

#### wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 09:01 am GMT

PDB ID : 4ALI

Title: Crystal structure of S. aureus FabI in complex with NADP and triclosan (P1)

Authors: Schiebel, J.; Chang, A.; Tonge, P.J.; Kisker, C.

Deposited on : 2012-03-04

Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

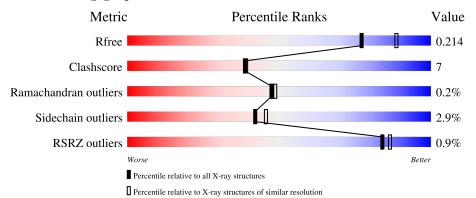
Validation Pipeline (wwPDB-VP) : 2.36

#### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}(\AA))$
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	282	77%	12%	10%
1	В	282	79%	11%	10%
1	С	282	81%	10%	10%
1	D	282	78%	9% •	10%
1	Е	282	76%	14%	• 10%



Continued from previous page...

Mol	Chain	Length	Quality of chain		
1	F	282	78%	12%	10%
1	G	282	79%	11%	• 10%
1	Н	282	79%	9% •	10%

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
4	GLU	В	1259	-	-	X	-
4	GLU	Е	1259	-	-	X	-
4	GLU	F	1259	-	-	X	-
4	GLU	G	1259	-	-	X	-



#### 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18131 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	254	Total	С	N	О	S	0	13	0
1	A	204	2052	1289	359	399	5	0	10	
1	В	255	Total	С	N	О	S	0	15	0
1	Б	255	2072	1304	363	400	5	0	10	U
1	С	255	Total	С	N	О	S	0	13	0
1		255	2059	1294	361	399	5	U	15	
1	D	254	Total	С	N	О	S	0	4	0
1	ש	204	1976	1245	341	385	5			U
1	E	255	Total	С	N	О	S	0	14	0
1	12	255	2063	1297	359	402	5	0	14	
1	F	255	Total	С	N	О	S	0	13	0
1	I.	255	2057	1293	358	401	5	0	15	0
1	G	255	Total	С	N	О	S	0	12	0
1	I G	255	2051	1289	357	400	5	0	12	0
1	Н	255	Total	С	N	О	S	0	3	0
1	11	200	1978	1246	341	387	4			U

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	=	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	=	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	_	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	_	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	_	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
В	-25	MET	-	expression tag	UNP Q7A6D8
В	-24	LYS	-	expression tag	UNP Q7A6D8
В	-23	HIS	-	expression tag	UNP Q7A6D8
В	-22	HIS	-	expression tag	UNP Q7A6D8
В	-21	HIS	-	expression tag	UNP Q7A6D8
В	-20	HIS	-	expression tag	UNP Q7A6D8
В	-19	HIS	-	expression tag	UNP Q7A6D8
В	-18	HIS	-	expression tag	UNP Q7A6D8
В	-17	PRO	-	expression tag	UNP Q7A6D8
В	-16	MET	-	expression tag	UNP Q7A6D8
В	-15	SER	_	expression tag	UNP Q7A6D8
В	-14	ASP	-	expression tag	UNP Q7A6D8
В	-13	TYR	-	expression tag	UNP Q7A6D8
В	-12	ASP	_	expression tag	UNP Q7A6D8
В	-11	ILE	-	expression tag	UNP Q7A6D8
В	-10	PRO	-	expression tag	UNP Q7A6D8
В	-9	THR	_	expression tag	UNP Q7A6D8
В	-8	THR	-	expression tag	UNP Q7A6D8
В	-7	GLU	_	expression tag	UNP Q7A6D8
В	-6	ASN	-	expression tag	UNP Q7A6D8
В	-5	LEU	-	expression tag	UNP Q7A6D8
В	-4	TYR	-	expression tag	UNP Q7A6D8
В	-3	PHE	-	expression tag	UNP Q7A6D8
В	-2	GLN	-	expression tag	UNP Q7A6D8
В	-1	GLY	-	expression tag	UNP Q7A6D8
В	0	ALA	-	expression tag	UNP Q7A6D8
В	2	VAL	LEU	engineered mutation	UNP Q7A6D8



Continued from previous page...

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
С	-25	MET	-	expression tag	UNP Q7A6D8
С	-24	LYS	-	expression tag	UNP Q7A6D8
С	-23	HIS	-	expression tag	UNP Q7A6D8
С	-22	HIS	-	expression tag	UNP Q7A6D8
С	-21	HIS	-	expression tag	UNP Q7A6D8
С	-20	HIS	-	expression tag	UNP Q7A6D8
С	-19	HIS	-	expression tag	UNP Q7A6D8
С	-18	HIS	-	expression tag	UNP Q7A6D8
С	-17	PRO	-	expression tag	UNP Q7A6D8
С	-16	MET	-	expression tag	UNP Q7A6D8
С	-15	SER	-	expression tag	UNP Q7A6D8
С	-14	ASP	-	expression tag	UNP Q7A6D8
С	-13	TYR	_	expression tag	UNP Q7A6D8
С	-12	ASP	-	expression tag	UNP Q7A6D8
С	-11	ILE	-	expression tag	UNP Q7A6D8
С	-10	PRO	-	expression tag	UNP Q7A6D8
С	-9	THR	-	expression tag	UNP Q7A6D8
С	-8	THR	-	expression tag	UNP Q7A6D8
С	-7	GLU	-	expression tag	UNP Q7A6D8
С	-6	ASN	-	expression tag	UNP Q7A6D8
С	-5	LEU	-	expression tag	UNP Q7A6D8
С	-4	TYR	-	expression tag	UNP Q7A6D8
С	-3	PHE	-	expression tag	UNP Q7A6D8
С	-2	GLN	-	expression tag	UNP Q7A6D8
С	-1	GLY	-	expression tag	UNP Q7A6D8
С	0	ALA	-	expression tag	UNP Q7A6D8
С	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS		expression tag	UNP Q7A6D8
D	-18	HIS		expression tag	UNP Q7A6D8
D	-17	PRO		expression tag	UNP Q7A6D8
D	-16	MET		expression tag	UNP Q7A6D8
D	-15	SER		expression tag	UNP Q7A6D8
D	-14	ASP		expression tag	UNP Q7A6D8
D	-13	TYR		expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE		expression tag	UNP Q7A6D8



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	_	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	_	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
Е	-25	MET	-	expression tag	UNP Q7A6D8
Е	-24	LYS	-	expression tag	UNP Q7A6D8
Е	-23	HIS	-	expression tag	UNP Q7A6D8
Е	-22	HIS	-	expression tag	UNP Q7A6D8
Е	-21	HIS	-	expression tag	UNP Q7A6D8
Е	-20	HIS	-	expression tag	UNP Q7A6D8
Е	-19	HIS	-	expression tag	UNP Q7A6D8
Е	-18	HIS	-	expression tag	UNP Q7A6D8
E	-17	PRO	-	expression tag	UNP Q7A6D8
E	-16	MET	-	expression tag	UNP Q7A6D8
E	-15	SER	_	expression tag	UNP Q7A6D8
E	-14	ASP	-	expression tag	UNP Q7A6D8
E	-13	TYR	-	expression tag	UNP Q7A6D8
Ε	-12	ASP	-	expression tag	UNP Q7A6D8
E	-11	ILE	_	expression tag	UNP Q7A6D8
E	-10	PRO	-	expression tag	UNP Q7A6D8
E	-9	THR	-	expression tag	UNP Q7A6D8
Е	-8	THR	-	expression tag	UNP Q7A6D8
Е	-7	GLU	-	expression tag	UNP Q7A6D8
Е	-6	ASN	-	expression tag	UNP Q7A6D8
Е	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
Е	-3	PHE	-	expression tag	UNP Q7A6D8
Е	-2	GLN	-	expression tag	UNP Q7A6D8
Е	-1	GLY	-	expression tag	UNP Q7A6D8
Е	0	ALA	-	expression tag	UNP Q7A6D8
Е	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	-25	MET	-	expression tag	UNP Q7A6D8
F	-24	LYS	-	expression tag	UNP Q7A6D8
F	-23	HIS	-	expression tag	UNP Q7A6D8



Continued from previous page...

