



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:06 PM UTC

PDB ID : 3QMN / pdb_00003qmn
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

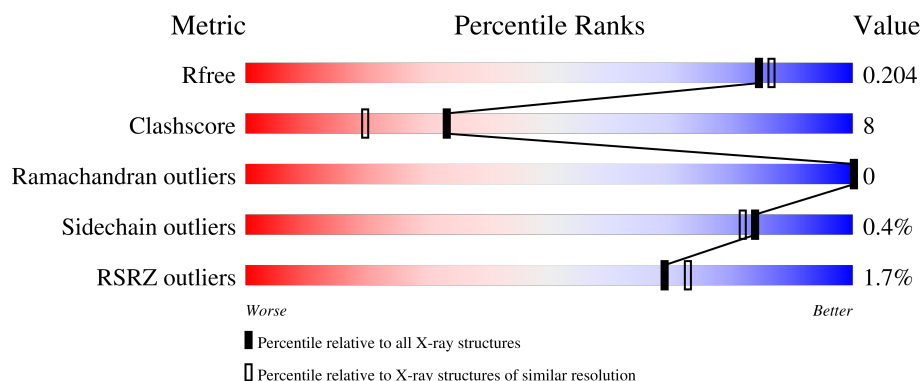
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	129	
1	B	129	
1	C	129	
1	D	129	

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Mol	Chain	Length	Quality of chain
1	E	129	
1	F	129	
1	G	129	
1	H	129	
1	I	129	
1	J	129	
1	K	129	
1	L	129	
1	M	129	
1	N	129	
1	O	129	
1	P	129	
1	Q	129	
1	R	129	
1	S	129	
1	T	129	
1	U	129	
1	V	129	
1	W	129	
1	X	129	

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	R	2595	-	-	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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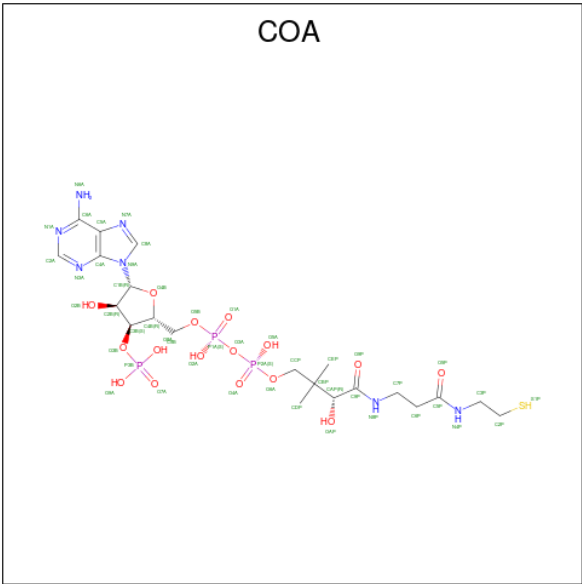
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	expression tag	UNP Q9KPB6
I	-2	SER	-	expression tag	UNP Q9KPB6
I	-1	ASN	-	expression tag	UNP Q9KPB6
I	0	ALA	-	expression tag	UNP Q9KPB6
J	-2	SER	-	expression tag	UNP Q9KPB6
J	-1	ASN	-	expression tag	UNP Q9KPB6
J	0	ALA	-	expression tag	UNP Q9KPB6
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 (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	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 (CCD ID: CL) (formula: Cl).

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

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

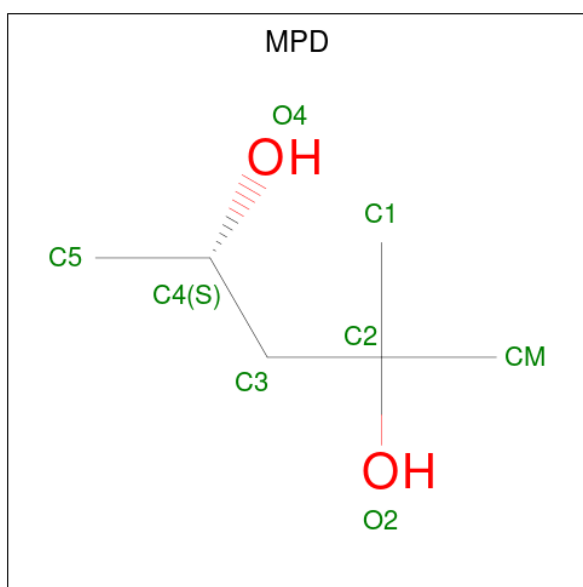
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0
4	B	2	Total 2	Ca 2	0	0
4	C	2	Total 2	Ca 2	0	0
4	D	2	Total 2	Ca 2	0	0
4	E	2	Total 2	Ca 2	0	0
4	F	2	Total 2	Ca 2	0	0
4	G	2	Total 2	Ca 2	0	0
4	H	2	Total 2	Ca 2	0	0
4	I	2	Total 2	Ca 2	0	0
4	J	2	Total 2	Ca 2	0	0
4	K	2	Total 2	Ca 2	0	0
4	L	2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

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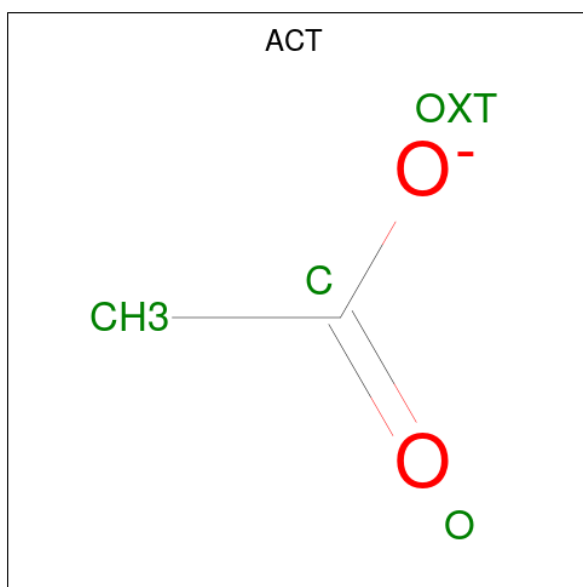
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total 1 Ca 1	0	0
4	O	1	Total 1 Ca 1	0	0
4	P	2	Total 2 Ca 2	0	0
4	Q	2	Total 2 Ca 2	0	0
4	R	2	Total 2 Ca 2	0	0
4	S	2	Total 2 Ca 2	0	0
4	T	2	Total 2 Ca 2	0	0
4	U	2	Total 2 Ca 2	0	0
4	V	2	Total 2 Ca 2	0	0
4	W	2	Total 2 Ca 2	0	0
4	X	2	Total 2 Ca 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



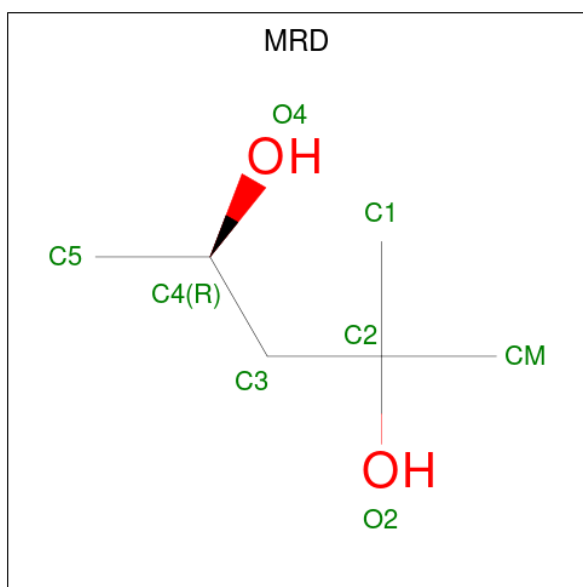
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	H	1	Total C O 8 6 2	0	0
5	I	1	Total C O 8 6 2	0	0
5	M	1	Total C O 8 6 2	0	0
5	O	1	Total C O 8 6 2	0	0
5	P	1	Total C O 8 6 2	0	0
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 (CCD ID: ACT) (formula: C₂H₃O₂).



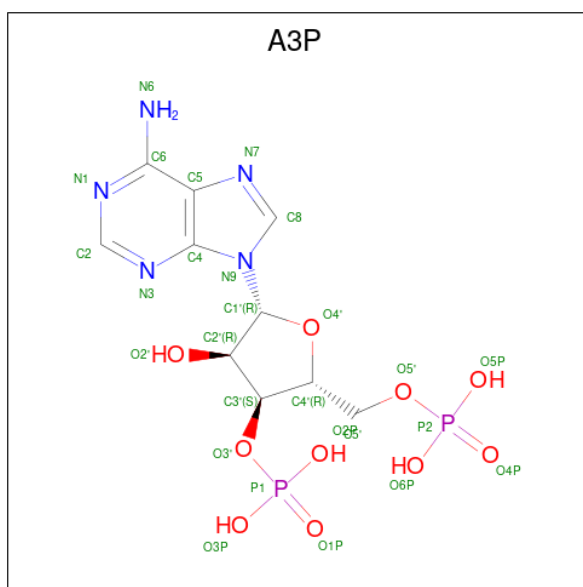
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total	C	O	0	0
			4	2	2		
6	R	1	Total	C	O	0	0
			4	2	2		
6	T	1	Total	C	O	0	0
			4	2	2		
6	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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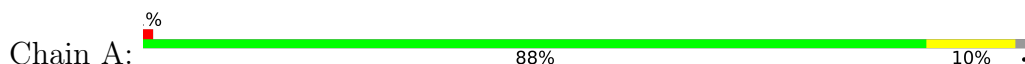
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	134	Total 137	O 137	0	4
9	M	103	Total 105	O 105	0	4
9	N	127	Total 132	O 132	0	11
9	O	101	Total 105	O 105	0	6
9	P	106	Total 110	O 110	0	6
9	Q	103	Total 104	O 104	0	3
9	R	99	Total 100	O 100	0	1
9	S	110	Total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

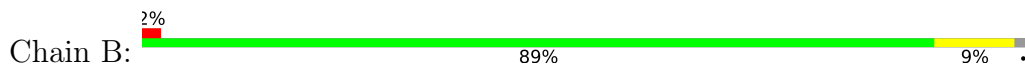
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

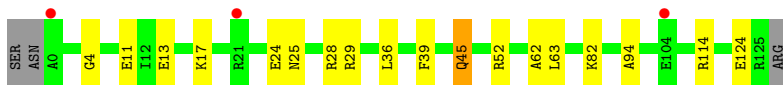
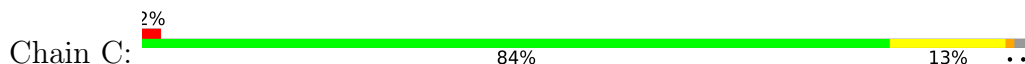
- Molecule 1: Holo-[acyl-carrier-protein] synthase



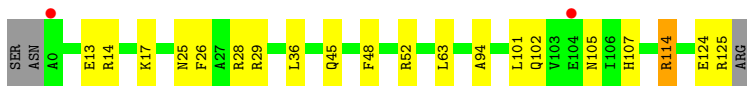
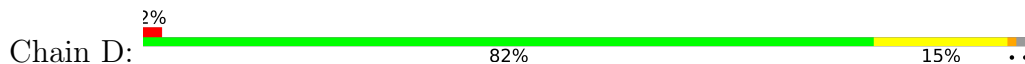
- Molecule 1: Holo-[acyl-carrier-protein] synthase



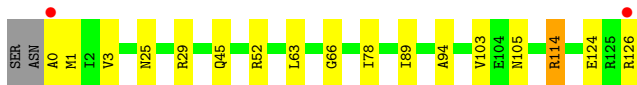
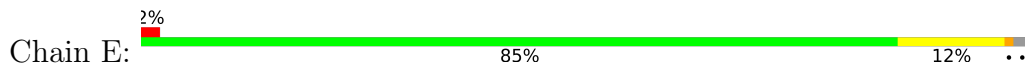
- Molecule 1: Holo-[acyl-carrier-protein] synthase



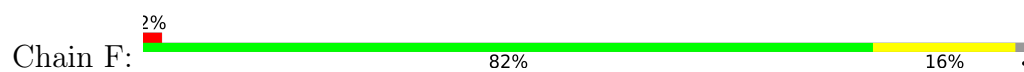
- Molecule 1: Holo-[acyl-carrier-protein] synthase



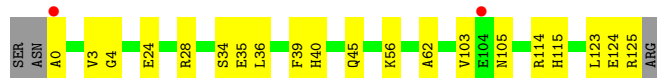
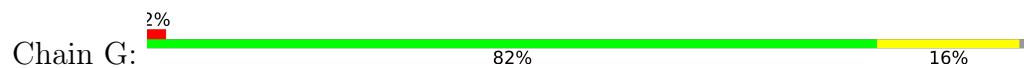
- Molecule 1: Holo-[acyl-carrier-protein] synthase



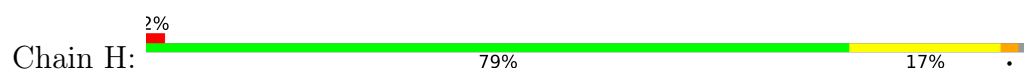
- Molecule 1: Holo-[acyl-carrier-protein] synthase



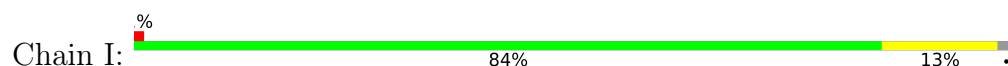
- Molecule 1: Holo-[acyl-carrier-protein] synthase



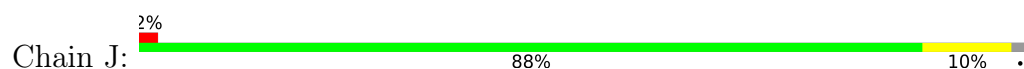
- Molecule 1: Holo-[acyl-carrier-protein] synthase



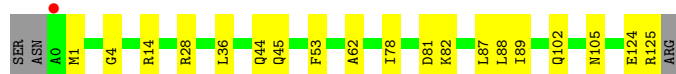
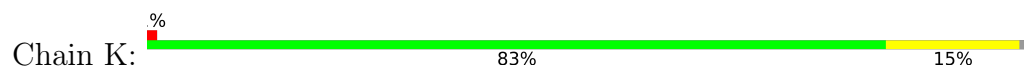
- Molecule 1: Holo-[acyl-carrier-protein] synthase



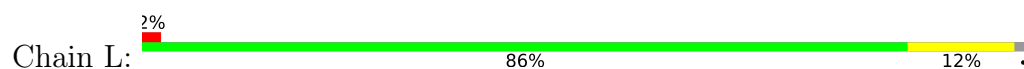
- Molecule 1: Holo-[acyl-carrier-protein] synthase



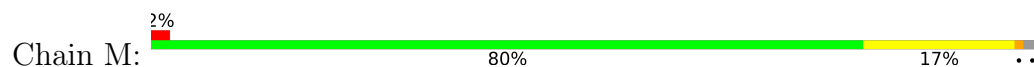
- Molecule 1: Holo-[acyl-carrier-protein] synthase



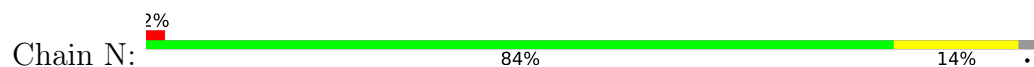
- Molecule 1: Holo-[acyl-carrier-protein] synthase



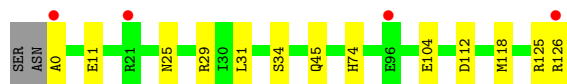
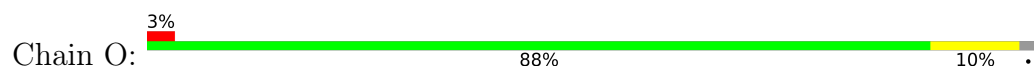
- Molecule 1: Holo-[acyl-carrier-protein] synthase



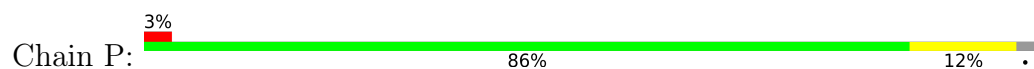
- Molecule 1: Holo-[acyl-carrier-protein] synthase



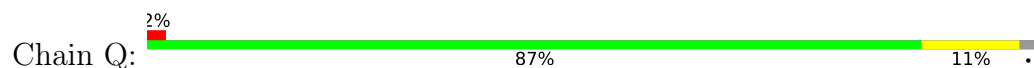
- Molecule 1: Holo-[acyl-carrier-protein] synthase



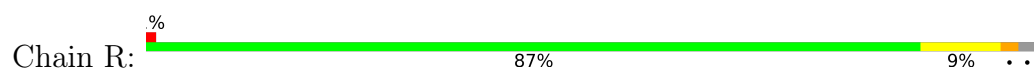
- Molecule 1: Holo-[acyl-carrier-protein] synthase



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



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

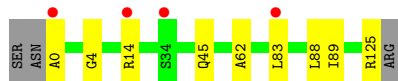
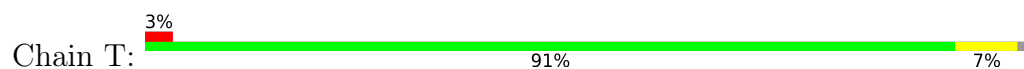


- Molecule 1: Holo-[acyl-carrier-protein] synthase

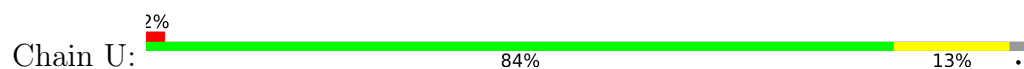




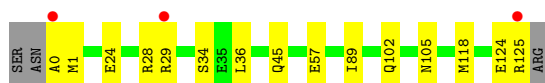
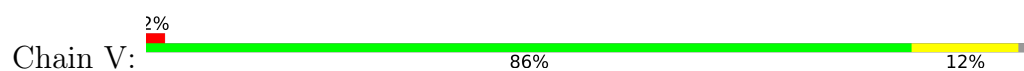
- Molecule 1: Holo-[acyl-carrier-protein] synthase



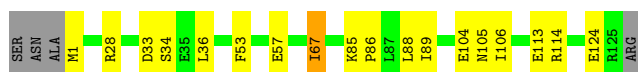
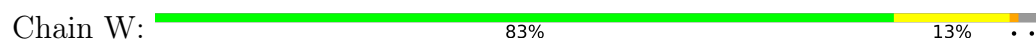
- Molecule 1: Holo-[acyl-carrier-protein] synthase



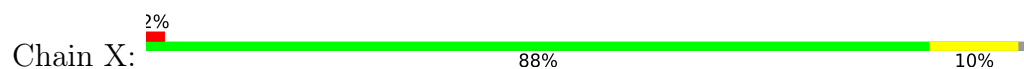
- Molecule 1: Holo-[acyl-carrier-protein] synthase



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



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



4 Data and refinement statistics

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 29.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.89-1.85) 99.2 (29.89-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.156 , 0.191 0.170 , 0.204	Depositor DCC
R_{free} test set	15148 reflections (5.01%)	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)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.69	0/1045	0.93	1/1397 (0.1%)
1	B	0.68	0/1016	0.96	2/1359 (0.1%)
1	C	0.73	0/1043	0.95	2/1395 (0.1%)
1	D	0.69	0/1066	0.93	2/1425 (0.1%)
1	E	0.67	0/1039	0.91	3/1388 (0.2%)
1	F	0.69	0/1032	0.92	0/1380
1	G	0.59	0/1005	0.92	0/1346
1	H	0.64	0/1053	0.92	2/1408 (0.1%)
1	I	0.64	0/1028	0.90	0/1375
1	J	0.75	0/1009	0.96	1/1350 (0.1%)
1	K	0.70	1/1030 (0.1%)	0.93	1/1377 (0.1%)
1	L	0.73	0/1032	0.90	1/1381 (0.1%)
1	M	0.69	0/1032	0.92	1/1380 (0.1%)
1	N	0.75	0/1034	0.92	0/1383
1	O	0.65	0/1034	0.93	1/1382 (0.1%)
1	P	0.64	0/1036	0.92	1/1386 (0.1%)
1	Q	0.66	0/1021	0.93	1/1365 (0.1%)
1	R	0.64	0/1034	0.92	0/1383
1	S	0.71	0/1073	0.95	3/1436 (0.2%)
1	T	0.63	0/1034	0.90	1/1384 (0.1%)
1	U	0.70	0/1055	0.93	1/1411 (0.1%)
1	V	0.64	0/1019	0.93	2/1363 (0.1%)
1	W	0.70	0/1011	0.97	1/1355 (0.1%)
1	X	0.66	0/1033	0.93	2/1381 (0.1%)
All	All	0.68	1/24814 (0.0%)	0.93	29/33190 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	78	ILE	CA-CB	5.09	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	45	GLN	N-CA-C	6.85	118.75	111.28
1	B	45	GLN	N-CA-C	6.79	118.68	111.28
1	E	45	GLN	N-CA-C	6.67	118.55	111.28
1	P	1	MSE	N-CA-C	6.50	120.13	109.85
1	A	45	GLN	N-CA-C	6.26	118.11	111.28
1	S	66	GLY	N-CA-C	-6.21	101.00	112.62
1	H	115	HIS	N-CA-C	6.06	121.50	113.73
1	D	114	ARG	N-CA-C	5.85	118.41	111.33
1	O	45	GLN	N-CA-C	5.79	117.58	111.28
1	W	67	ILE	N-CA-C	-5.71	100.10	106.21
1	L	45	GLN	N-CA-C	5.66	117.47	111.31
1	J	45	GLN	N-CA-C	5.64	117.43	111.28
1	M	45	GLN	N-CA-C	5.63	117.42	111.28
1	E	114	ARG	N-CA-C	5.63	117.42	111.28
1	X	66	GLY	N-CA-C	-5.59	102.16	112.62
1	H	45	GLN	N-CA-C	5.55	117.33	111.28
1	U	45	GLN	N-CA-C	5.53	117.30	111.28
1	B	66	GLY	N-CA-C	-5.50	102.26	112.37
1	E	66	GLY	N-CA-C	-5.49	102.36	112.62
1	X	115	HIS	N-CA-C	5.44	120.19	113.50
1	K	45	GLN	N-CA-C	5.36	117.12	111.28
1	S	115	HIS	N-CA-C	5.30	120.25	113.73
1	C	114	ARG	N-CA-C	5.25	117.00	111.28
1	Q	45	GLN	N-CA-C	5.15	117.56	111.33
1	D	45	GLN	N-CA-C	5.09	116.83	111.28
1	C	45	GLN	N-CA-C	5.07	116.81	111.28
1	V	1	MSE	N-CA-C	5.06	118.26	110.42
1	V	45	GLN	N-CA-C	5.06	116.79	111.28
1	T	45	GLN	N-CA-C	5.00	117.39	111.33

