



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:11 PM GMT

PDB ID : 4BNG  
Title : Crystal structure of S. aureus FabI in complex with NADP and 5-pentyl- 2-phenoxyphenol  
Authors : Schiebel, J.; Chang, A.; Bommineni, G.R.; Tonge, P.J.; Kisker, C.  
Deposited on : 2013-05-15  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

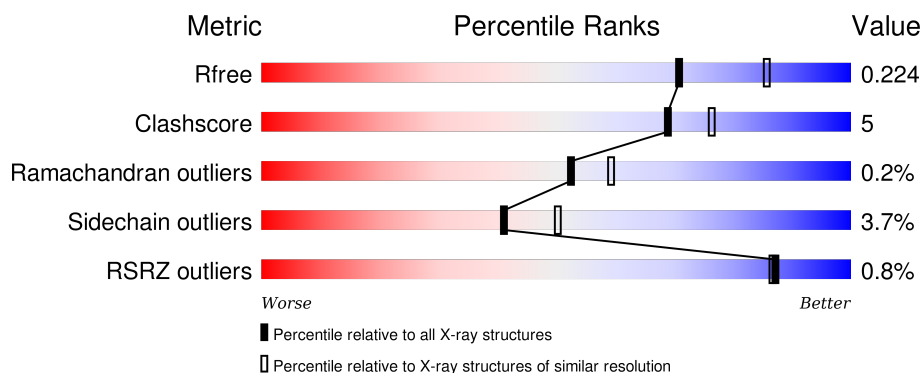
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>84%</div> <div>6%</div> <div>10%</div> </div>
1	B	282	<div> <div>%</div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div>
1	C	282	<div> <div>%</div> <div>80%</div> <div>9%</div> <div>• 10%</div> </div>
1	D	282	<div> <div>%</div> <div>79%</div> <div>10%</div> <div>• 10%</div> </div>
1	E	282	<div> <div>%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	282	 % 77% 13% • 10%
1	G	282	 % 77% 11% • 10%
1	H	282	 % 78% 11% • 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	B	1259	-	-	-	X
4	GLU	C	1259	-	-	-	X
4	GLU	E	1259	-	-	-	X
4	GLU	F	1259	-	-	-	X
4	GLU	G	1259	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17399 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	1	0
			1961	1236	338	383	4			
1	B	255	Total	C	N	O	S	0	3	0
			1977	1245	342	386	4			
1	C	254	Total	C	N	O	S	0	1	0
			1961	1236	338	383	4			
1	D	254	Total	C	N	O	S	0	3	0
			1973	1242	343	384	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	3	0
			1978	1246	341	387	4			
1	G	254	Total	C	N	O	S	0	4	0
			1980	1246	341	389	4			
1	H	254	Total	C	N	O	S	0	2	0
			1965	1237	340	384	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

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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

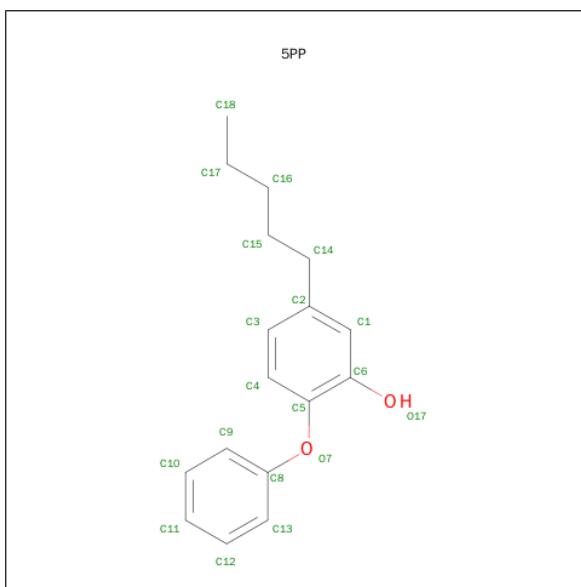
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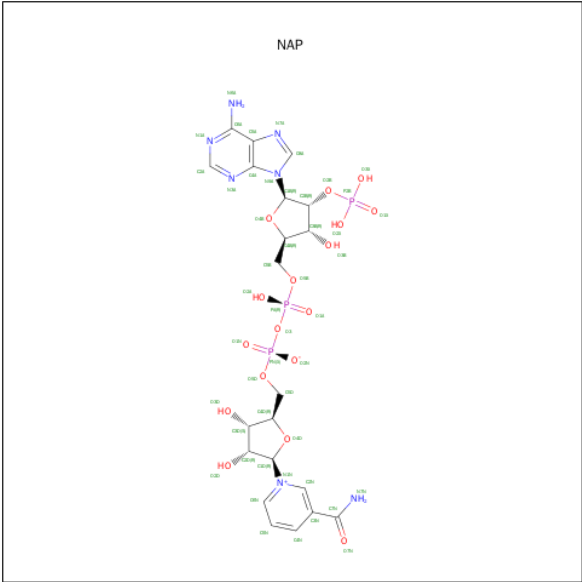
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
G	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
G	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
G	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
G	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
G	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
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 5-PENTYL-2-PHENOXYPHENOL (three-letter code: 5PP) (formula:  $C_{17}H_{20}O_2$ ).



