



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:09 PM GMT

PDB ID : 4BNF
Title : Crystal structure of *S. aureus* FabI in complex with NADP and 2- phenoxy-5
-propylphenol
Authors : Schiebel, J.; Chang, A.; Bommineni, G.R.; Tonge, P.J.; Kisker, C.
Deposited on : 2013-05-15
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

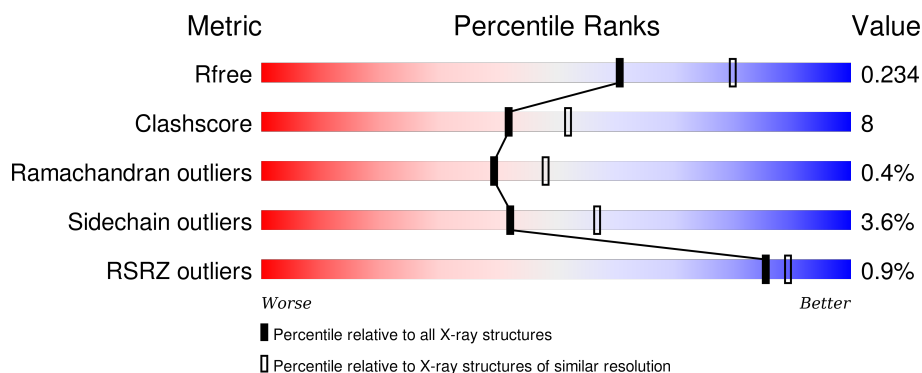
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>71%</div> <div>18%</div> <div>10%</div> </div>
1	B	282	<div> <div>77%</div> <div>12%</div> <div>10%</div> </div>
1	C	282	<div> <div>75%</div> <div>15%</div> <div>10%</div> </div>
1	D	282	<div> <div>76%</div> <div>13%</div> <div>10%</div> </div>
1	E	282	<div> <div>78%</div> <div>12%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	1259	-	-	X	X
2	GLU	B	1000	-	-	X	-
2	GLU	C	1000	-	-	X	-
2	GLU	E	1000	-	-	X	X
2	GLU	F	1000	-	-	X	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17895 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	12	0
			2044	1284	356	399	5			
1	B	255	Total	C	N	O	S	0	11	0
			2043	1284	354	400	5			
1	C	255	Total	C	N	O	S	0	5	0
			1994	1256	347	387	4			
1	D	254	Total	C	N	O	S	0	2	0
			1965	1237	340	384	4			
1	E	254	Total	C	N	O	S	0	11	0
			2036	1279	353	399	5			
1	F	255	Total	C	N	O	S	0	10	0
			2039	1281	357	396	5			
1	G	255	Total	C	N	O	S	0	3	0
			1980	1247	344	385	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

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...

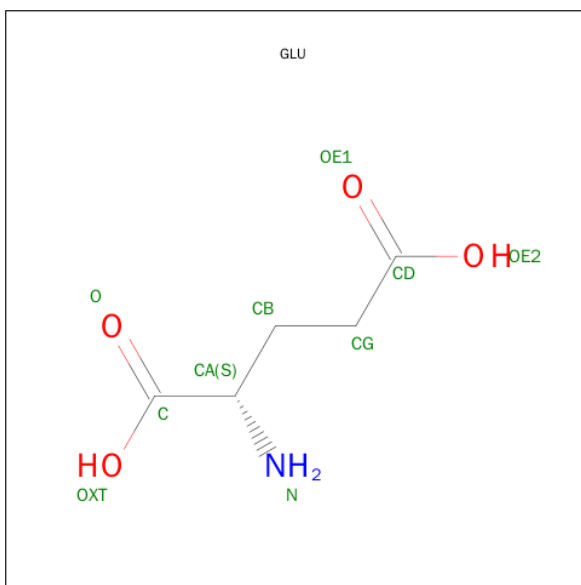
Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
F	-16	MET	-	EXPRESSION TAG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

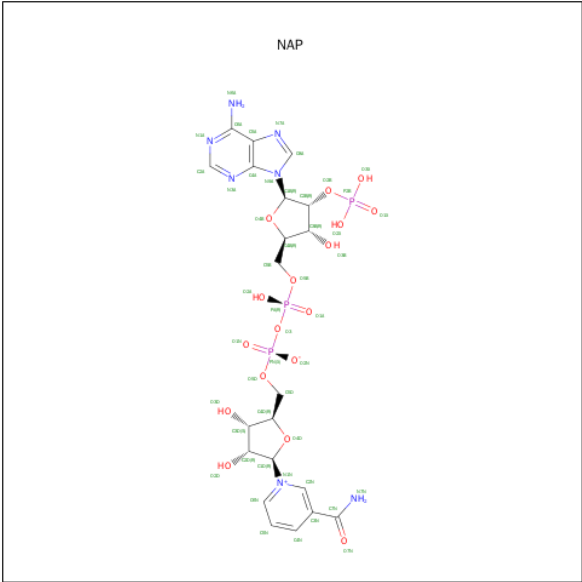
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
G	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
G	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
G	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
G	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
G	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
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 GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



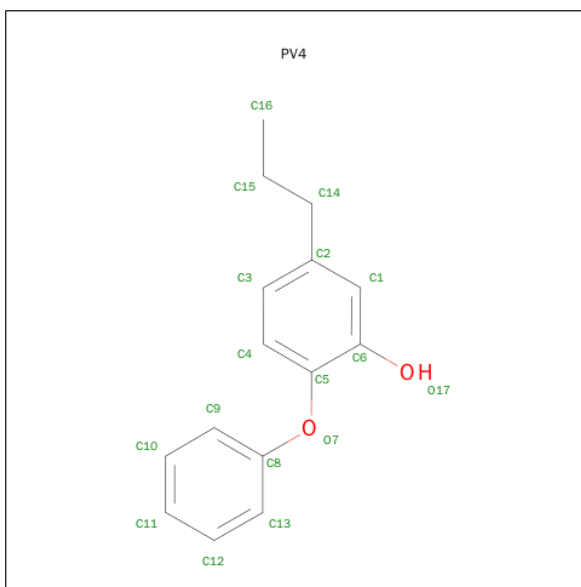
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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 2-PHENOXY-5-PROPYL-PHENOL (three-letter code: PV4) (formula: C₁₅H₁₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 15 2	0	0
4	B	1	Total C O 17 15 2	0	0
4	C	1	Total C O 17 15 2	0	0
4	D	1	Total C O 17 15 2	0	0
4	E	1	Total C O 17 15 2	0	0
4	F	1	Total C O 17 15 2	0	0
4	G	1	Total C O 17 15 2	0	0
4	H	1	Total C O 17 15 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	193	Total O 193 193	0	0
5	B	176	Total O 176 176	0	0
5	C	161	Total O 161 161	0	0
5	D	104	Total O 104 104	0	0

Continued on next page...

