



# Full wwPDB X-ray Structure Validation Report

Aug 8, 2014 – 01:37 AM EDT

PDB ID : 4CV1  
Title : Crystal structure of *S. aureus* FabI in complex with NADPH and CG400549  
Authors : Schiebel, J.; Chang, A.; Shah, S.; Tonge, P.J.; Kisker, C.  
Deposited on : 2014-03-22  
Resolution : 1.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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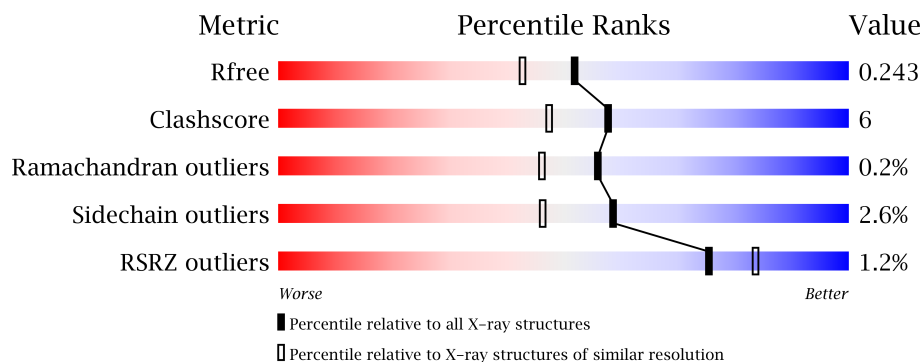
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	
1	F	282	
1	G	282	
1	H	282	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	G	1358	-	X
5	EDO	H	1257	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17795 atoms, of which 0 are hydrogen and 0 are deuterium.

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 [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	7	0
			2060	1301	353	401	5			
1	B	256	Total	C	N	O	S	0	13	0
			2057	1299	352	401	5			
1	C	262	Total	C	N	O	S	0	4	0
			2047	1295	350	397	5			
1	D	256	Total	C	N	O	S	0	6	0
			2007	1269	344	389	5			
1	E	256	Total	C	N	O	S	0	13	0
			2063	1303	357	398	5			
1	F	262	Total	C	N	O	S	0	2	0
			2028	1282	347	394	5			
1	G	257	Total	C	N	O	S	0	5	0
			2007	1264	347	390	6			
1	H	263	Total	C	N	O	S	0	3	0
			2047	1294	353	395	5			

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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

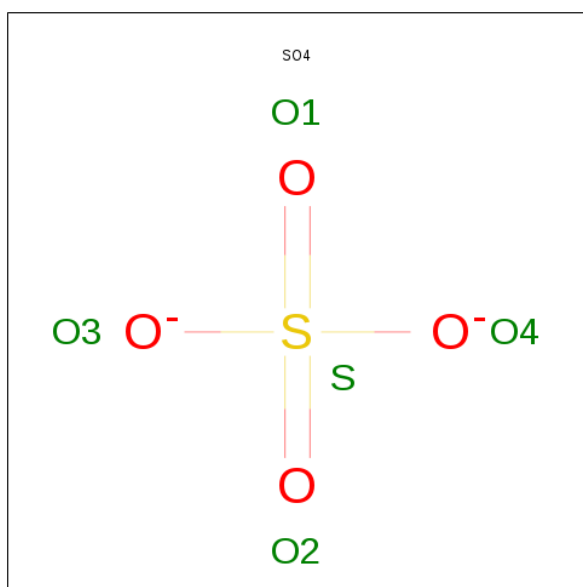
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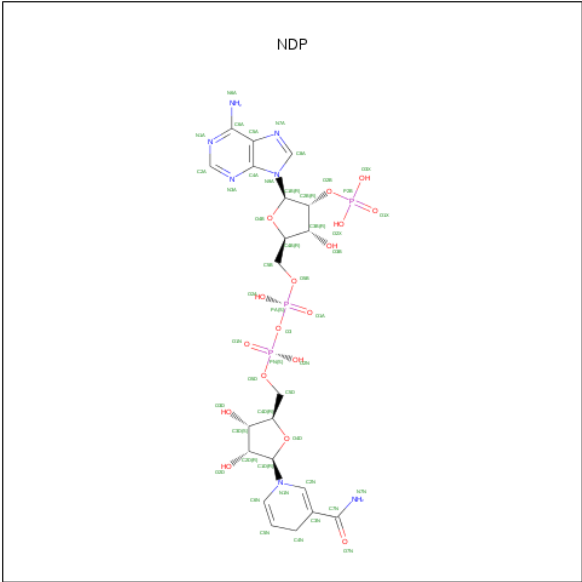
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
G	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
G	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
G	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
G	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
G	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



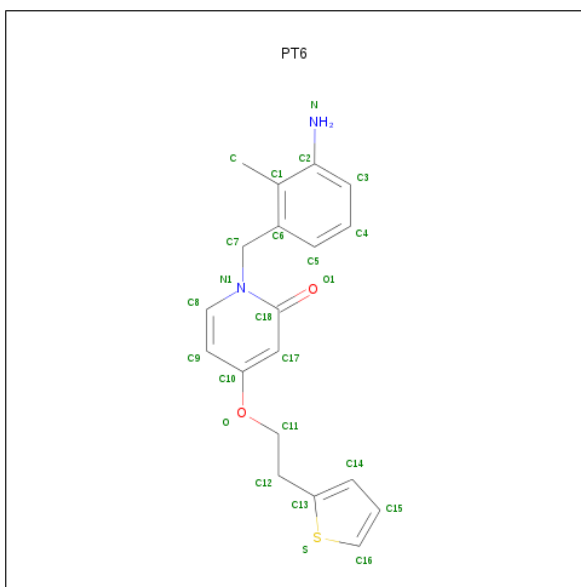
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



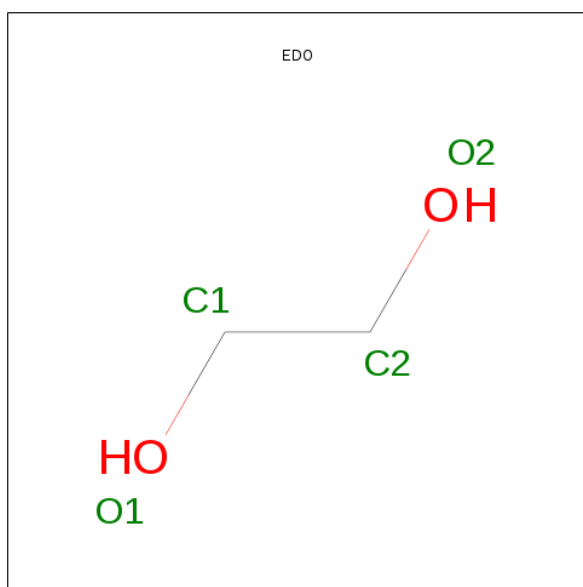
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	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 1-(3-AMINO-2-METHYLBENZYL)-4-[2-(THIOPHEN-2-YL)ETHOXY]PYRIDIN-2(1H)-ONE (three-letter code: PT6) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	C	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	E	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	F	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	G	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	H	1	Total	C	N	O	S	0	0
			24	19	2	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		

