



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:36 PM UTC

PDB ID : 4BNK / pdb_00004bnk
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

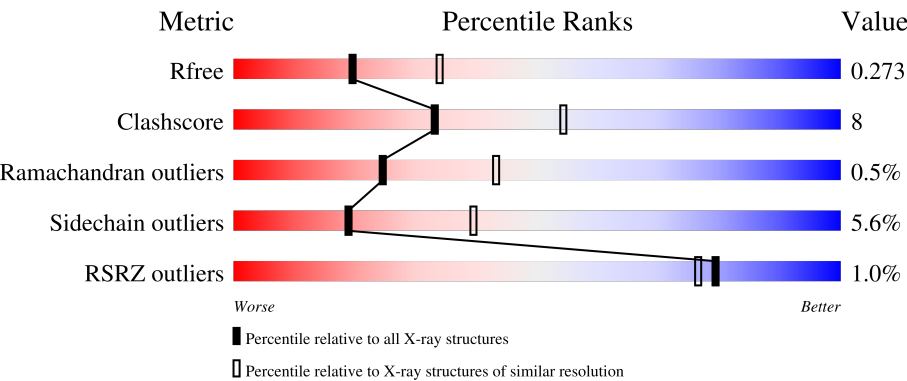
1 Overall quality at a glance i

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	77%12%• 10%
1	B	282	% 71%18%• 10%
1	C	282	2% 67%21%• 10%
1	D	282	% 71%18%• 10%
1	E	282	77%12%• 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	282	 71% 17% 10%
1	G	282	 65% 22% 10%
1	H	282	 74% 14% 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

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
1	A	254	Total	C	N	O	S	0	2	0
			1967	1240	338	385	4			
1	B	255	Total	C	N	O	S	0	1	0
			1968	1241	339	384	4			
1	C	255	Total	C	N	O	S	0	1	0
			1970	1242	342	382	4			
1	D	254	Total	C	N	O	S	0	0	0
			1955	1232	338	381	4			
1	E	254	Total	C	N	O	S	0	2	0
			1967	1240	338	385	4			
1	F	255	Total	C	N	O	S	0	0	0
			1962	1237	339	382	4			
1	G	255	Total	C	N	O	S	0	1	0
			1968	1241	339	384	4			
1	H	254	Total	C	N	O	S	0	0	0
			1955	1232	338	381	4			

There are 216 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
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

Continued on next page...

Continued from previous page...

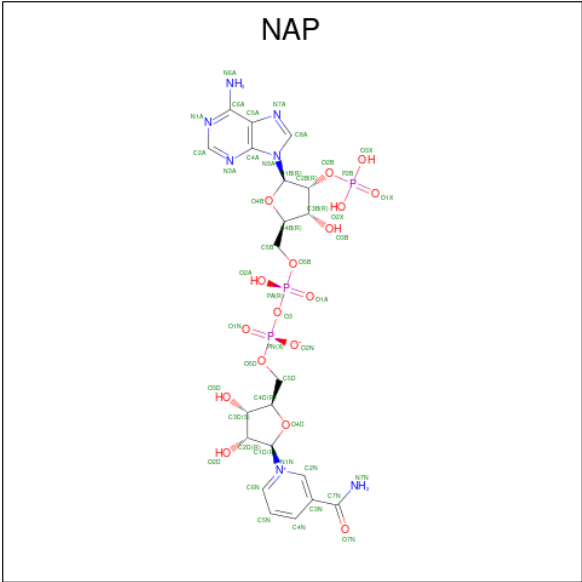
Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	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

Continued on next page...

Continued from previous page...

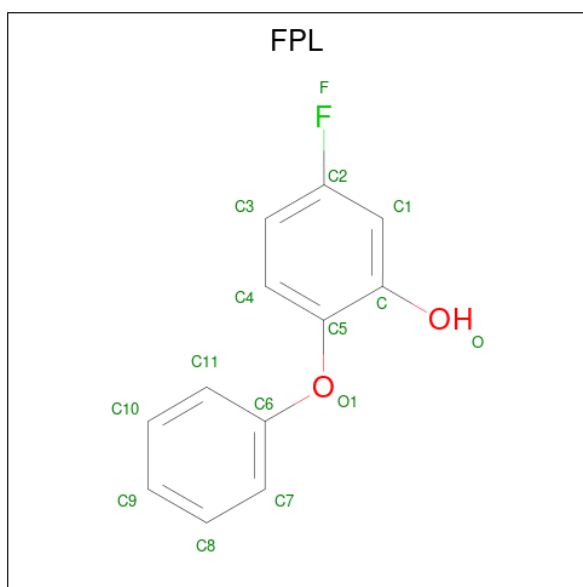
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



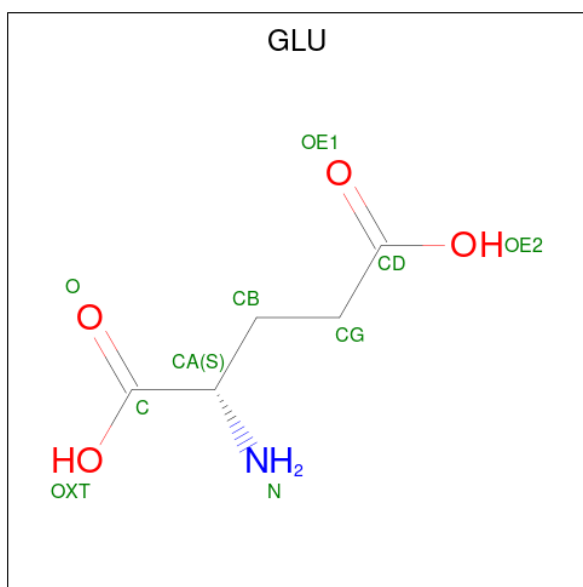
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	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-fluoro-2-phenoxyphenol (CCD ID: FPL) (formula: C₁₂H₉FO₂).



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

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

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

Continued on next page...

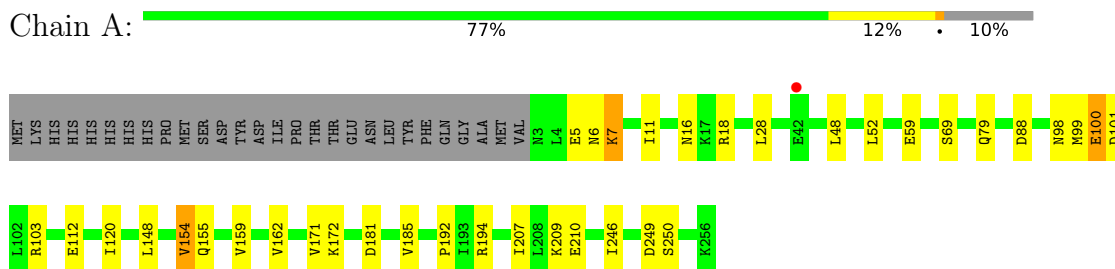
Continued from previous page...

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

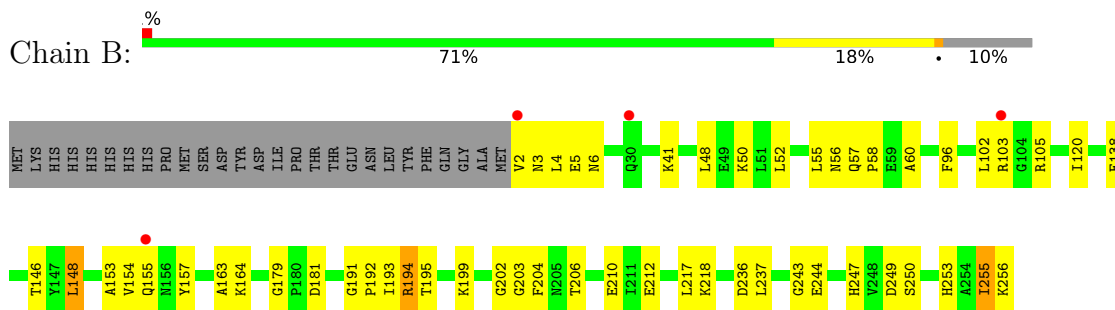
3 Residue-property plots

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.

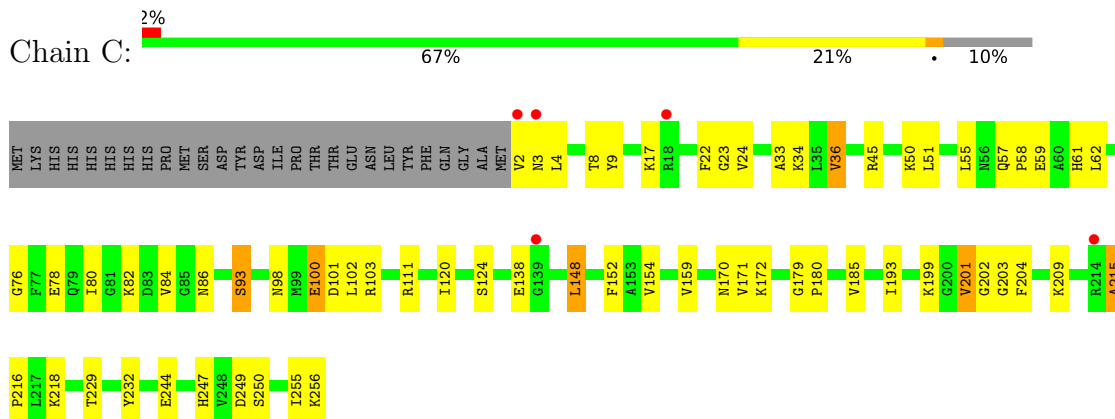
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



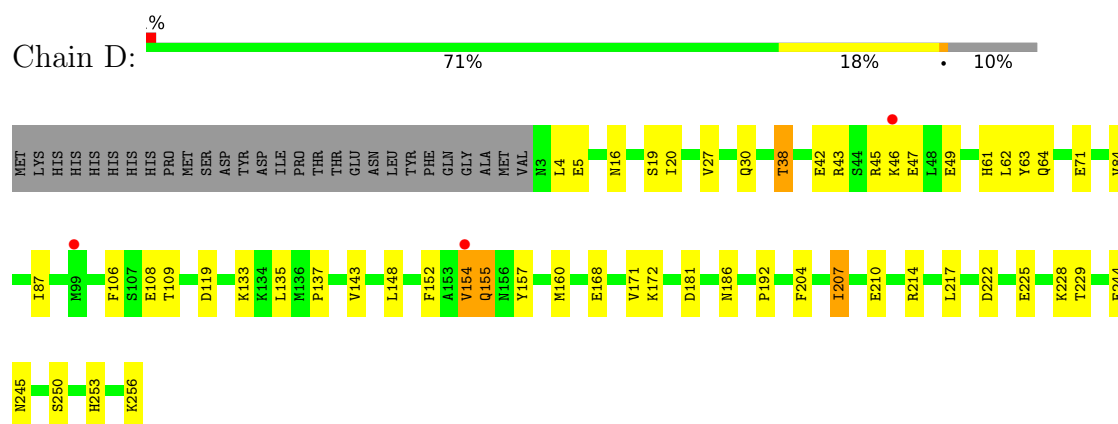
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



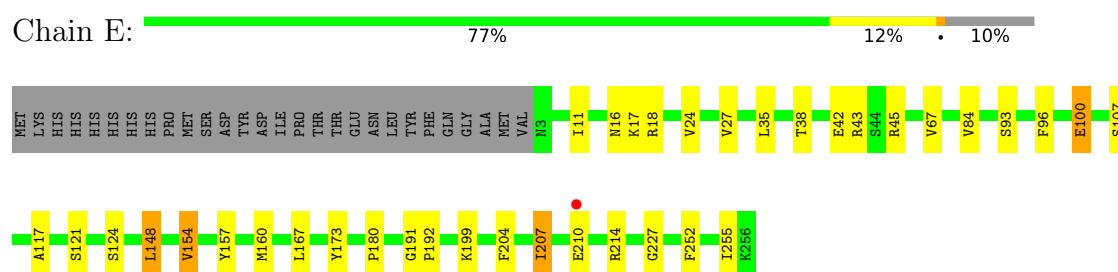
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



