Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:06 am GMT

PDB ID	:	4BNK
Title	:	Crystal structure of S. aureus FabI in complex with NADP and 5-fluoro- 2-phenoxyphenol
Authors	:	Schiebel, J.; Chang, A.; Bommineni, G.R.; Tonge, P.J.; Kisker, C.
Deposited on	:	2013-05-15
Resolution	:	2.50 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 (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 (i)) were used in the production of this report:

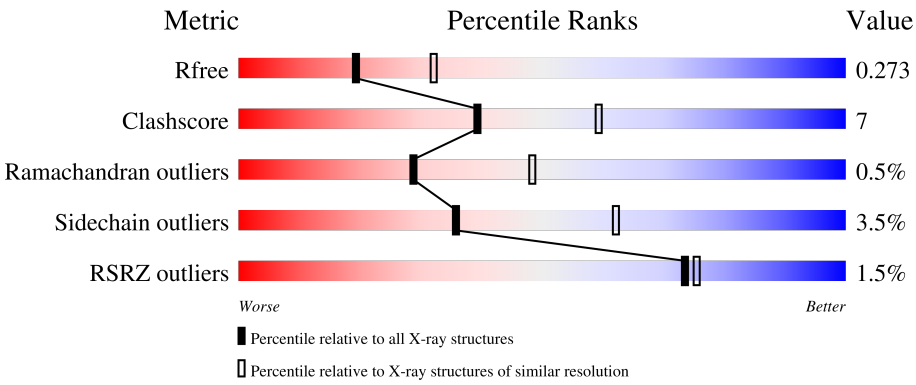
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	% 78% 11% • 10%
1	B	282	% 74% 15% • 10%
1	C	282	% 70% 20% • 10%
1	D	282	% 74% 15% • 10%
1	E	282	% 79% 10% 10%

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Mol	Chain	Length	Quality of chain
1	F	282	%, 74%, 15%, 10%
1	G	282	%, 69%, 19%, 10%
1	H	282	4%, 76%, 13%, 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	C	1259	-	-	X	-
4	GLU	D	1259	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17055 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	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	1967	1240	338	385	4	0	2	0
1	B	255	1968	1241	339	384	4	0	1	0
1	C	255	1970	1242	342	382	4	0	1	0
1	D	254	1955	1232	338	381	4	0	0	0
1	E	254	1967	1240	338	385	4	0	2	0
1	F	255	1962	1237	339	382	4	0	0	0
1	G	255	1968	1241	339	384	4	0	1	0
1	H	254	1955	1232	338	381	4	0	0	0

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

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

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

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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
E	-25	MET	-	expression tag	UNP Q7A6D8
E	-24	LYS	-	expression tag	UNP Q7A6D8
E	-23	HIS	-	expression tag	UNP Q7A6D8
E	-22	HIS	-	expression tag	UNP Q7A6D8
E	-21	HIS	-	expression tag	UNP Q7A6D8
E	-20	HIS	-	expression tag	UNP Q7A6D8
E	-19	HIS	-	expression tag	UNP Q7A6D8
E	-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
E	-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
E	-8	THR	-	expression tag	UNP Q7A6D8
E	-7	GLU	-	expression tag	UNP Q7A6D8
E	-6	ASN	-	expression tag	UNP Q7A6D8
E	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
E	-3	PHE	-	expression tag	UNP Q7A6D8
E	-2	GLN	-	expression tag	UNP Q7A6D8
E	-1	GLY	-	expression tag	UNP Q7A6D8
E	0	ALA	-	expression tag	UNP Q7A6D8
E	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

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Chain	Residue	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

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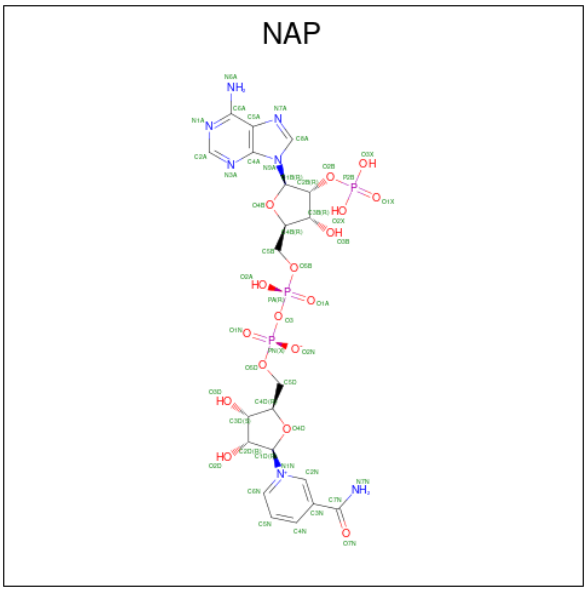
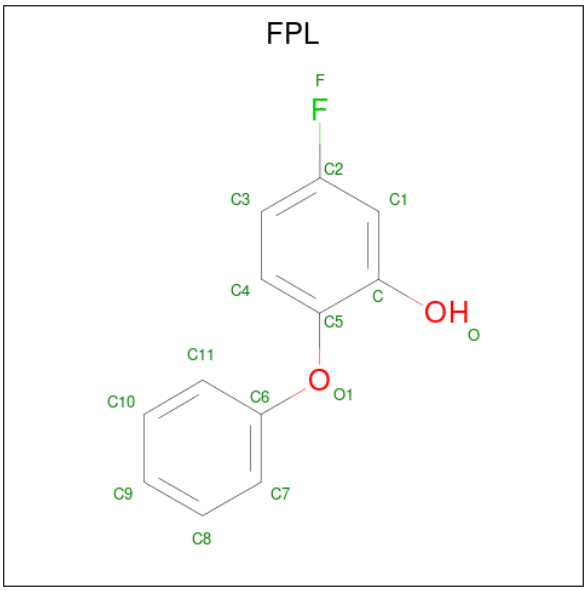
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8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

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



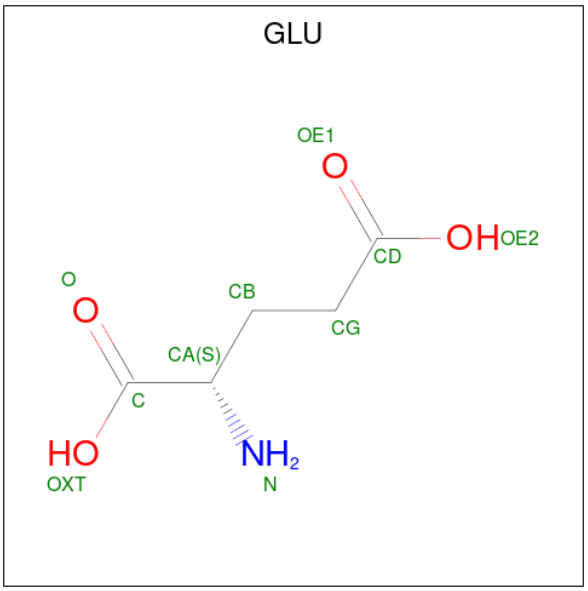
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0
2	C	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0
2	E	1	48	21	7	17	3	0	0
2	F	1	48	21	7	17	3	0	0
2	G	1	48	21	7	17	3	0	0
2	H	1	48	21	7	17	3	0	0

- Molecule 3 is 5-fluoro-2-phenoxyphenol (three-letter code: FPL) (formula: $C_{12}H_9FO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
3	A	1	15	12	1	2	0	0
			Total	C	F	O		
3	B	1	15	12	1	2	0	0
			Total	C	F	O		
3	C	1	15	12	1	2	0	0
			Total	C	F	O		
3	D	1	15	12	1	2	0	0
			Total	C	F	O		
3	E	1	15	12	1	2	0	0
			Total	C	F	O		
3	F	1	15	12	1	2	0	0
			Total	C	F	O		
3	G	1	15	12	1	2	0	0
			Total	C	F	O		
3	H	1	15	12	1	2	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	5	1	4	0	0
			Total	C	N	O		
4	C	1	10	5	1	4	0	0
			Total	C	N	O		
4	D	1	10	5	1	4	0	0
			Total	C	N	O		
4	E	1	10	5	1	4	0	0
			Total	C	N	O		
4	G	1	10	5	1	4	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	E	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	82	82	82	0	0
			Total	O		
6	B	116	116	116	0	0
			Total	O		
6	C	109	109	109	0	0

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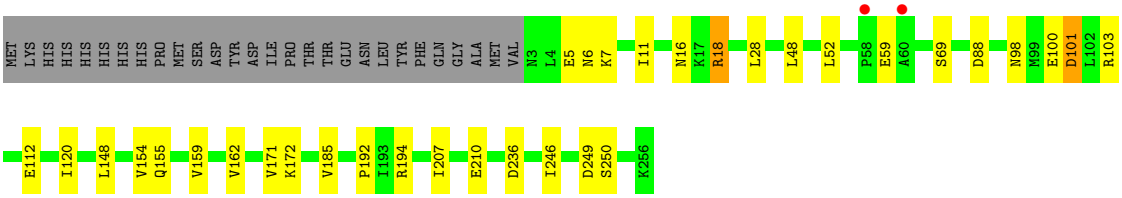
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	60	60	60	0	0
			Total	O		
6	E	89	89	89	0	0
			Total	O		
6	F	104	104	104	0	0
			Total	O		
6	G	105	105	105	0	0
			Total	O		
6	H	123	123	123	0	0

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.

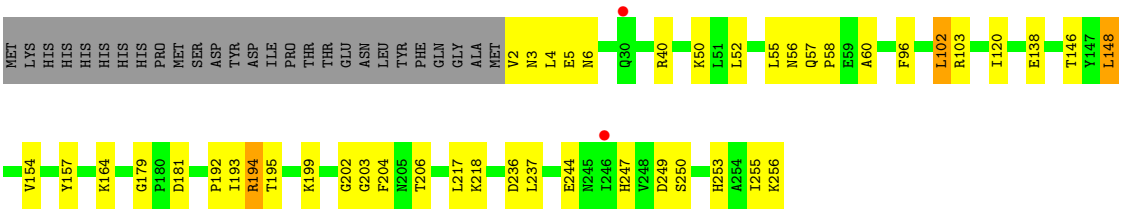
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain A:



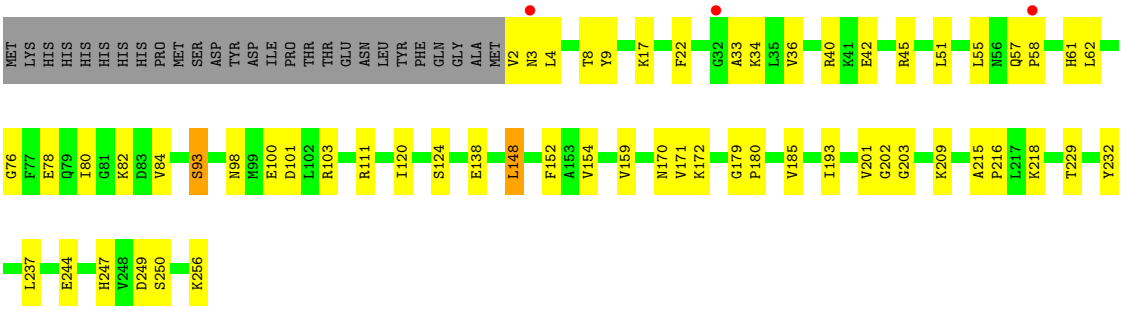
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain B:



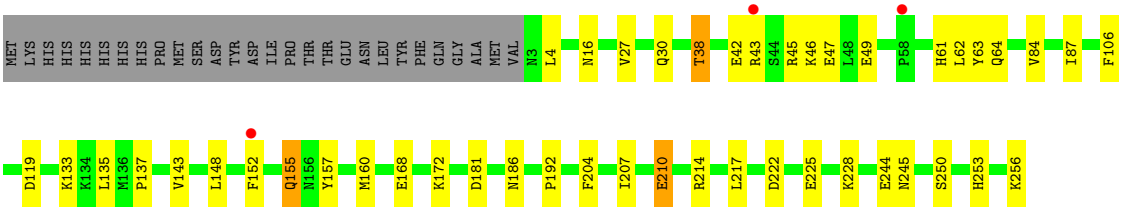
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain C:



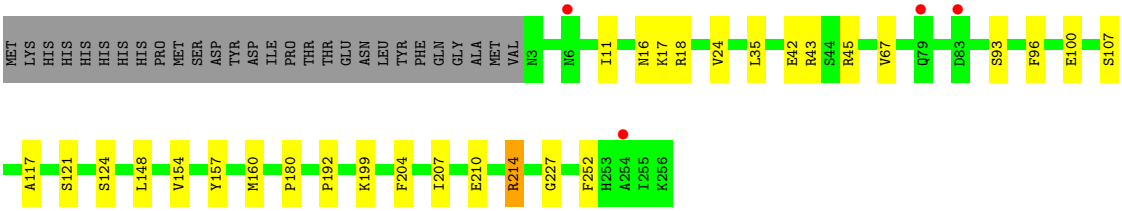
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain D:



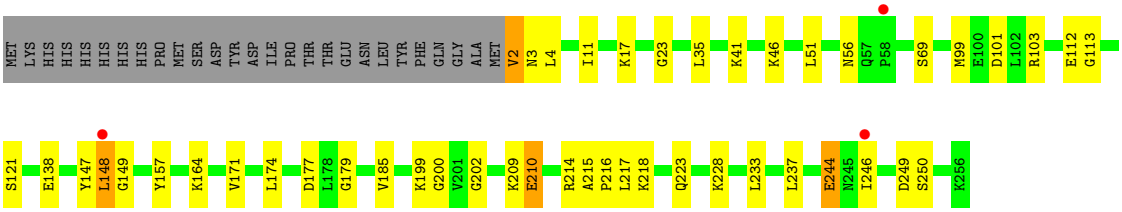
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain E:



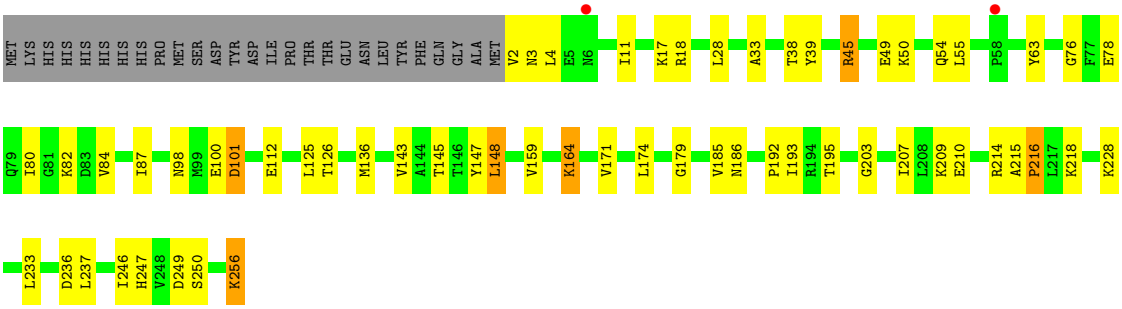
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F:



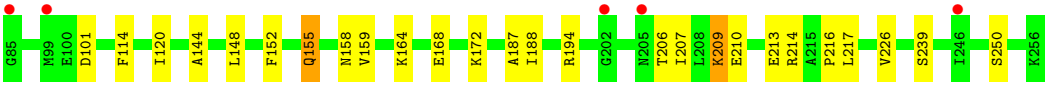
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G:



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

Chain H:


G85
M99
E100
D101
F114
I120
A144
L148
F152
Q155
N158
V159
K164
E168
K172
A187
I188
R194
G202
N205
T206
I207
L208
K209
E210
E213
R214
A215
P216
L217
V226
S239
I246
S250
K256

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.61Å 95.01Å 94.95Å 98.12° 97.00° 112.79°	Depositor
Resolution (Å)	46.11 – 2.50 46.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (46.11-2.50) 96.6 (46.11-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.250 0.206 , 0.273	Depositor DCC
R_{free} test set	4746 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17055	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7037e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FPL, 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	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.85	1/2000 (0.1%)	0.83	3/2695 (0.1%)
1	B	0.90	0/1998	0.90	2/2693 (0.1%)
1	C	0.91	1/2000 (0.1%)	0.88	3/2695 (0.1%)
1	D	0.77	0/1982	0.77	0/2671
1	E	0.86	0/2000	0.81	0/2695
1	F	0.90	1/1989 (0.1%)	0.88	0/2681
1	G	0.89	0/1998	0.88	1/2693 (0.0%)
1	H	0.73	0/1982	0.77	0/2671
All	All	0.85	3/15949 (0.0%)	0.84	9/21494 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	CB-CG1	-6.65	1.38	1.52
1	C	42	GLU	CG-CD	5.26	1.59	1.51
1	F	244	GLU	CG-CD	5.03	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	40	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	102	LEU	CA-CB-CG	6.45	130.14	115.30
1	C	40	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	G	237	LEU	CB-CG-CD1	-6.16	100.52	111.00
1	A	18	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	103	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	40	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	237	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	A	101	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1967	0	1980	19	0
1	B	1968	0	1983	41	0
1	C	1970	0	1990	43	0
1	D	1955	0	1968	33	0
1	E	1967	0	1980	26	0
1	F	1962	0	1977	32	0
1	G	1968	0	1983	43	0
1	H	1955	0	1968	25	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	2	0
2	H	48	0	25	3	0
3	A	15	0	8	0	0
3	B	15	0	9	0	0
3	C	15	0	8	0	0
3	D	15	0	8	0	0
3	E	15	0	8	1	0
3	F	15	0	9	0	0
3	G	15	0	8	1	0
3	H	15	0	8	0	0
4	A	10	0	5	1	0
4	C	10	0	5	4	0
4	D	10	0	5	4	0
4	E	10	0	5	1	0
4	G	10	0	5	2	0
5	E	1	0	0	0	0
6	A	82	0	0	4	0
6	B	116	0	0	7	0
6	C	109	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	60	0	0	7	0
6	E	89	0	0	3	0
6	F	104	0	0	4	0
6	G	105	0	0	5	0
6	H	123	0	0	4	0
All	All	17055	0	16120	239	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 7.

