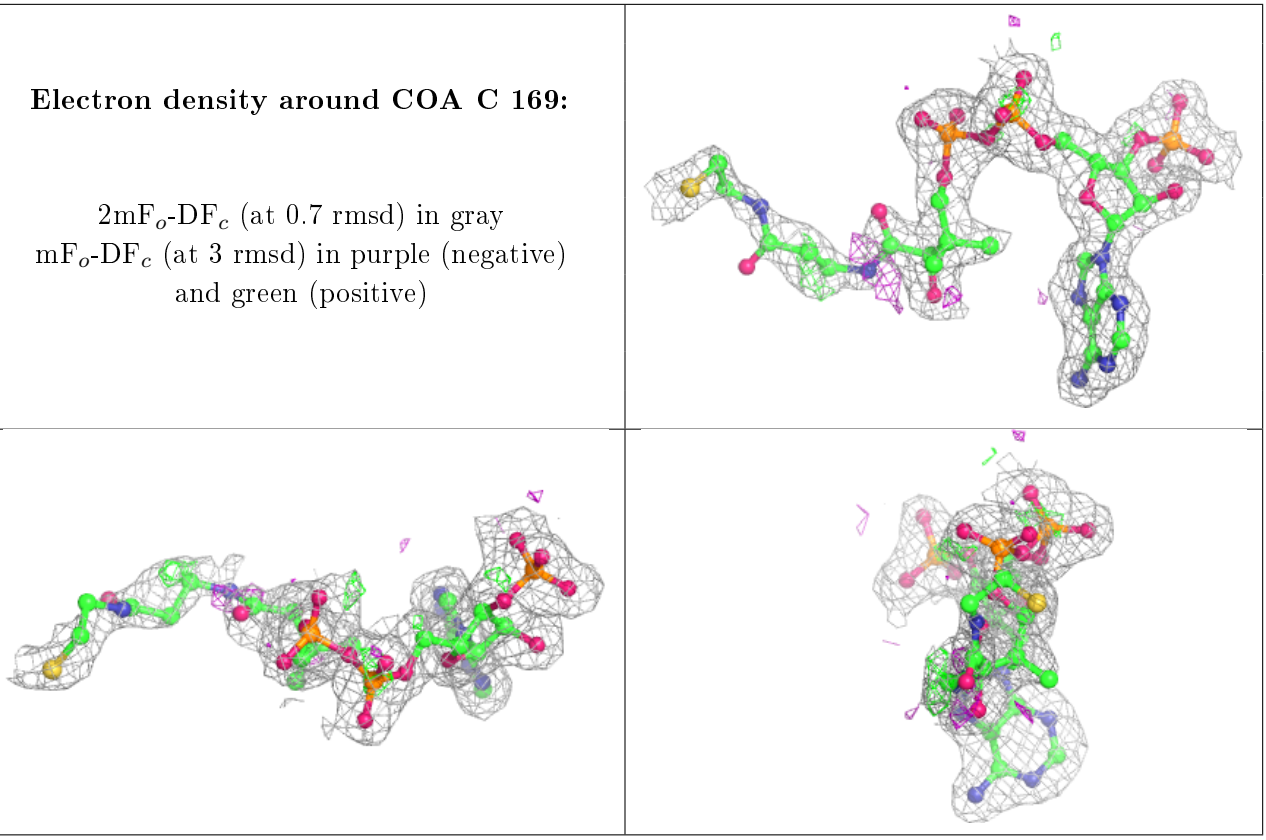
Electron density around COA X 1944:

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



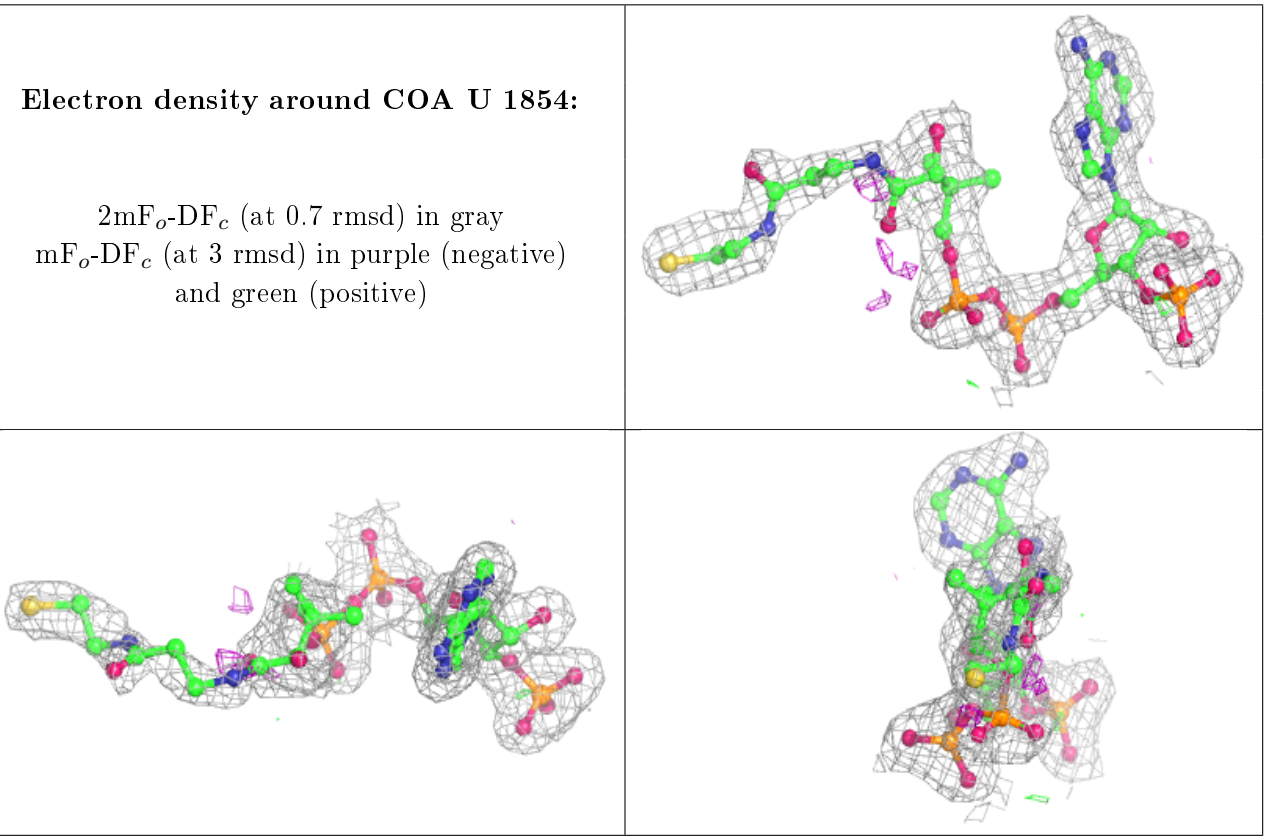
Electron density around COA C 169:

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



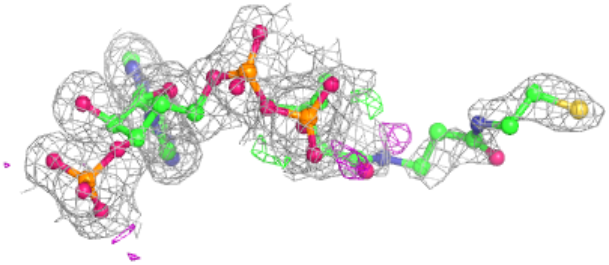
Electron density around COA U 1854:

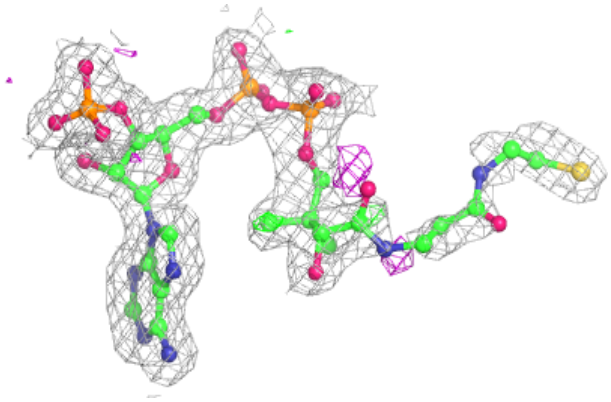
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA N 1221:

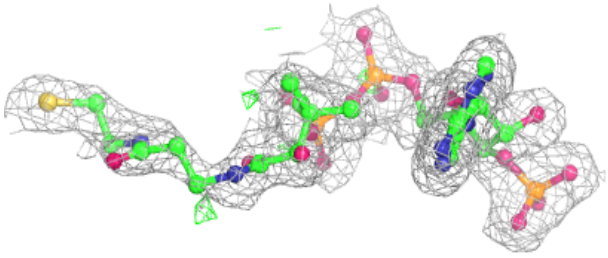
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

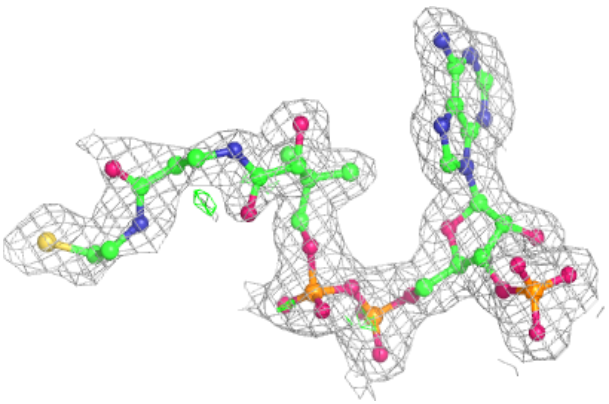


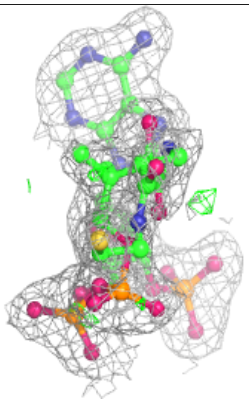


Electron density around COA R 1606:

