Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:38 PM GMT

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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

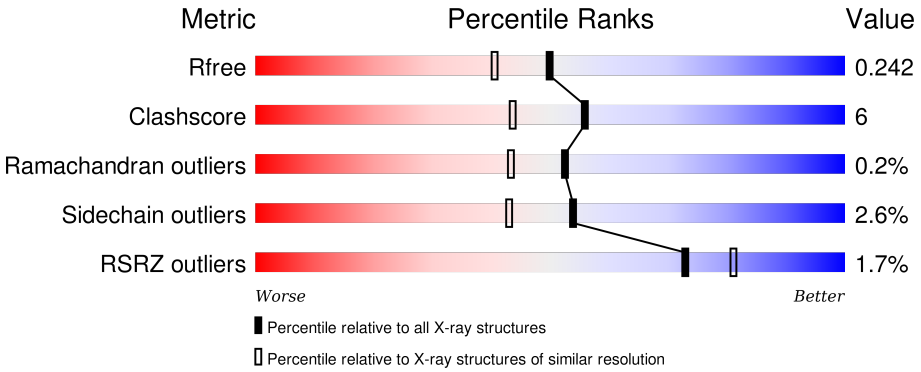
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 >=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 <=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	82% 11% 7%
1	B	282	% 80% 10% • 9%
1	C	282	% 79% 12% • 7%
1	D	282	% 80% 10% • 9%
1	E	282	2% 79% 11% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	282	85% 7% 7%
1	G	282	4% 75% 15% • 9%
1	H	282	% 80% 11% • 7%

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
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 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 [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

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...

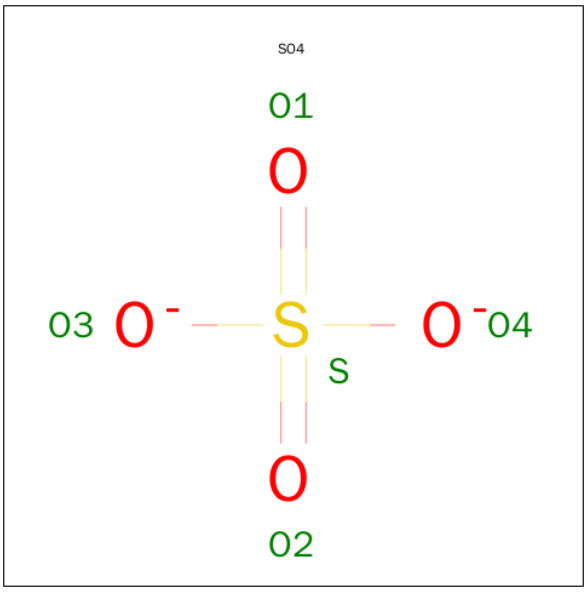
Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
F	-16	MET	-	EXPRESSION TAG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

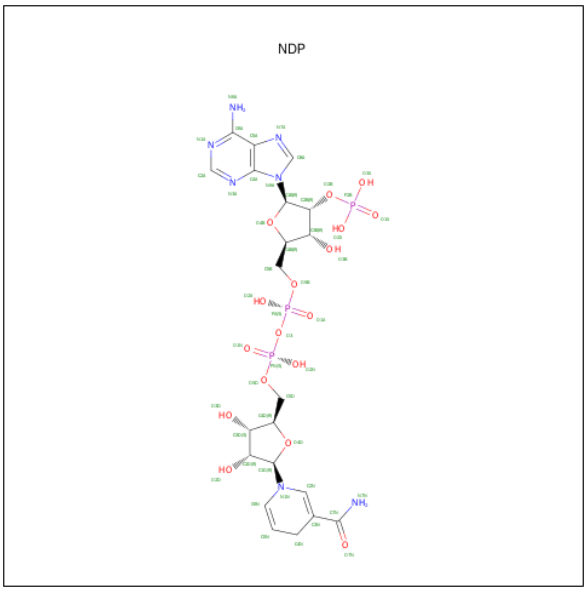
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
G	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
G	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
G	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
G	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
G	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