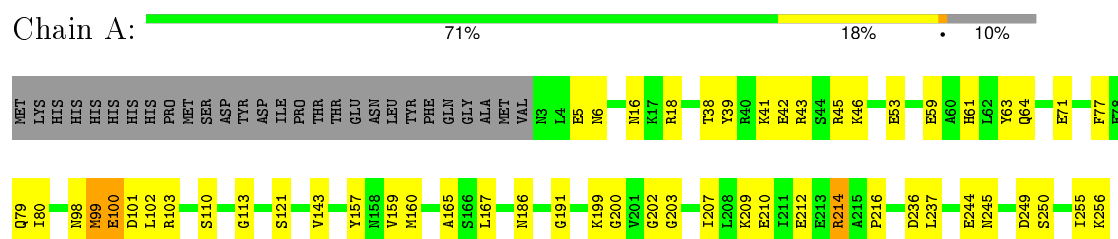
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	171	Total 171	O 171	0	0
5	F	166	Total 166	O 166	0	0
5	G	149	Total 149	O 149	0	0
5	H	129	Total 129	O 129	0	0

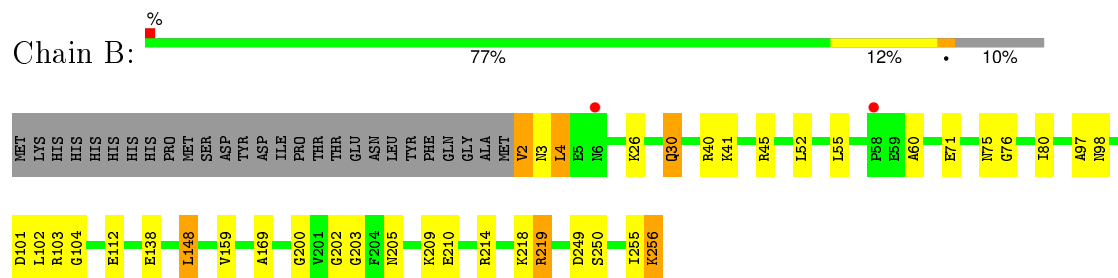
3 Residue-property plots

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.

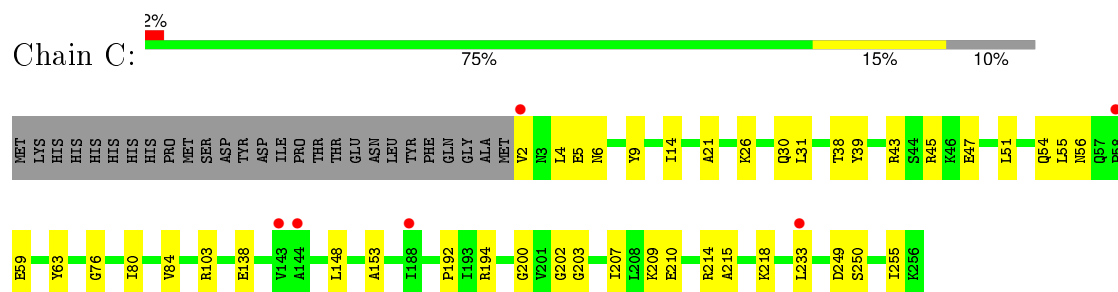
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



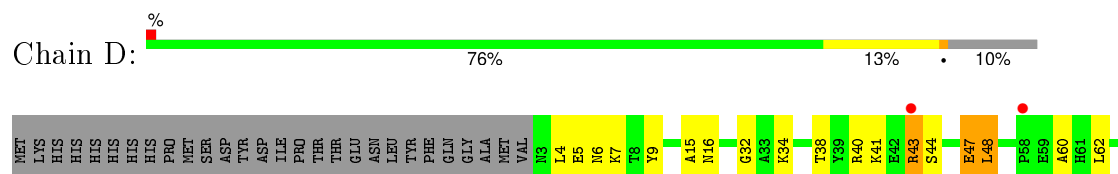
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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



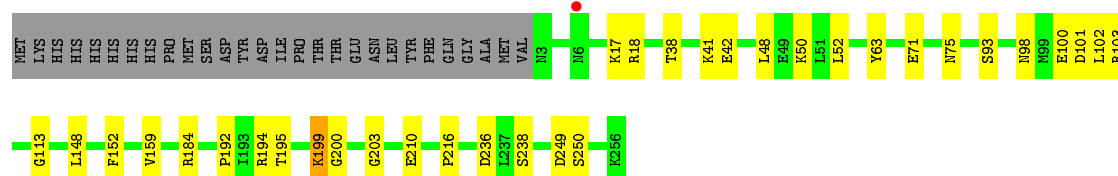
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





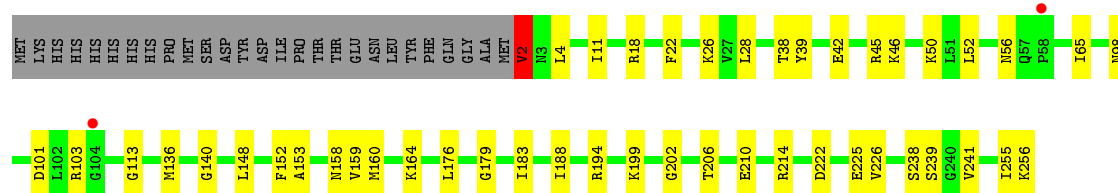
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain E: 78% 12% 10%



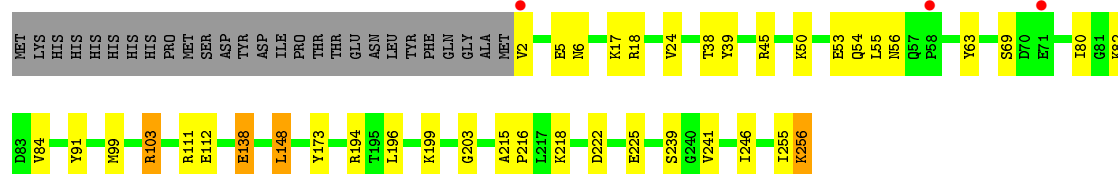
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F: 74% 16% 10%



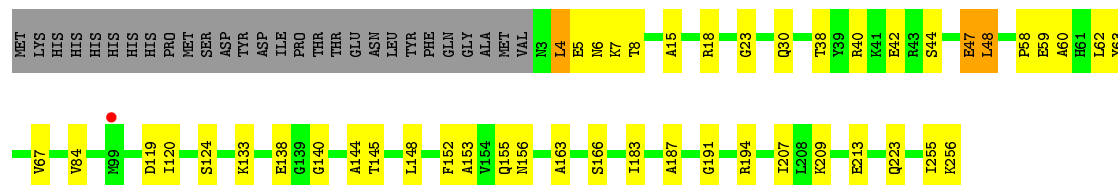
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G: 76% 13% 10%



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

Chain H: 73% 16% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.05Å 94.89Å 94.83Å 98.08° 97.29° 112.29°	Depositor
Resolution (Å)	37.10 – 2.30 37.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.10-2.30) 90.8 (37.10-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.158 , 0.219 0.177 , 0.234	Depositor DCC
R_{free} test set	6180 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 122747 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17895	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, PV4

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	0.52	0/2080	0.80	0/2799
1	B	0.56	0/2076	0.80	0/2795
1	C	0.51	0/2030	0.80	0/2734
1	D	0.47	0/1992	0.76	0/2684
1	E	0.53	0/2069	0.80	0/2785
1	F	0.56	0/2069	0.80	0/2785
1	G	0.53	0/2010	0.79	0/2708
1	H	0.47	0/1992	0.73	0/2684
All	All	0.52	0/16318	0.79	0/21974