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

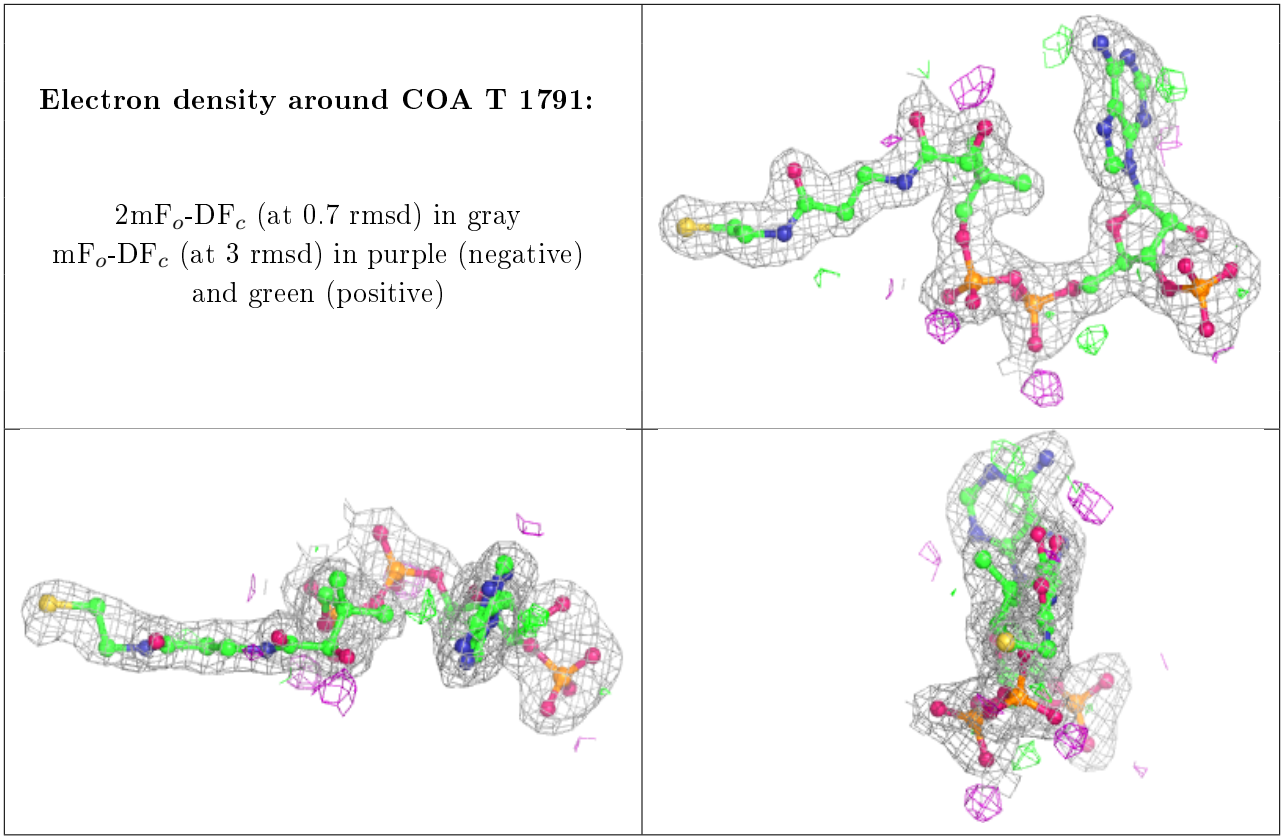






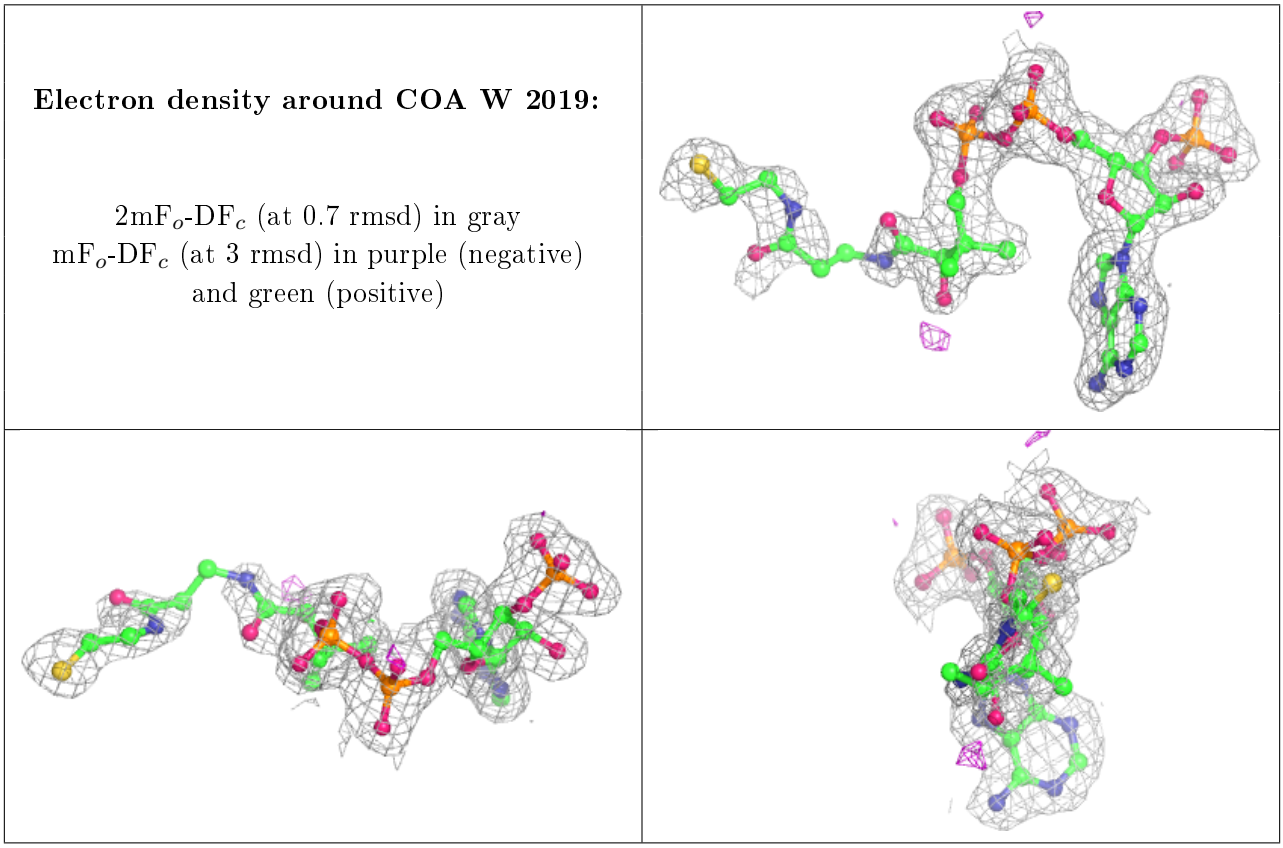