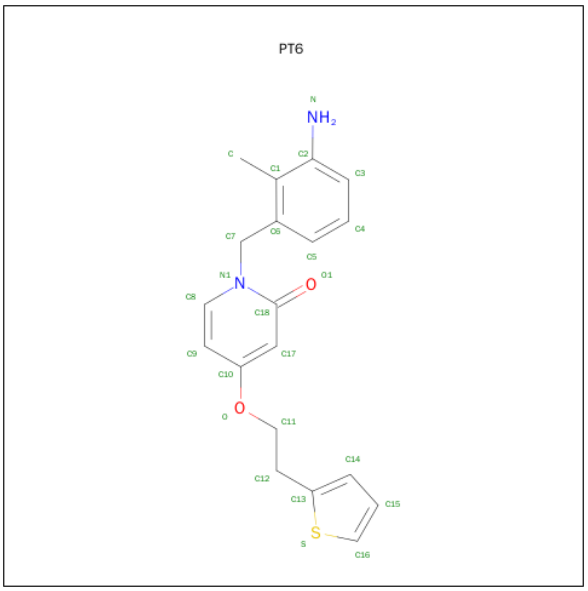
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

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



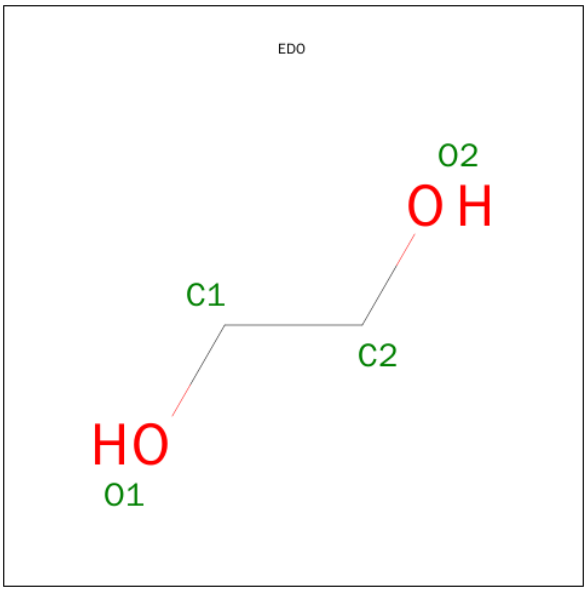
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	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: $C_{19}H_{20}N_2O_2S$).



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: $C_2H_6O_2$).



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

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

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

- Molecule 7 is water.

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

Continued on next page...

Continued from previous page...

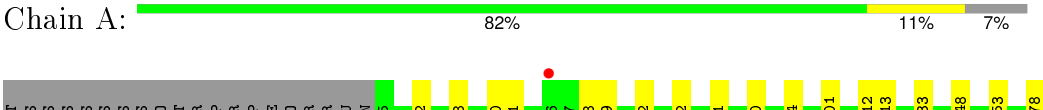
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	110	Total O 110 110	0	0
7	C	106	Total O 106 106	0	0
7	D	87	Total O 87 87	0	0
7	E	138	Total O 138 138	0	0
7	F	112	Total O 112 112	0	0
7	G	82	Total O 82 82	0	0
7	H	80	Total O 80 80	0	0

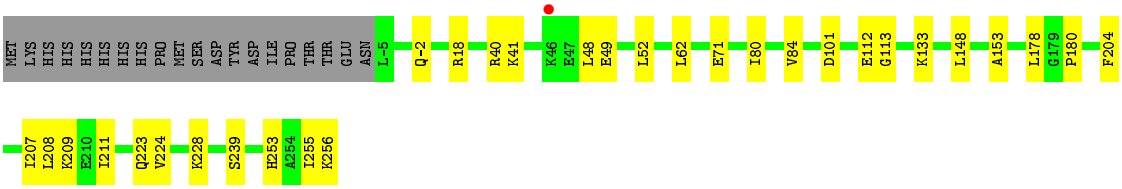
3 Residue-property plots (i)

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

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

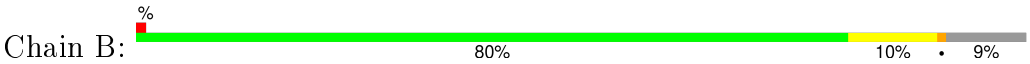
Chain A:

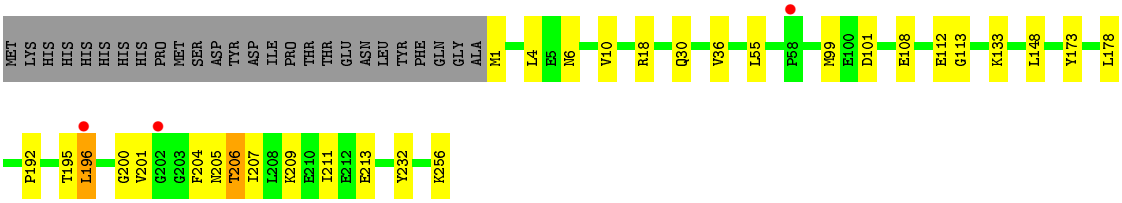




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

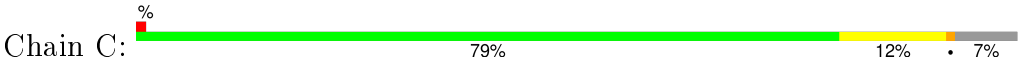
Chain B:

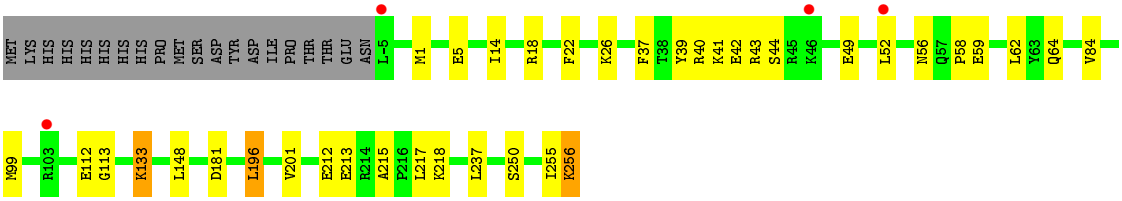




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

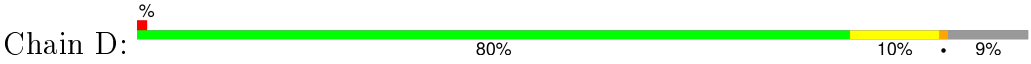
Chain C:

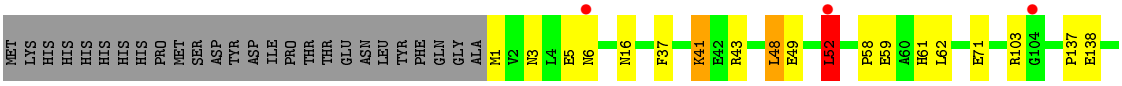


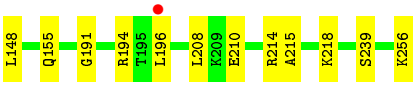


• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain D:

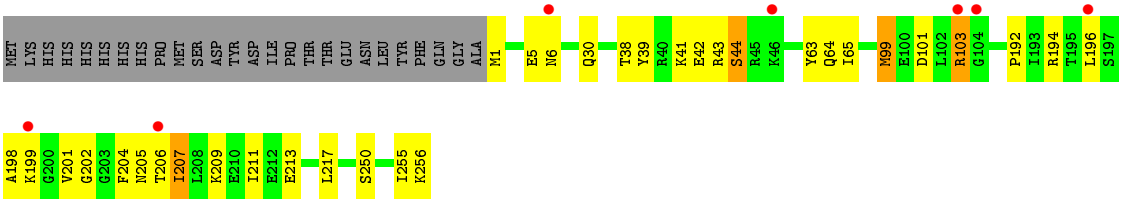






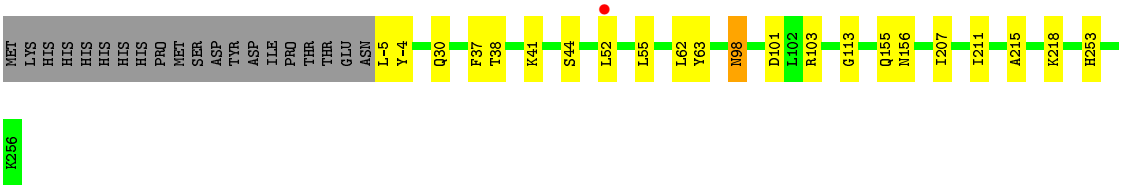
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain E:



