



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 03:27 PM BST

PDB ID : 4ALK
Title : Crystal structure of S. aureus FabI in complex with NADP and 5-ethyl- 2-phenoxyphe

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nol
Authors : Schiebel, J.; Chang, A.; Tonge, P.J.; Kisker, C.
Deposited on : 2012-03-04
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

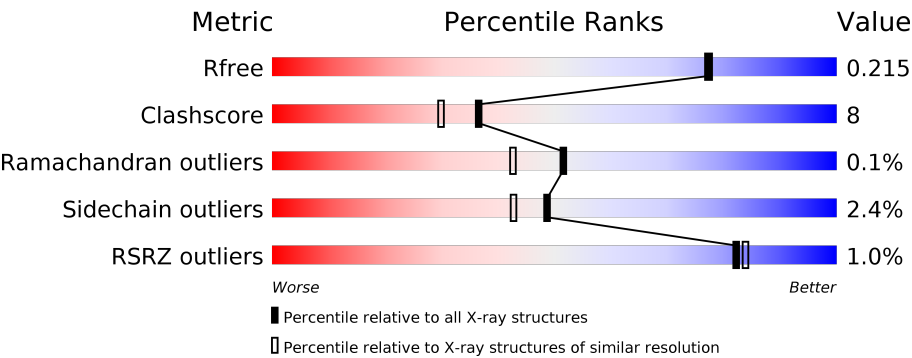
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	<div><div></div><div>80%8%10%</div></div>
1	B	282	<div><div></div><div>79%11%10%</div></div>
1	C	282	<div><div></div><div>81%9%10%</div></div>
1	D	282	<div><div>3%</div><div></div><div>79%9%10%</div></div>
1	E	282	<div><div></div><div>79%10%10%</div></div>
1	F	282	<div><div>%</div><div></div><div>78%12%9%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	282	
1	H	282	

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	A	1002[B]	-	-	X	-
4	GLU	B	1002[A]	-	-	X	-
4	GLU	E	1002[B]	-	-	X	-
4	GLU	G	1002[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18573 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
1	A	254	Total	C	N	O	S	0	16	0
			2068	1302	360	401	5			
1	B	255	Total	C	N	O	S	0	19	0
			2098	1323	369	401	5			
1	C	255	Total	C	N	O	S	0	13	0
			2059	1295	361	398	5			
1	D	254	Total	C	N	O	S	0	12	0
			2041	1282	355	399	5			
1	E	255	Total	C	N	O	S	0	18	0
			2089	1318	365	401	5			
1	F	256	Total	C	N	O	S	0	14	0
			2074	1305	364	399	6			
1	G	254	Total	C	N	O	S	0	13	0
			2050	1289	357	399	5			
1	H	255	Total	C	N	O	S	0	12	0
			2051	1289	357	400	5			

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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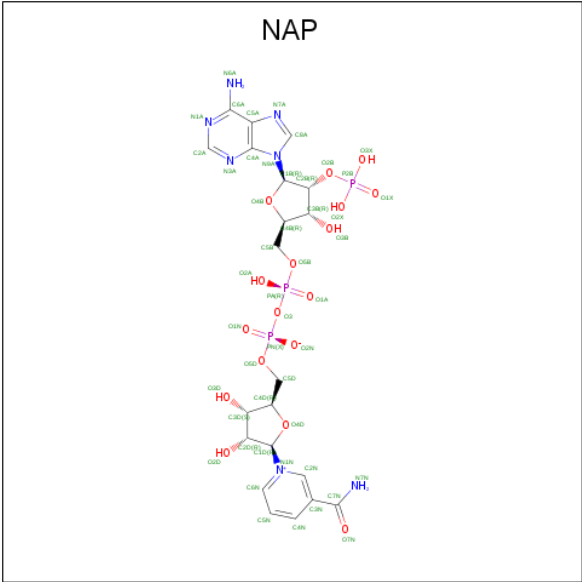
Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	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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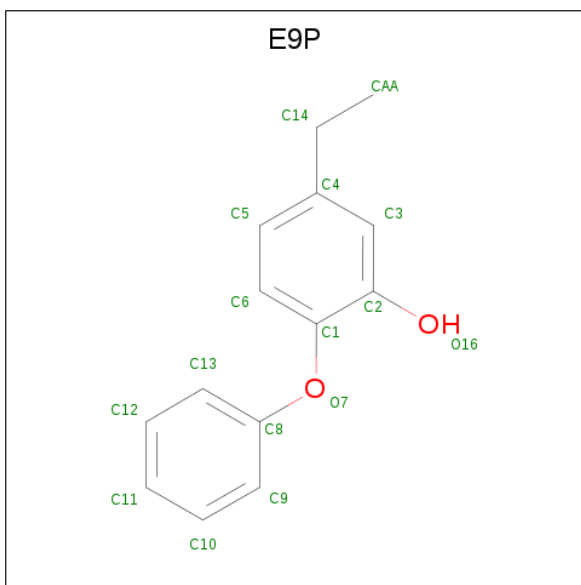
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
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: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 5-ETHYL-2-PHENOXYPHENOL (three-letter code: E9P) (formula: C₁₄H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	14	2		
3	B	1	Total	C	O	0	0
			16	14	2		
3	C	1	Total	C	O	0	0
			16	14	2		
3	D	1	Total	C	O	0	0
			16	14	2		
3	E	1	Total	C	O	0	0
			16	14	2		
3	F	1	Total	C	O	0	0
			16	14	2		
3	G	1	Total	C	O	0	0
			16	14	2		
3	H	1	Total	C	O	0	0
			16	14	2		

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			20	10	2	8		
4	B	1	Total	C	N	O	0	1
			20	10	2	8		
4	C	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	1
			20	10	2	8		
4	E	1	Total	C	N	O	0	1
			20	10	2	8		
4	F	1	Total	C	N	O	0	1
			20	10	2	8		
4	F	1	Total	C	N	O	0	0
			10	5	1	4		
4	G	1	Total	C	N	O	0	1
			20	10	2	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	235	Total	O	0	0
			235	235		
5	B	202	Total	O	0	0
			202	202		
5	C	174	Total	O	0	0
			174	174		
5	D	113	Total	O	0	0
			113	113		

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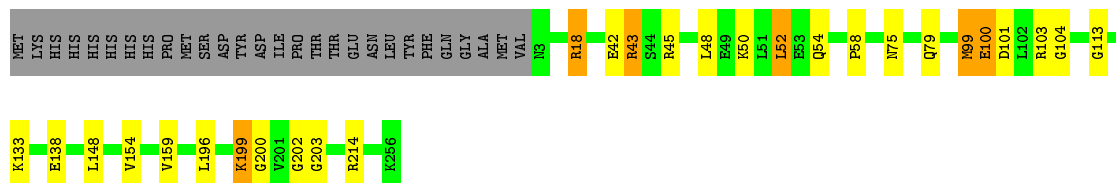
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	202	Total 202	O 202	0	0
5	F	180	Total 180	O 180	0	0
5	G	170	Total 170	O 170	0	0
5	H	115	Total 115	O 115	0	0

3 Residue-property plots


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

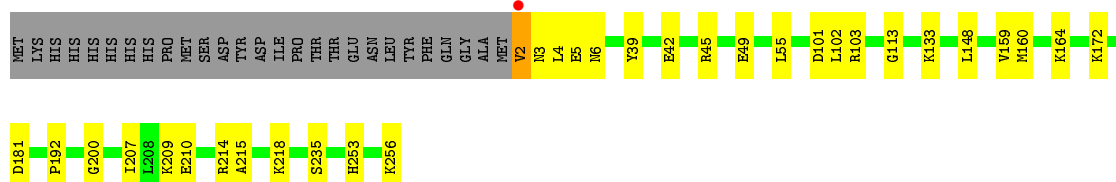
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain A: 




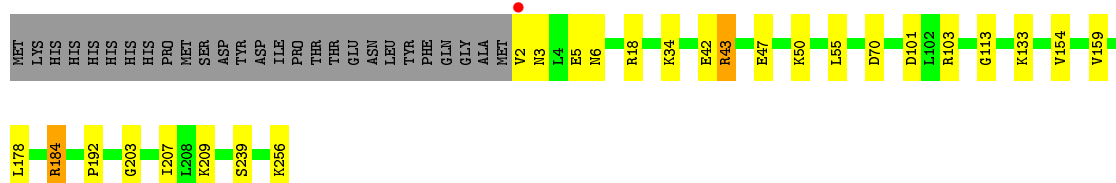
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain B: 




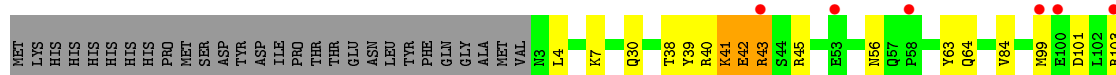
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

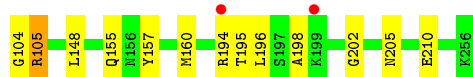
Chain C: 



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

Chain D: 





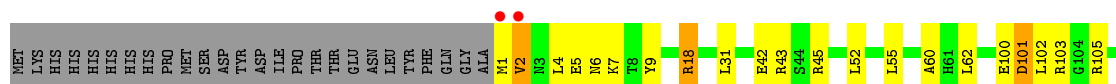
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain E: 79% 10% 10%



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

Chain F: 78% 12% 9%



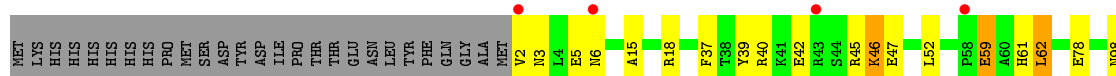
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G: 74% 15% 10%



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

Chain H: 80% 9% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.23Å 95.14Å 95.34Å 98.24° 112.27° 97.27°	Depositor
Resolution (Å)	40.93 – 1.90 40.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (40.93-1.90) 91.8 (40.93-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.150 , 0.193 0.176 , 0.215	Depositor DCC
R_{free} test set	10405 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18573	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E9P, 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	0.76	0/2116	0.85	2/2845 (0.1%)
1	B	0.72	0/2155	0.81	1/2896 (0.0%)
1	C	0.72	0/2098	0.84	3/2822 (0.1%)
1	D	0.63	0/2077	0.73	0/2796
1	E	0.73	0/2143	0.84	4/2882 (0.1%)
1	F	0.72	0/2116	0.86	5/2846 (0.2%)
1	G	0.70	0/2089	0.83	3/2810 (0.1%)
1	H	0.63	0/2087	0.79	0/2809
All	All	0.70	0/16881	0.82	18/22706 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	101[A]	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	F	101[B]	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	E	43	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	G	43	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	18	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	43	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	F	101[A]	ASP	CB-CG-OD1	6.17	123.85	118.30
1	F	101[B]	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	70	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	43	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	184	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	148	LEU	CA-CB-CG	5.37	127.65	115.30
1	G	228	LYS	CD-CE-NZ	-5.28	99.56	111.70
1	F	18	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	G	70	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	18[A]	ARG	NE-CZ-NH2	-5.15	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18[B]	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	E	7	LYS	CD-CE-NZ	-5.10	99.97	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2068	0	2100	33	0
1	B	2098	0	2151	37	0
1	C	2059	0	2087	31	0
1	D	2041	0	2053	23	0
1	E	2089	0	2136	41	0
1	F	2074	0	2110	37	0
1	G	2050	0	2071	50	1
1	H	2051	0	2067	30	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	H	48	0	25	1	0
3	A	16	0	14	0	0
3	B	16	0	14	0	0
3	C	16	0	13	0	0
3	D	16	0	13	0	0
3	E	16	0	14	0	0
3	F	16	0	14	1	0
3	G	16	0	13	0	0
3	H	16	0	14	0	0
4	A	20	0	10	9	0
4	B	20	0	10	9	0
4	C	10	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	20	0	10	2	0
4	E	20	0	10	7	0
4	F	30	0	15	1	0
4	G	20	0	10	10	0
5	A	235	0	0	14	1
5	B	202	0	0	11	0
5	C	174	0	0	10	0
5	D	113	0	0	5	0
5	E	202	0	0	8	0
5	F	180	0	0	10	0
5	G	170	0	0	7	0
5	H	115	0	0	3	0
All	All	18573	0	17154	270	1