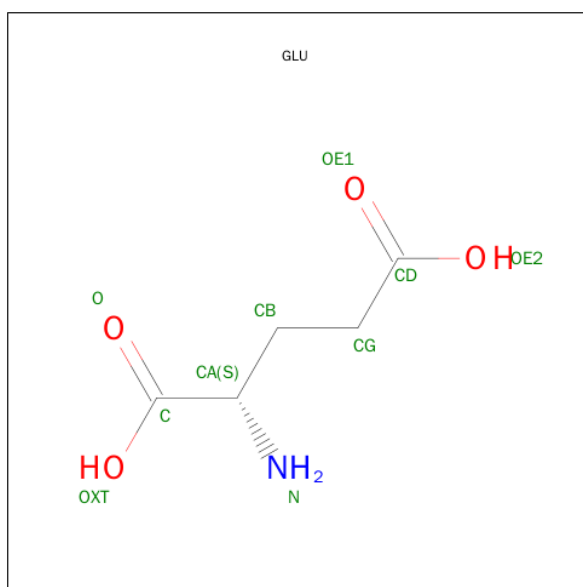
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	17	2		
2	B	1	Total	C	O	0	0
			19	17	2		
2	C	1	Total	C	O	0	0
			19	17	2		
2	D	1	Total	C	O	0	0
			19	17	2		
2	E	1	Total	C	O	0	0
			19	17	2		
2	F	1	Total	C	O	0	0
			19	17	2		
2	G	1	Total	C	O	0	0
			19	17	2		
2	H	1	Total	C	O	0	0
			19	17	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	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	E	1	Total	C	N	O	0	0
			10	5	1	4		
4	F	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total	O	0	0
			167	167		
5	B	135	Total	O	0	0
			135	135		
5	C	120	Total	O	0	0
			120	120		
5	D	118	Total	O	0	0
			118	118		
5	E	127	Total	O	0	0
			127	127		
5	F	140	Total	O	0	0
			140	140		
5	G	136	Total	O	0	0
			136	136		

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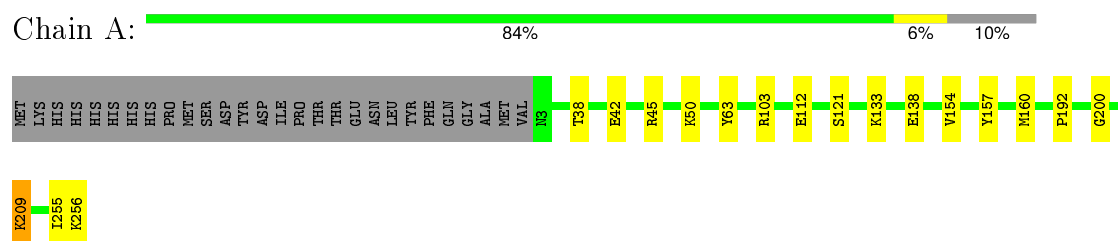
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	108	Total 108	O 108	0	0

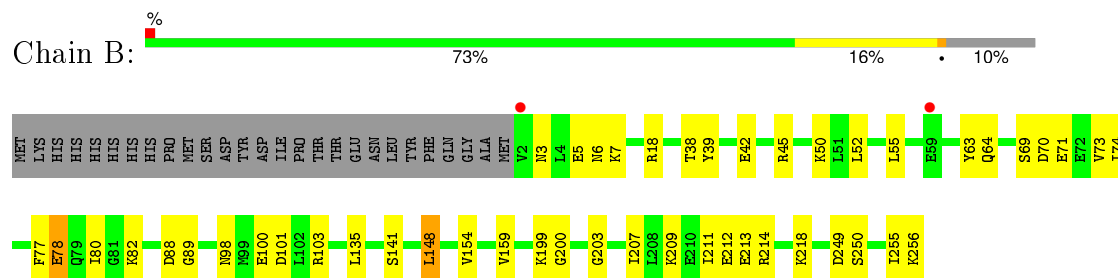
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

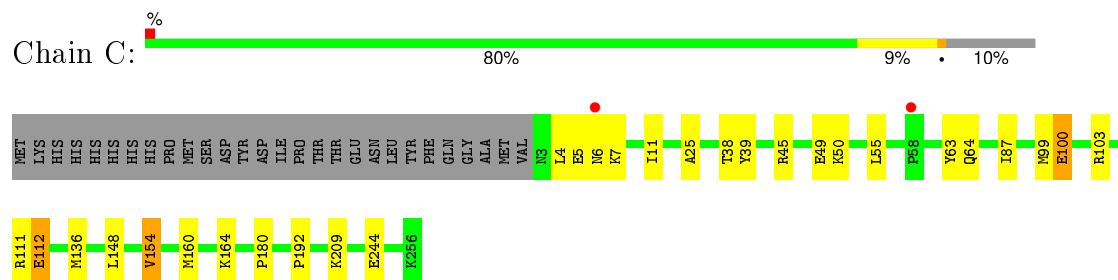
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



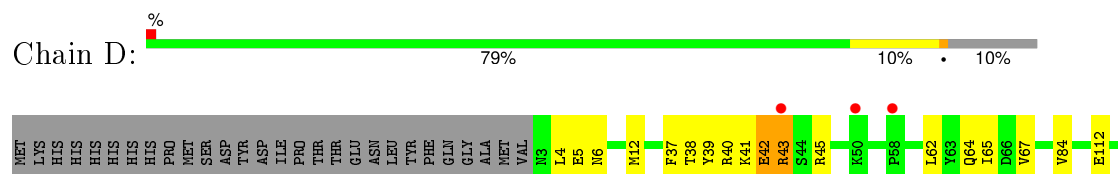
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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

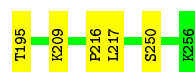
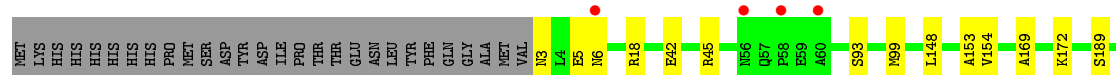
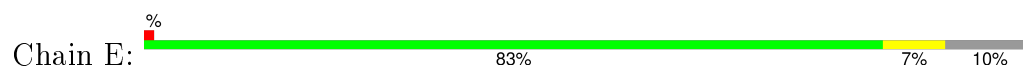


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

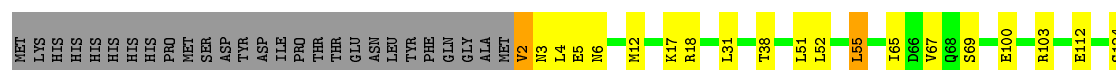
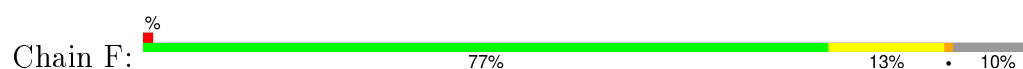