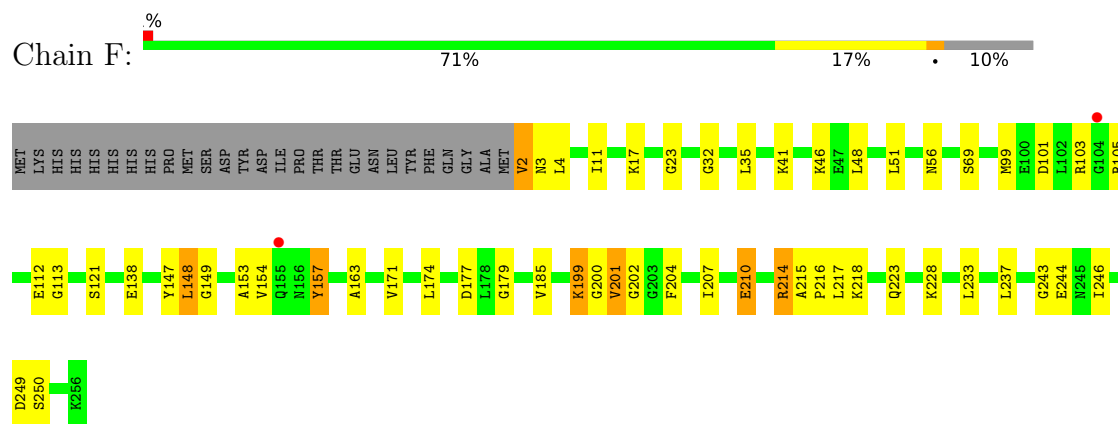
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



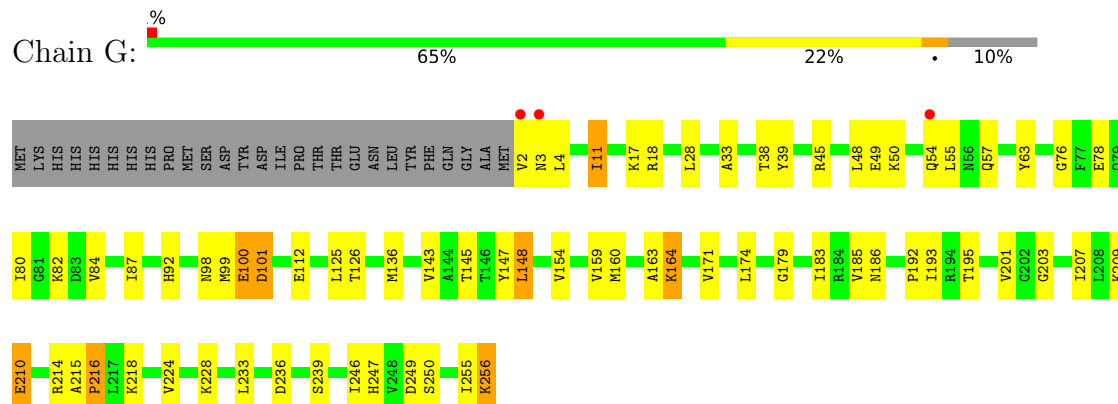
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



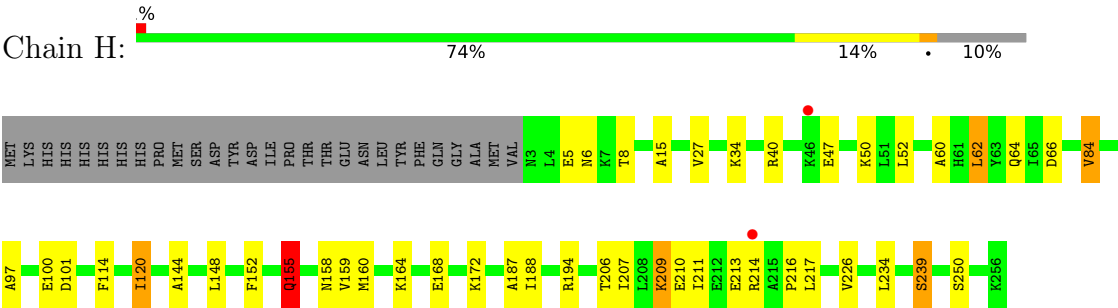
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.250 0.207 , 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)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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: FPL, CL, 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	1.07	1/2000 (0.1%)	1.14	2/2695 (0.1%)
1	B	1.09	1/1998 (0.1%)	1.21	6/2693 (0.2%)
1	C	1.11	1/2000 (0.1%)	1.21	7/2695 (0.3%)
1	D	0.96	0/1982	1.06	0/2671
1	E	1.08	3/2000 (0.1%)	1.11	2/2695 (0.1%)
1	F	1.11	1/1989 (0.1%)	1.23	8/2681 (0.3%)
1	G	1.12	2/1998 (0.1%)	1.21	7/2693 (0.3%)
1	H	0.93	1/1982 (0.1%)	1.07	3/2671 (0.1%)
All	All	1.06	10/15949 (0.1%)	1.16	35/21494 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	CA-CB	-5.95	1.46	1.54
1	H	27	VAL	CA-CB	5.91	1.61	1.54
1	G	224	VAL	CA-CB	5.82	1.61	1.54
1	G	183	ILE	CA-CB	5.81	1.61	1.53
1	E	167	LEU	N-CA	5.46	1.52	1.46
1	C	215	ALA	CA-CB	-5.37	1.45	1.53
1	E	207	ILE	CA-CB	5.30	1.60	1.54
1	F	207	ILE	CA-CB	5.18	1.60	1.54
1	E	27	VAL	CA-CB	5.17	1.60	1.54
1	B	153	ALA	CA-CB	-5.05	1.46	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	57	GLN	CA-C-N	7.34	126.97	119.56
1	G	57	GLN	C-N-CA	7.34	126.97	119.56
1	C	201	VAL	N-CA-C	6.62	117.27	107.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	163	ALA	N-CA-C	-6.53	104.24	111.82
1	F	105	ARG	N-CA-C	-6.50	99.10	109.76
1	B	105	ARG	N-CA-C	-6.45	98.72	109.24
1	G	239	SER	CA-C-N	-6.43	114.39	123.08
1	G	239	SER	C-N-CA	-6.43	114.39	123.08
1	B	191	GLY	CA-C-N	6.34	126.70	119.92
1	B	191	GLY	C-N-CA	6.34	126.70	119.92
1	F	243	GLY	N-CA-C	-6.23	106.33	115.30
1	H	239	SER	CA-C-N	-6.13	112.92	122.86
1	H	239	SER	C-N-CA	-6.13	112.92	122.86
1	C	204	PHE	N-CA-C	5.93	118.23	111.11
1	F	201	VAL	N-CA-C	5.89	116.17	107.15
1	G	201	VAL	N-CA-C	5.79	116.72	107.98
1	F	157	TYR	N-CA-C	-5.76	106.09	113.23
1	B	243	GLY	N-CA-C	-5.72	106.08	114.90
1	B	163	ALA	N-CA-C	-5.58	105.35	111.82
1	F	153	ALA	N-CA-C	-5.55	100.14	108.96
1	C	215	ALA	CA-C-N	5.51	125.86	119.47
1	C	215	ALA	C-N-CA	5.51	125.86	119.47
1	G	163	ALA	N-CA-C	-5.50	105.29	111.28
1	E	148	LEU	N-CA-C	5.46	118.74	111.75
1	B	191	GLY	N-CA-C	-5.38	105.48	112.10
1	C	86	ASN	N-CA-C	5.31	117.15	110.24
1	E	191	GLY	N-CA-C	-5.22	105.74	112.00
1	A	181	ASP	N-CA-C	-5.21	106.24	112.59
1	F	32	GLY	N-CA-C	5.19	122.48	115.32
1	G	160	MET	N-CA-C	5.17	117.65	111.71
1	C	36	VAL	N-CA-C	-5.15	100.64	108.17
1	A	103	ARG	N-CA-C	5.13	115.11	107.88
1	C	102	LEU	N-CA-C	5.05	118.97	112.41
1	H	234	LEU	N-CA-C	-5.03	107.15	113.28
1	F	204	PHE	N-CA-C	5.02	117.13	111.11

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	1967	0	1980	21	0
1	B	1968	0	1983	42	0
1	C	1970	0	1990	44	0
1	D	1955	0	1968	36	0
1	E	1967	0	1980	27	0
1	F	1962	0	1977	34	0
1	G	1968	0	1983	46	0
1	H	1955	0	1968	26	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
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	252	0

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

All (252) 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
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: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:D:244:GLU:HG3	1:D:245:ASN:N	2.14	0.61
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:HIS:C	1:D:62:LEU:HD12	2.35	0.52
1:E:173:TYR:OH	1:F:149:GLY:O	2.22	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:201:VAL:O	1:C:202:GLY:C	2.51	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
1:D:204:PHE:HA	1:D:207:ILE:HG13	1.94	0.48
1:E:100:GLU:CD	1:E:100:GLU:H	2.21	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:F:147:TYR:O	1:F:148:LEU:C	2.56	0.48
6:F:2001:HOH:O	1:G:2:VAL:C	2.57	0.48
1:D:135:LEU:C	1:D:137:PRO:HD3	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:GLU:CD	1:F:214:ARG:HH21	2.22	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: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
6:B:2001:HOH:O	1:C:2:VAL:C	2.58	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:B:217:LEU:O	1:B:218:LYS:C	2.57	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:F:217:LEU:O	1:F:218:LYS:C	2.60	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:148:LEU:HD12	1:G:148:LEU:HA	1.87	0.43
1:H:66:ASP:OD1	1:H:66:ASP:C	2.60	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:B:103:ARG:CZ	4:D:1259:GLU:OXT	2.66	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:19:SER:O	1:D:20:ILE:C	2.61	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: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
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: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:G:48:LEU:O	1:G:49:GLU:C	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:108:GLU:O	1:D:109:THR:C	2.63	0.41
1:D:154:VAL:O	1:D:155:GLN:C	2.61	0.41
1:B:2:VAL:N	1:C:2:VAL:N	2.68	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:97:ALA:HB2	1:H:160:MET:HE2	2.03	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:92:HIS:ND1	1:G:92:HIS:C	2.78	0.41
1:G:218:LYS:CE	6:G:2093:HOH:O	2.68	0.41
1:B:192:PRO:C	1:B:193:ILE:HG13	2.45	0.41
1:C:23:GLY:O	1:C:24:VAL:C	2.64	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:G:99:MET:O	1:G:100:GLU:C	2.62	0.40
1:A:11:ILE:HD11	1:A:28:LEU:HD12	2.02	0.40
1:A:99:MET:O	1:A:100:GLU:C	2.64	0.40
1:A:100:GLU:CD	1:A:100:GLU:H	2.28	0.40
1:C:216:PRO:HD2	1:C:250:SER:O	2.21	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
1:C:101:ASP:HB3	1:C:159:VAL:HG11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:VAL:O	1:F:202:GLY:C	2.64	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%)	16	31
1	C	254/282 (90%)	236 (93%)	17 (7%)	1 (0%)	30	49
1	D	252/282 (89%)	234 (93%)	17 (7%)	1 (0%)	30	49
1	E	254/282 (90%)	236 (93%)	18 (7%)	0	100	100
1	F	253/282 (90%)	233 (92%)	19 (8%)	1 (0%)	30	49
1	G	254/282 (90%)	242 (95%)	10 (4%)	2 (1%)	16	31
1	H	252/282 (89%)	236 (94%)	13 (5%)	3 (1%)	10	20
All	All	2027/2256 (90%)	1887 (93%)	130 (6%)	10 (0%)	24	43