Electron density around COA T 1791:

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



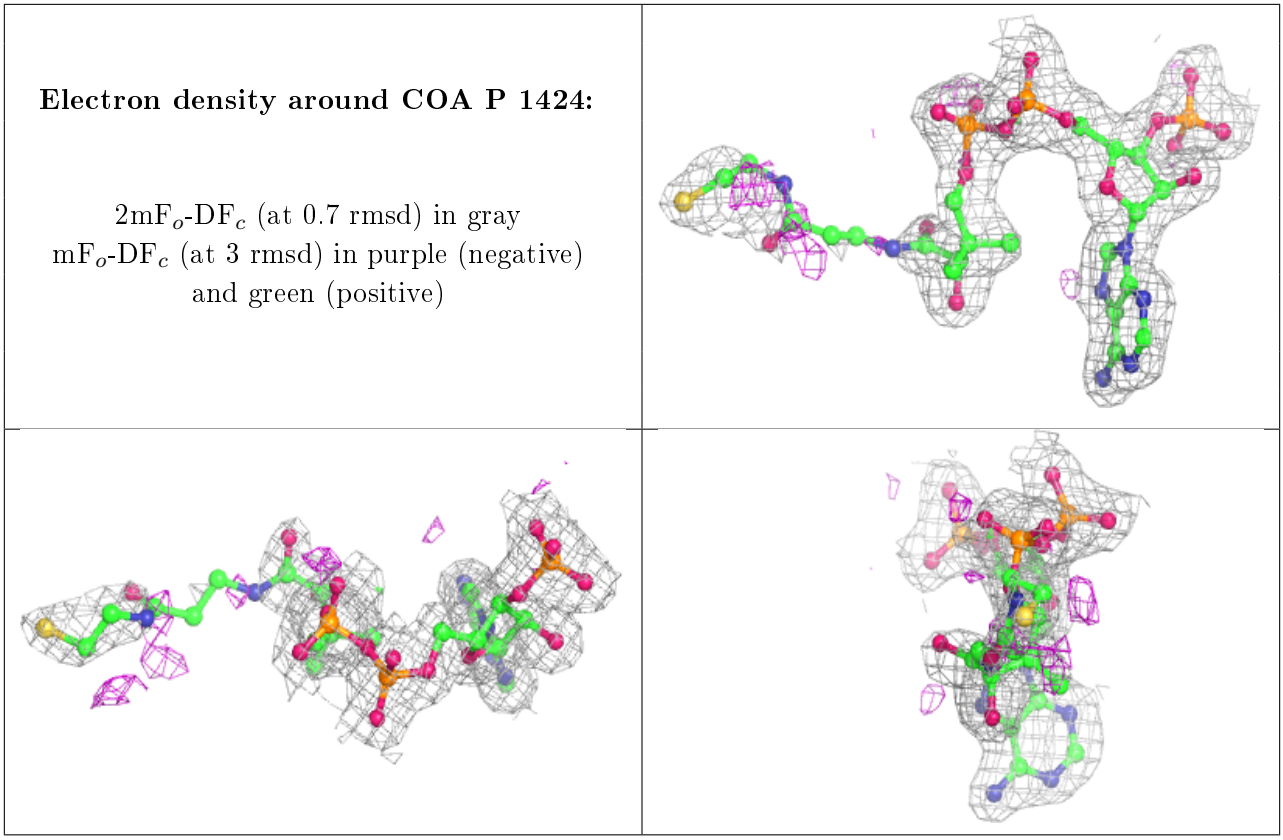
Electron density around COA W 2019:

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



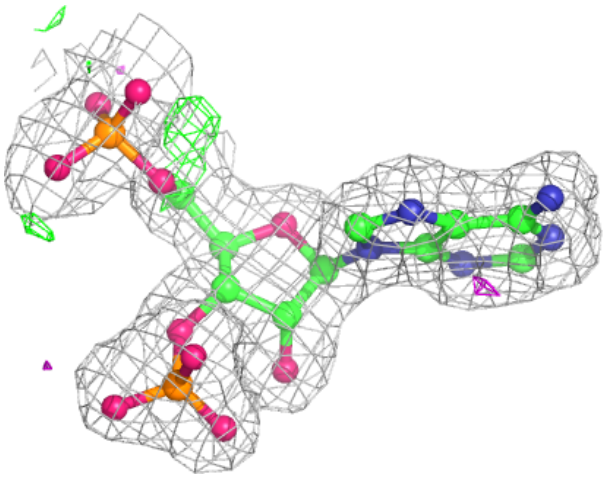
Electron density around COA P 1424:

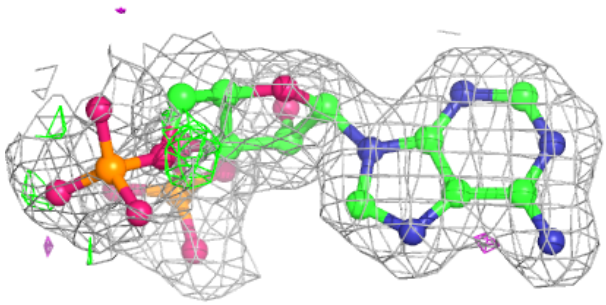
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

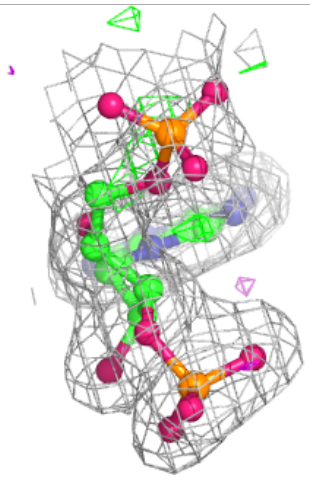


Electron density around A3P O 2575 (B):