All (239) 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:C:103:ARG:HH12	4:C:1259:GLU:HA	1.21	1.03
1:B:103:ARG:HH21	1:B:202:GLY:CA	1.80	0.94
1:G:203:GLY:H	4:G:1259:GLU:HB2	1.30	0.94
1:A:155:GLN:OE1	6:A:2046:HOH:O	1.89	0.89
1:D:253:HIS:HD2	6:D:2059:HOH:O	1.53	0.89
1:H:194:ARG:HD2	6:H:2010:HOH:O	1.74	0.88
1:B:103:ARG:HH21	1:B:202:GLY:HA3	1.40	0.87
1:G:215:ALA:O	1:G:218:LYS:HD3	1.80	0.82
1:B:253:HIS:HD2	6:B:2114:HOH:O	1.61	0.81
1:E:148:LEU:HD21	1:G:256:LYS:HD2	1.63	0.79
1:C:203:GLY:H	4:C:1259:GLU:HB3	1.48	0.78
1:E:199:LYS:HE2	4:E:1260:GLU:O	1.83	0.78
1:F:171:VAL:HG13	1:F:185:VAL:HG12	1.65	0.78
1:B:203:GLY:H	4:D:1259:GLU:HB3	1.51	0.76
1:D:214:ARG:NH2	1:D:256:LYS:OXT	2.19	0.76
1:G:249:ASP:O	1:G:250:SER:HB2	1.86	0.73
1:H:155:GLN:OE1	6:H:2033:HOH:O	2.06	0.73
1:B:103:ARG:HH21	1:B:202:GLY:HA2	1.54	0.72
1:F:11:ILE:CD1	1:F:35:LEU:HD22	2.23	0.69
1:D:46:LYS:HA	1:D:49:GLU:HG2	1.76	0.68
1:F:11:ILE:HD11	1:F:35:LEU:HD22	1.76	0.66
1:C:4:LEU:HD13	1:C:9:TYR:HE2	1.61	0.66
1:C:103:ARG:NH1	4:C:1259:GLU:HA	2.03	0.66
1:D:210:GLU:OE2	1:D:214:ARG:NH1	2.28	0.66
1:G:233:LEU:HD21	1:G:246:ILE:HD12	1.79	0.65
1:B:194:ARG:HB2	6:B:2091:HOH:O	1.97	0.65
1:D:214:ARG:HD2	6:D:2054:HOH:O	1.97	0.64
1:C:101:ASP:O	1:C:159:VAL:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:HE2	1:D:148:LEU:HD21	1.81	0.63
1:H:172:LYS:NZ	6:H:2037:HOH:O	2.31	0.63
1:F:2:VAL:HA	1:G:2:VAL:HG12	1.80	0.62
1:D:244:GLU:HG3	1:D:245:ASN:N	2.14	0.62
1:G:171:VAL:HG13	1:G:185:VAL:HG12	1.81	0.62
1:E:210[A]:GLU:HG3	1:E:214:ARG:HD3	1.82	0.62
1:A:16:ASN:HD21	1:A:18:ARG:HH11	1.49	0.61
1:F:215:ALA:O	1:F:218:LYS:HD3	2.02	0.59
1:C:218:LYS:HE3	6:C:2052:HOH:O	2.03	0.59
1:G:50:LYS:HB2	6:G:2038:HOH:O	2.03	0.59
1:G:203:GLY:N	4:G:1259:GLU:HB2	2.11	0.59
1:C:215:ALA:O	1:C:218:LYS:HD3	2.02	0.58
1:C:17:LYS:NZ	6:C:2023:HOH:O	2.35	0.58
1:E:18:ARG:HH12	1:E:199:LYS:NZ	2.01	0.58
1:E:204:PHE:HA	1:E:207:ILE:HD12	1.86	0.58
1:B:255:ILE:O	1:D:256:LYS:HE2	2.04	0.57
1:A:148:LEU:HD21	1:C:256:LYS:HE3	1.86	0.57
1:E:11:ILE:CD1	1:E:35:LEU:HD22	2.34	0.57
1:D:42:GLU:O	1:D:45:ARG:N	2.38	0.57
1:H:5:GLU:O	1:H:6:ASN:HB2	2.04	0.57
1:A:120:ILE:HD13	2:A:1257:NAP:H61A	1.68	0.57
1:D:155:GLN:HA	6:D:2037:HOH:O	2.04	0.57
1:D:244:GLU:HG3	1:D:245:ASN:H	1.69	0.57
6:A:2079:HOH:O	1:C:152:PHE:CD1	2.52	0.57
1:B:2:VAL:O	6:B:2003:HOH:O	2.17	0.56
1:F:103:ARG:HH12	1:F:202:GLY:HA2	1.70	0.56
1:A:5:GLU:O	1:A:6:ASN:HB2	2.04	0.56
1:C:76:GLY:O	1:C:80:ILE:HG13	2.04	0.56
1:F:23:GLY:HA3	1:F:223:GLN:HB3	1.88	0.56
1:F:237:LEU:HD23	1:G:228:LYS:HB3	1.87	0.56
1:D:217:LEU:HB2	1:D:250:SER:HB3	1.88	0.56
1:A:101:ASP:O	1:A:159:VAL:HG12	2.05	0.56
1:B:2:VAL:HG23	1:C:2:VAL:N	2.21	0.55
1:B:203:GLY:N	4:D:1259:GLU:HB3	2.21	0.55
1:D:16:ASN:HA	1:D:47:GLU:HG2	1.89	0.55
1:G:50:LYS:HE3	6:G:2035:HOH:O	2.06	0.55
1:F:249:ASP:O	1:F:250:SER:HB2	2.06	0.55
1:B:103:ARG:NH2	1:B:202:GLY:HA2	2.22	0.54
1:B:179:GLY:HA3	1:C:216:PRO:O	2.07	0.54
1:D:222:ASP:OD1	1:D:225:GLU:HG3	2.08	0.54
1:F:179:GLY:HA3	1:G:216:PRO:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LYS:NZ	6:D:2042:HOH:O	2.41	0.54
1:F:233:LEU:HD21	1:F:246:ILE:HD12	1.90	0.53
1:G:101:ASP:O	1:G:159:VAL:HG12	2.08	0.53
1:B:199:LYS:NZ	6:B:2024:HOH:O	2.41	0.53
1:C:171:VAL:HG13	1:C:185:VAL:HG12	1.90	0.53
1:H:60:ALA:HB1	1:H:62:LEU:HD11	1.90	0.53
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH1	2.41	0.53
1:D:133:LYS:HD3	6:D:2033:HOH:O	2.09	0.52
1:B:244:GLU:OE2	1:C:247:HIS:ND1	2.29	0.52
1:H:209:LYS:O	1:H:213:GLU:HG3	2.10	0.52
1:B:103:ARG:NH2	1:B:202:GLY:HA3	2.19	0.52
1:E:180:PRO:HG2	6:E:2067:HOH:O	2.08	0.52
1:C:103:ARG:HH12	4:C:1259:GLU:CA	2.08	0.52
1:B:193:ILE:O	1:B:195:THR:HG23	2.09	0.52
1:B:206:THR:HG23	4:D:1259:GLU:OE2	2.09	0.52
1:C:4:LEU:HD13	1:C:9:TYR:CE2	2.43	0.51
1:C:120:ILE:O	1:C:124:SER:OG	2.24	0.51
1:B:249:ASP:O	1:B:250:SER:HB2	2.11	0.51
1:E:210[A]:GLU:HG3	1:E:214:ARG:CD	2.41	0.51
4:A:1259:GLU:O	1:F:103:ARG:NH1	2.44	0.51
1:B:148:LEU:CD2	1:D:256:LYS:HG2	2.41	0.51
1:E:192:PRO:HG3	1:E:207:ILE:HG22	1.92	0.50
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.76	0.50
1:B:52:LEU:HD13	1:B:60:ALA:HB2	1.93	0.50
1:A:192:PRO:HG3	1:A:207:ILE:HG22	1.94	0.50
1:G:98:ASN:HB3	1:G:100:GLU:HG2	1.93	0.50
1:C:4:LEU:HB3	1:C:33:ALA:HB2	1.94	0.50
1:B:5:GLU:O	1:B:6:ASN:HB2	2.12	0.49
1:G:147:TYR:HB2	2:G:1257:NAP:C5N	2.42	0.49
1:G:210:GLU:OE2	1:G:214:ARG:HD3	2.12	0.49
1:H:40:ARG:HB2	2:H:1257:NAP:C2A	2.43	0.49
1:G:2:VAL:HG13	1:G:2:VAL:O	2.12	0.49
1:G:78:GLU:O	1:G:82:LYS:HG3	2.11	0.49
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.94	0.49
1:D:192:PRO:HG3	1:D:207:ILE:HG22	1.93	0.49
1:F:103:ARG:NH1	1:F:202:GLY:HA2	2.27	0.49
1:A:7:LYS:HA	1:A:88:ASP:OD2	2.13	0.49
1:A:154:VAL:HG13	6:A:2044:HOH:O	2.12	0.49
1:F:103:ARG:HA	6:F:2064:HOH:O	2.12	0.49
1:G:11:ILE:HD11	1:G:28:LEU:HD12	1.95	0.49
1:F:147:TYR:O	1:F:149:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:HA	1:D:207:ILE:HG13	1.94	0.48
1:E:11:ILE:HD11	1:E:35:LEU:HD22	1.94	0.48
1:C:229:THR:O	1:C:232:TYR:HB3	2.13	0.48
1:B:253:HIS:CD2	6:B:2114:HOH:O	2.48	0.48
1:G:45:ARG:NH1	1:G:49:GLU:OE2	2.47	0.48
1:B:56:ASN:HD22	1:B:56:ASN:N	2.11	0.47
1:D:61:HIS:C	1:D:62:LEU:HD12	2.35	0.47
1:A:48:LEU:O	1:A:52:LEU:HD23	2.14	0.47
1:B:96:PHE:HB3	1:B:120:ILE:HD12	1.95	0.47
1:B:181:ASP:HA	6:B:2087:HOH:O	2.15	0.47
1:C:3:ASN:O	1:C:4:LEU:HD23	2.15	0.47
1:C:201:VAL:O	1:C:202:GLY:C	2.51	0.47
1:E:107:SER:HB3	1:F:177:ASP:OD2	2.14	0.47
1:F:216:PRO:O	1:G:179:GLY:HA3	2.14	0.47
1:E:157:TYR:CZ	1:E:160:MET:HG3	2.50	0.47
1:H:213:GLU:HB2	1:H:214:ARG:HG3	1.96	0.47
1:G:80:ILE:O	1:G:84:VAL:HG22	2.15	0.46
1:G:101:ASP:HB3	1:G:159:VAL:CG1	2.46	0.46
1:C:172:LYS:HE2	6:C:2107:HOH:O	2.15	0.46
1:E:11:ILE:HD12	1:E:35:LEU:HD22	1.96	0.46
1:G:3:ASN:HB2	6:G:2001:HOH:O	2.15	0.46
1:C:98:ASN:HB3	1:C:100:GLU:HG2	1.98	0.46
6:E:2083:HOH:O	1:H:239:SER:HB2	2.15	0.46
1:G:76:GLY:O	1:G:80:ILE:HG13	2.16	0.46
1:C:249:ASP:O	1:C:250:SER:HB2	2.16	0.46
1:H:209:LYS:HE2	1:H:209:LYS:HB3	1.58	0.46
1:F:11:ILE:HD12	1:F:35:LEU:HD22	1.96	0.46
1:D:46:LYS:HA	1:D:49:GLU:CG	2.44	0.45
1:D:133:LYS:HE2	1:D:181:ASP:OD2	2.16	0.45
1:F:2:VAL:HB	1:F:3:ASN:H	1.58	0.45
1:A:249:ASP:O	1:A:250:SER:HB2	2.16	0.45
1:B:2:VAL:HG12	1:B:3:ASN:H	1.81	0.45
1:F:244:GLU:OE2	1:G:247:HIS:ND1	2.32	0.45
1:E:24:VAL:HA	1:E:227:GLY:HA2	1.97	0.45
1:G:143:VAL:HA	1:G:186:ASN:O	2.17	0.45
1:F:17:LYS:HB3	1:F:51:LEU:HD21	1.98	0.45
1:B:247:HIS:ND1	1:C:244:GLU:OE2	2.38	0.45
1:D:143:VAL:HA	1:D:186:ASN:O	2.17	0.45
1:H:40:ARG:HD3	2:H:1257:NAP:C6A	2.47	0.45
1:A:172:LYS:HE3	6:A:2051:HOH:O	2.16	0.45
1:E:107:SER:CB	1:F:177:ASP:OD2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:LEU:HG	1:G:174:LEU:HD11	1.98	0.45
1:C:111:ARG:HD3	1:D:119:ASP:OD1	2.17	0.44
1:G:193:ILE:O	1:G:195:THR:HG23	2.18	0.44
1:H:120:ILE:HD13	2:H:1257:NAP:H61A	1.80	0.44
1:B:103:ARG:NH2	1:B:202:GLY:CA	2.63	0.44
1:G:39:TYR:CZ	1:G:45:ARG:HB2	2.53	0.44
1:H:15:ALA:O	1:H:47:GLU:HG2	2.17	0.44
1:D:38:THR:HA	1:D:63:TYR:O	2.17	0.44
1:H:155:GLN:HA	6:H:2033:HOH:O	2.18	0.44
1:E:100:GLU:CD	1:E:100:GLU:H	2.21	0.44
1:G:148:LEU:HD12	1:G:148:LEU:HA	1.87	0.43
1:A:112:GLU:HB3	1:E:42[A]:GLU:OE1	2.18	0.43
1:C:209:LYS:HB2	1:C:209:LYS:HE3	1.88	0.43
1:F:147:TYR:O	1:F:148:LEU:C	2.56	0.43
1:B:103:ARG:CZ	4:D:1259:GLU:OXT	2.66	0.43
6:F:2001:HOH:O	1:G:2:VAL:C	2.57	0.43
1:G:101:ASP:HB3	1:G:159:VAL:HG11	2.01	0.43
1:E:117:ALA:O	1:E:121:SER:HB2	2.19	0.43
1:H:101:ASP:HB3	1:H:159:VAL:HG11	1.99	0.43
1:H:148:LEU:HD11	1:H:152:PHE:HE2	1.82	0.43
1:H:217:LEU:HB2	1:H:250:SER:HB3	2.01	0.43
1:C:170:ASN:OD1	1:D:106:PHE:HE2	2.01	0.43
1:E:16:ASN:HD21	1:E:18:ARG:HH21	1.66	0.43
1:G:126:THR:HA	1:G:174:LEU:HD21	2.00	0.43
1:A:171:VAL:HG13	1:A:185:VAL:HG12	1.99	0.43
1:D:135:LEU:C	1:D:137:PRO:HD3	2.39	0.43
1:D:27:VAL:HG11	1:D:228:LYS:HA	2.01	0.43
1:E:210[A]:GLU:CG	1:E:214:ARG:HD3	2.48	0.43
1:E:252:PHE:O	1:G:256:LYS:NZ	2.50	0.43
1:H:8:THR:HA	1:H:34:LYS:O	2.19	0.43
1:B:5:GLU:O	1:B:6:ASN:CB	2.67	0.42
1:B:192:PRO:HA	2:B:1257:NAP:O7N	2.19	0.42
1:F:210:GLU:CD	1:F:214:ARG:HH21	2.22	0.42
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.19	0.42
1:F:174:LEU:HD23	1:F:174:LEU:HA	1.88	0.42
1:A:98:ASN:HB3	1:A:100:GLU:HG2	2.01	0.42
1:D:157:TYR:CZ	1:D:160:MET:HG3	2.55	0.42
1:C:57:GLN:HA	1:C:58:PRO:HD2	1.85	0.42
1:F:147:TYR:HD2	1:F:157:TYR:CE2	2.37	0.42
1:G:192:PRO:HG3	1:G:207:ILE:HG22	2.00	0.42
1:A:101:ASP:HB2	1:A:159:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLN:HG3	6:D:2037:HOH:O	2.20	0.42
1:B:193:ILE:H	1:B:204:PHE:HZ	1.67	0.42
1:B:217:LEU:O	1:B:218:LYS:C	2.57	0.42
1:H:8:THR:HG21	1:H:84:VAL:HG11	2.00	0.42
1:A:100:GLU:HB2	1:E:43:ARG:HG2	2.01	0.42
1:C:193:ILE:HA	6:C:2095:HOH:O	2.20	0.42
1:E:96:PHE:HA	3:E:1259:FPL:H8	2.01	0.42
1:G:17:LYS:HD3	6:G:2040:HOH:O	2.19	0.42
1:B:146:THR:O	2:B:1257:NAP:H6N	2.20	0.42
1:C:45:ARG:HG3	1:C:62:LEU:HD13	2.02	0.41
1:B:2:VAL:N	1:C:2:VAL:N	2.68	0.41
6:B:2001:HOH:O	1:C:2:VAL:C	2.58	0.41
1:G:4:LEU:O	1:G:33:ALA:HA	2.21	0.41
1:B:154:VAL:HG23	1:B:157:TYR:HB2	2.02	0.41
1:H:114:PHE:HA	1:H:159:VAL:HG21	2.02	0.41
1:B:57:GLN:HA	1:B:58:PRO:HD2	1.70	0.41
1:G:145:THR:O	1:G:164:LYS:NZ	2.53	0.41
2:G:1257:NAP:C7N	3:G:1258:FPL:C3	2.98	0.41
1:H:144:ALA:O	1:H:187:ALA:HA	2.20	0.41
1:B:52:LEU:HD13	1:B:60:ALA:CB	2.49	0.41
1:G:218:LYS:CE	6:G:2093:HOH:O	2.68	0.41
1:C:179:GLY:N	1:C:180:PRO:CD	2.84	0.41
1:F:199:LYS:NZ	6:F:2026:HOH:O	2.11	0.41
1:F:228:LYS:HB2	1:F:228:LYS:HE3	1.84	0.41
1:G:3:ASN:O	1:G:4:LEU:HD23	2.21	0.41
1:H:188:ILE:HG21	1:H:226:VAL:HG13	2.03	0.41
1:C:8:THR:HA	1:C:34:LYS:O	2.20	0.41
1:C:36:VAL:HA	1:C:61:HIS:HB2	2.02	0.41
1:D:168:GLU:OE1	6:D:2041:HOH:O	2.21	0.41
1:H:164:LYS:O	1:H:168:GLU:HG3	2.21	0.41
1:B:256:LYS:HG2	1:D:152:PHE:CG	2.56	0.40
1:C:22:PHE:CZ	1:C:51:LEU:HD22	2.56	0.40
1:C:78:GLU:O	1:C:82:LYS:HG3	2.20	0.40
1:E:154:VAL:HG13	6:E:2056:HOH:O	2.21	0.40
1:H:66:ASP:C	1:H:66:ASP:OD1	2.60	0.40
1:A:11:ILE:HD11	1:A:28:LEU:HD12	2.02	0.40
1:C:216:PRO:HD2	1:C:250:SER:O	2.21	0.40
1:F:217:LEU:O	1:F:218:LYS:C	2.60	0.40
1:F:218:LYS:HB3	6:F:2092:HOH:O	2.21	0.40
1:H:210:GLU:HA	1:H:213:GLU:HG3	2.03	0.40
1:C:93:SER:O	2:C:1257:NAP:H52N	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASP:HB3	1:C:159:VAL:HG11	2.02	0.40
1:G:38:THR:HA	1:G:63:TYR:O	2.20	0.40
1:G:87:ILE:O	1:G:136:MET:HG2	2.22	0.40
1:C:80:ILE:O	1:C:84:VAL:HG22	2.21	0.40
1:E:67:VAL:HG21	1:E:124:SER:CB	2.51	0.40
1:F:99:MET:SD	1:F:200:GLY:HA2	2.61	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	254/282 (90%)	241 (95%)	13 (5%)	0	100	100
1	B	254/282 (90%)	229 (90%)	23 (9%)	2 (1%)	19	35
1	C	254/282 (90%)	236 (93%)	17 (7%)	1 (0%)	34	54
1	D	252/282 (89%)	234 (93%)	17 (7%)	1 (0%)	34	54
1	E	254/282 (90%)	236 (93%)	18 (7%)	0	100	100
1	F	253/282 (90%)	233 (92%)	19 (8%)	1 (0%)	34	54
1	G	254/282 (90%)	242 (95%)	10 (4%)	2 (1%)	19	35
1	H	252/282 (89%)	236 (94%)	13 (5%)	3 (1%)	13	24
All	All	2027/2256 (90%)	1887 (93%)	130 (6%)	10 (0%)	29	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	148	LEU
1	B	148	LEU
1	B	194	ARG
1	C	148	LEU