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	200 (95%)	10 (5%)	23	46
1	B	210/234 (90%)	196 (93%)	14 (7%)	15	31
1	C	210/234 (90%)	200 (95%)	10 (5%)	23	46
1	D	208/234 (89%)	195 (94%)	13 (6%)	16	34
1	E	210/234 (90%)	203 (97%)	7 (3%)	33	61
1	F	209/234 (89%)	195 (93%)	14 (7%)	15	31
1	G	210/234 (90%)	196 (93%)	14 (7%)	15	31
1	H	208/234 (89%)	196 (94%)	12 (6%)	18	38
All	All	1675/1872 (90%)	1581 (94%)	94 (6%)	19	39

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	59	GLU
1	A	69	SER
1	A	79	GLN
1	A	100	GLU
1	A	154	VAL
1	A	209	LYS
1	A	210[A]	GLU
1	A	210[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	246	ILE
1	B	4	LEU
1	B	41	LYS
1	B	48	LEU
1	B	50	LYS
1	B	55	LEU
1	B	102	LEU
1	B	138	GLU
1	B	155	GLN
1	B	164	LYS
1	B	210	GLU
1	B	212	GLU
1	B	236	ASP
1	B	237	LEU
1	B	255	ILE
1	C	50	LYS
1	C	55	LEU
1	C	59	GLU
1	C	93	SER
1	C	100	GLU
1	C	138	GLU
1	C	148	LEU
1	C	154	VAL
1	C	199	LYS
1	C	255	ILE
1	D	4	LEU
1	D	5	GLU
1	D	30	GLN
1	D	38	THR
1	D	64	GLN
1	D	71	GLU
1	D	84	VAL
1	D	87	ILE
1	D	154	VAL
1	D	155	GLN
1	D	171	VAL
1	D	207	ILE
1	D	229	THR
1	E	17	LYS
1	E	38	THR
1	E	84	VAL
1	E	93	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	100	GLU
1	E	154	VAL
1	E	255	ILE
1	F	2	VAL
1	F	4	LEU
1	F	41	LYS
1	F	46	LYS
1	F	48	LEU
1	F	56	ASN
1	F	69	SER
1	F	112	GLU
1	F	121	SER
1	F	138	GLU
1	F	154	VAL
1	F	199	LYS
1	F	210	GLU
1	F	214	ARG
1	G	11	ILE
1	G	18	ARG
1	G	54	GLN
1	G	55	LEU
1	G	100	GLU
1	G	112	GLU
1	G	154	VAL
1	G	164	LYS
1	G	209	LYS
1	G	210	GLU
1	G	216	PRO
1	G	236	ASP
1	G	255	ILE
1	G	256	LYS
1	H	50	LYS
1	H	52	LEU
1	H	62	LEU
1	H	64	GLN
1	H	84	VAL
1	H	100	GLU
1	H	120	ILE
1	H	155	GLN
1	H	206	THR
1	H	209	LYS
1	H	211	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	216	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	253	HIS
1	B	56	ASN
1	B	253	HIS
1	C	6	ASN
1	C	30	GLN
1	C	79	GLN
1	C	155	GLN
1	C	220	ASN
1	C	253	HIS
1	D	56	ASN
1	D	68	GLN
1	D	170	ASN
1	D	220	ASN
1	D	253	HIS
1	E	3	ASN
1	E	16	ASN
1	E	54	GLN
1	E	56	ASN
1	E	75	ASN
1	E	98	ASN
1	E	253	HIS
1	F	3	ASN
1	F	61	HIS
1	F	98	ASN
1	F	220	ASN
1	G	155	GLN
1	G	220	ASN
1	G	253	HIS
1	H	30	GLN
1	H	64	GLN
1	H	155	GLN
1	H	253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	NAP	B	1257	-	50,52,52	1.61	7 (14%)	71,80,80	1.99	18 (25%)
2	NAP	G	1257	-	50,52,52	1.49	5 (10%)	71,80,80	1.71	16 (22%)
3	FPL	F	1258	-	16,16,16	0.51	0	21,21,21	0.59	0
2	NAP	F	1257	-	50,52,52	1.58	5 (10%)	71,80,80	1.75	14 (19%)
4	GLU	A	1259	-	8,9,9	1.61	1 (12%)	8,11,11	1.13	1 (12%)
3	FPL	H	1258	-	16,16,16	0.17	0	21,21,21	0.42	0
2	NAP	E	1258	-	50,52,52	1.46	4 (8%)	71,80,80	2.02	18 (25%)
3	FPL	D	1258	-	16,16,16	0.37	0	21,21,21	0.60	0
2	NAP	D	1257	-	50,52,52	1.78	6 (12%)	71,80,80	1.67	16 (22%)
3	FPL	A	1258	-	16,16,16	0.39	0	21,21,21	0.58	0
3	FPL	C	1258	-	16,16,16	0.45	0	21,21,21	0.66	1 (4%)
2	NAP	A	1257	-	50,52,52	1.62	8 (16%)	71,80,80	1.90	18 (25%)
3	FPL	G	1258	-	16,16,16	0.33	0	21,21,21	0.61	0
4	GLU	C	1259	-	8,9,9	1.58	1 (12%)	8,11,11	0.90	0
4	GLU	D	1259	-	8,9,9	1.53	1 (12%)	8,11,11	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	H	1257	-	50,52,52	1.79	7 (14%)	71,80,80	1.63	17 (23%)
4	GLU	E	1260	-	8,9,9	1.21	0	8,11,11	1.15	1 (12%)
4	GLU	G	1259	-	8,9,9	1.64	1 (12%)	8,11,11	1.06	0
3	FPL	B	1258	-	16,16,16	0.30	0	21,21,21	0.53	0
3	FPL	E	1259	-	16,16,16	0.32	0	21,21,21	0.68	1 (4%)
2	NAP	C	1257	-	50,52,52	1.59	4 (8%)	71,80,80	1.83	17 (23%)

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
2	NAP	B	1257	-	-	5/35/67/67	0/5/5/5
2	NAP	G	1257	-	-	8/35/67/67	0/5/5/5
3	FPL	F	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	F	1257	-	-	7/35/67/67	0/5/5/5
4	GLU	A	1259	-	-	6/9/9/9	-
3	FPL	H	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	E	1258	-	-	5/35/67/67	0/5/5/5
3	FPL	D	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	D	1257	-	-	6/35/67/67	0/5/5/5
3	FPL	A	1258	-	-	0/4/4/4	0/2/2/2
3	FPL	C	1258	-	-	0/4/4/4	0/2/2/2
2	NAP	A	1257	-	-	6/35/67/67	0/5/5/5
3	FPL	G	1258	-	-	0/4/4/4	0/2/2/2
4	GLU	C	1259	-	-	5/9/9/9	-
4	GLU	D	1259	-	-	7/9/9/9	-
2	NAP	H	1257	-	-	5/35/67/67	0/5/5/5
4	GLU	E	1260	-	-	2/9/9/9	-
4	GLU	G	1259	-	-	6/9/9/9	-
3	FPL	B	1258	-	-	0/4/4/4	0/2/2/2
3	FPL	E	1259	-	-	0/4/4/4	0/2/2/2
2	NAP	C	1257	-	-	6/35/67/67	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1257	NAP	O7N-C7N	8.80	1.40	1.24
2	D	1257	NAP	O7N-C7N	8.71	1.40	1.24
2	F	1257	NAP	O7N-C7N	7.99	1.39	1.24
2	C	1257	NAP	O7N-C7N	7.36	1.37	1.24
2	G	1257	NAP	O7N-C7N	7.31	1.37	1.24
2	A	1257	NAP	O7N-C7N	7.18	1.37	1.24
2	E	1258	NAP	O7N-C7N	7.06	1.37	1.24
2	B	1257	NAP	O7N-C7N	6.87	1.36	1.24
2	D	1257	NAP	C2A-N3A	3.82	1.40	1.33
2	A	1257	NAP	C2A-N3A	3.53	1.40	1.33
2	D	1257	NAP	C2A-N1A	3.42	1.40	1.33
2	B	1257	NAP	PA-O3	3.42	1.63	1.59
2	H	1257	NAP	C2A-N1A	3.40	1.40	1.33
4	C	1259	GLU	CG-CD	3.37	1.58	1.50
2	H	1257	NAP	PN-O3	3.26	1.63	1.59
2	E	1258	NAP	C2A-N3A	3.21	1.39	1.33
2	H	1257	NAP	C2A-N3A	3.20	1.39	1.33
2	D	1257	NAP	PA-O3	3.13	1.62	1.59
4	G	1259	GLU	CG-CD	3.10	1.57	1.50
2	G	1257	NAP	C2A-N1A	3.09	1.39	1.33
4	A	1259	GLU	CG-CD	3.05	1.57	1.50
2	C	1257	NAP	C2A-N3A	2.89	1.39	1.33
2	B	1257	NAP	PN-O3	2.79	1.62	1.59
4	D	1259	GLU	CG-CD	2.78	1.57	1.50
2	A	1257	NAP	C2A-N1A	2.71	1.38	1.33
2	C	1257	NAP	C2A-N1A	2.70	1.38	1.33
2	H	1257	NAP	PA-O3	2.70	1.62	1.59
2	F	1257	NAP	P2B-O2B	2.65	1.64	1.59
2	B	1257	NAP	C2A-N1A	2.64	1.38	1.33
2	E	1258	NAP	PA-O3	2.60	1.62	1.59
2	F	1257	NAP	C2A-N1A	2.58	1.38	1.33
2	A	1257	NAP	PN-O3	-2.57	1.56	1.59
2	B	1257	NAP	C2N-C3N	2.56	1.43	1.39
2	F	1257	NAP	PA-O3	2.54	1.62	1.59
2	E	1258	NAP	C2A-N1A	2.49	1.38	1.33
2	A	1257	NAP	C2N-N1N	2.46	1.37	1.35
2	A	1257	NAP	P2B-O2B	2.41	1.63	1.59
2	B	1257	NAP	O4D-C4D	-2.38	1.39	1.45
2	C	1257	NAP	C2N-N1N	-2.36	1.32	1.35
2	B	1257	NAP	C2A-N3A	2.34	1.38	1.33
2	D	1257	NAP	PN-O3	2.31	1.62	1.59
2	F	1257	NAP	PN-O3	2.28	1.62	1.59
2	H	1257	NAP	O4B-C4B	-2.25	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1257	NAP	C8A-N7A	2.19	1.35	1.31
2	G	1257	NAP	C3N-C7N	-2.10	1.47	1.50
2	D	1257	NAP	C8A-N7A	2.09	1.35	1.31
2	A	1257	NAP	C5A-N7A	-2.07	1.35	1.39
2	A	1257	NAP	O4B-C4B	-2.06	1.40	1.45
2	G	1257	NAP	C2A-N3A	2.03	1.37	1.33
2	G	1257	NAP	C5A-N7A	-2.01	1.35	1.39