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	UNP Q7A6D8
F	-15	SER	-	expression tag	UNP Q7A6D8
F	-14	ASP	-	expression tag	UNP Q7A6D8
F	-13	TYR	-	expression tag	UNP Q7A6D8
F	-12	ASP	-	expression tag	UNP Q7A6D8
F	-11	ILE	-	expression tag	UNP Q7A6D8
F	-10	PRO	-	expression tag	UNP Q7A6D8
F	-9	THR	-	expression tag	UNP Q7A6D8
F	-8	THR	-	expression tag	UNP Q7A6D8
F	-7	GLU	-	expression tag	UNP Q7A6D8
F	-6	ASN	-	expression tag	UNP Q7A6D8
F	-5	LEU	-	expression tag	UNP Q7A6D8
F	-4	TYR	-	expression tag	UNP Q7A6D8
F	-3	PHE	-	expression tag	UNP Q7A6D8
F	-2	GLN	-	expression tag	UNP Q7A6D8
F	-1	GLY	-	expression tag	UNP Q7A6D8
F	0	ALA	-	expression tag	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	-25	MET	-	expression tag	UNP Q7A6D8
G	-24	LYS	-	expression tag	UNP Q7A6D8
G	-23	HIS	-	expression tag	UNP Q7A6D8
G	-22	HIS	-	expression tag	UNP Q7A6D8
G	-21	HIS	-	expression tag	UNP Q7A6D8
G	-20	HIS	-	expression tag	UNP Q7A6D8
G	-19	HIS	-	expression tag	UNP Q7A6D8
G	-18	HIS	-	expression tag	UNP Q7A6D8
G	-17	PRO	-	expression tag	UNP Q7A6D8
G	-16	MET	-	expression tag	UNP Q7A6D8
G	-15	SER	-	expression tag	UNP Q7A6D8
G	-14	ASP	-	expression tag	UNP Q7A6D8
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8

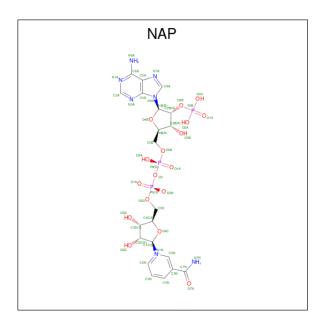


 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
Н	-25	MET	-	expression tag	UNP Q7A6D8
Н	-24	LYS	-	expression tag	UNP Q7A6D8
Н	-23	HIS	-	expression tag	UNP Q7A6D8
Н	-22	HIS	-	expression tag	UNP Q7A6D8
Н	-21	HIS	-	expression tag	UNP Q7A6D8
Н	-20	HIS	-	expression tag	UNP Q7A6D8
Н	-19	HIS	-	expression tag	UNP Q7A6D8
Н	-18	HIS	-	expression tag	UNP Q7A6D8
Н	-17	PRO	-	expression tag	UNP Q7A6D8
Н	-16	MET	-	expression tag	UNP Q7A6D8
Н	-15	SER	-	expression tag	UNP Q7A6D8
Н	-14	ASP	-	expression tag	UNP Q7A6D8
Н	-13	TYR	-	expression tag	UNP Q7A6D8
Н	-12	ASP	-	expression tag	UNP Q7A6D8
Н	-11	ILE	-	expression tag	UNP Q7A6D8
Н	-10	PRO	-	expression tag	UNP Q7A6D8
Н	-9	THR	-	expression tag	UNP Q7A6D8
Н	-8	THR	-	expression tag	UNP Q7A6D8
H	-7	GLU	-	expression tag	UNP Q7A6D8
Н	-6	ASN	-	expression tag	UNP Q7A6D8
Н	-5	LEU	-	expression tag	UNP Q7A6D8
Н	-4	TYR	-	expression tag	UNP Q7A6D8
H	-3	PHE	-	expression tag	UNP Q7A6D8
H	-2	GLN	-	expression tag	UNP Q7A6D8
Н	-1	GLY	-	expression tag	UNP Q7A6D8
H	0	ALA	-	expression tag	UNP Q7A6D8
Н	2	VAL	LEU	engineered mutation	UNP Q7A6D8

• Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).

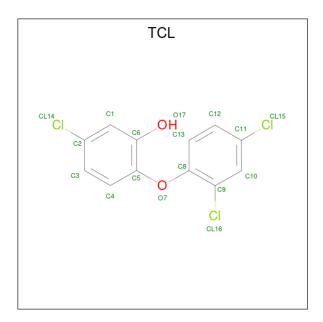




Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	Р	0	0		
	2 A	1	48	21	7	17	3	U	U		
2	В	1	Total	С	N	О	Р	0	0		
2	Б	1	48	21	7	17	3	U	U		
2	С	1	Total	С	N	О	Р	0	0		
2			2   C	1	48	21	7	17	3	U	U
2	2 D	1	Total	С	N	О	Р	0	0		
2		1	48	21	7	17	3	0	U		
2	E	1	Total	С	N	О	Р	0	0		
	ינו	1	48	21	7	17	3	U	U		
2	F	1	Total	С	N	О	Р	0	0		
	I.	1	48	21	7	17	3	U	U		
2	G	1	Total	С	N	Ο	Р	0	0		
	2 G	1	48	21	7	17	3	0	U		
2	2 H	1	Total	С	N	О	Р	0	0		
		1	48	21	7	17	3	U	U		

 $\bullet$  Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula:  $\mathrm{C_{12}H_7Cl_3O_2}).$ 

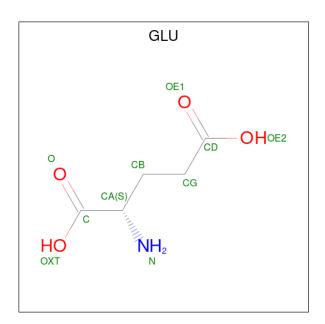




Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf		
3	A	1	Total	С	Cl	О	0	0		
3	A	1	17	12	3	2	0	0		
3	В	1	Total	С	Cl	О	0	0		
J	Ъ	1	17	12	3	2	U	U		
3	С	1	Total	С	Cl	Ο	0	0		
		1	17	12	3	2	0	U		
3	D	1	Total	С	Cl	O	0	0		
	D	1	17	12	3	2	U			
3	E	E 1	Total	$\mathbf{C}$	$\operatorname{Cl}$	Ο	0	0		
	Ш		17	12	3	2	O	0		
3	F	1	Total	$\mathbf{C}$	$\operatorname{Cl}$	Ο	0	0		
	I.	1	17	12	3	2	O			
3	C	G	С	1	Total	$\mathbf{C}$	Cl	Ο	0	0
	J	1	17	12	3	2	0	0		
3	H	1	Total	$\mathbf{C}$	Cl	Ο	0	0		
3	Н	1	17	12	3	2				

 $\bullet$  Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 10 5 1 4	0	0
4	В	1	Total C N O 10 5 1 4	0	0
4	С	1	Total C N O 10 5 1 4	0	0
4	E	1	Total C N O 10 5 1 4	0	0
4	Е	1	Total C N O 10 5 1 4	0	0
4	F	1	Total C N O 10 5 1 4	0	0
4	G	1	Total C N O 10 5 1 4	0	0

#### • Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	202	Total O 202 202	0	0
5	В	161	Total O 161 161	0	0
5	С	148	Total O 148 148	0	0
5	D	108	Total O 108 108	0	0
5	E	161	Total O 161 161	0	0



Continued from previous page...