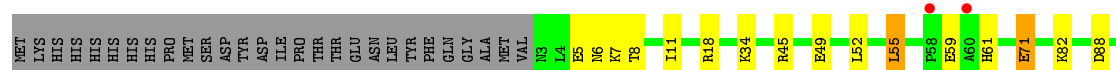
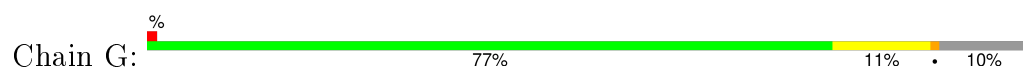
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



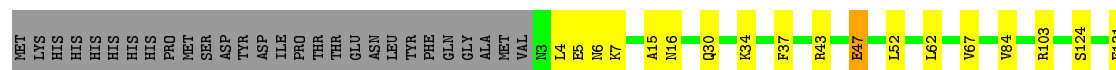
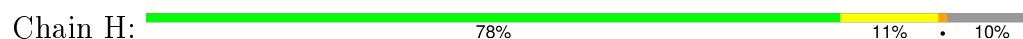
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



- 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, $\alpha$ , $\beta$ , $\gamma$	89.12Å 94.44Å 94.88Å 98.56° 97.22° 111.35°	Depositor
Resolution (Å)	46.01 – 2.20 46.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.01-2.20) 87.0 (46.01-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.208 0.175 , 0.224	Depositor DCC
$R_{free}$ test set	6647 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 132674 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, 5PP

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	0.60	0/1991	0.82	0/2683
1	B	0.59	0/2007	0.81	1/2705 (0.0%)
1	C	0.56	0/1991	0.80	0/2683
1	D	0.54	0/2003	0.78	0/2698
1	E	0.60	0/2000	0.82	0/2695
1	F	0.61	0/2008	0.85	2/2706 (0.1%)
1	G	0.61	0/2010	0.87	1/2708 (0.0%)
1	H	0.60	0/1992	0.85	0/2684
All	All	0.59	0/16002	0.83	4/21562 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	208	LEU	CA-CB-CG	6.12	129.38	115.30
1	F	208	LEU	CA-CB-CG	6.07	129.27	115.30
1	B	52	LEU	CA-CB-CG	-5.43	102.80	115.30
1	F	177	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	43	ARG	Peptide

## 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	1961	0	1974	12	0
1	B	1977	0	1990	29	0
1	C	1961	0	1974	20	1
1	D	1973	0	1988	18	0
1	E	1967	0	1980	9	0
1	F	1978	0	1990	22	0
1	G	1980	0	1986	29	0
1	H	1965	0	1975	19	0
2	A	19	0	20	0	0
2	B	19	0	20	0	0
2	C	19	0	20	0	0
2	D	19	0	20	1	0
2	E	19	0	20	1	0
2	F	19	0	20	0	0
2	G	19	0	19	1	0
2	H	19	0	20	0	0
3	A	48	0	25	1	0
3	B	48	0	25	0	0
3	C	48	0	25	1	0
3	D	48	0	25	4	0
3	E	48	0	25	1	0
3	F	48	0	25	1	0
3	G	48	0	25	2	0
3	H	48	0	25	0	0
4	B	10	0	5	1	0
4	C	10	0	5	1	0
4	E	10	0	5	0	0
4	F	10	0	5	1	0
4	G	10	0	5	4	0
5	A	167	0	0	4	0
5	B	135	0	0	2	0
5	C	120	0	0	6	0
5	D	118	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	127	0	0	1	0
5	F	140	0	0	1	1
5	G	136	0	0	5	0
5	H	108	0	0	2	0
All	All	17399	0	16241	150	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 5.