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

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	16	0
1	B	1006	0	1020	7	0
1	C	1033	0	1039	20	0
1	D	1056	0	1069	23	0
1	E	1029	0	1044	12	0
1	F	1022	0	1032	20	0
1	G	995	0	1004	20	0
1	H	1043	0	1053	20	0
1	I	1018	0	1026	20	0
1	J	999	0	1021	16	0
1	K	1020	0	1041	18	0
1	L	1022	0	1028	13	0
1	M	1022	0	1034	28	0
1	N	1024	0	1044	19	0
1	O	1023	0	1033	15	0
1	P	1025	0	1040	12	0
1	Q	1011	0	1028	11	0
1	R	1024	0	1034	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	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	2	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	2	0
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	3	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	3	0
9	H	87	0	0	4	0
9	I	105	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	137	0	0	2	0
9	K	116	0	0	6	0
9	L	137	0	0	4	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	409	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 (409) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2	7:N:2565:MRD:C5	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
2:S:1696:COA:H142	1:U:57[B]:GLU:OE2	1.85	0.77
7:D:2573:MRD:O2	7:D:2573:MRD:H5C3	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:K:88:LEU:C	1:K:89:ILE:HD12	2.13	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:O2	7:N:2565:MRD:H5C3	1.87	0.73
5:B:127:MPD:O2	5:B:127:MPD:H52	1.90	0.72
1:R:88:LEU:C	1:R:89:ILE:HD12	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:104:GLU:CD	1:X:126:ARG:HB2	2.15	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:S:88:LEU:C	1:S:89:ILE:HD12	2.16	0.70
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: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:W:89:ILE:HD13	9:W:2088:HOH:O	1.93	0.68
1:R:89:ILE:HD12	1:R:89:ILE:N	2.08	0.68
1:A:104:GLU:CG	9:A:164:HOH:O	2.41	0.68
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
6:C:2598:ACT:H3	9:C:2501:HOH:O	1.88	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:HN8	2:W:2105:COA:H121	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:NE2	1:M:38[B]:GLN:N	2.45	0.64
1:T:88:LEU:C	1:T:89:ILE:HD12	2.22	0.64
1:N:7[B]:THR:HG22	1:O:118:MSE:HE3	1.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:88:LEU:C	1:F:89:ILE:HD12	2.23	0.63
1:H:89:ILE:N	1:H:89:ILE:HD12	2.12	0.63
7:N:2565:MRD:O2	7:N:2565:MRD:H5C2	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:HD12	1:U:89:ILE:N	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: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:M:14:ARG:NH1	5:M:2572:MPD:HO4	1.99	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: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:OE2	1:S:96[A]:GLU:HA	2.01	0.59
1:V:0:ALA:N	1:V:125:ARG:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD12	1:S:89:ILE:N	2.19	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:HG2	1:R:14:ARG:HH11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:2572:MPD:O4	5:M:2572:MPD:O2	2.21	0.54
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:HD12	1:F:89:ILE:N	2.24	0.53
1:O:25:ASN:O	1:O:29:ARG:HG3	2.09	0.53
7:D:2573:MRD:O2	7:D:2573:MRD:C5	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:L:85:LYS:NZ	9:L:1103:HOH:O	2.42	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
1:T:89:ILE:HD12	1:T:89:ILE:N	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:O9P	2:F:477:COA:H121	2.10	0.52
1:S:105:ASN:HB2	1:S:124[A]:GLU:HG3	1.92	0.51
2:S:1696:COA:O9P	2:S:1696:COA:C6P	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:H121	2:W:2019:COA:O9P	2.11	0.51
2:S:1696:COA:CEP	1:U:57[B]:GLU:OE2	2.58	0.50
1:U:88:LEU:C	1:U:89:ILE:HD12	2.36	0.50
2:W:2105:COA:H121	2:W:2105:COA:N8P	2.24	0.50
1:I:29:ARG:NH2	9:I:760:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:105:ASN:HB2	1:A:124:GLU:CG	2.42	0.50
1:A:114[B]:ARG:NH1	1:C:11:GLU:OE1	2.43	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
1:N:21:ARG:NH1	9:N:1299:HOH:O	2.32	0.49
2:N:1221:COA:O1A	9:N:1259[B]:HOH:O	2.20	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
1:S:47[A]:ARG:HD2	9:S:2481[A]:HOH:O	2.12	0.49
1:S:102[A]:GLN:OE1	1:S:125:ARG:NH1	2.45	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:G:35:GLU:OE1	1:G:56:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:125:ARG:NH2	9:R:1682:HOH:O	2.43	0.48
1:R:89:ILE:N	1:R:89:ILE:CD1	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:R:51:LYS:NZ	6:R:2595:ACT:O	2.39	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:U:97:LEU:HD11	9:U:1937:HOH:O	2.16	0.46
1:E:78:ILE:HD12	1:E:78:ILE:N	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:OE1	1:W:104:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:S:78:ILE:N	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:H52	5:S:1697:MPD:HM1	1.98	0.44
5:Q:2567:MPD:O4	5:Q:2567:MPD:O2	2.32	0.44
2:W:2105:COA:HN8	2:W:2105:COA:CCP	2.27	0.44
2:H:630:COA:O9P	2:H:630:COA:O6A	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:O2P	8:O:2575[B]:A3P:O2'	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:N	1:M:78:ILE:HD12	2.34	0.43
1:S:89:ILE:N	1:S:89:ILE:CD1	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
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:O	1:M:44[B]:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:X:44[B]:GLN:O	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: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:C:13[B]:GLU:CD	1:C:17:LYS:HZ3	2.25	0.41
1:H:88:LEU:C	1:H:89:ILE:HD12	2.45	0.41
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:G:24:GLU:CD	9:G:603:HOH:O	2.63	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
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:O9P	2:H:630:COA:CCP	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:105[B]:ASN:ND2	1:H:124[B]:GLU:OE2	2.53	0.41
1:S:63[A]:LEU:HD11	1:S:94:ALA:HB1	2.03	0.41
2:S:1696:COA:S1P	1:U:29[B]:ARG:HD3	2.61	0.41
1:W:34:SER:HB3	9:W:2100:HOH:O	2.21	0.41
1:D:13:GLU:CD	1:D:17:LYS:NZ	2.79	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:N	1:H:89:ILE:CD1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	103 (100%)	0	100	100
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%)	104 (97%)	3 (3%)	38	23
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%)	68	60
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%)	104 (99%)	1 (1%)	68	60
1	Q	103/100 (103%)	103 (100%)	0	100	100
1	R	105/100 (105%)	102 (97%)	3 (3%)	37	22
1	S	110/100 (110%)	108 (98%)	2 (2%)	51	40
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
All	All	2519/2400 (105%)	2509 (100%)	10 (0%)	84	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	VAL
1	H	89	ILE
1	H	90	LEU
1	M	1	MSE
1	P	3	VAL
1	R	14	ARG

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Mol	Chain	Res	Type
1	R	89	ILE
1	R	97	LEU
1	S	89	ILE
1	S	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	B	69	GLN
1	B	105	ASN
1	C	102	GLN
1	H	69	GLN
1	I	93	GLN
1	I	105	ASN
1	J	102	GLN
1	O	38	GLN
1	O	100	GLN
1	O	105	ASN
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	105	ASN
1	W	69	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
6	ACT	A	2597	4	3,3,3	0.83	0	3,3,3	1.38	0
6	ACT	R	2595	4	3,3,3	0.85	0	3,3,3	1.47	0
7	MRD	F	2559	-	7,7,7	0.29	0	9,10,10	0.27	0
7	MRD	L	2562	-	7,7,7	0.37	0	9,10,10	0.30	0
2	COA	N	1221	4	47,50,50	1.10	2 (4%)	69,75,75	1.91	19 (27%)
2	COA	T	1791	4	47,50,50	1.17	4 (8%)	69,75,75	1.53	12 (17%)
5	MPD	R	2566	-	7,7,7	0.25	0	9,10,10	0.25	0
2	COA	N	1333[A]	-	47,50,50	1.10	2 (4%)	69,75,75	1.72	12 (17%)
2	COA	S	1696	4	47,50,50	1.15	4 (8%)	69,75,75	1.79	17 (24%)
5	MPD	S	1697	-	7,7,7	0.27	0	9,10,10	0.24	0
5	MPD	V	1945	-	7,7,7	0.26	0	9,10,10	0.24	0
2	COA	J	780	4	47,50,50	1.20	3 (6%)	69,75,75	1.66	13 (18%)
5	MPD	W	2106	-	7,7,7	0.32	0	9,10,10	0.25	0
2	COA	A	129	4	47,50,50	1.18	2 (4%)	69,75,75	1.66	14 (20%)
2	COA	A	127	4	47,50,50	1.19	4 (8%)	69,75,75	1.86	20 (28%)
2	COA	F	477	4	47,50,50	1.04	1 (2%)	69,75,75	1.97	20 (28%)
2	COA	O	1127	4	47,50,50	1.09	1 (2%)	69,75,75	1.87	20 (28%)
5	MPD	Q	2567	-	7,7,7	0.30	0	9,10,10	0.40	0
2	COA	E	387	4	47,50,50	1.23	3 (6%)	69,75,75	1.63	15 (21%)
6	ACT	E	2594	4	3,3,3	0.86	0	3,3,3	1.39	0
2	COA	Q	1515	4	47,50,50	1.15	2 (4%)	69,75,75	1.74	16 (23%)
5	MPD	G	571	-	7,7,7	0.27	0	9,10,10	0.26	0
5	MPD	P	1425	-	7,7,7	0.30	0	9,10,10	0.24	0
5	MPD	C	2571	-	7,7,7	0.30	0	9,10,10	0.33	0
5	MPD	H	631	-	7,7,7	0.26	0	9,10,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	K	900	4	47,50,50	1.18	5 (10%)	69,75,75	1.77	16 (23%)
2	COA	H	630	4	47,50,50	1.10	3 (6%)	69,75,75	1.74	17 (24%)
2	COA	X	1944	4	47,50,50	1.10	2 (4%)	69,75,75	1.69	15 (21%)
5	MPD	M	2572	-	7,7,7	0.31	0	9,10,10	0.25	0
7	MRD	N	2565	-	7,7,7	0.23	0	9,10,10	0.40	0
5	MPD	A	2570	-	7,7,7	0.30	0	9,10,10	0.18	0
5	MPD	E	2560	-	7,7,7	0.40	0	9,10,10	0.25	0
2	COA	G	570	4	47,50,50	1.11	2 (4%)	69,75,75	1.67	19 (27%)
6	ACT	W	2596	4	3,3,3	0.78	0	3,3,3	1.61	0
7	MRD	T	2569	-	7,7,7	0.31	0	9,10,10	0.18	0
2	COA	W	2019	4	47,50,50	1.08	2 (4%)	69,75,75	1.78	18 (26%)
6	ACT	C	2598	-	3,3,3	1.03	0	3,3,3	0.89	0
6	ACT	K	629	4	3,3,3	0.88	0	3,3,3	1.31	0
2	COA	C	169	4	47,50,50	1.10	2 (4%)	69,75,75	1.81	18 (26%)
2	COA	R	1606	4	47,50,50	1.10	2 (4%)	69,75,75	1.72	17 (24%)
5	MPD	O	1334	-	7,7,7	0.28	0	9,10,10	0.27	0
5	MPD	U	1698	-	7,7,7	0.34	0	9,10,10	0.28	0
6	ACT	T	2568	4	3,3,3	0.85	0	3,3,3	1.27	0
7	MRD	K	2564	-	7,7,7	0.29	0	9,10,10	0.49	0
2	COA	P	1424	4	47,50,50	1.19	4 (8%)	69,75,75	1.66	15 (21%)
2	COA	D	283	4	47,50,50	1.14	5 (10%)	69,75,75	1.66	16 (23%)
7	MRD	D	2573	-	7,7,7	0.26	0	9,10,10	0.28	0
6	ACT	K	2563	-	3,3,3	0.81	0	3,3,3	1.31	0
8	A3P	O	2575[B]	-	29,29,29	1.34	3 (10%)	44,45,45	1.87	12 (27%)
2	COA	I	699	4	47,50,50	1.08	3 (6%)	69,75,75	1.76	19 (27%)
2	COA	U	1854	4	47,50,50	1.08	3 (6%)	69,75,75	1.61	12 (17%)
2	COA	W	2105	4	47,50,50	1.17	3 (6%)	69,75,75	1.70	14 (20%)
2	COA	L	1008	4	47,50,50	1.19	4 (8%)	69,75,75	1.78	22 (31%)
5	MPD	I	2561	-	7,7,7	0.32	0	9,10,10	0.19	0
5	MPD	B	127	-	7,7,7	0.26	0	9,10,10	0.17	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
7	MRD	F	2559	-	-	0/5/5/5	-
7	MRD	L	2562	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	N	1221	4	-	8/48/64/64	0/3/3/3
2	COA	T	1791	4	-	4/48/64/64	0/3/3/3
5	MPD	R	2566	-	-	0/5/5/5	-
2	COA	N	1333[A]	-	-	17/48/64/64	0/3/3/3
2	COA	S	1696	4	-	13/48/64/64	0/3/3/3
5	MPD	S	1697	-	-	2/5/5/5	-
5	MPD	V	1945	-	-	0/5/5/5	-
2	COA	J	780	4	-	5/48/64/64	0/3/3/3
5	MPD	W	2106	-	-	3/5/5/5	-
2	COA	A	129	4	-	10/48/64/64	0/3/3/3
2	COA	A	127	4	-	7/48/64/64	0/3/3/3
2	COA	F	477	4	-	9/48/64/64	0/3/3/3
2	COA	O	1127	4	-	10/48/64/64	0/3/3/3
5	MPD	Q	2567	-	-	3/5/5/5	-
2	COA	E	387	4	-	8/48/64/64	0/3/3/3
2	COA	Q	1515	4	-	7/48/64/64	0/3/3/3
5	MPD	G	571	-	-	1/5/5/5	-
5	MPD	P	1425	-	-	0/5/5/5	-
5	MPD	C	2571	-	-	1/5/5/5	-
5	MPD	H	631	-	-	2/5/5/5	-
2	COA	K	900	4	-	5/48/64/64	0/3/3/3
2	COA	H	630	4	-	12/48/64/64	0/3/3/3
2	COA	X	1944	4	-	8/48/64/64	0/3/3/3
5	MPD	M	2572	-	-	3/5/5/5	-
7	MRD	N	2565	-	-	4/5/5/5	-
5	MPD	A	2570	-	-	0/5/5/5	-
5	MPD	E	2560	-	-	0/5/5/5	-
2	COA	G	570	4	-	4/48/64/64	0/3/3/3
7	MRD	T	2569	-	-	0/5/5/5	-
2	COA	W	2019	4	-	13/48/64/64	0/3/3/3
2	COA	C	169	4	-	7/48/64/64	0/3/3/3
2	COA	R	1606	4	-	4/48/64/64	0/3/3/3
5	MPD	O	1334	-	-	2/5/5/5	-
5	MPD	U	1698	-	-	3/5/5/5	-
7	MRD	K	2564	-	-	3/5/5/5	-
2	COA	P	1424	4	-	14/48/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	D	283	4	-	6/48/64/64	0/3/3/3
7	MRD	D	2573	-	-	1/5/5/5	-
8	A3P	O	2575[B]	-	-	8/15/31/31	0/3/3/3
2	COA	I	699	4	-	5/48/64/64	0/3/3/3
2	COA	U	1854	4	-	8/48/64/64	0/3/3/3
2	COA	W	2105	4	-	8/48/64/64	0/3/3/3
2	COA	L	1008	4	-	4/48/64/64	0/3/3/3
5	MPD	I	2561	-	-	0/5/5/5	-
5	MPD	B	127	-	-	4/5/5/5	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1515	COA	O9P-C9P	5.54	1.34	1.23
2	A	129	COA	O9P-C9P	5.54	1.34	1.23
2	E	387	COA	O9P-C9P	5.40	1.33	1.23
2	P	1424	COA	O9P-C9P	5.36	1.33	1.23
2	N	1333[A]	COA	O9P-C9P	5.32	1.33	1.23
2	N	1221	COA	O9P-C9P	5.31	1.33	1.23
2	G	570	COA	O9P-C9P	5.26	1.33	1.23
2	S	1696	COA	O9P-C9P	5.25	1.33	1.23
2	T	1791	COA	O9P-C9P	5.25	1.33	1.23
2	A	127	COA	O9P-C9P	5.23	1.33	1.23
2	I	699	COA	O9P-C9P	5.21	1.33	1.23
2	W	2019	COA	O9P-C9P	5.17	1.33	1.23
2	X	1944	COA	O9P-C9P	5.16	1.33	1.23
2	W	2105	COA	O9P-C9P	5.15	1.33	1.23
2	O	1127	COA	O9P-C9P	5.12	1.33	1.23
2	H	630	COA	O9P-C9P	5.09	1.33	1.23
2	R	1606	COA	O9P-C9P	5.07	1.33	1.23
2	C	169	COA	O9P-C9P	5.04	1.33	1.23
2	J	780	COA	O9P-C9P	5.03	1.33	1.23
2	L	1008	COA	O9P-C9P	4.97	1.32	1.23
2	F	477	COA	O9P-C9P	4.93	1.32	1.23
2	U	1854	COA	O9P-C9P	4.88	1.32	1.23
2	D	283	COA	O9P-C9P	4.77	1.32	1.23
8	O	2575[B]	A3P	C5-C4	4.54	1.47	1.39
2	K	900	COA	P1A-O3A	3.86	1.63	1.59
2	K	900	COA	O9P-C9P	3.81	1.30	1.23
2	T	1791	COA	P1A-O3A	3.30	1.63	1.59
2	E	387	COA	C4A-N9A	-2.98	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	2105	COA	C8A-N7A	2.82	1.37	1.31
2	U	1854	COA	C8A-N7A	2.77	1.37	1.31
2	A	127	COA	C8A-N7A	2.70	1.36	1.31
2	X	1944	COA	C4A-N9A	-2.70	1.32	1.37
2	H	630	COA	C8A-N7A	2.70	1.36	1.31
2	J	780	COA	C8A-N7A	2.70	1.36	1.31
2	S	1696	COA	C8A-N7A	2.67	1.36	1.31
2	D	283	COA	P3B-O3B	2.64	1.64	1.59
8	O	2575[B]	A3P	C5-C6	2.62	1.48	1.41
2	A	129	COA	C8A-N7A	2.60	1.36	1.31
2	L	1008	COA	C4A-N9A	-2.57	1.32	1.37
8	O	2575[B]	A3P	C8-N7	2.56	1.36	1.31
2	G	570	COA	C8A-N7A	2.54	1.36	1.31
2	K	900	COA	C8A-N7A	2.53	1.36	1.31
2	A	127	COA	P2A-O3A	-2.43	1.56	1.59
2	I	699	COA	C8A-N7A	2.41	1.36	1.31
2	W	2105	COA	C5A-N7A	-2.41	1.34	1.39
2	P	1424	COA	C8A-N7A	2.39	1.36	1.31
2	P	1424	COA	C5A-N7A	-2.36	1.34	1.39
2	L	1008	COA	P1A-O3A	-2.36	1.56	1.59
2	N	1221	COA	C8A-N7A	2.35	1.36	1.31
2	J	780	COA	P1A-O3A	-2.29	1.57	1.59
2	K	900	COA	P2A-O3A	2.29	1.62	1.59
2	N	1333[A]	COA	C8A-N7A	2.27	1.36	1.31
2	W	2019	COA	C8A-N7A	2.26	1.36	1.31
2	D	283	COA	C4A-N9A	-2.23	1.33	1.37
2	D	283	COA	C5A-N7A	-2.23	1.35	1.39
2	L	1008	COA	C8A-N7A	2.19	1.35	1.31
2	E	387	COA	C8A-N7A	2.19	1.35	1.31
2	K	900	COA	C4A-N9A	-2.19	1.33	1.37
2	U	1854	COA	C4A-N9A	-2.16	1.33	1.37
2	S	1696	COA	C5A-N7A	-2.14	1.35	1.39
2	R	1606	COA	C8A-N7A	2.11	1.35	1.31
2	T	1791	COA	C8A-N7A	2.11	1.35	1.31
2	T	1791	COA	C4A-N9A	-2.10	1.33	1.37
2	Q	1515	COA	C4A-N9A	-2.09	1.33	1.37
2	P	1424	COA	C4A-N9A	-2.07	1.33	1.37
2	S	1696	COA	C4A-N9A	-2.07	1.33	1.37
2	A	127	COA	P3B-O3B	2.05	1.63	1.59
2	D	283	COA	C8A-N7A	2.05	1.35	1.31
2	I	699	COA	C4A-N9A	-2.05	1.33	1.37
2	H	630	COA	C4A-N9A	-2.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	169	COA	C8A-N7A	2.01	1.35	1.31