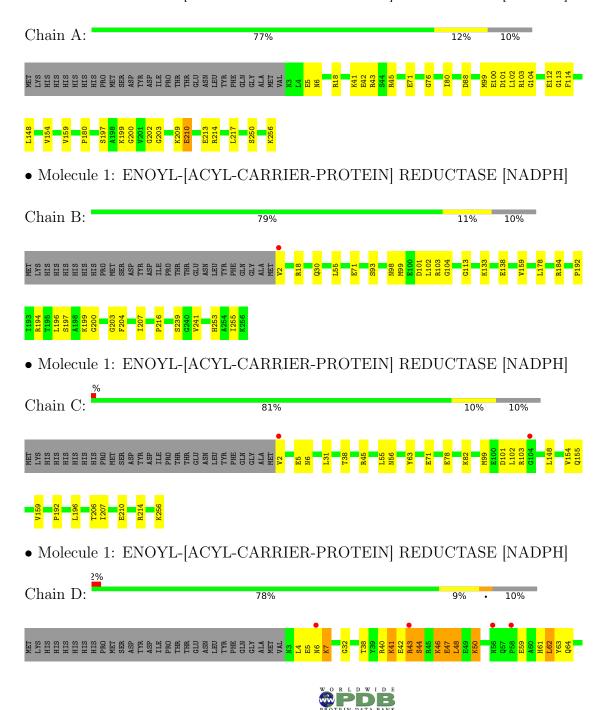
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	175	Total O 175 175	0	0
5	G	163	Total O 163 163	0	0
5	Н	115	Total O 115 115	0	0



#### 3 Residue-property plots (i)

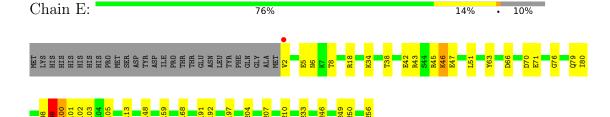
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



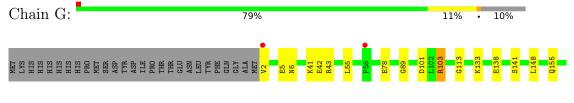
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F: 78% 12% 10%

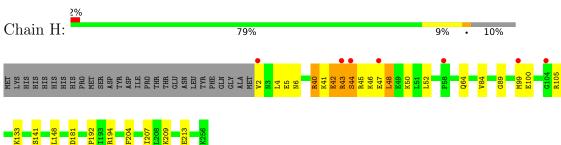
EXERCISE SERVICE SERVICE

H184 H192 K199 K199 H200 H200 H2100 H2100

• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



 $\bullet$  Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





#### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	89.96Å 94.81Å 94.88Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.13° 111.98° 97.25°	Depositor
Resolution (Å)	38.47 - 2.10	Depositor
rtesolution (A)	38.47 - 2.10	EDS
% Data completeness	97.8 (38.47-2.10)	Depositor
(in resolution range)	97.9 (38.47-2.10)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.149 , 0.197	Depositor
$R, R_{free}$	0.169 , $0.214$	DCC
$R_{free}$ test set	8072 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 38.0	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

#### 5 Model quality (i)

#### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TCL, NAP

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	Bo	nd lengths	Bo	ond angles
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	0.67	0/2091	0.90	1/2813 (0.0%)
1	В	0.63	0/2117	0.83	0/2848
1	С	0.61	0/2098	0.85	0/2823
1	D	0.61	0/2009	0.86	0/2706
1	Е	0.67	1/2105~(0.0%)	0.87	0/2833
1	F	0.65	0/2096	0.83	0/2821
1	G	0.63	0/2087	0.86	0/2809
1	Н	0.59	0/2008	0.85	$2/2706 \ (0.1\%)$
All	All	0.63	1/16611 (0.0%)	0.86	$3/22359 \ (0.0\%)$

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

$\mathbf{Mol}$	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	Е	168	GLU	CB-CG	5.43	1.62	1.52

#### All (3) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	Н	40	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	88	ASP	CB-CG-OD2	5.24	123.02	118.30
1	Н	48	LEU	CA-CB-CG	5.09	127.01	115.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	46	LYS	Peptide

#### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2052	0	2071	40	0
1	В	2072	0	2104	36	0
1	С	2059	0	2082	25	1
1	D	1976	0	1992	26	0
1	Е	2063	0	2083	53	0
1	F	2057	0	2075	37	0
1	G	2051	0	2067	34	3
1	Н	1978	0	1990	21	0
2	A	48	0	25	0	0
2	В	48	0	25	0	0
2	С	48	0	25	0	0
2	D	48	0	25	2	0
2	Ε	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	Н	48	0	25	2	0
3	A	17	0	6	1	0
3	В	17	0	6	3	0
3	С	17	0	6	1	0
3	D	17	0	7	2	0
3	Е	17	0	6	2	0
3	F	17	0	6	0	0
3	G	17	0	6	1	0
3	Н	17	0	7	1	0
4	A	10	0	5	2	0
4	В	10	0	5	9	0
4	С	10	0	5	2	0
4	Е	20	0	10	8	0
4	F	10	0	5	7	0



$\alpha \cdots$	, r	•	
Continued	trom	mromonie	maaa
-	110116	DICULUUS	Duuc
	J	1	1

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	G	10	0	5	6	0
5	A	202	0	0	10	1
5	В	161	0	0	5	1
5	С	148	0	0	6	0
5	D	108	0	0	4	0
5	Ε	161	0	0	7	0
5	F	175	0	0	12	0
5	G	163	0	0	1	0
5	Н	115	0	0	0	0
All	All	18131	0	16749	252	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 252 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:H:44:SER:O	1:H:48:LEU:HB2	1.25	1.30	
1:G:103[B]:ARG:HH12	4:G:1259:GLU:HB2	1.17	1.05	
1:C:103[B]:ARG:HH22	4:C:1259:GLU:HG3	1.27	0.99	
1:F:103[A]:ARG:HH22	4:F:1259:GLU:HG2	1.27	0.98	
1:E:103[A]:ARG:HH12	4:E:1259:GLU:HA	1.25	0.96	

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:82:LYS:NZ	1:G:78:GLU:OE2[1_564]	2.07	0.13
1:G:43:ARG:NH1	5:B:2082:HOH:O[1_545]	2.14	0.06
1:G:42[B]:GLU:OE2	5:A:2066:HOH:O[1_545]	2.15	0.05