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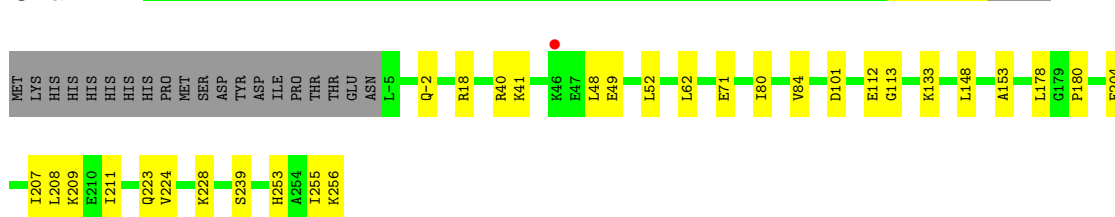
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	110	Total 110	O 110	0	0
7	C	106	Total 106	O 106	0	0
7	D	87	Total 87	O 87	0	0
7	E	138	Total 138	O 138	0	0
7	F	112	Total 112	O 112	0	0
7	G	82	Total 82	O 82	0	0
7	H	80	Total 80	O 80	0	0

### 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.

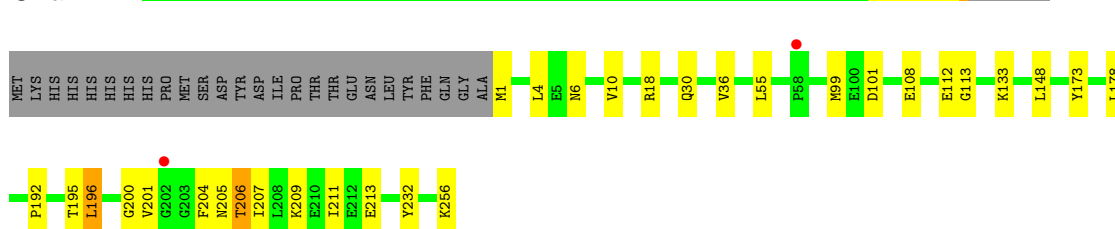
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain A:



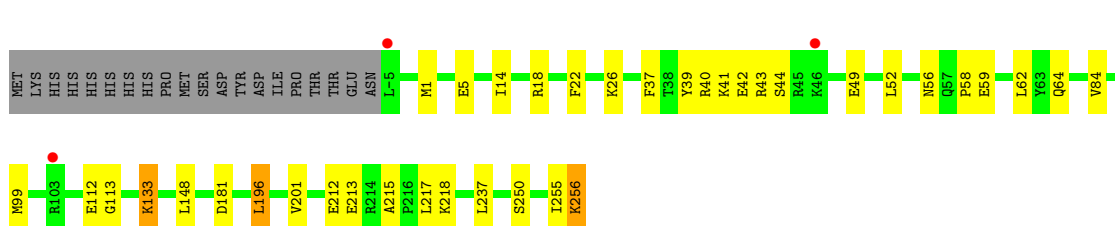
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain B:



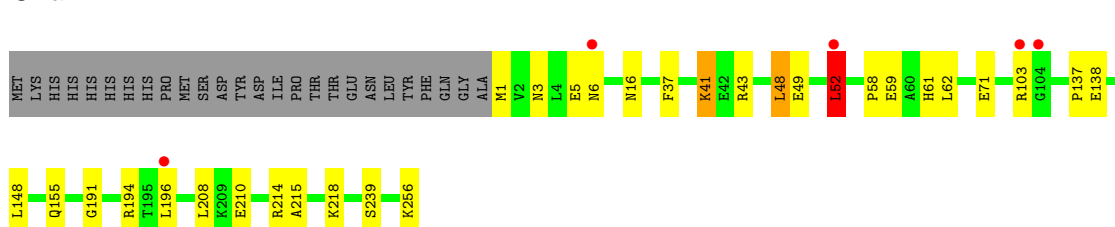
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain C:



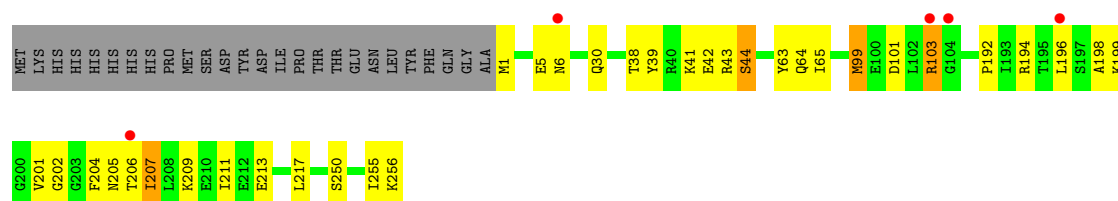
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain D:



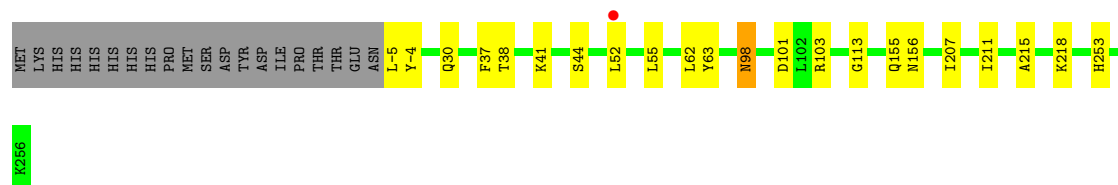
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain E: 



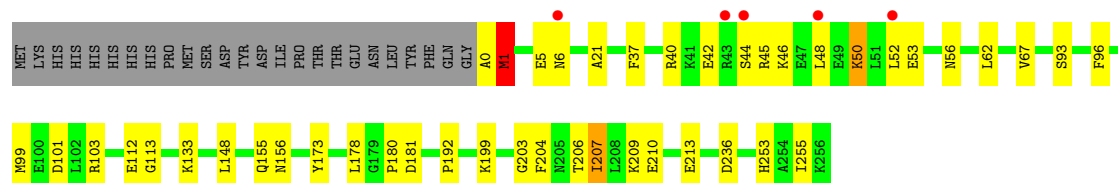
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain F: 



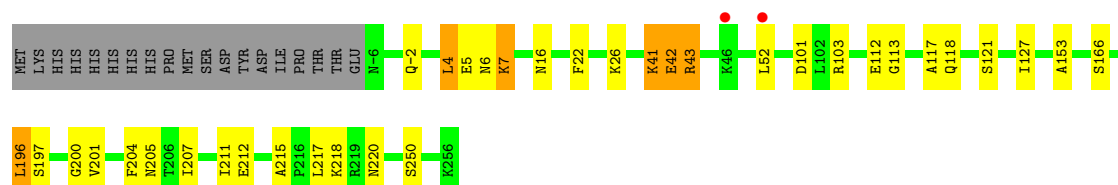
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN]REDUCTASE [NADH]

Chain G: 