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

All (270) 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:A:103[B]:ARG:HH12	4:A:1002[B]:GLU:HB2	1.03	1.15
5:B:2001:HOH:O	1:C:2:VAL:HG12	1.45	1.15
1:A:103[B]:ARG:NH1	4:A:1002[B]:GLU:HB2	1.60	1.14
1:G:103[B]:ARG:HH12	4:G:1002[B]:GLU:CA	1.65	1.08
1:E:42[B]:GLU:HG3	1:E:45[B]:ARG:HH21	0.92	1.06
4:E:1002[A]:GLU:CG	4:E:1002[A]:GLU:O	2.03	1.05
1:E:42[B]:GLU:HG3	1:E:45[B]:ARG:NH2	1.72	1.03
1:E:42[B]:GLU:CG	1:E:45[B]:ARG:HH21	1.75	0.98
1:H:101[B]:ASP:OD1	5:H:2050:HOH:O	1.84	0.95
1:F:154:VAL:HG11	5:F:2108:HOH:O	1.70	0.91
1:H:101[B]:ASP:O	1:H:103[B]:ARG:N	2.04	0.91
1:B:103[B]:ARG:NH2	1:B:200:GLY:O	2.04	0.90
1:B:103[A]:ARG:HH12	4:B:1002[A]:GLU:HA	1.35	0.90
1:B:103[A]:ARG:HH22	4:B:1002[A]:GLU:HG2	1.39	0.87
1:A:148:LEU:HD21	1:C:256:LYS:HD2	1.55	0.86
1:G:154:VAL:HG11	5:G:2115:HOH:O	1.72	0.86
4:E:1002[A]:GLU:HG3	4:E:1002[A]:GLU:O	1.75	0.86
4:E:1002[A]:GLU:HG2	4:E:1002[A]:GLU:O	1.75	0.84
1:C:47:GLU:OE2	1:C:50[B]:LYS:NZ	2.10	0.84
1:D:101[B]:ASP:OD2	5:D:2056:HOH:O	1.96	0.84
1:F:1:MET:HG2	1:G:3:ASN:N	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:VAL:CG1	5:G:2115:HOH:O	2.25	0.84
1:H:100[B]:GLU:OE1	1:H:100[B]:GLU:N	2.11	0.83
1:G:103[B]:ARG:HH12	4:G:1002[B]:GLU:C	1.82	0.83
1:C:154:VAL:HG11	5:C:2120:HOH:O	1.76	0.83
1:A:75:ASN:O	1:A:79[B]:GLN:HG3	1.78	0.82
1:E:42[A]:GLU:OE2	5:E:2032:HOH:O	1.97	0.82
1:G:42[B]:GLU:OE1	1:G:45[B]:ARG:NH2	2.12	0.82
1:C:43:ARG:NH1	5:C:2043:HOH:O	2.04	0.81
4:E:1002[B]:GLU:HG2	4:E:1002[B]:GLU:O	1.82	0.79
1:A:101[B]:ASP:OD1	1:E:43:ARG:HD3	1.83	0.79
1:E:155[A]:GLN:NE2	5:E:2126:HOH:O	2.16	0.79
1:A:203:GLY:H	4:A:1002[B]:GLU:HG3	1.47	0.79
1:G:89:GLY:HA2	1:G:136:MET:CE	2.12	0.78
1:C:154:VAL:CG1	5:C:2120:HOH:O	2.33	0.77
1:B:103[A]:ARG:HH12	4:B:1002[A]:GLU:CA	1.99	0.76
1:B:2:VAL:O	1:B:3:ASN:OD1	2.03	0.75
1:E:101[B]:ASP:OD2	5:E:2087:HOH:O	2.04	0.75
1:C:184:ARG:HH21	4:C:1002:GLU:HG2	1.51	0.74
1:F:103[B]:ARG:NH1	5:F:2088:HOH:O	2.20	0.74
1:G:89:GLY:HA2	1:G:136:MET:HE1	1.67	0.74
1:D:104[B]:GLY:O	1:D:105[B]:ARG:O	2.06	0.73
5:B:2001:HOH:O	1:C:2:VAL:CG1	2.19	0.73
1:G:103[B]:ARG:HH12	4:G:1002[B]:GLU:HA	1.49	0.73
1:B:101[B]:ASP:HB3	1:B:159:VAL:CG1	2.17	0.73
1:F:154:VAL:CG1	5:F:2108:HOH:O	2.34	0.73
1:C:101[B]:ASP:OD2	5:C:2093:HOH:O	2.06	0.72
1:A:43:ARG:NH1	5:A:2048:HOH:O	2.05	0.72
1:G:103[A]:ARG:NH2	1:G:200:GLY:O	2.23	0.71
1:B:3:ASN:HB3	5:B:2003:HOH:O	1.91	0.71
1:F:101[B]:ASP:O	1:F:102[B]:LEU:HD23	1.89	0.71
1:F:18:ARG:HH22	1:F:199:LYS:HZ2	1.35	0.71
1:G:103[B]:ARG:NH1	4:G:1002[B]:GLU:C	2.44	0.71
1:E:18[A]:ARG:HH12	1:E:199:LYS:NZ	1.87	0.70
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH2	2.22	0.70
1:A:101[B]:ASP:OD2	1:A:113:GLY:HA3	1.91	0.70
1:B:103[B]:ARG:HD3	4:B:1002[B]:GLU:O	1.92	0.69
4:A:1002[B]:GLU:OXT	5:C:2174:HOH:O	2.09	0.69
1:B:103[A]:ARG:NH1	4:B:1002[A]:GLU:HA	2.05	0.69
1:B:253:HIS:HD2	5:B:2055:HOH:O	1.76	0.69
1:A:154:VAL:HG11	5:A:2146:HOH:O	1.91	0.69
1:G:101[B]:ASP:OD2	5:G:2084:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103[B]:ARG:HH22	4:E:1002[B]:GLU:HB2	1.57	0.69
1:F:206:THR:HG23	5:F:2144:HOH:O	1.93	0.69
1:C:42[B]:GLU:OE1	5:C:2039:HOH:O	2.10	0.68
1:H:101[B]:ASP:OD1	5:H:2048:HOH:O	2.12	0.67
5:B:2198:HOH:O	1:F:9:TYR:OH	1.80	0.67
1:A:103[B]:ARG:HH12	4:A:1002[B]:GLU:CB	1.96	0.67
1:C:42[B]:GLU:OE2	5:C:2038:HOH:O	2.13	0.66
1:C:50[A]:LYS:HG3	5:C:2045:HOH:O	1.93	0.66
1:C:5:GLU:O	1:C:6:ASN:HB2	1.95	0.66
1:A:214[B]:ARG:NH2	5:A:2199:HOH:O	2.28	0.66
1:F:18:ARG:HH22	1:F:199:LYS:NZ	1.94	0.66
1:B:210:GLU:HG3	1:B:214[A]:ARG:HD3	1.77	0.66
1:B:103[A]:ARG:NH2	4:B:1002[A]:GLU:HG2	2.10	0.65
1:F:101[A]:ASP:OD2	1:F:113:GLY:HA3	1.97	0.65
1:A:154:VAL:CG1	5:A:2146:HOH:O	2.44	0.65
1:E:202:GLY:HA2	4:E:1002[B]:GLU:HG3	1.78	0.65
1:A:196:LEU:O	1:A:199[A]:LYS:HG2	1.97	0.65
5:A:2151:HOH:O	1:B:172[A]:LYS:HE2	1.95	0.64
1:D:205[B]:ASN:ND2	1:D:205[B]:ASN:H	1.95	0.64
1:E:45[A]:ARG:NH1	1:E:49:GLU:OE2	2.31	0.64
1:G:101[B]:ASP:OD2	1:G:113:GLY:HA3	1.97	0.64
1:E:18[A]:ARG:HH12	1:E:199:LYS:HZ2	1.44	0.64
1:E:148:LEU:HD21	1:G:256:LYS:HG2	1.79	0.63
1:H:3:ASN:OD1	1:H:5:GLU:HG3	1.99	0.63
1:E:101[B]:ASP:OD2	1:E:113:GLY:HA3	1.99	0.63
1:A:100[A]:GLU:HB3	1:E:196:LEU:HD21	1.81	0.62
1:F:253:HIS:HD2	5:F:2074:HOH:O	1.81	0.62
1:G:103[B]:ARG:HH12	4:G:1002[B]:GLU:N	1.98	0.62
1:E:133[B]:LYS:HZ2	1:F:105[B]:ARG:HH22	1.48	0.62
1:F:2:VAL:HG21	1:F:235:SER:CB	2.30	0.61
1:B:101[B]:ASP:HB3	1:B:159:VAL:HG12	1.81	0.61
1:G:89:GLY:CA	1:G:136:MET:CE	2.78	0.61
5:B:2172:HOH:O	1:C:239[B]:SER:O	2.16	0.61
1:A:79[B]:GLN:NE2	5:A:2089:HOH:O	2.33	0.61
1:D:99[B]:MET:O	1:D:103[B]:ARG:HG2	2.00	0.61
1:H:18:ARG:HH12	1:H:194:ARG:HD2	1.66	0.61
1:B:101[A]:ASP:OD2	1:B:113:GLY:HA3	2.01	0.61
1:G:103[B]:ARG:NH1	4:G:1002[B]:GLU:CA	2.51	0.61
1:B:101[A]:ASP:OD2	5:B:2098:HOH:O	2.15	0.60
1:F:42[B]:GLU:HG3	5:F:2042:HOH:O	2.00	0.60
1:G:103[B]:ARG:HH22	4:G:1002[B]:GLU:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HD3	5:A:2135:HOH:O	2.02	0.59
1:D:194:ARG:HD2	5:D:2016:HOH:O	2.02	0.59
4:B:1002[A]:GLU:N	5:D:2113:HOH:O	2.35	0.59
1:A:100[A]:GLU:HG3	1:E:43:ARG:HG2	1.83	0.59
1:F:2:VAL:HG21	1:F:235:SER:HB2	1.84	0.59
1:F:103[B]:ARG:HB2	5:F:2088:HOH:O	2.01	0.58
1:B:101[B]:ASP:HB3	1:B:159:VAL:HG11	1.84	0.58
1:F:101[B]:ASP:O	1:F:159:VAL:HG12	2.05	0.57
1:G:215:ALA:O	1:G:218:LYS:HD3	2.04	0.57
1:C:2:VAL:HG13	1:C:2:VAL:O	2.04	0.57
1:B:2:VAL:C	1:B:3:ASN:OD1	2.43	0.57
1:H:101[B]:ASP:C	1:H:103[B]:ARG:H	2.08	0.57
1:E:203:GLY:H	4:E:1002[B]:GLU:HG2	1.69	0.56
1:G:89:GLY:HA2	1:G:136:MET:HE3	1.85	0.56
1:F:210:GLU:HG3	1:F:214[B]:ARG:HD2	1.88	0.56
1:E:2:VAL:HG13	1:E:2:VAL:O	2.05	0.56
1:A:104[B]:GLY:HA3	1:E:43:ARG:HH21	1.71	0.56
1:E:101[A]:ASP:HB3	1:E:159:VAL:CG1	2.35	0.56
1:G:89:GLY:N	1:G:136:MET:CE	2.68	0.56
1:H:100[B]:GLU:CD	1:H:100[B]:GLU:N	2.60	0.55
1:D:42[B]:GLU:HG3	5:D:2029:HOH:O	2.06	0.55
1:G:203:GLY:H	4:G:1002[B]:GLU:HB3	1.71	0.55
1:H:103[A]:ARG:NH2	1:H:200:GLY:O	2.40	0.55
1:E:43:ARG:HG3	1:E:43:ARG:HH11	1.70	0.55
1:A:48:LEU:O	1:A:52:LEU:HD23	2.07	0.54
1:F:18:ARG:NH2	1:F:199:LYS:NZ	2.54	0.54
1:B:103[A]:ARG:HH22	4:B:1002[A]:GLU:CG	2.15	0.54
1:F:101[B]:ASP:HB3	1:F:159:VAL:CG1	2.38	0.54
5:E:2166:HOH:O	1:G:155:GLN:OE1	2.19	0.54
1:H:37:PHE:HB2	1:H:62:LEU:HD12	1.90	0.54
1:A:202:GLY:HA2	4:A:1002[B]:GLU:HG3	1.90	0.54
5:B:2202:HOH:O	4:F:1003:GLU:OXT	2.19	0.54
1:F:210:GLU:OE2	1:F:214[B]:ARG:HD2	2.07	0.54
5:B:2074:HOH:O	1:E:45[B]:ARG:NH1	2.40	0.53
1:G:59:GLU:HG3	1:G:61:HIS:CE1	2.43	0.53
1:E:102[A]:LEU:CB	1:E:200:GLY:O	2.56	0.53
1:G:89:GLY:CA	1:G:136:MET:HE3	2.38	0.53
1:H:15:ALA:O	1:H:47:GLU:HG2	2.08	0.53
1:C:34:LYS:HD3	5:C:2060:HOH:O	2.09	0.53
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.90	0.53
1:E:5:GLU:O	1:E:6:ASN:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101[B]:ASP:HB3	1:F:159:VAL:HG11	1.91	0.52
1:F:194:ARG:HG3	5:F:2018:HOH:O	2.10	0.52
1:H:101[B]:ASP:C	1:H:103[B]:ARG:N	2.63	0.52
1:G:202:GLY:HA2	4:G:1002[B]:GLU:HA	1.91	0.52
1:C:203:GLY:H	4:D:1002[B]:GLU:HB2	1.75	0.51
5:E:2156:HOH:O	1:G:214:ARG:CD	2.57	0.51
1:E:210:GLU:HG3	1:E:214[A]:ARG:HD3	1.91	0.51
1:G:88:ASP:C	1:G:136:MET:CE	2.79	0.51
5:B:2198:HOH:O	1:F:7:LYS:HD2	2.08	0.51
1:A:203:GLY:H	4:A:1002[A]:GLU:HB3	1.74	0.51
1:C:103[A]:ARG:NH1	4:D:1002[A]:GLU:O	2.37	0.51
1:D:205[B]:ASN:H	1:D:205[B]:ASN:HD22	1.58	0.51
1:G:192:PRO:HG3	1:G:207:ILE:HG22	1.92	0.51
1:D:84:VAL:O	1:D:84:VAL:HG12	2.11	0.51
1:B:39:TYR:OH	1:B:45[A]:ARG:HD2	2.11	0.50
1:B:102[B]:LEU:HB2	1:B:200:GLY:O	2.11	0.50
1:B:215:ALA:O	1:B:218:LYS:HD2	2.11	0.50
1:B:42[B]:GLU:OE1	1:B:45[B]:ARG:NH2	2.44	0.50
1:E:102[A]:LEU:HB2	1:E:200:GLY:O	2.12	0.50
1:A:203:GLY:N	4:A:1002[B]:GLU:HG3	2.22	0.50
1:A:54:GLN:HG3	5:A:2065:HOH:O	2.11	0.50
1:A:101[A]:ASP:HB3	1:A:159:VAL:CG1	2.42	0.49
1:B:214[B]:ARG:NH2	5:B:2165:HOH:O	2.44	0.49
1:C:133:LYS:HE3	1:D:105[B]:ARG:HH12	1.76	0.49
1:A:203:GLY:H	4:A:1002[B]:GLU:CG	2.22	0.49
1:G:103[B]:ARG:NH1	4:G:1002[B]:GLU:HA	2.21	0.49
1:C:101[A]:ASP:O	1:C:159:VAL:HG12	2.13	0.49
1:H:18:ARG:NH1	1:H:194:ARG:HD2	2.27	0.49
1:B:103[A]:ARG:NH1	4:B:1002[A]:GLU:O	2.46	0.48
1:A:50:LYS:HE2	5:A:2057:HOH:O	2.12	0.48
1:G:8:THR:HG21	1:G:84:VAL:HG11	1.94	0.48
1:C:5:GLU:O	1:C:6:ASN:CB	2.60	0.48
1:B:102[B]:LEU:CB	1:B:200:GLY:O	2.61	0.48
1:B:2:VAL:HG11	1:B:235:SER:CB	2.44	0.48
1:C:184:ARG:NH2	4:C:1002:GLU:HG2	2.27	0.48
1:E:43:ARG:HG3	1:E:43:ARG:NH1	2.28	0.47
1:G:59:GLU:HG3	1:G:61:HIS:NE2	2.28	0.47
1:A:196:LEU:HD21	1:E:100[A]:GLU:HB3	1.96	0.47
1:B:192:PRO:HG3	1:B:207:ILE:HG22	1.96	0.47
1:C:101[B]:ASP:OD2	1:C:113:GLY:HA3	2.14	0.47
1:D:41:LYS:HG3	1:D:43:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100[A]:GLU:H	1:G:100[A]:GLU:CD	2.18	0.47
1:C:133:LYS:HD2	1:C:178:LEU:HD22	1.97	0.47
1:E:101[A]:ASP:HB3	1:E:159:VAL:HG11	1.96	0.47
5:E:2156:HOH:O	1:G:214:ARG:HD2	2.14	0.47
1:H:5:GLU:O	1:H:6:ASN:HB2	2.15	0.46
1:D:40:ARG:HD3	2:D:400:NAP:C6A	2.45	0.46
1:G:41:LYS:HE3	5:G:2034:HOH:O	2.15	0.46
1:B:214[A]:ARG:NH2	1:D:210:GLU:OE2	2.48	0.46
1:G:42[B]:GLU:OE1	1:G:45[B]:ARG:NE	2.48	0.46
1:F:5:GLU:O	1:F:6:ASN:HB2	2.15	0.46
1:G:42[B]:GLU:OE1	1:G:45[B]:ARG:CZ	2.63	0.46
1:F:255:ILE:O	1:H:256:LYS:HE2	2.16	0.46
1:E:99[B]:MET:SD	1:E:200:GLY:HA2	2.56	0.46
1:H:104[B]:GLY:CA	5:H:2049:HOH:O	2.64	0.46
1:H:42[B]:GLU:H	1:H:42[B]:GLU:CD	2.18	0.45
1:G:101[A]:ASP:HB3	1:G:159:VAL:CG1	2.46	0.45
1:D:7:LYS:NZ	5:D:2006:HOH:O	2.50	0.45
1:G:16:ASN:HA	1:G:47:GLU:HG2	1.97	0.45
1:G:154:VAL:HG13	5:G:2115:HOH:O	2.02	0.45
1:F:102[B]:LEU:HD13	3:F:1001:E9P:H10	1.98	0.45
1:G:43:ARG:NH1	5:G:2044:HOH:O	2.17	0.45
1:H:101[B]:ASP:O	1:H:102[B]:LEU:C	2.53	0.45
1:F:42[A]:GLU:OE1	5:F:2042:HOH:O	2.21	0.45
1:A:99[B]:MET:SD	1:A:200:GLY:HA2	2.57	0.45
5:A:2233:HOH:O	1:D:196:LEU:HD23	2.17	0.45
1:G:38:THR:HA	1:G:63:TYR:O	2.17	0.45
1:H:59:GLU:HG3	1:H:61:HIS:NE2	2.31	0.44
1:F:2:VAL:CG2	1:F:4:LEU:HD21	2.47	0.44
1:C:101[A]:ASP:HB3	1:C:159:VAL:CG1	2.47	0.44
1:B:45[B]:ARG:HD2	1:B:49:GLU:OE2	2.18	0.44
1:G:214:ARG:NH1	5:G:2149:HOH:O	2.26	0.44
1:H:98:ASN:O	1:H:102[B]:LEU:HD12	2.18	0.44
1:H:40:ARG:HD3	2:H:400:NAP:C6A	2.48	0.44
1:D:103[B]:ARG:NH1	1:D:202:GLY:HA2	2.32	0.44
1:F:43[A]:ARG:HG3	1:F:43[A]:ARG:HH11	1.83	0.44
1:H:101[B]:ASP:OD2	1:H:113:GLY:HA3	2.18	0.43
1:E:98:ASN:HB3	1:E:100[B]:GLU:HG3	2.00	0.43
1:H:46:LYS:HB3	1:H:46:LYS:HE3	1.46	0.43
1:C:184:ARG:HH21	4:C:1002:GLU:CG	2.25	0.43
1:F:2:VAL:O	1:F:31:LEU:HD22	2.19	0.43
1:C:192:PRO:HG3	1:C:207:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ASN:HD21	1:C:5:GLU:HG3	1.84	0.43
1:E:2:VAL:HG12	1:H:2:VAL:N	2.34	0.43
1:F:155:GLN:NE2	5:F:2120:HOH:O	2.51	0.43
1:B:210:GLU:OE2	1:B:214[A]:ARG:NE	2.51	0.43
1:C:133:LYS:HE3	1:D:105[B]:ARG:NH1	2.34	0.43
1:E:102[A]:LEU:HB3	1:E:200:GLY:O	2.18	0.43
1:H:18:ARG:HH11	1:H:194:ARG:HG2	1.84	0.43
1:D:157:TYR:CZ	1:D:160:MET:HG3	2.53	0.43
1:A:58:PRO:HD2	5:A:2066:HOH:O	2.19	0.43
1:H:42[A]:GLU:HA	1:H:42[A]:GLU:OE1	2.19	0.42
1:D:38:THR:HA	1:D:63:TYR:O	2.19	0.42
1:E:18[A]:ARG:NH1	1:E:199:LYS:NZ	2.62	0.42
1:C:103[A]:ARG:HB3	1:C:103[A]:ARG:CZ	2.49	0.42
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.54	0.42
1:B:101[B]:ASP:O	1:B:159:VAL:HG12	2.19	0.42
1:A:101[B]:ASP:OD2	5:A:2106:HOH:O	2.20	0.42
1:B:101[B]:ASP:CB	1:B:159:VAL:HG11	2.47	0.42
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.54	0.42
1:E:16:ASN:HD21	1:E:18[A]:ARG:HH21	1.68	0.42
1:E:214[A]:ARG:NH2	5:E:2161:HOH:O	2.53	0.42
1:G:39:TYR:CE2	1:G:45[A]:ARG:HB2	2.55	0.42
1:B:160:MET:O	1:B:164:LYS:HG2	2.20	0.42
1:F:42[B]:GLU:OE1	1:F:45[B]:ARG:NH2	2.49	0.42
1:C:18[A]:ARG:HD2	5:C:2016:HOH:O	2.20	0.42
1:G:39:TYR:CE2	1:G:45[B]:ARG:HB2	2.54	0.41
1:A:100[A]:GLU:HB2	5:A:2110:HOH:O	2.20	0.41
1:A:18:ARG:HD3	5:A:2016:HOH:O	2.21	0.41
1:D:39:TYR:CZ	1:D:64:GLN:HB2	2.56	0.41
1:E:100[A]:GLU:HA	1:E:103[A]:ARG:HD2	2.02	0.41
1:F:43[A]:ARG:HG3	1:F:43[A]:ARG:NH1	2.36	0.41
5:E:2156:HOH:O	1:G:214:ARG:NH1	2.54	0.41
1:B:5:GLU:O	1:B:6:ASN:HB2	2.20	0.41
1:E:18[A]:ARG:HH12	1:E:199:LYS:HZ1	1.66	0.41
1:E:256:LYS:HE3	1:G:148:LEU:HD21	2.02	0.41
1:B:133:LYS:HE2	1:B:181:ASP:OD2	2.21	0.41
1:B:256:LYS:HE3	1:D:148:LEU:HD21	2.03	0.41
1:H:39:TYR:OH	1:H:45:ARG:NH1	2.47	0.40
1:G:237:LEU:HD23	1:G:237:LEU:HA	1.89	0.40
1:F:52:LEU:HD13	1:F:60:ALA:HB2	2.03	0.40
1:D:195:THR:H	1:D:198:ALA:HB3	1.86	0.40
1:H:209:LYS:HE3	1:H:209:LYS:HB2	1.86	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:G:42[A]:GLU:OE2	5:A:2084:HOH:O[1_554]	1.94	0.26