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1221	COA	O2A-P1A-O3A	6.48	124.78	107.27
2	F	477	COA	O3A-P1A-O1A	-5.99	92.70	110.70
2	N	1333[A]	COA	C7P-N8P-C9P	5.93	133.19	122.55
2	F	477	COA	O2A-P1A-O3A	5.63	122.48	107.27
8	O	2575[B]	A3P	C5-C4-N3	-5.48	119.17	126.72
2	O	1127	COA	C5A-C4A-N3A	-5.23	119.51	126.72
2	O	1127	COA	O2A-P1A-O3A	5.22	121.37	107.27
2	R	1606	COA	N3A-C2A-N1A	-5.20	120.72	128.58
2	W	2105	COA	N3A-C2A-N1A	-5.20	120.72	128.58
2	S	1696	COA	C5A-C4A-N3A	-5.15	119.62	126.72
2	J	780	COA	N3A-C2A-N1A	-5.15	120.79	128.58
2	U	1854	COA	N3A-C2A-N1A	-5.09	120.88	128.58
2	K	900	COA	N3A-C2A-N1A	-5.08	120.89	128.58
2	I	699	COA	N3A-C2A-N1A	-5.07	120.90	128.58
2	C	169	COA	C5A-C4A-N3A	-5.04	119.78	126.72
2	N	1221	COA	N3A-C2A-N1A	-5.04	120.96	128.58
2	W	2019	COA	C5A-C4A-N3A	-5.03	119.80	126.72
2	L	1008	COA	C5A-C4A-N3A	-5.01	119.82	126.72
2	A	129	COA	C7P-N8P-C9P	5.01	131.54	122.55
2	C	169	COA	N3A-C2A-N1A	-5.00	121.02	128.58
2	H	630	COA	N3A-C2A-N1A	-4.94	121.10	128.58
2	A	127	COA	C5A-C4A-N3A	-4.85	120.04	126.72
2	D	283	COA	C5A-C4A-N3A	-4.84	120.06	126.72
2	N	1333[A]	COA	C5A-C4A-N3A	-4.84	120.06	126.72
2	P	1424	COA	C5A-C4A-N3A	-4.82	120.08	126.72
2	W	2105	COA	C5A-C4A-N3A	-4.82	120.08	126.72
2	S	1696	COA	N3A-C2A-N1A	-4.81	121.31	128.58
2	A	127	COA	N3A-C2A-N1A	-4.72	121.44	128.58
2	Q	1515	COA	N3A-C2A-N1A	-4.72	121.44	128.58
2	A	129	COA	C5A-C4A-N3A	-4.71	120.24	126.72
2	F	477	COA	N3A-C2A-N1A	-4.61	121.61	128.58
2	H	630	COA	C5A-C4A-N3A	-4.59	120.40	126.72
2	Q	1515	COA	C5A-C4A-N3A	-4.58	120.41	126.72
2	W	2019	COA	N3A-C2A-N1A	-4.55	121.69	128.58
2	T	1791	COA	N3A-C2A-N1A	-4.53	121.72	128.58
2	F	477	COA	C5A-C4A-N3A	-4.53	120.48	126.72
2	N	1221	COA	C5A-C4A-N3A	-4.50	120.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1606	COA	C5A-C4A-N3A	-4.44	120.60	126.72
2	E	387	COA	N3A-C2A-N1A	-4.44	121.86	128.58
2	G	570	COA	N3A-C2A-N1A	-4.43	121.88	128.58
2	T	1791	COA	C5A-C4A-N3A	-4.40	120.65	126.72
2	A	129	COA	N3A-C2A-N1A	-4.40	121.91	128.58
2	N	1333[A]	COA	N3A-C2A-N1A	-4.40	121.92	128.58
2	G	570	COA	C5A-C4A-N3A	-4.38	120.68	126.72
2	O	1127	COA	N3A-C2A-N1A	-4.37	121.96	128.58
8	O	2575[B]	A3P	N3-C4-N9	4.36	134.58	127.17
2	X	1944	COA	C5A-C4A-N3A	-4.34	120.73	126.72
2	A	127	COA	N9A-C8A-N7A	-4.33	107.79	113.94
2	H	630	COA	C6P-C7P-N8P	-4.32	102.80	112.00
2	X	1944	COA	N3A-C2A-N1A	-4.32	122.04	128.58
2	W	2105	COA	CAP-C9P-N8P	4.28	124.61	116.48
2	P	1424	COA	N3A-C2A-N1A	-4.27	122.11	128.58
2	S	1696	COA	C7P-N8P-C9P	4.27	130.22	122.55
2	I	699	COA	C5A-C4A-N3A	-4.26	120.86	126.72
2	E	387	COA	C5A-C4A-N3A	-4.26	120.86	126.72
2	U	1854	COA	C5A-C4A-N3A	-4.25	120.87	126.72
2	K	900	COA	C2P-C3P-N4P	-4.14	102.90	112.31
2	Q	1515	COA	C7P-N8P-C9P	4.11	129.93	122.55
2	K	900	COA	C5A-C4A-N3A	-4.05	121.13	126.72
2	L	1008	COA	N3A-C2A-N1A	-4.03	122.48	128.58
2	J	780	COA	C5A-C4A-N3A	-4.00	121.20	126.72
2	X	1944	COA	N9A-C8A-N7A	-4.00	108.27	113.94
2	S	1696	COA	N9A-C8A-N7A	-3.99	108.28	113.94
2	W	2019	COA	C3P-N4P-C5P	3.96	130.19	122.82
2	G	570	COA	N9A-C8A-N7A	-3.95	108.33	113.94
2	F	477	COA	N9A-C8A-N7A	-3.94	108.34	113.94
2	N	1221	COA	O3A-P1A-O1A	-3.90	98.96	110.70
2	L	1008	COA	N9A-C8A-N7A	-3.88	108.43	113.94
2	E	387	COA	O2A-P1A-O3A	3.84	117.66	107.27
2	W	2019	COA	N9A-C8A-N7A	-3.80	108.55	113.94
2	D	283	COA	N3A-C2A-N1A	-3.76	122.89	128.58
2	C	169	COA	C7P-N8P-C9P	3.73	129.25	122.55
2	I	699	COA	N9A-C8A-N7A	-3.72	108.66	113.94
2	A	127	COA	O2A-P1A-O3A	-3.70	97.28	107.27
8	O	2575[B]	A3P	C2-N3-C4	3.67	120.80	111.83
2	N	1221	COA	N9A-C8A-N7A	-3.63	108.79	113.94
2	A	127	COA	C2A-N3A-C4A	3.61	120.66	111.83
2	S	1696	COA	C2A-N3A-C4A	3.61	120.65	111.83
2	L	1008	COA	O5A-P2A-O4A	3.61	129.23	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	630	COA	N9A-C8A-N7A	-3.60	108.83	113.94
2	X	1944	COA	C7P-N8P-C9P	3.58	128.98	122.55
2	A	127	COA	C4A-C5A-N7A	-3.55	106.53	110.58
2	O	1127	COA	N9A-C8A-N7A	-3.53	108.93	113.94
2	O	1127	COA	C2A-N3A-C4A	3.53	120.45	111.83
2	D	283	COA	C7P-N8P-C9P	3.50	128.84	122.55
2	C	169	COA	N9A-C8A-N7A	-3.48	109.00	113.94
2	X	1944	COA	C4A-N9A-C8A	3.48	109.39	105.74
2	K	900	COA	N9A-C8A-N7A	-3.47	109.01	113.94
2	J	780	COA	N9A-C8A-N7A	-3.45	109.04	113.94
2	T	1791	COA	N9A-C8A-N7A	-3.43	109.07	113.94
2	D	283	COA	N9A-C8A-N7A	-3.42	109.08	113.94
2	N	1333[A]	COA	N9A-C8A-N7A	-3.42	109.09	113.94
2	W	2019	COA	C2A-N3A-C4A	3.40	120.14	111.83
2	R	1606	COA	N9A-C8A-N7A	-3.40	109.11	113.94
2	A	127	COA	C5A-N7A-C8A	3.40	108.80	103.45
2	K	900	COA	C4A-N9A-C8A	3.40	109.31	105.74
2	W	2019	COA	N3A-C4A-N9A	3.38	132.92	127.17
2	Q	1515	COA	C6P-C7P-N8P	-3.38	104.82	112.00
2	P	1424	COA	C7P-N8P-C9P	3.37	128.59	122.55
2	C	169	COA	C2A-N3A-C4A	3.36	120.05	111.83
2	P	1424	COA	N9A-C8A-N7A	-3.36	109.17	113.94
8	O	2575[B]	A3P	N3-C2-N1	-3.36	123.50	128.58
2	W	2019	COA	C4A-N9A-C8A	3.36	109.26	105.74
2	W	2105	COA	C2A-N3A-C4A	3.35	120.01	111.83
2	K	900	COA	CEP-CBP-CAP	3.34	114.47	108.77
2	W	2105	COA	N9A-C8A-N7A	-3.34	109.20	113.94
2	A	129	COA	N9A-C8A-N7A	-3.34	109.20	113.94
2	N	1221	COA	C2A-N3A-C4A	3.33	119.98	111.83
2	F	477	COA	C2A-N3A-C4A	3.33	119.97	111.83
2	U	1854	COA	N9A-C8A-N7A	-3.30	109.25	113.94
2	R	1606	COA	C2A-N3A-C4A	3.30	119.88	111.83
2	I	699	COA	C2A-N3A-C4A	3.29	119.87	111.83
8	O	2575[B]	A3P	C4-C5-N7	-3.29	106.82	110.58
2	H	630	COA	C2A-N3A-C4A	3.29	119.86	111.83
2	O	1127	COA	N3A-C4A-N9A	3.27	132.73	127.17
2	N	1333[A]	COA	C2A-N3A-C4A	3.24	119.76	111.83
2	Q	1515	COA	N9A-C8A-N7A	-3.24	109.34	113.94
2	O	1127	COA	C6P-C7P-N8P	-3.24	105.10	112.00
2	T	1791	COA	C2P-C3P-N4P	-3.23	104.98	112.31
2	J	780	COA	O4B-C1B-N9A	3.22	114.28	108.09
2	N	1221	COA	C3P-N4P-C5P	3.22	128.81	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	169	COA	O4B-C1B-N9A	3.21	114.25	108.09
2	D	283	COA	O2A-P1A-O3A	3.20	115.93	107.27
2	R	1606	COA	C6P-C7P-N8P	-3.20	105.19	112.00
2	C	169	COA	C3P-N4P-C5P	3.20	128.77	122.82
2	J	780	COA	O5A-P2A-O4A	3.18	127.25	112.44
2	X	1944	COA	C4A-C5A-N7A	-3.18	106.94	110.58
2	E	387	COA	C3P-N4P-C5P	3.18	128.74	122.82
2	E	387	COA	N9A-C8A-N7A	-3.17	109.44	113.94
2	N	1221	COA	C6P-C7P-N8P	-3.17	105.25	112.00
2	Q	1515	COA	C2A-N3A-C4A	3.13	119.46	111.83
2	U	1854	COA	C2A-N3A-C4A	3.11	119.42	111.83
2	L	1008	COA	N3A-C4A-N9A	3.10	132.44	127.17
8	O	2575[B]	A3P	C4-N9-C8	3.10	108.99	105.74
2	L	1008	COA	C2A-N3A-C4A	3.09	119.38	111.83
2	C	169	COA	O2A-P1A-O3A	3.09	115.63	107.27
2	T	1791	COA	C2A-N3A-C4A	3.09	119.38	111.83
2	R	1606	COA	N3A-C4A-N9A	3.09	132.43	127.17
2	C	169	COA	N3A-C4A-N9A	3.08	132.41	127.17
2	K	900	COA	CDP-CBP-CAP	-3.08	103.52	108.77
2	H	630	COA	C3P-N4P-C5P	3.08	128.56	122.82
2	G	570	COA	C4A-N9A-C8A	3.08	108.97	105.74
2	J	780	COA	C4A-N9A-C8A	3.07	108.96	105.74
2	L	1008	COA	C4A-N9A-C8A	3.05	108.94	105.74
2	N	1221	COA	C4A-N9A-C8A	3.05	108.94	105.74
2	O	1127	COA	C4A-C5A-N7A	-3.04	107.10	110.58
2	P	1424	COA	N3A-C4A-N9A	3.04	132.34	127.17
2	P	1424	COA	C2A-N3A-C4A	3.04	119.25	111.83
2	C	169	COA	O5A-P2A-O4A	3.03	126.56	112.44
2	A	129	COA	C2A-N3A-C4A	3.03	119.23	111.83
2	F	477	COA	C4A-N9A-C8A	3.02	108.91	105.74
2	K	900	COA	C2A-N3A-C4A	3.02	119.20	111.83
2	S	1696	COA	N3A-C4A-N9A	3.02	132.29	127.17
2	W	2105	COA	N3A-C4A-N9A	3.01	132.28	127.17
2	N	1333[A]	COA	C2P-C3P-N4P	-3.00	105.50	112.31
2	T	1791	COA	C4A-C5A-N7A	-2.99	107.16	110.58
2	S	1696	COA	C4A-C5A-N7A	-2.99	107.16	110.58
2	C	169	COA	C4A-C5A-N7A	-2.99	107.16	110.58
2	R	1606	COA	O5A-P2A-O4A	2.99	126.34	112.44
2	W	2019	COA	O4B-C1B-N9A	2.98	113.82	108.09
2	F	477	COA	C2P-C3P-N4P	-2.98	105.54	112.31
2	F	477	COA	N3A-C4A-N9A	2.97	132.22	127.17
2	X	1944	COA	C3P-N4P-C5P	2.97	128.34	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	630	COA	C4A-N9A-C8A	2.96	108.84	105.74
2	I	699	COA	C4A-N9A-C8A	2.93	108.82	105.74
2	N	1333[A]	COA	N3A-C4A-N9A	2.92	132.14	127.17
2	D	283	COA	C2A-N3A-C4A	2.92	118.95	111.83
2	G	570	COA	O2A-P1A-O1A	2.90	125.93	112.44
2	D	283	COA	N3A-C4A-N9A	2.90	132.10	127.17
2	D	283	COA	C4A-C5A-N7A	-2.90	107.27	110.58
2	W	2019	COA	C7P-N8P-C9P	2.90	127.75	122.55
2	O	1127	COA	C2P-C3P-N4P	-2.89	105.74	112.31
2	Q	1515	COA	O5A-P2A-O4A	2.89	125.90	112.44
2	A	129	COA	N3A-C4A-N9A	2.89	132.08	127.17
2	G	570	COA	C2A-N3A-C4A	2.89	118.88	111.83
2	J	780	COA	C2A-N3A-C4A	2.88	118.86	111.83
2	U	1854	COA	C4A-N9A-C8A	2.87	108.75	105.74
2	O	1127	COA	O4B-C1B-N9A	2.87	113.60	108.09
2	A	127	COA	O9P-C9P-N8P	-2.87	116.91	122.98
2	Q	1515	COA	N3A-C4A-N9A	2.86	132.03	127.17
2	L	1008	COA	C7P-N8P-C9P	2.86	127.68	122.55
2	H	630	COA	N3A-C4A-N9A	2.86	132.02	127.17
2	E	387	COA	C4A-N9A-C8A	2.84	108.72	105.74
2	Q	1515	COA	O2A-P1A-O1A	2.83	125.59	112.44
2	X	1944	COA	C2P-C3P-N4P	-2.82	105.90	112.31
2	N	1221	COA	O4B-C1B-N9A	2.82	113.51	108.09
2	N	1221	COA	N3A-C4A-N9A	2.82	131.96	127.17
2	U	1854	COA	O5A-P2A-O4A	2.82	125.55	112.44
2	X	1944	COA	C2A-N3A-C4A	2.81	118.70	111.83
2	S	1696	COA	C3P-N4P-C5P	2.81	128.06	122.82
2	I	699	COA	C3P-N4P-C5P	2.80	128.04	122.82
2	E	387	COA	C2A-N3A-C4A	2.80	118.67	111.83
2	S	1696	COA	C5A-N7A-C8A	2.80	107.84	103.45
2	F	477	COA	C5A-N7A-C8A	2.78	107.82	103.45
2	R	1606	COA	C3P-N4P-C5P	2.78	128.00	122.82
2	X	1944	COA	C5A-N7A-C8A	2.76	107.79	103.45
2	R	1606	COA	C4A-N9A-C8A	2.76	108.64	105.74
2	S	1696	COA	C4A-N9A-C8A	2.76	108.63	105.74
2	A	129	COA	C4A-N9A-C8A	2.74	108.62	105.74
2	L	1008	COA	C4A-C5A-N7A	-2.74	107.45	110.58
2	K	900	COA	C7P-N8P-C9P	2.73	127.45	122.55
2	F	477	COA	O3B-P3B-O7A	-2.73	99.61	109.33
2	N	1221	COA	C4A-C5A-N7A	-2.72	107.47	110.58
2	W	2105	COA	OAP-CAP-CBP	-2.72	103.88	110.18
2	E	387	COA	C4A-C5A-N7A	-2.72	107.47	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1127	COA	C5A-N7A-C8A	2.71	107.71	103.45
2	U	1854	COA	N3A-C4A-N9A	2.71	131.77	127.17
2	I	699	COA	O5A-P2A-O4A	2.71	125.04	112.44
2	W	2105	COA	C3P-N4P-C5P	2.70	127.86	122.82
2	W	2019	COA	O5A-P2A-O4A	2.70	125.01	112.44
2	C	169	COA	C5A-N7A-C8A	2.70	107.69	103.45
2	X	1944	COA	O5A-P2A-O4A	2.70	124.98	112.44
2	N	1333[A]	COA	C4A-N9A-C8A	2.69	108.57	105.74
8	O	2575[B]	A3P	O4'-C1'-N9	2.69	113.26	108.09
2	N	1333[A]	COA	C4A-C5A-N7A	-2.69	107.51	110.58
2	C	169	COA	C2P-C3P-N4P	-2.68	106.22	112.31
2	T	1791	COA	C4A-N9A-C8A	2.68	108.55	105.74
2	K	900	COA	N3A-C4A-N9A	2.67	131.72	127.17
2	G	570	COA	C4A-C5A-N7A	-2.67	107.53	110.58
2	L	1008	COA	O2A-P1A-O1A	2.67	124.85	112.44
2	S	1696	COA	C2P-C3P-N4P	-2.67	106.26	112.31
2	H	630	COA	O6A-CCP-CBP	2.67	114.83	110.55
2	K	900	COA	O4B-C1B-N9A	2.66	113.19	108.09
2	Q	1515	COA	C4A-C5A-N7A	-2.65	107.55	110.58
2	G	570	COA	N3A-C4A-N9A	2.65	131.67	127.17
2	I	699	COA	C2P-C3P-N4P	-2.65	106.30	112.31
2	S	1696	COA	O3A-P2A-O4A	-2.65	102.74	110.70
2	J	780	COA	C3P-N4P-C5P	2.65	127.75	122.82
2	X	1944	COA	N3A-C4A-N9A	2.65	131.67	127.17
2	W	2105	COA	O2A-P1A-O3A	2.64	114.41	107.27
2	H	630	COA	C2B-C1B-N9A	-2.64	106.75	113.30
2	O	1127	COA	C2B-C1B-N9A	-2.64	106.75	113.30
2	S	1696	COA	O5A-P2A-O4A	2.63	124.69	112.44
2	O	1127	COA	C4A-N9A-C8A	2.63	108.50	105.74
2	D	283	COA	O4B-C1B-N9A	2.62	113.12	108.09
2	Q	1515	COA	O3A-P2A-O4A	-2.62	102.83	110.70
2	P	1424	COA	C3P-N4P-C5P	2.61	127.69	122.82
2	U	1854	COA	C3P-N4P-C5P	2.60	127.67	122.82
2	J	780	COA	N3A-C4A-N9A	2.60	131.59	127.17
2	L	1008	COA	O4B-C1B-N9A	2.60	113.09	108.09
2	U	1854	COA	C6P-C7P-N8P	-2.60	106.47	112.00
2	A	129	COA	C3P-N4P-C5P	2.60	127.66	122.82
2	H	630	COA	C4A-C5A-N7A	-2.60	107.61	110.58
2	F	477	COA	C4A-C5A-N7A	-2.60	107.61	110.58
2	Q	1515	COA	C4A-N9A-C8A	2.59	108.46	105.74
2	K	900	COA	CDP-CBP-CCP	2.59	112.50	108.22
2	G	570	COA	C5A-N7A-C8A	2.58	107.51	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	283	COA	C5A-N7A-C8A	2.58	107.51	103.45
2	A	127	COA	C4A-N9A-C8A	2.58	108.45	105.74
2	I	699	COA	C4A-C5A-N7A	-2.58	107.63	110.58
2	P	1424	COA	C2P-C3P-N4P	-2.58	106.46	112.31
2	U	1854	COA	C7P-N8P-C9P	2.57	127.16	122.55
2	L	1008	COA	O3A-P2A-O4A	-2.57	102.98	110.70
2	I	699	COA	C2B-C3B-C4B	-2.56	98.75	103.24
2	Q	1515	COA	C3P-N4P-C5P	2.56	127.58	122.82
2	A	127	COA	N3A-C4A-N9A	2.56	131.51	127.17
8	O	2575[B]	A3P	C2'-C1'-N9	-2.55	106.96	113.30
2	A	127	COA	CAP-C9P-N8P	2.55	121.32	116.48
2	L	1008	COA	C5A-N7A-C8A	2.53	107.43	103.45
2	R	1606	COA	C3B-C2B-C1B	2.53	105.45	99.89
2	I	699	COA	N3A-C4A-N9A	2.53	131.46	127.17
2	A	127	COA	O5A-P2A-O4A	2.52	124.19	112.44
2	A	129	COA	C4A-C5A-N7A	-2.52	107.70	110.58
2	F	477	COA	C7P-N8P-C9P	2.52	127.07	122.55
2	C	169	COA	C4A-N9A-C8A	2.52	108.38	105.74
2	T	1791	COA	N3A-C4A-N9A	2.52	131.45	127.17
2	S	1696	COA	O4B-C1B-N9A	2.51	112.92	108.09
2	T	1791	COA	C3P-N4P-C5P	2.51	127.50	122.82
2	L	1008	COA	O3B-P3B-O7A	-2.51	100.40	109.33
2	E	387	COA	C7P-N8P-C9P	2.50	127.05	122.55
2	O	1127	COA	C3P-N4P-C5P	2.50	127.48	122.82
2	U	1854	COA	C2P-C3P-N4P	-2.50	106.64	112.31
2	L	1008	COA	C2B-C3B-C4B	-2.50	98.87	103.24
2	A	127	COA	C2P-C3P-N4P	-2.50	106.64	112.31
2	A	129	COA	O2A-P1A-O3A	2.49	114.01	107.27
2	G	570	COA	C6P-C7P-N8P	-2.49	106.70	112.00
2	T	1791	COA	C5A-N7A-C8A	2.48	107.35	103.45
2	R	1606	COA	C2P-C3P-N4P	-2.48	106.69	112.31
2	I	699	COA	O2A-P1A-O1A	2.47	123.95	112.44
2	R	1606	COA	C2B-C3B-C4B	-2.47	98.92	103.24
2	A	127	COA	C7P-C6P-C5P	-2.46	108.30	112.39
2	J	780	COA	C6P-C7P-N8P	-2.46	106.77	112.00
2	F	477	COA	O3A-P2A-O4A	-2.46	103.31	110.70
2	F	477	COA	C3P-N4P-C5P	2.45	127.38	122.82
2	D	283	COA	C4A-N9A-C8A	2.43	108.29	105.74
2	J	780	COA	O2A-P1A-O1A	2.43	123.75	112.44
2	X	1944	COA	C7P-C6P-C5P	-2.43	108.35	112.39
2	W	2019	COA	C4A-C5A-N7A	-2.42	107.82	110.58
2	N	1221	COA	C5A-N7A-C8A	2.42	107.25	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	570	COA	O5A-P2A-O4A	2.41	123.67	112.44
2	A	127	COA	C5A-C4A-N9A	2.40	108.43	105.81
2	D	283	COA	C3P-N4P-C5P	2.40	127.29	122.82
2	A	127	COA	C2B-C3B-C4B	-2.40	99.04	103.24
2	E	387	COA	N3A-C4A-N9A	2.39	131.24	127.17
2	P	1424	COA	C4A-N9A-C8A	2.39	108.25	105.74
2	W	2105	COA	C5A-N7A-C8A	2.39	107.20	103.45
2	I	699	COA	C5A-N7A-C8A	2.39	107.20	103.45
2	W	2105	COA	O3B-P3B-O7A	-2.38	100.84	109.33
2	G	570	COA	C7P-N8P-C9P	2.38	126.81	122.55
2	W	2019	COA	C6P-C7P-N8P	-2.38	106.94	112.00
2	H	630	COA	O5A-P2A-O4A	2.36	123.44	112.44
2	W	2105	COA	C4A-C5A-N7A	-2.36	107.89	110.58
2	H	630	COA	C5A-N7A-C8A	2.35	107.14	103.45
2	R	1606	COA	O2A-P1A-O1A	2.34	123.34	112.44
2	R	1606	COA	C5A-N7A-C8A	2.34	107.12	103.45
8	O	2575[B]	A3P	C5-N7-C8	2.34	107.12	103.45
2	P	1424	COA	C4A-C5A-N7A	-2.33	107.92	110.58
2	N	1221	COA	C2P-C3P-N4P	-2.33	107.03	112.31
2	F	477	COA	CAP-C9P-N8P	2.33	120.90	116.48
2	P	1424	COA	O5A-P2A-O4A	2.32	123.25	112.44
2	Q	1515	COA	C5A-N7A-C8A	2.32	107.09	103.45
2	J	780	COA	CAP-C9P-N8P	2.32	120.88	116.48
2	W	2019	COA	O2A-P1A-O1A	2.31	123.21	112.44
2	W	2019	COA	C5A-N7A-C8A	2.31	107.09	103.45
2	P	1424	COA	C5A-N7A-C8A	2.31	107.08	103.45
2	W	2105	COA	O9P-C9P-N8P	-2.31	118.09	122.98
2	L	1008	COA	C2P-C3P-N4P	-2.30	107.09	112.31
2	X	1944	COA	O2A-P1A-O1A	2.29	123.09	112.44
2	D	283	COA	O5A-P2A-O4A	2.28	123.05	112.44
2	Q	1515	COA	C2B-C3B-C4B	-2.28	99.25	103.24
2	N	1333[A]	COA	C5A-N7A-C8A	2.28	107.03	103.45
2	C	169	COA	C6P-C7P-N8P	-2.28	107.16	112.00
8	O	2575[B]	A3P	C3'-C2'-C1'	2.27	104.89	99.89
2	K	900	COA	C2B-C3B-C4B	-2.27	99.26	103.24
2	L	1008	COA	C7P-C6P-C5P	-2.26	108.64	112.39
2	H	630	COA	O2A-P1A-O1A	2.25	122.91	112.44
2	I	699	COA	C6P-C7P-N8P	-2.25	107.21	112.00
2	G	570	COA	C3P-N4P-C5P	2.25	127.01	122.82
2	I	699	COA	O4B-C1B-N9A	2.25	112.41	108.09
2	E	387	COA	CAP-C9P-N8P	2.24	120.74	116.48
2	C	169	COA	C3B-C2B-C1B	2.24	104.81	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1944	COA	C2B-C3B-C4B	-2.24	99.32	103.24
2	I	699	COA	CEP-CBP-CCP	-2.23	104.54	108.22
2	N	1221	COA	C7P-N8P-C9P	2.23	126.55	122.55
2	W	2105	COA	C4A-N9A-C8A	2.23	108.08	105.74
2	N	1221	COA	CAP-C9P-N8P	2.22	120.70	116.48
2	G	570	COA	C2P-C3P-N4P	-2.21	107.30	112.31
2	E	387	COA	O5A-P2A-O4A	2.21	122.71	112.44
2	T	1791	COA	C7P-C6P-C5P	-2.20	108.72	112.39
2	W	2019	COA	C3B-C2B-C1B	2.20	104.73	99.89
8	O	2575[B]	A3P	N9-C8-N7	-2.20	110.82	113.94
2	O	1127	COA	C7P-N8P-C9P	2.19	126.49	122.55
2	A	127	COA	CEP-CBP-CAP	2.19	112.50	108.77
2	R	1606	COA	CAP-C9P-N8P	2.19	120.63	116.48
2	D	283	COA	C3B-C2B-C1B	2.19	104.70	99.89
2	S	1696	COA	O2A-P1A-O1A	2.19	122.61	112.44
2	F	477	COA	C2B-C1B-N9A	-2.18	107.89	113.30
2	P	1424	COA	C6P-C7P-N8P	-2.17	107.37	112.00
2	D	283	COA	O2A-P1A-O1A	2.17	122.53	112.44
2	W	2019	COA	O2A-P1A-O3A	2.17	113.13	107.27
2	I	699	COA	O6A-CCP-CBP	2.16	114.03	110.55
2	R	1606	COA	O9P-C9P-N8P	-2.16	118.41	122.98
2	C	169	COA	C2B-C3B-C4B	-2.16	99.46	103.24
2	N	1333[A]	COA	CDP-CBP-CAP	2.16	112.45	108.77
2	N	1221	COA	O9P-C9P-N8P	-2.15	118.42	122.98
2	A	127	COA	C6P-C7P-N8P	-2.15	107.41	112.00
2	F	477	COA	O5A-P2A-O4A	2.15	122.46	112.44
2	O	1127	COA	O5B-C5B-C4B	-2.15	101.67	108.99
2	R	1606	COA	C4A-C5A-N7A	-2.14	108.13	110.58
2	G	570	COA	C2B-C1B-N9A	-2.14	107.98	113.30
2	A	129	COA	C2B-C1B-N9A	-2.14	108.00	113.30
2	W	2019	COA	O5B-C5B-C4B	-2.14	101.72	108.99
2	D	283	COA	C2P-C3P-N4P	-2.13	107.46	112.31
2	Q	1515	COA	C3B-C2B-C1B	2.13	104.58	99.89
2	A	129	COA	C5A-N7A-C8A	2.13	106.80	103.45
8	O	2575[B]	A3P	C6-C5-N7	2.13	136.19	132.09
2	W	2019	COA	C2B-C3B-C4B	-2.13	99.52	103.24
2	G	570	COA	O5B-C5B-C4B	-2.12	101.78	108.99
2	O	1127	COA	O3B-P3B-O7A	-2.11	101.80	109.33
2	I	699	COA	C7P-N8P-C9P	2.11	126.34	122.55
2	O	1127	COA	O3A-P1A-O1A	-2.11	104.36	110.70
2	H	630	COA	C2B-C3B-C4B	-2.11	99.55	103.24
2	N	1333[A]	COA	O4B-C1B-N9A	2.11	112.14	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	900	COA	O2A-P1A-O3A	2.10	112.96	107.27
2	H	630	COA	C2P-C3P-N4P	-2.10	107.54	112.31
2	A	129	COA	C2B-C3B-C4B	-2.10	99.56	103.24
2	A	127	COA	C2B-C1B-N9A	-2.10	108.09	113.30
2	O	1127	COA	C2B-C3B-C4B	-2.10	99.56	103.24
2	G	570	COA	O3A-P2A-O4A	-2.10	104.39	110.70
2	F	477	COA	C6P-C7P-N8P	-2.10	107.54	112.00
2	G	570	COA	O4B-C1B-N9A	2.10	112.11	108.09
2	I	699	COA	O9P-C9P-N8P	-2.09	118.55	122.98
2	C	169	COA	O2A-P1A-O1A	2.09	122.17	112.44
2	A	127	COA	C3P-N4P-C5P	2.09	126.71	122.82
2	S	1696	COA	C5A-C4A-N9A	2.09	108.08	105.81
2	E	387	COA	O6A-CCP-CBP	2.08	113.89	110.55
2	U	1854	COA	C2B-C3B-C4B	-2.08	99.60	103.24
2	L	1008	COA	C3P-N4P-C5P	2.08	126.69	122.82
2	A	129	COA	O2A-P1A-O1A	2.07	122.08	112.44
2	O	1127	COA	C3B-C2B-C1B	2.07	104.44	99.89
2	P	1424	COA	O4B-C1B-N9A	2.07	112.06	108.09
2	K	900	COA	C4A-C5A-N7A	-2.06	108.23	110.58
2	N	1221	COA	O2A-P1A-O1A	2.06	122.00	112.44
2	G	570	COA	O6A-CCP-CBP	2.05	113.85	110.55
2	J	780	COA	C2P-C3P-N4P	-2.05	107.65	112.31
2	K	900	COA	C3B-C2B-C1B	2.05	104.40	99.89
2	N	1221	COA	O5A-P2A-O4A	2.05	121.98	112.44
2	L	1008	COA	O8A-P3B-O7A	2.04	118.79	110.83
2	T	1791	COA	O9A-P3B-O8A	2.04	115.45	107.80
2	E	387	COA	C2P-C3P-N4P	-2.04	107.68	112.31
2	P	1424	COA	C2B-C3B-C4B	-2.04	99.67	103.24
2	S	1696	COA	C2B-C3B-C4B	-2.03	99.68	103.24
2	F	477	COA	O4B-C1B-N9A	2.03	111.98	108.09
2	L	1008	COA	O9P-C9P-N8P	-2.02	118.70	122.98
2	H	630	COA	C7P-N8P-C9P	2.02	126.18	122.55
2	L	1008	COA	O5B-C5B-C4B	-2.02	102.11	108.99
2	L	1008	COA	C3B-C2B-C1B	2.01	104.32	99.89
2	E	387	COA	O5B-C5B-C4B	-2.00	102.17	108.99