#### 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	Perce	$\mathbf{ntiles}$
1	A	265/282~(94%)	251 (95%)	14 (5%)	0	100	100
1	В	$268/282 \ (95\%)$	257 (96%)	11 (4%)	0	100	100
1	С	266/282 (94%)	259 (97%)	7 (3%)	0	100	100
1	D	256/282 (91%)	239 (93%)	14 (6%)	3 (1%)	13	8
1	E	$267/282 \ (95\%)$	254 (95%)	11 (4%)	2 (1%)	22	18
1	F	266/282 (94%)	247 (93%)	19 (7%)	0	100	100
1	G	$265/282 \ (94\%)$	254 (96%)	11 (4%)	0	100	100
1	Н	256/282 (91%)	240 (94%)	16 (6%)	0	100	100
All	All	2109/2256 (94%)	2001 (95%)	103 (5%)	5 (0%)	47	49

#### All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	47	GLU
1	D	48	LEU
1	D	46	LYS
1	Е	99[A]	MET
1	Ε	99[B]	MET

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Rotameric Outliers	
1	A	$219/234\ (94\%)$	218 (100%)	1 (0%)	88 92
1	В	$222/234\ (95\%)$	218 (98%)	4 (2%)	59 65
1	С	220/234 (94%)	216 (98%)	4 (2%)	59 65
1	D	$211/234\ (90\%)$	202 (96%)	9 (4%)	29 29
1	Е	221/234 (94%)	214 (97%)	7 (3%)	39 41
1	F	220/234~(94%)	214 (97%)	6 (3%)	44 48
1	G	219/234 (94%)	214 (98%)	5 (2%)	50 55



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	Н	211/234 (90%)	199 (94%)	12 (6%)	20 18		
All	All	1743/1872 (93%)	1695 (97%)	48 (3%)	42 47		

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	138	GLU
1	G	209	LYS
1	F	209	LYS
1	G	103[A]	ARG
1	Н	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	3	ASN
1	F	253	HIS
1	Н	155	GLN
1	В	253	HIS
1	В	56	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



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

Mol	Type	Chain	Res	Link	Во	Bond lengths		В	Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
3	TCL	A	1258	-	18,18,18	1.66	3 (16%)	25,25,25	0.73	0		
4	GLU	A	1259	-	8,9,9	1.29	1 (12%)	10,11,11	1.29	1 (10%)		
4	GLU	G	1259	-	8,9,9	1.38	1 (12%)	10,11,11	1.11	0		
2	NAP	В	1258	-	45,52,52	1.54	4 (8%)	56,80,80	1.54	6 (10%)		
4	GLU	Е	1259	-	8,9,9	1.34	1 (12%)	10,11,11	1.21	1 (10%)		
3	TCL	F	1258	-	18,18,18	1.45	3 (16%)	25,25,25	0.74	0		
2	NAP	G	1257	-	45,52,52	1.54	3 (6%)	56,80,80	1.80	8 (14%)		
2	NAP	F	1257	-	45,52,52	1.50	4 (8%)	56,80,80	1.76	6 (10%)		
3	TCL	Е	1258	-	18,18,18	1.57	4 (22%)	25,25,25	0.74	1 (4%)		
4	GLU	С	1259	-	8,9,9	1.26	1 (12%)	10,11,11	1.05	0		
2	NAP	С	1257	-	45,52,52	1.44	3 (6%)	56,80,80	1.78	8 (14%)		
3	TCL	В	1257	-	18,18,18	1.42	3 (16%)	25,25,25	0.73	0		
3	TCL	Н	1258	-	18,18,18	1.71	5 (27%)	25,25,25	0.74	1 (4%)		
2	NAP	Н	1257	-	45,52,52	1.62	3 (6%)	56,80,80	1.86	10 (17%)		
4	GLU	В	1259	-	8,9,9	1.23	0	10,11,11	2.24	5 (50%)		
4	GLU	F	1259	-	8,9,9	1.29	1 (12%)	10,11,11	1.14	1 (10%)		
2	NAP	D	1257	-	45,52,52	1.59	3 (6%)	56,80,80	1.61	10 (17%)		
3	TCL	D	1258	-	18,18,18	1.57	4 (22%)	25,25,25	0.74	1 (4%)		
2	NAP	A	1257	-	45,52,52	1.66	5 (11%)	56,80,80	1.69	7 (12%)		
3	TCL	С	1258	-	18,18,18	1.60	6 (33%)	25,25,25	0.73	0		
2	NAP	Е	1257	-	45,52,52	1.68	4 (8%)	56,80,80	1.60	8 (14%)		
4	GLU	Е	1260	-	8,9,9	1.11	0	10,11,11	1.44	2 (20%)		
3	TCL	G	1258	-	18,18,18	1.52	3 (16%)	25,25,25	0.73	1 (4%)		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCL	A	1258	-	-	0/4/4/4	0/2/2/2



 $Continued\ from\ previous\ page...$ 

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLU	A	1259	-	-	4/9/9/9	-
4	GLU	G	1259	-	-	6/9/9/9	-
2	NAP	В	1258	-	-	6/31/67/67	0/5/5/5
4	GLU	Е	1259	-	-	7/9/9/9	-
3	TCL	F	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	G	1257	-	-	8/31/67/67	0/5/5/5
2	NAP	F	1257	-	-	6/31/67/67	0/5/5/5
3	TCL	E	1258	-	-	0/4/4/4	0/2/2/2
4	GLU	С	1259	-	-	3/9/9/9	-
2	NAP	С	1257	-	-	5/31/67/67	0/5/5/5
3	TCL	В	1257	-	-	0/4/4/4	0/2/2/2
3	TCL	Н	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	Н	1257	-	-	7/31/67/67	0/5/5/5
4	GLU	В	1259	-	-	5/9/9/9	-
4	GLU	F	1259	-	-	5/9/9/9	-
2	NAP	D	1257	-	-	6/31/67/67	0/5/5/5
3	TCL	D	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	A	1257	-	-	6/31/67/67	0/5/5/5
3	TCL	С	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	Е	1257	-	-	4/31/67/67	0/5/5/5
4	GLU	Е	1260	-	-	2/9/9/9	-
3	TCL	G	1258	-	-	0/4/4/4	0/2/2/2

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	Н	1257	NAP	O7N-C7N	8.22	1.39	1.24
2	Е	1257	NAP	O7N-C7N	7.92	1.39	1.24
2	D	1257	NAP	O7N-C7N	7.87	1.39	1.24
2	A	1257	NAP	O7N-C7N	7.86	1.39	1.24
2	G	1257	NAP	O7N-C7N	7.52	1.38	1.24

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	F	1257	NAP	C3N-C7N-N7N	7.05	126.21	117.75
2	G	1257	NAP	N3A-C2A-N1A	-7.00	117.74	128.68
2	Н	1257	NAP	O7N-C7N-C3N	-6.63	111.70	119.63
2	A	1257	NAP	N3A-C2A-N1A	-6.41	118.66	128.68



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	D	1257	NAP	N3A-C2A-N1A	-6.34	118.77	128.68

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1257	NAP	C5D-O5D-PN-O1N
2	A	1257	NAP	C5D-O5D-PN-O2N
2	A	1257	NAP	O4D-C1D-N1N-C2N
2	В	1258	NAP	C5D-O5D-PN-O1N
2	В	1258	NAP	C5D-O5D-PN-O2N

There are no ring outliers.