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Mol	Chain	Res	Type
1	D	43	ARG
1	H	158	ASN
1	G	101	ASP
1	H	155	GLN
1	G	148	LEU
1	H	207	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/234 (90%)	204 (97%)	6 (3%)	42	69
1	B	210/234 (90%)	202 (96%)	8 (4%)	33	58
1	C	210/234 (90%)	205 (98%)	5 (2%)	49	74
1	D	208/234 (89%)	200 (96%)	8 (4%)	33	58
1	E	210/234 (90%)	207 (99%)	3 (1%)	67	86
1	F	209/234 (89%)	197 (94%)	12 (6%)	20	39
1	G	210/234 (90%)	200 (95%)	10 (5%)	25	48
1	H	208/234 (89%)	202 (97%)	6 (3%)	42	69
All	All	1675/1872 (90%)	1617 (96%)	58 (4%)	36	62

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	69	SER
1	A	210[A]	GLU
1	A	210[B]	GLU
1	A	236	ASP
1	A	246	ILE
1	B	4	LEU
1	B	50	LYS
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	138	GLU
1	B	164	LYS
1	B	236	ASP
1	B	237	LEU
1	C	55	LEU
1	C	93	SER
1	C	138	GLU
1	C	148	LEU
1	C	154	VAL
1	D	4	LEU
1	D	30	GLN
1	D	38	THR
1	D	64	GLN
1	D	84	VAL
1	D	87	ILE
1	D	155	GLN
1	D	210	GLU
1	E	17	LYS
1	E	93	SER
1	E	214	ARG
1	F	2	VAL
1	F	4	LEU
1	F	41	LYS
1	F	46	LYS
1	F	56	ASN
1	F	69	SER
1	F	112	GLU
1	F	121	SER
1	F	138	GLU
1	F	164	LYS
1	F	209	LYS
1	F	210	GLU
1	G	18	ARG
1	G	45	ARG
1	G	54	GLN
1	G	55	LEU
1	G	112	GLU
1	G	164	LYS
1	G	209	LYS
1	G	216	PRO
1	G	236	ASP

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Mol	Chain	Res	Type
1	G	256	LYS
1	H	45	ARG
1	H	50	LYS
1	H	84	VAL
1	H	206	THR
1	H	209	LYS
1	H	216	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	56	ASN
1	B	253	HIS
1	C	6	ASN
1	C	79	GLN
1	C	253	HIS
1	D	6	ASN
1	D	253	HIS
1	E	3	ASN
1	E	75	ASN
1	F	3	ASN
1	G	155	GLN
1	H	30	GLN
1	H	155	GLN

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)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FPL	E	1259	-	16,16,16	0.31	0	21,21,21	0.67	1 (4%)
4	GLU	G	1259	-	8,9,9	1.61	1 (12%)	10,11,11	1.06	0
2	NAP	E	1258	-	45,52,52	1.55	3 (6%)	56,80,80	1.76	11 (19%)
2	NAP	H	1257	-	45,52,52	1.76	4 (8%)	56,80,80	1.30	9 (16%)
3	FPL	G	1258	-	16,16,16	0.32	0	21,21,21	0.58	0
3	FPL	A	1258	-	16,16,16	0.40	0	21,21,21	0.55	0
2	NAP	D	1257	-	45,52,52	1.78	3 (6%)	56,80,80	1.30	7 (12%)
4	GLU	C	1259	-	8,9,9	1.56	1 (12%)	10,11,11	1.02	0
3	FPL	H	1258	-	16,16,16	0.18	0	21,21,21	0.43	0
3	FPL	D	1258	-	16,16,16	0.37	0	21,21,21	0.60	0
2	NAP	G	1257	-	45,52,52	1.53	4 (8%)	56,80,80	1.52	8 (14%)
3	FPL	C	1258	-	16,16,16	0.44	0	21,21,21	0.63	1 (4%)
2	NAP	F	1257	-	45,52,52	1.57	4 (8%)	56,80,80	1.54	8 (14%)
3	FPL	B	1258	-	16,16,16	0.29	0	21,21,21	0.50	0
2	NAP	B	1257	-	45,52,52	1.59	5 (11%)	56,80,80	1.81	10 (17%)
3	FPL	F	1258	-	16,16,16	0.50	0	21,21,21	0.56	0
4	GLU	A	1259	-	8,9,9	1.58	1 (12%)	10,11,11	1.13	1 (10%)
4	GLU	D	1259	-	8,9,9	1.51	1 (12%)	10,11,11	1.00	0
2	NAP	A	1257	-	45,52,52	1.67	6 (13%)	56,80,80	1.68	11 (19%)
2	NAP	C	1257	-	45,52,52	1.62	4 (8%)	56,80,80	1.66	8 (14%)
4	GLU	E	1260	-	8,9,9	1.18	0	10,11,11	1.14	1 (10%)

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	FPL	E	1259	-	-	0/4/4/4	0/2/2/2
4	GLU	G	1259	-	-	6/9/9/9	-
2	NAP	E	1258	-	-	5/31/67/67	0/5/5/5
2	NAP	H	1257	-	-	6/31/67/67	0/5/5/5
3	FPL	G	1258	-	-	0/4/4/4	0/2/2/2
3	FPL	A	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	D	1257	-	-	6/31/67/67	0/5/5/5
4	GLU	C	1259	-	-	6/9/9/9	-
3	FPL	H	1258	-	-	0/4/4/4	0/2/2/2
3	FPL	D	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	G	1257	-	-	7/31/67/67	0/5/5/5
3	FPL	C	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	F	1257	-	-	6/31/67/67	0/5/5/5
3	FPL	B	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	B	1257	-	-	5/31/67/67	0/5/5/5
3	FPL	F	1258	-	-	0/4/4/4	0/2/2/2
4	GLU	A	1259	-	-	5/9/9/9	-
4	GLU	D	1259	-	-	7/9/9/9	-
2	NAP	A	1257	-	-	6/31/67/67	0/5/5/5
2	NAP	C	1257	-	-	6/31/67/67	0/5/5/5
4	GLU	E	1260	-	-	3/9/9/9	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1257	NAP	O7N-C7N	8.54	1.40	1.24
2	D	1257	NAP	O7N-C7N	8.46	1.40	1.24
2	F	1257	NAP	O7N-C7N	7.76	1.39	1.24
2	C	1257	NAP	O7N-C7N	7.14	1.37	1.24
2	G	1257	NAP	O7N-C7N	7.10	1.37	1.24
2	A	1257	NAP	O7N-C7N	6.97	1.37	1.24
2	E	1258	NAP	O7N-C7N	6.86	1.37	1.24
2	B	1257	NAP	O7N-C7N	6.67	1.36	1.24
2	D	1257	NAP	C2A-N3A	5.34	1.40	1.32
2	A	1257	NAP	C2A-N3A	5.02	1.40	1.32
2	E	1258	NAP	C2A-N3A	4.68	1.39	1.32
2	H	1257	NAP	C2A-N3A	4.67	1.39	1.32
2	C	1257	NAP	C2A-N3A	4.33	1.39	1.32
2	B	1257	NAP	C2A-N3A	3.72	1.38	1.32
2	G	1257	NAP	C2A-N3A	3.38	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1259	GLU	CG-CD	3.36	1.58	1.50
2	D	1257	NAP	C2A-N1A	3.28	1.40	1.33
2	H	1257	NAP	C2A-N1A	3.26	1.40	1.33
2	F	1257	NAP	C2A-N3A	3.25	1.37	1.32
4	G	1259	GLU	CG-CD	3.09	1.57	1.50
4	A	1259	GLU	CG-CD	3.04	1.57	1.50
2	G	1257	NAP	C2A-N1A	2.96	1.39	1.33
4	D	1259	GLU	CG-CD	2.77	1.57	1.50
2	B	1257	NAP	C2N-C3N	2.61	1.43	1.39
2	A	1257	NAP	C2A-N1A	2.60	1.38	1.33
2	C	1257	NAP	C2A-N1A	2.59	1.38	1.33
2	F	1257	NAP	P2B-O2B	2.58	1.64	1.59
2	B	1257	NAP	C2A-N1A	2.54	1.38	1.33
2	F	1257	NAP	C2A-N1A	2.48	1.38	1.33
2	E	1258	NAP	C2A-N1A	2.39	1.38	1.33
2	B	1257	NAP	O4D-C4D	-2.37	1.39	1.45
2	A	1257	NAP	P2B-O2B	2.36	1.63	1.59
2	H	1257	NAP	O4B-C4B	-2.24	1.40	1.45
2	A	1257	NAP	C2N-N1N	2.24	1.37	1.35
2	C	1257	NAP	C2N-N1N	-2.10	1.32	1.35
2	G	1257	NAP	C3N-C7N	-2.07	1.47	1.50
2	A	1257	NAP	O4B-C4B	-2.05	1.40	1.45

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1258	NAP	N3A-C2A-N1A	-6.12	119.11	128.68
2	B	1257	NAP	O7N-C7N-C3N	-6.11	112.32	119.63
2	F	1257	NAP	N3A-C2A-N1A	-5.87	119.51	128.68
2	B	1257	NAP	N3A-C2A-N1A	-5.85	119.53	128.68
2	B	1257	NAP	C3N-C7N-N7N	5.69	124.58	117.75
2	A	1257	NAP	C3N-C7N-N7N	5.66	124.54	117.75
2	C	1257	NAP	N3A-C2A-N1A	-5.36	120.29	128.68
2	E	1258	NAP	C3N-C7N-N7N	5.36	124.18	117.75
2	A	1257	NAP	N3A-C2A-N1A	-5.32	120.36	128.68
2	G	1257	NAP	N3A-C2A-N1A	-5.17	120.60	128.68
2	C	1257	NAP	O7N-C7N-C3N	-5.08	113.55	119.63
2	C	1257	NAP	C2N-C3N-C4N	4.83	123.73	118.26
2	D	1257	NAP	N3A-C2A-N1A	-4.68	121.36	128.68
2	G	1257	NAP	O7N-C7N-C3N	-4.59	114.14	119.63
2	E	1258	NAP	O7N-C7N-C3N	-4.30	114.48	119.63
2	H	1257	NAP	N3A-C2A-N1A	-4.12	122.24	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1257	NAP	C6N-N1N-C2N	-4.07	118.26	121.97
2	F	1257	NAP	C3N-C7N-N7N	3.98	122.53	117.75
2	G	1257	NAP	C3N-C7N-N7N	3.90	122.43	117.75
2	F	1257	NAP	O7N-C7N-C3N	-3.85	115.03	119.63
2	C	1257	NAP	C3N-C7N-N7N	3.66	122.14	117.75
2	H	1257	NAP	C3N-C7N-N7N	3.59	122.06	117.75
2	E	1258	NAP	C2N-C3N-C4N	3.41	122.12	118.26
2	D	1257	NAP	O4B-C1B-C2B	-3.34	100.79	106.59
2	G	1257	NAP	C2N-C3N-C4N	3.32	122.02	118.26
2	F	1257	NAP	O4B-C1B-C2B	-3.20	101.03	106.59
2	H	1257	NAP	O4D-C1D-C2D	-3.19	102.26	106.93
2	E	1258	NAP	O4D-C1D-C2D	-3.15	102.32	106.93
2	B	1257	NAP	C2N-C3N-C4N	3.11	121.79	118.26
2	A	1257	NAP	O7N-C7N-N7N	-3.04	118.26	122.58
2	E	1258	NAP	C6N-N1N-C2N	-2.95	119.28	121.97
2	A	1257	NAP	O4D-C1D-C2D	-2.85	102.76	106.93
2	C	1257	NAP	C5N-C4N-C3N	-2.73	117.11	120.34
2	F	1257	NAP	O4D-C1D-C2D	-2.59	103.13	106.93
2	H	1257	NAP	O3D-C3D-C4D	-2.55	103.68	111.05
2	A	1257	NAP	C5N-C6N-N1N	2.53	124.04	120.40
2	B	1257	NAP	O2N-PN-O1N	2.50	124.58	112.24
2	F	1257	NAP	O2N-PN-O1N	2.49	124.53	112.24
2	D	1257	NAP	C3N-C7N-N7N	2.48	120.73	117.75
2	F	1257	NAP	C2N-C3N-C4N	2.48	121.07	118.26
2	G	1257	NAP	O4B-C1B-C2B	-2.48	102.29	106.59
2	E	1258	NAP	C1B-N9A-C4A	-2.46	122.31	126.64
2	A	1257	NAP	C5A-C6A-N6A	-2.43	116.66	120.35
2	B	1257	NAP	C5N-C4N-C3N	-2.37	117.53	120.34
2	B	1257	NAP	C6N-N1N-C2N	-2.37	119.82	121.97
3	E	1259	FPL	C5-O1-C6	2.36	123.90	118.00
2	D	1257	NAP	O4D-C1D-C2D	-2.33	103.52	106.93
2	H	1257	NAP	O5B-C5B-C4B	-2.33	100.97	108.99
2	A	1257	NAP	N6A-C6A-N1A	2.32	123.39	118.57
2	A	1257	NAP	C2N-C3N-C4N	2.30	120.86	118.26
2	H	1257	NAP	C1B-N9A-C4A	-2.29	122.61	126.64
2	D	1257	NAP	C6N-N1N-C2N	-2.27	119.91	121.97
2	B	1257	NAP	N6A-C6A-N1A	2.26	123.27	118.57
4	A	1259	GLU	CG-CB-CA	2.24	119.06	113.84
4	E	1260	GLU	OE1-CD-CG	-2.24	115.89	123.08
2	B	1257	NAP	O5B-C5B-C4B	-2.23	101.31	108.99
2	G	1257	NAP	O4D-C1D-C2D	-2.23	103.67	106.93
2	E	1258	NAP	O3X-P2B-O1X	-2.22	101.99	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1257	NAP	O4B-C1B-C2B	-2.21	102.75	106.59
2	H	1257	NAP	C3B-C2B-C1B	-2.19	98.77	102.89
2	G	1257	NAP	C5N-C4N-C3N	-2.15	117.80	120.34
2	H	1257	NAP	O2N-PN-O1N	2.15	122.87	112.24
2	E	1258	NAP	O2N-PN-O1N	2.13	122.79	112.24
2	E	1258	NAP	O3X-P2B-O2B	2.11	115.46	105.99
2	D	1257	NAP	O7N-C7N-C3N	-2.11	117.11	119.63
2	A	1257	NAP	O2N-PN-O1N	2.11	122.65	112.24
2	E	1258	NAP	C5N-C6N-N1N	2.09	123.40	120.40
3	C	1258	FPL	C5-O1-C6	2.09	123.22	118.00
2	C	1257	NAP	N6A-C6A-N1A	2.09	122.91	118.57
2	F	1257	NAP	O3X-P2B-O2B	2.09	115.34	105.99
2	D	1257	NAP	O2N-PN-O1N	2.08	122.51	112.24
2	G	1257	NAP	O2N-PN-O1N	2.06	122.43	112.24
2	C	1257	NAP	O2N-PN-O1N	2.05	122.37	112.24
2	A	1257	NAP	O7N-C7N-C3N	-2.04	117.19	119.63
2	B	1257	NAP	O4D-C1D-C2D	-2.03	103.96	106.93
2	H	1257	NAP	O7N-C7N-C3N	-2.02	117.21	119.63

There are no chirality outliers.