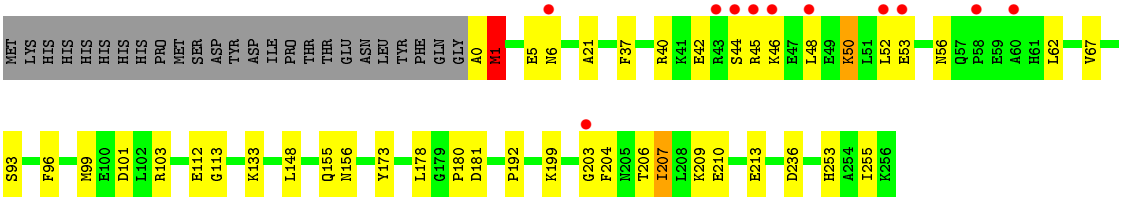
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain F:



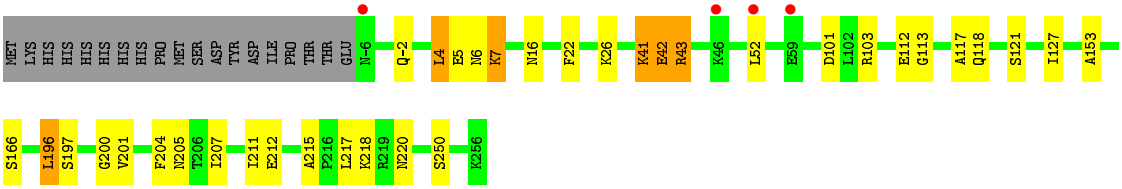
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.231 0.182 , 0.242	Depositor DCC
R_{free} test set	7320 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	2060	0	2078	26	0
1	B	2057	0	2079	29	0
1	C	2047	0	2071	34	0
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	20	0	0
4	B	24	0	20	0	0
4	C	24	0	20	0	0
4	D	24	0	20	0	0
4	E	24	0	20	0	0
4	F	24	0	20	0	0
4	G	24	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	24	0	20	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	16922	211	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 6.

All (211) 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: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:H:205:ASN:O	7:H:2068:HOH:O	2.01	0.77
1:G:0:ALA:O	1:G:1[A]:MET:HB3	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204[A]:PHE:O	1:E:207[A]:ILE:HG23	1.86	0.75
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:201[B]:VAL:HG13	1:E:204[B]:PHE:HB2	1.86	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: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:D:48:LEU:O	1:D:52:LEU:HD12	2.05	0.57
1:A:256:LYS:HD2	1:C:256[B]:LYS:HE3	1.86	0.57
1:E:205[B]:ASN:O	1:E:206[B]:THR:C	2.41	0.57
1:C:41:LYS:HD2	1:C:43:ARG:NH2	2.19	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:D:16:ASN:HD22	1:D:196[B]:LEU:HD22	1.72	0.55
1:A:112[A]:GLU:HG2	7:A:2067:HOH:O	2.07	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:H	1:D:71:GLU:CD	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:G:0:ALA:O	1:G:1[B]:MET:CB	2.54	0.53
1:F:218:LYS:HD3	1:G:180:PRO:HG3	1.90	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:H:118:GLN:HE22	1:H:166:SER:CB	2.21	0.53
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.09	0.53
1:A:239[B]:SER:O	7:A:2124:HOH:O	2.19	0.53
1:A:207:ILE:O	1:A:211:ILE:HG12	2.08	0.53