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

Chain H: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.90Å 108.47Å 296.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 1.95 47.24 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.56-1.95) 99.9 (47.24-1.95)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.168 , 0.231 0.183 , 0.243	Depositor DCC
$R_{free}$ test set	7315 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 146545 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, SO4, PT6, EDO, CL

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	0.59	0/2104	0.78	1/2834 (0.0%)
1	B	0.56	0/2094	0.76	1/2821 (0.0%)
1	C	0.53	0/2084	0.75	1/2803 (0.0%)
1	D	0.57	0/2052	0.79	2/2763 (0.1%)
1	E	0.56	0/2097	0.74	0/2823
1	F	0.56	0/2063	0.76	0/2780
1	G	0.51	0/2040	0.74	0/2747
1	H	0.51	0/2085	0.74	0/2808
All	All	0.55	0/16619	0.76	5/22379 (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	B	0	1
1	E	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	LEU	CA-CB-CG	6.70	130.71	115.30
1	D	52	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	208	LEU	CA-CB-CG	5.96	129.00	115.30
1	D	239	SER	C-N-CA	-5.28	111.21	122.30
1	C	196	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200[A]	GLY	Peptide
1	E	103[A]	ARG	Peptide
1	E	103[B]	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2060	0	2078	26	0
1	B	2057	0	2079	29	3
1	C	2047	0	2071	34	3
1	D	2007	0	2044	27	0
1	E	2063	0	2095	42	0
1	F	2028	0	2045	15	0
1	G	2007	0	2028	37	0
1	H	2047	0	2072	24	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	E	5	0	0	0	0
2	H	5	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	0	0
3	C	48	0	26	1	0
3	D	48	0	26	0	0
3	E	48	0	26	1	0
3	F	48	0	26	0	0
3	G	48	0	26	2	0
3	H	48	0	26	2	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
4	C	24	0	0	0	0
4	D	24	0	0	0	0
4	E	24	0	0	0	0
4	F	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	24	0	0	0	0
4	H	24	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
5	E	4	0	6	2	0
5	G	8	0	12	3	0
5	H	4	0	6	0	0
6	F	1	0	0	0	0
7	A	134	0	0	6	0
7	B	110	0	0	5	0
7	C	106	0	0	3	0
7	D	87	0	0	2	0
7	E	138	0	0	5	0
7	F	112	0	0	2	0
7	G	82	0	0	4	0
7	H	80	0	0	4	0
All	All	17795	0	16762	211	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (211) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:112[B]:GLU:OE1	7:B:2051:HOH:O	1.55	1.24
1:A:40:ARG:HH11	1:A:41:LYS:HD2	1.32	0.93
1:E:101:ASP:OD1	7:E:2062:HOH:O	1.86	0.93
1:G:112[A]:GLU:HG3	7:G:2046:HOH:O	1.71	0.89
1:E:207[B]:ILE:O	1:E:211:ILE:HG12	1.73	0.88
1:C:215:ALA:O	1:C:218[A]:LYS:HD3	1.73	0.88
7:E:2121:HOH:O	1:G:210:GLU:HG3	1.75	0.85
1:D:49:GLU:HA	1:D:52:LEU:CD1	2.07	0.84
1:B:209[B]:LYS:O	1:B:213:GLU:HG3	1.78	0.84
1:B:30:GLN:HE22	1:F:-4:TYR:H	1.26	0.84
1:E:256:LYS:HG2	1:G:148:LEU:HD21	1.61	0.82
1:B:204[A]:PHE:O	1:B:207[A]:ILE:HG22	1.81	0.81
1:C:1:MET:HE2	1:C:237:LEU:HD21	1.66	0.78
1:G:0:ALA:O	1:G:1[A]:MET:HB3	1.83	0.77
1:H:205:ASN:O	7:H:2068:HOH:O	2.01	0.77
1:A:40:ARG:NH1	1:A:41:LYS:HD2	1.99	0.76
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.67	0.76
1:E:204[A]:PHE:O	1:E:207[A]:ILE:HG23	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:ILE:O	1:C:256[B]:LYS:HE2	1.87	0.74
1:B:6:ASN:HB2	7:B:2004:HOH:O	1.88	0.74
1:A:101:ASP:OD2	1:A:113:GLY:HA3	1.88	0.74
1:H:43:ARG:HG2	7:H:2015:HOH:O	1.88	0.73
1:B:204[A]:PHE:HA	1:B:207[A]:ILE:HG22	1.69	0.72
1:A:180:PRO:HG3	1:D:218[B]:LYS:HD2	1.70	0.72
1:G:0:ALA:O	1:G:1[B]:MET:HB2	1.89	0.71
1:B:206[A]:THR:HG22	7:B:2087:HOH:O	1.92	0.70
1:G:0:ALA:O	1:G:1[A]:MET:CB	2.40	0.69
1:C:18:ARG:HD2	7:C:2018:HOH:O	1.92	0.69
1:G:112[B]:GLU:HG2	1:G:113:GLY:N	2.07	0.69
1:H:204:PHE:O	1:H:207:ILE:HG22	1.93	0.68
1:D:5:GLU:O	1:D:6:ASN:HB2	1.93	0.68
1:C:18:ARG:HG2	7:C:2021:HOH:O	1.93	0.68
1:E:256:LYS:HG2	1:G:148:LEU:CD2	2.24	0.67
1:C:213:GLU:O	1:C:218[A]:LYS:HE3	1.95	0.67
1:C:49:GLU:HG2	1:C:62:LEU:HD11	1.77	0.67
1:D:41:LYS:HG3	1:D:43:ARG:HG3	1.75	0.66
1:A:41:LYS:NZ	7:A:2022:HOH:O	2.27	0.65
1:A:256:LYS:HG2	1:C:148:LEU:CD2	2.25	0.65
1:D:49:GLU:HA	1:D:52:LEU:HD12	1.79	0.64
1:G:1[A]:MET:HE1	1:G:236:ASP:H	1.62	0.64
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.79	0.64
1:F:207:ILE:O	1:F:211:ILE:HD13	1.98	0.63
1:C:49:GLU:HG2	1:C:62:LEU:CD1	2.29	0.63
1:B:204[A]:PHE:CA	1:B:207[A]:ILE:HG22	2.29	0.62
1:D:16:ASN:ND2	1:D:196[B]:LEU:HD22	2.15	0.61
1:D:41:LYS:HE2	1:D:43:ARG:NE	2.16	0.61
1:H:22:PHE:CE2	1:H:26:LYS:HE3	2.35	0.61
1:B:204[A]:PHE:O	1:B:207[A]:ILE:CG2	2.48	0.60