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	268/282 (95%)	255 (95%)	13 (5%)	0	100	100
1	B	272/282 (96%)	258 (95%)	14 (5%)	0	100	100
1	C	266/282 (94%)	256 (96%)	10 (4%)	0	100	100
1	D	264/282 (94%)	249 (94%)	13 (5%)	2 (1%)	19	9
1	E	271/282 (96%)	261 (96%)	10 (4%)	0	100	100
1	F	268/282 (95%)	258 (96%)	10 (4%)	0	100	100
1	G	265/282 (94%)	257 (97%)	8 (3%)	0	100	100
1	H	265/282 (94%)	251 (95%)	10 (4%)	4 (2%)	10	3
All	All	2139/2256 (95%)	2045 (96%)	88 (4%)	6 (0%)	51	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105[A]	ARG
1	D	105[B]	ARG
1	H	102[A]	LEU
1	H	102[B]	LEU
1	H	101[A]	ASP
1	H	101[B]	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/234 (95%)	214 (96%)	8 (4%)	35	26
1	B	226/234 (97%)	222 (98%)	4 (2%)	59	55
1	C	220/234 (94%)	218 (99%)	2 (1%)	78	79
1	D	218/234 (93%)	209 (96%)	9 (4%)	30	21
1	E	225/234 (96%)	221 (98%)	4 (2%)	59	55
1	F	222/234 (95%)	215 (97%)	7 (3%)	39	30
1	G	219/234 (94%)	213 (97%)	6 (3%)	44	38
1	H	219/234 (94%)	214 (98%)	5 (2%)	50	45
All	All	1771/1872 (95%)	1726 (98%)	45 (2%)	49	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	99[A]	MET
1	A	99[B]	MET
1	A	100[A]	GLU
1	A	100[B]	GLU
1	A	138	GLU
1	A	199[A]	LYS
1	A	199[B]	LYS
1	B	2	VAL
1	B	4	LEU
1	B	55	LEU
1	B	209	LYS
1	C	55	LEU
1	C	209	LYS
1	D	4	LEU
1	D	30	GLN
1	D	41	LYS
1	D	42[A]	GLU
1	D	42[B]	GLU

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Mol	Chain	Res	Type
1	D	43	ARG
1	D	56	ASN
1	D	155[A]	GLN
1	D	155[B]	GLN
1	E	35	LEU
1	E	103[A]	ARG
1	E	103[B]	ARG
1	E	112	GLU
1	F	2	VAL
1	F	55	LEU
1	F	62	LEU
1	F	100[A]	GLU
1	F	100[B]	GLU
1	F	112	GLU
1	F	218	LYS
1	G	30	GLN
1	G	55	LEU
1	G	62	LEU
1	G	99[A]	MET
1	G	99[B]	MET
1	G	112	GLU
1	H	46	LYS
1	H	52	LEU
1	H	59	GLU
1	H	62	LEU
1	H	78	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	B	253	HIS
1	C	3	ASN
1	C	253	HIS
1	E	253	HIS
1	F	155	GLN
1	F	253	HIS
1	G	30	GLN
1	G	56	ASN
1	G	79	GLN
1	G	155	GLN
1	H	64	GLN

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Mol	Chain	Res	Type
1	H	253	HIS