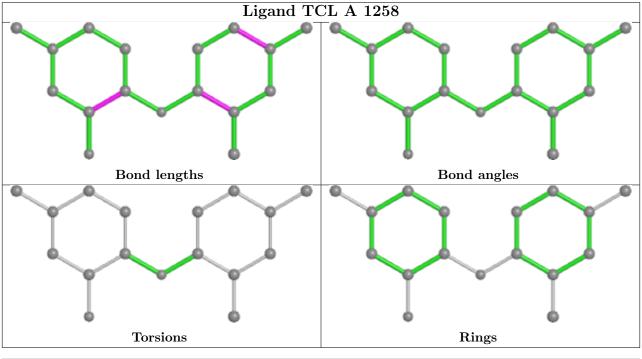
15 monomers are involved in 47 short contacts:

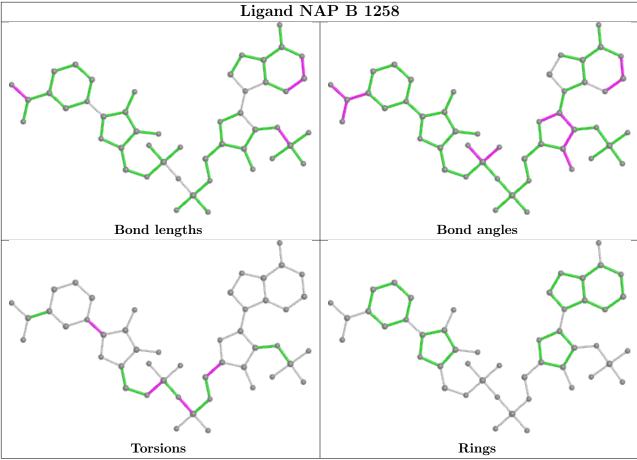
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1258	TCL	1	0
4	A	1259	GLU	2	0
4	G	1259	GLU	6	0
4	Е	1259	GLU	8	0
3	Е	1258	TCL	2	0
4	С	1259	GLU	2	0
3	В	1257	TCL	3	0
3	Н	1258	TCL	1	0
2	Н	1257	NAP	2	0
4	В	1259	GLU	9	0
4	F	1259	GLU	7	0
2	D	1257	NAP	2	0
3	D	1258	TCL	2	0
3	С	1258	TCL	1	0
3	G	1258	TCL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

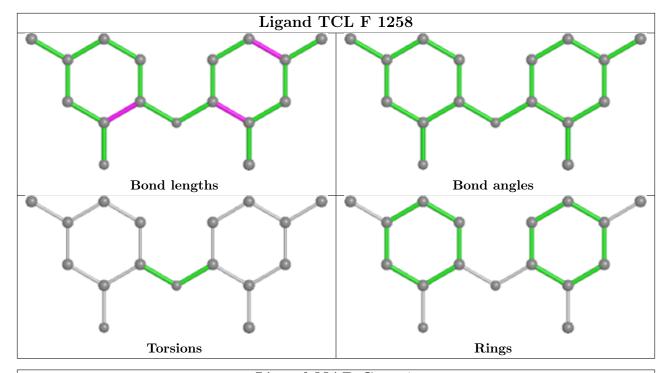


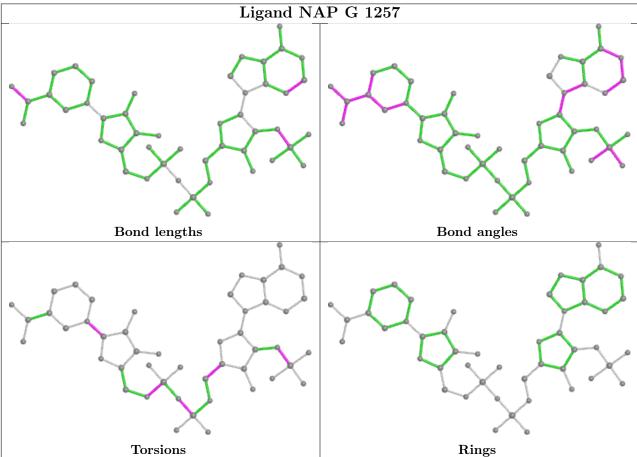
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