All (74) 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	B	1257	NAP	C5D-O5D-PN-O1N
2	B	1257	NAP	C5D-O5D-PN-O2N
2	B	1257	NAP	O4D-C1D-N1N-C2N
2	C	1257	NAP	C5D-O5D-PN-O1N
2	C	1257	NAP	O4D-C1D-N1N-C2N
2	D	1257	NAP	PN-O3-PA-O5B
2	D	1257	NAP	C5D-O5D-PN-O1N
2	D	1257	NAP	C5D-O5D-PN-O2N
2	D	1257	NAP	O4D-C1D-N1N-C2N
2	E	1258	NAP	C5D-O5D-PN-O1N
2	E	1258	NAP	C5D-O5D-PN-O2N
2	E	1258	NAP	O4D-C1D-N1N-C2N
2	F	1257	NAP	C5D-O5D-PN-O1N
2	F	1257	NAP	C5D-O5D-PN-O2N
2	G	1257	NAP	C5D-O5D-PN-O1N
2	G	1257	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	H	1257	NAP	C5D-O5D-PN-O1N
2	H	1257	NAP	C5D-O5D-PN-O2N
2	H	1257	NAP	O4D-C1D-N1N-C2N
4	A	1259	GLU	N-CA-CB-CG
4	A	1259	GLU	C-CA-CB-CG
4	C	1259	GLU	O-C-CA-N
4	D	1259	GLU	O-C-CA-N
4	C	1259	GLU	OXT-C-CA-N
4	D	1259	GLU	OXT-C-CA-N
4	G	1259	GLU	O-C-CA-CB
4	C	1259	GLU	OXT-C-CA-CB
4	G	1259	GLU	OXT-C-CA-CB
4	A	1259	GLU	CA-CB-CG-CD
4	C	1259	GLU	O-C-CA-CB
4	D	1259	GLU	O-C-CA-CB
4	D	1259	GLU	OXT-C-CA-CB
2	A	1257	NAP	PN-O3-PA-O5B
2	C	1257	NAP	PN-O3-PA-O5B
2	F	1257	NAP	PN-O3-PA-O5B
2	G	1257	NAP	PN-O3-PA-O5B
2	A	1257	NAP	C5D-O5D-PN-O3
2	C	1257	NAP	C5D-O5D-PN-O3
2	E	1258	NAP	C5D-O5D-PN-O3
2	F	1257	NAP	O4B-C4B-C5B-O5B
4	E	1260	GLU	OE1-CD-CG-CB
4	E	1260	GLU	OE2-CD-CG-CB
2	G	1257	NAP	PA-O3-PN-O1N
2	G	1257	NAP	PA-O3-PN-O2N
2	C	1257	NAP	O4B-C4B-C5B-O5B
4	G	1259	GLU	OE2-CD-CG-CB
4	A	1259	GLU	OE2-CD-CG-CB
4	E	1260	GLU	CA-CB-CG-CD
4	A	1259	GLU	OE1-CD-CG-CB
4	D	1259	GLU	OE2-CD-CG-CB
4	D	1259	GLU	OE1-CD-CG-CB
2	G	1257	NAP	O4B-C4B-C5B-O5B
4	G	1259	GLU	C-CA-CB-CG
4	G	1259	GLU	OE1-CD-CG-CB
2	B	1257	NAP	C5D-O5D-PN-O3
2	D	1257	NAP	C5D-O5D-PN-O3
2	F	1257	NAP	C5D-O5D-PN-O3
2	G	1257	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	H	1257	NAP	C2B-O2B-P2B-O2X
2	H	1257	NAP	C5D-O5D-PN-O3
2	A	1257	NAP	O4B-C4B-C5B-O5B
2	B	1257	NAP	O4B-C4B-C5B-O5B
2	E	1258	NAP	O4B-C4B-C5B-O5B
2	F	1257	NAP	PA-O3-PN-O2N
4	C	1259	GLU	CA-CB-CG-CD
2	C	1257	NAP	C5D-O5D-PN-O2N
2	D	1257	NAP	O4B-C4B-C5B-O5B
2	H	1257	NAP	O4B-C4B-C5B-O5B
4	C	1259	GLU	N-CA-CB-CG
4	D	1259	GLU	N-CA-CB-CG
4	G	1259	GLU	N-CA-CB-CG

There are no ring outliers.

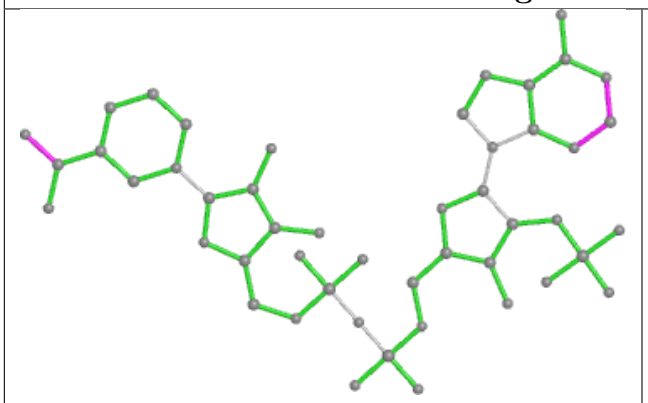
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1259	FPL	1	0
4	G	1259	GLU	2	0
2	H	1257	NAP	3	0
3	G	1258	FPL	1	0
4	C	1259	GLU	4	0
2	G	1257	NAP	2	0
2	B	1257	NAP	2	0
4	A	1259	GLU	1	0
4	D	1259	GLU	4	0
2	A	1257	NAP	1	0
2	C	1257	NAP	1	0
4	E	1260	GLU	1	0

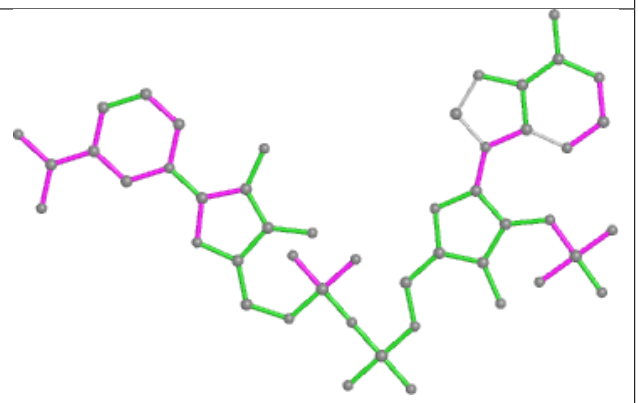
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

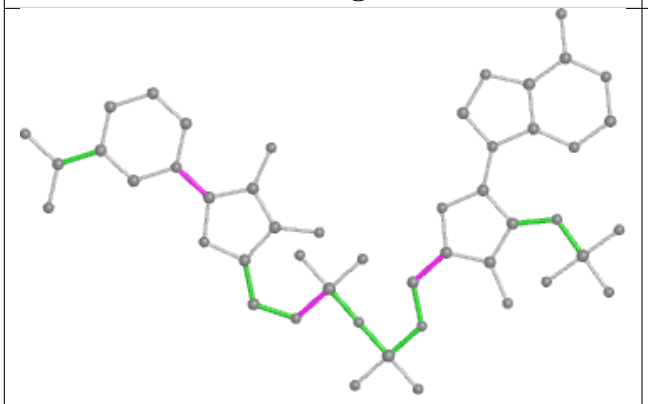
Ligand NAP E 1258



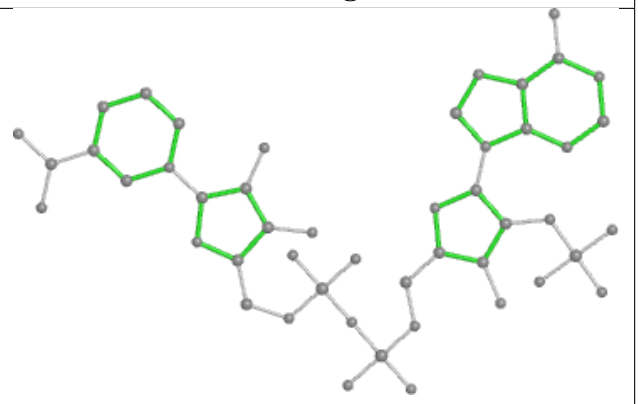
Bond lengths



Bond angles

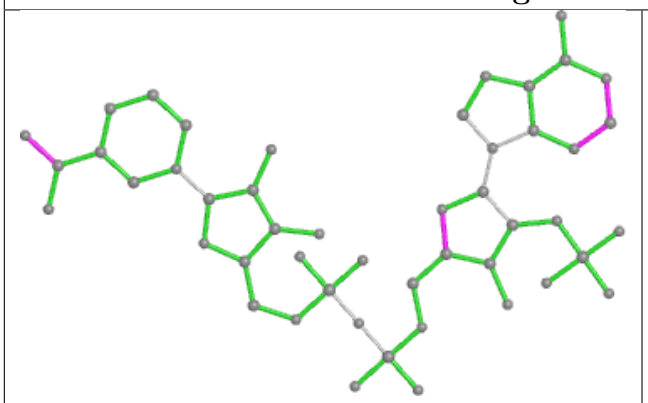


Torsions



Rings

Ligand NAP H 1257



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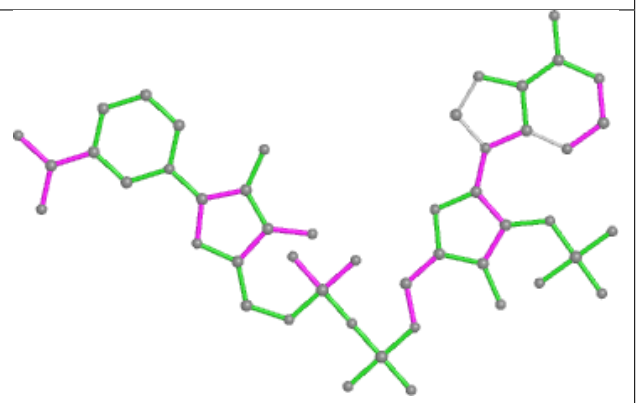

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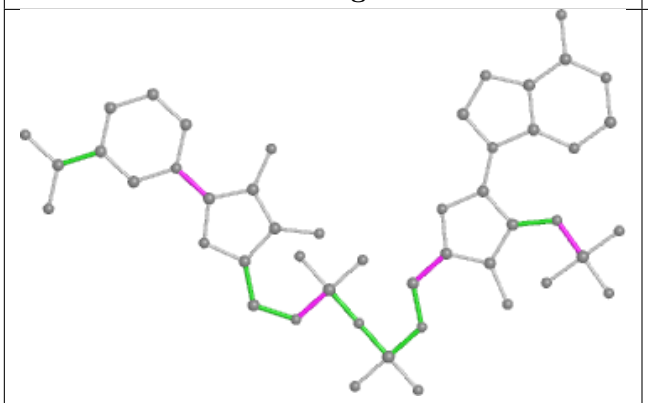