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](#)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GLU	F	1002[A]	-	2,9,9	0.30	0	2,11,11	0.66	0
2	NAP	D	400	-	45,52,52	1.75	4 (8%)	56,80,80	1.58	9 (16%)
2	NAP	E	400	-	45,52,52	1.74	5 (11%)	56,80,80	1.68	7 (12%)
4	GLU	D	1002[B]	-	2,9,9	0.65	0	2,11,11	1.41	0
4	GLU	F	1003	-	2,9,9	0.18	0	2,11,11	2.50	2 (100%)
2	NAP	C	400	-	45,52,52	1.45	5 (11%)	56,80,80	1.81	10 (17%)
4	GLU	D	1002[A]	-	2,9,9	0.32	0	2,11,11	0.78	0
2	NAP	F	400	-	45,52,52	1.59	5 (11%)	56,80,80	1.64	8 (14%)
3	E9P	A	1001	-	17,17,17	0.87	1 (5%)	22,22,22	0.95	1 (4%)
3	E9P	G	1001	-	17,17,17	0.86	0	22,22,22	1.10	3 (13%)
2	NAP	H	400	-	45,52,52	1.65	5 (11%)	56,80,80	1.79	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLU	C	1002	-	2,9,9	0.27	0	2,11,11	2.16	1 (50%)
2	NAP	A	400	-	45,52,52	1.65	6 (13%)	56,80,80	1.96	7 (12%)
2	NAP	G	400	-	45,52,52	1.45	5 (11%)	56,80,80	1.95	9 (16%)
3	E9P	C	1001	-	17,17,17	0.91	0	22,22,22	1.00	0
3	E9P	E	1001	-	17,17,17	0.84	1 (5%)	22,22,22	0.87	1 (4%)
4	GLU	A	1002[A]	-	2,9,9	0.23	0	2,11,11	1.10	0
4	GLU	A	1002[B]	-	2,9,9	0.32	0	2,11,11	0.84	0
4	GLU	E	1002[A]	-	2,9,9	0.27	0	2,11,11	0.66	0
4	GLU	E	1002[B]	-	2,9,9	0.16	0	2,11,11	0.55	0
3	E9P	B	1001	-	17,17,17	0.64	0	22,22,22	0.80	0
3	E9P	D	1001	-	17,17,17	0.61	0	22,22,22	0.67	0
3	E9P	H	1001	-	17,17,17	0.66	0	22,22,22	1.05	2 (9%)
2	NAP	B	400	-	45,52,52	1.69	6 (13%)	56,80,80	1.67	8 (14%)
3	E9P	F	1001	-	17,17,17	0.91	0	22,22,22	0.77	0
4	GLU	G	1002[B]	-	2,9,9	0.29	0	2,11,11	0.63	0
4	GLU	G	1002[A]	-	2,9,9	0.25	0	2,11,11	0.85	0
4	GLU	B	1002[B]	-	2,9,9	0.24	0	2,11,11	0.16	0
4	GLU	B	1002[A]	-	2,9,9	0.21	0	2,11,11	1.41	0
4	GLU	F	1002[B]	-	2,9,9	0.40	0	2,11,11	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLU	F	1002[A]	-	-	3/3/9/9	-
2	NAP	D	400	-	-	6/31/67/67	0/5/5/5
2	NAP	E	400	-	-	7/31/67/67	0/5/5/5
4	GLU	D	1002[B]	-	-	2/3/9/9	-
4	GLU	F	1003	-	-	0/3/9/9	-
2	NAP	C	400	-	-	6/31/67/67	0/5/5/5
4	GLU	D	1002[A]	-	-	2/3/9/9	-
2	NAP	F	400	-	-	6/31/67/67	0/5/5/5
3	E9P	A	1001	-	-	0/6/6/6	0/2/2/2
3	E9P	G	1001	-	-	0/6/6/6	0/2/2/2
2	NAP	H	400	-	-	9/31/67/67	0/5/5/5
4	GLU	C	1002	-	-	3/3/9/9	-
2	NAP	A	400	-	-	6/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	G	400	-	-	5/31/67/67	0/5/5/5
3	E9P	C	1001	-	-	0/6/6/6	0/2/2/2
3	E9P	E	1001	-	-	0/6/6/6	0/2/2/2
4	GLU	A	1002[A]	-	-	1/3/9/9	-
4	GLU	A	1002[B]	-	-	1/3/9/9	-
4	GLU	E	1002[A]	-	-	2/3/9/9	-
4	GLU	E	1002[B]	-	-	3/3/9/9	-
3	E9P	B	1001	-	-	0/6/6/6	0/2/2/2
3	E9P	D	1001	-	-	0/6/6/6	0/2/2/2
3	E9P	H	1001	-	-	0/6/6/6	0/2/2/2
2	NAP	B	400	-	-	6/31/67/67	0/5/5/5
3	E9P	F	1001	-	-	0/6/6/6	0/2/2/2
4	GLU	G	1002[B]	-	-	3/3/9/9	-
4	GLU	G	1002[A]	-	-	3/3/9/9	-
4	GLU	B	1002[B]	-	-	0/3/9/9	-
4	GLU	B	1002[A]	-	-	3/3/9/9	-
4	GLU	F	1002[B]	-	-	3/3/9/9	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAP	O7N-C7N	8.87	1.41	1.24
2	H	400	NAP	O7N-C7N	7.63	1.38	1.24
2	E	400	NAP	O7N-C7N	7.57	1.38	1.24
2	B	400	NAP	O7N-C7N	6.87	1.37	1.24
2	A	400	NAP	O7N-C7N	6.75	1.37	1.24
2	F	400	NAP	O7N-C7N	6.67	1.36	1.24
2	G	400	NAP	O7N-C7N	6.63	1.36	1.24
2	C	400	NAP	O7N-C7N	6.32	1.36	1.24
2	B	400	NAP	C2A-N3A	5.33	1.40	1.32
2	D	400	NAP	C2A-N3A	4.60	1.39	1.32
2	F	400	NAP	C2A-N3A	4.52	1.39	1.32
2	A	400	NAP	C2A-N3A	4.41	1.39	1.32
2	E	400	NAP	C2A-N3A	4.19	1.38	1.32
2	H	400	NAP	C2A-N3A	4.18	1.38	1.32
2	C	400	NAP	P2B-O2B	3.32	1.65	1.59
2	E	400	NAP	C2N-N1N	3.31	1.39	1.35
2	E	400	NAP	P2B-O2B	3.27	1.65	1.59
2	B	400	NAP	P2B-O2B	3.21	1.65	1.59
2	A	400	NAP	C2N-N1N	3.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	NAP	C2A-N3A	3.15	1.37	1.32
2	F	400	NAP	C2N-N1N	3.05	1.38	1.35
2	F	400	NAP	P2B-O2B	3.05	1.65	1.59
2	H	400	NAP	C2N-N1N	3.02	1.38	1.35
2	D	400	NAP	C2A-N1A	2.91	1.39	1.33
2	C	400	NAP	C2A-N3A	2.91	1.36	1.32
2	A	400	NAP	P2B-O2B	2.81	1.64	1.59
2	E	400	NAP	C2A-N1A	2.74	1.39	1.33
2	B	400	NAP	C2N-N1N	2.63	1.38	1.35
2	C	400	NAP	C2N-N1N	2.63	1.38	1.35
2	B	400	NAP	C2A-N1A	2.61	1.38	1.33
2	A	400	NAP	C2A-N1A	2.54	1.38	1.33
2	H	400	NAP	C2A-N1A	2.52	1.38	1.33
2	G	400	NAP	P2B-O2B	2.49	1.64	1.59
2	G	400	NAP	C2N-N1N	2.47	1.38	1.35
3	A	1001	E9P	O7-C8	-2.45	1.34	1.39
3	E	1001	E9P	O7-C8	-2.43	1.34	1.39
2	H	400	NAP	P2B-O2B	2.40	1.63	1.59
2	C	400	NAP	C2A-N1A	2.36	1.38	1.33
2	A	400	NAP	PN-O2N	-2.26	1.44	1.55
2	F	400	NAP	C2A-N1A	2.26	1.38	1.33
2	D	400	NAP	P2B-O2B	2.20	1.63	1.59
2	B	400	NAP	C3N-C7N	2.08	1.53	1.50
2	G	400	NAP	C2A-N1A	2.02	1.37	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	400	NAP	C3N-C7N-N7N	8.99	128.54	117.75
2	A	400	NAP	C3N-C7N-N7N	8.14	127.52	117.75
2	A	400	NAP	O7N-C7N-C3N	-7.77	110.33	119.63
2	H	400	NAP	N3A-C2A-N1A	-7.12	117.54	128.68
2	C	400	NAP	C3N-C7N-N7N	6.76	125.86	117.75
2	B	400	NAP	C3N-C7N-N7N	6.54	125.60	117.75
2	E	400	NAP	C3N-C7N-N7N	6.23	125.23	117.75
2	F	400	NAP	C3N-C7N-N7N	6.02	124.98	117.75
2	F	400	NAP	N3A-C2A-N1A	-5.99	119.31	128.68
2	H	400	NAP	O7N-C7N-C3N	-5.92	112.54	119.63
2	G	400	NAP	O7N-C7N-C3N	-5.42	113.14	119.63
2	G	400	NAP	N3A-C2A-N1A	-5.18	120.58	128.68
2	C	400	NAP	O7N-C7N-C3N	-5.18	113.43	119.63
2	A	400	NAP	N3A-C2A-N1A	-5.17	120.61	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	NAP	N3A-C2A-N1A	-5.15	120.63	128.68
2	D	400	NAP	O7N-C7N-C3N	-5.05	113.58	119.63
2	H	400	NAP	C3N-C7N-N7N	4.89	123.62	117.75
2	C	400	NAP	C2N-C3N-C4N	4.74	123.63	118.26
2	D	400	NAP	N3A-C2A-N1A	-4.62	121.46	128.68
2	B	400	NAP	N3A-C2A-N1A	-4.46	121.71	128.68
2	D	400	NAP	C3N-C7N-N7N	4.25	122.85	117.75
2	C	400	NAP	N3A-C2A-N1A	-3.83	122.69	128.68
2	F	400	NAP	O2N-PN-O1N	3.39	129.00	112.24
2	C	400	NAP	C5N-C4N-C3N	-3.38	116.34	120.34
2	E	400	NAP	O7N-C7N-N7N	-3.35	117.82	122.58
2	B	400	NAP	O7N-C7N-N7N	-3.29	117.91	122.58
3	H	1001	E9P	O7-C1-C2	3.27	122.34	116.22
2	F	400	NAP	O7N-C7N-N7N	-3.10	118.17	122.58
2	G	400	NAP	O7N-C7N-N7N	-3.07	118.21	122.58
2	D	400	NAP	O4D-C1D-C2D	-3.07	102.43	106.93
2	E	400	NAP	O3X-P2B-O2X	3.07	119.38	107.64
4	C	1002	GLU	CG-CB-CA	-3.04	106.76	113.84
2	D	400	NAP	O4B-C1B-C2B	-3.00	101.38	106.59
2	B	400	NAP	O2N-PN-O1N	2.91	126.64	112.24
2	F	400	NAP	O3X-P2B-O2X	2.87	118.59	107.64
2	G	400	NAP	O4B-C1B-C2B	-2.85	101.64	106.59
4	F	1003	GLU	CG-CB-CA	-2.79	107.34	113.84
2	B	400	NAP	C1B-N9A-C4A	-2.75	121.81	126.64
2	E	400	NAP	O7N-C7N-C3N	-2.69	116.42	119.63
3	H	1001	E9P	C1-O7-C8	-2.66	111.36	118.00
2	B	400	NAP	O7N-C7N-C3N	-2.64	116.48	119.63
2	H	400	NAP	C1B-N9A-C4A	-2.55	122.16	126.64
2	H	400	NAP	O4B-C1B-C2B	-2.54	102.17	106.59
2	A	400	NAP	C3N-C2N-N1N	-2.49	117.99	120.43
2	H	400	NAP	C2A-N1A-C6A	2.49	123.01	118.75
2	B	400	NAP	C4A-C5A-N7A	-2.48	106.81	109.40
2	D	400	NAP	O2B-P2B-O1X	-2.46	99.91	109.39
2	A	400	NAP	O4D-C1D-C2D	-2.42	103.38	106.93
2	E	400	NAP	C6N-N1N-C2N	-2.42	119.77	121.97
2	C	400	NAP	C6N-N1N-C2N	-2.41	119.78	121.97
2	F	400	NAP	O7N-C7N-C3N	-2.40	116.75	119.63
2	A	400	NAP	O4B-C1B-C2B	-2.36	102.48	106.59
2	F	400	NAP	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	400	NAP	O3X-P2B-O1X	2.36	119.92	110.68
2	H	400	NAP	O2N-PN-O1N	2.36	123.90	112.24
2	G	400	NAP	C1B-N9A-C4A	-2.32	122.57	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	400	NAP	O2X-P2B-O1X	-2.25	101.87	110.68
3	E	1001	E9P	C2-C3-C4	-2.24	118.44	120.83
3	G	1001	E9P	C6-C1-C2	-2.21	117.10	119.86
2	G	400	NAP	C5N-C4N-C3N	-2.20	117.74	120.34
2	D	400	NAP	C2N-C3N-C4N	2.20	120.75	118.26
3	A	1001	E9P	C2-C3-C4	-2.19	118.51	120.83
4	F	1003	GLU	CB-CG-CD	-2.18	108.91	113.59
2	D	400	NAP	C5N-C4N-C3N	-2.17	117.77	120.34
2	C	400	NAP	C3N-C2N-N1N	-2.14	118.33	120.43
3	G	1001	E9P	O7-C1-C2	2.13	120.20	116.22
2	G	400	NAP	C2N-C3N-C4N	2.12	120.66	118.26
2	C	400	NAP	C1B-N9A-C4A	-2.11	122.93	126.64
3	G	1001	E9P	C3-C2-C1	2.11	121.97	119.81
2	C	400	NAP	O4D-C1D-C2D	-2.10	103.85	106.93
2	A	400	NAP	O2N-PN-O1N	2.08	122.52	112.24
2	C	400	NAP	O4B-C1B-C2B	-2.08	102.98	106.59
2	G	400	NAP	C6N-N1N-C2N	-2.07	120.09	121.97
2	F	400	NAP	C1B-N9A-C4A	-2.07	123.01	126.64
2	H	400	NAP	C2N-C3N-C4N	2.05	120.58	118.26
2	H	400	NAP	O3X-P2B-O1X	2.04	118.66	110.68
2	D	400	NAP	O2N-PN-O1N	2.02	122.25	112.24
2	E	400	NAP	O2D-C2D-C3D	2.02	118.34	111.82