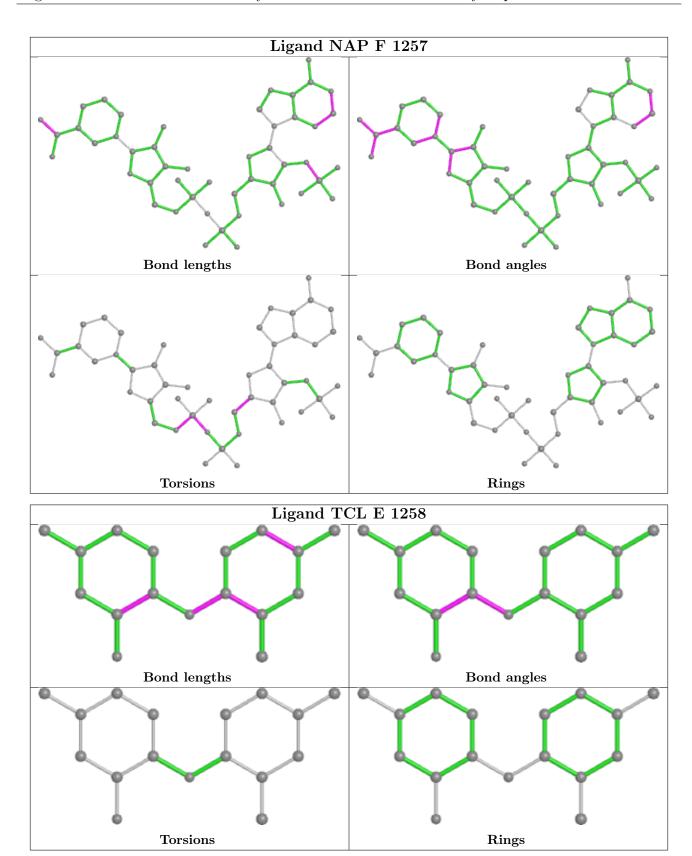




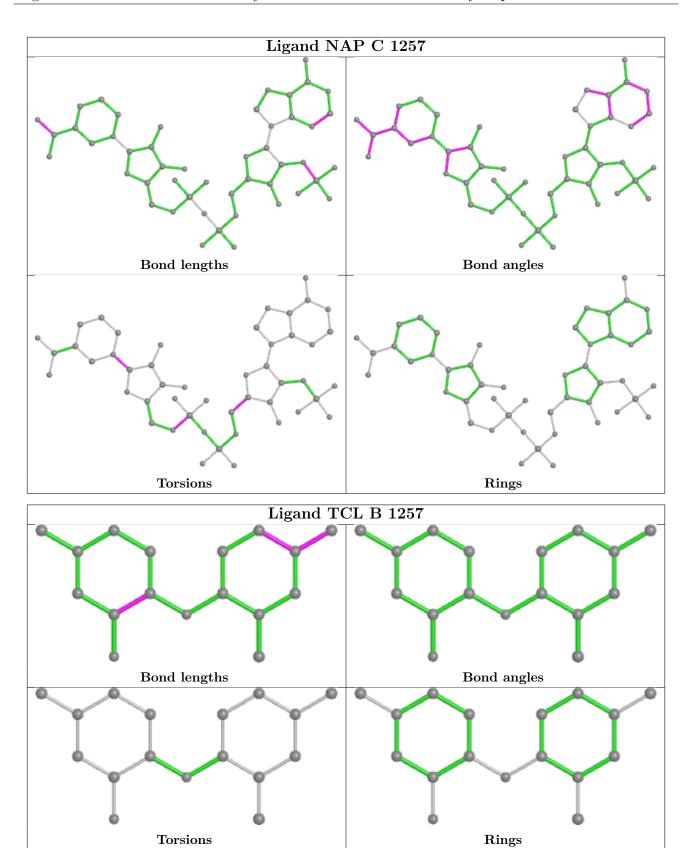




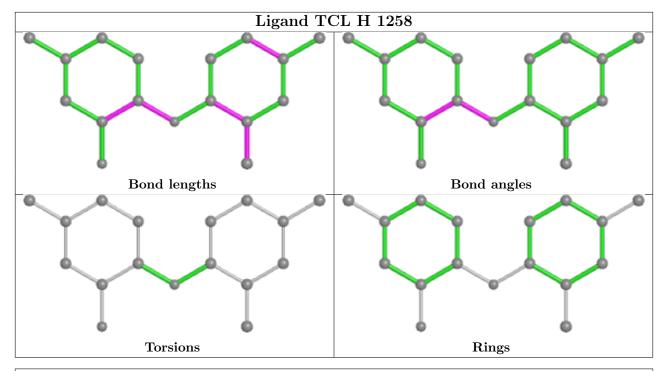


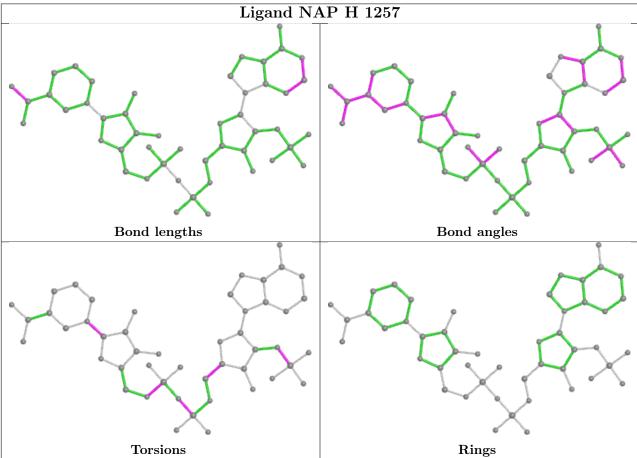




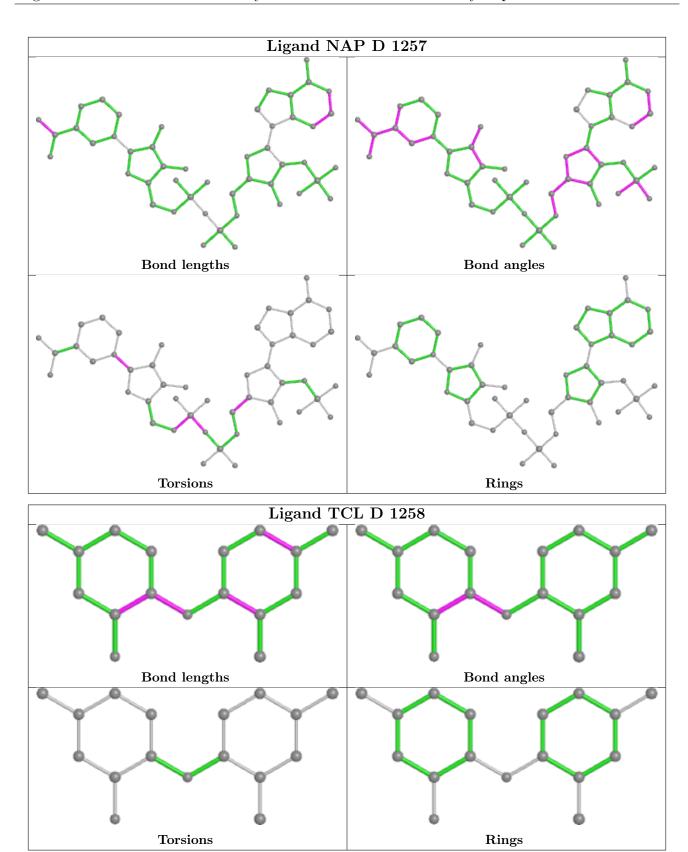




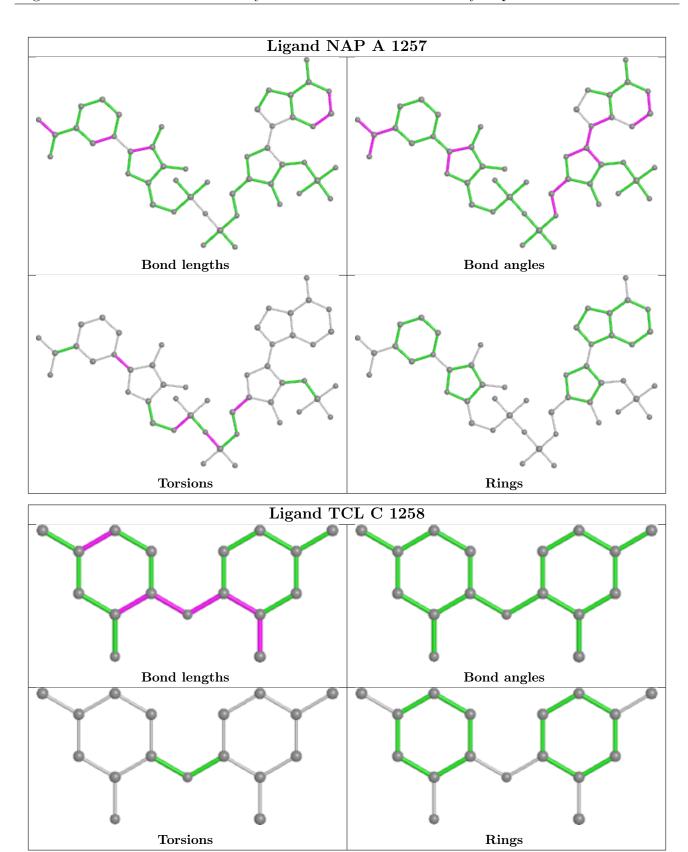




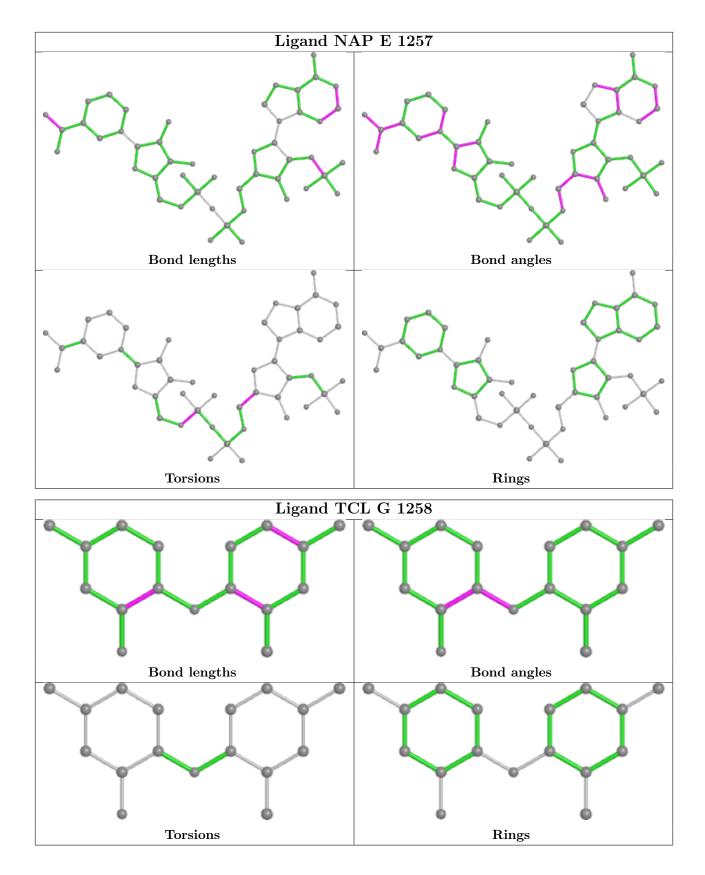












#### 5.7 Other polymers (i)

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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ} {>} 2$	$OWAB(A^2)$	Q < 0.9
1	A	$254/282 \ (90\%)$	-0.56	0 100 100	15, 25, 47, 59	0
1	В	255/282~(90%)	-0.49	1 (0%) 92 93	15, 27, 51, 72	0
1	С	$255/282 \ (90\%)$	-0.28	2 (0%) 86 88	16, 29, 52, 70	0
1	D	254/282 (90%)	-0.36	5 (1%) 65 69	17, 33, 65, 87	0
1	E	$255/282 \ (90\%)$	-0.44	1 (0%) 92 93	15, 25, 47, 64	0
1	F	255/282~(90%)	-0.56	1 (0%) 92 93	16, 26, 49, 67	0
1	G	255/282~(90%)	-0.35	2 (0%) 86 88	18, 28, 52, 62	0
1	Н	255/282 (90%)	-0.22	7 (2%) 54 60	15, 32, 67, 89	0
All	All	2038/2256 (90%)	-0.41	19 (0%) 84 86	15, 28, 54, 89	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	2	VAL	4.3
1	G	2	VAL	4.0
1	Е	2	VAL	3.7
1	F	2	VAL	3.6
1	Н	2	VAL	3.5

#### 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 monosaccharides in this entry.



#### 6.4 Ligands (i)

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

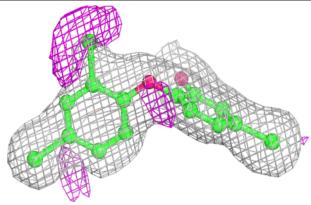
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B ext{-}factors}({f \AA}^2)$	Q<0.9
4	GLU	В	1259	10/10	0.66	0.25	62,66,69,70	0
4	GLU	G	1259	10/10	0.70	0.31	60,63,70,73	0
4	GLU	A	1259	10/10	0.72	0.21	57,59,65,67	0
4	GLU	Е	1259	10/10	0.77	0.20	60,62,63,63	0
4	GLU	Е	1260	10/10	0.80	0.21	63,72,76,77	0
4	GLU	С	1259	10/10	0.84	0.23	59,63,76,82	0
4	GLU	F	1259	10/10	0.88	0.27	60,65,72,72	0
3	TCL	Н	1258	17/17	0.94	0.12	30,34,53,78	0
3	TCL	D	1258	17/17	0.95	0.12	33,37,51,74	0
3	TCL	Е	1258	17/17	0.97	0.10	19,24,38,54	0
3	TCL	G	1258	17/17	0.97	0.09	21,28,45,58	0
3	TCL	В	1257	17/17	0.97	0.09	20,26,44,51	0