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	127	COA	S1P-C2P-C3P-N4P
2	A	129	COA	N8P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	A	129	COA	C5P-C6P-C7P-N8P
2	D	283	COA	C2B-C3B-O3B-P3B
2	E	387	COA	C2B-C3B-O3B-P3B
2	E	387	COA	S1P-C2P-C3P-N4P
2	F	477	COA	CCP-O6A-P2A-O3A
2	F	477	COA	CCP-O6A-P2A-O4A
2	F	477	COA	S1P-C2P-C3P-N4P
2	G	570	COA	S1P-C2P-C3P-N4P
2	H	630	COA	C2P-C3P-N4P-C5P
2	I	699	COA	S1P-C2P-C3P-N4P
2	J	780	COA	C2B-C3B-O3B-P3B
2	J	780	COA	S1P-C2P-C3P-N4P
2	N	1221	COA	CCP-O6A-P2A-O3A
2	N	1221	COA	CCP-O6A-P2A-O4A
2	N	1221	COA	S1P-C2P-C3P-N4P
2	N	1333[A]	COA	CCP-O6A-P2A-O4A
2	N	1333[A]	COA	CCP-O6A-P2A-O5A
2	N	1333[A]	COA	CDP-CBP-CCP-O6A
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	O	1127	COA	CCP-O6A-P2A-O3A
2	O	1127	COA	CCP-O6A-P2A-O4A
2	O	1127	COA	S1P-C2P-C3P-N4P
2	P	1424	COA	OAP-CAP-CBP-CCP
2	P	1424	COA	C9P-CAP-CBP-CCP
2	P	1424	COA	OAP-CAP-CBP-CDP
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	Q	1515	COA	S1P-C2P-C3P-N4P
2	R	1606	COA	S1P-C2P-C3P-N4P
2	S	1696	COA	C5B-O5B-P1A-O1A
2	S	1696	COA	C5B-O5B-P1A-O3A
2	S	1696	COA	N8P-C9P-CAP-OAP
2	S	1696	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
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	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
5	S	1697	MPD	C2-C3-C4-O4
5	S	1697	MPD	C2-C3-C4-C5
7	N	2565	MRD	C2-C3-C4-C5
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	N	1333[A]	COA	C6P-C7P-N8P-C9P
2	S	1696	COA	C6P-C7P-N8P-C9P
2	A	129	COA	C2B-C3B-O3B-P3B
2	C	169	COA	C2B-C3B-O3B-P3B
2	F	477	COA	C2B-C3B-O3B-P3B
2	G	570	COA	C2B-C3B-O3B-P3B
2	I	699	COA	C2B-C3B-O3B-P3B
2	K	900	COA	C2B-C3B-O3B-P3B
2	N	1221	COA	C2B-C3B-O3B-P3B
2	N	1333[A]	COA	C2B-C3B-O3B-P3B
2	P	1424	COA	C2B-C3B-O3B-P3B
2	S	1696	COA	C2B-C3B-O3B-P3B
2	T	1791	COA	C2B-C3B-O3B-P3B
2	U	1854	COA	C2B-C3B-O3B-P3B
2	W	2019	COA	C2B-C3B-O3B-P3B
2	W	2105	COA	C2B-C3B-O3B-P3B
8	O	2575[B]	A3P	C2'-C3'-O3'-P1
2	C	169	COA	C6P-C7P-N8P-C9P
2	A	127	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	Q	1515	COA	C2B-C3B-O3B-P3B
2	R	1606	COA	C2B-C3B-O3B-P3B
2	X	1944	COA	C2B-C3B-O3B-P3B
2	A	129	COA	C6P-C7P-N8P-C9P
8	O	2575[B]	A3P	O4'-C4'-C5'-O5'
8	O	2575[B]	A3P	C3'-C4'-C5'-O5'
2	A	127	COA	C4B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
2	G	570	COA	C4B-C3B-O3B-P3B
2	H	630	COA	C4B-C3B-O3B-P3B
2	L	1008	COA	C4B-C3B-O3B-P3B
2	N	1333[A]	COA	C4B-C3B-O3B-P3B
2	O	1127	COA	C4B-C3B-O3B-P3B
2	Q	1515	COA	C4B-C3B-O3B-P3B
2	R	1606	COA	C4B-C3B-O3B-P3B
2	W	2019	COA	C4B-C3B-O3B-P3B
2	X	1944	COA	C4B-C3B-O3B-P3B
2	A	129	COA	C4B-C3B-O3B-P3B
2	F	477	COA	C4B-C3B-O3B-P3B
2	A	129	COA	O9P-C9P-CAP-OAP
2	N	1333[A]	COA	O9P-C9P-CAP-OAP
2	S	1696	COA	O9P-C9P-CAP-OAP
2	W	2019	COA	O9P-C9P-CAP-OAP
2	F	477	COA	C6P-C7P-N8P-C9P
2	C	169	COA	C4B-C3B-O3B-P3B
2	D	283	COA	C4B-C3B-O3B-P3B
2	E	387	COA	C4B-C3B-O3B-P3B
2	I	699	COA	C4B-C3B-O3B-P3B
2	J	780	COA	C4B-C3B-O3B-P3B
2	K	900	COA	C4B-C3B-O3B-P3B
2	N	1221	COA	C4B-C3B-O3B-P3B
2	P	1424	COA	C4B-C3B-O3B-P3B
2	T	1791	COA	C4B-C3B-O3B-P3B
2	U	1854	COA	C4B-C3B-O3B-P3B
2	W	2105	COA	C4B-C3B-O3B-P3B
8	O	2575[B]	A3P	C4'-C3'-O3'-P1
2	A	129	COA	O9P-C9P-CAP-CBP
2	S	1696	COA	O9P-C9P-CAP-CBP
2	W	2019	COA	O9P-C9P-CAP-CBP
2	A	127	COA	C3B-O3B-P3B-O9A
2	A	129	COA	N8P-C9P-CAP-CBP
2	C	169	COA	N8P-C9P-CAP-CBP
2	H	630	COA	N8P-C9P-CAP-CBP
2	S	1696	COA	N8P-C9P-CAP-CBP
2	W	2019	COA	N8P-C9P-CAP-CBP
2	W	2105	COA	N8P-C9P-CAP-OAP
2	F	477	COA	P1A-O3A-P2A-O6A
2	H	630	COA	C5P-C6P-C7P-N8P
2	E	387	COA	C6P-C7P-N8P-C9P
2	A	127	COA	P1A-O3A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
2	E	387	COA	CDP-CBP-CCP-O6A
2	H	630	COA	CDP-CBP-CCP-O6A
2	U	1854	COA	CDP-CBP-CCP-O6A
5	M	2572	MPD	C1-C2-C3-C4
5	M	2572	MPD	CM-C2-C3-C4
5	U	1698	MPD	CM-C2-C3-C4
5	W	2106	MPD	C1-C2-C3-C4
7	K	2564	MRD	CM-C2-C3-C4
7	N	2565	MRD	CM-C2-C3-C4
2	E	387	COA	CAP-CBP-CCP-O6A
2	H	630	COA	CAP-CBP-CCP-O6A
2	H	630	COA	S1P-C2P-C3P-N4P
2	U	1854	COA	CAP-CBP-CCP-O6A
2	U	1854	COA	S1P-C2P-C3P-N4P
2	W	2019	COA	S1P-C2P-C3P-N4P
2	A	127	COA	C5B-O5B-P1A-O3A
2	F	477	COA	CCP-O6A-P2A-O5A
2	K	900	COA	C5B-O5B-P1A-O1A
2	N	1221	COA	CCP-O6A-P2A-O5A
2	N	1333[A]	COA	CCP-O6A-P2A-O3A
2	O	1127	COA	CCP-O6A-P2A-O5A
2	P	1424	COA	C5B-O5B-P1A-O1A
2	T	1791	COA	C5B-O5B-P1A-O1A
5	B	127	MPD	C2-C3-C4-C5
7	D	2573	MRD	C2-C3-C4-C5
2	S	1696	COA	C4B-C3B-O3B-P3B
2	N	1333[A]	COA	C5P-C6P-C7P-N8P
2	X	1944	COA	OAP-CAP-CBP-CEP
2	C	169	COA	O9P-C9P-CAP-CBP
2	N	1333[A]	COA	O9P-C9P-CAP-CBP
2	A	129	COA	C3B-O3B-P3B-O9A
2	C	169	COA	C3B-O3B-P3B-O9A
2	D	283	COA	C3B-O3B-P3B-O9A
2	E	387	COA	C3B-O3B-P3B-O9A
2	F	477	COA	C3B-O3B-P3B-O9A
2	G	570	COA	C3B-O3B-P3B-O9A
2	I	699	COA	C3B-O3B-P3B-O9A
2	J	780	COA	C3B-O3B-P3B-O9A
2	K	900	COA	C3B-O3B-P3B-O9A
2	N	1221	COA	C3B-O3B-P3B-O9A
2	O	1127	COA	C3B-O3B-P3B-O9A
2	Q	1515	COA	C3B-O3B-P3B-O9A

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Mol	Chain	Res	Type	Atoms
2	S	1696	COA	C3B-O3B-P3B-O9A
2	T	1791	COA	C3B-O3B-P3B-O9A
2	U	1854	COA	C3B-O3B-P3B-O9A
2	W	2019	COA	C3B-O3B-P3B-O9A
2	W	2105	COA	C3B-O3B-P3B-O9A
2	X	1944	COA	C3B-O3B-P3B-O9A
8	O	2575[B]	A3P	C3'-O3'-P1-O2P
2	N	1333[A]	COA	N8P-C9P-CAP-CBP
2	U	1854	COA	N8P-C9P-CAP-CBP
2	N	1333[A]	COA	N8P-C9P-CAP-OAP
2	S	1696	COA	C3B-C4B-C5B-O5B
2	W	2019	COA	O5P-C5P-C6P-C7P
2	H	630	COA	OAP-CAP-CBP-CEP
2	X	1944	COA	OAP-CAP-CBP-CDP
2	A	127	COA	P1A-O3A-P2A-O5A
2	N	1221	COA	P1A-O3A-P2A-O4A
2	Q	1515	COA	P2A-O3A-P1A-O2A
2	S	1696	COA	P1A-O3A-P2A-O4A
2	H	630	COA	O9P-C9P-CAP-CBP
2	U	1854	COA	O9P-C9P-CAP-CBP
5	B	127	MPD	O2-C2-C3-C4
5	M	2572	MPD	O2-C2-C3-C4
5	W	2106	MPD	O2-C2-C3-C4
7	K	2564	MRD	O2-C2-C3-C4
2	R	1606	COA	C3B-O3B-P3B-O8A
2	X	1944	COA	C3B-O3B-P3B-O8A
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	A	129	COA	CDP-CBP-CCP-O6A
2	D	283	COA	C9P-CAP-CBP-CCP
2	E	387	COA	CEP-CBP-CCP-O6A
2	H	630	COA	CEP-CBP-CCP-O6A
2	H	630	COA	C9P-CAP-CBP-CCP
2	I	699	COA	CDP-CBP-CCP-O6A
2	O	1127	COA	C9P-CAP-CBP-CCP
2	Q	1515	COA	CDP-CBP-CCP-O6A
2	Q	1515	COA	C9P-CAP-CBP-CCP
2	W	2019	COA	CDP-CBP-CCP-O6A
2	X	1944	COA	C9P-CAP-CBP-CCP
5	B	127	MPD	C1-C2-C3-C4
5	B	127	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	C	2571	MPD	C1-C2-C3-C4
5	G	571	MPD	C1-C2-C3-C4
5	H	631	MPD	C1-C2-C3-C4
5	H	631	MPD	CM-C2-C3-C4
5	O	1334	MPD	C1-C2-C3-C4
5	O	1334	MPD	CM-C2-C3-C4
5	Q	2567	MPD	C1-C2-C3-C4
5	Q	2567	MPD	CM-C2-C3-C4
5	U	1698	MPD	C1-C2-C3-C4
5	W	2106	MPD	CM-C2-C3-C4
7	K	2564	MRD	C1-C2-C3-C4
7	N	2565	MRD	C1-C2-C3-C4
2	J	780	COA	C6P-C7P-N8P-C9P
2	K	900	COA	N8P-C9P-CAP-OAP
2	C	169	COA	S1P-C2P-C3P-N4P
2	D	283	COA	S1P-C2P-C3P-N4P
2	L	1008	COA	S1P-C2P-C3P-N4P
2	X	1944	COA	S1P-C2P-C3P-N4P
2	W	2019	COA	N4P-C5P-C6P-C7P
2	D	283	COA	C6P-C7P-N8P-C9P
2	L	1008	COA	P2A-O3A-P1A-O2A
2	N	1333[A]	COA	P2A-O3A-P1A-O2A
2	O	1127	COA	P2A-O3A-P1A-O2A
2	O	1127	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

31 monomers are involved in 75 short contacts:

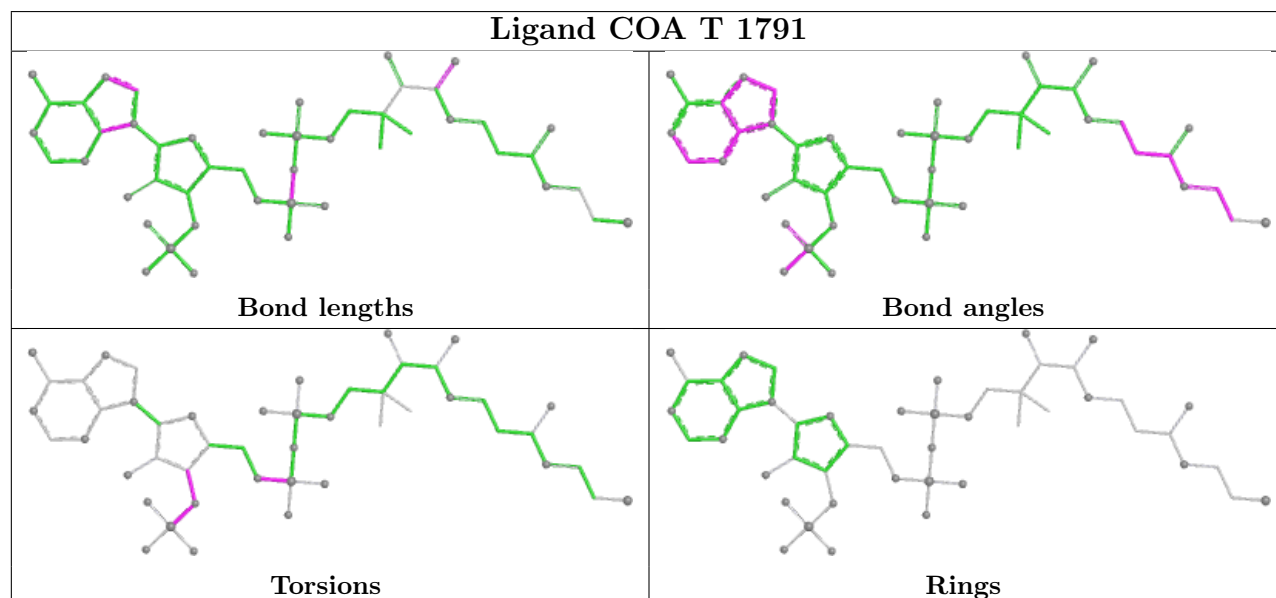
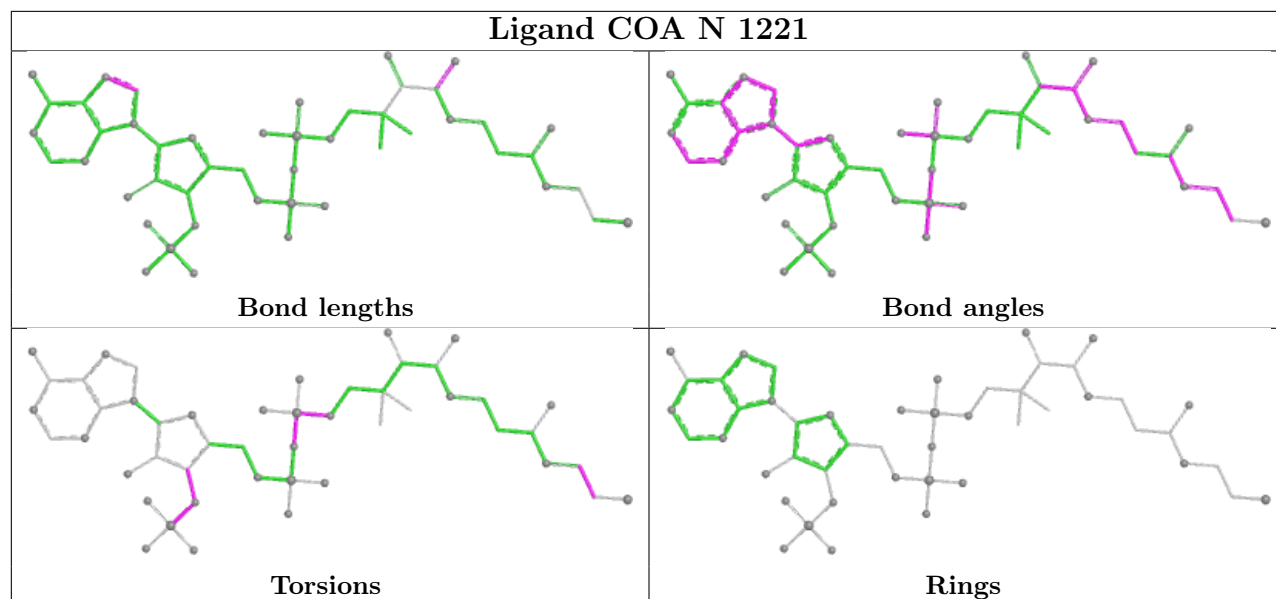
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2597	ACT	2	0
6	R	2595	ACT	2	0
7	F	2559	MRD	3	0
2	N	1221	COA	5	0
2	N	1333[A]	COA	3	0
2	S	1696	COA	4	0
5	S	1697	MPD	2	0
2	A	129	COA	2	0
2	A	127	COA	2	0
2	F	477	COA	1	0
5	Q	2567	MPD	1	0
6	E	2594	ACT	1	0
5	H	631	MPD	2	0

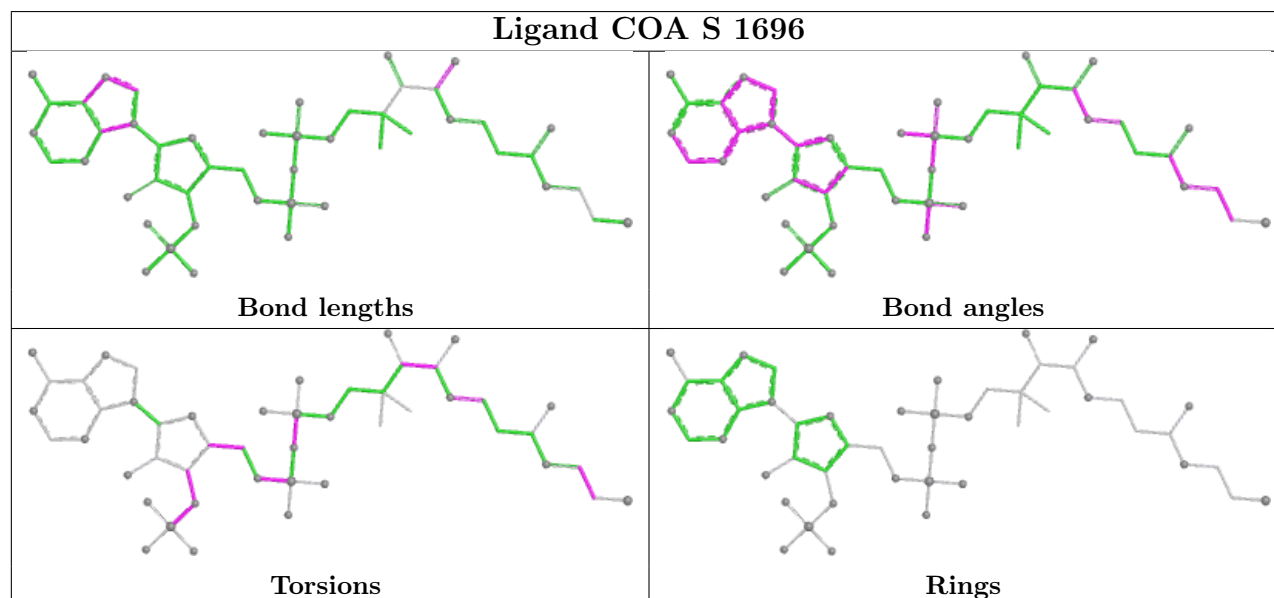
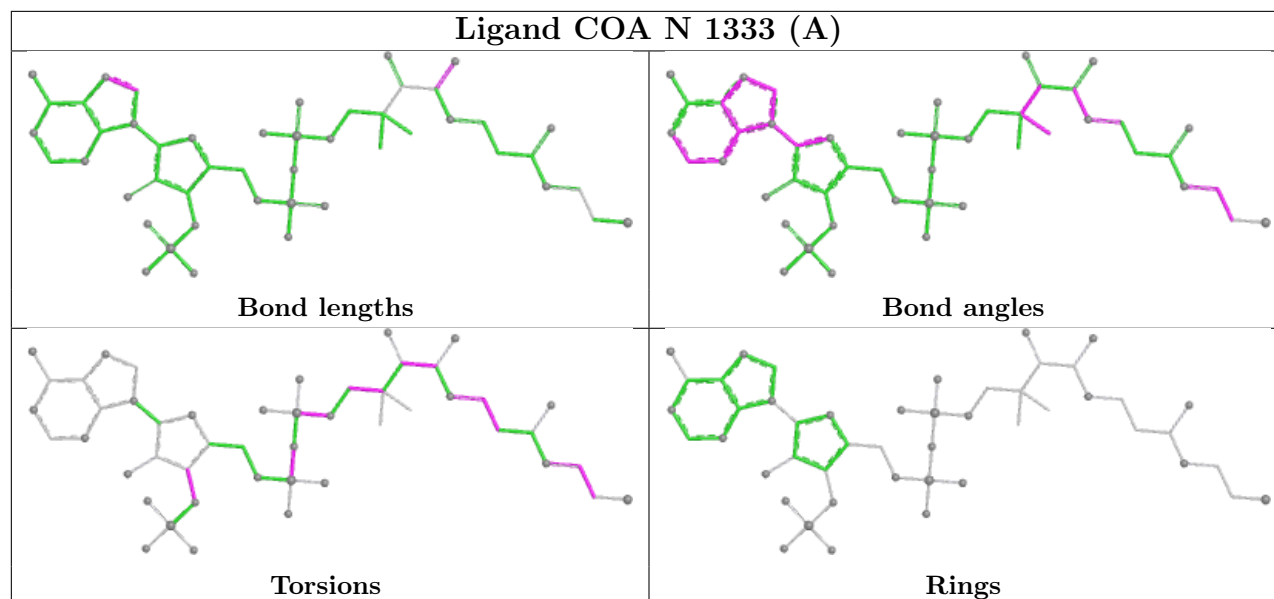
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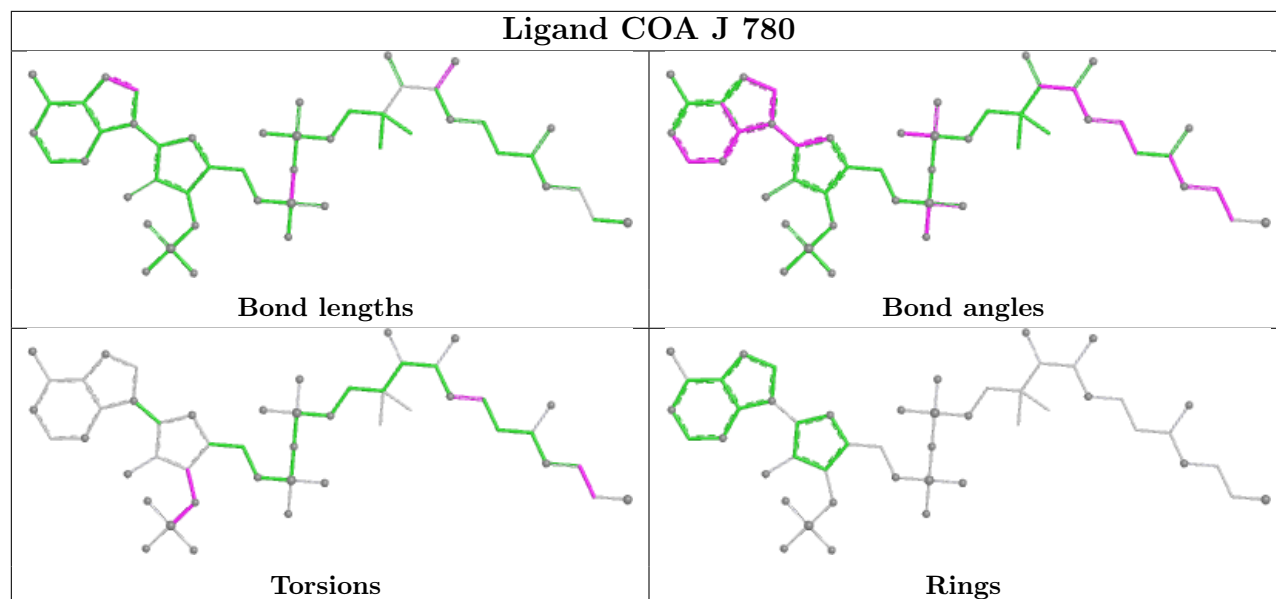
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	630	COA	2	0
2	X	1944	COA	3	0
5	M	2572	MPD	7	0
7	N	2565	MRD	3	0
5	A	2570	MPD	2	0
2	W	2019	COA	5	0
6	C	2598	ACT	3	0
6	K	629	ACT	1	0
5	U	1698	MPD	1	0
6	T	2568	ACT	1	0
7	K	2564	MRD	3	0
2	D	283	COA	2	0
7	D	2573	MRD	4	0
8	O	2575[B]	A3P	1	0
2	I	699	COA	1	0
2	W	2105	COA	7	0
5	I	2561	MPD	1	0
5	B	127	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