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1258	NAP	N3A-C2A-N1A	-6.26	119.11	128.58
2	F	1257	NAP	N3A-C2A-N1A	-5.99	119.51	128.58
2	B	1257	NAP	N3A-C2A-N1A	-5.98	119.53	128.58
2	B	1257	NAP	O7N-C7N-C3N	-5.95	112.32	119.60
2	B	1257	NAP	C3N-C7N-N7N	5.56	124.58	117.74
2	A	1257	NAP	C3N-C7N-N7N	5.52	124.54	117.74
2	C	1257	NAP	N3A-C2A-N1A	-5.48	120.29	128.58
2	E	1258	NAP	N9A-C8A-N7A	-5.44	106.21	113.94
2	A	1257	NAP	N3A-C2A-N1A	-5.43	120.36	128.58
2	G	1257	NAP	N3A-C2A-N1A	-5.27	120.60	128.58
2	E	1258	NAP	C3N-C7N-N7N	5.23	124.18	117.74
2	C	1257	NAP	O7N-C7N-C3N	-4.95	113.55	119.60
2	D	1257	NAP	N3A-C2A-N1A	-4.77	121.36	128.58
2	C	1257	NAP	C2N-C3N-C4N	4.71	123.73	118.26
2	H	1257	NAP	N9A-C8A-N7A	-4.63	107.37	113.94
2	D	1257	NAP	C5A-C4A-N3A	-4.46	120.57	126.72
2	G	1257	NAP	O7N-C7N-C3N	-4.46	114.14	119.60
2	A	1257	NAP	C6N-N1N-C2N	-4.25	118.26	121.88
2	H	1257	NAP	N3A-C2A-N1A	-4.19	122.24	128.58
2	E	1258	NAP	O7N-C7N-C3N	-4.18	114.48	119.60
2	A	1257	NAP	C5A-C4A-N3A	-4.18	120.97	126.72
2	E	1258	NAP	C5A-N7A-C8A	4.12	109.93	103.45
2	B	1257	NAP	C5A-C4A-N3A	-4.11	121.06	126.72
2	F	1257	NAP	C5A-C4A-N3A	-4.10	121.07	126.72
2	D	1257	NAP	N9A-C8A-N7A	-3.98	108.29	113.94
2	E	1258	NAP	C4A-N9A-C8A	3.97	109.90	105.74
2	A	1257	NAP	N9A-C8A-N7A	-3.94	108.34	113.94
2	E	1258	NAP	C5A-C4A-N3A	-3.93	121.30	126.72
2	B	1257	NAP	N9A-C8A-N7A	-3.89	108.41	113.94
2	F	1257	NAP	C3N-C7N-N7N	3.89	122.53	117.74
2	G	1257	NAP	C3N-C7N-N7N	3.81	122.43	117.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1257	NAP	O4B-C1B-N9A	3.74	115.27	108.09
2	F	1257	NAP	O7N-C7N-C3N	-3.74	115.03	119.60
2	B	1257	NAP	N3A-C4A-N9A	3.71	133.48	127.17
2	C	1257	NAP	C4D-O4D-C1D	-3.70	106.53	109.92
2	E	1258	NAP	C2A-N3A-C4A	3.65	120.75	111.83
2	G	1257	NAP	C5A-C4A-N3A	-3.65	121.69	126.72
2	C	1257	NAP	N9A-C8A-N7A	-3.59	108.84	113.94
2	H	1257	NAP	C5A-C4A-N3A	-3.58	121.78	126.72
2	C	1257	NAP	C3N-C7N-N7N	3.57	122.14	117.74
2	D	1257	NAP	C5A-N7A-C8A	3.52	108.98	103.45
2	H	1257	NAP	C3N-C7N-N7N	3.51	122.06	117.74
2	F	1257	NAP	N9A-C8A-N7A	-3.49	108.98	113.94
2	B	1257	NAP	O4B-C1B-N9A	3.47	114.74	108.09
2	F	1257	NAP	O4B-C1B-N9A	3.45	114.72	108.09
2	H	1257	NAP	C5A-N7A-C8A	3.44	108.86	103.45
2	F	1257	NAP	C2A-N3A-C4A	3.41	120.15	111.83
2	A	1257	NAP	N3A-C4A-N9A	3.38	132.92	127.17
2	A	1257	NAP	C2A-N3A-C4A	3.38	120.09	111.83
2	D	1257	NAP	O4B-C1B-C2B	-3.37	100.79	106.59
2	H	1257	NAP	O4B-C1B-N9A	3.33	114.48	108.09
2	E	1258	NAP	C2N-C3N-C4N	3.32	122.12	118.26
2	C	1257	NAP	C5N-C4N-C3N	-3.31	117.11	120.36
2	D	1257	NAP	N3A-C4A-N9A	3.29	132.75	127.17
2	B	1257	NAP	C2A-N3A-C4A	3.25	119.78	111.83
2	G	1257	NAP	C2N-C3N-C4N	3.23	122.02	118.26
2	F	1257	NAP	O4B-C1B-C2B	-3.23	101.03	106.59
2	H	1257	NAP	C4A-N9A-C8A	3.22	109.12	105.74
2	D	1257	NAP	C2A-N3A-C4A	3.20	119.65	111.83
2	C	1257	NAP	C5A-C4A-N3A	-3.19	122.32	126.72
2	B	1257	NAP	C5A-N7A-C8A	3.18	108.44	103.45
2	E	1258	NAP	N3A-C4A-N9A	3.14	132.51	127.17
2	D	1257	NAP	O4B-C1B-N9A	3.14	114.11	108.09
2	F	1257	NAP	N3A-C4A-N9A	3.13	132.49	127.17
2	H	1257	NAP	C2B-C1B-N9A	-3.08	108.68	113.75
2	C	1257	NAP	C4A-N9A-C8A	3.08	108.97	105.74
2	F	1257	NAP	C5A-N7A-C8A	3.07	108.28	103.45
2	E	1258	NAP	C6N-N1N-C2N	-3.05	119.28	121.88
2	B	1257	NAP	C2N-C3N-C4N	3.04	121.79	118.26
2	A	1257	NAP	O7N-C7N-N7N	-3.01	118.26	122.62
2	B	1257	NAP	C4A-N9A-C8A	2.94	108.83	105.74
2	C	1257	NAP	C2A-N3A-C4A	2.92	118.97	111.83
2	B	1257	NAP	C5N-C4N-C3N	-2.88	117.53	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1257	NAP	C4D-O4D-C1D	-2.86	107.30	109.92
2	C	1257	NAP	N3A-C4A-N9A	2.86	132.03	127.17
2	A	1257	NAP	O4B-C1B-N9A	2.77	113.40	108.09
2	A	1257	NAP	C5A-N7A-C8A	2.75	107.78	103.45
2	G	1257	NAP	N3A-C4A-N9A	2.74	131.82	127.17
2	G	1257	NAP	C2A-N3A-C4A	2.73	118.51	111.83
2	A	1257	NAP	C4A-N9A-C8A	2.73	108.61	105.74
2	G	1257	NAP	N9A-C8A-N7A	-2.69	110.11	113.94
2	A	1257	NAP	C5N-C6N-N1N	2.68	124.04	120.38
2	A	1257	NAP	C5A-C6A-N6A	-2.68	116.66	123.29
2	G	1257	NAP	C5N-C4N-C3N	-2.61	117.80	120.36
2	B	1257	NAP	O2N-PN-O1N	2.61	124.58	112.44
2	G	1257	NAP	O3-PN-O1N	-2.60	102.87	110.70
2	H	1257	NAP	C4A-C5A-N7A	-2.60	107.61	110.58
2	F	1257	NAP	O2N-PN-O1N	2.60	124.53	112.44
2	H	1257	NAP	O3D-C3D-C4D	-2.58	103.68	111.08
2	D	1257	NAP	C4A-C5A-N7A	-2.50	107.72	110.58
2	G	1257	NAP	O4B-C1B-C2B	-2.49	102.29	106.59
2	H	1257	NAP	C2A-N3A-C4A	2.48	117.89	111.83
2	D	1257	NAP	C4A-N9A-C8A	2.48	108.34	105.74
2	E	1258	NAP	C4A-C5A-N7A	-2.47	107.76	110.58
2	G	1257	NAP	C5A-N7A-C8A	2.47	107.33	103.45
2	E	1258	NAP	O3X-P2B-O2B	2.47	115.46	105.85
3	E	1259	FPL	C5-O1-C6	2.46	123.90	117.95
2	F	1257	NAP	O3X-P2B-O2B	2.43	115.34	105.85
2	D	1257	NAP	C3N-C7N-N7N	2.43	120.73	117.74
2	A	1257	NAP	O3-PN-O1N	-2.42	103.41	110.70
2	B	1257	NAP	C6N-N1N-C2N	-2.42	119.82	121.88
2	F	1257	NAP	C2N-C3N-C4N	2.42	121.07	118.26
2	C	1257	NAP	O3-PN-O1N	-2.41	103.46	110.70
2	H	1257	NAP	N3A-C4A-N9A	2.36	131.18	127.17
2	H	1257	NAP	O5B-C5B-C4B	-2.36	100.97	108.99
2	D	1257	NAP	C6N-N1N-C2N	-2.32	119.91	121.88
2	C	1257	NAP	C5A-N7A-C8A	2.31	107.09	103.45
2	E	1258	NAP	O3X-P2B-O1X	-2.27	101.99	110.83
4	E	1260	GLU	OE1-CD-CG	-2.27	115.89	123.09
4	A	1259	GLU	CG-CB-CA	2.27	119.06	113.86
2	B	1257	NAP	O5B-C5B-C4B	-2.26	101.31	108.99
2	A	1257	NAP	N6A-C6A-N1A	2.25	123.39	118.38
2	E	1258	NAP	C4B-O4B-C1B	-2.25	104.50	109.47
2	H	1257	NAP	O2N-PN-O1N	2.24	122.87	112.44
2	A	1257	NAP	C2N-C3N-C4N	2.24	120.86	118.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1257	NAP	O4B-C1B-C2B	-2.23	102.75	106.59
2	E	1258	NAP	O2N-PN-O1N	2.22	122.79	112.44
2	E	1258	NAP	C5N-C6N-N1N	2.21	123.40	120.38
2	B	1257	NAP	N6A-C6A-N1A	2.19	123.27	118.38
2	A	1257	NAP	O2N-PN-O1N	2.19	122.65	112.44
2	D	1257	NAP	C4D-O4D-C1D	-2.19	107.92	109.92
2	G	1257	NAP	C6A-C5A-C4A	2.18	120.16	117.18
3	C	1258	FPL	C5-O1-C6	2.17	123.22	117.95
2	D	1257	NAP	O2N-PN-O1N	2.16	122.51	112.44
2	G	1257	NAP	O2N-PN-O1N	2.15	122.43	112.44
2	C	1257	NAP	O2N-PN-O1N	2.13	122.37	112.44
2	H	1257	NAP	C6A-C5A-C4A	2.11	120.06	117.18
2	H	1257	NAP	C3B-C2B-C1B	-2.11	98.77	102.81
2	B	1257	NAP	C5A-C6A-N6A	-2.07	118.15	123.29
2	F	1257	NAP	C4A-N9A-C8A	2.06	107.91	105.74
2	H	1257	NAP	C4B-O4B-C1B	-2.06	104.92	109.47
2	E	1258	NAP	O3-PN-O1N	-2.06	104.52	110.70
2	D	1257	NAP	O7N-C7N-C3N	-2.04	117.11	119.60
2	C	1257	NAP	N6A-C6A-N1A	2.03	122.91	118.38
2	A	1257	NAP	O5B-C5B-C4B	-2.02	102.13	108.99
2	B	1257	NAP	C6A-C5A-C4A	2.02	119.93	117.18
2	D	1257	NAP	C6A-C5A-C4A	2.01	119.92	117.18
2	C	1257	NAP	C5A-C6A-N6A	-2.00	118.32	123.29

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1257	NAP	C5D-O5D-PN-O3
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-O3
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-O3
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-O3
2	D	1257	NAP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1257	NAP	C5D-O5D-PN-O2N
2	D	1257	NAP	O4D-C1D-N1N-C2N
2	E	1258	NAP	C5D-O5D-PN-O3
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-O3
2	F	1257	NAP	C5D-O5D-PN-O1N
2	F	1257	NAP	C5D-O5D-PN-O2N
2	G	1257	NAP	C5D-O5D-PN-O3
2	G	1257	NAP	C5D-O5D-PN-O1N
2	G	1257	NAP	O4D-C1D-N1N-C2N
2	H	1257	NAP	C5D-O5D-PN-O3
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	A	1259	GLU	CA-CB-CG-CD
4	G	1259	GLU	O-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
4	C	1259	GLU	O-C-CA-CB
4	C	1259	GLU	OXT-C-CA-CB
4	D	1259	GLU	O-C-CA-CB
4	G	1259	GLU	OXT-C-CA-CB
4	D	1259	GLU	OXT-C-CA-CB
4	E	1260	GLU	OE1-CD-CG-CB
4	E	1260	GLU	OE2-CD-CG-CB
2	A	1257	NAP	O4D-C1D-N1N-C6N
2	B	1257	NAP	O4D-C1D-N1N-C6N
2	C	1257	NAP	O4D-C1D-N1N-C6N
2	D	1257	NAP	O4D-C1D-N1N-C6N
2	E	1258	NAP	O4D-C1D-N1N-C6N
2	F	1257	NAP	O4D-C1D-N1N-C6N
2	G	1257	NAP	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	1257	NAP	O4D-C1D-N1N-C6N
2	G	1257	NAP	PA-O3-PN-O1N
2	G	1257	NAP	PA-O3-PN-O2N
4	G	1259	GLU	OE2-CD-CG-CB
4	A	1259	GLU	OE2-CD-CG-CB
4	D	1259	GLU	OE1-CD-CG-CB
4	D	1259	GLU	OE2-CD-CG-CB
4	A	1259	GLU	OE1-CD-CG-CB
4	G	1259	GLU	C-CA-CB-CG
4	G	1259	GLU	OE1-CD-CG-CB
2	F	1257	NAP	O4B-C4B-C5B-O5B
2	F	1257	NAP	PA-O3-PN-O2N
4	A	1259	GLU	OXT-C-CA-CB
2	C	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
2	G	1257	NAP	O4B-C4B-C5B-O5B