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	2	VAL	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	2044	0	2058	58	0
1	B	2043	0	2054	44	0
1	C	1994	0	2016	36	0
1	D	1965	0	1975	23	0
1	E	2036	0	2045	36	0
1	F	2039	0	2055	46	0
1	G	1980	0	1997	33	0
1	H	1965	0	1975	29	0
2	A	10	0	5	5	0
2	B	10	0	5	9	0
2	C	10	0	5	8	0
2	E	10	0	5	4	0
2	F	10	0	5	9	0
2	G	10	0	5	3	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
3	E	48	0	25	1	0
3	F	48	0	25	0	0
3	G	48	0	25	0	0
3	H	48	0	25	2	0
4	A	17	0	15	1	0
4	B	17	0	16	0	0
4	C	17	0	15	0	0
4	D	17	0	15	0	0
4	E	17	0	15	0	0
4	F	17	0	16	0	0
4	G	17	0	15	0	0
4	H	17	0	16	0	0
5	A	193	0	0	9	0
5	B	176	0	0	8	0
5	C	161	0	0	1	0
5	D	104	0	0	2	0
5	E	171	0	0	2	0
5	F	166	0	0	7	0
5	G	149	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	129	0	0	5	0
All	All	17895	0	16528	278	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 (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH1	1.83	1.11
1:B:2:VAL:CG2	1:B:3:ASN:H	1.65	1.10
1:B:103[B]:ARG:NH2	1:B:200:GLY:O	1.88	1.05
1:A:103[B]:ARG:NH1	2:A:1259:GLU:OE1	1.91	1.04
1:B:2:VAL:HG22	1:B:3:ASN:H	1.21	1.02
1:A:100[B]:GLU:HG3	1:E:41:LYS:HZ3	1.23	1.02
1:C:210:GLU:HG3	1:C:214[B]:ARG:HD2	1.44	0.99
1:F:206:THR:HG23	5:F:2127:HOH:O	1.65	0.96
1:H:42:GLU:HB2	5:H:2026:HOH:O	1.70	0.90
1:A:103[A]:ARG:NH1	2:A:1259:GLU:OE1	2.05	0.90
1:C:103:ARG:HH12	2:C:1000:GLU:CG	1.87	0.88
1:B:2:VAL:HG22	1:B:3:ASN:N	1.89	0.87
1:C:103:ARG:HH12	2:C:1000:GLU:HG3	1.40	0.86
1:G:203:GLY:H	2:G:1000:GLU:HA	1.40	0.86
1:F:101[B]:ASP:HB3	1:F:159:VAL:CG1	2.06	0.85
1:B:2:VAL:CG2	1:B:3:ASN:N	2.36	0.85
1:F:101[B]:ASP:HB3	1:F:159:VAL:HG11	1.57	0.83
2:E:1000:GLU:N	2:E:1000:GLU:CD	2.33	0.82
2:A:1259:GLU:O	5:A:2152:HOH:O	1.97	0.81
1:F:101[A]:ASP:OD2	1:F:113:GLY:HA3	1.81	0.80
1:F:103[B]:ARG:NH1	2:F:1000:GLU:OE2	2.14	0.80
1:D:5:GLU:O	1:D:6:ASN:HB2	1.82	0.78
1:E:103[B]:ARG:NH1	2:E:1000:GLU:OE1	2.16	0.76
1:G:18[A]:ARG:NH2	1:G:194:ARG:HD2	2.01	0.74
1:B:104[B]:GLY:O	5:B:2096:HOH:O	2.04	0.74
1:B:2:VAL:HG23	1:B:3:ASN:H	1.53	0.73
1:B:205:ASN:ND2	5:B:2142:HOH:O	2.20	0.73
1:A:100[B]:GLU:HG3	1:E:41:LYS:NZ	2.01	0.73
1:A:101[B]:ASP:OD2	5:A:2094:HOH:O	2.08	0.72
1:G:54:GLN:HG3	5:G:2047:HOH:O	1.90	0.71
1:D:224:VAL:HG23	5:D:2094:HOH:O	1.91	0.71
1:E:148:LEU:HD21	1:G:256:LYS:HD3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101[A]:ASP:HB3	1:E:159:VAL:CG1	2.21	0.71
2:E:1000:GLU:N	2:E:1000:GLU:OE2	2.24	0.71
1:D:222:ASP:OD1	1:D:225:GLU:HG3	1.91	0.70
1:E:102[A]:LEU:HB2	1:E:200:GLY:O	1.90	0.69
1:C:103:ARG:NH1	2:C:1000:GLU:CG	2.56	0.68
1:A:212:GLU:OE2	5:A:2160:HOH:O	2.10	0.68
1:A:101[B]:ASP:OD2	1:A:113:GLY:HA3	1.93	0.68
5:F:2139:HOH:O	1:G:239[B]:SER:O	2.11	0.68
1:F:256:LYS:HE3	1:H:148:LEU:HD21	1.75	0.68
1:C:5:GLU:O	1:C:6:ASN:HB2	1.93	0.67
1:E:148:LEU:HD21	1:G:256:LYS:CD	2.25	0.66
1:B:101[B]:ASP:HB3	1:B:159:VAL:HG11	1.75	0.66
1:A:255:ILE:HG22	1:C:153:ALA:HB3	1.76	0.66
1:H:18:ARG:NH2	5:H:2017:HOH:O	2.27	0.66
1:E:48:LEU:O	1:E:52:LEU:HD23	1.95	0.66
1:A:18[A]:ARG:NH2	1:A:199:LYS:NZ	2.44	0.66
1:H:40:ARG:HD3	3:H:1257:NAP:C6A	2.27	0.65
1:A:100[B]:GLU:CG	1:E:41:LYS:HZ3	2.03	0.65
1:C:103:ARG:NH1	2:C:1000:GLU:HG3	2.10	0.65
1:E:101[A]:ASP:HB3	1:E:159:VAL:HG11	1.80	0.64
1:H:60:ALA:HB1	1:H:62:LEU:HD11	1.79	0.64
1:G:50:LYS:O	1:G:53:GLU:HG2	1.98	0.64
1:F:103[A]:ARG:HH12	2:F:1000:GLU:CD	2.00	0.64
1:A:214:ARG:HD3	5:A:2155:HOH:O	1.98	0.64
1:B:103[A]:ARG:HH12	2:B:1000:GLU:HA	1.63	0.63