1:E:194:ARG:HH11	1:E:194:ARG:HG2	1.64	0.60
1:H:5:GLU:O	1:H:6:ASN:HB2	2.00	0.60
1:A:253:HIS:HD2	7:A:2131:HOH:O	1.84	0.60
1:H:103:ARG:NH2	1:H:200:GLY:O	2.34	0.60
1:D:41:LYS:HB3	7:D:2016:HOH:O	2.01	0.60
1:G:204:PHE:O	1:G:207:ILE:HG22	2.01	0.60
1:G:209:LYS:O	1:G:213:GLU:HG3	2.02	0.60
1:D:59:GLU:HG3	1:D:61:HIS:NE2	2.17	0.60
1:F:37:PHE:HB2	1:F:62:LEU:HD23	1.84	0.59
1:H:201:VAL:O	7:H:3135:HOH:O	2.16	0.59
1:A:148:LEU:HD21	1:C:256[A]:LYS:HD2	1.85	0.59
1:C:56:ASN:ND2	1:F:30:GLN:OE1	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:253:HIS:HD2	7:F:2031:HOH:O	1.86	0.59
1:E:204[A]:PHE:HA	1:E:207[A]:ILE:CG2	2.33	0.58
1:E:43:ARG:HD3	5:E:1261:EDO:H12	1.85	0.58
1:B:148:LEU:CD2	1:D:256:LYS:HG2	2.33	0.58
1:B:204[A]:PHE:HA	1:B:207[A]:ILE:CG2	2.32	0.58
1:C:58:PRO:O	1:C:59:GLU:HB3	2.03	0.58
1:E:201[B]:VAL:HG13	1:E:204[B]:PHE:HB2	1.86	0.58
1:B:204[A]:PHE:C	1:B:207[A]:ILE:HG22	2.23	0.58
1:E:41:LYS:HD2	1:E:43:ARG:CZ	2.34	0.58
1:B:30:GLN:NE2	1:F:-4:TYR:H	1.97	0.57
1:E:103[A]:ARG:HH11	1:E:103[A]:ARG:HG2	1.69	0.57
1:G:5:GLU:O	1:G:6:ASN:HB2	2.05	0.57
1:A:256:LYS:HD2	1:C:256[B]:LYS:HE3	1.86	0.57
1:D:48:LEU:O	1:D:52:LEU:HD12	2.05	0.57
1:C:41:LYS:HD2	1:C:43:ARG:NH2	2.19	0.57
1:E:205[B]:ASN:O	1:E:206[B]:THR:C	2.41	0.57
1:D:49:GLU:HA	1:D:52:LEU:HD11	1.85	0.56
1:D:37:PHE:HB2	1:D:62:LEU:HD23	1.88	0.56
1:A:112[A]:GLU:HG2	7:A:2067:HOH:O	2.07	0.55
1:D:16:ASN:HD22	1:D:196[B]:LEU:HD22	1.72	0.55
1:H:207:ILE:O	1:H:211:ILE:HG12	2.07	0.55
1:G:96:PHE:HD1	7:G:2032:HOH:O	1.88	0.55
1:D:71:GLU:CD	1:D:71:GLU:H	2.10	0.55
1:F:98:ASN:ND2	7:F:2040:HOH:O	2.40	0.55
1:G:37:PHE:HB2	1:G:62:LEU:HD23	1.89	0.55
1:G:101:ASP:OD2	1:G:113:GLY:HA3	2.07	0.54
1:H:41:LYS:HE3	3:H:1258:NDP:O2X	2.07	0.54
1:C:42[A]:GLU:OE1	1:C:64:GLN:NE2	2.40	0.54
1:G:99:MET:O	1:G:103[A]:ARG:HG3	2.08	0.54
1:F:218:LYS:HD3	1:G:180:PRO:HG3	1.90	0.53
1:G:0:ALA:O	1:G:1[B]:MET:CB	2.54	0.53
1:A:255:ILE:O	1:C:256[B]:LYS:CE	2.56	0.53
1:H:112:GLU:CD	1:H:112:GLU:H	2.12	0.53
1:E:43:ARG:CD	5:E:1261:EDO:H12	2.39	0.53
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.09	0.53
1:H:118:GLN:HE22	1:H:166:SER:CB	2.21	0.53
1:A:207:ILE:O	1:A:211:ILE:HG12	2.08	0.53
1:A:239[B]:SER:O	7:A:2124:HOH:O	2.19	0.53
1:B:112[A]:GLU:CD	1:B:112[A]:GLU:H	2.12	0.52
1:C:5:GLU:OE2	1:G:1[B]:MET:HA	2.10	0.52
1:E:41:LYS:HG2	7:E:2022:HOH:O	2.10	0.52
1:D:210:GLU:HG2	1:D:214:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:198:ALA:O	1:E:201[B]:VAL:HG12	2.09	0.52
1:E:256:LYS:HE2	1:G:255:ILE:O	2.10	0.52
1:G:50:LYS:O	1:G:53:GLU:HG3	2.10	0.52
1:D:215:ALA:O	1:D:218[A]:LYS:HD2	2.10	0.52
1:H:101:ASP:OD2	1:H:113:GLY:HA3	2.10	0.52
1:A:133:LYS:HD2	1:A:178:LEU:HD22	1.92	0.50
1:E:5:GLU:O	1:E:6:ASN:HB2	2.11	0.50
1:H:212:GLU:HG3	1:H:220:ASN:ND2	2.26	0.50
1:A:256:LYS:HE2	1:C:255:ILE:O	2.12	0.50
1:D:16:ASN:HD21	1:D:196[A]:LEU:HB2	1.77	0.50
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.46	0.50
1:G:155:GLN:O	1:G:156:ASN:HB2	2.12	0.50
1:G:253:HIS:HD2	7:G:2016:HOH:O	1.93	0.50
1:B:232:TYR:HA	1:C:1:MET:HE1	1.92	0.50
1:C:112[B]:GLU:HG2	1:C:113:GLY:N	2.27	0.49
1:B:192:PRO:HG2	1:B:207[B]:ILE:CG2	2.42	0.49
1:E:194:ARG:HG2	1:E:194:ARG:NH1	2.27	0.49
1:B:205[A]:ASN:HB3	7:B:2087:HOH:O	2.11	0.49
1:D:16:ASN:HD21	1:D:196[B]:LEU:CB	2.26	0.49
1:C:37:PHE:HB2	1:C:62:LEU:HD23	1.94	0.49
1:C:49:GLU:CG	1:C:62:LEU:CD1	2.89	0.49
1:G:206:THR:HG23	5:G:1257:EDO:H11	1.95	0.48
1:E:205[B]:ASN:O	1:E:207[B]:ILE:N	2.46	0.48
1:C:37:PHE:CD2	1:C:52:LEU:HD21	2.49	0.48
1:C:52:LEU:HD22	1:C:62:LEU:HD21	1.96	0.48
1:E:103[A]:ARG:HG2	1:E:103[A]:ARG:NH1	2.29	0.48
1:H:4:LEU:O	1:H:7:LYS:HB2	2.14	0.48
1:A:18[A]:ARG:NE	1:A:223:GLN:HE22	2.12	0.47
1:G:67:VAL:HG22	3:G:1259:NDP:N1A	2.29	0.47
1:E:38:THR:HG21	1:E:65:ILE:HD12	1.96	0.47
1:B:207[B]:ILE:O	1:B:211:ILE:HG12	2.15	0.47
1:H:117:ALA:O	1:H:121:SER:HB2	2.15	0.47
1:A:18[A]:ARG:CZ	1:A:223:GLN:HE22	2.27	0.47
1:E:41:LYS:O	1:E:44:SER:HB2	2.14	0.47
1:F:41:LYS:HE2	1:F:44:SER:OG	2.14	0.47
1:H:5:GLU:O	1:H:6:ASN:CB	2.61	0.47
1:B:99:MET:HE1	1:B:201[B]:VAL:HG22	1.97	0.47
1:E:41:LYS:HE2	3:E:1259:NDP:O2X	2.15	0.47
1:A:224:VAL:O	1:A:228:LYS:HG3	2.15	0.47
1:D:16:ASN:HD21	1:D:196[B]:LEU:HB2	1.79	0.47
1:E:196:LEU:HB3	7:E:2010:HOH:O	2.14	0.46
1:G:203:GLY:O	1:G:207:ILE:HB	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:99:MET:CE	1:E:201[B]:VAL:HB	2.44	0.46
1:F:-5:LEU:HD22	1:G:56:ASN:ND2	2.30	0.46
1:B:112[A]:GLU:HG2	7:B:2050:HOH:O	2.14	0.46
1:G:133:LYS:HE3	1:G:181:ASP:OD2	2.15	0.46