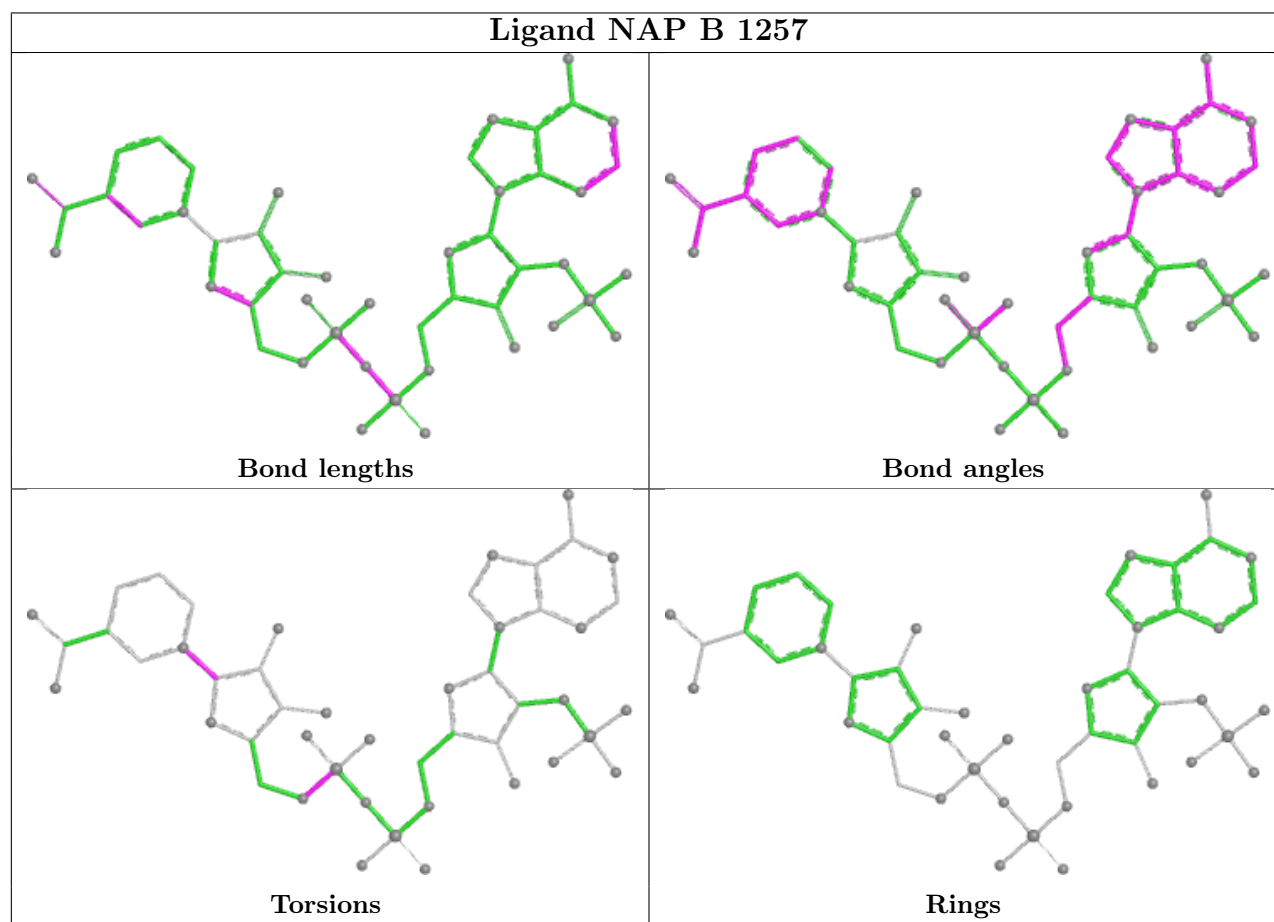
There are no ring outliers.

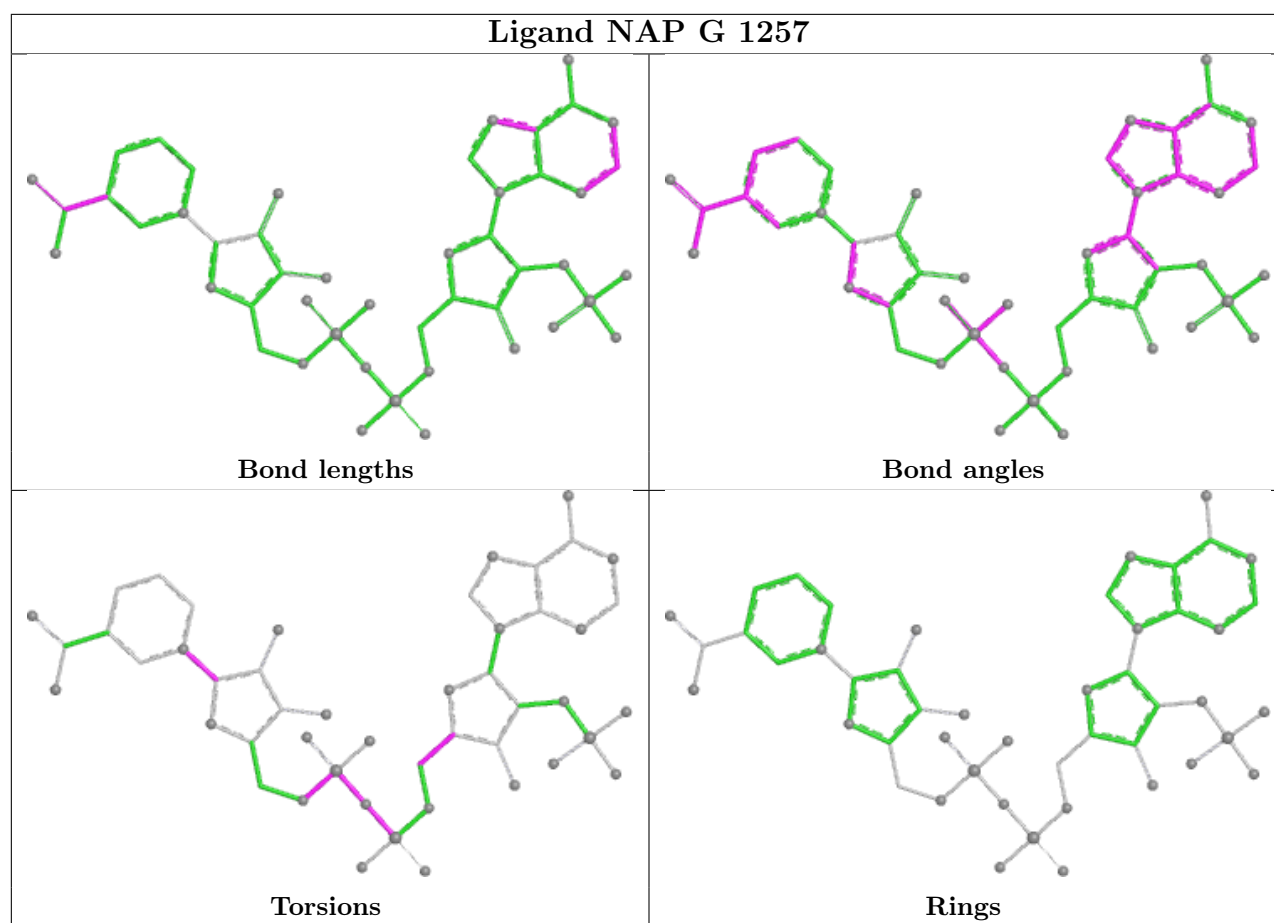
12 monomers are involved in 22 short contacts:

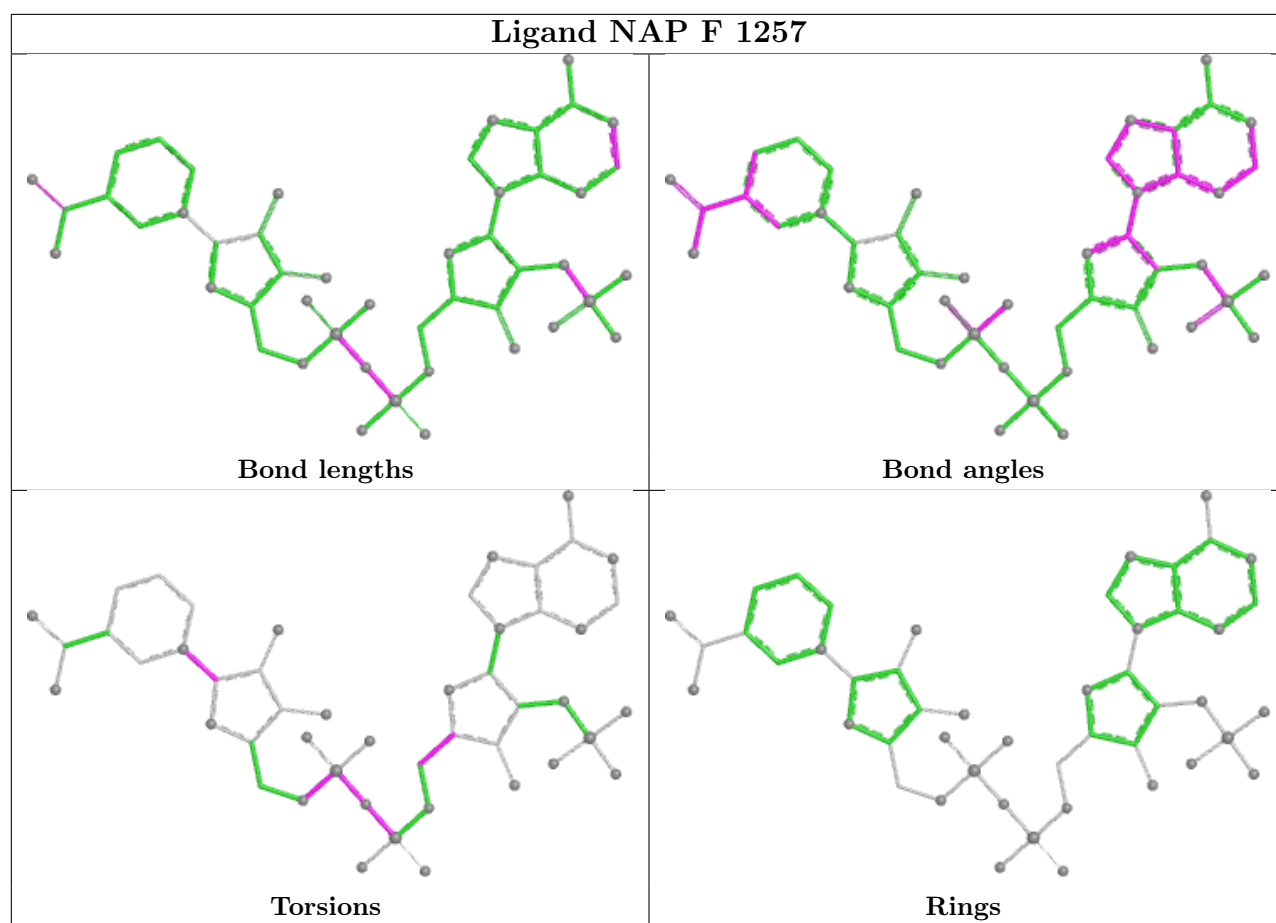
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1257	NAP	2	0
2	G	1257	NAP	2	0
4	A	1259	GLU	1	0
2	A	1257	NAP	1	0
3	G	1258	FPL	1	0
4	C	1259	GLU	4	0
4	D	1259	GLU	4	0
2	H	1257	NAP	3	0
4	E	1260	GLU	1	0
4	G	1259	GLU	2	0
3	E	1259	FPL	1	0
2	C	1257	NAP	1	0