3	TCL	С	1258	17/17	0.97	0.11	21,29,46,59	0
2	NAP	Н	1257	48/48	0.97	0.08	22,30,56,61	0
3	TCL	F	1258	17/17	0.98	0.07	20,26,40,51	0
2	NAP	D	1257	48/48	0.98	0.07	21,30,47,50	0
2	NAP	G	1257	48/48	0.98	0.10	20,26,30,36	0
2	NAP	С	1257	48/48	0.98	0.12	18,26,33,37	0
3	TCL	A	1258	17/17	0.98	0.09	20,25,39,51	0
2	NAP	В	1258	48/48	0.99	0.10	19,25,31,32	0
2	NAP	Е	1257	48/48	0.99	0.10	18,23,28,33	0
2	NAP	F	1257	48/48	0.99	0.08	18,25,32,33	0
2	NAP	A	1257	48/48	0.99	0.08	17,23,29,34	0

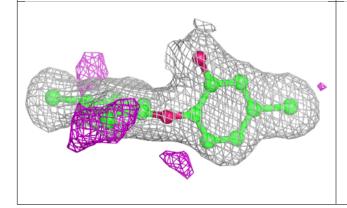
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

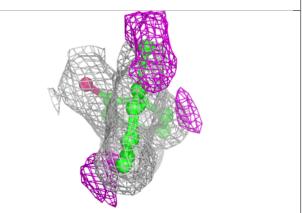


#### Electron density around TCL H 1258:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

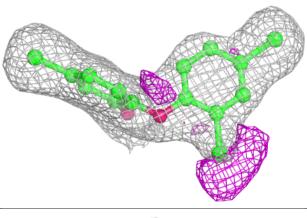


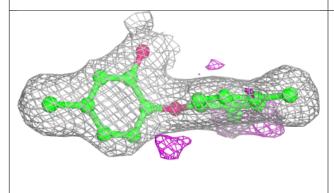


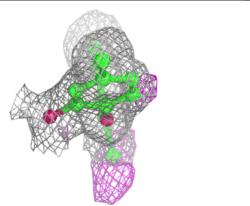


#### Electron density around TCL D 1258:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



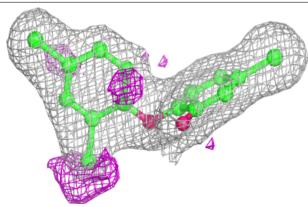


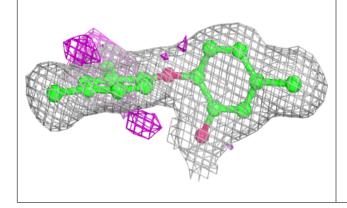


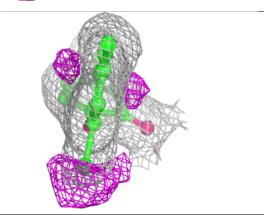


#### Electron density around TCL E 1258:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

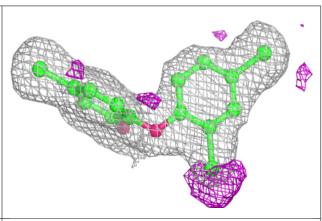


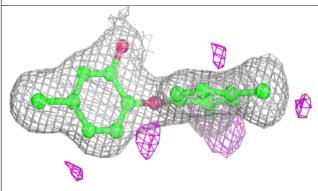


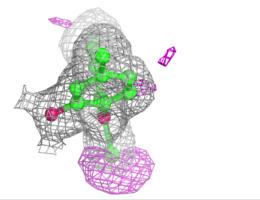


#### Electron density around TCL G 1258:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



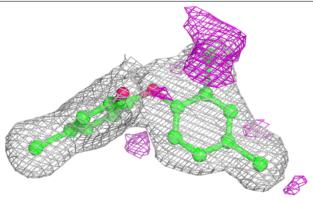


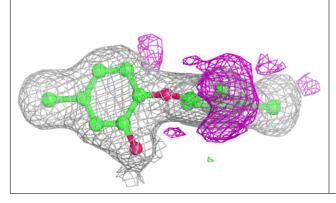


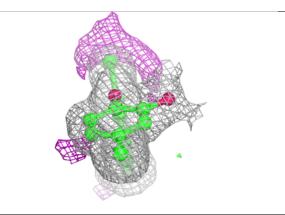


### Electron density around TCL B 1257:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

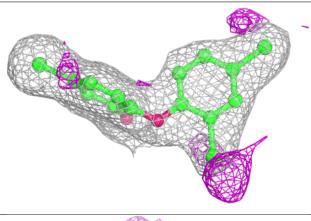


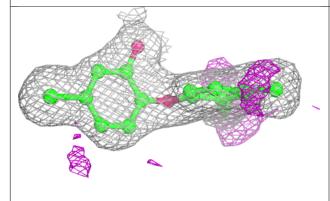


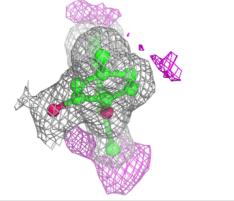


#### Electron density around TCL C 1258:

 $2 \text{mF}_o\text{-DF}_c$  (at 0.7 rmsd) in gray  $\text{mF}_o\text{-DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