All (150) 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:G:99:MET:HE1	1:G:200:GLY:HA2	1.13	1.11
1:G:99:MET:CE	1:G:200:GLY:HA2	1.90	1.00
1:B:45:ARG:HD3	5:B:2027:HOH:O	1.66	0.95
1:E:148:LEU:HD21	1:G:256:LYS:HD2	1.58	0.85
1:B:199:LYS:HE2	4:G:1259:GLU:O	1.75	0.85
1:C:100[A]:GLU:OE1	5:C:2057:HOH:O	1.93	0.84
1:G:99:MET:HE1	1:G:200:GLY:CA	2.04	0.83
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH2	2.18	0.77
1:B:42:GLU:HG3	5:G:2076:HOH:O	1.86	0.75
1:A:103:ARG:NH2	1:A:200:GLY:O	2.21	0.73
1:H:210:GLU:HG3	1:H:214:ARG:CD	2.18	0.73
1:D:40:ARG:HB3	3:D:1258:NAP:O2X	1.91	0.71
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.74	0.70
4:G:1259:GLU:N	4:G:1259:GLU:OE1	2.25	0.69
1:D:40:ARG:HD3	3:D:1258:NAP:C6A	2.23	0.68
1:E:3:ASN:HD21	1:E:5:GLU:HB2	1.59	0.68
1:G:99:MET:CE	1:G:200:GLY:CA	2.66	0.67
4:C:1259:GLU:OXT	5:C:2060:HOH:O	2.12	0.67
1:H:210:GLU:HG3	1:H:214:ARG:HD2	1.76	0.67
1:D:39:TYR:CZ	1:D:45:ARG:HG3	2.33	0.64
1:F:103:ARG:NH2	1:F:200:GLY:O	2.30	0.64
1:D:42:GLU:O	1:D:45:ARG:N	2.24	0.64
1:F:5:GLU:O	1:F:6:ASN:HB2	1.98	0.64
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.80	0.63
1:C:112:GLU:HB3	5:C:2068:HOH:O	2.01	0.60
1:C:244:GLU:OE1	5:C:2119:HOH:O	2.16	0.60
1:H:210:GLU:HG3	1:H:214:ARG:HD3	1.84	0.59
1:G:71[B]:GLU:HG3	5:G:2051:HOH:O	2.04	0.58
1:F:239[A]:SER:OG	1:G:225:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLU:O	1:C:6:ASN:HB2	2.04	0.57
1:G:5:GLU:O	1:G:6:ASN:HB2	2.05	0.57
1:C:50:LYS:HG3	5:C:2027:HOH:O	2.03	0.57
1:H:5:GLU:O	1:H:6:ASN:HB2	2.03	0.56
1:F:17:LYS:HB3	1:F:51:LEU:HD21	1.87	0.56
1:H:133:LYS:HE3	1:H:181:ASP:OD2	2.07	0.55
1:D:37:PHE:HB2	1:D:62:LEU:HD23	1.90	0.54
1:G:45:ARG:HD3	1:G:49:GLU:OE2	2.08	0.54
1:H:67:VAL:HB	1:H:124:SER:HB2	1.89	0.53
1:F:207:ILE:O	1:F:211:ILE:HG12	2.09	0.53
1:B:255:ILE:HA	1:D:153:ALA:O	2.08	0.53
1:C:11:ILE:HD13	1:C:25:ALA:HB2	1.91	0.53
1:H:154:VAL:HG13	5:H:2070:HOH:O	2.08	0.53
1:C:192:PRO:HA	3:C:1258:NAP:O7N	2.09	0.53
1:H:155:GLN:O	1:H:156:ASN:HB2	2.08	0.53
1:G:154:VAL:HG13	5:G:2093:HOH:O	2.10	0.52
1:A:50:LYS:NZ	5:A:2037:HOH:O	2.43	0.52
1:A:133:LYS:HD3	5:A:2097:HOH:O	2.09	0.51
1:B:77:PHE:HA	1:B:80:ILE:HD12	1.92	0.51
1:E:172:LYS:HE3	5:E:2086:HOH:O	2.10	0.51
1:C:154:VAL:HG13	5:C:2087:HOH:O	2.11	0.51
1:F:239[A]:SER:HG	1:G:225:GLU:HG2	1.77	0.50
1:H:34:LYS:HD2	5:H:2002:HOH:O	2.11	0.50
1:G:52:LEU:HD23	1:G:55:LEU:HD22	1.92	0.50
1:B:5:GLU:O	1:B:6:ASN:HB2	2.11	0.50
1:D:5:GLU:O	1:D:6:ASN:HB2	2.12	0.50
1:A:256:LYS:HG2	1:C:148:LEU:CD2	2.41	0.49
4:G:1259:GLU:CD	4:G:1259:GLU:N	2.66	0.49
1:C:111:ARG:NH1	1:D:119:ASP:OD1	2.42	0.49
1:C:5:GLU:O	1:C:6:ASN:CB	2.60	0.49
1:G:7:LYS:HA	1:G:88:ASP:OD2	2.13	0.49
1:H:37:PHE:HB2	1:H:62:LEU:HD23	1.94	0.49
1:H:215:ALA:O	1:H:218:LYS:HD2	2.12	0.48
1:B:214:ARG:HH12	1:D:214[B]:ARG:HH12	1.62	0.48
1:C:45:ARG:O	1:C:49:GLU:HG3	2.13	0.48
1:A:154:VAL:HG12	1:A:157:TYR:HB2	1.96	0.48
1:G:249:ASP:O	1:G:250:SER:HB2	2.14	0.47
1:H:131:GLU:O	1:H:134:LYS:HB2	2.13	0.47
1:G:101:ASP:HB3	1:G:159:VAL:CG1	2.44	0.47
1:G:101:ASP:O	1:G:159:VAL:HG12	2.15	0.47
1:D:38:THR:HG21	1:D:65:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:THR:HG21	1:F:65:ILE:HD12	1.97	0.46
1:B:42:GLU:CG	5:G:2076:HOH:O	2.55	0.46
1:G:52:LEU:HD23	1:G:52:LEU:HA	1.55	0.46
1:G:207:ILE:O	1:G:211:ILE:HG12	2.15	0.46
2:E:1257:5PP:O7	3:E:1258:NAP:H2D	2.16	0.46