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1002[A]	GLU	N-CA-CB-CG
4	F	1002[A]	GLU	C-CA-CB-CG
2	D	400	NAP	C5D-O5D-PN-O1N
2	D	400	NAP	C5D-O5D-PN-O2N
2	D	400	NAP	O4D-C1D-N1N-C2N
2	E	400	NAP	PN-O3-PA-O5B
2	E	400	NAP	C5D-O5D-PN-O1N
2	E	400	NAP	C5D-O5D-PN-O2N
2	E	400	NAP	O4D-C1D-N1N-C2N
2	E	400	NAP	O4D-C1D-N1N-C6N
4	D	1002[B]	GLU	N-CA-CB-CG
4	D	1002[B]	GLU	C-CA-CB-CG
2	C	400	NAP	C5D-O5D-PN-O1N
2	C	400	NAP	C5D-O5D-PN-O2N
2	C	400	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	D	1002[A]	GLU	N-CA-CB-CG
4	D	1002[A]	GLU	C-CA-CB-CG
2	F	400	NAP	C5D-O5D-PN-O1N
2	F	400	NAP	C5D-O5D-PN-O2N
2	F	400	NAP	O4D-C1D-N1N-C2N
2	H	400	NAP	C5B-O5B-PA-O2A
2	H	400	NAP	C5D-O5D-PN-O1N
2	H	400	NAP	C5D-O5D-PN-O2N
2	H	400	NAP	O4D-C1D-N1N-C2N
4	C	1002	GLU	N-CA-CB-CG
4	C	1002	GLU	C-CA-CB-CG
4	C	1002	GLU	CA-CB-CG-CD
2	A	400	NAP	C5D-O5D-PN-O3
2	A	400	NAP	C5D-O5D-PN-O1N
2	A	400	NAP	O4D-C1D-N1N-C2N
2	G	400	NAP	PN-O3-PA-O5B
2	G	400	NAP	C5D-O5D-PN-O3
2	G	400	NAP	C5D-O5D-PN-O1N
2	G	400	NAP	O4D-C1D-N1N-C2N
4	A	1002[B]	GLU	C-CA-CB-CG
4	E	1002[A]	GLU	C-CA-CB-CG
4	E	1002[B]	GLU	C-CA-CB-CG
4	E	1002[B]	GLU	CA-CB-CG-CD
2	B	400	NAP	C5D-O5D-PN-O1N
2	B	400	NAP	C5D-O5D-PN-O2N
2	B	400	NAP	O4D-C1D-N1N-C2N
4	G	1002[B]	GLU	N-CA-CB-CG
4	G	1002[B]	GLU	C-CA-CB-CG
4	G	1002[A]	GLU	N-CA-CB-CG
4	G	1002[A]	GLU	C-CA-CB-CG
4	G	1002[A]	GLU	CA-CB-CG-CD
4	B	1002[A]	GLU	N-CA-CB-CG
4	B	1002[A]	GLU	C-CA-CB-CG
4	F	1002[B]	GLU	C-CA-CB-CG
4	F	1002[A]	GLU	CA-CB-CG-CD
4	B	1002[A]	GLU	CA-CB-CG-CD
2	H	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	PN-O3-PA-O5B
2	H	400	NAP	PN-O3-PA-O5B
2	A	400	NAP	PN-O3-PA-O5B
2	B	400	NAP	PN-O3-PA-O5B
2	E	400	NAP	C5D-O5D-PN-O3

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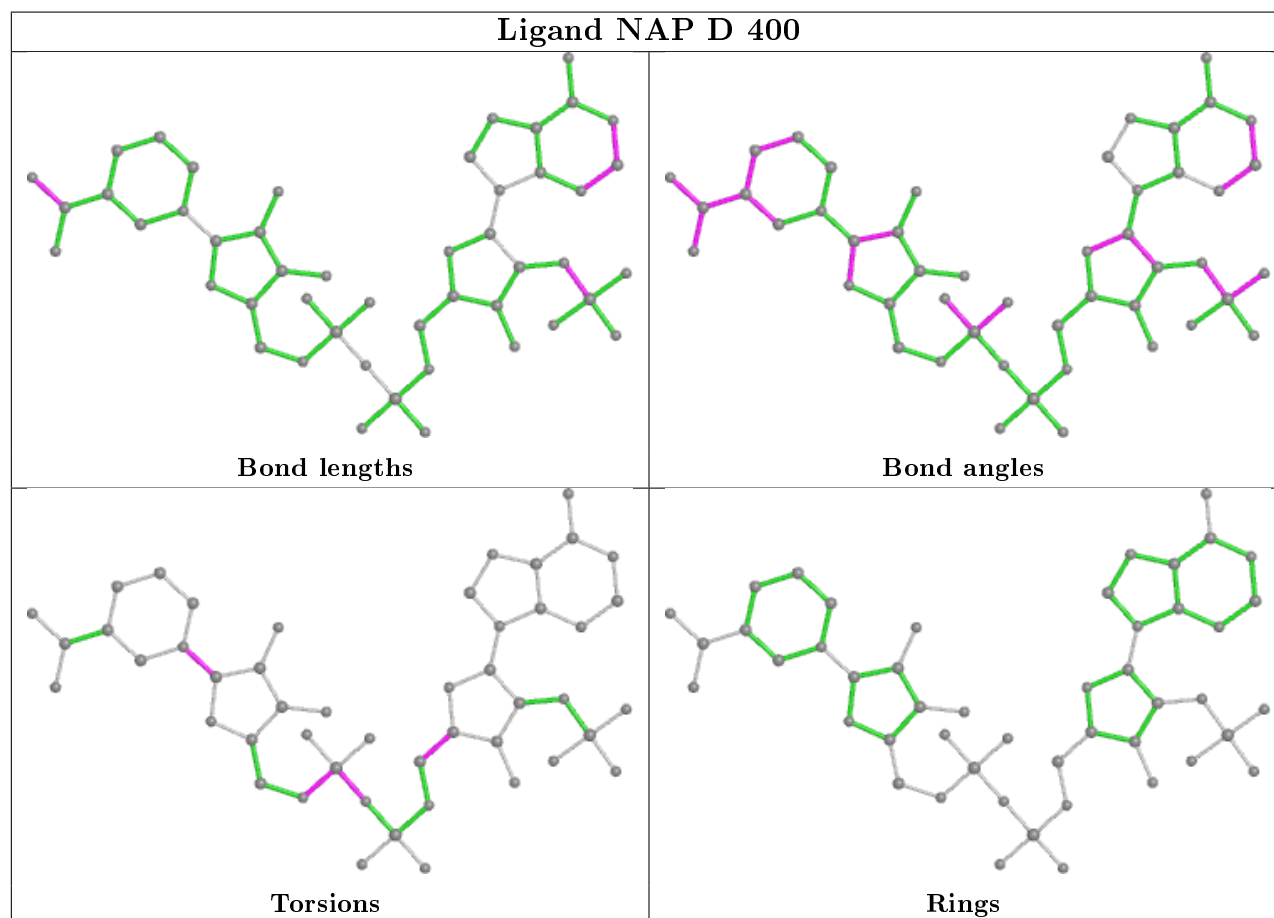
Mol	Chain	Res	Type	Atoms
2	C	400	NAP	C5D-O5D-PN-O3
4	E	1002[A]	GLU	N-CA-CB-CG
4	F	1002[B]	GLU	N-CA-CB-CG
4	F	1002[B]	GLU	CA-CB-CG-CD
4	G	1002[B]	GLU	CA-CB-CG-CD
2	D	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	O4B-C4B-C5B-O5B
2	H	400	NAP	C3B-C4B-C5B-O5B
2	D	400	NAP	C5D-O5D-PN-O3
2	F	400	NAP	C5D-O5D-PN-O3
2	H	400	NAP	C5D-O5D-PN-O3
2	A	400	NAP	C2D-C1D-N1N-C6N
2	B	400	NAP	C5D-O5D-PN-O3
2	F	400	NAP	O4B-C4B-C5B-O5B
2	B	400	NAP	O4B-C4B-C5B-O5B
2	D	400	NAP	PA-O3-PN-O2N
2	F	400	NAP	PA-O3-PN-O2N
2	H	400	NAP	C5B-O5B-PA-O1A
2	E	400	NAP	O4B-C4B-C5B-O5B
2	A	400	NAP	O4B-C4B-C5B-O5B
2	G	400	NAP	O4B-C4B-C5B-O5B
4	A	1002[A]	GLU	N-CA-CB-CG
4	E	1002[B]	GLU	N-CA-CB-CG

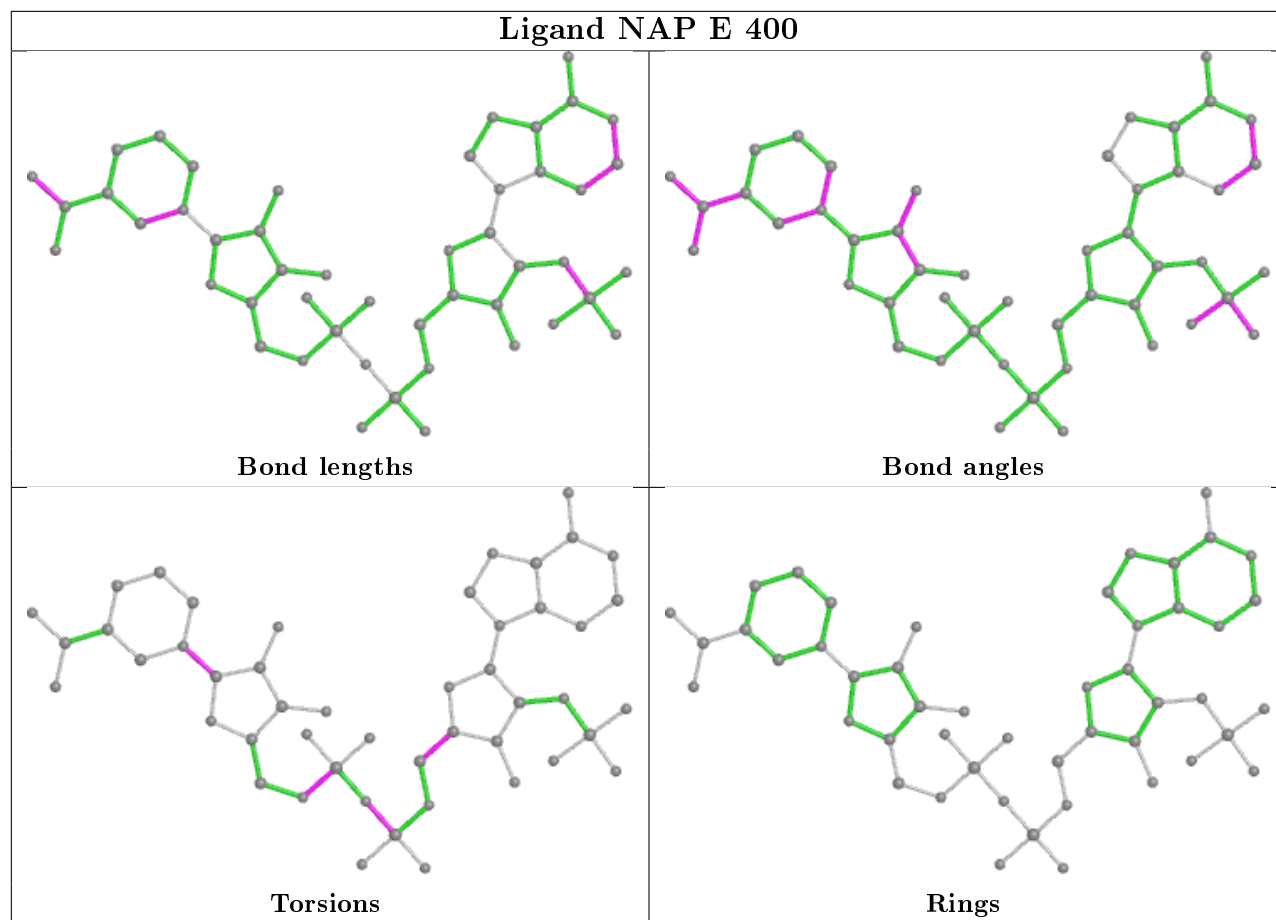
There are no ring outliers.

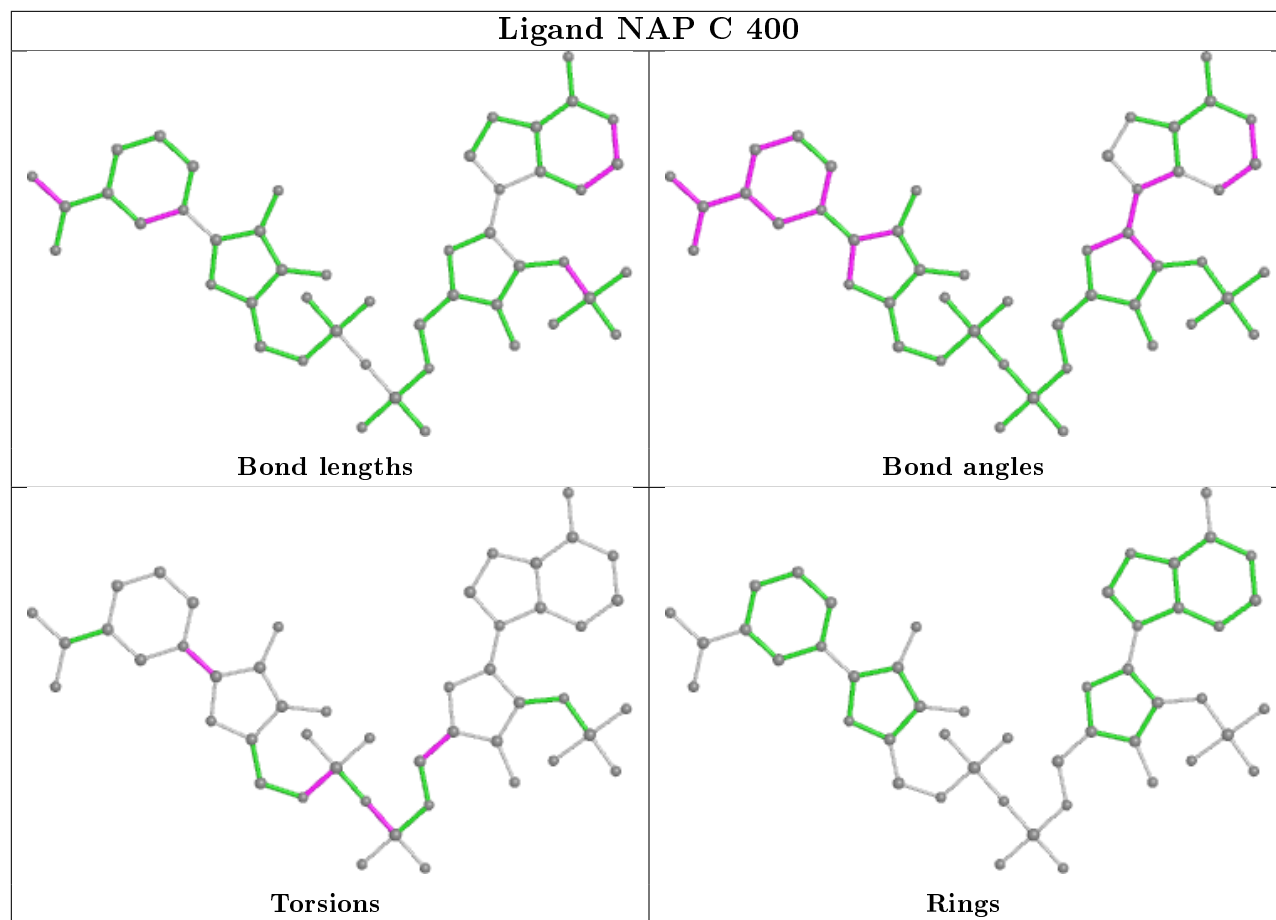
14 monomers are involved in 44 short contacts:

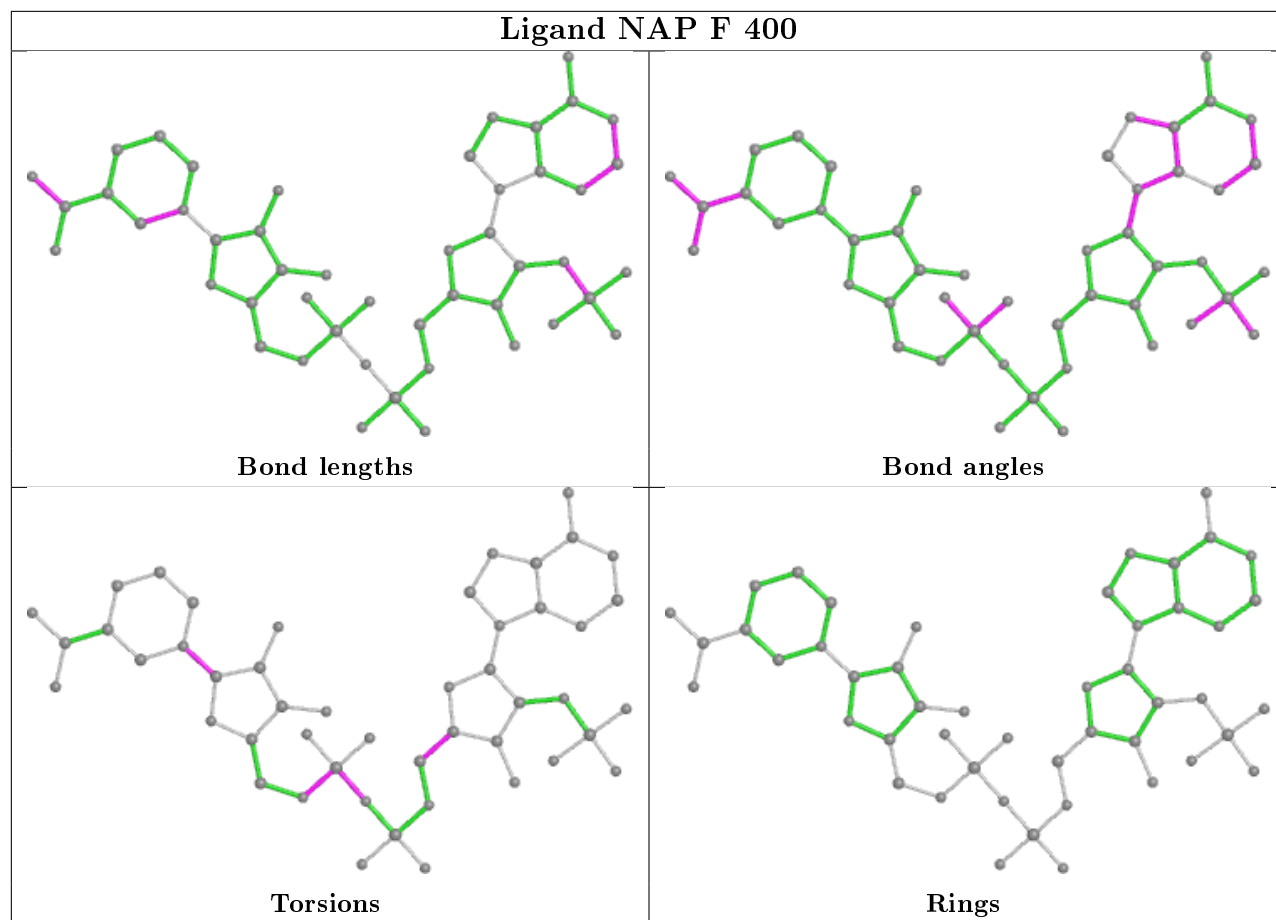
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	NAP	1	0
4	D	1002[B]	GLU	1	0
4	F	1003	GLU	1	0
4	D	1002[A]	GLU	1	0
2	H	400	NAP	1	0
4	C	1002	GLU	3	0
4	A	1002[A]	GLU	1	0
4	A	1002[B]	GLU	8	0
4	E	1002[A]	GLU	3	0
4	E	1002[B]	GLU	4	0
3	F	1001	E9P	1	0
4	G	1002[B]	GLU	10	0
4	B	1002[B]	GLU	1	0
4	B	1002[A]	GLU	8	0

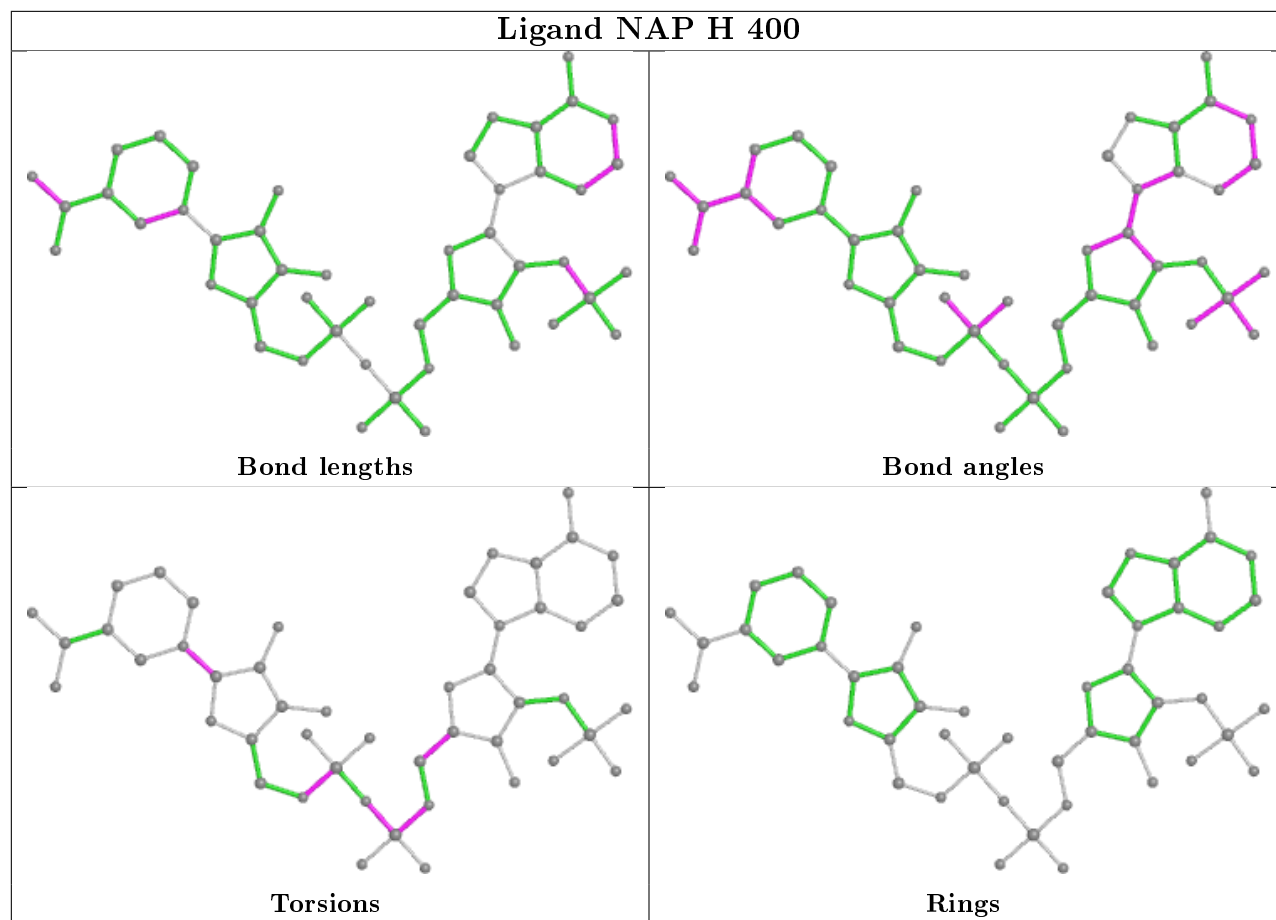
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