1:H:16:ASN:HD21	1:H:196:LEU:HB2	1.81	0.46
1:H:42:GLU:HB2	7:H:2015:HOH:O	2.15	0.46
1:D:3:ASN:OD1	1:D:5:GLU:HB2	2.16	0.46
1:G:21:ALA:HB2	1:G:93:SER:CB	2.46	0.46
7:A:2073:HOH:O	1:B:108:GLU:OE2	2.21	0.46
1:C:99:MET:HE1	1:C:201:VAL:HA	1.98	0.46
1:E:196:LEU:HD13	1:E:199[B]:LYS:NZ	2.31	0.46
1:F:38:THR:HA	1:F:63:TYR:O	2.15	0.46
1:H:-2:GLN:CD	1:H:-2:GLN:H	2.19	0.46
1:E:103[B]:ARG:CZ	1:E:202[B]:GLY:CA	2.95	0.45
1:B:99:MET:CE	1:B:201[B]:VAL:HG22	2.46	0.45
1:G:42:GLU:O	1:G:45:ARG:N	2.48	0.45
1:E:217:LEU:HD12	1:E:250:SER:HA	1.99	0.45
1:H:215:ALA:O	1:H:218[A]:LYS:HD3	2.16	0.44
1:G:1[A]:MET:CE	1:G:236:ASP:H	2.30	0.44
1:B:133:LYS:HD2	1:B:178:LEU:HD22	1.98	0.44
1:E:41:LYS:HD2	1:E:43:ARG:NH2	2.32	0.44
1:G:0:ALA:HB2	5:G:1358:EDO:H22	2.00	0.44
1:G:133:LYS:HD2	1:G:178:LEU:HD22	2.00	0.44
1:F:155:GLN:O	1:F:156:ASN:HB2	2.18	0.44
1:B:101:ASP:OD2	1:B:113:GLY:HA3	2.17	0.44
1:C:22:PHE:O	1:C:26:LYS:HG3	2.18	0.43
1:E:201[B]:VAL:HG13	1:E:201[B]:VAL:O	2.18	0.43
1:A:253:HIS:CD2	7:A:2131:HOH:O	2.65	0.43
1:B:10:VAL:HG22	1:B:36:VAL:HB	2.01	0.43
1:F:215:ALA:O	1:F:218:LYS:HD2	2.18	0.43
1:F:41:LYS:HG2	1:F:44:SER:OG	2.18	0.43
1:D:191:GLY:HA3	7:D:2082:HOH:O	2.18	0.43
1:E:103[B]:ARG:CZ	1:E:202[B]:GLY:HA2	2.48	0.43
1:H:7:LYS:HD3	1:H:7:LYS:HA	1.75	0.43
1:C:217:LEU:HD12	1:C:250:SER:HA	2.00	0.43
1:D:137:PRO:HB2	1:D:138:GLU:OE1	2.19	0.43
1:G:40:ARG:HB3	3:G:1259:NDP:O2X	2.19	0.42
1:E:38:THR:HA	1:E:63:TYR:O	2.20	0.42
1:D:210:GLU:OE2	1:D:214:ARG:NH1	2.45	0.42
1:C:1:MET:CE	1:C:237:LEU:HD21	2.43	0.42
1:E:207[B]:ILE:HD12	1:E:211:ILE:HD11	2.02	0.42
1:C:39:TYR:HA	7:C:2015:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1:MET:N	7:E:2002:HOH:O	2.29	0.41
1:G:206:THR:H	5:G:1257:EDO:H11	1.85	0.41
1:A:204:PHE:O	1:A:207:ILE:HG22	2.20	0.41
1:E:209[A]:LYS:O	1:E:213:GLU:HG3	2.20	0.41
1:E:196:LEU:HD13	1:E:199[B]:LYS:HZ3	1.85	0.41
1:H:197:SER:HB3	3:H:1258:NDP:O1A	2.21	0.41
1:A:153:ALA:HA	1:B:173:TYR:CZ	2.56	0.41
1:C:133:LYS:HE2	1:C:181:ASP:OD2	2.20	0.41
1:A:48:LEU:HD11	1:A:52:LEU:HD11	2.02	0.41
1:A:49:GLU:HG2	1:A:62:LEU:HD11	2.03	0.41
1:A:80:ILE:O	1:A:84:VAL:HG22	2.21	0.41
1:C:212:GLU:O	1:C:218[B]:LYS:HD2	2.19	0.41
1:G:253:HIS:CD2	7:G:2016:HOH:O	2.70	0.41
1:H:217:LEU:HB2	1:H:250:SER:HB3	2.02	0.41
1:C:14:ILE:HD12	1:C:37:PHE:CD1	2.56	0.41
1:C:40:ARG:HD3	3:C:1258:NDP:C5A	2.51	0.41
1:D:194:ARG:NH1	1:D:208:LEU:HD13	2.36	0.41
1:E:99:MET:HE1	1:E:201[B]:VAL:HB	2.03	0.41
1:B:256:LYS:HE3	1:D:148:LEU:HD21	2.02	0.40
1:E:39:TYR:OH	1:E:42:GLU:OE2	2.28	0.40
1:B:18:ARG:O	1:B:195:THR:HG22	2.21	0.40
1:E:192:PRO:HG3	1:E:207[B]:ILE:HG23	2.03	0.40
1:E:204[A]:PHE:HA	1:E:207[A]:ILE:HG22	2.03	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:B:209[B]:LYS:NZ	1:C:112[B]:GLU:OE1[3_555]	1.91	0.29
1:B:209[B]:LYS:NZ	1:C:112[B]:GLU:OE2[3_555]	1.92	0.28
1:B:209[B]:LYS:NZ	1:C:112[B]:GLU:CD[3_555]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	267/282 (95%)	256 (96%)	10 (4%)	1 (0%)	43	30
1	B	267/282 (95%)	259 (97%)	8 (3%)	0	100	100
1	C	263/282 (93%)	257 (98%)	6 (2%)	0	100	100
1	D	260/282 (92%)	248 (95%)	11 (4%)	1 (0%)	43	30
1	E	267/282 (95%)	250 (94%)	17 (6%)	0	100	100
1	F	262/282 (93%)	253 (97%)	9 (3%)	0	100	100
1	G	260/282 (92%)	250 (96%)	8 (3%)	2 (1%)	27	12
1	H	264/282 (94%)	252 (96%)	11 (4%)	1 (0%)	43	30
All	All	2110/2256 (94%)	2025 (96%)	80 (4%)	5 (0%)	56	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1[A]	MET
1	G	1[B]	MET
1	H	42	GLU
1	D	58	PRO
1	A	-2	GLN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/234 (94%)	218 (99%)	2 (1%)	87	86
1	B	220/234 (94%)	214 (97%)	6 (3%)	57	45
1	C	218/234 (93%)	212 (97%)	6 (3%)	56	43
1	D	216/234 (92%)	209 (97%)	7 (3%)	51	37
1	E	220/234 (94%)	213 (97%)	7 (3%)	51	37
1	F	216/234 (92%)	212 (98%)	4 (2%)	69	62
1	G	214/234 (92%)	204 (95%)	10 (5%)	36	18
1	H	218/234 (93%)	211 (97%)	7 (3%)	51	37
All	All	1742/1872 (93%)	1693 (97%)	49 (3%)	59	43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	209	LYS
1	B	1	MET
1	B	4	LEU
1	B	55	LEU
1	B	196	LEU
1	B	206[A]	THR
1	B	206[B]	THR
1	C	44	SER
1	C	84	VAL
1	C	133	LYS
1	C	196	LEU
1	C	256[A]	LYS
1	C	256[B]	LYS
1	D	1	MET
1	D	41	LYS
1	D	48	LEU
1	D	52	LEU
1	D	103[A]	ARG
1	D	103[B]	ARG
1	D	155	GLN
1	E	30	GLN
1	E	44	SER
1	E	64	GLN
1	E	99	MET
1	E	207[A]	ILE
1	E	207[B]	ILE
1	E	255	ILE
1	F	52	LEU
1	F	55	LEU
1	F	98	ASN
1	F	103	ARG
1	G	1[A]	MET
1	G	1[B]	MET
1	G	44	SER
1	G	46	LYS
1	G	48	LEU
1	G	50	LYS
1	G	52	LEU
1	G	192	PRO
1	G	199	LYS
1	G	207	ILE