1:E:5:GLU:O	1:E:6:ASN:HB2	2.16	0.45
1:B:78:GLU:O	1:B:82:LYS:HG3	2.16	0.45
1:B:212:GLU:O	1:B:218:LYS:HA	2.16	0.45
1:B:103:ARG:NH2	1:B:200:GLY:O	2.49	0.45
1:F:12:MET:HG2	1:F:38:THR:OG1	2.16	0.45
5:A:2145:HOH:O	1:D:239[A]:SER:O	2.21	0.45
1:H:15:ALA:O	1:H:47:GLU:HG2	2.16	0.45
1:H:103:ARG:CZ	1:H:103:ARG:HB3	2.47	0.45
1:H:16:ASN:HA	1:H:47:GLU:HG3	1.99	0.45
1:F:146:THR:O	3:F:1258:NAP:H6N	2.17	0.44
1:C:100[B]:GLU:H	1:C:100[B]:GLU:CD	2.20	0.44
1:G:52:LEU:HD23	1:G:55:LEU:CD2	2.47	0.44
1:A:192:PRO:HA	3:A:1258:NAP:O7N	2.18	0.44
1:G:8:THR:HA	1:G:34:LYS:O	2.16	0.44
1:G:99:MET:HE2	1:G:200:GLY:CA	2.47	0.44
1:F:184:ARG:HD2	1:F:241:VAL:O	2.18	0.44
1:G:157:TYR:CZ	1:G:160:MET:HG3	2.53	0.44
1:B:39:TYR:O	1:B:64:GLN:HA	2.17	0.44
1:B:38:THR:HA	1:B:63:TYR:O	2.17	0.44
1:C:87:ILE:O	1:C:136:MET:HG2	2.18	0.44
1:A:154:VAL:HG13	5:A:2113:HOH:O	2.18	0.43
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH2	2.35	0.43
1:F:203:GLY:H	4:F:1259:GLU:HB2	1.84	0.43
1:B:77:PHE:O	1:B:135:LEU:HD11	2.19	0.43
1:H:7:LYS:HA	1:H:7:LYS:HD3	1.66	0.43
1:B:256:LYS:HB3	1:B:256:LYS:HE3	1.87	0.43
1:F:18:ARG:O	1:F:195:THR:HG22	2.19	0.43
1:D:112:GLU:H	1:D:112:GLU:CD	2.22	0.43
1:G:101:ASP:HB3	1:G:159:VAL:HG11	2.00	0.43
1:D:12:MET:HG2	1:D:38:THR:OG1	2.18	0.43
2:G:1257:5PP:O7	3:G:1258:NAP:H2D	2.18	0.43
1:A:38:THR:HA	1:A:63:TYR:O	2.19	0.43
1:B:70:ASP:O	1:B:74:ILE:HG13	2.19	0.43
1:B:218:LYS:HD3	1:C:180:PRO:HG3	1.99	0.43
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.54	0.42
1:B:101:ASP:HB3	1:B:159:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASP:O	1:B:250:SER:HB2	2.18	0.42
1:G:192:PRO:HA	3:G:1258:NAP:O7N	2.19	0.42
1:D:117:ALA:O	1:D:121:SER:HB2	2.19	0.42
1:C:39:TYR:CZ	1:C:64:GLN:HB2	2.54	0.42
1:B:7:LYS:HA	1:B:88:ASP:OD2	2.19	0.42
1:B:89:GLY:HA3	1:B:141:SER:O	2.20	0.42
1:G:18:ARG:NE	5:G:2023:HOH:O	2.50	0.42
1:B:71:GLU:HB2	5:B:2048:HOH:O	2.20	0.42
1:F:67:VAL:HB	1:F:124:SER:HB2	2.02	0.42
1:E:169:ALA:HB2	1:F:165:ALA:CB	2.49	0.42
1:F:52:LEU:HA	1:F:52:LEU:HD23	1.72	0.42
1:F:55:LEU:HD12	1:F:55:LEU:HA	1.82	0.42
1:B:69:SER:O	1:B:73:VAL:HG23	2.20	0.42
1:G:59:GLU:HG3	1:G:61:HIS:NE2	2.34	0.42
1:F:214:ARG:NH2	5:F:2121:HOH:O	2.52	0.42
1:B:209:LYS:HE2	1:B:213:GLU:OE2	2.20	0.42
1:H:155:GLN:OE1	1:H:155:GLN:HA	2.19	0.41
1:G:209:LYS:O	1:G:213:GLU:HG3	2.20	0.41
1:E:217:LEU:HB2	1:E:250:SER:HB3	2.01	0.41
1:G:8:THR:HG23	1:G:34:LYS:HG2	2.03	0.41
1:B:203:GLY:H	4:B:1259:GLU:HB2	1.86	0.41
2:D:1257:5PP:O7	3:D:1258:NAP:H2D	2.20	0.41
1:A:157:TYR:CZ	1:A:160:MET:HG3	2.55	0.41
1:C:160:MET:O	1:C:164:LYS:HG2	2.21	0.41
1:B:148:LEU:HD21	1:D:256:LYS:HE3	2.03	0.41
1:A:209:LYS:HB3	1:A:209:LYS:HE2	1.70	0.41
1:B:207:ILE:O	1:B:211:ILE:HG12	2.20	0.41
1:F:256:LYS:HE2	1:H:148:LEU:HD21	2.02	0.41
1:C:4:LEU:HD22	1:C:7:LYS:HG3	2.02	0.41
1:G:11:ILE:HG21	1:G:11:ILE:HD13	1.79	0.40
1:B:98:ASN:HB3	1:B:100:GLU:OE1	2.22	0.40
1:F:2:VAL:HB	1:F:31:LEU:HD13	2.02	0.40
1:B:199:LYS:HD3	4:G:1259:GLU:HB3	2.03	0.40
1:D:130:HIS:HE1	5:D:2073:HOH:O	2.03	0.40
1:C:38:THR:HA	1:C:63:TYR:O	2.21	0.40
1:D:120:ILE:HD13	3:D:1258:NAP:H61A	1.86	0.40
1:F:124:SER:O	1:F:128:VAL:HG23	2.22	0.40
1:E:18:ARG:O	1:E:195:THR:HG22	2.21	0.40
1:D:67:VAL:HG21	1:D:124:SER:CB	2.52	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:C:100[B]:GLU:OE1	5:F:2038:HOH:O[1_566]	2.02	0.18