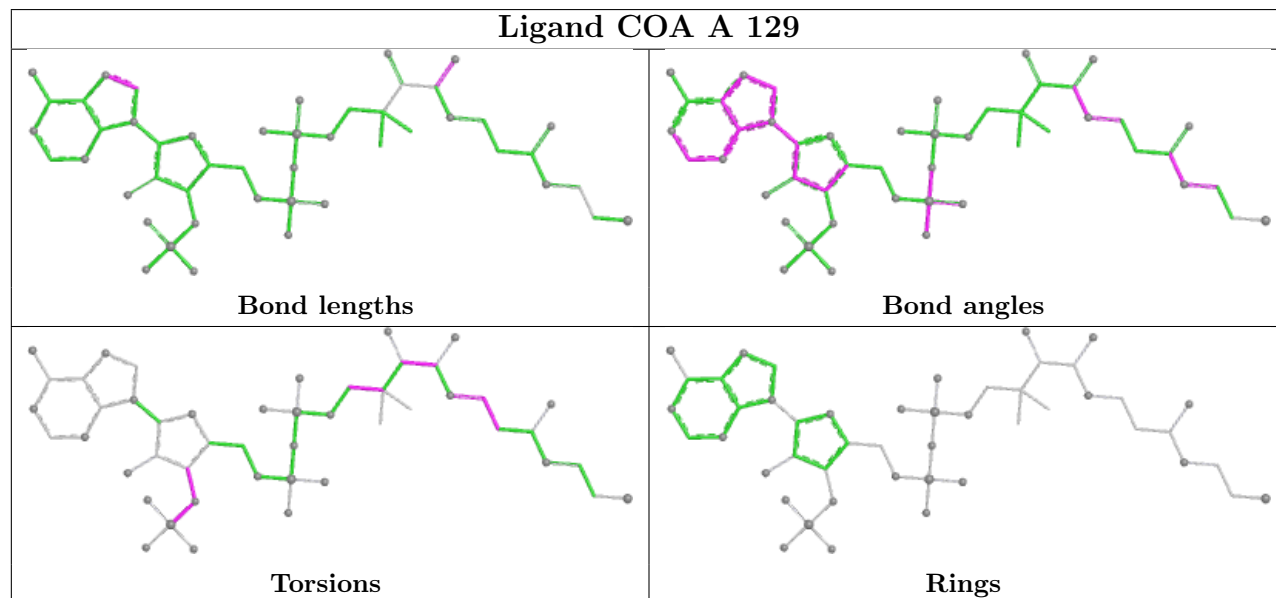


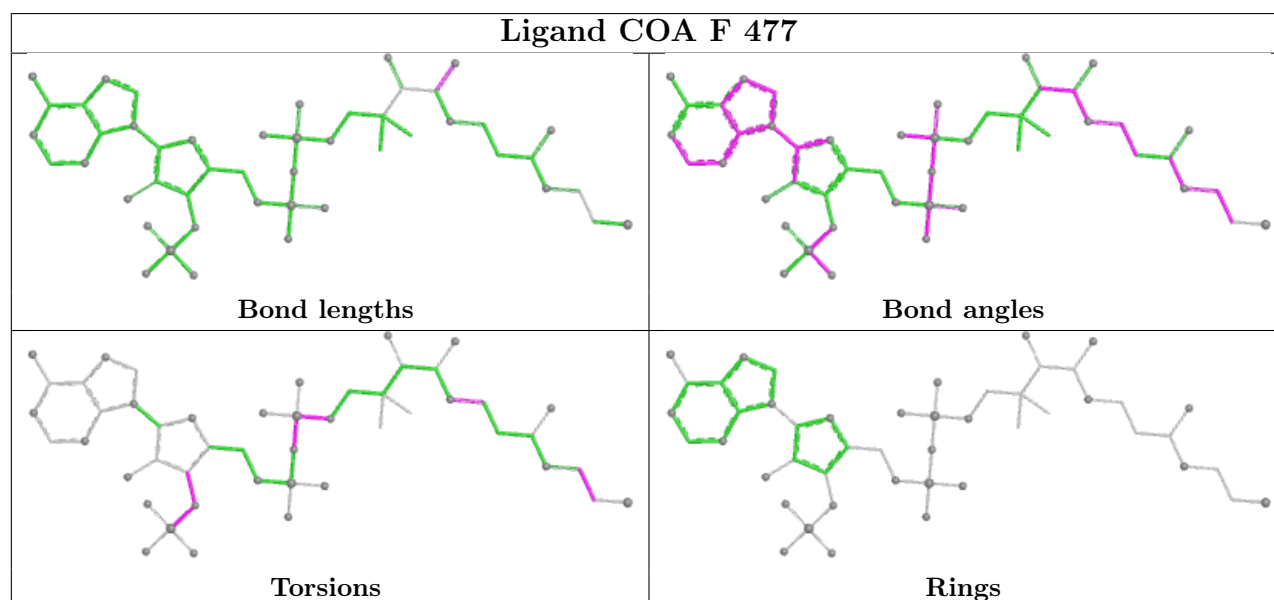
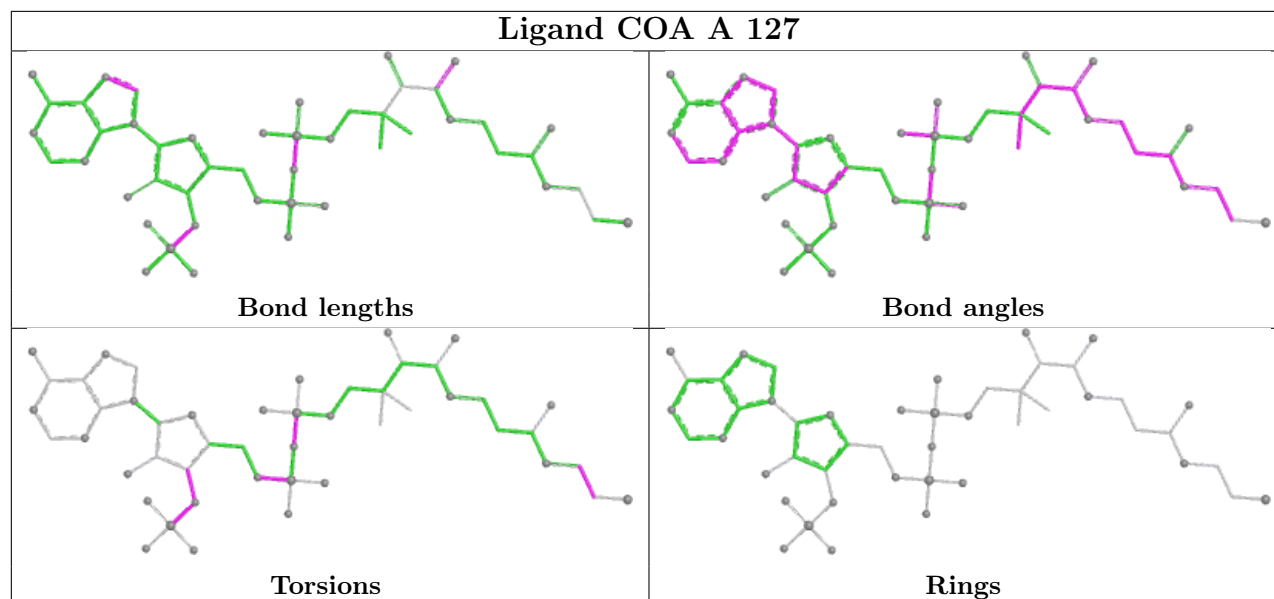


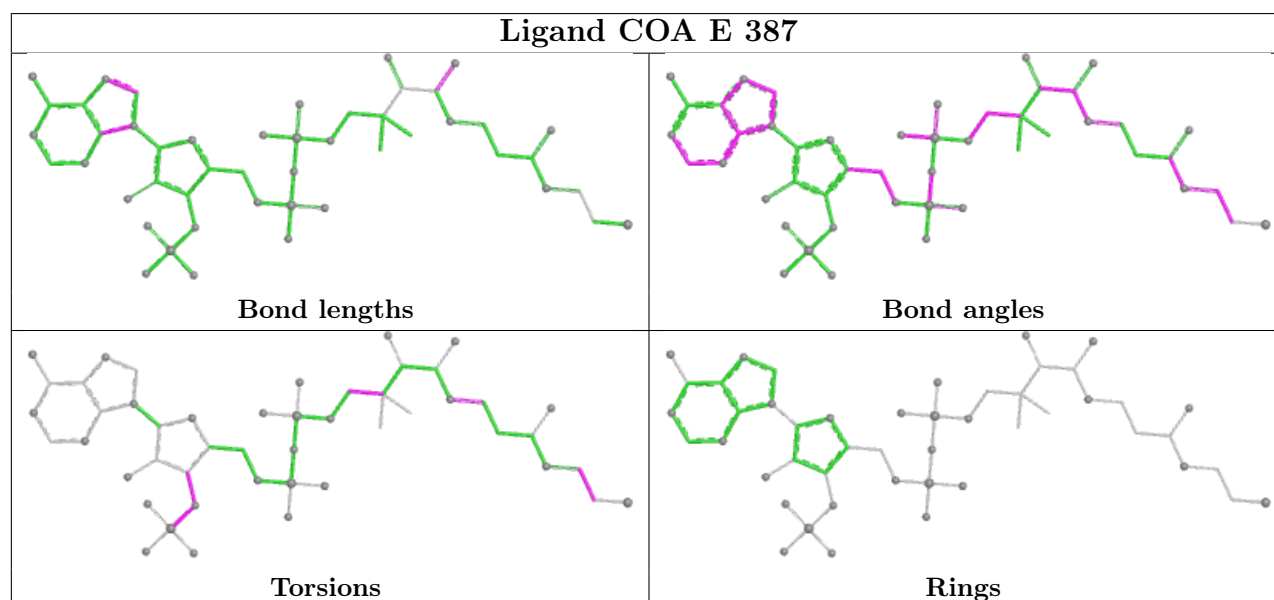
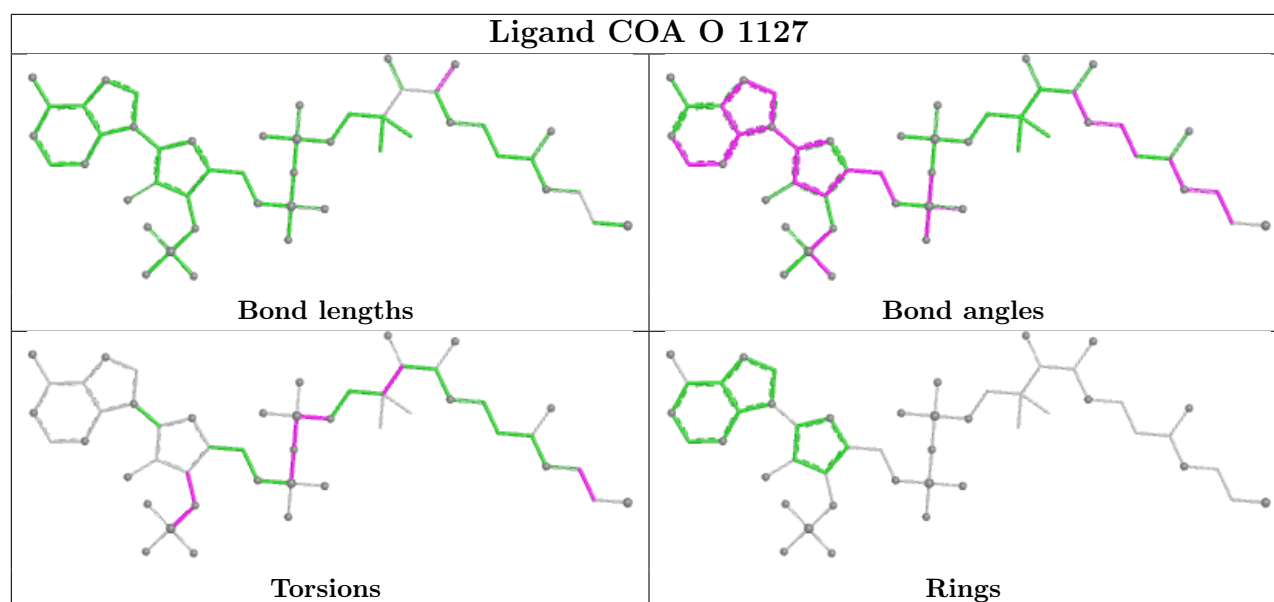
Ligand COA J 780

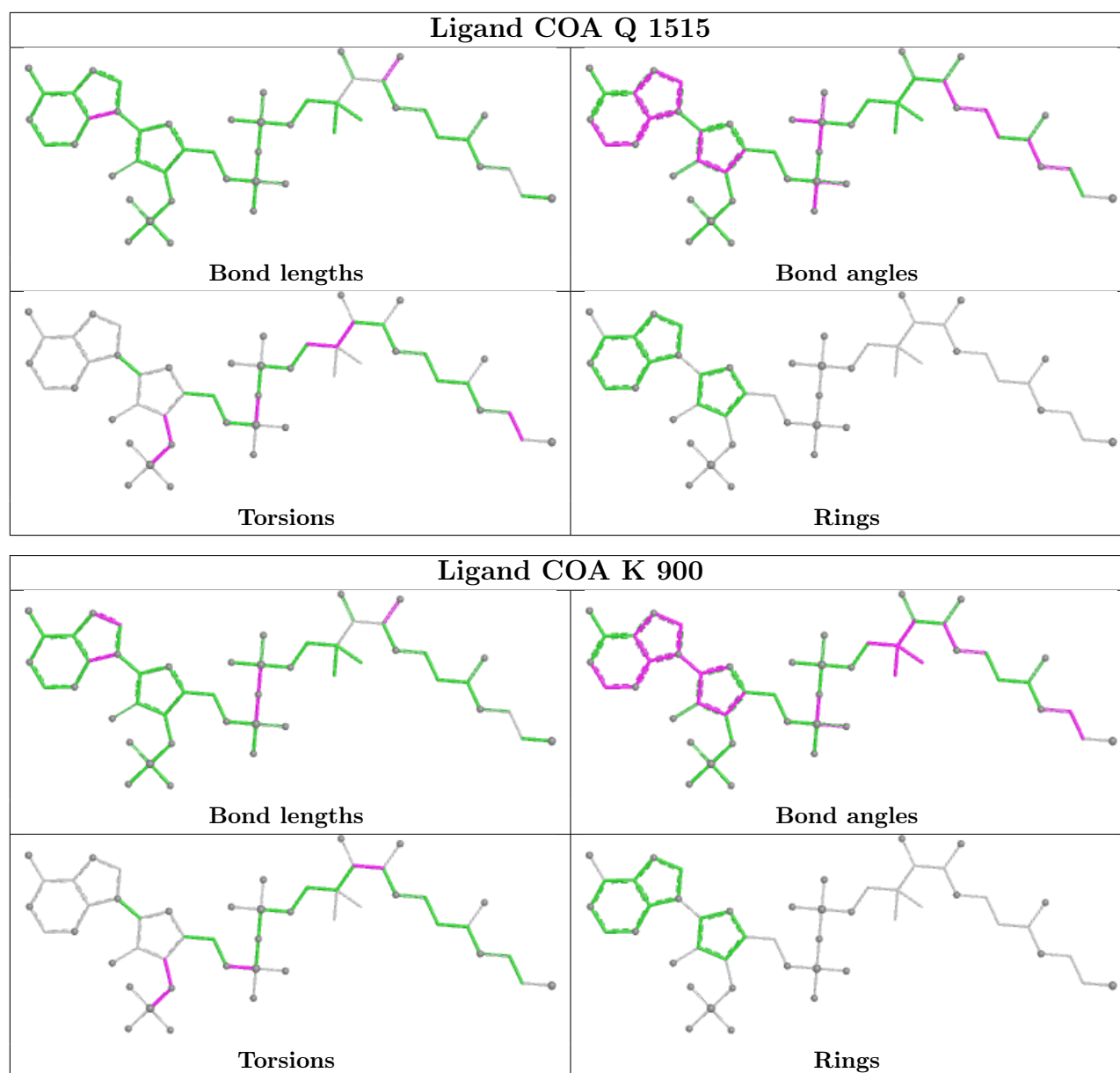


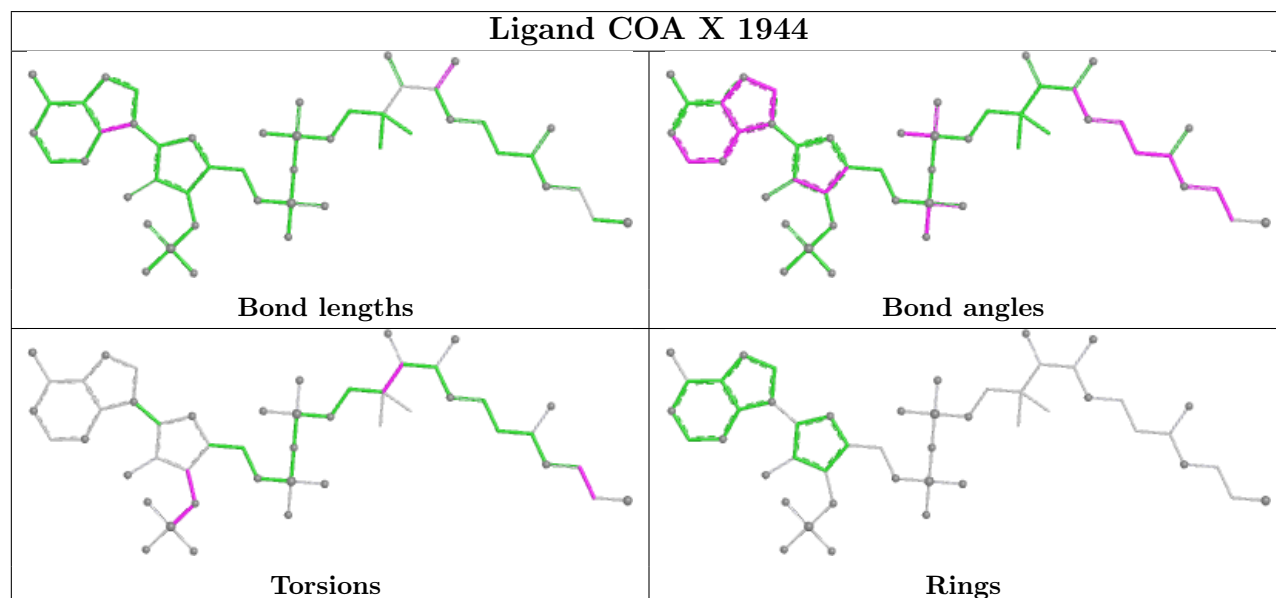
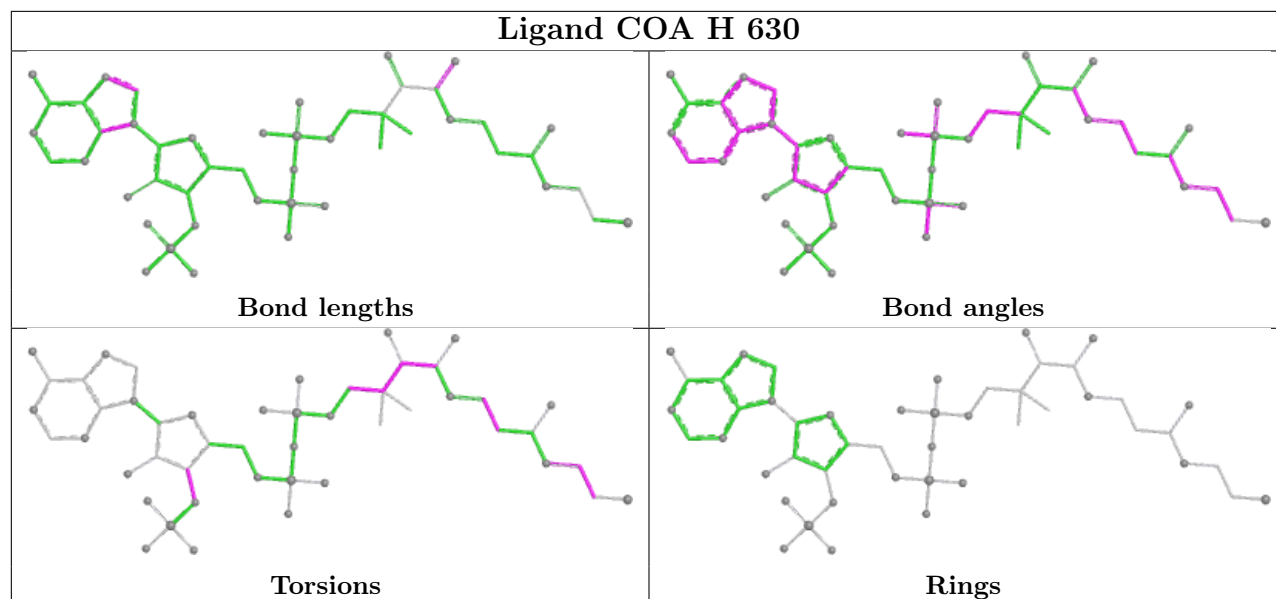
Ligand COA A 129

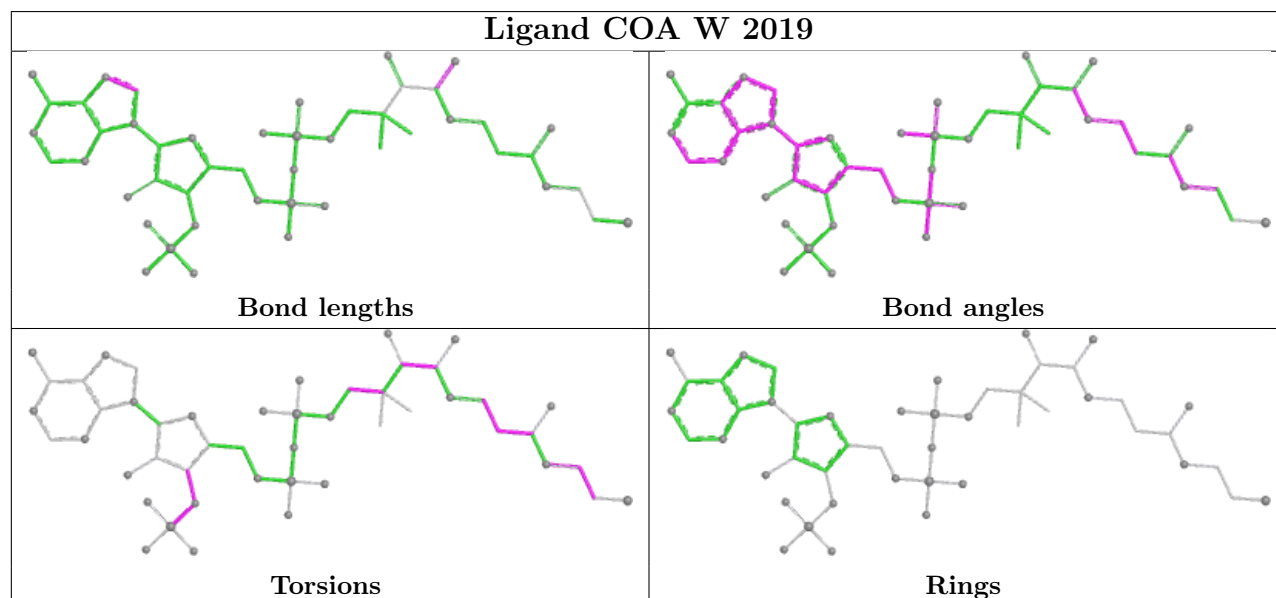
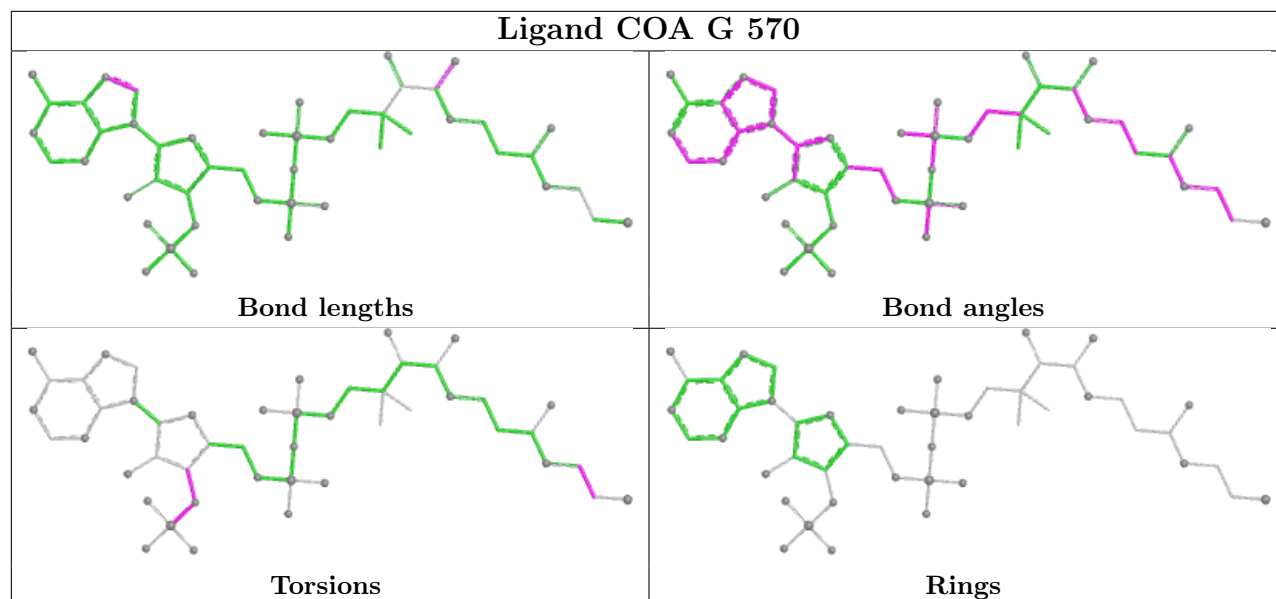