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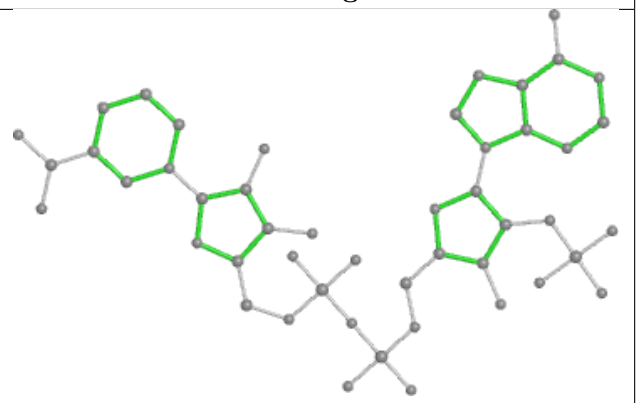
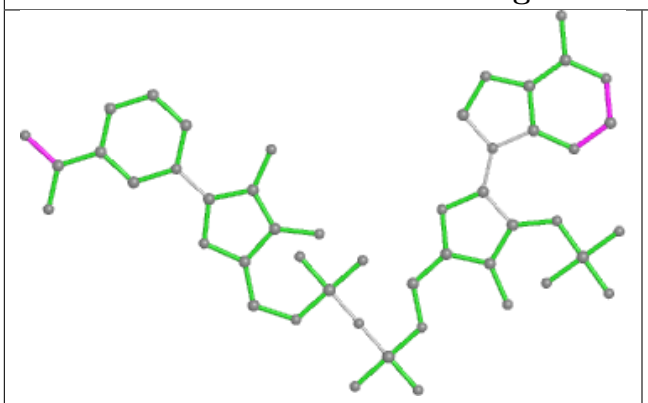
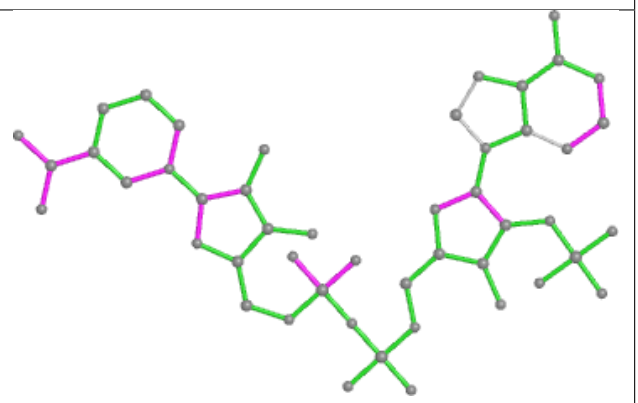


Rings

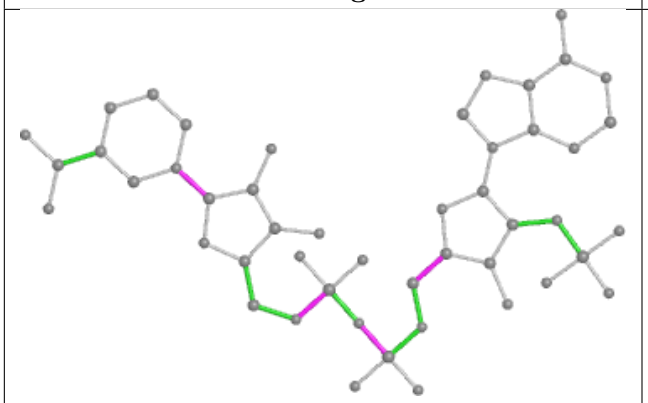
Ligand NAP D 1257



Bond lengths



Bond angles



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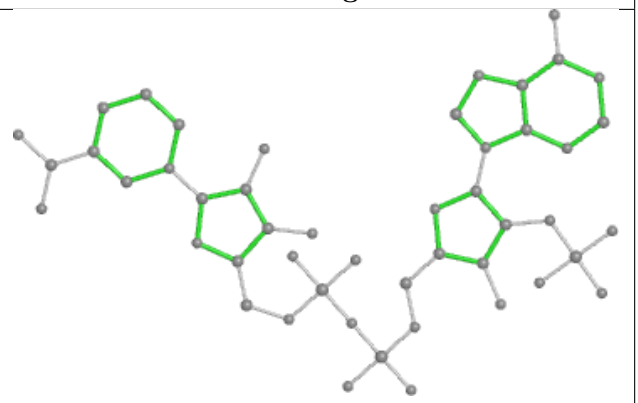
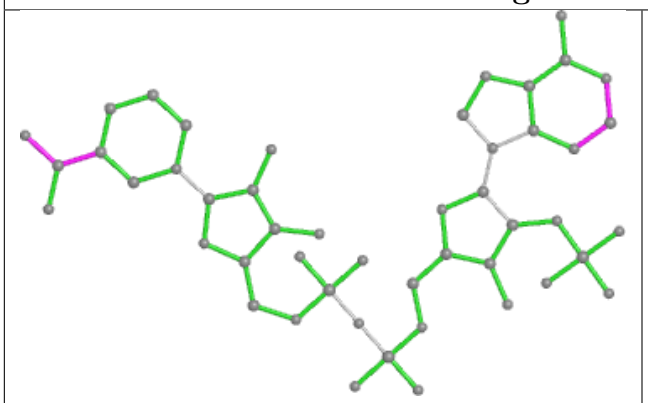


Rings

Ligand NAP G 1257



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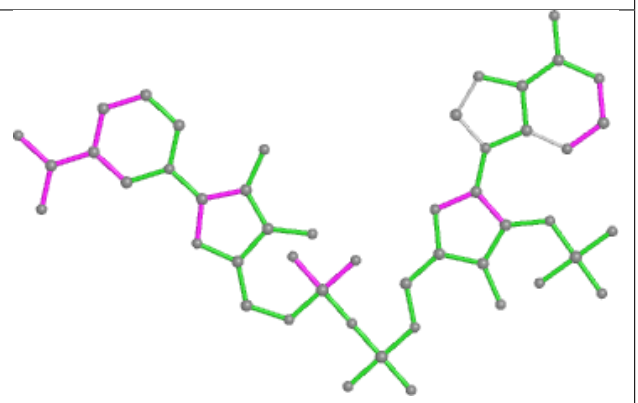
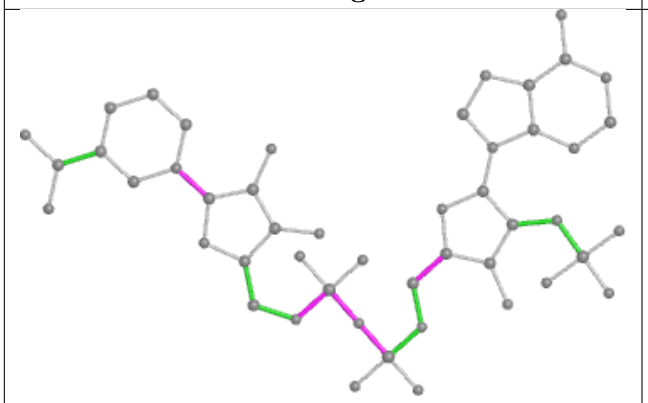


Bond angles



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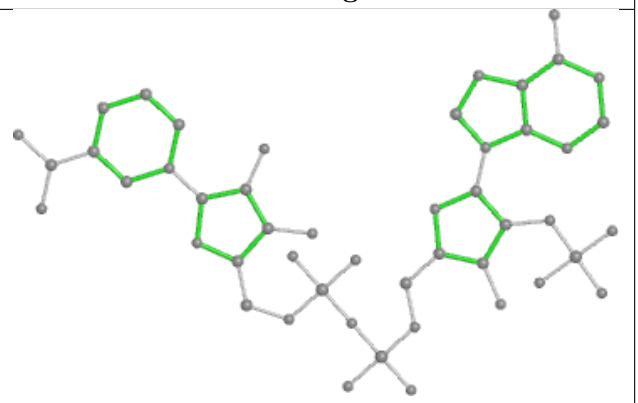
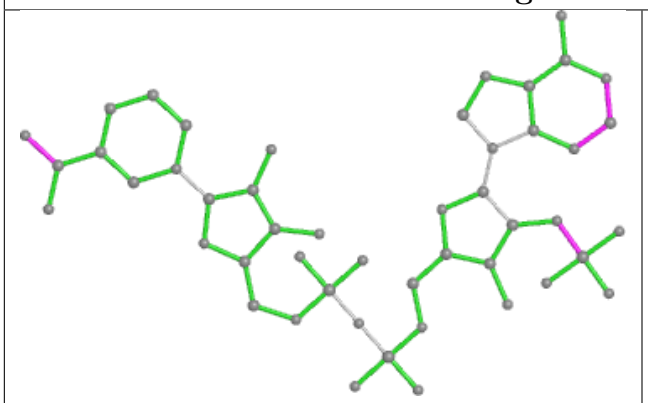


Rings

Ligand NAP F 1257



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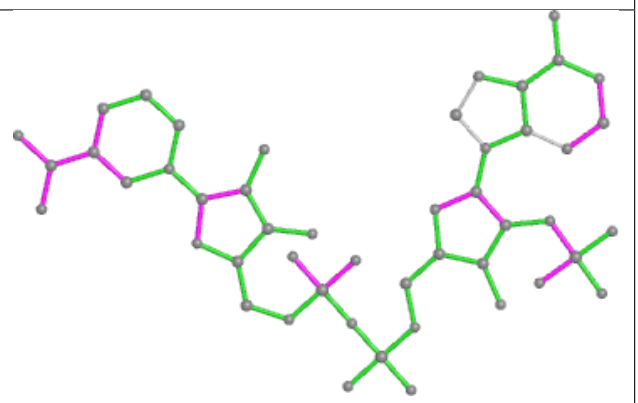
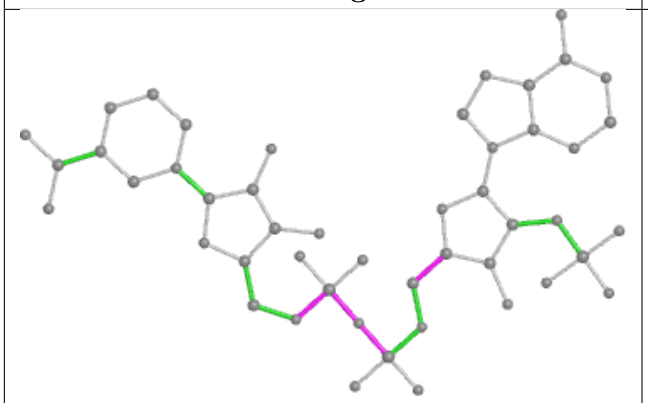
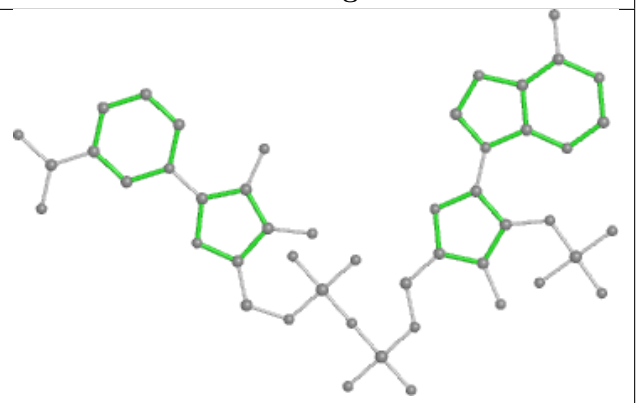