## 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	253/282 (90%)	244 (96%)	9 (4%)	0	100	100
1	B	256/282 (91%)	243 (95%)	12 (5%)	1 (0%)	39	42
1	C	253/282 (90%)	242 (96%)	11 (4%)	0	100	100
1	D	255/282 (90%)	242 (95%)	12 (5%)	1 (0%)	39	42
1	E	254/282 (90%)	242 (95%)	12 (5%)	0	100	100
1	F	256/282 (91%)	244 (95%)	11 (4%)	1 (0%)	39	42
1	G	256/282 (91%)	242 (94%)	13 (5%)	1 (0%)	39	42
1	H	254/282 (90%)	239 (94%)	15 (6%)	0	100	100
All	All	2037/2256 (90%)	1938 (95%)	95 (5%)	4 (0%)	52	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	LEU
1	D	43	ARG
1	F	100	GLU
1	G	148	LEU

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/234 (89%)	204 (98%)	5 (2%)	57	69
1	B	211/234 (90%)	204 (97%)	7 (3%)	45	56
1	C	209/234 (89%)	201 (96%)	8 (4%)	40	49
1	D	210/234 (90%)	202 (96%)	8 (4%)	40	49
1	E	210/234 (90%)	204 (97%)	6 (3%)	50	62
1	F	211/234 (90%)	204 (97%)	7 (3%)	45	56
1	G	211/234 (90%)	203 (96%)	8 (4%)	40	49
1	H	209/234 (89%)	196 (94%)	13 (6%)	23	25
All	All	1680/1872 (90%)	1618 (96%)	62 (4%)	41	50

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	121	SER
1	A	138	GLU
1	A	209	LYS
1	A	255	ILE
1	B	3[A]	ASN
1	B	3[B]	ASN
1	B	18	ARG
1	B	50	LYS
1	B	55	LEU
1	B	78	GLU
1	B	154	VAL
1	C	55	LEU
1	C	99	MET
1	C	100[A]	GLU
1	C	100[B]	GLU
1	C	103	ARG
1	C	112	GLU
1	C	154	VAL
1	C	209	LYS
1	D	4	LEU
1	D	41	LYS
1	D	42	GLU
1	D	64	GLN
1	D	84	VAL