1:B:112[A]:GLU:CD	1:B:112[A]:GLU:H	2.12	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:5:GLU:O	1:H:6:ASN:CB	2.61	0.47
1:E:41:LYS:O	1:E:44:SER:HB2	2.14	0.47
1:A:18[A]:ARG:CZ	1:A:223:GLN:HE22	2.27	0.47
1:F:41:LYS:HE2	1:F:44:SER:OG	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:203:GLY:O	1:G:207:ILE:HB	2.14	0.46
1:E:196:LEU:HB3	7:E:2010:HOH:O	2.14	0.46
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:E:196:LEU:HD13	1:E:199[B]:LYS:NZ	2.31	0.46
1:H:-2:GLN:CD	1:H:-2:GLN:H	2.19	0.46
1:C:99:MET:HE1	1:C:201:VAL:HA	1.98	0.46
1:F:38:THR:HA	1:F:63:TYR:O	2.15	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:E:41:LYS:HD2	1:E:43:ARG:NH2	2.32	0.44
1:B:133:LYS:HD2	1:B:178:LEU:HD22	1.98	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:E:201[B]:VAL:HG13	1:E:201[B]:VAL:O	2.18	0.43
1:C:22:PHE:O	1:C:26:LYS:HG3	2.18	0.43
1:A:253:HIS:CD2	7:A:2131:HOH:O	2.65	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:B:10:VAL:HG22	1:B:36:VAL:HB	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:207[B]:ILE:HD12	1:E:211:ILE:HD11	2.02	0.42
1:C:1:MET:CE	1:C:237:LEU:HD21	2.43	0.42
1:C:39:TYR:HA	7:C:2015:HOH:O	2.20	0.42
1:G:206:THR:H	5:G:1257:EDO:H11	1.85	0.41
1:E:1:MET:N	7:E:2002:HOH:O	2.29	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:H:197:SER:HB3	3:H:1258:NDP:O1A	2.21	0.41
1:E:196:LEU:HD13	1:E:199[B]:LYS:HZ3	1.85	0.41
1:C:133:LYS:HE2	1:C:181:ASP:OD2	2.20	0.41
1:A:153:ALA:HA	1:B:173:TYR:CZ	2.56	0.41
1:C:212:GLU:O	1:C:218[B]:LYS:HD2	2.19	0.41
1:A:80:ILE:O	1:A:84:VAL:HG22	2.21	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:G:253:HIS:CD2	7:G:2016:HOH:O	2.70	0.41
1:C:14:ILE:HD12	1:C:37:PHE:CD1	2.56	0.41
1:H:217:LEU:HB2	1:H:250:SER:HB3	2.02	0.41
1:E:99:MET:HE1	1:E:201[B]:VAL:HB	2.03	0.41
1:D:194:ARG:NH1	1:D:208:LEU:HD13	2.36	0.41
1:C:40:ARG:HD3	3:C:1258:NDP:C5A	2.51	0.41
1:E:39:TYR:OH	1:E:42:GLU:OE2	2.28	0.40
1:B:256:LYS:HE3	1:D:148:LEU:HD21	2.02	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