1:A:99[B]:MET:HE3	1:A:103[B]:ARG:CG	2.29	0.63
1:B:101[B]:ASP:HB3	1:B:159:VAL:CG1	2.28	0.63
1:B:103[B]:ARG:CZ	1:B:103[B]:ARG:HB3	2.30	0.62
1:A:100[B]:GLU:CG	1:E:41:LYS:NZ	2.62	0.61
1:H:44:SER:O	1:H:48:LEU:HB2	1.99	0.61
1:E:101[B]:ASP:OD2	1:E:113:GLY:HA3	2.00	0.61
1:B:71[B]:GLU:HG2	1:B:75:ASN:HD21	1.67	0.60
1:A:207:ILE:HD12	4:A:1258:PV4:H161	1.83	0.60
1:E:71[B]:GLU:HG3	1:E:75:ASN:ND2	2.16	0.59
1:C:2:VAL:HG13	1:C:2:VAL:O	2.03	0.59
1:B:103[A]:ARG:HH22	2:B:1000:GLU:HA	1.67	0.59
1:A:249:ASP:O	1:A:250:SER:HB2	2.03	0.59
1:A:101[A]:ASP:HB3	1:A:159:VAL:CG1	2.33	0.59
1:B:97:ALA:HB3	1:B:102[A]:LEU:HD11	1.84	0.59
1:B:45:ARG:HD3	5:B:2043:HOH:O	2.03	0.58
1:B:103[A]:ARG:HH12	2:B:1000:GLU:CD	2.06	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102[A]:LEU:CB	1:E:200:GLY:O	2.51	0.58
1:H:15:ALA:O	1:H:47:GLU:HG2	2.03	0.58
1:C:4:LEU:HD13	1:C:9:TYR:HE2	1.68	0.58
1:B:256:LYS:HE3	1:D:148:LEU:HD21	1.85	0.58
1:A:99[B]:MET:HE3	1:A:103[B]:ARG:HG2	1.85	0.57
1:B:26:LYS:O	1:B:30:GLN:HB3	2.04	0.57
1:F:101[B]:ASP:HB3	1:F:159:VAL:HG12	1.85	0.57
1:E:101[A]:ASP:HB3	1:E:159:VAL:HG12	1.87	0.57
1:G:215:ALA:O	1:G:218:LYS:HD3	2.04	0.57
1:C:194:ARG:HG2	1:C:194:ARG:HH11	1.69	0.57
1:E:50:LYS:HG3	5:E:2035:HOH:O	2.05	0.57
1:C:210:GLU:CG	1:C:214[B]:ARG:HD2	2.28	0.56
1:E:194:ARG:HG2	1:E:194:ARG:NH1	2.20	0.56
1:F:103[B]:ARG:CZ	1:F:103[B]:ARG:HB3	2.30	0.56
1:F:202:GLY:HA2	2:F:1000:GLU:HA	1.88	0.56
1:A:98:ASN:O	1:A:101[A]:ASP:HB2	2.05	0.56
1:C:249:ASP:O	1:C:250:SER:HB2	2.04	0.56
1:F:98:ASN:O	1:F:101[B]:ASP:HB2	2.06	0.56
1:E:194:ARG:HH11	1:E:194:ARG:HG2	1.71	0.55
1:A:102[A]:LEU:HB2	1:A:200:GLY:O	2.06	0.55
1:C:5:GLU:O	1:C:6:ASN:CB	2.55	0.55
1:D:15:ALA:O	1:D:47:GLU:HG2	2.08	0.55
1:F:22:PHE:CE2	1:F:26:LYS:HE2	2.42	0.55
1:E:18:ARG:NH2	1:E:199:LYS:HE3	2.22	0.55
1:D:44:SER:O	1:D:48:LEU:HB2	2.07	0.54
1:H:67:VAL:HB	1:H:124:SER:HB2	1.90	0.54
1:H:60:ALA:HB1	1:H:62:LEU:CD1	2.37	0.54
1:F:103[A]:ARG:HH12	2:F:1000:GLU:CG	2.20	0.54
1:G:222:ASP:OD1	1:G:225:GLU:HG3	2.08	0.53
1:B:101[B]:ASP:O	1:B:159:VAL:HG12	2.09	0.53
1:D:120:ILE:HD13	3:D:1257:NAP:H61A	1.74	0.53
1:B:71[B]:GLU:HG2	1:B:75:ASN:ND2	2.25	0.52
1:A:256:LYS:HE2	1:C:255:ILE:O	2.09	0.52
1:F:103[A]:ARG:NH1	2:F:1000:GLU:CD	2.62	0.52
1:E:98:ASN:O	1:E:101[A]:ASP:HB2	2.10	0.52
1:A:99[A]:MET:C	1:A:101[A]:ASP:H	2.13	0.52
1:D:5:GLU:HA	1:D:32:GLY:O	2.09	0.52
1:A:18[A]:ARG:HD3	5:A:2015:HOH:O	2.10	0.52
1:B:2:VAL:N	1:C:2:VAL:N	2.57	0.52
1:C:2:VAL:O	1:C:31:LEU:HD22	2.09	0.51
1:C:80:ILE:O	1:C:84:VAL:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HE3	1:E:103[A]:ARG:NH1	2.24	0.51
1:H:133:LYS:HD3	5:H:2059:HOH:O	2.10	0.51
1:A:101[A]:ASP:HB3	1:A:159:VAL:HG12	1.92	0.51
1:F:153:ALA:HB3	1:H:255:ILE:HG22	1.93	0.51
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.46	0.51
1:B:255:ILE:O	1:D:256:LYS:HE2	2.10	0.51
1:F:45:ARG:HD3	5:F:2050:HOH:O	2.11	0.51
1:A:18[A]:ARG:NH2	1:A:199:LYS:HZ1	2.08	0.51
1:C:14:ILE:HG12	1:C:21:ALA:HB3	1.93	0.51
1:A:18[A]:ARG:HH21	1:A:199:LYS:HZ3	1.58	0.50
1:C:26:LYS:O	1:C:30:GLN:HB3	2.12	0.50
1:A:77:PHE:HA	1:A:80:ILE:HD12	1.93	0.50
1:H:8:THR:HG21	1:H:84:VAL:HG11	1.93	0.50
1:F:18[A]:ARG:NH2	1:F:194:ARG:HD2	2.26	0.50
1:H:209:LYS:O	1:H:213:GLU:HG3	2.10	0.50
1:A:41:LYS:HE2	1:E:100[B]:GLU:OE1	2.12	0.50
1:F:22:PHE:CD2	1:F:26:LYS:HE2	2.47	0.49
1:F:18[B]:ARG:NH2	1:F:199:LYS:NZ	2.60	0.49
1:F:179:GLY:HA3	1:G:216:PRO:O	2.12	0.49
1:C:103:ARG:NH1	2:C:1000:GLU:OE2	2.45	0.49