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Mol	Chain	Res	Type
1	D	154	VAL
1	D	155	GLN
1	D	256	LYS
1	E	93	SER
1	E	99	MET
1	E	154	VAL
1	E	189	SER
1	E	209	LYS
1	E	216	PRO
1	F	2	VAL
1	F	3	ASN
1	F	4	LEU
1	F	55	LEU
1	F	69	SER
1	F	112	GLU
1	F	213	GLU
1	G	55	LEU
1	G	71[A]	GLU
1	G	71[B]	GLU
1	G	82	LYS
1	G	100	GLU
1	G	103	ARG
1	G	154	VAL
1	G	256	LYS
1	H	4	LEU
1	H	30	GLN
1	H	43	ARG
1	H	47	GLU
1	H	52	LEU
1	H	84	VAL
1	H	138	GLU
1	H	154	VAL
1	H	155	GLN
1	H	164	LYS
1	H	205	ASN
1	H	214	ARG
1	H	216	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN

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Mol	Chain	Res	Type
1	B	56	ASN
1	B	155	GLN
1	C	155	GLN
1	D	30	GLN
1	D	253	HIS
1	E	3	ASN
1	F	56	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

21 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	$\# Z  > 2$
2	5PP	A	1257	-	20,20,20	1.25	2 (10%)	25,25,25	1.10	2 (8%)
3	NAP	A	1258	-	42,52,52	1.44	2 (4%)	54,80,80	2.25	9 (16%)
2	5PP	B	1257	-	20,20,20	1.16	1 (5%)	25,25,25	1.01	1 (4%)
3	NAP	B	1258	-	42,52,52	1.59	4 (9%)	54,80,80	2.01	10 (18%)
4	GLU	B	1259	-	3,9,9	0.34	0	2,11,11	0.22	0
2	5PP	C	1257	-	20,20,20	1.09	1 (5%)	25,25,25	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAP	C	1258	-	42,52,52	1.47	3 (7%)	54,80,80	2.31	11 (20%)
4	GLU	C	1259	-	3,9,9	0.32	0	2,11,11	0.17	0
2	5PP	D	1257	-	20,20,20	1.12	1 (5%)	25,25,25	0.90	0
3	NAP	D	1258	-	42,52,52	1.49	3 (7%)	54,80,80	2.10	8 (14%)
2	5PP	E	1257	-	20,20,20	1.09	1 (5%)	25,25,25	1.03	1 (4%)
3	NAP	E	1258	-	42,52,52	1.47	3 (7%)	54,80,80	2.45	7 (12%)
4	GLU	E	1259	-	3,9,9	0.23	0	2,11,11	0.47	0
2	5PP	F	1257	-	20,20,20	1.26	1 (5%)	25,25,25	0.76	1 (4%)
3	NAP	F	1258	-	42,52,52	1.42	3 (7%)	54,80,80	2.37	7 (12%)
4	GLU	F	1259	-	3,9,9	0.32	0	2,11,11	0.09	0
2	5PP	G	1257	-	20,20,20	1.09	1 (5%)	25,25,25	1.03	1 (4%)
3	NAP	G	1258	-	42,52,52	1.47	4 (9%)	54,80,80	2.25	8 (14%)
4	GLU	G	1259	-	3,9,9	0.18	0	2,11,11	0.55	0
2	5PP	H	1257	-	20,20,20	1.18	1 (5%)	25,25,25	0.91	1 (4%)
3	NAP	H	1258	-	42,52,52	1.50	3 (7%)	54,80,80	2.70	10 (18%)

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	5PP	A	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	A	1258	-	-	0/27/67/67	0/5/5/5
2	5PP	B	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	B	1258	-	-	0/27/67/67	0/5/5/5
4	GLU	B	1259	-	-	0/3/9/9	0/0/0/0
2	5PP	C	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	C	1258	-	-	0/27/67/67	0/5/5/5
4	GLU	C	1259	-	-	0/3/9/9	0/0/0/0
2	5PP	D	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	D	1258	-	-	0/27/67/67	0/5/5/5
2	5PP	E	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	E	1258	-	-	0/27/67/67	0/5/5/5
4	GLU	E	1259	-	-	0/3/9/9	0/0/0/0
2	5PP	F	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	F	1258	-	-	0/27/67/67	0/5/5/5
4	GLU	F	1259	-	-	0/3/9/9	0/0/0/0
2	5PP	G	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	G	1258	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLU	G	1259	-	-	0/3/9/9	0/0/0/0
2	5PP	H	1257	-	-	0/9/9/9	0/2/2/2
3	NAP	H	1258	-	-	0/27/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1257	5PP	C14-C2	-4.54	1.38	1.51
2	H	1257	5PP	C14-C2	-4.34	1.39	1.51
2	F	1257	5PP	C14-C2	-4.23	1.39	1.51
2	B	1257	5PP	C14-C2	-4.12	1.39	1.51
2	D	1257	5PP	C14-C2	-3.90	1.40	1.51
2	G	1257	5PP	C14-C2	-3.89	1.40	1.51
2	C	1257	5PP	C14-C2	-3.68	1.41	1.51
2	E	1257	5PP	C14-C2	-3.58	1.41	1.51
3	G	1258	NAP	PA-O2A	-2.25	1.45	1.54
3	B	1258	NAP	PA-O2A	-2.00	1.46	1.54
3	F	1258	NAP	C2A-N1A	2.04	1.37	1.33
2	A	1257	5PP	C1-C6	2.23	1.42	1.38
3	C	1258	NAP	C2A-N1A	2.38	1.38	1.33
3	G	1258	NAP	C2A-N1A	2.45	1.38	1.33
3	D	1258	NAP	C2A-N1A	2.54	1.38	1.33
3	E	1258	NAP	C2A-N1A	2.55	1.38	1.33
3	B	1258	NAP	C2A-N1A	2.81	1.39	1.33
3	H	1258	NAP	C2A-N1A	2.88	1.39	1.33
3	D	1258	NAP	C2A-N3A	3.01	1.37	1.32
3	C	1258	NAP	C2A-N3A	3.05	1.37	1.32
3	G	1258	NAP	C2A-N3A	3.10	1.37	1.32
3	F	1258	NAP	C2A-N3A	3.34	1.38	1.32
3	A	1258	NAP	C2A-N3A	3.35	1.38	1.32
3	E	1258	NAP	C2A-N3A	3.58	1.38	1.32
3	H	1258	NAP	C2A-N3A	3.62	1.38	1.32
3	B	1258	NAP	C2A-N3A	3.70	1.38	1.32
3	F	1258	NAP	O7N-C7N	6.94	1.39	1.24
3	H	1258	NAP	O7N-C7N	7.03	1.39	1.24
3	A	1258	NAP	O7N-C7N	7.07	1.39	1.24
3	E	1258	NAP	O7N-C7N	7.09	1.39	1.24
3	G	1258	NAP	O7N-C7N	7.29	1.39	1.24
3	C	1258	NAP	O7N-C7N	7.40	1.40	1.24
3	D	1258	NAP	O7N-C7N	7.43	1.40	1.24
3	B	1258	NAP	O7N-C7N	7.58	1.40	1.24