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Mol	Chain	Res	Type
1	H	4	LEU
1	H	7	LYS
1	H	41	LYS
1	H	43	ARG
1	H	52	LEU
1	H	127	ILE
1	H	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	98	ASN
1	A	156	ASN
1	A	253	HIS
1	B	30	GLN
1	B	86	ASN
1	C	30	GLN
1	C	64	GLN
1	C	155	GLN
1	C	253	HIS
1	D	56	ASN
1	D	253	HIS
1	E	98	ASN
1	F	-2	GLN
1	F	56	ASN
1	F	98	ASN
1	F	156	ASN
1	F	253	HIS
1	G	56	ASN
1	G	155	GLN
1	G	156	ASN
1	G	253	HIS
1	H	3	ASN
1	H	118	GLN
1	H	253	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	1257	-	4,4,4	0.03	0	6,6,6	0.13	0
2	SO4	A	1259	-	4,4,4	0.21	0	6,6,6	0.47	0
3	NDP	A	1260	-	52,52,52	0.78	1 (1%)	80,80,80	1.20	6 (7%)
4	PT6	A	1261	-	26,26,26	1.65	4 (15%)	33,35,35	0.96	1 (3%)
5	EDO	A	1270	-	3,3,3	0.43	0	2,2,2	0.85	0
2	SO4	B	1257	-	4,4,4	0.21	0	6,6,6	0.25	0
5	EDO	B	1258	-	3,3,3	0.51	0	2,2,2	0.45	0
3	NDP	B	1259	-	52,52,52	0.79	2 (3%)	80,80,80	1.29	7 (8%)
4	PT6	B	1260	-	26,26,26	1.32	2 (7%)	33,35,35	0.77	0
3	NDP	C	1258	-	52,52,52	0.78	2 (3%)	80,80,80	1.33	11 (13%)
4	PT6	C	1259	-	26,26,26	1.30	2 (7%)	33,35,35	0.87	1 (3%)
5	EDO	C	1270	-	3,3,3	0.57	0	2,2,2	0.44	0
3	NDP	D	1257	-	52,52,52	0.70	1 (1%)	80,80,80	1.28	8 (10%)
4	PT6	D	1258	-	26,26,26	1.33	2 (7%)	33,35,35	1.01	1 (3%)
2	SO4	E	1257	-	4,4,4	0.19	0	6,6,6	0.16	0
3	NDP	E	1259	-	52,52,52	0.71	1 (1%)	80,80,80	1.24	11 (13%)
4	PT6	E	1260	-	26,26,26	1.63	3 (11%)	33,35,35	0.93	1 (3%)
5	EDO	E	1261	-	3,3,3	0.50	0	2,2,2	0.80	0
3	NDP	F	1258	-	52,52,52	0.84	2 (3%)	80,80,80	1.29	8 (10%)
4	PT6	F	1259	-	26,26,26	1.38	2 (7%)	33,35,35	1.02	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	G	1257	-	3,3,3	0.51	0	2,2,2	0.83	0
3	NDP	G	1259	-	52,52,52	0.80	3 (5%)	80,80,80	1.46	11 (13%)
4	PT6	G	1260	-	26,26,26	1.51	3 (11%)	33,35,35	0.74	0
5	EDO	G	1358	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	H	1257	-	3,3,3	0.56	0	2,2,2	0.49	0
3	NDP	H	1258	-	52,52,52	0.69	1 (1%)	80,80,80	1.41	12 (15%)
4	PT6	H	1259	-	26,26,26	1.33	2 (7%)	33,35,35	0.80	1 (3%)
2	SO4	H	1358	-	4,4,4	0.14	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1257	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1259	-	-	0/0/0/0	0/0/0/0
3	NDP	A	1260	-	-	0/35/77/77	0/5/5/5
4	PT6	A	1261	-	-	0/10/10/10	0/3/3/3
5	EDO	A	1270	-	-	0/1/1/1	0/0/0/0
2	SO4	B	1257	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1258	-	-	0/1/1/1	0/0/0/0
3	NDP	B	1259	-	-	0/35/77/77	0/5/5/5
4	PT6	B	1260	-	-	0/10/10/10	0/3/3/3
3	NDP	C	1258	-	-	0/35/77/77	0/5/5/5
4	PT6	C	1259	-	-	0/10/10/10	0/3/3/3
5	EDO	C	1270	-	-	0/1/1/1	0/0/0/0
3	NDP	D	1257	-	-	0/35/77/77	0/5/5/5
4	PT6	D	1258	-	-	0/10/10/10	0/3/3/3
2	SO4	E	1257	-	-	0/0/0/0	0/0/0/0
3	NDP	E	1259	-	-	0/35/77/77	0/5/5/5
4	PT6	E	1260	-	-	0/10/10/10	0/3/3/3
5	EDO	E	1261	-	-	0/1/1/1	0/0/0/0
3	NDP	F	1258	-	-	0/35/77/77	0/5/5/5
4	PT6	F	1259	-	-	0/10/10/10	0/3/3/3
5	EDO	G	1257	-	-	0/1/1/1	0/0/0/0
3	NDP	G	1259	-	-	0/35/77/77	0/5/5/5
4	PT6	G	1260	-	-	0/10/10/10	0/3/3/3
5	EDO	G	1358	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1257	-	-	0/1/1/1	0/0/0/0
3	NDP	H	1258	-	-	0/35/77/77	0/5/5/5
4	PT6	H	1259	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	H	1358	-	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1260	PT6	C17-C18	5.94	1.44	1.37
4	G	1260	PT6	C17-C18	5.91	1.44	1.37
4	A	1261	PT6	C17-C18	5.90	1.44	1.37
4	D	1258	PT6	C17-C18	5.14	1.43	1.37
4	C	1259	PT6	C17-C18	4.87	1.42	1.37
4	H	1259	PT6	C17-C18	4.85	1.42	1.37
4	F	1259	PT6	C17-C18	4.76	1.42	1.37
4	B	1260	PT6	C17-C18	4.56	1.42	1.37
4	B	1260	PT6	C9-C10	3.49	1.45	1.38
3	A	1260	NDP	C2N-N1N	3.42	1.43	1.37
4	A	1261	PT6	C12-C13	3.33	1.52	1.51
3	F	1258	NDP	C7N-C3N	3.25	1.54	1.48
4	E	1260	PT6	C12-C13	3.22	1.52	1.51
4	H	1259	PT6	C9-C10	3.09	1.45	1.38
4	F	1259	PT6	C12-C13	3.07	1.52	1.51
4	C	1259	PT6	C9-C10	3.05	1.44	1.38
3	F	1258	NDP	C2N-N1N	2.89	1.42	1.37
3	B	1259	NDP	C2N-N1N	2.89	1.42	1.37
4	A	1261	PT6	C9-C10	2.83	1.44	1.38
4	E	1260	PT6	C9-C10	2.76	1.44	1.38
3	D	1257	NDP	C6N-N1N	2.73	1.45	1.37
3	B	1259	NDP	PN-O3	2.71	1.64	1.59
3	C	1258	NDP	C2N-N1N	2.68	1.42	1.37
3	G	1259	NDP	C6N-N1N	2.64	1.45	1.37
3	G	1259	NDP	C2N-N1N	2.61	1.42	1.37
4	G	1260	PT6	C12-C13	2.51	1.52	1.51
3	E	1259	NDP	C2N-N1N	2.48	1.41	1.37
3	C	1258	NDP	C7N-C3N	2.40	1.52	1.48
4	A	1261	PT6	C2-C1	2.39	1.47	1.39
4	D	1258	PT6	C9-C10	2.27	1.43	1.38
3	H	1258	NDP	PN-O3	2.25	1.63	1.59
4	G	1260	PT6	C9-C10	2.23	1.43	1.38
3	G	1259	NDP	PN-O3	2.18	1.63	1.59