1:F:239[B]:SER:O	5:F:2152:HOH:O	2.19	0.49
1:E:17:LYS:NZ	5:E:2015:HOH:O	2.38	0.49
1:G:38:THR:HA	1:G:63:TYR:O	2.12	0.49
1:A:216:PRO:O	1:D:179:GLY:HA3	2.13	0.49
1:A:5:GLU:O	1:A:6:ASN:HB2	2.12	0.48
1:C:194:ARG:CG	1:C:194:ARG:HH11	2.26	0.48
1:H:4:LEU:O	1:H:7:LYS:HB2	2.14	0.48
1:F:152:PHE:HE1	5:H:2099:HOH:O	1.96	0.48
1:C:4:LEU:HD13	1:C:9:TYR:CE2	2.49	0.48
1:F:158:ASN:HB3	5:F:2088:HOH:O	2.12	0.48
1:F:222:ASP:OD1	1:F:225:GLU:HG3	2.14	0.48
1:A:43:ARG:HG2	1:E:100[A]:GLU:HG3	1.95	0.48
1:B:40:ARG:HD3	3:B:1257:NAP:C6A	2.44	0.48
1:B:103[A]:ARG:NH1	2:B:1000:GLU:HA	2.29	0.48
1:G:111:ARG:NH1	1:H:119:ASP:OD1	2.42	0.47
1:G:18[A]:ARG:HH12	1:G:199:LYS:NZ	2.12	0.47
1:A:45:ARG:NH2	1:A:46:LYS:HE2	2.29	0.47
1:H:5:GLU:O	1:H:6:ASN:HB2	2.15	0.47
1:A:39:TYR:CZ	1:A:64:GLN:HB2	2.50	0.47
1:A:101[A]:ASP:HB3	1:A:159:VAL:HG11	1.97	0.47
1:E:203:GLY:H	2:E:1000:GLU:N	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ARG:NH1	1:E:238:SER:OG	2.45	0.47
1:H:144:ALA:O	1:H:187:ALA:HA	2.15	0.47
1:F:256:LYS:HG2	1:H:152:PHE:CG	2.50	0.46
2:B:1000:GLU:N	5:B:2175:HOH:O	2.48	0.46
1:B:30:GLN:HE21	1:B:30:GLN:HB2	1.44	0.46
1:G:5:GLU:O	1:G:6:ASN:CB	2.63	0.46
1:A:209:LYS:HE2	1:A:209:LYS:HB3	1.67	0.46
1:A:18[A]:ARG:NH2	1:A:199:LYS:HZ3	2.11	0.46
1:E:192:PRO:HA	3:E:1257:NAP:O7N	2.15	0.46
1:F:160:MET:O	1:F:164:LYS:HG2	2.16	0.46
1:G:5:GLU:O	1:G:6:ASN:HB2	2.15	0.46
1:G:24:VAL:HG21	1:G:91:TYR:CE2	2.51	0.46
1:C:103:ARG:NH1	2:C:1000:GLU:CD	2.69	0.46
1:D:60:ALA:HB1	1:D:62:LEU:CD1	2.45	0.46
1:F:2:VAL:N	1:G:2:VAL:N	2.64	0.46
1:F:103[B]:ARG:CB	1:F:103[B]:ARG:CZ	2.90	0.46
1:F:210:GLU:HG2	1:F:214:ARG:HD3	1.97	0.46
1:D:38:THR:HG21	1:D:65:ILE:HD12	1.97	0.45
1:F:103[A]:ARG:NH1	2:F:1000:GLU:CG	2.79	0.45
1:H:163:ALA:O	1:H:166:SER:HB3	2.15	0.45
1:D:192:PRO:HG3	1:D:207:ILE:HG22	1.97	0.45
1:G:203:GLY:N	2:G:1000:GLU:HA	2.20	0.45
1:A:100[B]:GLU:H	1:A:100[B]:GLU:HG2	1.50	0.45
1:E:148:LEU:HD21	1:G:256:LYS:HD2	1.98	0.45
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.98	0.45
1:B:219:ARG:HD3	5:B:2153:HOH:O	2.16	0.45
1:B:71[A]:GLU:HG2	5:B:2068:HOH:O	2.17	0.44
1:A:71[A]:GLU:H	1:A:71[A]:GLU:CD	2.19	0.44
1:D:43:ARG:HH11	1:D:43:ARG:HG3	1.83	0.44
1:B:41:LYS:HD3	5:B:2038:HOH:O	2.17	0.44
1:C:39:TYR:CE2	1:C:45:ARG:HB2	2.53	0.44
1:B:103[A]:ARG:HH22	2:B:1000:GLU:CA	2.31	0.44
1:H:38:THR:HA	1:H:63:TYR:O	2.18	0.44
1:H:155:GLN:O	1:H:156:ASN:HB2	2.17	0.44
1:A:100[A]:GLU:CD	1:A:100[A]:GLU:H	2.21	0.44
1:F:101[B]:ASP:O	1:F:159:VAL:HG12	2.17	0.44
1:A:191:GLY:HA3	5:A:2186:HOH:O	2.17	0.44
1:A:16:ASN:HB2	5:A:2017:HOH:O	2.17	0.44
1:B:98:ASN:O	1:B:101[B]:ASP:HB2	2.18	0.43
1:G:138:GLU:HG2	5:G:2103:HOH:O	2.18	0.43
1:H:140:GLY:O	1:H:183:ILE:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ARG:HH21	1:E:199:LYS:HE3	1.83	0.43
1:C:76:GLY:O	1:C:80:ILE:HG13	2.17	0.43
1:F:18[B]:ARG:NH2	1:F:199:LYS:HZ3	2.16	0.43
1:G:69:SER:HA	5:G:2063:HOH:O	2.17	0.43
1:B:103[A]:ARG:NH1	2:B:1000:GLU:CD	2.72	0.43
1:B:76:GLY:O	1:B:80:ILE:HG13	2.17	0.43
1:A:157:TYR:CZ	1:A:160:MET:HG3	2.53	0.43
1:A:18[A]:ARG:HH21	1:A:199:LYS:NZ	2.12	0.43
1:F:176:LEU:HD13	1:G:255:ILE:HG21	2.01	0.43
1:E:152:PHE:CD1	1:G:256:LYS:HG3	2.54	0.43
1:F:52:LEU:HD23	1:F:52:LEU:HA	1.74	0.43
1:F:188:ILE:HG21	1:F:226:VAL:HG13	2.01	0.43
1:D:16:ASN:HB2	5:D:2010:HOH:O	2.17	0.43
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.88	0.43
1:A:203:GLY:H	2:A:1259:GLU:N	2.17	0.43
1:D:9:TYR:CD1	1:D:234:LEU:HD22	2.54	0.43
1:H:191:GLY:HA3	5:H:2097:HOH:O	2.19	0.43