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1258	NAP	N3A-C2A-N1A	-13.67	118.43	128.89
3	E	1258	NAP	N3A-C2A-N1A	-13.40	118.64	128.89
3	F	1258	NAP	N3A-C2A-N1A	-12.50	119.32	128.89
3	D	1258	NAP	N3A-C2A-N1A	-12.30	119.48	128.89
3	G	1258	NAP	N3A-C2A-N1A	-12.13	119.61	128.89
3	H	1258	NAP	N3A-C2A-N1A	-12.09	119.64	128.89
3	A	1258	NAP	N3A-C2A-N1A	-11.66	119.97	128.89
3	B	1258	NAP	N3A-C2A-N1A	-10.79	120.63	128.89
3	H	1258	NAP	O7N-C7N-C3N	-8.49	110.32	119.59
3	E	1258	NAP	C4B-O4B-C1B	-7.18	101.83	109.72
3	F	1258	NAP	O7N-C7N-C3N	-6.22	112.80	119.59
3	A	1258	NAP	O7N-C7N-C3N	-5.20	113.91	119.59
3	B	1258	NAP	C4B-O4B-C1B	-4.45	104.83	109.72
3	F	1258	NAP	C4B-O4B-C1B	-4.41	104.87	109.72
3	H	1258	NAP	C4B-O4B-C1B	-4.32	104.97	109.72
3	H	1258	NAP	C1B-N9A-C4A	-3.67	121.41	126.94
3	A	1258	NAP	C4B-O4B-C1B	-3.60	105.76	109.72
3	B	1258	NAP	C1B-N9A-C4A	-3.38	121.84	126.94
3	D	1258	NAP	O4B-C1B-C2B	-3.24	100.74	106.60
3	A	1258	NAP	C1B-N9A-C4A	-3.21	122.10	126.94
3	E	1258	NAP	C1B-N9A-C4A	-3.16	122.18	126.94
3	C	1258	NAP	C1B-N9A-C4A	-3.04	122.36	126.94
3	C	1258	NAP	C4B-O4B-C1B	-2.86	106.58	109.72
3	C	1258	NAP	O7N-C7N-C3N	-2.74	116.60	119.59
3	H	1258	NAP	C4D-O4D-C1D	-2.71	106.74	109.72
3	G	1258	NAP	C1B-N9A-C4A	-2.63	122.97	126.94
3	D	1258	NAP	C4B-O4B-C1B	-2.54	106.93	109.72
3	B	1258	NAP	O7N-C7N-C3N	-2.51	116.84	119.59
3	E	1258	NAP	O4B-C1B-C2B	-2.48	102.11	106.60
3	A	1258	NAP	C4A-C5A-N7A	-2.44	107.23	109.48
3	H	1258	NAP	O3X-P2B-O1X	-2.42	102.79	110.58
3	G	1258	NAP	O7N-C7N-C3N	-2.40	116.97	119.59
3	C	1258	NAP	O4B-C1B-C2B	-2.34	102.38	106.60
3	H	1258	NAP	C4A-C5A-N7A	-2.31	107.35	109.48
3	D	1258	NAP	O3D-C3D-C2D	-2.31	104.32	111.83
3	G	1258	NAP	O4B-C1B-C2B	-2.26	102.51	106.60
3	A	1258	NAP	O4B-C1B-C2B	-2.18	102.66	106.60
2	A	1257	5PP	O17-C6-C5	-2.15	115.16	120.10
3	D	1258	NAP	O7N-C7N-N7N	-2.14	119.58	122.59
2	B	1257	5PP	O17-C6-C5	-2.07	115.33	120.10
2	A	1257	5PP	C11-C12-C13	-2.04	117.20	120.19
3	C	1258	NAP	C4A-C5A-N7A	-2.01	107.63	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1258	NAP	O4B-C1B-N9A	2.03	112.35	108.10
3	B	1258	NAP	O2N-PN-O1N	2.05	123.61	112.53
3	H	1258	NAP	O3X-P2B-O2X	2.06	115.21	107.38
3	A	1258	NAP	C2N-C3N-C4N	2.08	120.61	118.29
2	F	1257	5PP	O7-C5-C6	2.12	120.28	116.12
2	G	1257	5PP	C1-C6-C5	2.15	122.16	119.79
3	E	1258	NAP	C2A-N1A-C6A	2.23	122.75	118.77
3	B	1258	NAP	O2B-C2B-C1B	2.24	118.74	110.02
2	H	1257	5PP	C10-C9-C8	2.24	122.79	118.92
3	A	1258	NAP	O4B-C1B-N9A	2.28	112.86	108.10
3	F	1258	NAP	C2N-C3N-C4N	2.33	120.89	118.29
2	E	1257	5PP	C12-C13-C8	2.42	123.09	118.92
3	D	1258	NAP	C2A-N1A-C6A	2.43	123.10	118.77
3	B	1258	NAP	C2N-C3N-C4N	2.44	121.01	118.29
3	B	1258	NAP	C3N-C7N-N7N	2.46	120.51	117.82
3	C	1258	NAP	O4B-C1B-N9A	2.52	113.38	108.10
3	E	1258	NAP	C2N-C3N-C4N	2.57	121.16	118.29
3	C	1258	NAP	O4D-C1D-N1N	2.65	111.04	108.13
3	B	1258	NAP	O4D-C1D-N1N	2.66	111.05	108.13
3	H	1258	NAP	O4B-C1B-N9A	2.71	113.76	108.10
3	C	1258	NAP	C2N-C3N-C4N	2.79	121.39	118.29
3	G	1258	NAP	C2N-C3N-C4N	2.86	121.47	118.29
3	C	1258	NAP	C2A-N1A-C6A	2.89	123.93	118.77
3	D	1258	NAP	O4B-C1B-N9A	2.93	114.24	108.10
3	G	1258	NAP	O4B-C1B-N9A	3.03	114.44	108.10
3	D	1258	NAP	C3N-C7N-N7N	3.27	121.40	117.82
3	F	1258	NAP	O4B-C1B-N9A	3.31	115.02	108.10
3	F	1258	NAP	O4D-C1D-N1N	3.34	111.81	108.13
3	G	1258	NAP	C3N-C7N-N7N	3.98	122.17	117.82
3	C	1258	NAP	C3N-C7N-N7N	4.06	122.26	117.82
3	E	1258	NAP	C3N-C7N-N7N	4.38	122.61	117.82
3	F	1258	NAP	C3N-C7N-N7N	5.76	124.12	117.82
3	A	1258	NAP	C3N-C7N-N7N	6.04	124.43	117.82
3	G	1258	NAP	O4D-C1D-N1N	6.28	115.03	108.13
3	H	1258	NAP	C3N-C7N-N7N	8.62	127.25	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1258	NAP	1	0
4	B	1259	GLU	1	0
3	C	1258	NAP	1	0
4	C	1259	GLU	1	0
2	D	1257	5PP	1	0
3	D	1258	NAP	4	0
2	E	1257	5PP	1	0
3	E	1258	NAP	1	0
3	F	1258	NAP	1	0
4	F	1259	GLU	1	0
2	G	1257	5PP	1	0
3	G	1258	NAP	2	0
4	G	1259	GLU	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/282 (90%)	-0.18	0 <b>100</b> <b>100</b>	24, 33, 54, 67	0
1	B	255/282 (90%)	-0.20	2 (0%) <b>87</b> <b>87</b>	24, 34, 57, 71	0
1	C	254/282 (90%)	-0.32	2 (0%) <b>87</b> <b>87</b>	25, 35, 55, 70	0
1	D	254/282 (90%)	-0.12	3 (1%) <b>81</b> <b>80</b>	26, 38, 65, 96	0
1	E	254/282 (90%)	-0.31	4 (1%) <b>74</b> <b>73</b>	24, 32, 52, 68	0
1	F	255/282 (90%)	-0.39	2 (0%) <b>87</b> <b>87</b>	23, 32, 52, 69	0
1	G	254/282 (90%)	-0.23	2 (0%) <b>87</b> <b>87</b>	23, 33, 56, 68	0
1	H	254/282 (90%)	-0.32	1 (0%) <b>93</b> <b>93</b>	23, 33, 57, 73	0
All	All	2034/2256 (90%)	-0.26	16 (0%) <b>87</b> <b>87</b>	23, 34, 57, 96	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	43	ARG	4.0
1	D	58	PRO	3.5
1	F	209	LYS	2.6
1	E	60	ALA	2.6
1	C	6	ASN	2.5
1	E	58	PRO	2.4
1	B	59	GLU	2.4
1	B	2	VAL	2.2
1	E	56	ASN	2.2
1	D	50	LYS	2.2
1	E	6	ASN	2.2
1	G	58	PRO	2.2
1	H	150	GLY	2.2
1	F	187	ALA	2.0
1	G	60	ALA	2.0
1	C	58	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLU	E	1259	10/10	0.50	0.33	10.68	106,107,110,112	0
4	GLU	G	1259	10/10	0.82	0.21	4.62	94,96,97,99	0
4	GLU	C	1259	10/10	0.46	0.26	4.46	94,100,100,100	0
4	GLU	B	1259	10/10	0.64	0.18	4.17	87,88,92,93	0
4	GLU	F	1259	10/10	0.64	0.21	2.73	80,81,83,85	0
2	5PP	D	1257	19/19	0.96	0.13	0.83	31,34,39,40	0
2	5PP	E	1257	19/19	0.96	0.11	0.33	24,27,33,33	0
2	5PP	A	1257	19/19	0.96	0.13	0.27	29,31,36,36	0
2	5PP	G	1257	19/19	0.97	0.12	0.19	29,35,39,40	0
3	NAP	E	1258	48/48	0.98	0.10	0.02	24,32,38,41	0
2	5PP	H	1257	19/19	0.96	0.11	-0.01	32,35,39,42	0
2	5PP	B	1257	19/19	0.97	0.12	-0.05	29,33,37,37	0
3	NAP	A	1258	48/48	0.98	0.11	-0.25	24,32,38,42	0
3	NAP	H	1258	48/48	0.97	0.10	-0.39	28,36,49,57	0
3	NAP	F	1258	48/48	0.98	0.10	-0.40	28,33,37,39	0
2	5PP	C	1257	19/19	0.96	0.10	-0.42	28,34,41,43	0
3	NAP	B	1258	48/48	0.98	0.10	-0.54	26,34,38,40	0
3	NAP	G	1258	48/48	0.98	0.09	-0.56	23,33,38,42	0
3	NAP	D	1258	48/48	0.97	0.10	-0.60	29,36,55,65	0
2	5PP	F	1257	19/19	0.97	0.10	-0.76	27,32,35,36	0
3	NAP	C	1258	48/48	0.98	0.09	-0.84	29,35,40,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.