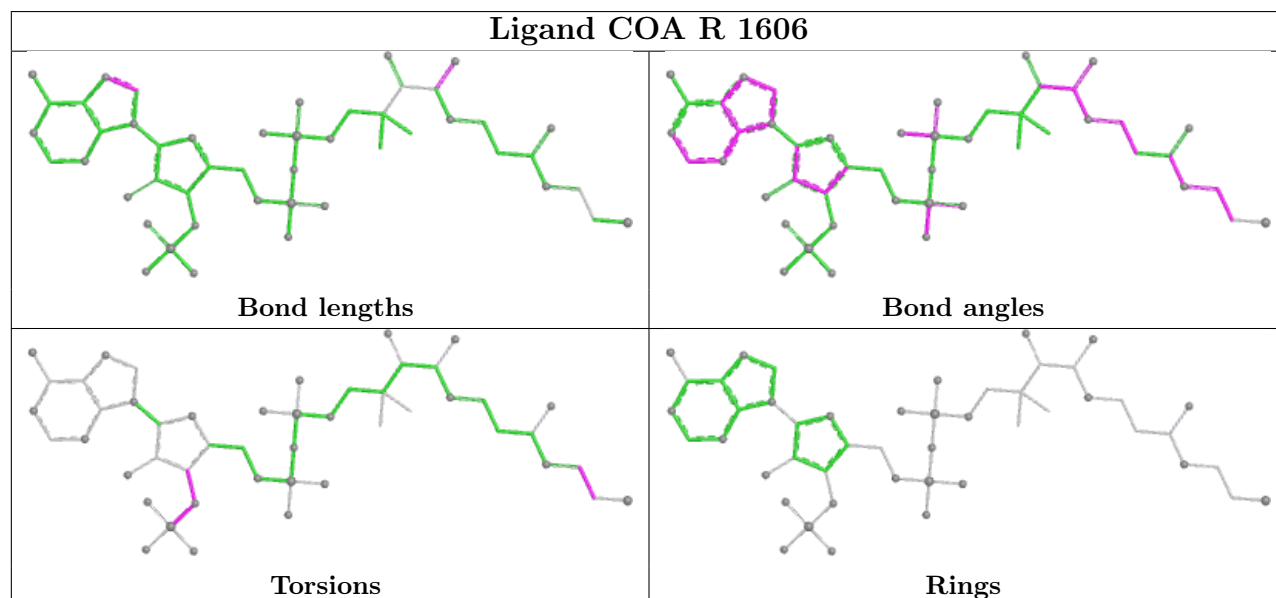
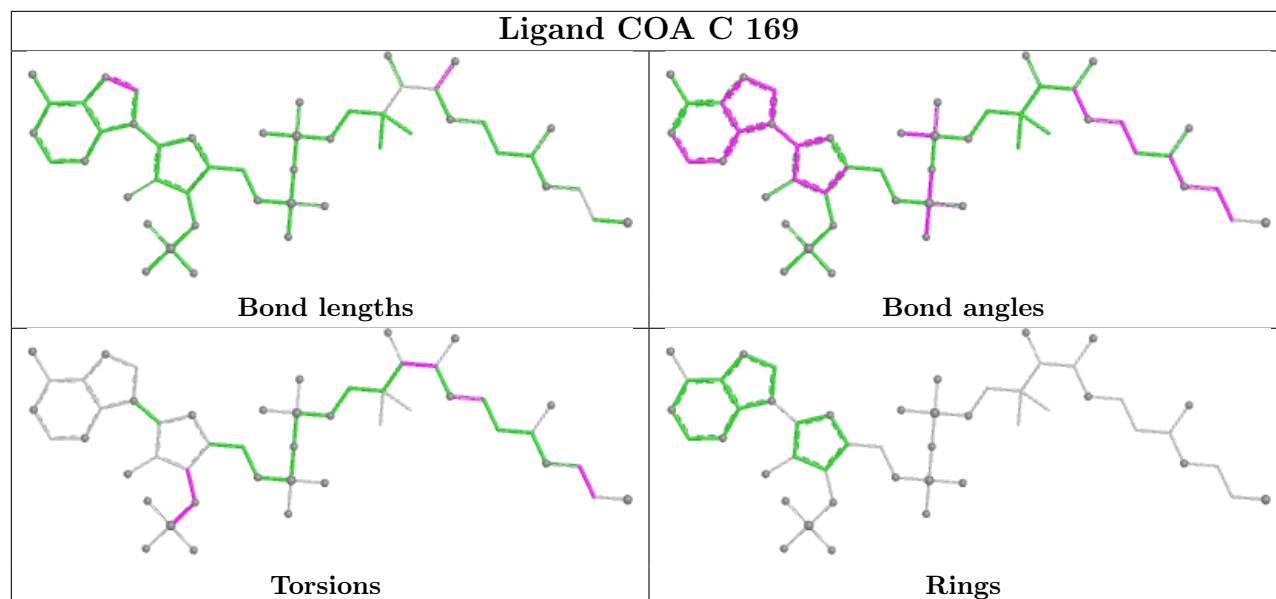


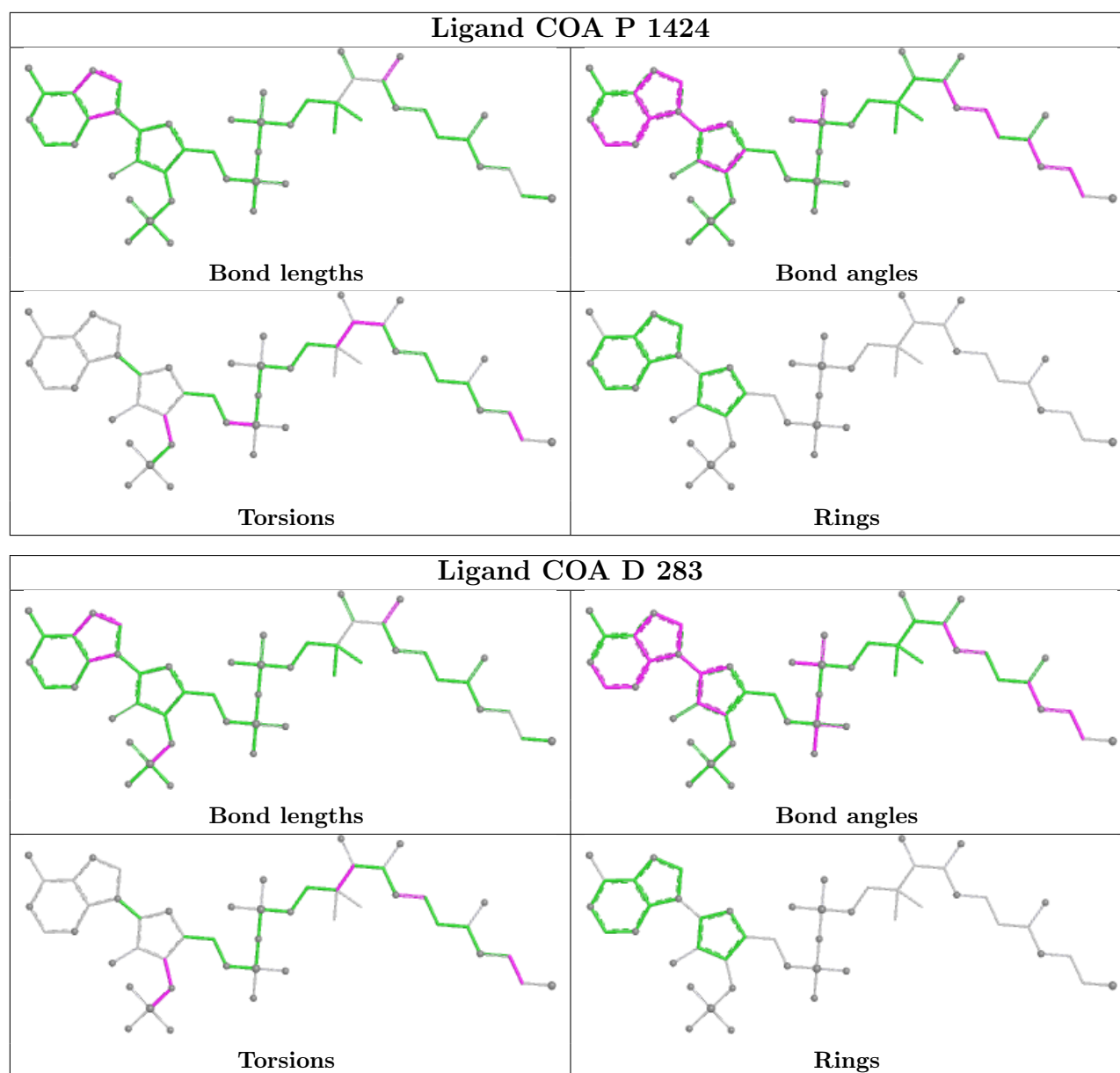




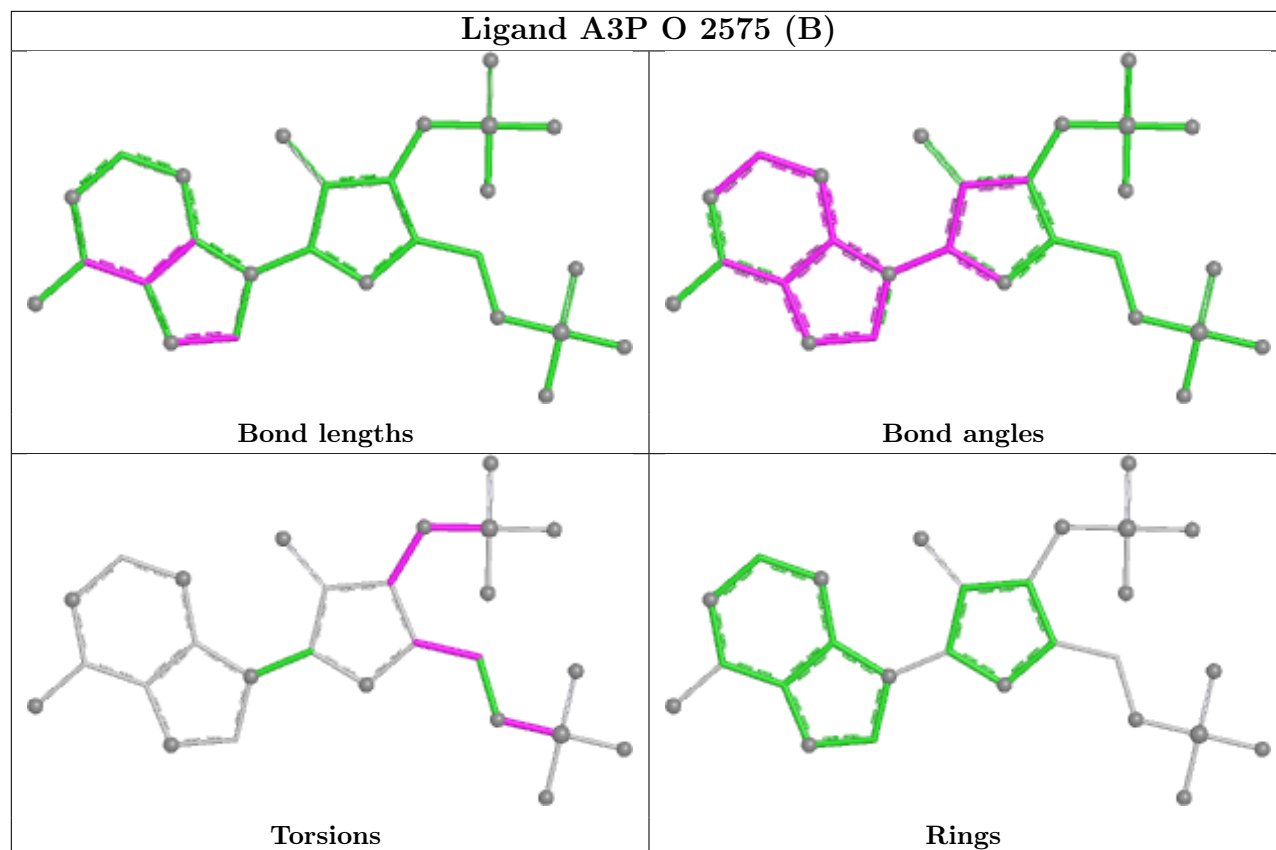




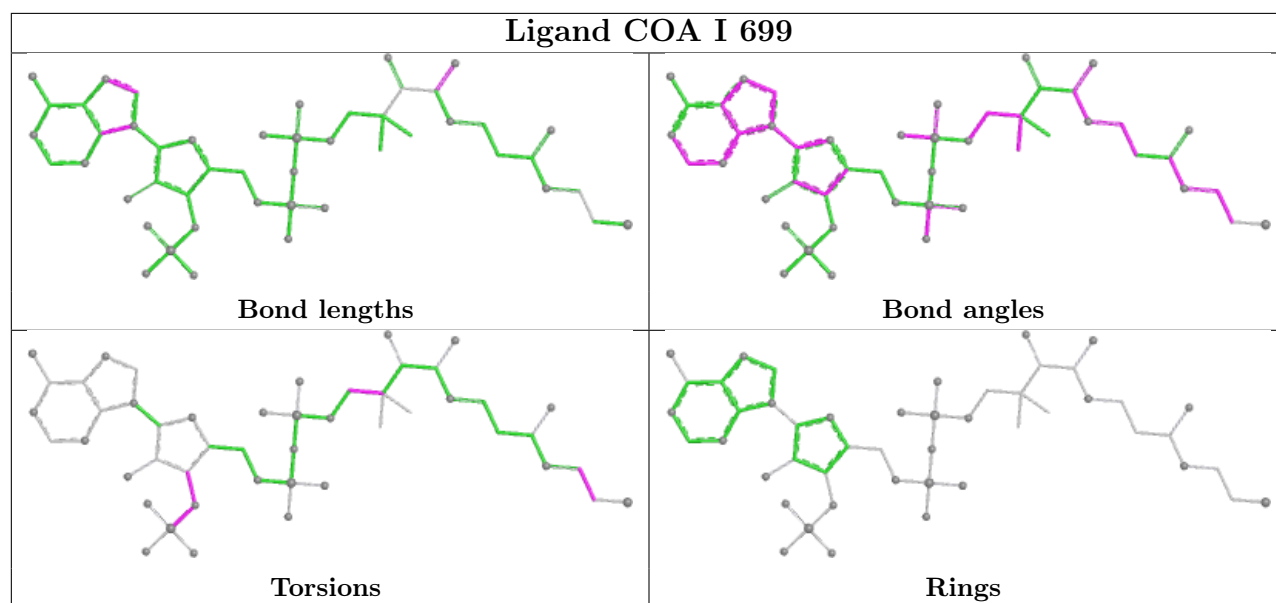


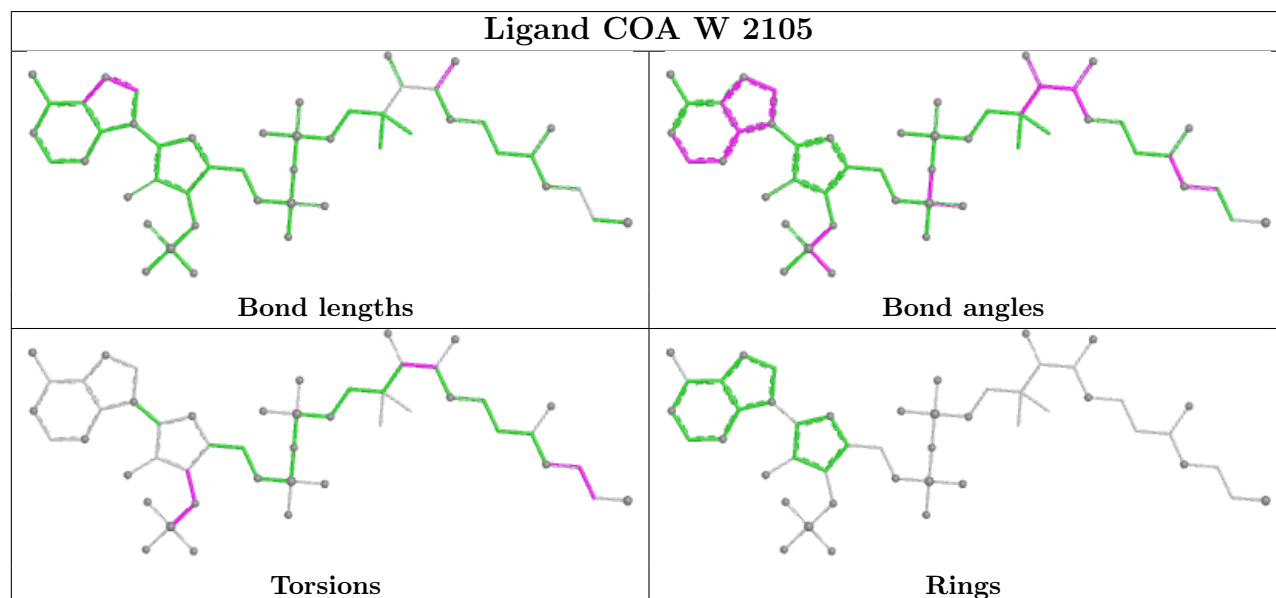
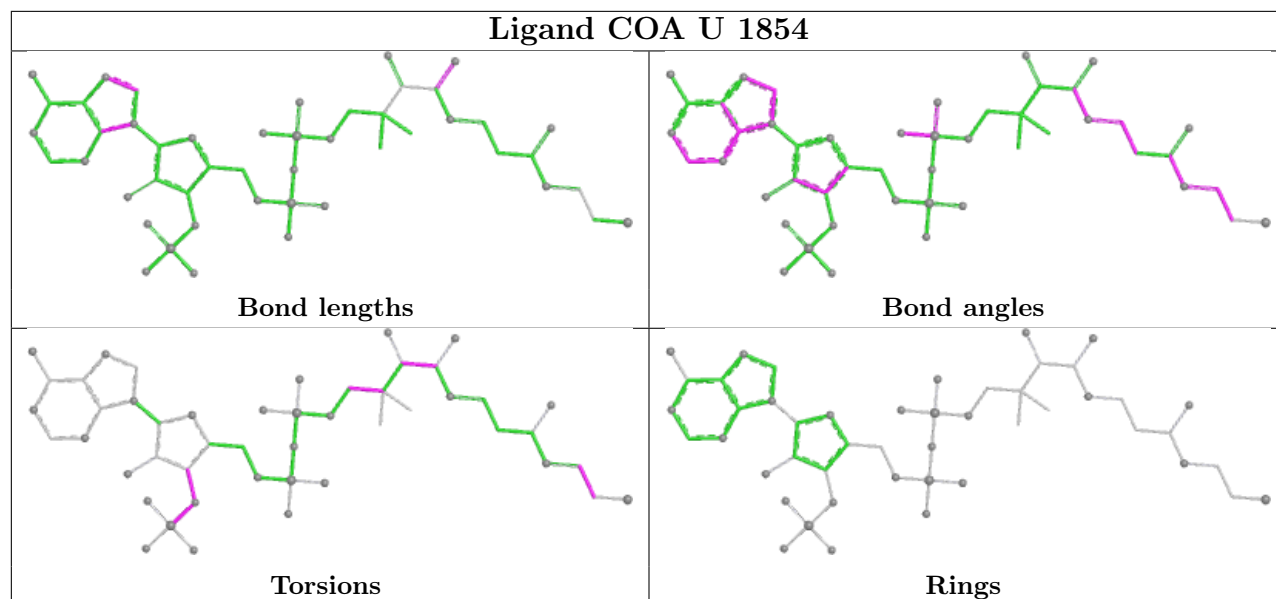


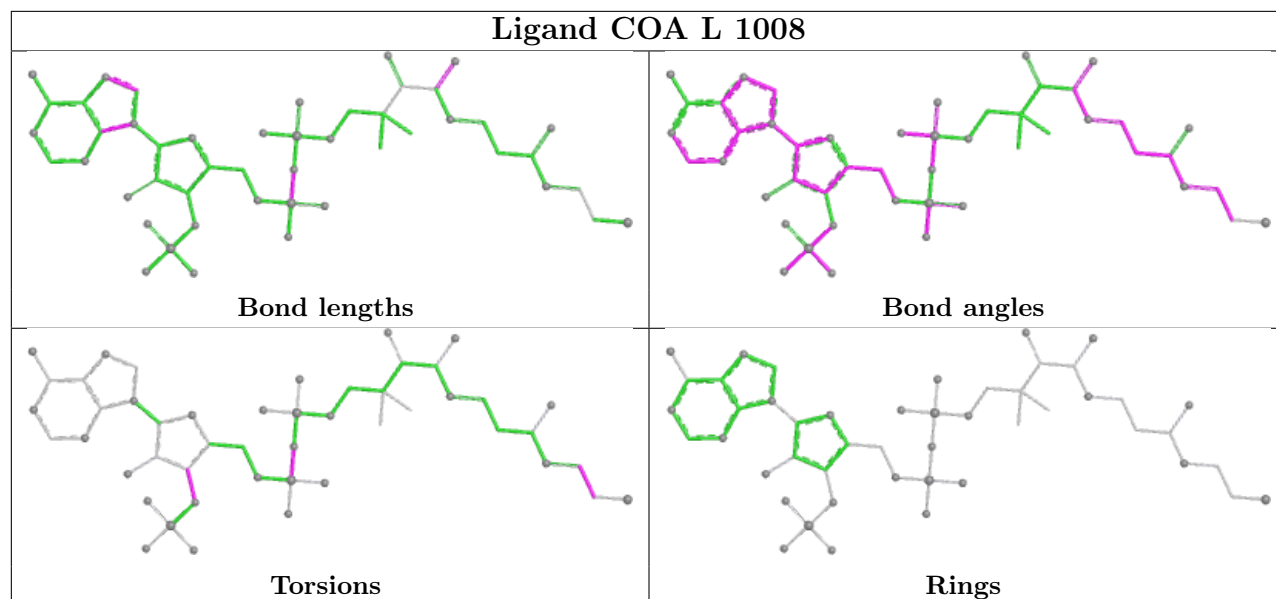
Ligand A3P O 2575 (B)