1:A:38:THR:HA	1:A:63:TYR:O	2.19	0.43
1:G:82:LYS:HB2	1:G:82:LYS:HE3	1.83	0.42
1:E:38:THR:HA	1:E:63:TYR:O	2.18	0.42
1:B:103[A]:ARG:NH2	1:B:202:GLY:HA2	2.34	0.42
1:C:38:THR:HA	1:C:63:TYR:O	2.18	0.42
5:F:2157:HOH:O	1:G:241:VAL:HA	2.19	0.42
1:A:99[B]:MET:HE3	1:A:103[B]:ARG:HG3	2.00	0.42
1:D:237:LEU:HD23	1:D:237:LEU:HA	1.88	0.42
1:A:100[B]:GLU:OE2	1:E:41:LYS:NZ	2.50	0.42
1:F:103[A]:ARG:HH12	2:F:1000:GLU:CB	2.33	0.42
1:D:7:LYS:N	1:D:7:LYS:CD	2.83	0.42
1:A:244:GLU:HG3	1:A:245:ASN:N	2.35	0.42
1:E:103[B]:ARG:HH21	1:E:200:GLY:HA2	1.84	0.42
1:E:195:THR:O	1:E:199:LYS:HD3	2.19	0.42
1:F:38:THR:HG21	1:F:65:ILE:HD12	2.02	0.42
1:H:207:ILE:H	1:H:207:ILE:HG12	1.66	0.42
1:F:255:ILE:O	1:H:256:LYS:HE2	2.19	0.42
1:A:165:ALA:CB	1:B:169:ALA:HB2	2.50	0.42
1:C:203:GLY:H	2:C:1000:GLU:N	2.17	0.42
1:C:14:ILE:HG12	1:C:21:ALA:CB	2.50	0.42
1:B:203:GLY:H	2:B:1000:GLU:N	2.18	0.41
1:G:246:ILE:HG21	1:G:246:ILE:HD13	1.75	0.41
1:C:51:LEU:O	1:C:54:GLN:HB2	2.20	0.41
1:B:2:VAL:HG23	1:B:3:ASN:N	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:ILE:HD13	3:H:1257:NAP:H61A	1.85	0.41
1:F:39:TYR:OH	1:F:45:ARG:NH1	2.50	0.41
1:E:249:ASP:O	1:E:250:SER:HB2	2.19	0.41
1:D:112:GLU:CD	1:D:112:GLU:H	2.23	0.41
1:A:110:SER:HB2	1:E:42[A]:GLU:OE2	2.20	0.41
1:H:58:PRO:HG2	1:H:59:GLU:HG2	2.02	0.41
1:B:52:LEU:HD13	1:B:60:ALA:HB2	2.03	0.41
1:C:148:LEU:HD22	5:C:2158:HOH:O	2.19	0.41
1:G:148:LEU:HD12	1:G:148:LEU:HA	1.85	0.41
1:G:39:TYR:CZ	1:G:45:ARG:HB2	2.56	0.41
1:A:18[B]:ARG:HD3	5:A:2150:HOH:O	2.20	0.41
1:G:80:ILE:O	1:G:84:VAL:HG22	2.20	0.41
1:C:215:ALA:O	1:C:218:LYS:HD3	2.19	0.41
1:D:5:GLU:O	1:D:6:ASN:CB	2.56	0.41
1:F:140:GLY:O	1:F:183:ILE:HA	2.20	0.41
1:F:136:MET:HA	5:F:2100:HOH:O	2.21	0.41
1:F:46:LYS:HE3	1:F:46:LYS:HB3	1.65	0.41
1:A:237:LEU:O	1:D:228:LYS:HB3	2.20	0.41
1:B:218:LYS:HD2	5:B:2071:HOH:O	2.21	0.41
1:F:11:ILE:HD11	1:F:28:LEU:HD12	2.03	0.41
1:B:103[A]:ARG:NH2	2:B:1000:GLU:HA	2.32	0.41
1:A:64:GLN:HG2	5:A:2064:HOH:O	2.21	0.41
1:A:121:SER:O	1:A:167:LEU:HD13	2.21	0.41
1:B:210:GLU:OE2	1:B:214:ARG:NH1	2.54	0.41
1:F:103[A]:ARG:NH1	2:F:1000:GLU:OE2	2.54	0.40
1:G:196:LEU:HA	1:G:196:LEU:HD12	1.86	0.40
1:C:202:GLY:HA2	2:C:1000:GLU:HA	2.02	0.40
1:G:103:ARG:CZ	1:G:103:ARG:HB3	2.52	0.40
1:C:43:ARG:HD2	1:C:43:ARG:HA	1.93	0.40
1:A:143:VAL:HA	1:A:186:ASN:O	2.20	0.40
1:C:103:ARG:NH2	1:C:200:GLY:O	2.49	0.40
1:H:23:GLY:HA3	1:H:223:GLN:HB3	2.03	0.40
1:B:249:ASP:O	1:B:250:SER:HB2	2.22	0.40
1:B:2:VAL:HG22	1:B:4:LEU:HD13	2.03	0.40
1:A:202:GLY:HA2	2:A:1259:GLU:HA	2.03	0.40
1:F:103[A]:ARG:NH2	2:F:1000:GLU:HB3	2.37	0.40
1:D:143:VAL:HA	1:D:186:ASN:O	2.21	0.40
1:A:59:GLU:HG3	1:A:61:HIS:CE1	2.56	0.40
1:F:238:SER:O	1:F:241:VAL:HB	2.21	0.40
1:C:192:PRO:HG3	1:C:207:ILE:HG22	2.03	0.40
1:G:103:ARG:NH1	2:G:1000:GLU:OE1	2.44	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	264/282 (94%)	252 (96%)	12 (4%)	0	100	100
1	B	264/282 (94%)	248 (94%)	15 (6%)	1 (0%)	39	48
1	C	258/282 (92%)	240 (93%)	18 (7%)	0	100	100
1	D	254/282 (90%)	236 (93%)	15 (6%)	3 (1%)	16	16
1	E	263/282 (93%)	249 (95%)	14 (5%)	0	100	100
1	F	263/282 (93%)	248 (94%)	14 (5%)	1 (0%)	39	48
1	G	256/282 (91%)	242 (94%)	13 (5%)	1 (0%)	39	48
1	H	254/282 (90%)	242 (95%)	10 (4%)	2 (1%)	24	27
All	All	2076/2256 (92%)	1957 (94%)	111 (5%)	8 (0%)	39	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	LEU
1	D	47	GLU
1	F	148	LEU
1	D	194	ARG
1	G	148	LEU
1	H	47	GLU
1	H	194	ARG
1	D	84	VAL