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1258	NDP	O2X-P2B-O2B	-5.16	92.22	107.09
3	B	1259	NDP	O3-PN-O5D	4.79	115.61	102.91
3	G	1259	NDP	O3-PN-O5D	4.77	115.55	102.91
3	H	1258	NDP	O3-PN-O5D	4.72	115.42	102.91
3	G	1259	NDP	O3-PA-O5B	4.63	115.18	102.91
3	D	1257	NDP	O3-PA-O5B	4.54	114.94	102.91
3	F	1258	NDP	O2X-P2B-O2B	-4.36	94.54	107.09
3	D	1257	NDP	O3-PN-O5D	4.09	113.75	102.91
3	G	1259	NDP	C4B-O4B-C1B	-4.00	105.32	109.72
3	A	1260	NDP	O3-PN-O5D	3.94	113.36	102.91
3	F	1258	NDP	C4B-O4B-C1B	-3.85	105.49	109.72
3	C	1258	NDP	O3-PA-O5B	3.71	112.75	102.91
3	C	1258	NDP	O2X-P2B-O2B	-3.58	96.78	107.09
3	B	1259	NDP	C4B-O4B-C1B	-3.55	105.82	109.72
3	C	1258	NDP	O3-PA-O1A	-3.39	87.19	110.43
3	E	1259	NDP	O7N-C7N-C3N	-3.39	113.99	120.96
3	H	1258	NDP	C4B-O4B-C1B	-3.30	106.09	109.72
3	C	1258	NDP	C4B-O4B-C1B	-3.30	106.09	109.72
3	G	1259	NDP	O2X-P2B-O2B	-3.20	97.89	107.09
3	E	1259	NDP	O2X-P2B-O2B	-3.18	97.93	107.09
3	B	1259	NDP	O3-PA-O5B	3.06	111.03	102.91
3	A	1260	NDP	O3-PA-O5B	3.01	110.88	102.91
3	H	1258	NDP	O2B-P2B-O1X	2.94	115.25	106.80
3	F	1258	NDP	O3-PN-O5D	2.94	110.69	102.91
3	E	1259	NDP	C4B-O4B-C1B	-2.93	106.49	109.72
4	E	1260	PT6	C7-N1-C18	2.92	119.74	117.30
3	F	1258	NDP	O3-PA-O5B	2.91	110.61	102.91
3	D	1257	NDP	O7N-C7N-C3N	-2.89	115.01	120.96
3	E	1259	NDP	O3-PN-O5D	2.89	110.57	102.91
3	G	1259	NDP	O2A-PA-O1A	2.86	127.95	112.14
3	D	1257	NDP	C4B-O4B-C1B	-2.80	106.64	109.72
3	G	1259	NDP	C3N-C2N-N1N	-2.77	119.21	123.17
3	H	1258	NDP	O7N-C7N-C3N	-2.75	115.31	120.96
3	G	1259	NDP	O7N-C7N-C3N	-2.74	115.32	120.96
3	F	1258	NDP	O4B-C1B-C2B	-2.72	101.64	106.60
3	A	1260	NDP	C4B-O4B-C1B	-2.71	106.74	109.72
3	G	1259	NDP	O4B-C1B-C2B	-2.70	101.68	106.60
3	E	1259	NDP	O4B-C1B-C2B	-2.67	101.73	106.60
3	E	1259	NDP	O2X-P2B-O1X	2.66	119.07	110.36
3	D	1257	NDP	C2D-C1D-N1N	2.66	120.50	113.29
3	E	1259	NDP	O3-PA-O5B	2.64	109.92	102.91
3	F	1258	NDP	O2B-P2B-O1X	2.57	114.17	106.80
3	B	1259	NDP	O7N-C7N-C3N	-2.51	115.79	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1258	NDP	O2A-PA-O1A	2.48	125.88	112.14
3	H	1258	NDP	O4B-C1B-C2B	-2.43	102.16	106.60
3	H	1258	NDP	O3-PA-O1A	-2.39	94.05	110.43
3	C	1258	NDP	O2X-P2B-O1X	2.39	118.19	110.36
3	A	1260	NDP	O4B-C1B-C2B	-2.39	102.25	106.60
3	D	1257	NDP	O3-PA-O1A	-2.36	94.29	110.43
3	H	1258	NDP	O3-PA-O5B	2.35	109.14	102.91
3	H	1258	NDP	O2N-PN-O3	-2.34	94.01	105.14
3	B	1259	NDP	P2B-O2B-C2B	2.33	127.16	121.77
3	E	1259	NDP	O2A-PA-O1A	2.32	124.98	112.14
3	F	1258	NDP	O2X-P2B-O1X	2.31	117.93	110.36
3	C	1258	NDP	O7N-C7N-C3N	-2.31	116.22	120.96
4	F	1259	PT6	C16-S-C13	2.30	93.21	91.94
3	G	1259	NDP	O2N-PN-O1N	2.27	124.71	112.14
3	H	1258	NDP	C3N-C2N-N1N	-2.25	119.96	123.17
3	A	1260	NDP	O2X-P2B-O1X	2.24	117.70	110.36
4	C	1259	PT6	C11-C12-C13	-2.22	108.54	113.01
3	D	1257	NDP	O2N-PN-O3	-2.19	94.74	105.14
4	F	1259	PT6	C7-N1-C18	2.19	119.13	117.30
3	E	1259	NDP	C3N-C7N-N7N	2.17	122.26	117.79
3	H	1258	NDP	O2N-PN-O1N	2.17	124.16	112.14
3	F	1258	NDP	C3B-C2B-C1B	-2.16	98.54	102.70
4	A	1261	PT6	C7-N1-C18	2.15	119.10	117.30
3	C	1258	NDP	O2N-PN-O1N	2.12	123.89	112.14