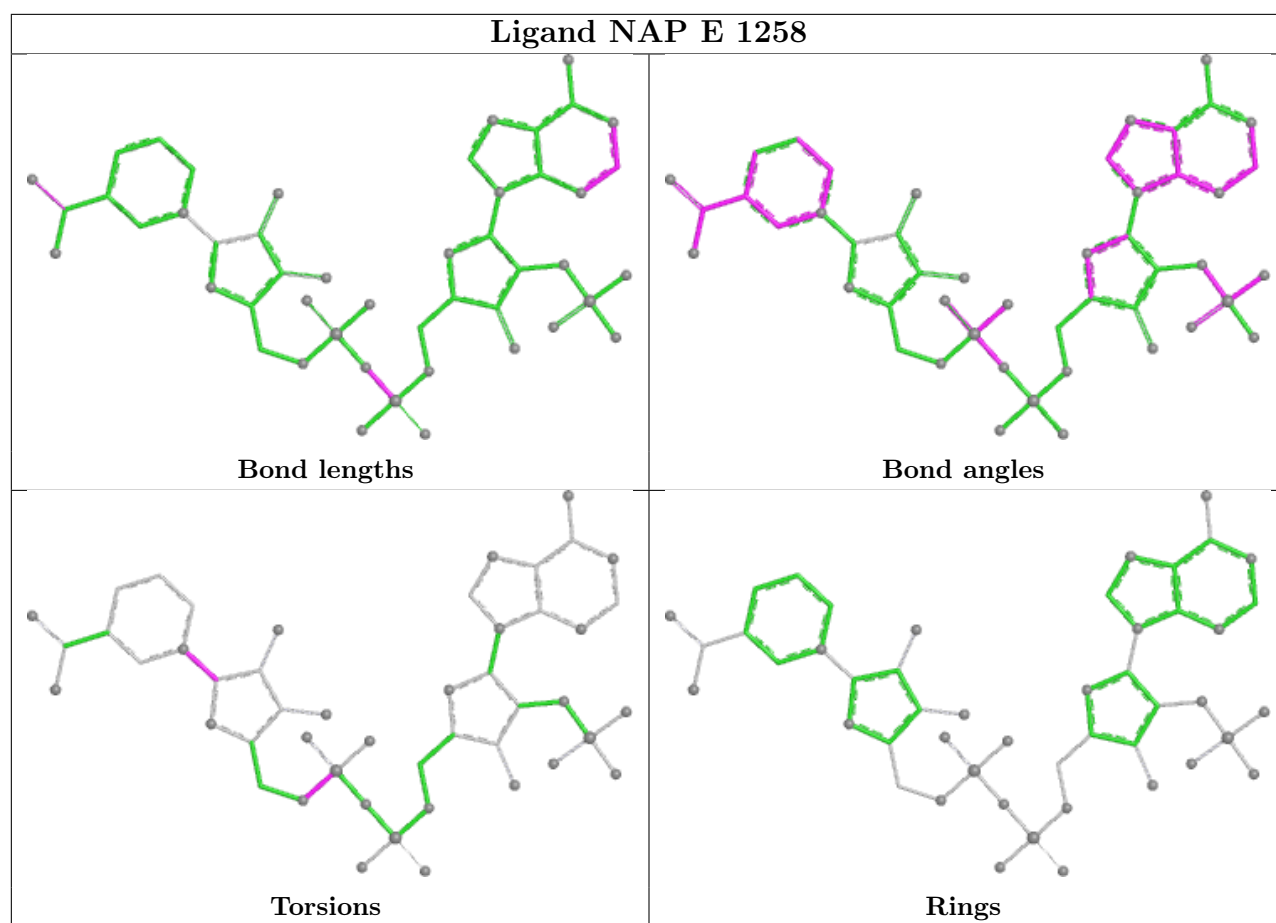
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

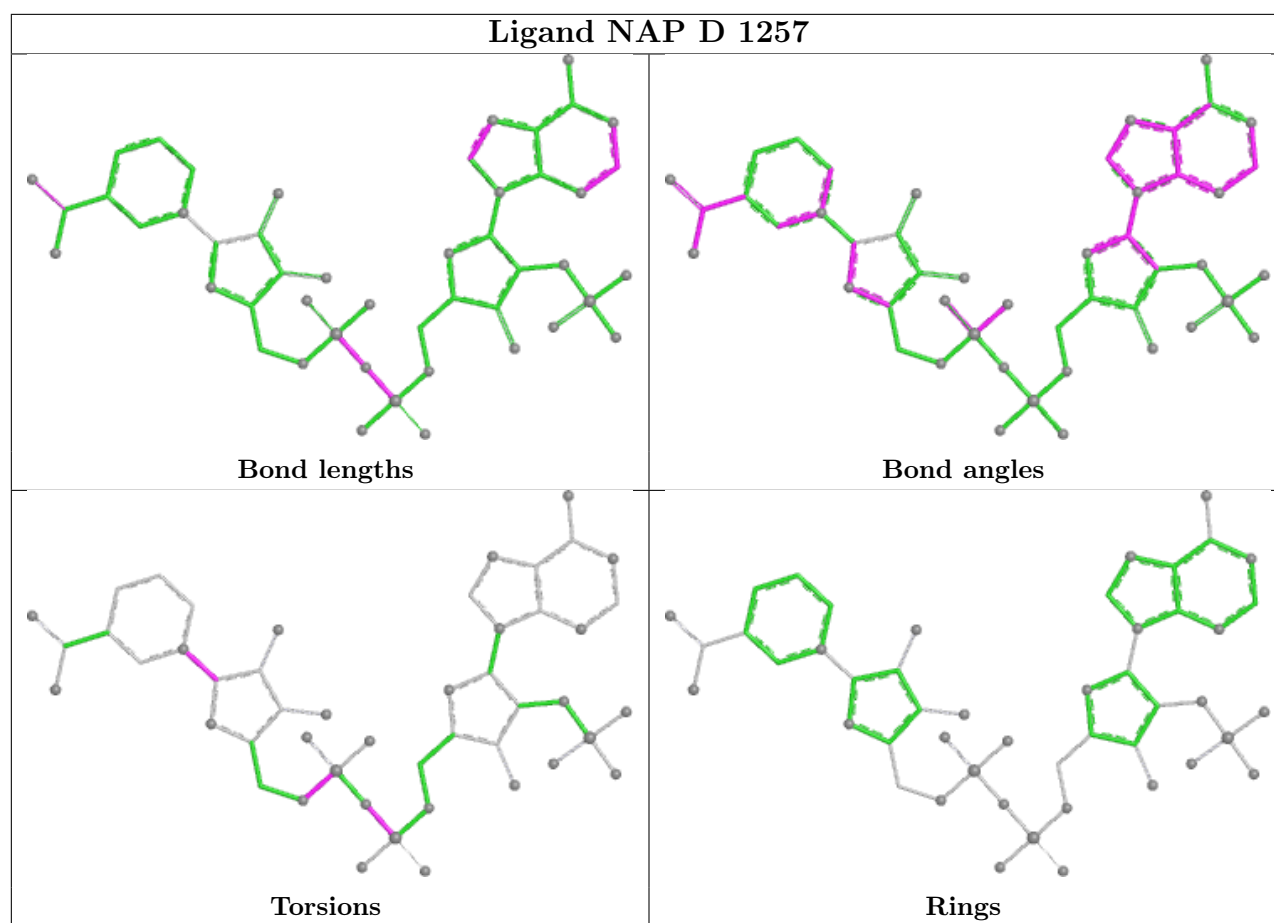
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