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	218/234 (93%)	209 (96%)	9 (4%)	37	50
1	B	218/234 (93%)	209 (96%)	9 (4%)	37	50
1	C	213/234 (91%)	207 (97%)	6 (3%)	51	68
1	D	209/234 (89%)	197 (94%)	12 (6%)	25	34
1	E	217/234 (93%)	212 (98%)	5 (2%)	58	75
1	F	217/234 (93%)	212 (98%)	5 (2%)	58	75
1	G	211/234 (90%)	203 (96%)	8 (4%)	40	54
1	H	209/234 (89%)	204 (98%)	5 (2%)	57	74
All	All	1712/1872 (92%)	1653 (97%)	59 (3%)	42	59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	79	GLN
1	A	99[A]	MET
1	A	99[B]	MET
1	A	100[A]	GLU
1	A	100[B]	GLU
1	A	210	GLU
1	A	214	ARG
1	A	236	ASP
1	B	2	VAL
1	B	4	LEU
1	B	30	GLN
1	B	55	LEU
1	B	112	GLU
1	B	138	GLU
1	B	209	LYS
1	B	219	ARG
1	B	256	LYS
1	C	47	GLU
1	C	55	LEU
1	C	56	ASN
1	C	59	GLU
1	C	138	GLU
1	C	209	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4	LEU
1	D	34	LYS
1	D	40	ARG
1	D	41	LYS
1	D	43	ARG
1	D	48	LEU
1	D	78	GLU
1	D	99	MET
1	D	100	GLU
1	D	155	GLN
1	D	208	LEU
1	D	237	LEU
1	E	93	SER
1	E	199	LYS
1	E	210	GLU
1	E	216	PRO
1	E	236	ASP
1	F	2	VAL
1	F	4	LEU
1	F	42	GLU
1	F	50	LYS
1	F	56	ASN
1	G	17	LYS
1	G	55	LEU
1	G	56	ASN
1	G	99	MET
1	G	103	ARG
1	G	112	GLU
1	G	138	GLU
1	G	256	LYS
1	H	4	LEU
1	H	30	GLN
1	H	48	LEU
1	H	138	GLU
1	H	145	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	56	ASN
1	B	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3	ASN
1	D	3	ASN
1	D	155	GLN
1	E	75	ASN
1	E	253	HIS
1	F	253	HIS
1	H	3	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
3	NAP	A	1257	-	42,52,52	1.52	3 (7%)	54,80,80	2.09	10 (18%)
4	PV4	A	1258	-	18,18,18	0.60	0	23,23,23	0.77	0
2	GLU	A	1259	-	3,9,9	0.16	0	2,11,11	0.54	0
2	GLU	B	1000	-	3,9,9	0.34	0	2,11,11	0.13	0
3	NAP	B	1257	-	42,52,52	1.45	3 (7%)	54,80,80	2.35	11 (20%)
4	PV4	B	1258	-	18,18,18	0.77	0	23,23,23	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	C	1000	-	3,9,9	0.26	0	2,11,11	1.00	0
3	NAP	C	1257	-	42,52,52	1.46	3 (7%)	54,80,80	2.04	10 (18%)
4	PV4	C	1258	-	18,18,18	0.73	0	23,23,23	1.05	2 (8%)
3	NAP	D	1257	-	42,52,52	1.57	3 (7%)	54,80,80	2.41	8 (14%)
4	PV4	D	1258	-	18,18,18	0.64	0	23,23,23	0.81	1 (4%)
2	GLU	E	1000	-	3,9,9	0.22	0	2,11,11	0.29	0
3	NAP	E	1257	-	42,52,52	1.47	3 (7%)	54,80,80	2.14	9 (16%)
4	PV4	E	1258	-	18,18,18	0.73	0	23,23,23	0.78	1 (4%)
2	GLU	F	1000	-	3,9,9	0.30	0	2,11,11	1.15	0
3	NAP	F	1257	-	42,52,52	1.51	3 (7%)	54,80,80	2.18	10 (18%)
4	PV4	F	1258	-	18,18,18	0.79	0	23,23,23	1.09	1 (4%)
2	GLU	G	1000	-	3,9,9	0.25	0	2,11,11	0.20	0
3	NAP	G	1257	-	42,52,52	1.46	3 (7%)	54,80,80	2.13	9 (16%)
4	PV4	G	1258	-	18,18,18	0.71	0	23,23,23	0.86	0
3	NAP	H	1257	-	42,52,52	1.49	2 (4%)	54,80,80	2.02	7 (12%)
4	PV4	H	1258	-	18,18,18	0.54	0	23,23,23	1.02	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	A	1258	-	-	0/7/7/7	0/2/2/2
2	GLU	A	1259	-	-	0/3/9/9	0/0/0/0
2	GLU	B	1000	-	-	0/3/9/9	0/0/0/0
3	NAP	B	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	B	1258	-	-	0/7/7/7	0/2/2/2
2	GLU	C	1000	-	-	0/3/9/9	0/0/0/0
3	NAP	C	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	C	1258	-	-	0/7/7/7	0/2/2/2
3	NAP	D	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	D	1258	-	-	0/7/7/7	0/2/2/2
2	GLU	E	1000	-	-	0/3/9/9	0/0/0/0
3	NAP	E	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	E	1258	-	-	0/7/7/7	0/2/2/2
2	GLU	F	1000	-	-	0/3/9/9	0/0/0/0
3	NAP	F	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	F	1258	-	-	0/7/7/7	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	G	1000	-	-	0/3/9/9	0/0/0/0
3	NAP	G	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	G	1258	-	-	0/7/7/7	0/2/2/2
3	NAP	H	1257	-	-	0/27/67/67	0/5/5/5
4	PV4	H	1258	-	-	0/7/7/7	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1257	NAP	C2A-N1A	2.03	1.37	1.33
3	B	1257	NAP	C2A-N1A	2.09	1.37	1.33
3	F	1257	NAP	C2A-N1A	2.34	1.38	1.33
3	A	1257	NAP	C2A-N1A	2.45	1.38	1.33
3	D	1257	NAP	C2A-N1A	2.54	1.38	1.33
3	G	1257	NAP	C2A-N1A	2.61	1.38	1.33
3	C	1257	NAP	C2A-N1A	2.68	1.39	1.33
3	H	1257	NAP	C2A-N3A	2.96	1.37	1.32
3	G	1257	NAP	C2A-N3A	3.25	1.37	1.32
3	C	1257	NAP	C2A-N3A	3.27	1.38	1.32
3	B	1257	NAP	C2A-N3A	3.39	1.38	1.32
3	E	1257	NAP	C2A-N3A	3.55	1.38	1.32
3	A	1257	NAP	C2A-N3A	3.66	1.38	1.32
3	D	1257	NAP	C2A-N3A	3.74	1.38	1.32
3	F	1257	NAP	C2A-N3A	4.00	1.39	1.32
3	G	1257	NAP	O7N-C7N	6.75	1.38	1.24
3	C	1257	NAP	O7N-C7N	6.90	1.38	1.24
3	B	1257	NAP	O7N-C7N	6.92	1.38	1.24
3	E	1257	NAP	O7N-C7N	7.09	1.39	1.24
3	F	1257	NAP	O7N-C7N	7.18	1.39	1.24
3	A	1257	NAP	O7N-C7N	7.18	1.39	1.24
3	D	1257	NAP	O7N-C7N	7.56	1.40	1.24
3	H	1257	NAP	O7N-C7N	7.68	1.40	1.24