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

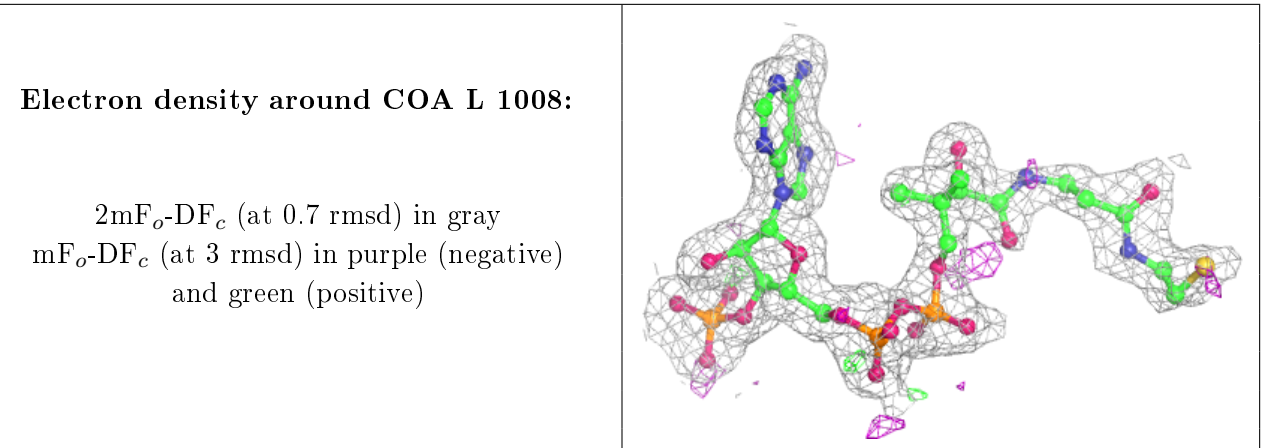


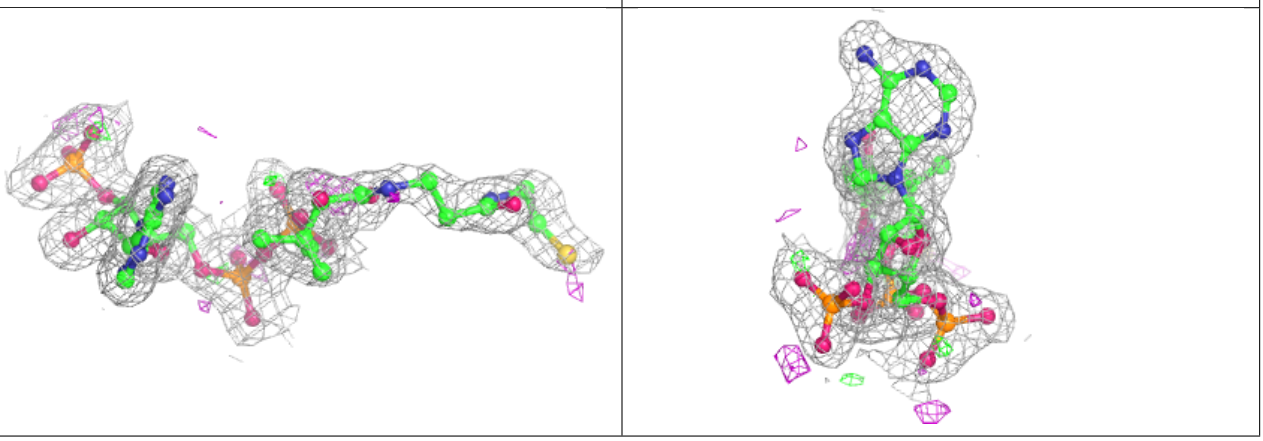




Electron density around COA L 1008:

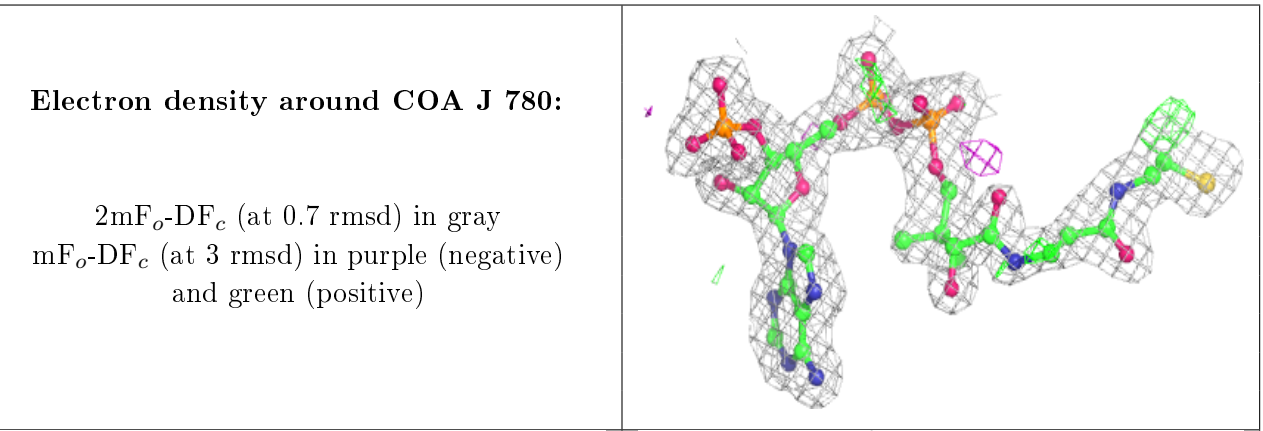
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

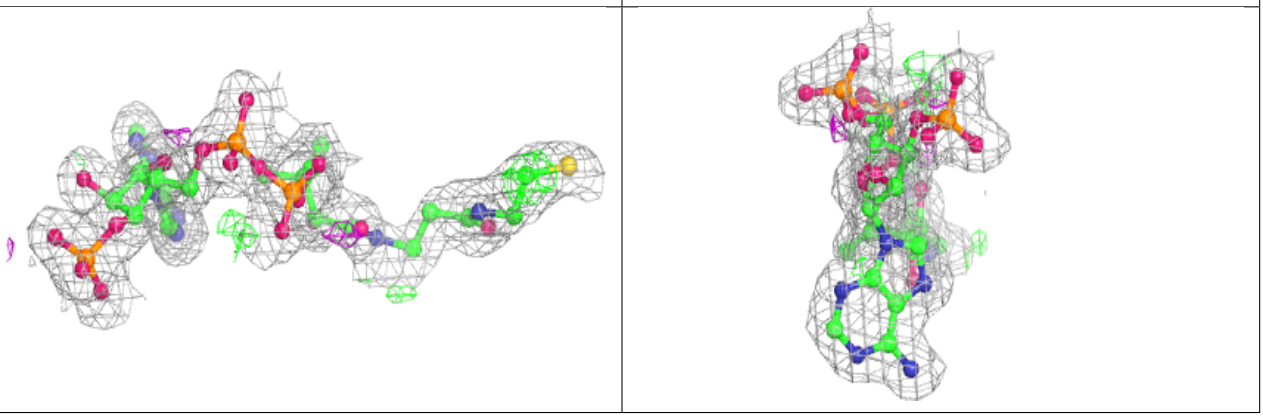




Electron density around COA J 780:

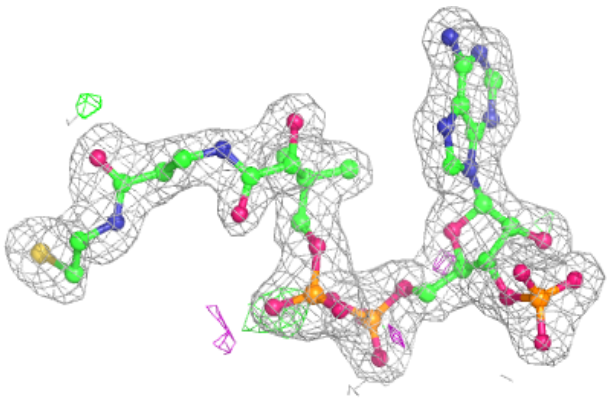
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

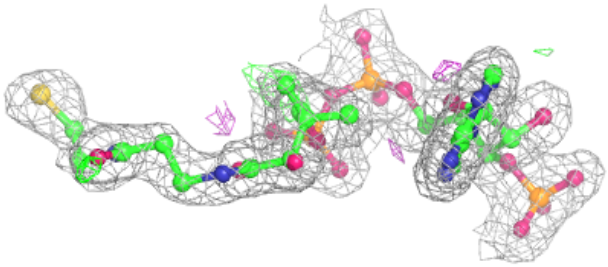


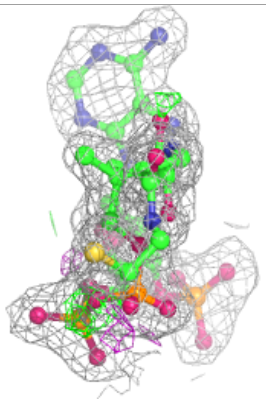


Electron density around COA A 127:

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

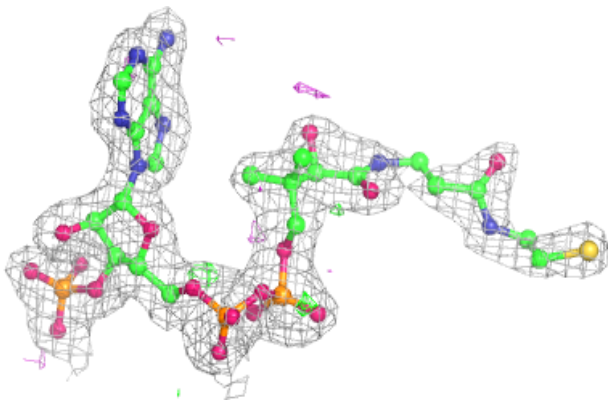


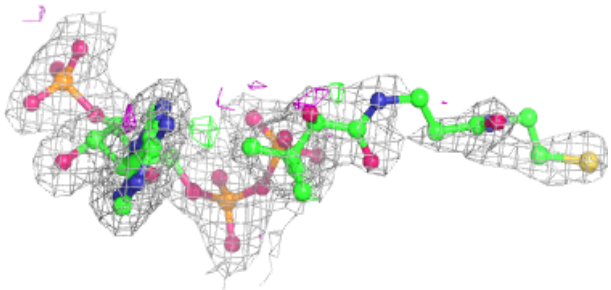




Electron density around COA S 1696:

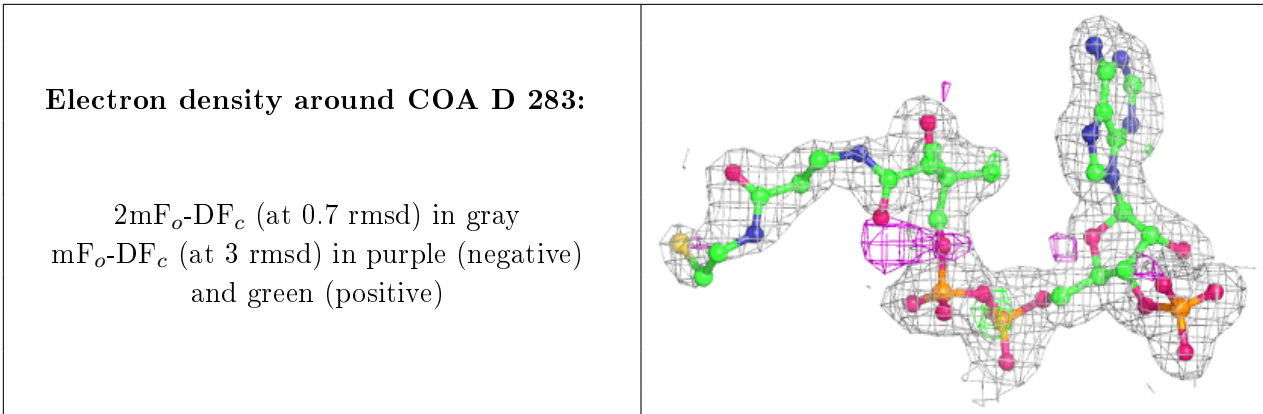
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