3	C	1258	NDP	PN-O3-PA	2.12	137.80	131.93
4	H	1259	PT6	O-C11-C12	-2.11	104.58	109.94
3	A	1260	NDP	O2X-P2B-O2B	-2.11	101.02	107.09
3	C	1258	NDP	C3N-C7N-N7N	2.09	122.09	117.79
3	E	1259	NDP	O3-PA-O1A	-2.08	96.21	110.43
3	H	1258	NDP	O2X-P2B-O1X	2.04	117.04	110.36
3	G	1259	NDP	C2D-C1D-N1N	2.04	118.82	113.29
3	B	1259	NDP	C3N-C7N-N7N	2.04	121.98	117.79
3	C	1258	NDP	O4B-C1B-N9A	2.03	112.52	108.10
3	B	1259	NDP	O4B-C1B-C2B	-2.03	102.90	106.60
3	E	1259	NDP	O2N-PN-O1N	2.03	123.35	112.14
3	D	1257	NDP	C3N-C7N-N7N	2.02	121.95	117.79
3	G	1259	NDP	P2B-O2B-C2B	2.01	126.41	121.77
4	D	1258	PT6	C1-C2-N	2.01	122.86	120.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	262/282 (92%)	-0.08	1 (0%) 90 94	13, 25, 50, 62	0
1	B	256/282 (90%)	0.01	2 (0%) 83 89	14, 25, 46, 57	0
1	C	262/282 (92%)	0.08	3 (1%) 77 85	13, 27, 50, 62	0
1	D	256/282 (90%)	-0.05	5 (1%) 62 70	14, 26, 52, 67	0
1	E	256/282 (90%)	0.04	5 (1%) 62 70	13, 25, 51, 64	0
1	F	262/282 (92%)	-0.00	1 (0%) 90 94	13, 26, 49, 59	0
1	G	257/282 (91%)	0.14	5 (1%) 64 72	17, 29, 56, 79	0
1	H	263/282 (93%)	0.10	2 (0%) 83 89	16, 29, 57, 78	0
All	All	2074/2256 (91%)	0.03	24 (1%) 75 83	13, 27, 52, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103[A]	ARG	3.7
1	C	-5	LEU	3.5
1	G	44	SER	3.3
1	H	46	LYS	3.2
1	E	104	GLY	3.2
1	D	52	LEU	3.0
1	C	46	LYS	3.0
1	B	58	PRO	2.8
1	G	48	LEU	2.8
1	E	206[A]	THR	2.7
1	C	103	ARG	2.6
1	E	6	ASN	2.6
1	A	46	LYS	2.6
1	G	43	ARG	2.5
1	G	6	ASN	2.5
1	B	202[A]	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	104	GLY	2.3
1	H	52	LEU	2.3
1	G	52	LEU	2.2
1	E	196	LEU	2.2
1	D	103[A]	ARG	2.1
1	F	52	LEU	2.1
1	D	196[A]	LEU	2.0
1	D	6	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	H	1257	4/4	0.15	5.86	40,42,44,45	0
5	EDO	G	1358	4/4	0.18	2.03	45,47,51,56	0
5	EDO	B	1258	4/4	0.15	1.89	43,45,51,52	0
5	EDO	C	1270	4/4	0.12	1.25	36,37,39,40	0
5	EDO	A	1270	4/4	0.15	1.01	49,49,51,53	0
4	PT6	F	1259	24/24	0.10	0.79	17,22,26,29	0
2	SO4	A	1257	5/5	0.12	0.20	47,50,53,54	0
4	PT6	A	1261	24/24	0.10	-0.05	23,26,29,30	0
5	EDO	G	1257	4/4	0.14	-0.07	43,44,45,46	0
4	PT6	H	1259	24/24	0.10	-0.27	23,28,31,33	0
3	NDP	H	1258	48/48	0.10	-0.29	22,31,46,54	0
2	SO4	A	1259	5/5	0.12	-0.39	51,51,54,54	0
3	NDP	D	1257	48/48	0.09	-0.40	17,26,41,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NDP	F	1258	48/48	0.09	-0.43	19,27,44,50	0
3	NDP	B	1259	48/48	0.09	-0.44	17,26,38,40	0
4	PT6	D	1258	24/24	0.09	-0.47	19,25,29,32	0
4	PT6	G	1260	24/24	0.10	-0.49	21,28,34,35	0
3	NDP	G	1259	48/48	0.09	-0.49	20,28,47,56	0
3	NDP	C	1258	48/48	0.09	-0.50	21,27,42,47	0
3	NDP	A	1260	48/48	0.08	-0.57	20,27,43,48	0
5	EDO	E	1261	4/4	0.20	-0.66	61,62,64,64	0
3	NDP	E	1259	48/48	0.08	-0.73	18,25,43,44	0
4	PT6	E	1260	24/24	0.09	-0.75	20,24,27,30	0
4	PT6	C	1259	24/24	0.09	-0.92	21,29,31,32	0
2	SO4	H	1358	5/5	0.11	-0.94	52,52,55,57	0
4	PT6	B	1260	24/24	0.08	-0.98	18,23,27,31	0
2	SO4	E	1257	5/5	0.08	-1.75	45,45,45,46	5
6	CL	F	1357	1/1	0.04	-2.64	60,60,60,60	0
2	SO4	B	1257	5/5	0.09	-3.13	33,34,36,36	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.