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1257	NAP	N3A-C2A-N1A	-14.21	118.01	128.89
3	B	1257	NAP	N3A-C2A-N1A	-12.94	118.99	128.89
3	F	1257	NAP	N3A-C2A-N1A	-11.48	120.11	128.89
3	E	1257	NAP	N3A-C2A-N1A	-11.18	120.33	128.89
3	A	1257	NAP	N3A-C2A-N1A	-10.74	120.67	128.89
3	C	1257	NAP	N3A-C2A-N1A	-10.69	120.71	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1257	NAP	N3A-C2A-N1A	-9.48	121.63	128.89
3	G	1257	NAP	N3A-C2A-N1A	-8.34	122.51	128.89
3	G	1257	NAP	O7N-C7N-C3N	-5.87	113.17	119.59
3	F	1257	NAP	C4B-O4B-C1B	-4.89	104.35	109.72
3	H	1257	NAP	O7N-C7N-C3N	-4.75	114.41	119.59
3	H	1257	NAP	C4B-O4B-C1B	-4.74	104.52	109.72
3	E	1257	NAP	C4B-O4B-C1B	-4.62	104.64	109.72
3	D	1257	NAP	C4B-O4B-C1B	-4.18	105.13	109.72
3	B	1257	NAP	C4B-O4B-C1B	-4.08	105.24	109.72
3	A	1257	NAP	C4B-O4B-C1B	-4.02	105.31	109.72
3	C	1257	NAP	O7N-C7N-C3N	-3.82	115.41	119.59
3	D	1257	NAP	O4B-C1B-C2B	-3.82	99.68	106.60
3	C	1257	NAP	C4B-O4B-C1B	-3.48	105.89	109.72
3	A	1257	NAP	C1B-N9A-C4A	-3.48	121.69	126.94
3	B	1257	NAP	C4D-O4D-C1D	-3.17	106.24	109.72
3	G	1257	NAP	C4B-O4B-C1B	-3.01	106.41	109.72
3	E	1257	NAP	O7N-C7N-C3N	-2.82	116.51	119.59
3	B	1257	NAP	O3B-C3B-C2B	-2.76	103.20	111.16
3	E	1257	NAP	C1B-N9A-C4A	-2.76	122.78	126.94
3	B	1257	NAP	O7N-C7N-C3N	-2.67	116.68	119.59
3	F	1257	NAP	O4B-C1B-C2B	-2.62	101.86	106.60
3	G	1257	NAP	C4A-C5A-N7A	-2.62	107.07	109.48
3	C	1257	NAP	C1B-N9A-C4A	-2.59	123.03	126.94
4	F	1258	PV4	C4-C3-C2	-2.46	117.66	121.04
3	A	1257	NAP	C4A-C5A-N7A	-2.45	107.22	109.48
3	G	1257	NAP	C3N-C2N-N1N	-2.42	117.58	120.36
3	C	1257	NAP	C3N-C2N-N1N	-2.40	117.59	120.36
3	D	1257	NAP	O7N-C7N-N7N	-2.34	119.30	122.59
3	C	1257	NAP	O4B-C1B-C2B	-2.29	102.47	106.60
3	H	1257	NAP	C1B-N9A-C4A	-2.23	123.57	126.94
4	C	1258	PV4	C6-C1-C2	-2.18	118.19	120.83
3	G	1257	NAP	C4N-C3N-C7N	-2.14	115.43	121.09
4	C	1258	PV4	C15-C14-C2	-2.10	103.65	113.86
3	A	1257	NAP	O7N-C7N-N7N	-2.09	119.66	122.59
3	D	1257	NAP	PN-O3-PA	-2.03	127.02	132.73
4	H	1258	PV4	C14-C2-C1	-2.02	117.17	120.56
3	A	1257	NAP	O7N-C7N-C3N	-2.02	117.39	119.59
3	H	1257	NAP	O2N-PN-O1N	2.02	123.47	112.53
3	E	1257	NAP	C2N-C3N-C4N	2.02	120.54	118.29
3	D	1257	NAP	O3X-P2B-O2X	2.05	115.20	107.38
4	E	1258	PV4	O7-C5-C6	2.07	120.19	116.12
3	B	1257	NAP	O4D-C1D-N1N	2.10	110.44	108.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1257	NAP	O2N-PN-O1N	2.13	124.09	112.53
3	F	1257	NAP	O3X-P2B-O2X	2.15	115.58	107.38
3	E	1257	NAP	O3X-P2B-O2X	2.18	115.69	107.38
3	B	1257	NAP	C2N-C3N-C4N	2.19	120.73	118.29
3	E	1257	NAP	O2B-P2B-O1X	2.25	112.73	107.11
3	A	1257	NAP	O4B-C1B-N9A	2.27	112.86	108.10
3	C	1257	NAP	O4B-C1B-N9A	2.30	112.92	108.10
4	D	1258	PV4	O7-C5-C6	2.38	120.80	116.12
3	C	1257	NAP	O3X-P2B-O2X	2.39	116.48	107.38
3	H	1257	NAP	O4B-C1B-N9A	2.46	113.25	108.10
3	B	1257	NAP	O3-PA-O5B	2.48	109.51	102.94
3	F	1257	NAP	C2N-C3N-C4N	2.52	121.09	118.29
3	E	1257	NAP	O4D-C1D-N1N	2.53	110.91	108.13
3	B	1257	NAP	O2B-P2B-O1X	2.54	113.44	107.11
3	A	1257	NAP	O3-PA-O5B	2.60	109.84	102.94
3	G	1257	NAP	C2N-C3N-C4N	2.97	121.59	118.29
3	D	1257	NAP	O2B-P2B-O1X	2.98	114.55	107.11
3	F	1257	NAP	O2B-P2B-O1X	3.06	114.74	107.11
3	F	1257	NAP	O4B-C1B-N9A	3.11	114.60	108.10
3	A	1257	NAP	C2N-C3N-C4N	3.13	121.77	118.29
3	C	1257	NAP	C2N-C3N-C4N	3.32	121.98	118.29
3	F	1257	NAP	O4D-C1D-N1N	3.32	111.78	108.13
3	B	1257	NAP	C3N-C7N-N7N	3.55	121.70	117.82
3	G	1257	NAP	O4B-C1B-N9A	3.84	116.14	108.10
3	F	1257	NAP	C3N-C7N-N7N	3.85	122.03	117.82
3	D	1257	NAP	C3N-C7N-N7N	3.93	122.11	117.82
3	B	1257	NAP	O4B-C1B-N9A	4.04	116.55	108.10
3	C	1257	NAP	C3N-C7N-N7N	4.14	122.35	117.82
3	A	1257	NAP	C3N-C7N-N7N	4.68	122.94	117.82
3	E	1257	NAP	C3N-C7N-N7N	4.70	122.96	117.82
3	H	1257	NAP	C3N-C7N-N7N	5.55	123.89	117.82
3	G	1257	NAP	C3N-C7N-N7N	7.39	125.90	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1258	PV4	1	0
2	A	1259	GLU	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	GLU	9	0
3	B	1257	NAP	1	0
2	C	1000	GLU	8	0
3	D	1257	NAP	1	0
2	E	1000	GLU	4	0
3	E	1257	NAP	1	0
2	F	1000	GLU	9	0
2	G	1000	GLU	3	0
3	H	1257	NAP	2	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, 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%)	-0.37	0 100 100	17, 26, 48, 64	0
1	B	255/282 (90%)	-0.26	2 (0%) 87 90	16, 30, 55, 70	0
1	C	255/282 (90%)	-0.06	6 (2%) 62 71	17, 31, 56, 71	0
1	D	254/282 (90%)	-0.19	3 (1%) 81 85	19, 34, 66, 94	0
1	E	254/282 (90%)	-0.39	1 (0%) 93 95	15, 26, 48, 63	0
1	F	255/282 (90%)	-0.44	2 (0%) 87 90	17, 28, 49, 63	0
1	G	255/282 (90%)	-0.21	3 (1%) 81 85	18, 31, 54, 70	0
1	H	254/282 (90%)	-0.19	1 (0%) 93 95	18, 36, 66, 83	0
All	All	2036/2256 (90%)	-0.26	18 (0%) 85 89	15, 30, 57, 94	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	VAL	6.0
1	C	2	VAL	4.2
1	D	58	PRO	3.5
1	G	71	GLU	3.0
1	C	143	VAL	2.9
1	C	58	PRO	2.9
1	D	43	ARG	2.8
1	B	58	PRO	2.8
1	G	58	PRO	2.8
1	H	99	MET	2.5
1	E	6	ASN	2.5
1	F	58	PRO	2.4
1	C	233	LEU	2.2
1	B	6	ASN	2.2
1	C	188	ILE	2.2
1	F	104[A]	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	144	ALA	2.1
1	D	104	GLY	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLU	A	1259	10/10	0.80	0.23	3.46	79,80,83,84	0
2	GLU	F	1000	10/10	0.61	0.27	2.39	74,77,78,78	0
2	GLU	E	1000	10/10	0.75	0.22	2.04	91,92,94,94	0
2	GLU	G	1000	10/10	0.84	0.18	1.79	80,81,82,83	0
2	GLU	C	1000	10/10	0.84	0.17	1.13	80,81,83,86	0
4	PV4	G	1258	17/17	0.97	0.13	0.60	17,27,37,39	0
2	GLU	B	1000	10/10	0.81	0.17	0.25	74,75,78,81	0
3	NAP	E	1257	48/48	0.98	0.10	0.14	19,24,29,31	0
4	PV4	C	1258	17/17	0.97	0.12	0.11	19,26,30,30	0
4	PV4	E	1258	17/17	0.96	0.11	0.07	20,25,27,30	0
4	PV4	A	1258	17/17	0.97	0.11	-0.07	18,22,28,29	0
3	NAP	A	1257	48/48	0.98	0.11	-0.23	19,25,31,34	0
3	NAP	G	1257	48/48	0.98	0.11	-0.25	17,27,33,37	0
3	NAP	D	1257	48/48	0.97	0.09	-0.34	28,35,53,55	0
4	PV4	H	1258	17/17	0.95	0.11	-0.36	36,42,48,50	0
4	PV4	F	1258	17/17	0.96	0.10	-0.37	19,27,33,33	0
4	PV4	D	1258	17/17	0.96	0.09	-0.40	31,35,39,39	0
3	NAP	B	1257	48/48	0.98	0.10	-0.43	19,27,32,36	0
3	NAP	F	1257	48/48	0.99	0.09	-0.63	18,25,30,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAP	C	1257	48/48	0.98	0.10	-0.68	23,28,33,35	0
3	NAP	H	1257	48/48	0.96	0.09	-0.82	29,38,52,56	0
4	PV4	B	1258	17/17	0.97	0.09	-1.20	19,25,27,28	0

6.5 Other polymers

There are no such residues in this entry.