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	267/282 (95%)	256 (96%)	10 (4%)	1 (0%)	39	27
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%)	39	27
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%)	24	11
1	H	264/282 (94%)	252 (96%)	11 (4%)	1 (0%)	39	27
All	All	2110/2256 (94%)	2025 (96%)	80 (4%)	5 (0%)	52	43

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 (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	220/234 (94%)	218 (99%)	2 (1%)	84	83
1	B	220/234 (94%)	214 (97%)	6 (3%)	52	41
1	C	218/234 (93%)	212 (97%)	6 (3%)	51	39
1	D	216/234 (92%)	209 (97%)	7 (3%)	46	33
1	E	220/234 (94%)	213 (97%)	7 (3%)	46	33
1	F	216/234 (92%)	212 (98%)	4 (2%)	65	58
1	G	214/234 (92%)	204 (95%)	10 (5%)	32	16
1	H	218/234 (93%)	211 (97%)	7 (3%)	46	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1742/1872 (93%)	1693 (97%)	49 (3%)	54 39

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	50	LYS
1	G	52	LEU
1	G	192	PRO
1	G	199	LYS
1	G	207	ILE
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	42,52,52	0.56	0	55,80,80	1.24	5 (9%)
4	PT6	A	1261	-	22,26,26	0.96	1 (4%)	26,35,35	0.89	0
5	EDO	A	1270	-	3,3,3	0.40	0	2,2,2	0.86	0
2	SO4	B	1257	-	4,4,4	0.22	0	6,6,6	0.26	0
5	EDO	B	1258	-	3,3,3	0.48	0	2,2,2	0.47	0
3	NDP	B	1259	-	42,52,52	0.59	0	55,80,80	1.35	6 (10%)
4	PT6	B	1260	-	22,26,26	1.03	1 (4%)	26,35,35	0.78	0
3	NDP	C	1258	-	42,52,52	0.61	0	55,80,80	1.29	7 (12%)
4	PT6	C	1259	-	22,26,26	0.94	1 (4%)	26,35,35	0.79	0
5	EDO	C	1270	-	3,3,3	0.53	0	2,2,2	0.46	0
3	NDP	D	1257	-	42,52,52	0.70	1 (2%)	55,80,80	1.33	6 (10%)
4	PT6	D	1258	-	22,26,26	0.82	1 (4%)	26,35,35	0.86	0
2	SO4	E	1257	-	4,4,4	0.19	0	6,6,6	0.17	0
3	NDP	E	1259	-	42,52,52	0.62	0	55,80,80	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PT6	E	1260	-	22,26,26	0.96	1 (4%)	26,35,35	0.73	0
5	EDO	E	1261	-	3,3,3	0.46	0	2,2,2	0.82	0
3	NDP	F	1258	-	42,52,52	0.58	0	55,80,80	1.31	7 (12%)
4	PT6	F	1259	-	22,26,26	0.83	0	26,35,35	0.87	0
5	EDO	G	1257	-	3,3,3	0.47	0	2,2,2	0.85	0
3	NDP	G	1259	-	42,52,52	0.65	1 (2%)	55,80,80	1.55	9 (16%)
4	PT6	G	1260	-	22,26,26	0.91	1 (4%)	26,35,35	0.70	0
5	EDO	G	1358	-	3,3,3	0.47	0	2,2,2	0.48	0
5	EDO	H	1257	-	3,3,3	0.52	0	2,2,2	0.51	0
3	NDP	H	1258	-	42,52,52	0.55	0	55,80,80	1.40	9 (16%)
4	PT6	H	1259	-	22,26,26	0.94	1 (4%)	26,35,35	0.73	1 (3%)
2	SO4	H	1358	-	4,4,4	0.14	0	6,6,6	0.28	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	-	-	0/30/77/77	0/5/5/5
4	PT6	A	1261	-	-	0/9/10/10	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	-	-	0/30/77/77	0/5/5/5
4	PT6	B	1260	-	-	0/9/10/10	0/3/3/3
3	NDP	C	1258	-	-	0/30/77/77	0/5/5/5
4	PT6	C	1259	-	-	0/9/10/10	0/3/3/3
5	EDO	C	1270	-	-	0/1/1/1	0/0/0/0
3	NDP	D	1257	-	-	0/30/77/77	0/5/5/5
4	PT6	D	1258	-	-	0/9/10/10	0/3/3/3
2	SO4	E	1257	-	-	0/0/0/0	0/0/0/0
3	NDP	E	1259	-	-	0/30/77/77	0/5/5/5
4	PT6	E	1260	-	-	0/9/10/10	0/3/3/3
5	EDO	E	1261	-	-	0/1/1/1	0/0/0/0
3	NDP	F	1258	-	-	0/30/77/77	0/5/5/5
4	PT6	F	1259	-	-	0/9/10/10	0/3/3/3
5	EDO	G	1257	-	-	0/1/1/1	0/0/0/0
3	NDP	G	1259	-	-	0/30/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PT6	G	1260	-	-	0/9/10/10	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	-	-	0/30/77/77	0/5/5/5
4	PT6	H	1259	-	-	0/9/10/10	0/3/3/3