Ligand COA I 699







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	124/129 (96%)	-0.14	1 (0%) 82 86	11, 24, 37, 43	7 (5%)
1	B	124/129 (96%)	-0.05	2 (1%) 70 74	12, 26, 41, 47	4 (3%)
1	C	124/129 (96%)	-0.29	3 (2%) 59 63	11, 20, 36, 45	7 (5%)
1	D	124/129 (96%)	-0.23	2 (1%) 70 74	11, 21, 35, 44	9 (7%)
1	E	125/129 (96%)	-0.12	2 (1%) 70 74	11, 23, 38, 56	5 (4%)
1	F	124/129 (96%)	-0.12	2 (1%) 70 74	13, 24, 37, 46	6 (4%)
1	G	124/129 (96%)	0.21	2 (1%) 70 74	16, 33, 52, 59	3 (2%)
1	H	124/129 (96%)	0.08	2 (1%) 70 74	13, 28, 47, 54	8 (6%)
1	I	124/129 (96%)	-0.09	1 (0%) 82 86	12, 26, 39, 49	5 (4%)
1	J	124/129 (96%)	-0.30	2 (1%) 70 74	9, 20, 35, 44	3 (2%)
1	K	124/129 (96%)	-0.16	1 (0%) 82 86	10, 23, 37, 46	6 (4%)
1	L	124/129 (96%)	-0.23	3 (2%) 59 63	10, 20, 34, 46	6 (4%)
1	M	124/129 (96%)	-0.15	3 (2%) 59 63	9, 23, 37, 44	6 (4%)
1	N	124/129 (96%)	-0.27	2 (1%) 70 74	8, 21, 34, 45	6 (4%)
1	O	125/129 (96%)	-0.03	4 (3%) 50 54	10, 26, 42, 59	5 (4%)
1	P	124/129 (96%)	-0.00	4 (3%) 50 54	13, 26, 39, 49	6 (4%)
1	Q	124/129 (96%)	-0.11	2 (1%) 70 74	12, 26, 37, 47	4 (3%)
1	R	124/129 (96%)	-0.12	1 (0%) 82 86	13, 26, 40, 48	6 (4%)
1	S	123/129 (95%)	-0.04	0 100 100	11, 24, 39, 46	11 (8%)
1	T	124/129 (96%)	0.19	4 (3%) 50 54	11, 29, 46, 52	6 (4%)
1	U	124/129 (96%)	-0.23	2 (1%) 70 74	10, 23, 37, 52	8 (6%)
1	V	124/129 (96%)	0.02	3 (2%) 59 63	11, 28, 42, 50	4 (3%)
1	W	123/129 (95%)	-0.14	0 100 100	10, 25, 38, 43	4 (3%)
1	X	124/129 (96%)	-0.09	2 (1%) 70 74	10, 26, 40, 63	5 (4%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2976/3096 (96%)	-0.10	50 (1%) 69 73	8, 24, 41, 63	140 (4%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	0	ALA	7.5
1	F	0	ALA	6.3
1	P	0	ALA	5.1
1	C	0	ALA	5.0
1	B	0	ALA	4.6
1	O	0	ALA	4.0
1	A	0	ALA	3.9
1	E	126	ARG	3.9
1	L	0	ALA	3.5
1	J	0	ALA	3.4
1	N	0	ALA	3.4
1	X	126	ARG	3.2
1	U	0	ALA	3.1
1	G	0	ALA	3.0
1	T	0	ALA	3.0
1	L	33	ASP	3.0
1	H	82[A]	LYS	3.0
1	C	21	ARG	2.9
1	M	21	ARG	2.7
1	O	126	ARG	2.7
1	I	0	ALA	2.7
1	R	0	ALA	2.7
1	X	114[A]	ARG	2.7
1	T	83	LEU	2.6
1	D	0	ALA	2.6
1	V	29[A]	ARG	2.6
1	M	0	ALA	2.5
1	V	125	ARG	2.4
1	K	0	ALA	2.4
1	P	104	GLU	2.4
1	B	125	ARG	2.3
1	P	114	ARG	2.3
1	D	104	GLU	2.3
1	F	28[A]	ARG	2.2
1	Q	125	ARG	2.2
1	N	114	ARG	2.2
1	C	104	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	104	GLU	2.2
1	Q	0	ALA	2.2
1	P	13	GLU	2.1
1	M	29	ARG	2.1
1	O	21	ARG	2.1
1	L	104	GLU	2.1
1	H	125	ARG	2.1
1	T	14	ARG	2.1
1	T	34	SER	2.0
1	E	0	ALA	2.0
1	J	13	GLU	2.0
1	O	96	GLU	2.0
1	U	96	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	K	2563	4/4	0.62	0.22	47,48,48,49	0
6	ACT	C	2598	4/4	0.67	0.16	47,48,48,48	0
5	MPD	S	1697	8/8	0.67	0.27	65,66,68,68	0
6	ACT	R	2595	4/4	0.75	0.18	39,39,39,40	4
7	MRD	L	2562	8/8	0.76	0.16	43,45,46,47	0
7	MRD	K	2564	8/8	0.78	0.17	57,59,59,59	0
6	ACT	A	2597	4/4	0.80	0.17	35,36,37,38	0
7	MRD	F	2559	8/8	0.81	0.17	73,73,74,74	0
5	MPD	Q	2567	8/8	0.81	0.15	47,49,50,51	0
6	ACT	E	2594	4/4	0.81	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	M	2572	8/8	0.82	0.15	63,63,64,64	0
5	MPD	A	2570	8/8	0.83	0.15	45,46,47,47	0
6	ACT	K	629	4/4	0.84	0.18	45,46,46,46	0
5	MPD	V	1945	8/8	0.85	0.13	53,54,54,54	0
5	MPD	H	631	8/8	0.85	0.15	55,57,57,57	0
5	MPD	P	1425	8/8	0.86	0.12	49,49,51,51	0
6	ACT	W	2596	4/4	0.86	0.14	50,50,50,50	0
5	MPD	U	1698	8/8	0.86	0.12	45,45,47,48	0
5	MPD	C	2571	8/8	0.86	0.12	52,53,54,54	0
5	MPD	R	2566	8/8	0.86	0.12	46,48,49,49	0
5	MPD	G	571	8/8	0.87	0.13	46,47,50,51	0
5	MPD	W	2106	8/8	0.88	0.14	47,48,49,49	0
4	CA	X	2550	1/1	0.88	0.12	50,50,50,50	1
7	MRD	D	2573	8/8	0.88	0.12	51,51,52,53	0
7	MRD	T	2569	8/8	0.88	0.12	46,48,49,49	0
5	MPD	O	1334	8/8	0.89	0.11	55,56,57,58	0
4	CA	N	2532	1/1	0.89	0.13	43,43,43,43	1
5	MPD	I	2561	8/8	0.90	0.11	48,50,51,52	0
6	ACT	T	2568	4/4	0.90	0.13	54,55,55,55	0
4	CA	X	2556	1/1	0.91	0.10	35,35,35,35	1
4	CA	M	2530	1/1	0.91	0.12	41,41,41,41	1
5	MPD	B	127	8/8	0.91	0.11	51,52,54,54	0
2	COA	N	1333[A]	48/48	0.91	0.15	24,44,68,69	48
5	MPD	E	2560	8/8	0.91	0.10	45,46,47,47	0
7	MRD	N	2565	8/8	0.91	0.11	45,46,47,48	0
3	CL	G	2574	1/1	0.91	0.12	51,51,51,51	0
4	CA	U	2537	1/1	0.93	0.13	34,34,34,34	1
4	CA	U	2546	1/1	0.93	0.08	27,27,27,27	1
4	CA	V	2557	1/1	0.93	0.10	47,47,47,47	0
4	CA	A	2514	1/1	0.93	0.14	36,36,36,36	1
4	CA	Q	2535	1/1	0.93	0.07	35,35,35,35	1
4	CA	A	2552	1/1	0.94	0.10	35,35,35,35	1
4	CA	C	2553	1/1	0.94	0.07	32,32,32,32	1
4	CA	E	2554	1/1	0.94	0.13	44,44,44,44	1
4	CA	F	2518	1/1	0.94	0.12	54,54,54,54	0
2	COA	W	2105	48/48	0.94	0.12	20,34,67,72	0
3	CL	A	128	1/1	0.94	0.15	48,48,48,48	0
8	A3P	O	2575[B]	27/27	0.94	0.07	5,9,22,23	27
2	COA	H	630	48/48	0.95	0.10	30,35,71,74	0
4	CA	P	2534	1/1	0.95	0.09	42,42,42,42	0
2	COA	X	1944	48/48	0.95	0.10	24,32,58,65	0
4	CA	T	2545	1/1	0.95	0.07	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	N	1221	48/48	0.95	0.10	18,28,68,72	0
3	CL	C	2558	1/1	0.95	0.09	41,41,41,41	0
2	COA	E	387	48/48	0.95	0.10	19,28,64,70	0
3	CL	L	2543	1/1	0.95	0.08	43,43,43,43	0
2	COA	Q	1515	48/48	0.96	0.09	23,32,70,75	0
4	CA	G	2520	1/1	0.96	0.07	44,44,44,44	0
4	CA	G	2523	1/1	0.96	0.11	42,42,42,42	1
4	CA	I	2525	1/1	0.96	0.06	31,31,31,31	1
4	CA	J	2542	1/1	0.96	0.10	29,29,29,29	1
4	CA	L	2528	1/1	0.96	0.09	31,31,31,31	1
2	COA	R	1606	48/48	0.96	0.08	21,29,65,70	0
2	COA	S	1696	48/48	0.96	0.09	21,29,66,72	0
2	COA	T	1791	48/48	0.96	0.08	23,28,45,55	0
2	COA	U	1854	48/48	0.96	0.09	21,29,67,72	0
4	CA	S	2538	1/1	0.96	0.12	36,36,36,36	1
2	COA	W	2019	48/48	0.96	0.09	22,32,72,75	0
2	COA	F	477	48/48	0.96	0.09	20,30,57,65	0
2	COA	G	570	48/48	0.96	0.09	25,33,68,74	0
2	COA	C	169	48/48	0.96	0.09	18,26,68,73	0
2	COA	I	699	48/48	0.96	0.09	22,30,66,69	0
3	CL	E	2591	1/1	0.96	0.08	42,42,42,42	0
2	COA	J	780	48/48	0.96	0.08	17,26,54,65	0
3	CL	J	2541	1/1	0.96	0.09	43,43,43,43	0
2	COA	L	1008	48/48	0.96	0.08	17,26,48,59	0
2	COA	D	283	48/48	0.96	0.09	18,28,53,65	0
2	COA	A	129	48/48	0.96	0.09	23,33,70,75	0
2	COA	O	1127	48/48	0.96	0.09	21,29,65,71	0
2	COA	P	1424	48/48	0.96	0.10	22,29,69,75	0
4	CA	F	2516	1/1	0.97	0.15	34,34,34,34	1
4	CA	L	2526	1/1	0.97	0.09	26,26,26,26	1
4	CA	B	2551	1/1	0.97	0.10	38,38,38,38	1
2	COA	A	127	48/48	0.97	0.07	17,25,40,54	0
4	CA	W	2548	1/1	0.97	0.10	38,38,38,38	1
4	CA	W	2549	1/1	0.97	0.13	35,35,35,35	1
4	CA	E	2519	1/1	0.97	0.07	26,26,26,26	1
4	CA	P	1426	1/1	0.97	0.13	36,36,36,36	1
4	CA	H	2522	1/1	0.97	0.06	48,48,48,48	0
4	CA	I	2521	1/1	0.97	0.11	43,43,43,43	0
4	CA	R	1607	1/1	0.97	0.10	34,34,34,34	1
4	CA	R	2512	1/1	0.97	0.06	36,36,36,36	1
3	CL	P	2544	1/1	0.97	0.07	49,49,49,49	0
3	CL	M	2555	1/1	0.98	0.11	48,48,48,48	0

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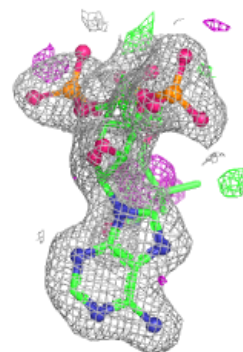
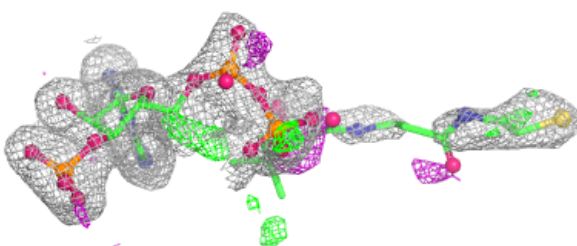
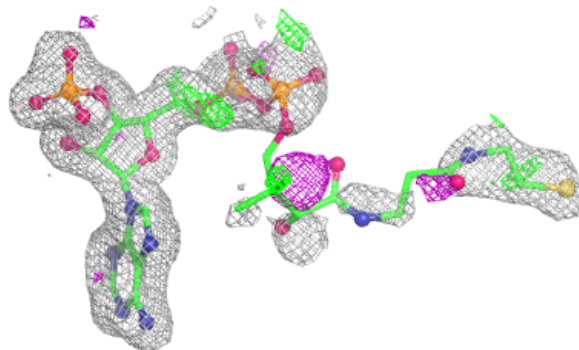
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	Q	2536	1/1	0.98	0.06	28,28,28,28	1
4	CA	K	569	1/1	0.98	0.04	20,20,20,20	1
4	CA	D	2517	1/1	0.98	0.08	27,27,27,27	1
4	CA	D	2540	1/1	0.98	0.05	30,30,30,30	1
2	COA	K	900	48/48	0.98	0.06	16,20,39,48	0
4	CA	M	2533	1/1	0.98	0.08	28,28,28,28	1
3	CL	T	2592	1/1	0.98	0.11	51,51,51,51	0
4	CA	O	2531	1/1	0.98	0.12	34,34,34,34	1
4	CA	C	2513	1/1	0.98	0.05	23,23,23,23	1
4	CA	J	2527	1/1	0.98	0.07	21,21,21,21	1
4	CA	S	2539	1/1	0.99	0.11	26,26,26,26	1
4	CA	T	1792	1/1	0.99	0.10	26,26,26,26	1
4	CA	B	2515	1/1	0.99	0.11	29,29,29,29	1
4	CA	K	2529	1/1	0.99	0.08	31,31,31,31	1
4	CA	H	2524	1/1	0.99	0.13	36,36,36,36	1
4	CA	V	2547	1/1	0.99	0.11	37,37,37,37	1

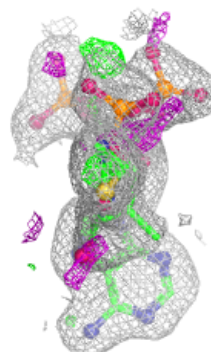
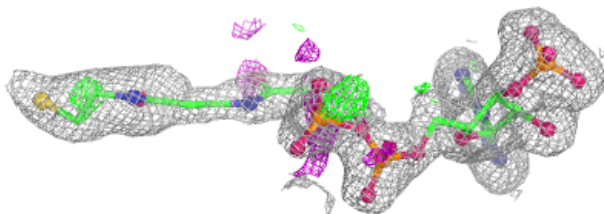
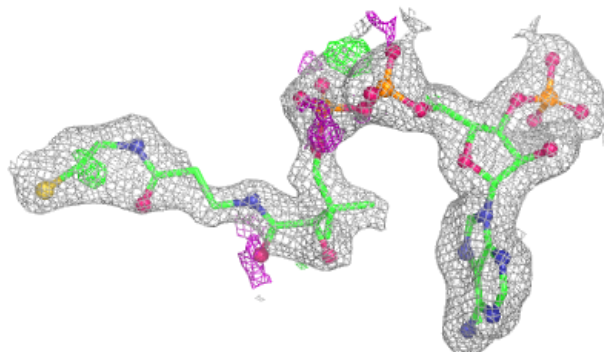
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

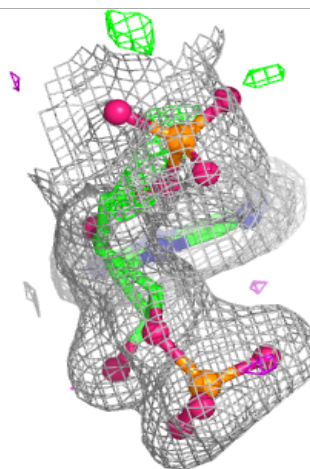
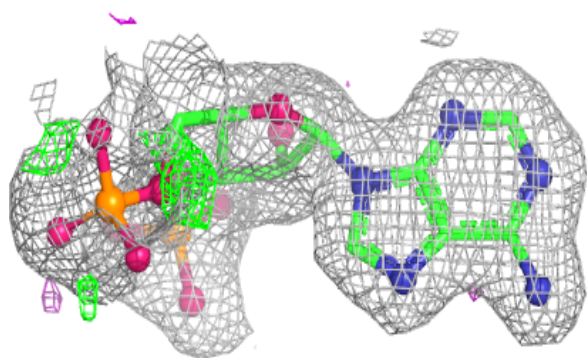
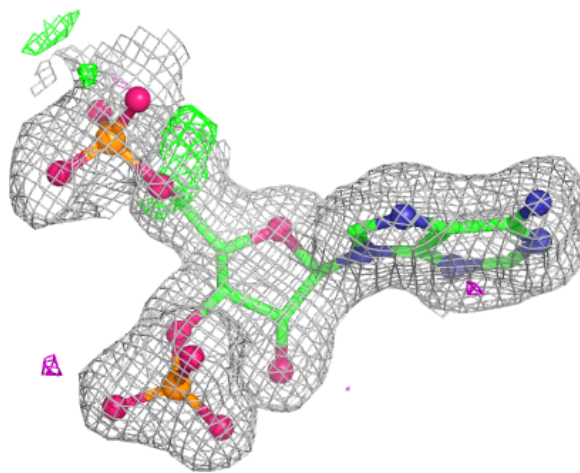
**Electron density around COA W 2105:**

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



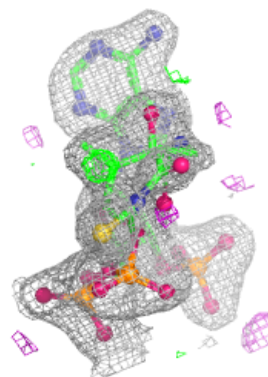
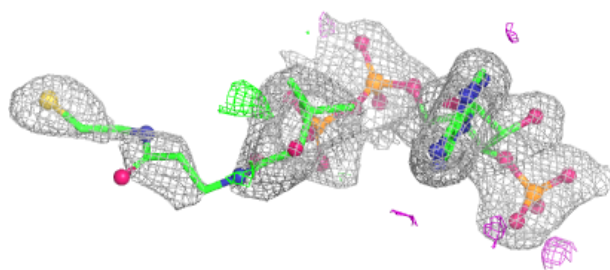
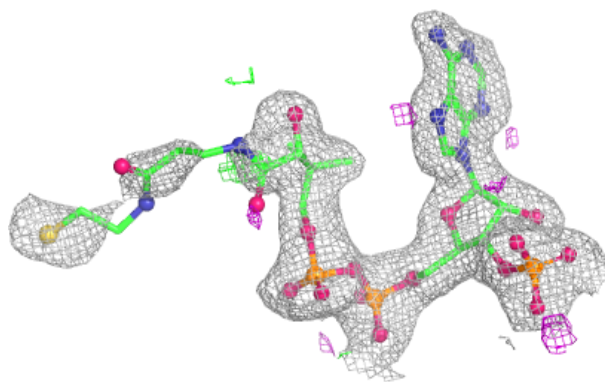
Electron density around A3P O 2575 (B):

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

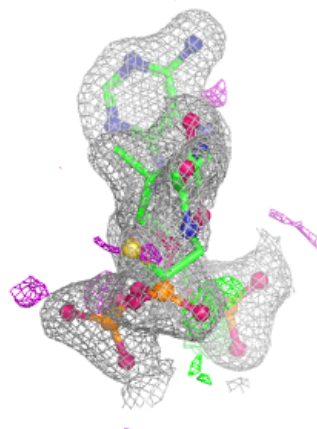
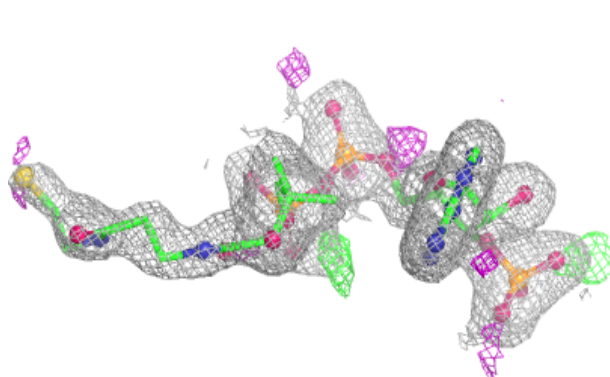
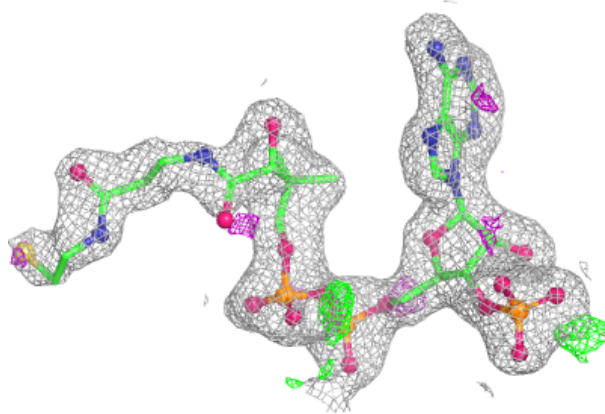


Electron density around COA H 630:

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

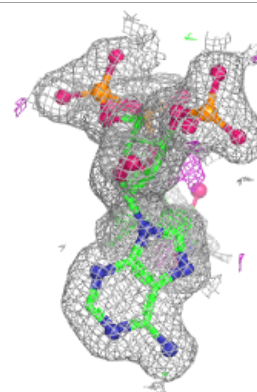
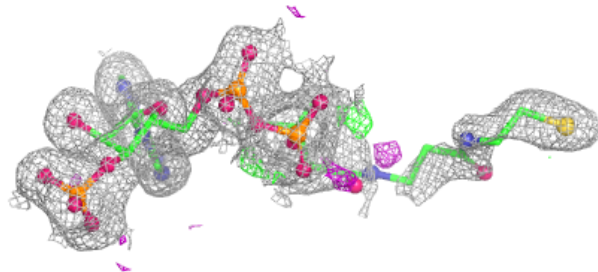
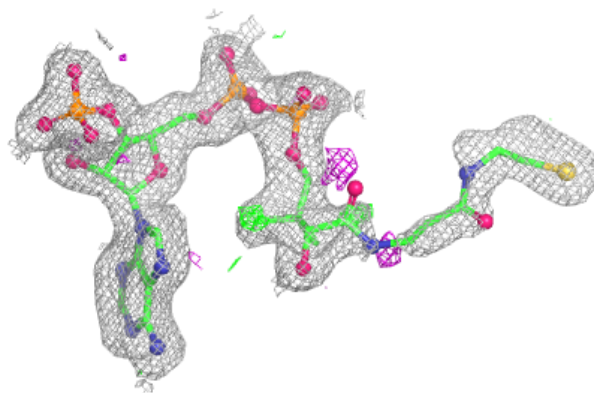
**Electron density around COA X 1944:**

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

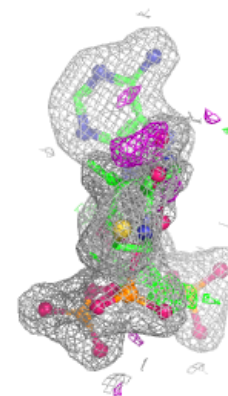
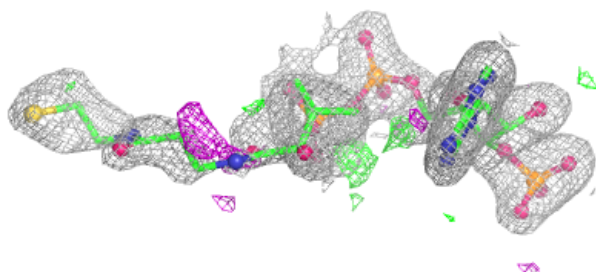
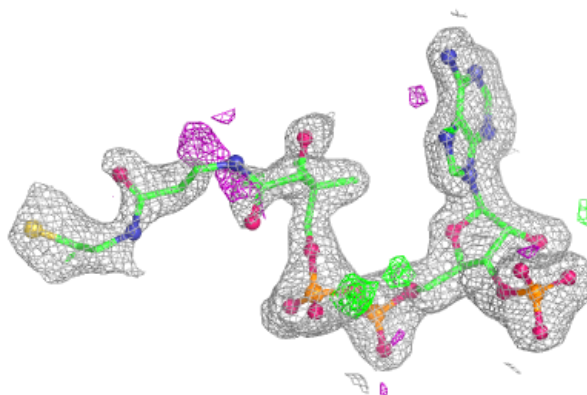


Electron density around COA N 1221:

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

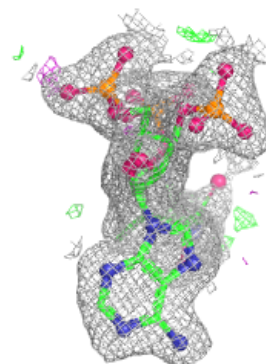
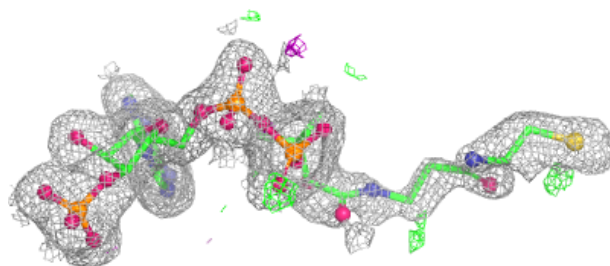
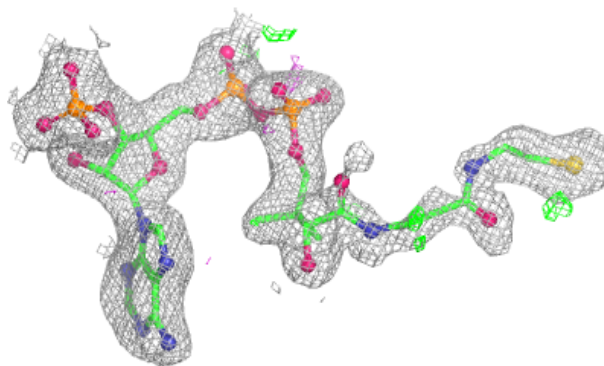
**Electron density around COA E 387:**

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

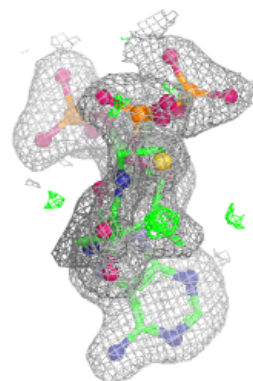
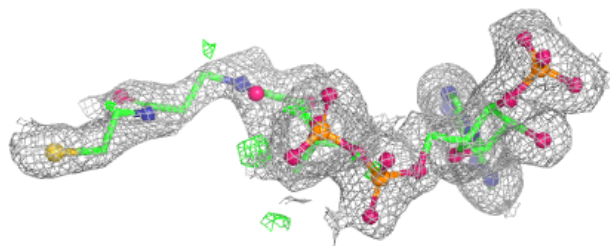
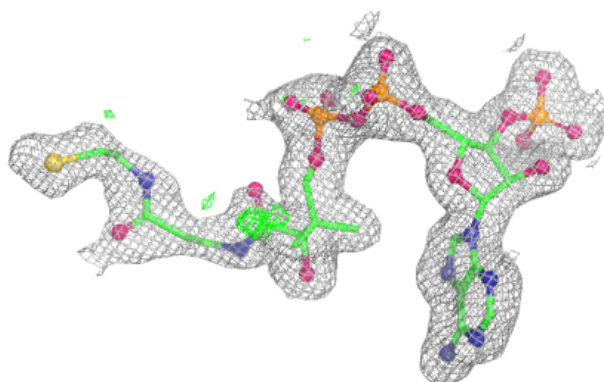


Electron density around COA Q 1515:

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

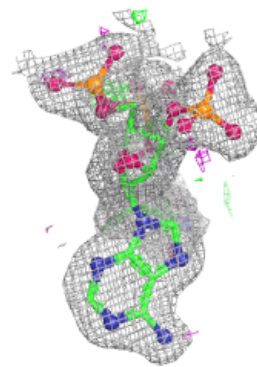
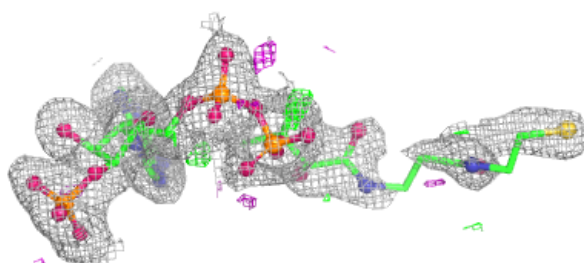
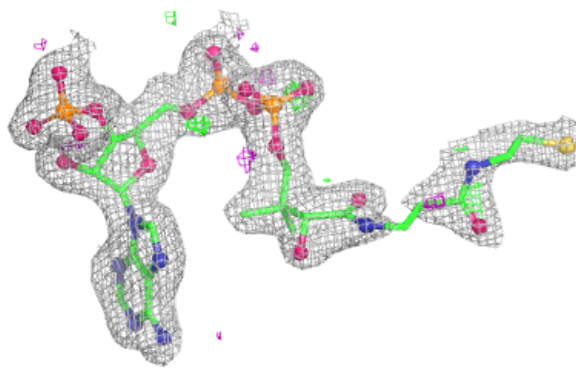
**Electron density around COA R 1606:**