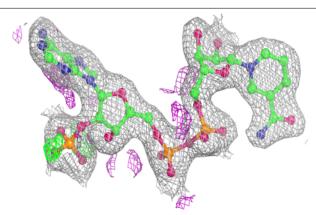


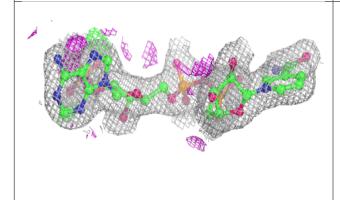


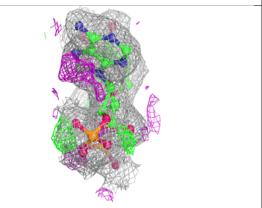


#### Electron density around NAP H 1257:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

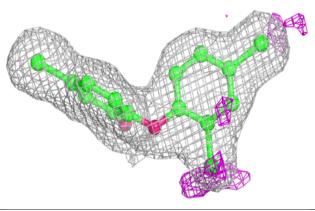


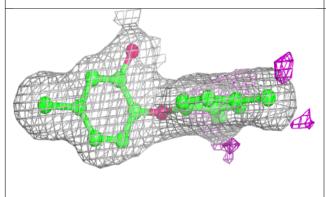


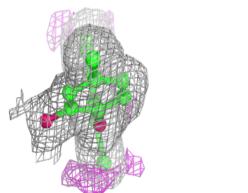


#### Electron density around TCL F 1258:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



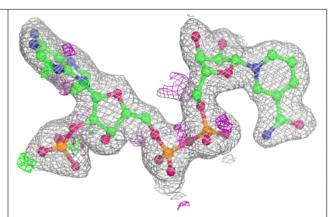


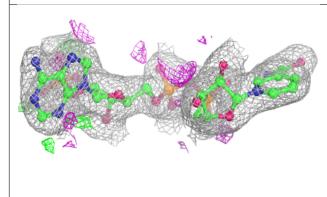


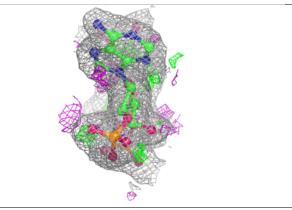


#### Electron density around NAP D 1257:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

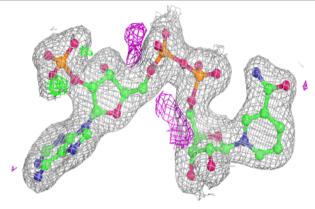


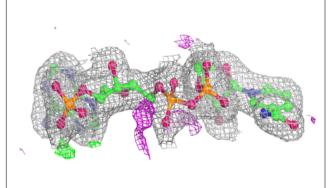


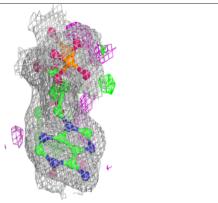


#### Electron density around NAP G 1257:

 $2 \text{mF}_o\text{-DF}_c$  (at 0.7 rmsd) in gray  $\text{mF}_o\text{-DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



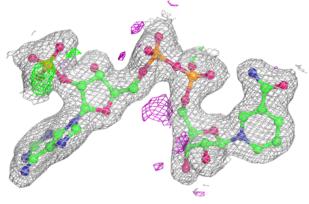


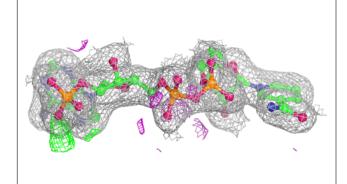


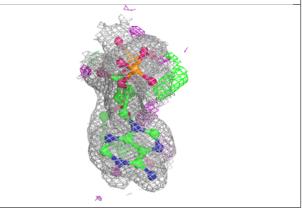


#### Electron density around NAP C 1257:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

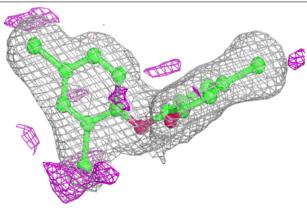


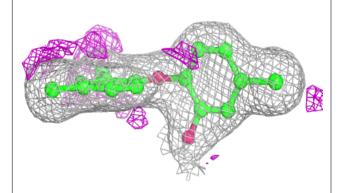


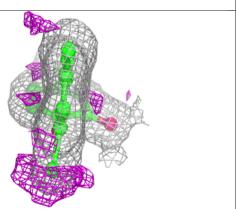


#### Electron density around TCL A 1258:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

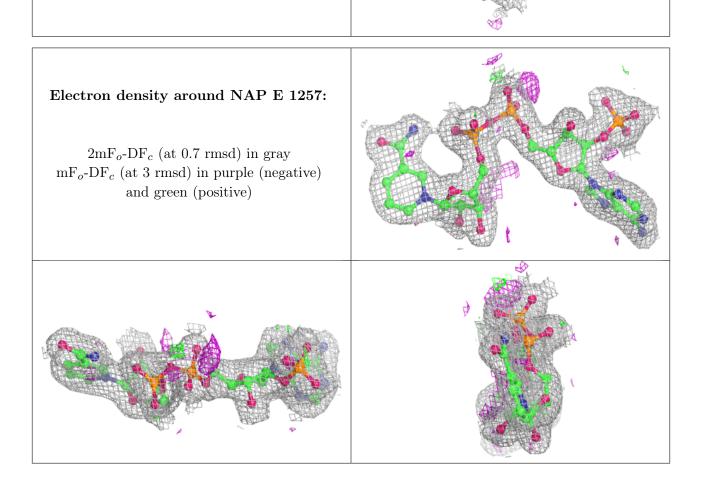








# Electron density around NAP B 1258: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

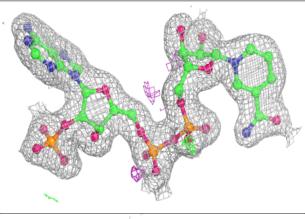


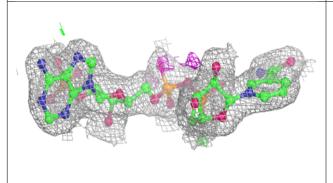


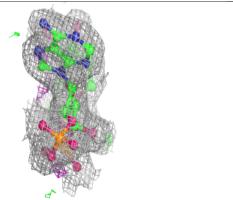
## 

#### Electron density around NAP A 1257:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)









#### 6.5 Other polymers (i)

There are no such residues in this entry.