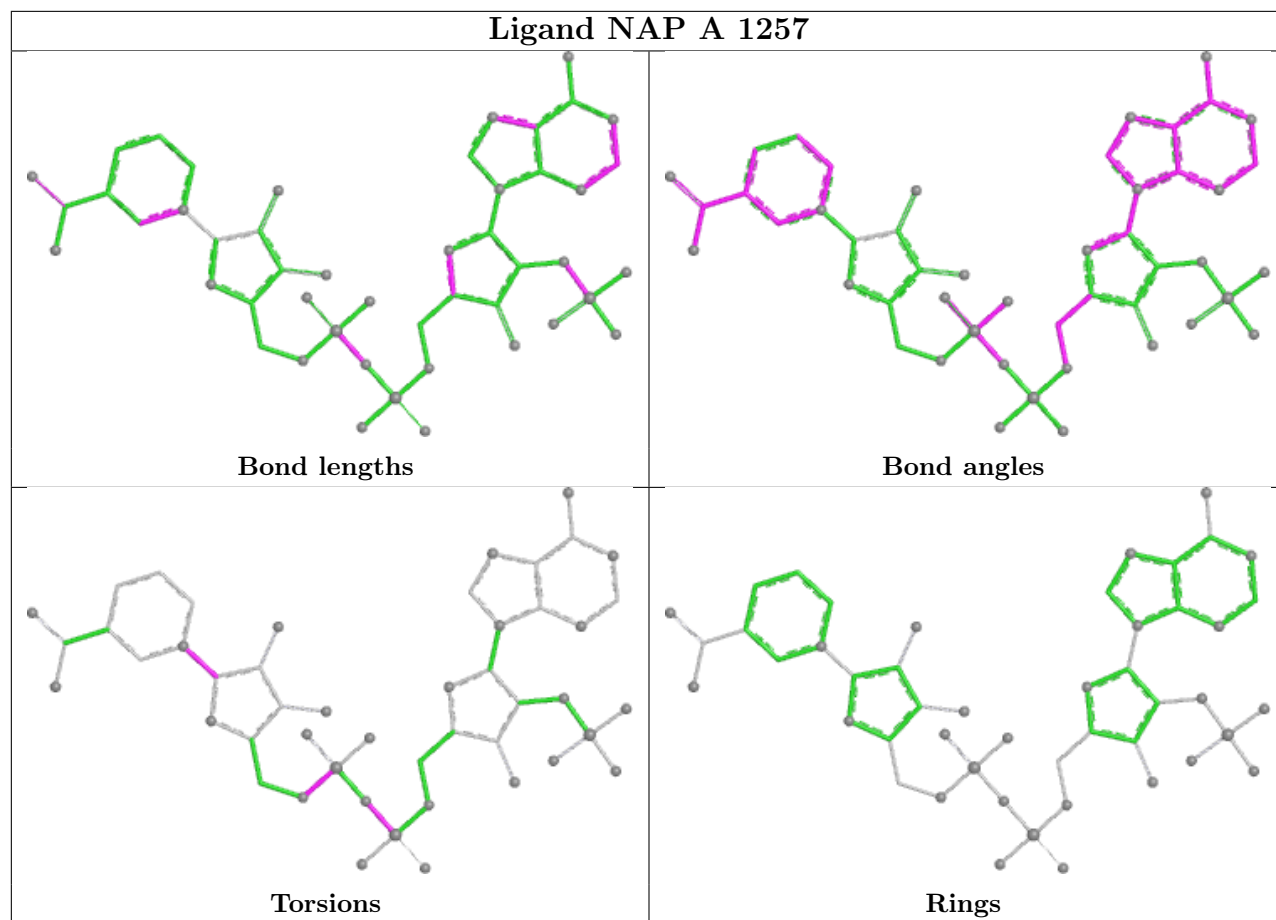


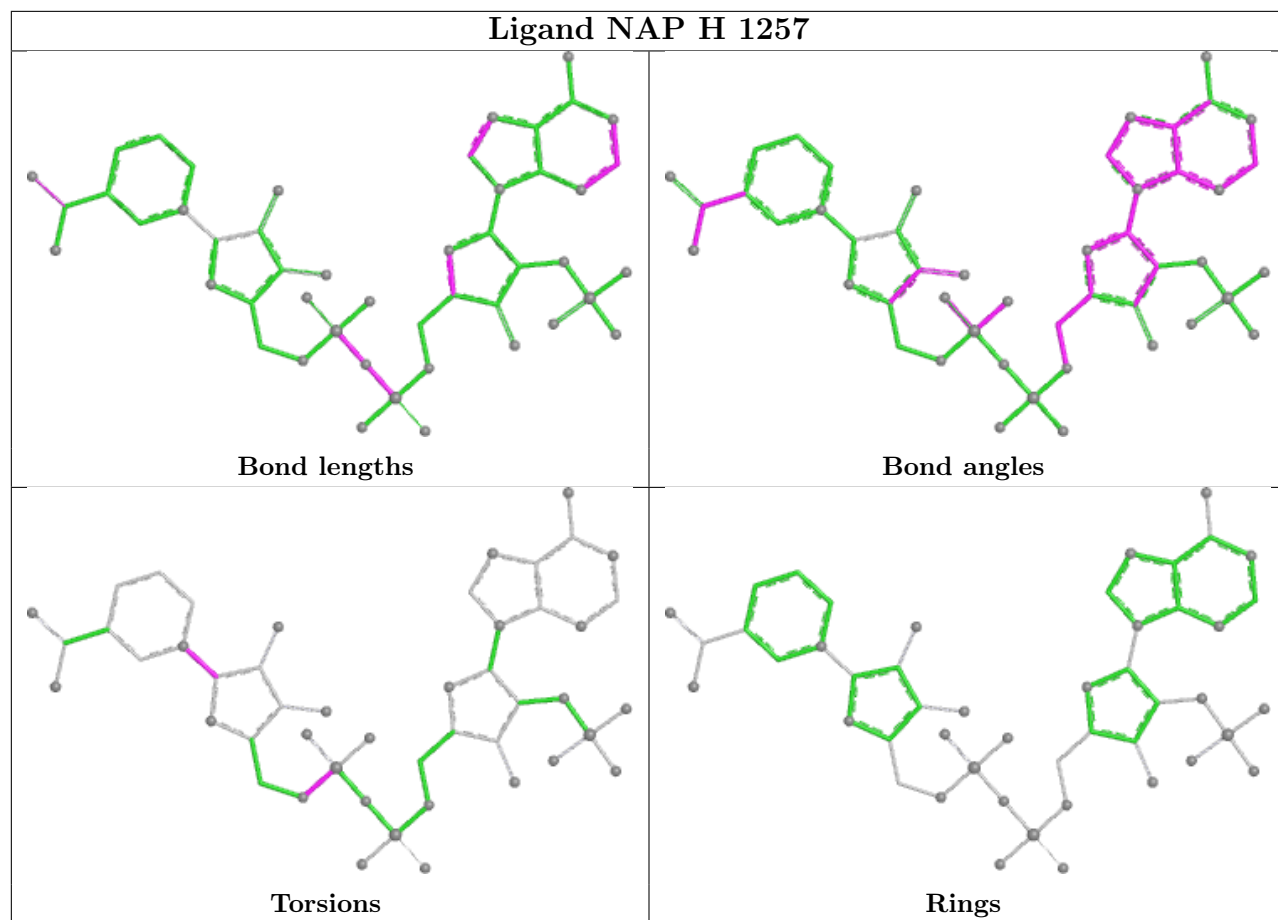


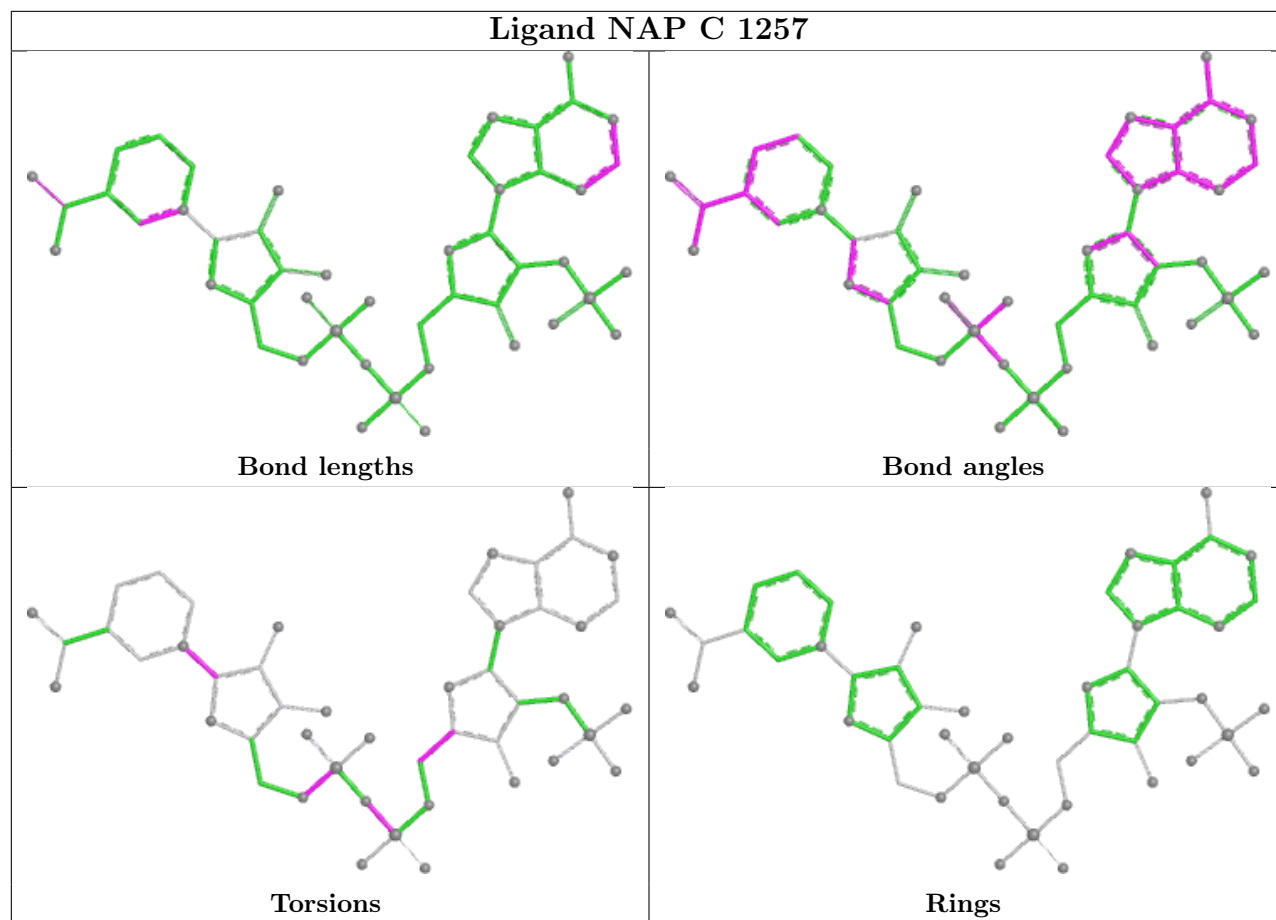












5.7 Other polymers [i](#)

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%)	-0.16	1 (0%) 88 86	27, 39, 62, 74	2 (0%)
1	B	255/282 (90%)	0.21	4 (1%) 70 67	27, 42, 65, 78	1 (0%)
1	C	255/282 (90%)	0.28	5 (1%) 65 61	23, 43, 67, 83	1 (0%)
1	D	254/282 (90%)	0.23	3 (1%) 76 73	32, 50, 79, 98	0
1	E	254/282 (90%)	-0.08	1 (0%) 88 86	28, 40, 62, 78	2 (0%)
1	F	255/282 (90%)	0.15	2 (0%) 82 80	27, 41, 62, 77	0
1	G	255/282 (90%)	0.23	3 (1%) 76 73	27, 43, 65, 86	1 (0%)
1	H	254/282 (90%)	0.15	2 (0%) 82 80	30, 50, 82, 97	0
All	All	2036/2256 (90%)	0.13	21 (1%) 79 76	23, 43, 70, 98	7 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ASN	4.4
1	G	2	VAL	3.5
1	F	104	GLY	3.3
1	B	2	VAL	3.2
1	G	3	ASN	3.1
1	C	2	VAL	3.0
1	C	18[A]	ARG	2.9
1	B	30	GLN	2.8
1	D	99	MET	2.6
1	D	154	VAL	2.3
1	C	214	ARG	2.3
1	H	46	LYS	2.3
1	B	155	GLN	2.3
1	C	139	GLY	2.3
1	B	103	ARG	2.2
1	F	155	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	42[A]	GLU	2.1
1	D	46	LYS	2.1
1	H	214	ARG	2.1
1	E	210[A]	GLU	2.0
1	G	54	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLU	A	1259	10/10	0.65	0.20	76,77,78,78	0
4	GLU	C	1259	10/10	0.71	0.21	81,83,83,83	0
4	GLU	D	1259	10/10	0.72	0.20	76,80,80,80	0
4	GLU	E	1260	10/10	0.75	0.25	95,96,101,102	0
4	GLU	G	1259	10/10	0.75	0.19	76,79,79,79	0
3	FPL	F	1258	15/15	0.92	0.11	37,40,41,43	0
3	FPL	B	1258	15/15	0.93	0.10	39,42,43,45	0
3	FPL	C	1258	15/15	0.93	0.11	39,42,47,48	0
5	CL	E	1257	1/1	0.93	0.20	64,64,64,64	0
2	NAP	H	1257	48/48	0.94	0.09	45,51,59,62	0
2	NAP	D	1257	48/48	0.94	0.09	42,49,61,62	0
3	FPL	G	1258	15/15	0.94	0.09	37,39,48,48	0
3	FPL	D	1258	15/15	0.95	0.10	50,51,55,55	0
3	FPL	E	1259	15/15	0.95	0.08	34,37,41,43	0
3	FPL	H	1258	15/15	0.95	0.10	57,58,59,59	0
3	FPL	A	1258	15/15	0.96	0.07	31,35,37,37	0
2	NAP	B	1257	48/48	0.96	0.07	27,41,45,46	0
2	NAP	C	1257	48/48	0.97	0.07	31,40,47,49	0

Continued on next page...

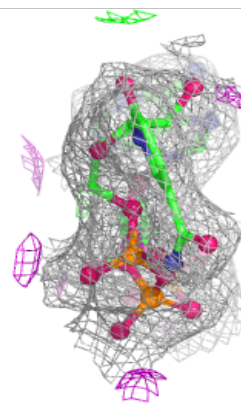
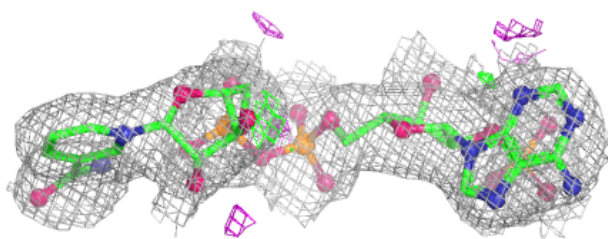
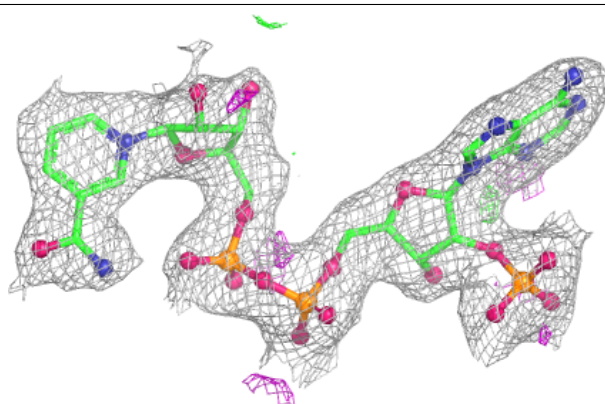
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	1257	48/48	0.97	0.07	32,37,42,43	0
2	NAP	E	1258	48/48	0.97	0.07	31,37,41,42	0
2	NAP	F	1257	48/48	0.97	0.07	31,38,43,44	0
2	NAP	G	1257	48/48	0.97	0.07	31,39,46,48	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.