Bond angles

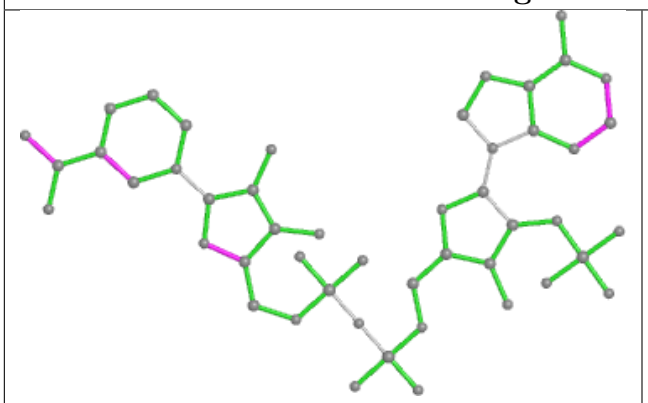


Torsions

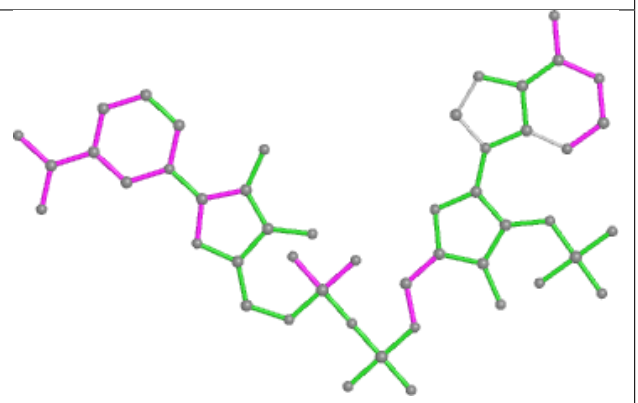


Rings

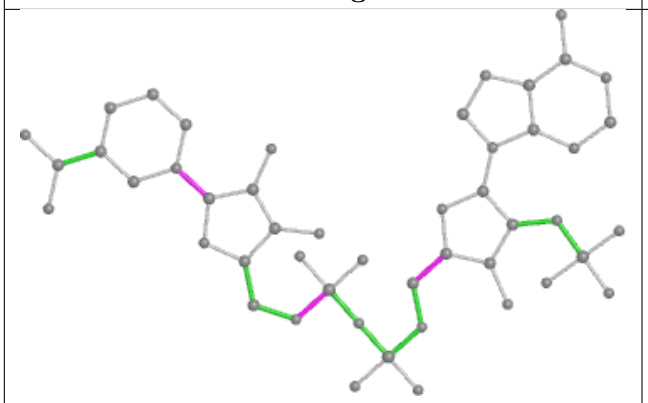
Ligand NAP B 1257



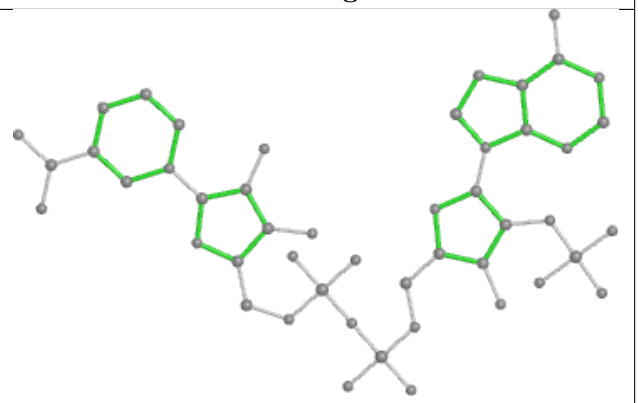
Bond lengths



Bond angles

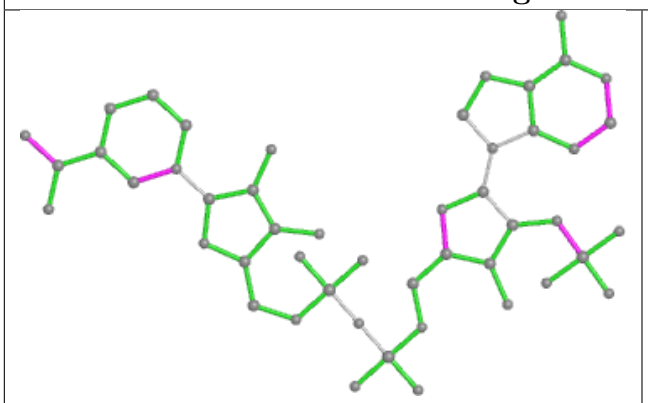


Torsions

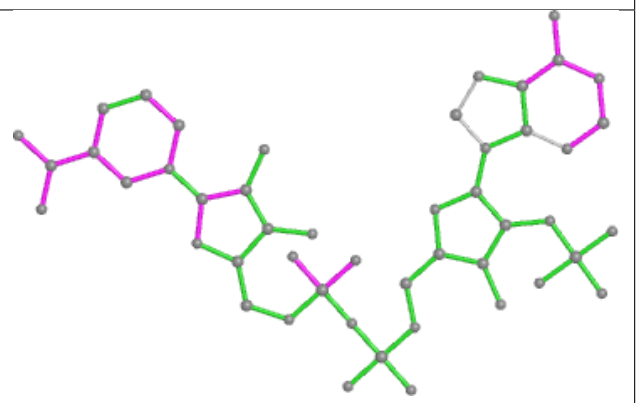


Rings

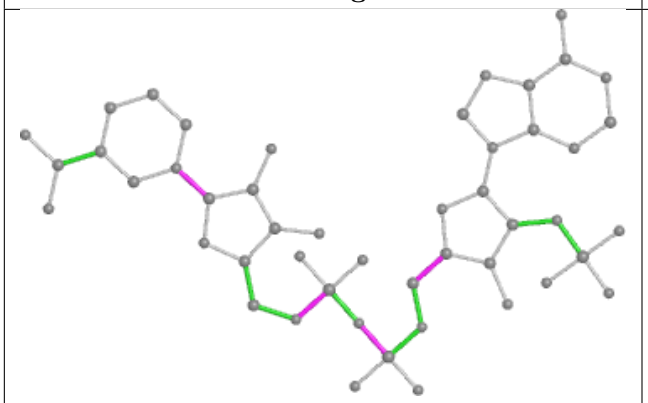
Ligand NAP A 1257



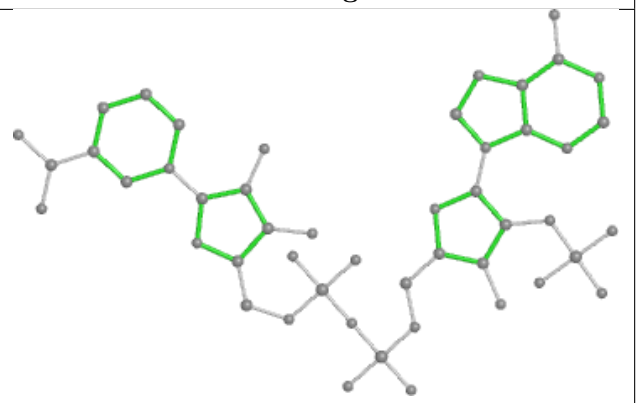
Bond lengths



Bond angles

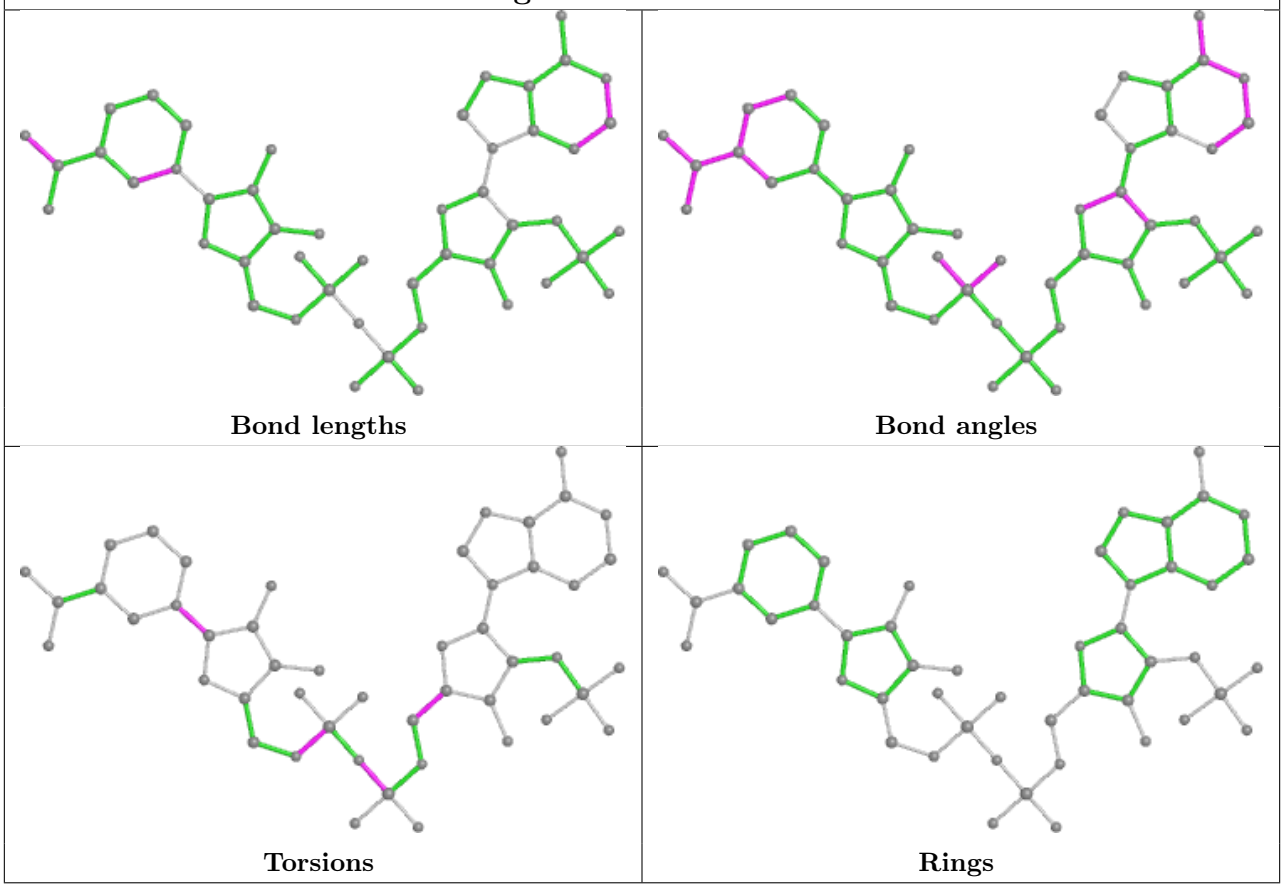


Torsions



Rings

Ligand NAP C 1257



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, 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	254/282 (90%)	-0.07	2 (0%)	86	87	28, 39, 62, 74	0
1	B	255/282 (90%)	-0.03	2 (0%)	86	87	27, 42, 65, 78	0
1	C	255/282 (90%)	0.07	3 (1%)	79	80	28, 43, 67, 83	0
1	D	254/282 (90%)	0.08	3 (1%)	79	80	32, 50, 79, 98	0
1	E	254/282 (90%)	0.05	4 (1%)	72	74	28, 40, 62, 78	0
1	F	255/282 (90%)	0.08	3 (1%)	79	80	27, 41, 62, 77	0
1	G	255/282 (90%)	0.02	2 (0%)	86	87	27, 43, 65, 86	0
1	H	254/282 (90%)	0.23	12 (4%)	31	33	30, 50, 82, 97	0
All	All	2036/2256 (90%)	0.05	31 (1%)	73	75	27, 43, 70, 98	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	PRO	3.7
1	C	58	PRO	3.4
1	F	58	PRO	3.2
1	D	43	ARG	3.2
1	G	58	PRO	3.1
1	A	58	PRO	3.1
1	H	99	MET	3.1
1	F	246	ILE	3.0
1	H	53	GLU	2.8
1	H	59	GLU	2.7
1	B	30	GLN	2.7
1	B	246	ILE	2.7
1	H	60	ALA	2.5
1	H	54	GLN	2.5
1	H	48	LEU	2.4
1	H	202	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	246	ILE	2.4
1	E	83	ASP	2.3
1	C	32	GLY	2.3
1	H	205	ASN	2.3
1	G	6	ASN	2.3
1	C	3	ASN	2.3
1	E	254	ALA	2.2
1	E	79	GLN	2.2
1	D	152	PHE	2.2
1	E	6	ASN	2.1
1	F	148	LEU	2.1
1	A	60	ALA	2.0
1	H	85	GLY	2.0
1	D	58	PRO	2.0
1	H	84	VAL	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 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, 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
4	GLU	E	1260	10/10	0.62	0.34	95,96,101,102	0
4	GLU	C	1259	10/10	0.70	0.24	81,83,83,83	0
4	GLU	D	1259	10/10	0.73	0.25	76,80,80,80	0
4	GLU	A	1259	10/10	0.77	0.19	76,77,78,78	0
4	GLU	G	1259	10/10	0.80	0.19	76,79,79,79	0
3	FPL	F	1258	15/15	0.92	0.16	37,40,41,43	0
2	NAP	D	1257	48/48	0.93	0.12	42,49,61,62	0
3	FPL	B	1258	15/15	0.93	0.15	39,42,43,45	0

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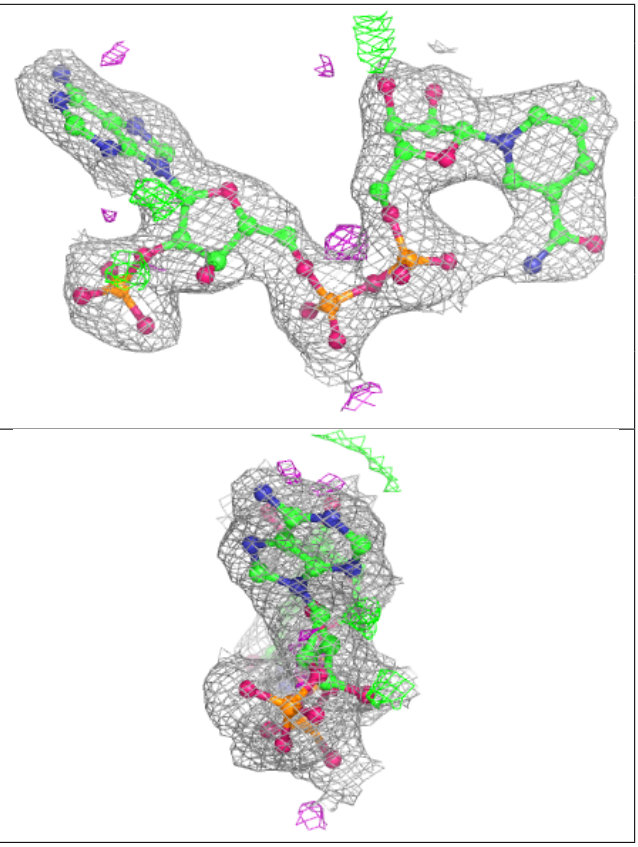
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FPL	D	1258	15/15	0.93	0.15	50,51,55,55	0
3	FPL	H	1258	15/15	0.94	0.14	57,58,59,59	0
5	CL	E	1257	1/1	0.94	0.20	64,64,64,64	0
3	FPL	C	1258	15/15	0.95	0.16	39,42,47,48	0
3	FPL	G	1258	15/15	0.95	0.12	37,39,48,48	0
2	NAP	H	1257	48/48	0.95	0.14	45,51,59,62	0
3	FPL	E	1259	15/15	0.96	0.14	34,37,41,43	0
3	FPL	A	1258	15/15	0.96	0.15	31,35,37,37	0
2	NAP	B	1257	48/48	0.96	0.12	27,41,45,46	0
2	NAP	G	1257	48/48	0.96	0.12	31,39,46,48	0
2	NAP	C	1257	48/48	0.96	0.13	31,40,47,49	0
2	NAP	E	1258	48/48	0.97	0.12	31,37,41,42	0
2	NAP	F	1257	48/48	0.97	0.12	31,38,43,44	0
2	NAP	A	1257	48/48	0.97	0.13	32,37,42,43	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.