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

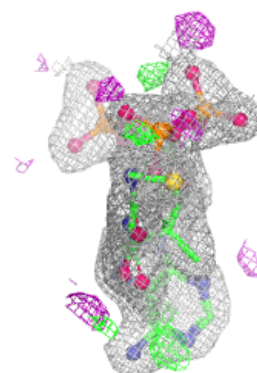
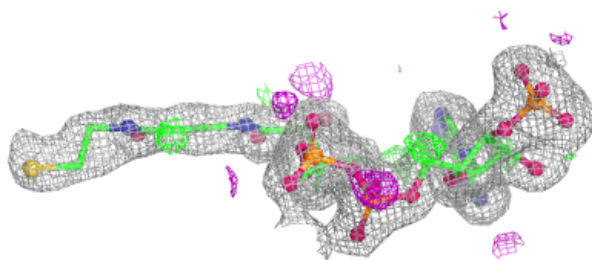
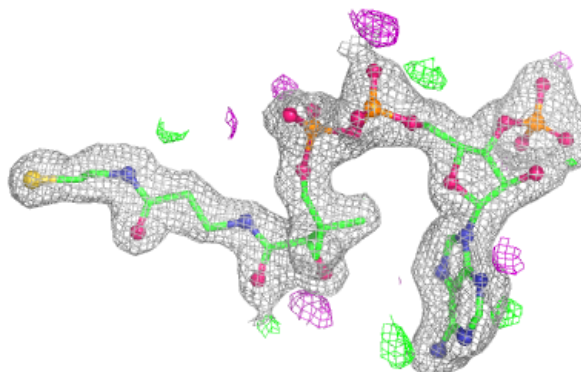


Electron density around COA S 1696:

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

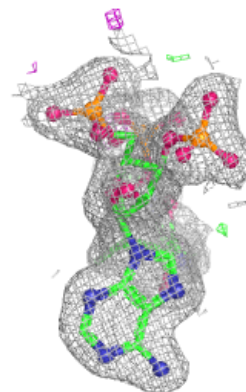
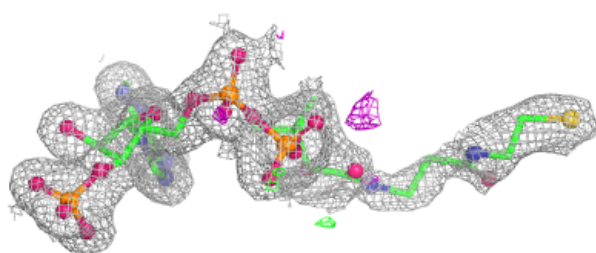
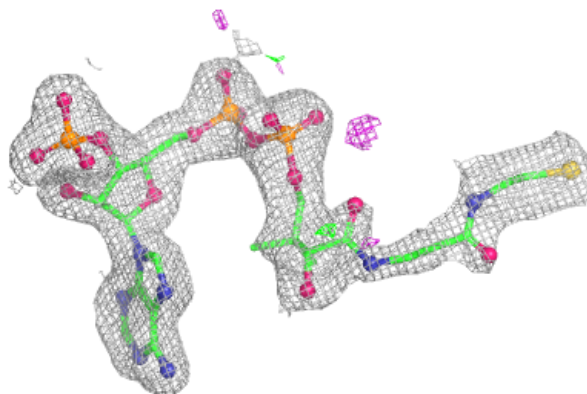
**Electron density around COA T 1791:**

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

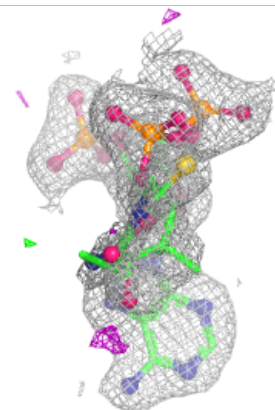
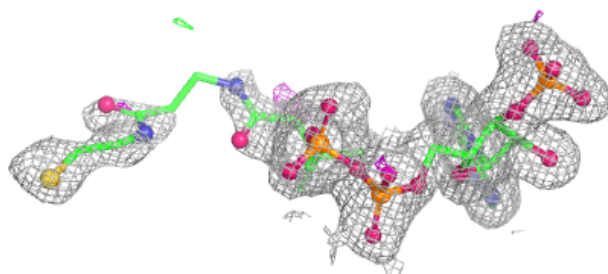
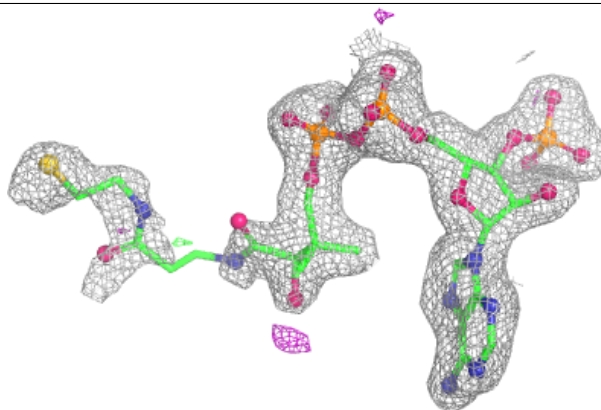


Electron density around COA U 1854:

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

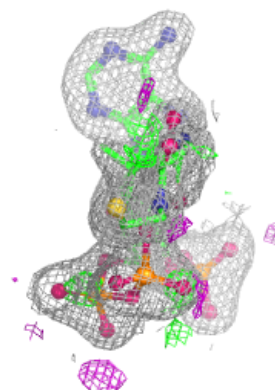
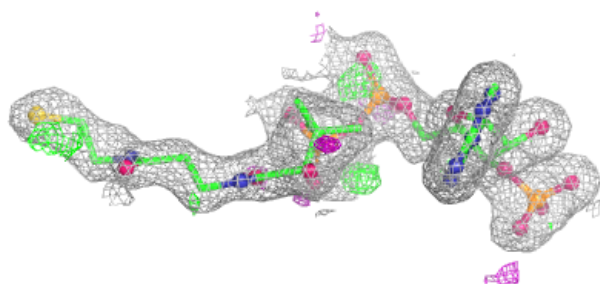
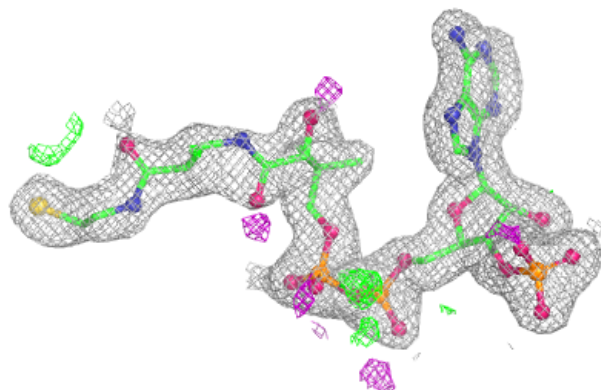
**Electron density around COA W 2019:**

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

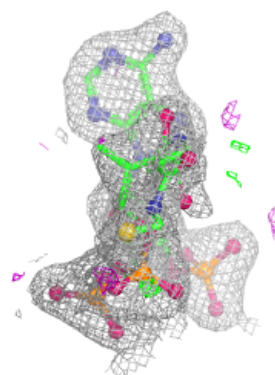
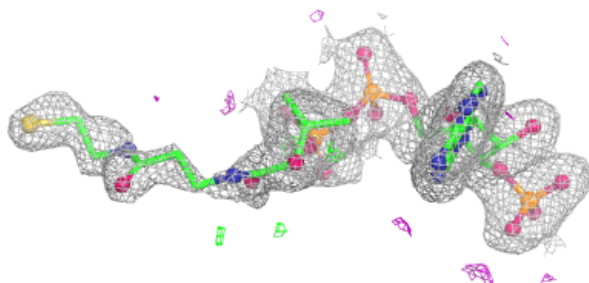
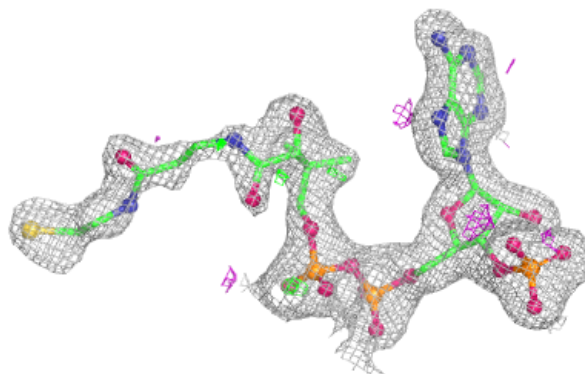


Electron density around COA F 477:

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

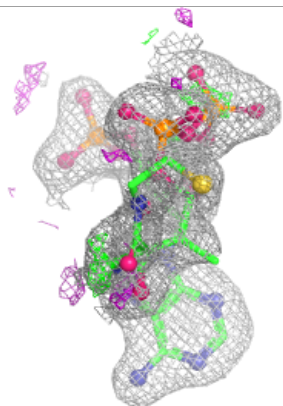
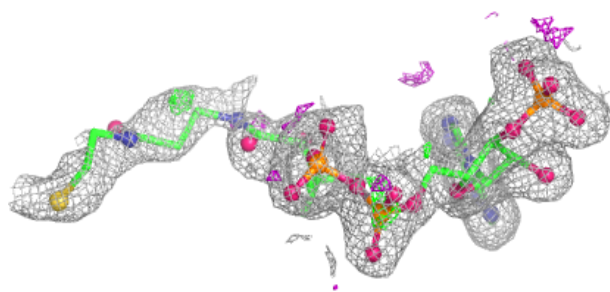
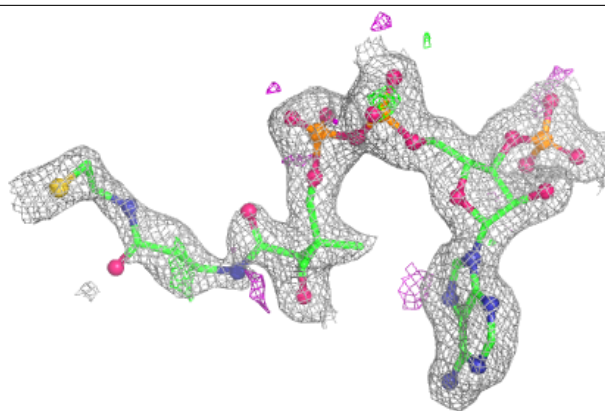
**Electron density around COA G 570:**

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

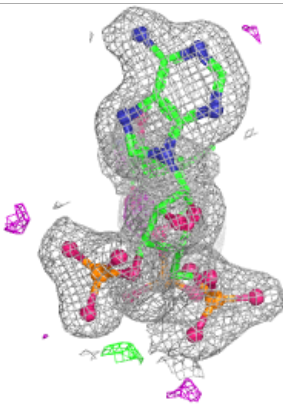
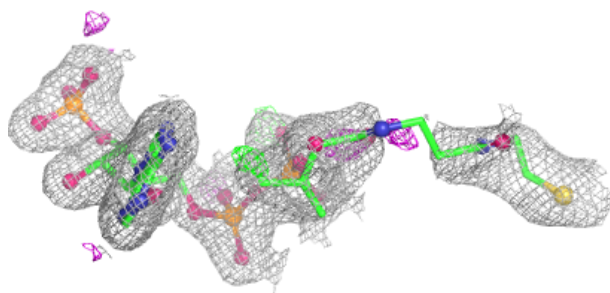
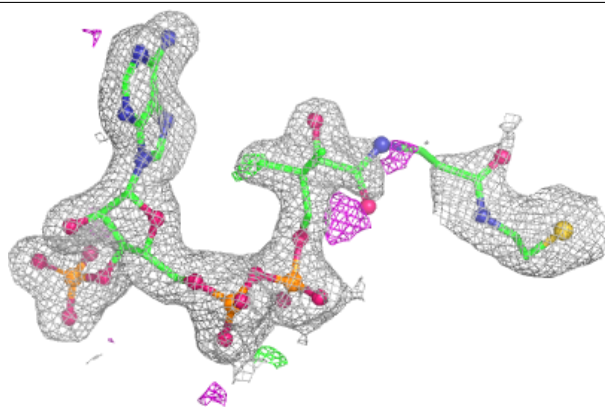


Electron density around COA C 169:

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

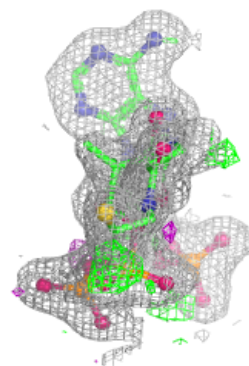
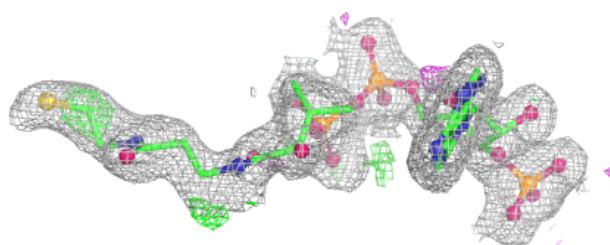
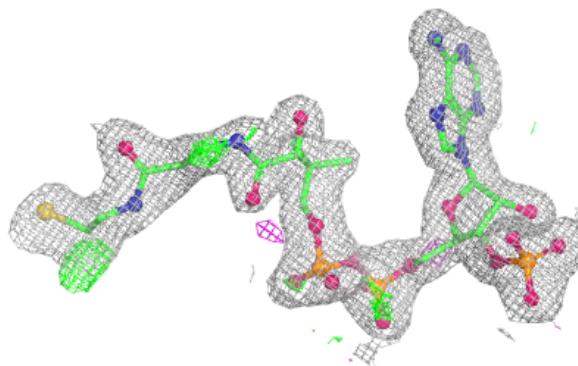
**Electron density around COA I 699:**

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

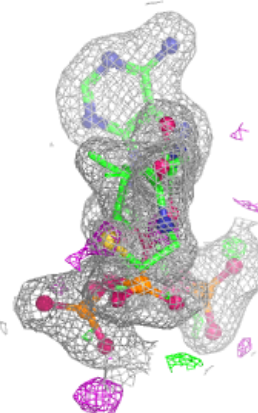
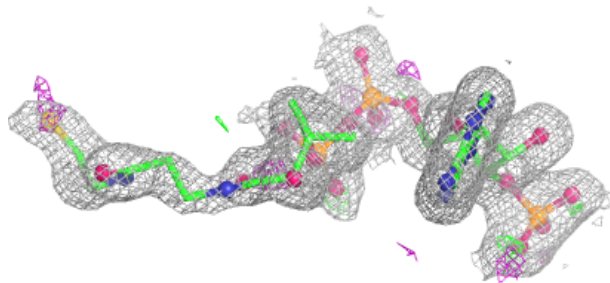
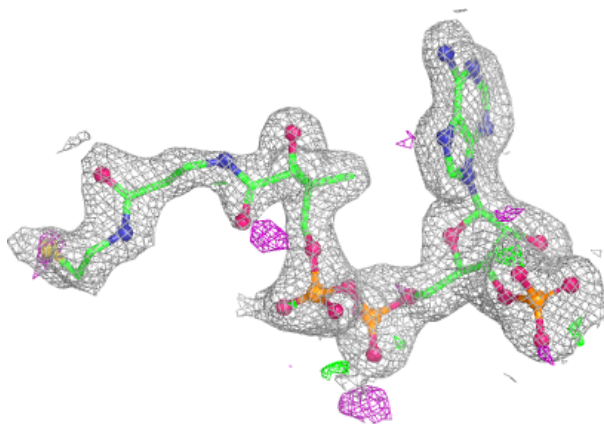


Electron density around COA J 780:

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

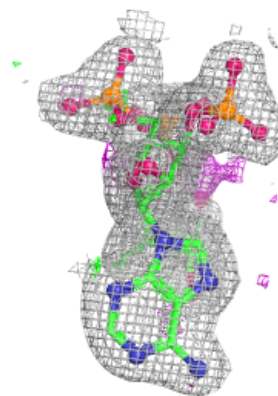
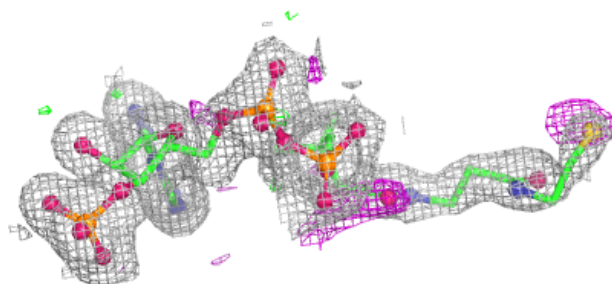
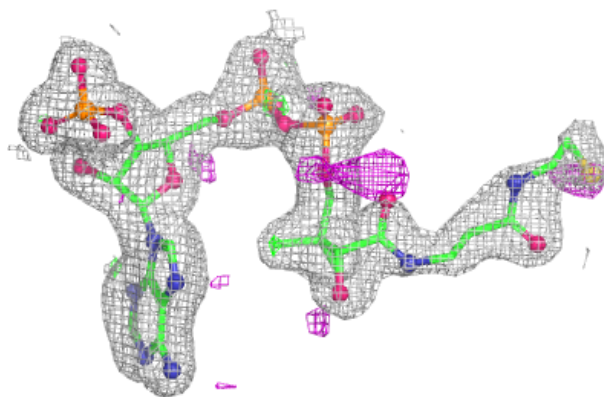
**Electron density around COA L 1008:**

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

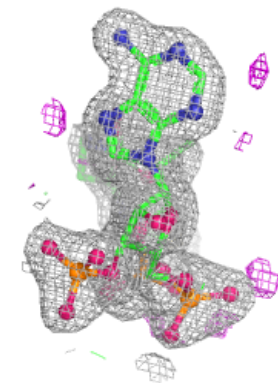
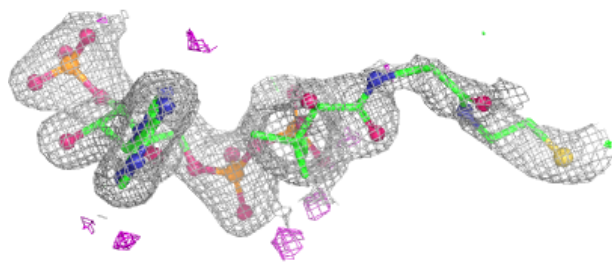
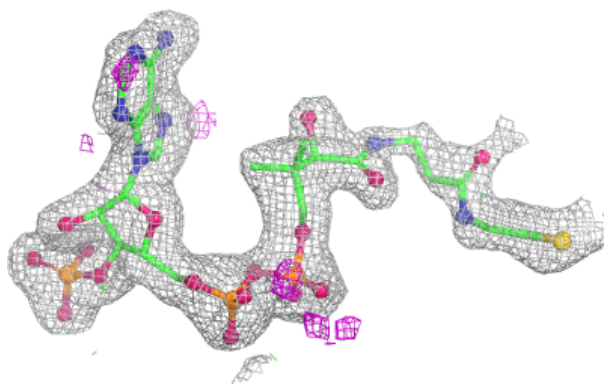


Electron density around COA D 283:

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

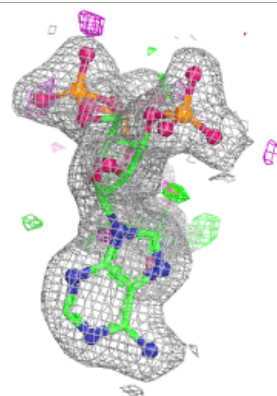
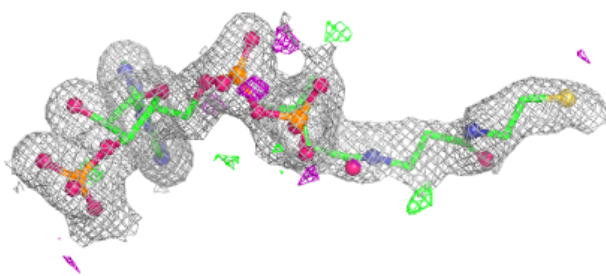
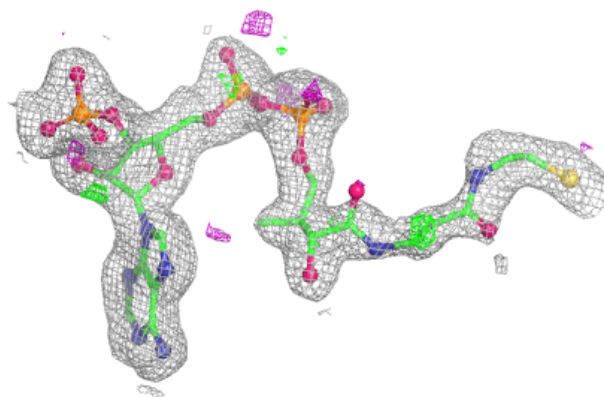
**Electron density around COA A 129:**

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

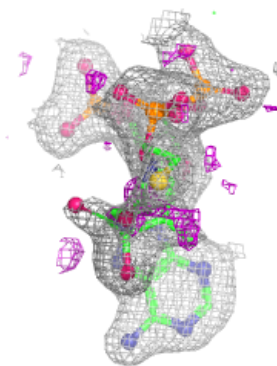
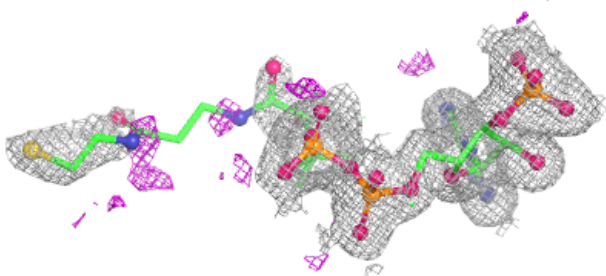
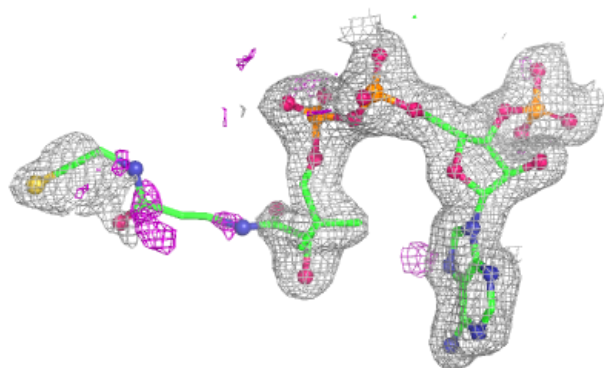


Electron density around COA O 1127:

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

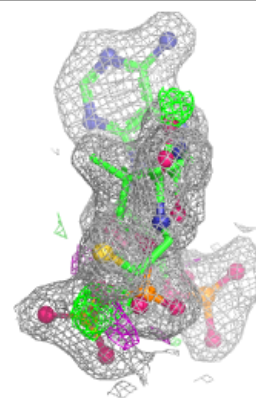
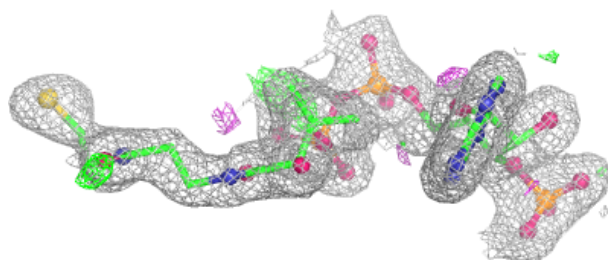
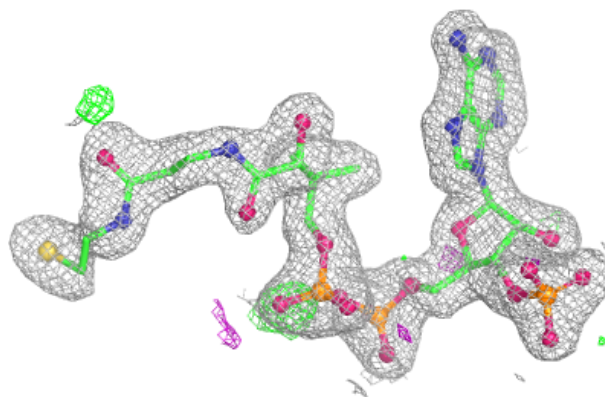
**Electron density around COA P 1424:**

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

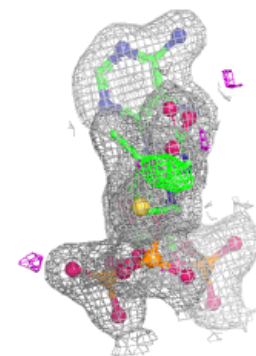
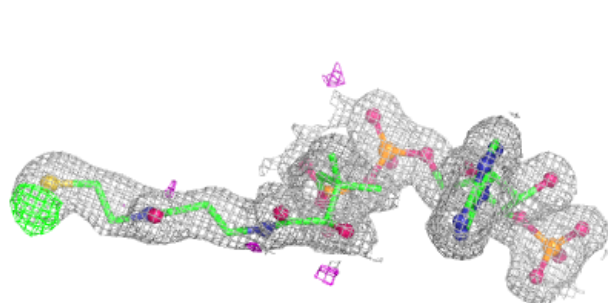
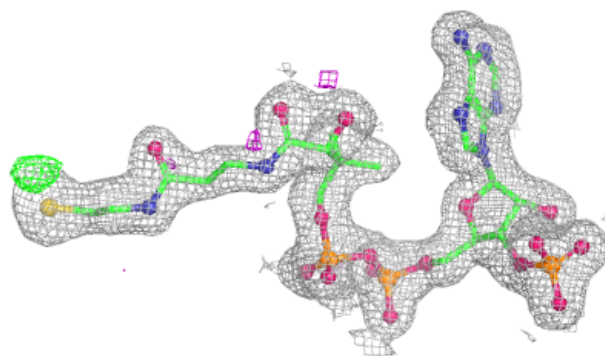


Electron density around COA A 127:

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

**Electron density around COA 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.