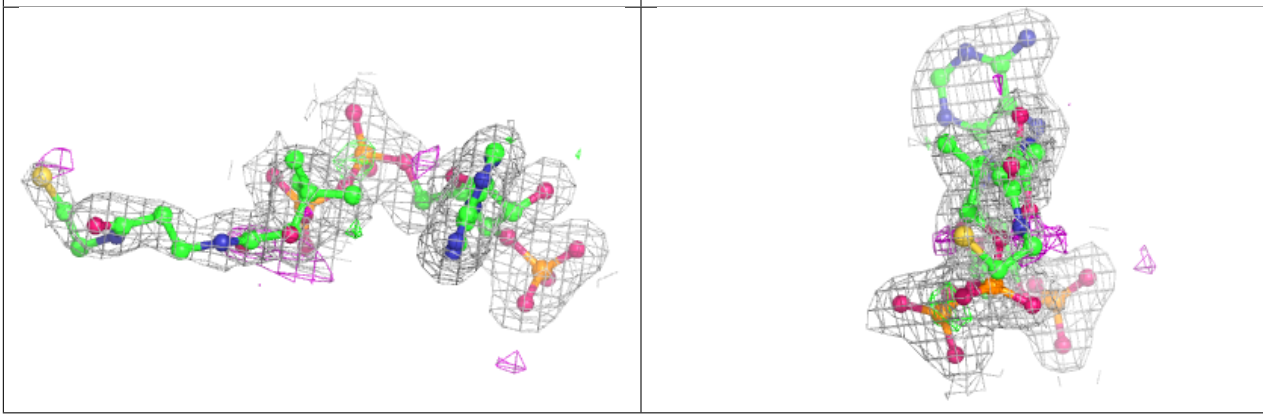




Electron density around COA D 283:

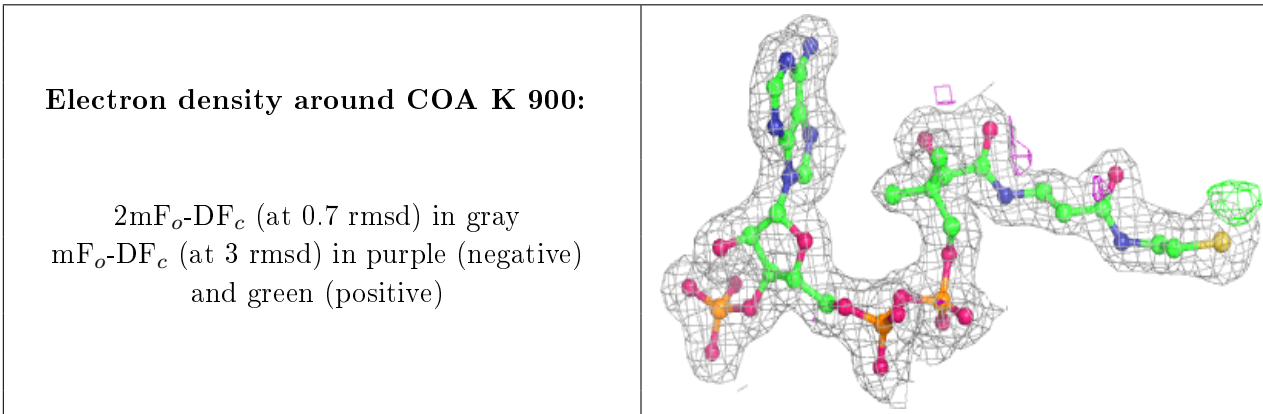
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

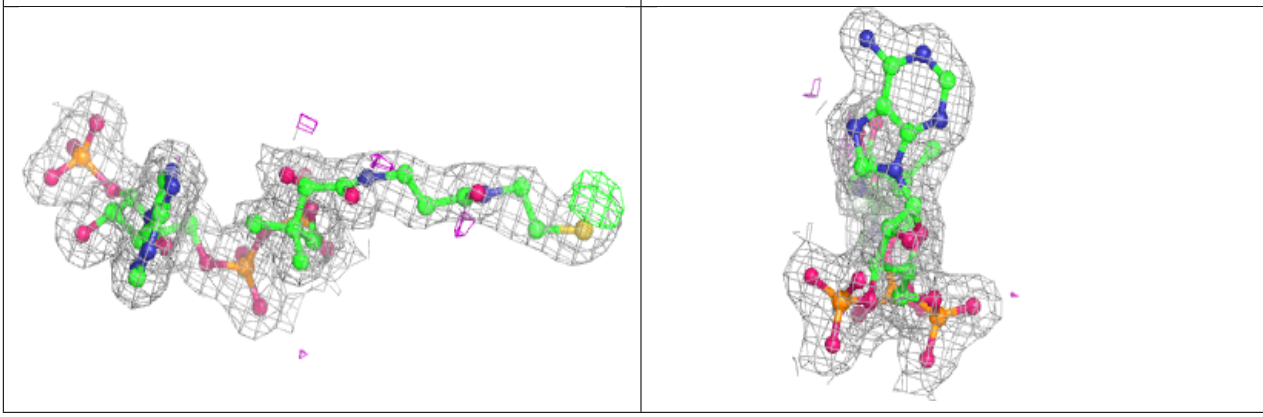




Electron density around COA K 900:

$2mF_o$-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.