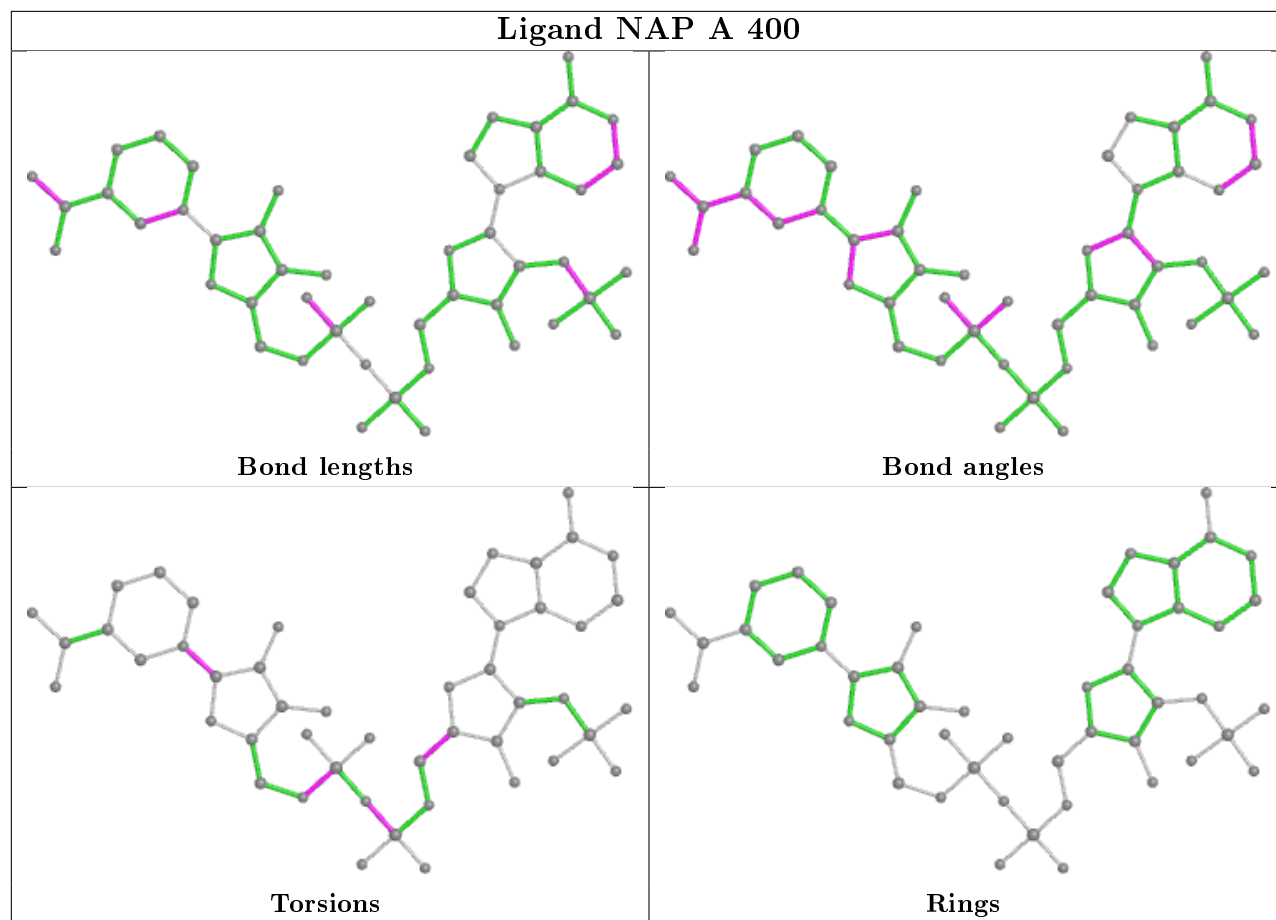


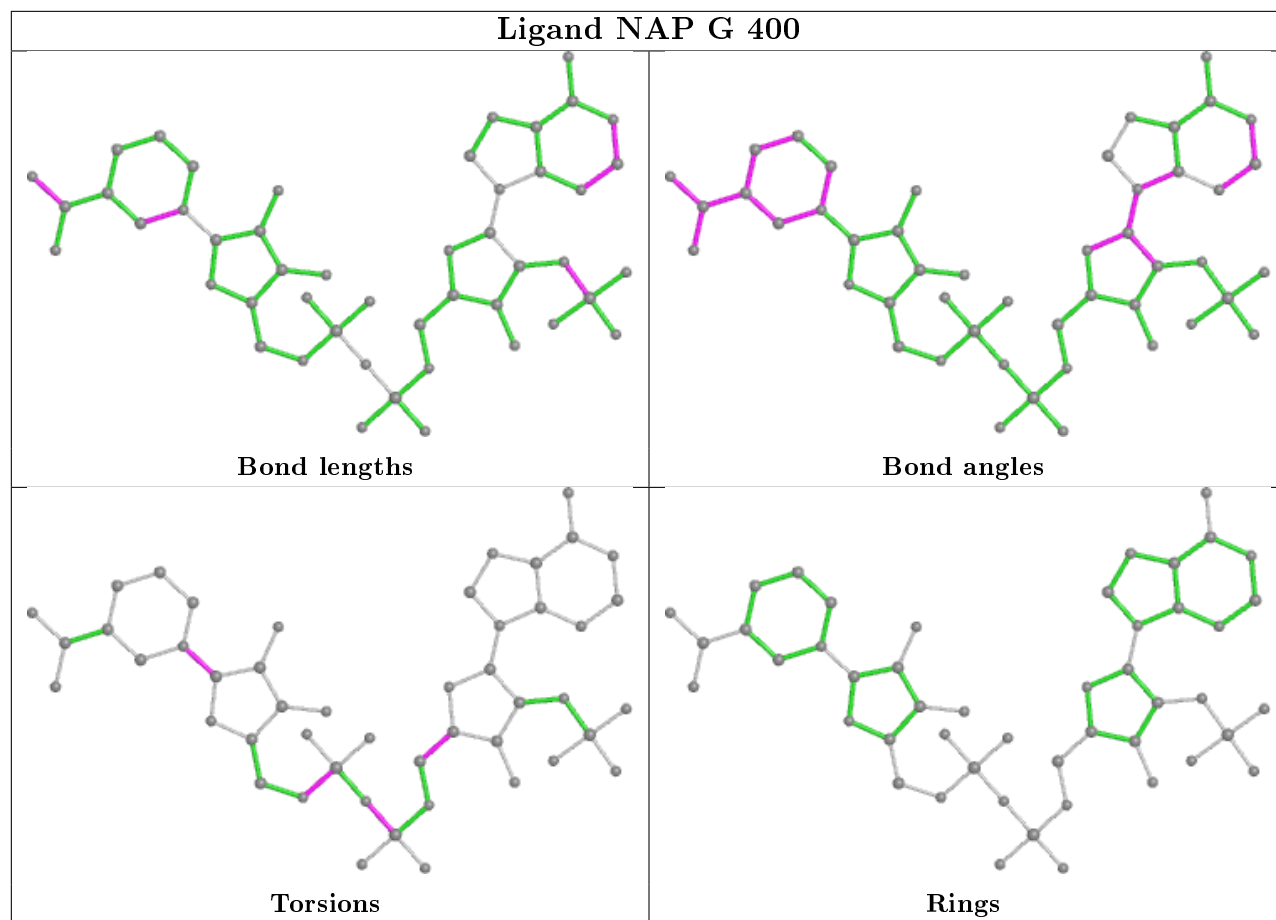


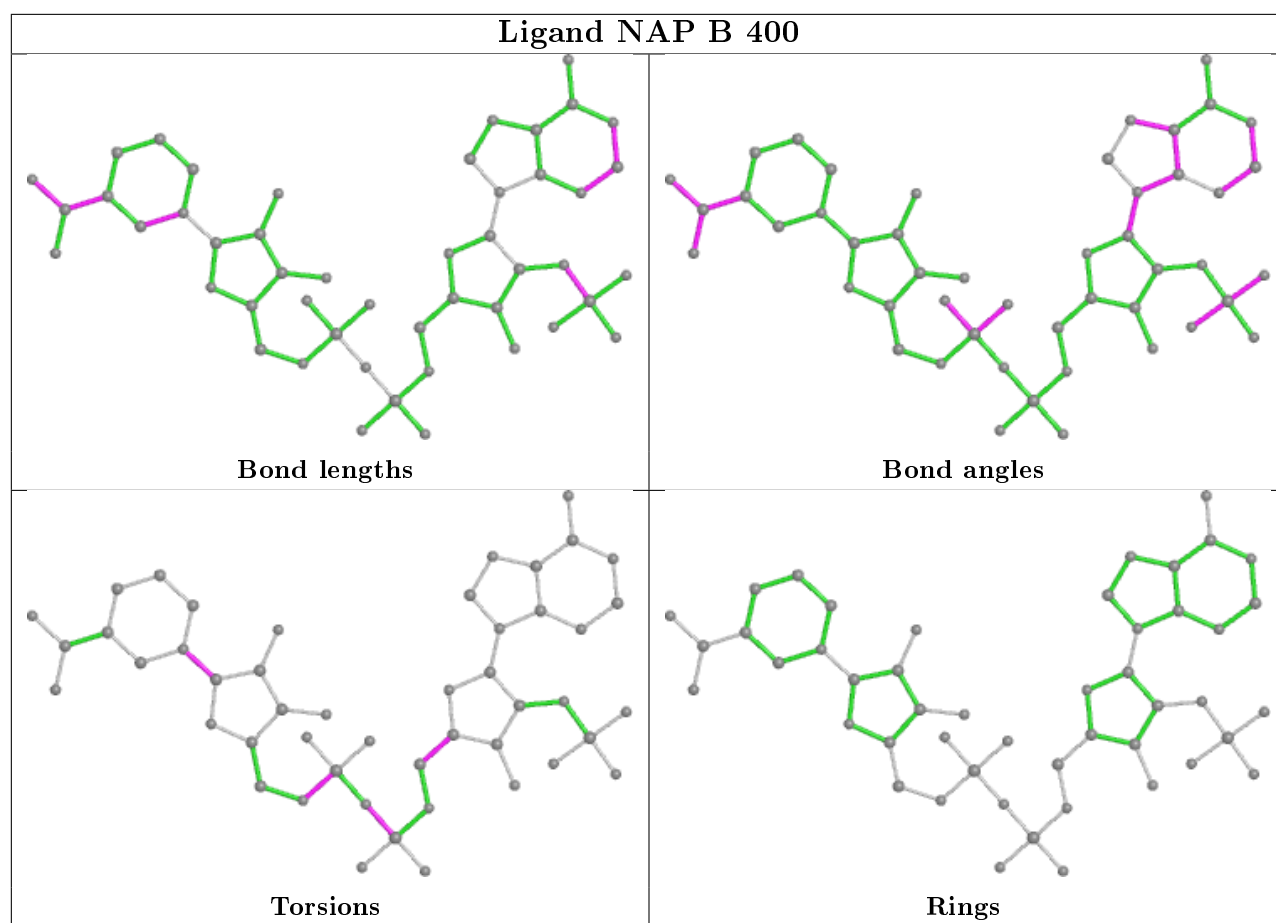












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/282 (90%)	-0.51	0 100 100	13, 24, 43, 59	0
1	B	255/282 (90%)	-0.39	1 (0%) 92 93	14, 25, 47, 63	0
1	C	255/282 (90%)	-0.39	1 (0%) 92 93	17, 27, 49, 63	0
1	D	254/282 (90%)	-0.10	8 (3%) 49 51	17, 32, 61, 78	0
1	E	255/282 (90%)	-0.40	1 (0%) 92 93	13, 23, 45, 61	0
1	F	256/282 (90%)	-0.49	2 (0%) 86 87	14, 26, 50, 65	0
1	G	254/282 (90%)	-0.34	2 (0%) 86 87	16, 27, 49, 65	0
1	H	255/282 (90%)	-0.32	5 (1%) 65 68	17, 31, 58, 85	0
All	All	2038/2256 (90%)	-0.37	20 (0%) 82 84	13, 27, 52, 85	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	VAL	4.3
1	C	2	VAL	4.2
1	D	103[A]	ARG	4.1
1	D	99[A]	MET	4.0
1	H	2	VAL	4.0
1	E	2	VAL	3.8
1	H	43	ARG	3.6
1	B	2	VAL	2.8
1	G	58	PRO	2.6
1	H	58	PRO	2.6
1	D	43	ARG	2.5
1	D	199	LYS	2.4
1	H	6	ASN	2.3
1	D	100[A]	GLU	2.3
1	D	53	GLU	2.3
1	F	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	59	GLU	2.2
1	D	58	PRO	2.2
1	D	194	ARG	2.2
1	H	103[A]	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

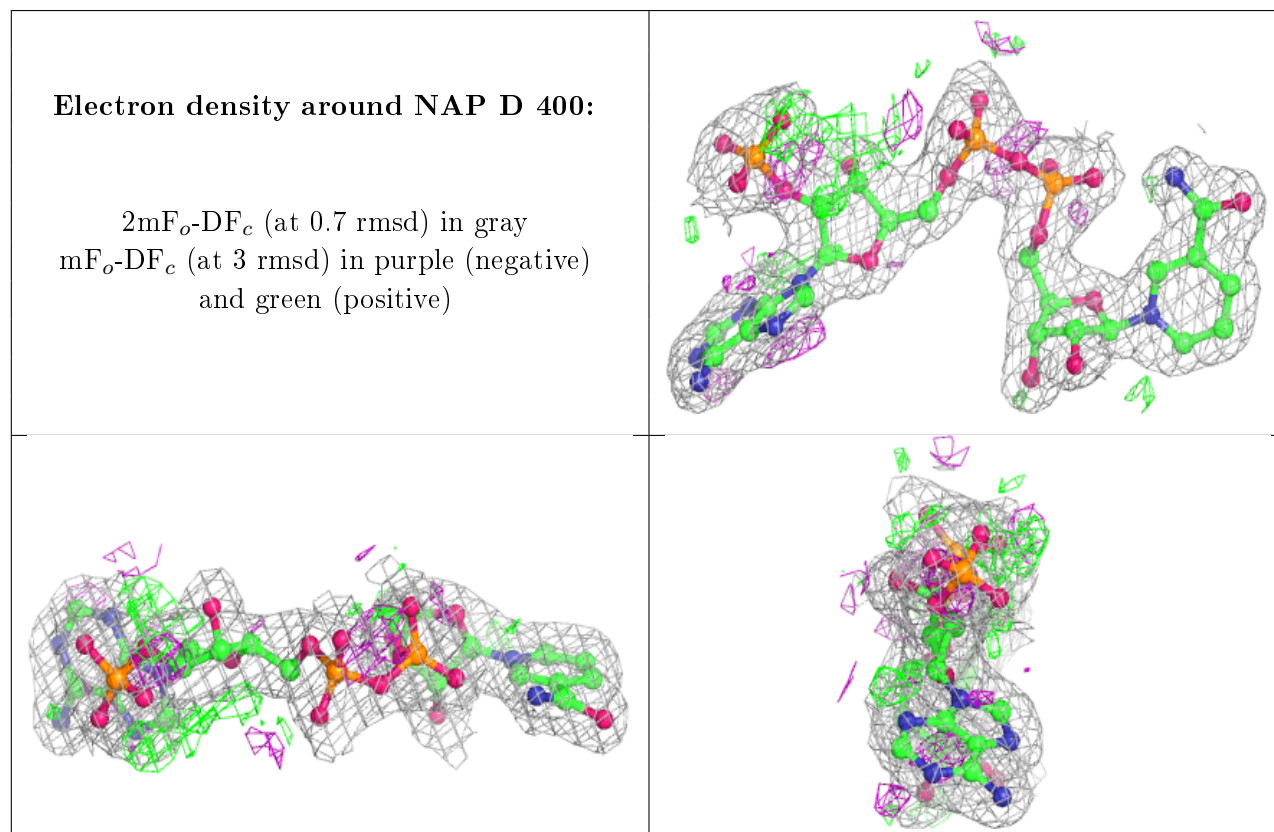
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLU	A	1002[A]	10/10	0.67	0.28	35,52,55,56	10
4	GLU	A	1002[B]	10/10	0.67	0.28	49,51,52,56	10
4	GLU	G	1002[B]	10/10	0.79	0.22	46,55,57,57	10
4	GLU	G	1002[A]	10/10	0.79	0.22	46,56,57,57	10
4	GLU	C	1002	10/10	0.81	0.19	57,71,73,74	0
4	GLU	D	1002[A]	10/10	0.82	0.25	42,51,51,52	10
4	GLU	F	1002[A]	10/10	0.82	0.29	80,82,83,83	10
4	GLU	D	1002[B]	10/10	0.82	0.25	69,72,72,73	10
4	GLU	F	1002[B]	10/10	0.82	0.29	36,46,47,47	10
4	GLU	B	1002[A]	10/10	0.85	0.18	44,54,55,56	10
4	GLU	B	1002[B]	10/10	0.85	0.18	55,56,58,58	10
4	GLU	E	1002[B]	10/10	0.86	0.25	28,49,52,52	10
4	GLU	E	1002[A]	10/10	0.86	0.25	47,51,53,53	10
4	GLU	F	1003	10/10	0.89	0.21	51,63,66,66	0
3	E9P	D	1001	16/16	0.92	0.13	29,38,42,44	0
3	E9P	H	1001	16/16	0.93	0.09	26,30,36,40	0
3	E9P	F	1001	16/16	0.96	0.07	20,23,27,29	0
2	NAP	D	400	48/48	0.96	0.07	26,35,49,52	0
3	E9P	B	1001	16/16	0.97	0.09	19,23,28,28	0

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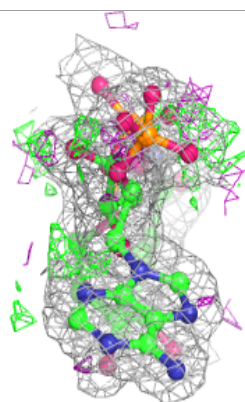
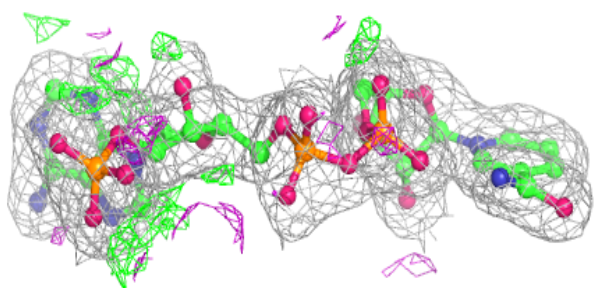
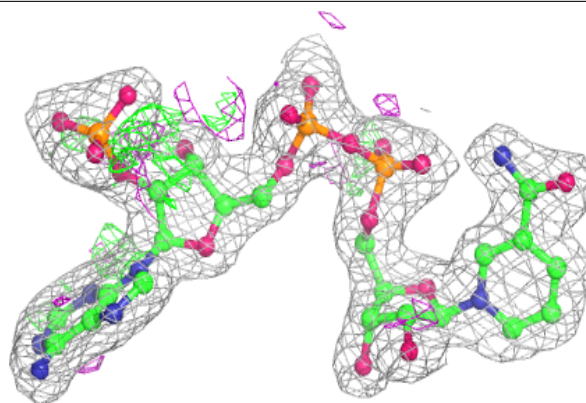
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	H	400	48/48	0.97	0.07	22,28,43,47	0
3	E9P	A	1001	16/16	0.97	0.08	14,19,26,28	0
2	NAP	F	400	48/48	0.98	0.07	19,23,30,32	0
2	NAP	C	400	48/48	0.98	0.07	17,24,30,34	0
2	NAP	G	400	48/48	0.98	0.08	16,22,32,35	0
3	E9P	C	1001	16/16	0.98	0.08	19,22,27,31	0
3	E9P	E	1001	16/16	0.98	0.12	12,18,25,27	0
3	E9P	G	1001	16/16	0.98	0.10	17,20,25,27	0
2	NAP	E	400	48/48	0.99	0.10	14,19,23,28	0
2	NAP	A	400	48/48	0.99	0.06	14,19,26,26	0
2	NAP	B	400	48/48	0.99	0.08	17,21,28,29	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.