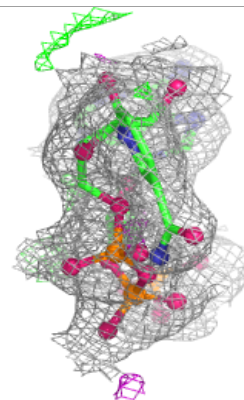
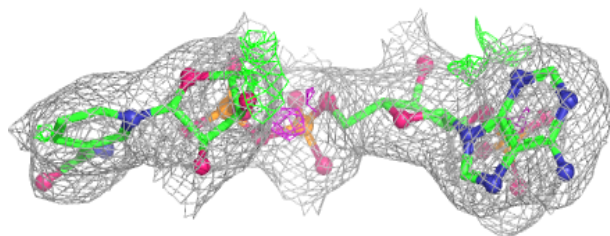
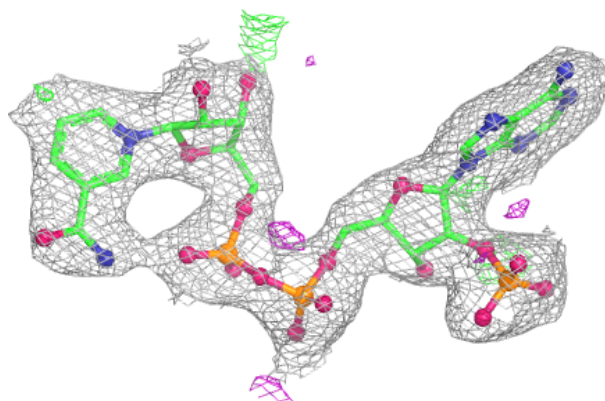
Electron density around NAP H 1257:

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

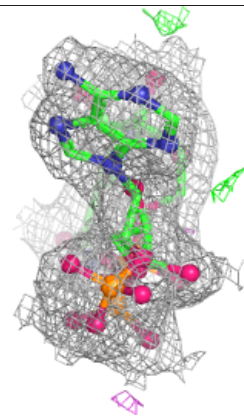
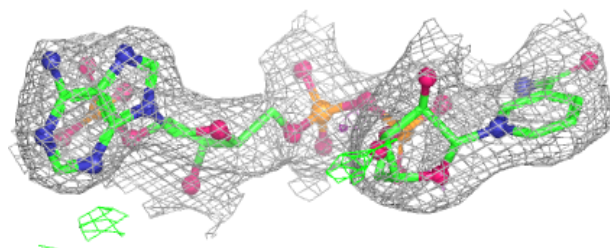
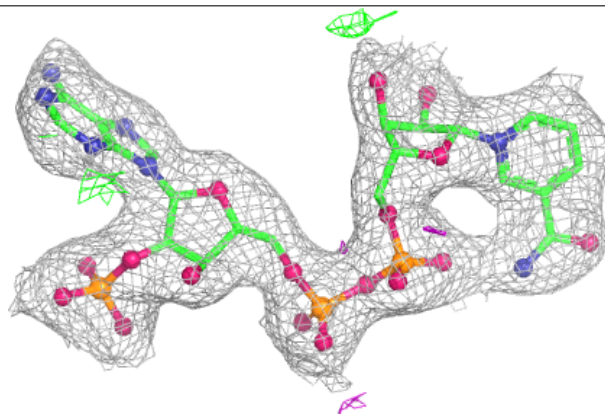


Electron density around NAP D 1257:

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

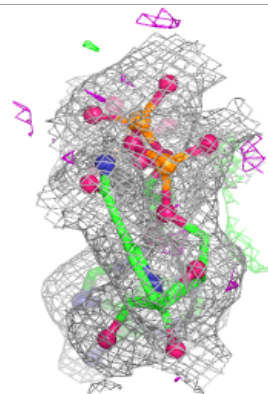
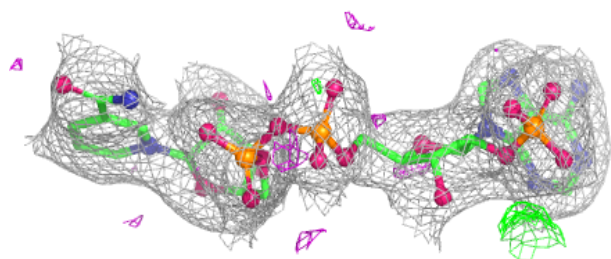
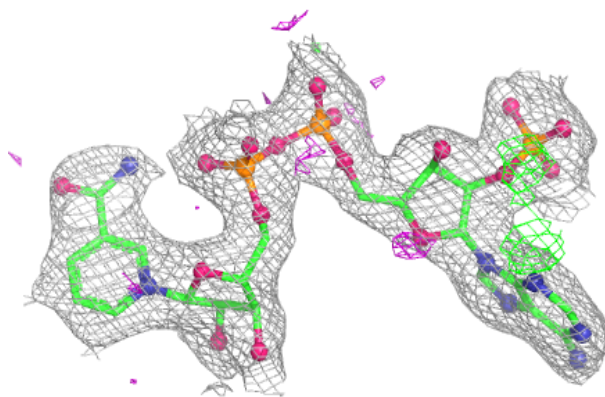
**Electron density around NAP B 1257:**

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

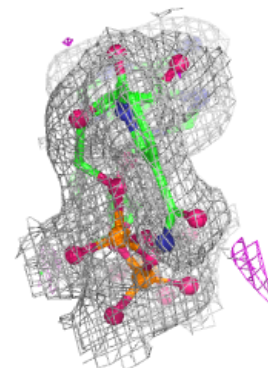
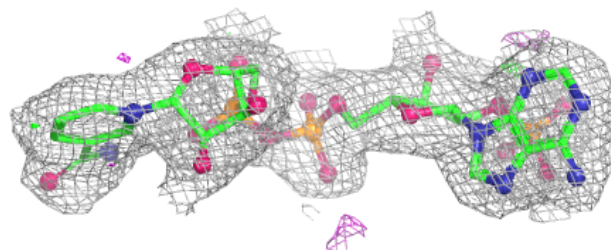
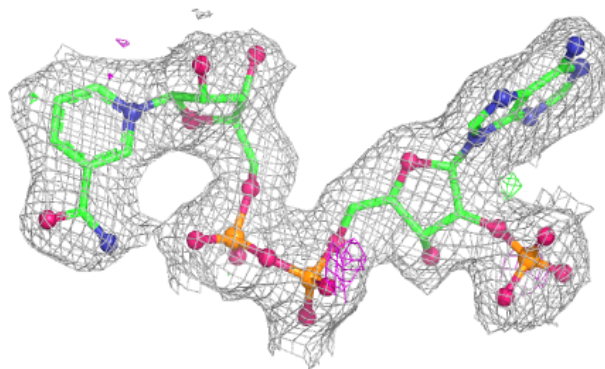


Electron density around NAP C 1257:

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

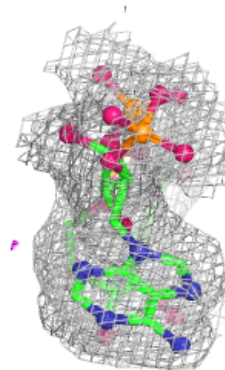
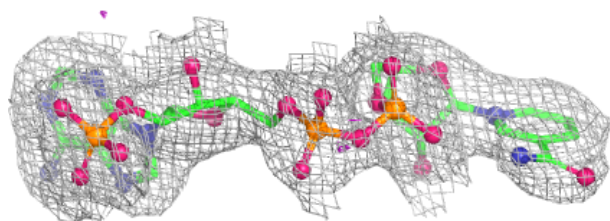
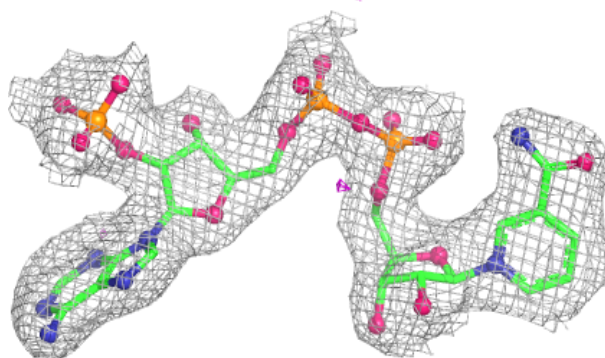
**Electron density around NAP A 1257:**

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

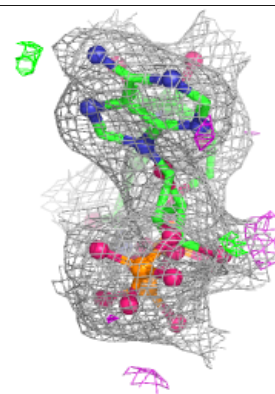
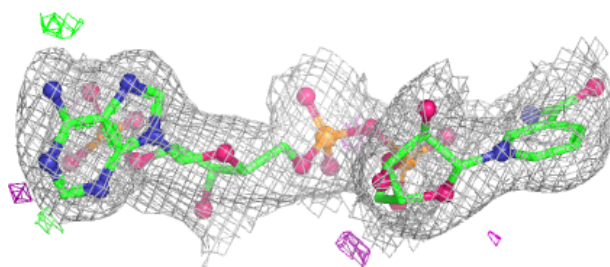
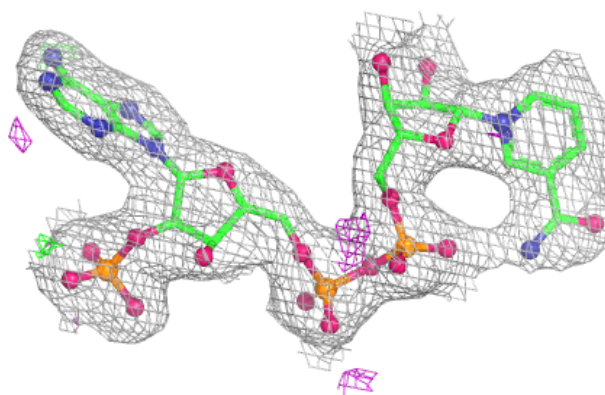


Electron density around NAP E 1258:

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

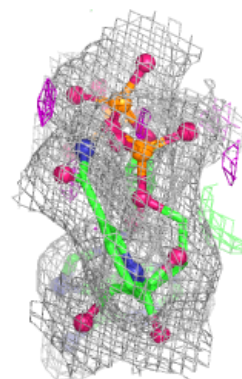
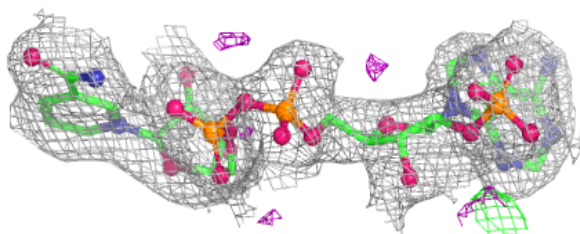
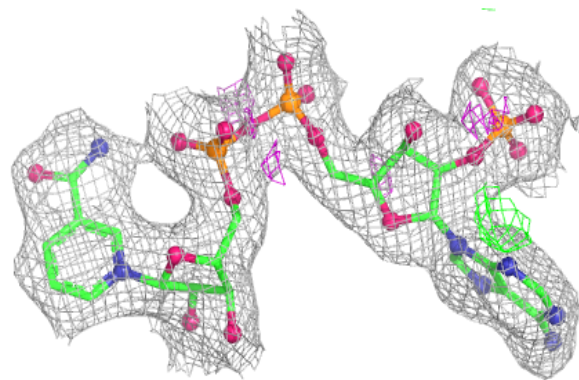
**Electron density around NAP F 1257:**

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



Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.