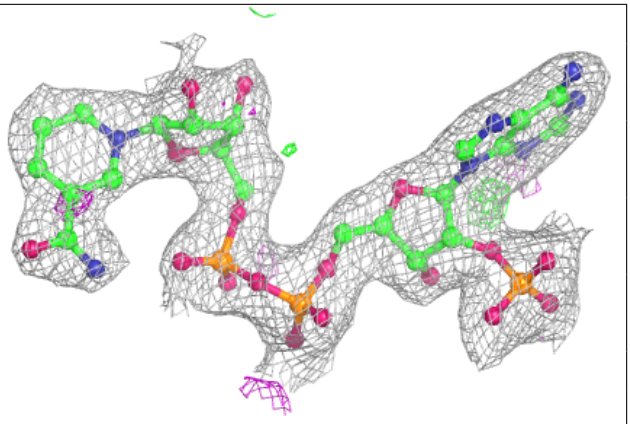
Electron density around NAP D 1257:

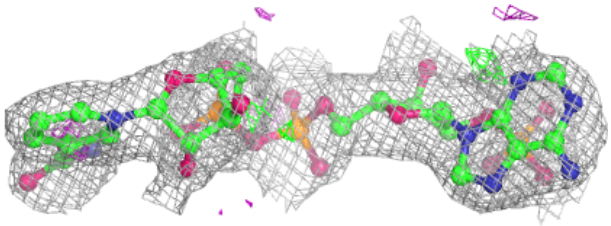
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

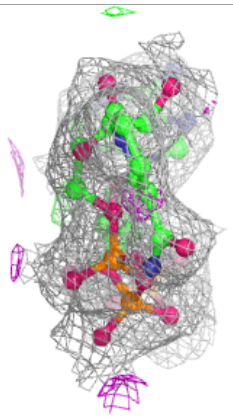


Electron density around NAP H 1257:

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

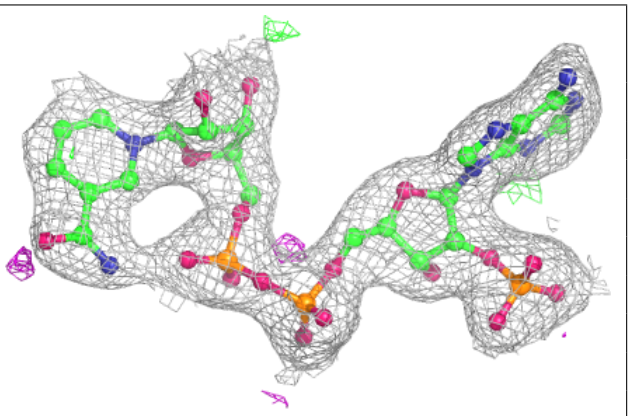


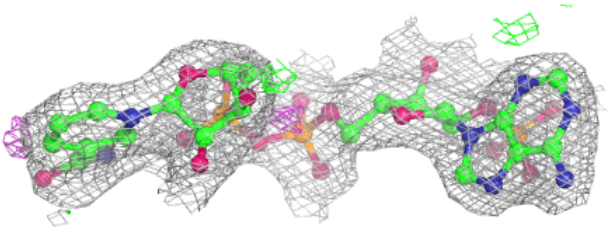


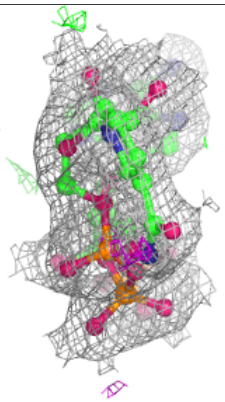


Electron density around NAP B 1257:

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

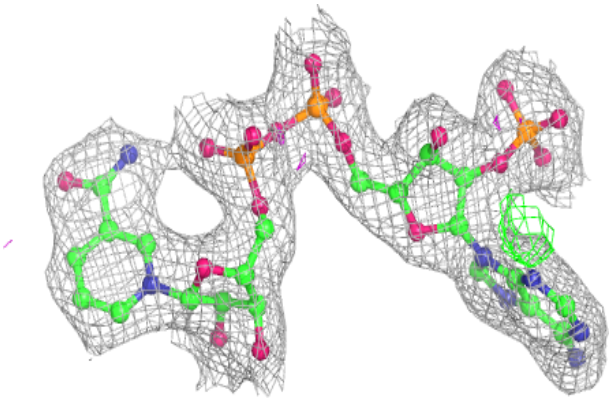


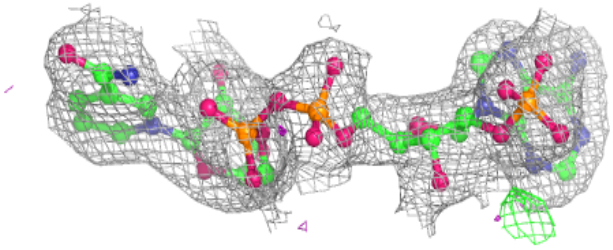


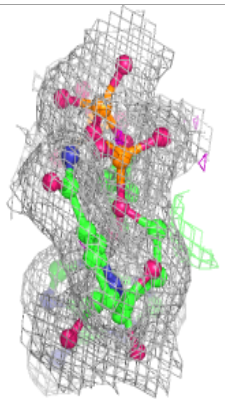


Electron density around NAP G 1257:

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

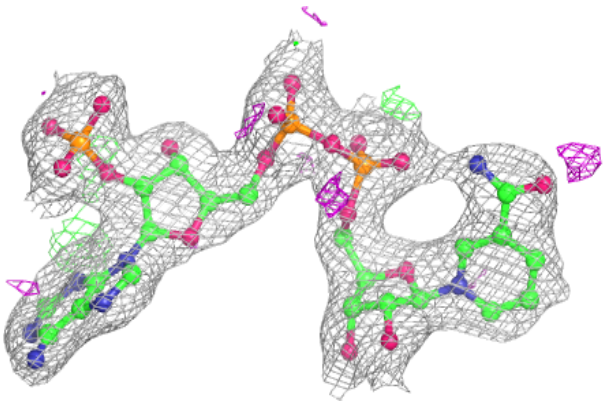


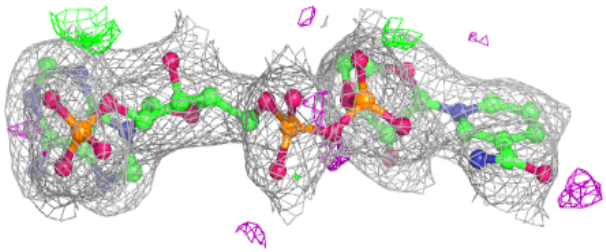


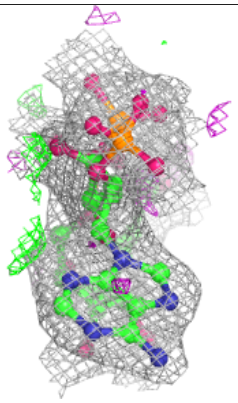


Electron density around NAP C 1257:

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

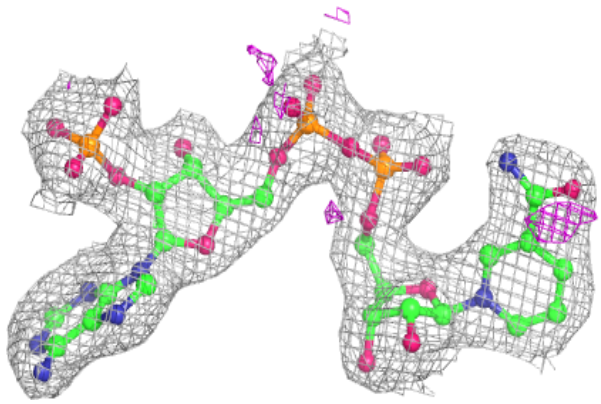


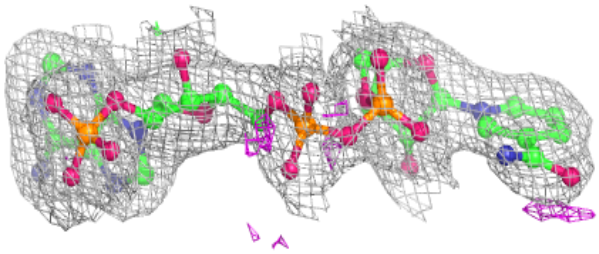


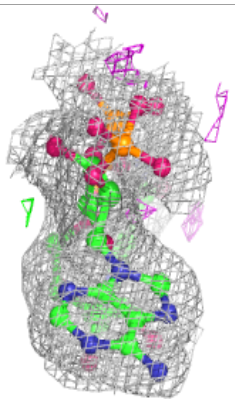


Electron density around NAP E 1258:

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

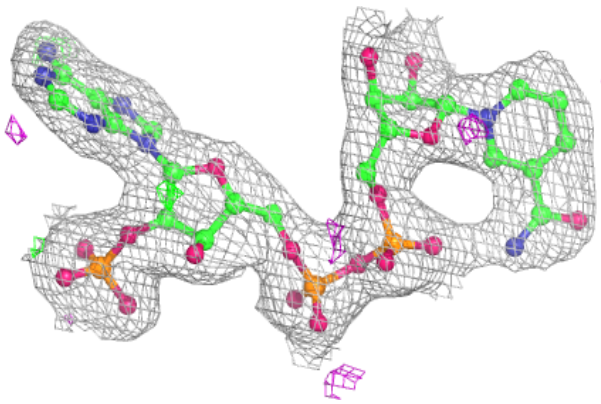


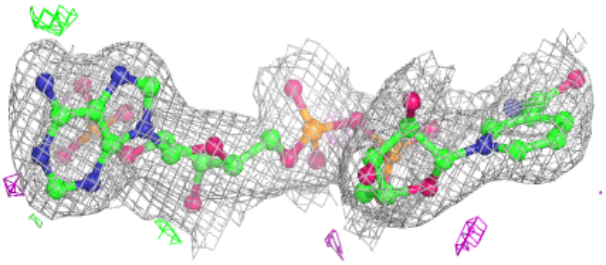


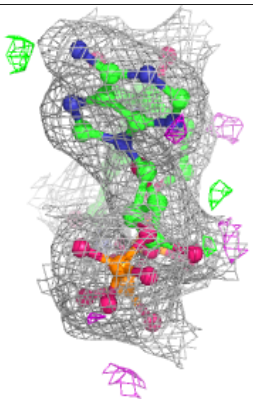


Electron density around NAP F 1257:

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

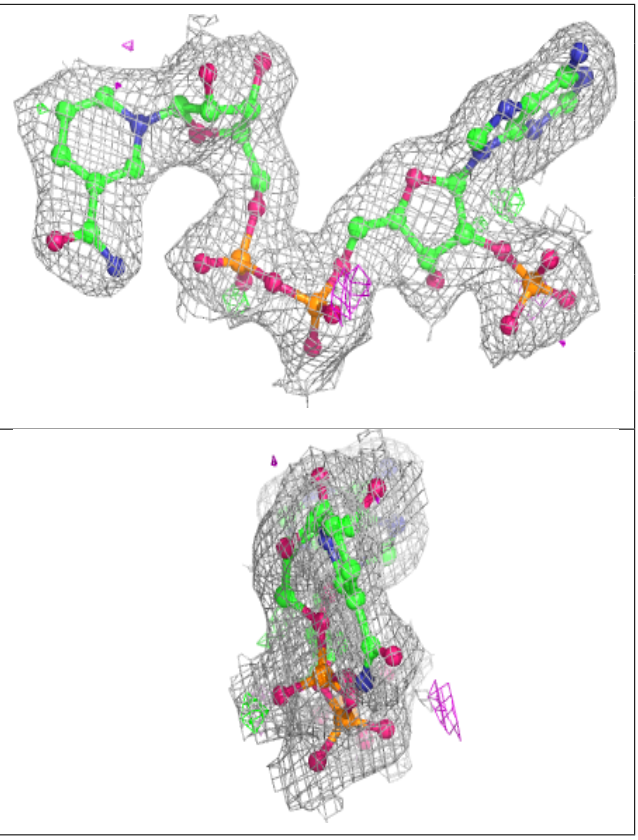






Electron density around NAP A 1257:

$2mF_o$-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.