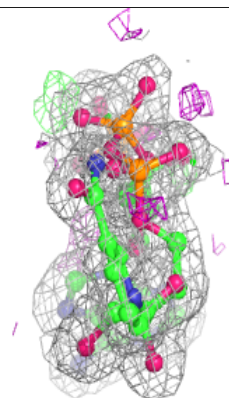
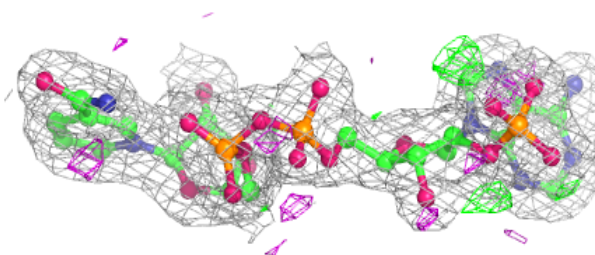
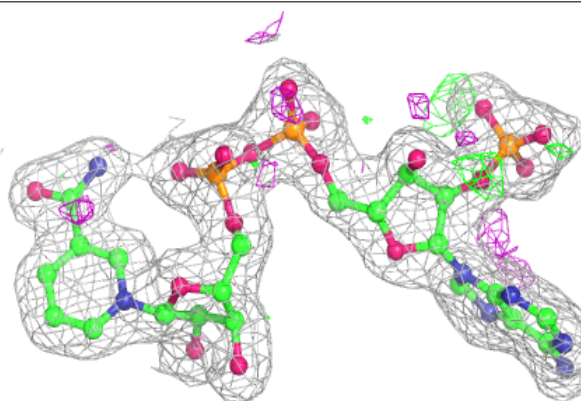


Electron density around NAP H 400:

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

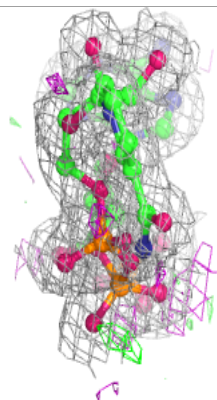
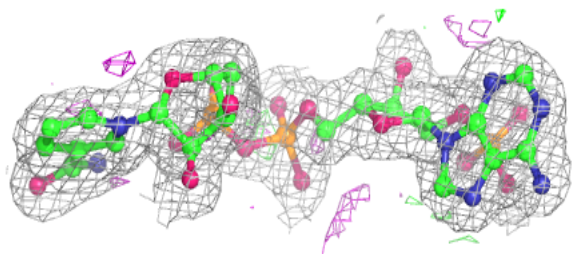
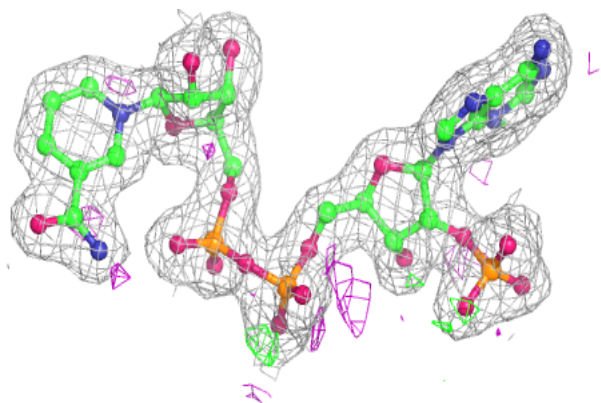
**Electron density around NAP F 400:**

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

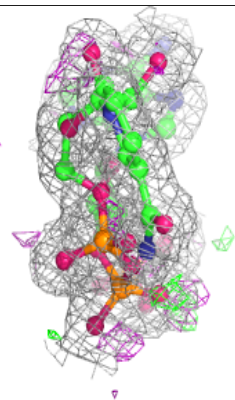
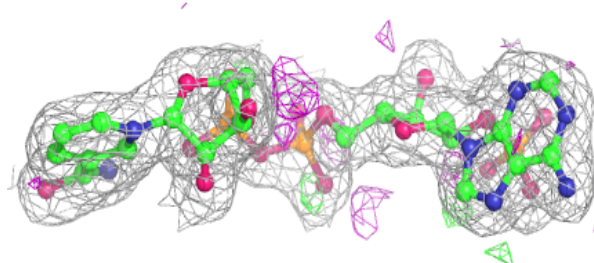
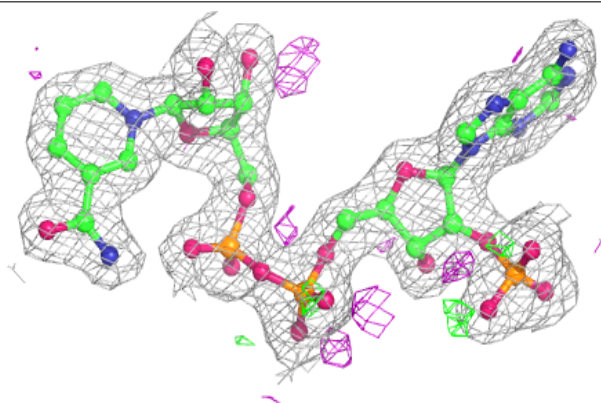


Electron density around NAP C 400:

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

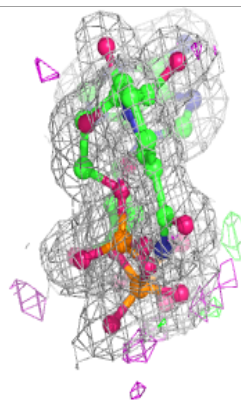
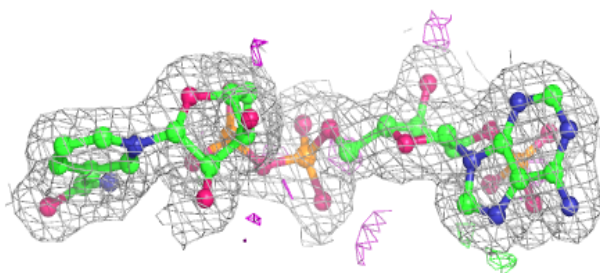
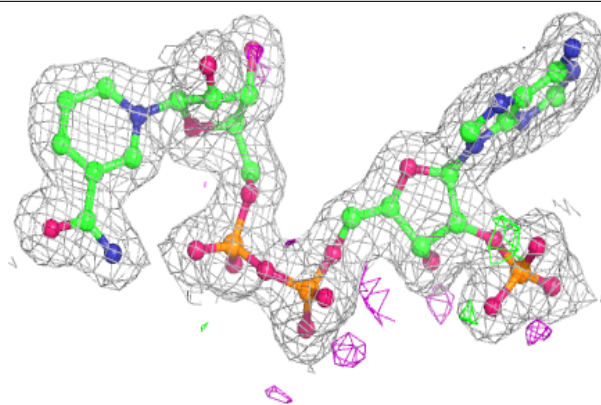
**Electron density around NAP G 400:**

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

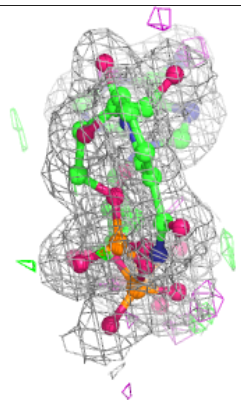
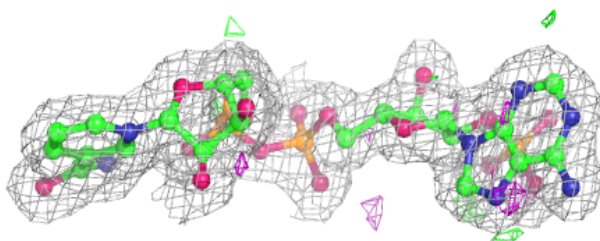
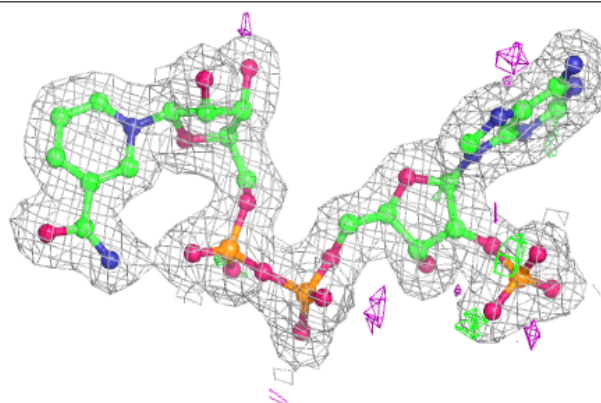


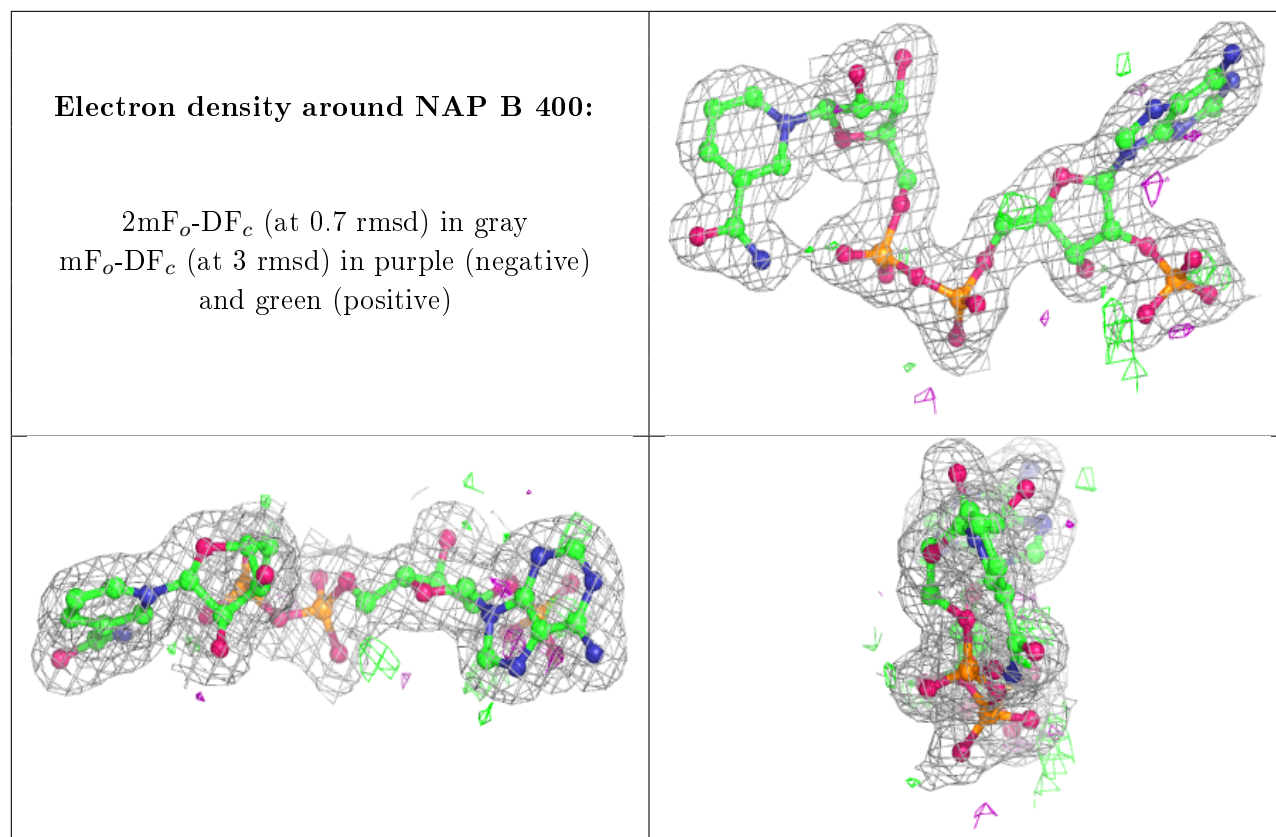
Electron density around NAP E 400:

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

**Electron density around NAP A 400:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.