2	SO4	H	1358	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1260	PT6	C9-C10	2.25	1.43	1.38
4	D	1258	PT6	C9-C10	2.29	1.43	1.38
3	G	1259	NDP	C6N-N1N	2.71	1.45	1.37
4	E	1260	PT6	C9-C10	2.79	1.44	1.38
3	D	1257	NDP	C6N-N1N	2.82	1.45	1.37
4	A	1261	PT6	C9-C10	2.86	1.44	1.38
4	C	1259	PT6	C9-C10	3.09	1.44	1.38
4	H	1259	PT6	C9-C10	3.13	1.45	1.38
4	B	1260	PT6	C9-C10	3.53	1.45	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1259	NDP	C4B-O4B-C1B	-4.00	105.32	109.72
3	F	1258	NDP	C4B-O4B-C1B	-3.85	105.49	109.72
3	B	1259	NDP	C4B-O4B-C1B	-3.55	105.82	109.72
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	E	1259	NDP	C4B-O4B-C1B	-2.93	106.49	109.72
3	D	1257	NDP	C4B-O4B-C1B	-2.80	106.64	109.72
3	F	1258	NDP	O4B-C1B-C2B	-2.74	101.64	106.60
3	G	1259	NDP	C3N-C2N-N1N	-2.74	119.21	123.14
3	G	1259	NDP	O4B-C1B-C2B	-2.72	101.68	106.60
3	A	1260	NDP	C4B-O4B-C1B	-2.71	106.74	109.72
3	E	1259	NDP	O4B-C1B-C2B	-2.69	101.73	106.60
3	H	1258	NDP	O4B-C1B-C2B	-2.45	102.16	106.60
3	H	1258	NDP	O2N-PN-O3	-2.44	94.01	105.09
3	A	1260	NDP	O4B-C1B-C2B	-2.41	102.25	106.60
3	D	1257	NDP	O2N-PN-O3	-2.28	94.74	105.09
3	H	1258	NDP	C3N-C2N-N1N	-2.22	119.96	123.14
3	F	1258	NDP	C3B-C2B-C1B	-2.17	98.54	102.73
4	H	1259	PT6	O-C11-C12	-2.05	104.58	109.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1259	NDP	O4B-C1B-C2B	-2.05	102.90	106.60
3	C	1258	NDP	C1B-N9A-C4A	-2.03	123.88	126.94
3	B	1259	NDP	PN-O3-PA	-2.01	127.09	132.73
3	H	1258	NDP	O2X-P2B-O1X	2.01	117.04	110.58
3	G	1259	NDP	P2B-O2B-C2B	2.02	126.41	121.56
3	G	1259	NDP	C2D-C1D-N1N	2.03	118.82	113.34
3	D	1257	NDP	O2B-P2B-O1X	2.05	112.23	107.11
3	C	1258	NDP	O2N-PN-O1N	2.10	123.89	112.53
3	C	1258	NDP	O4B-C1B-N9A	2.11	112.52	108.10
3	H	1258	NDP	O2N-PN-O1N	2.15	124.16	112.53
3	A	1260	NDP	O2X-P2B-O1X	2.21	117.70	110.58
3	G	1259	NDP	O2N-PN-O1N	2.25	124.71	112.53
3	F	1258	NDP	O2X-P2B-O1X	2.28	117.93	110.58
3	E	1259	NDP	O2A-PA-O1A	2.30	124.98	112.53
3	B	1259	NDP	P2B-O2B-C2B	2.33	127.16	121.56
3	H	1258	NDP	O3-PA-O5B	2.34	109.14	102.94
3	C	1258	NDP	O2X-P2B-O1X	2.36	118.19	110.58
3	C	1258	NDP	O2A-PA-O1A	2.46	125.88	112.53
3	E	1259	NDP	O3-PA-O5B	2.63	109.92	102.94
3	E	1259	NDP	O2X-P2B-O1X	2.64	119.07	110.58
3	D	1257	NDP	C2D-C1D-N1N	2.65	120.50	113.34
3	F	1258	NDP	O2B-P2B-O1X	2.83	114.17	107.11
3	G	1259	NDP	O2A-PA-O1A	2.85	127.95	112.53
3	E	1259	NDP	O3-PN-O5D	2.88	110.57	102.94
3	F	1258	NDP	O3-PA-O5B	2.89	110.61	102.94
3	F	1258	NDP	O3-PN-O5D	2.92	110.69	102.94
3	A	1260	NDP	O3-PA-O5B	2.99	110.88	102.94
3	B	1259	NDP	O3-PA-O5B	3.05	111.03	102.94
3	H	1258	NDP	O2B-P2B-O1X	3.26	115.25	107.11
3	C	1258	NDP	O3-PA-O5B	3.70	112.75	102.94
3	A	1260	NDP	O3-PN-O5D	3.93	113.36	102.94
3	D	1257	NDP	O3-PN-O5D	4.08	113.75	102.94
3	D	1257	NDP	O3-PA-O5B	4.53	114.94	102.94
3	G	1259	NDP	O3-PA-O5B	4.61	115.18	102.94
3	H	1258	NDP	O3-PN-O5D	4.71	115.42	102.94
3	G	1259	NDP	O3-PN-O5D	4.75	115.55	102.94
3	B	1259	NDP	O3-PN-O5D	4.78	115.61	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1258	NDP	1	0
3	E	1259	NDP	1	0
5	E	1261	EDO	2	0
5	G	1257	EDO	2	0
3	G	1259	NDP	2	0
5	G	1358	EDO	1	0
3	H	1258	NDP	2	0

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^{th} 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	262/282 (92%)	-0.00	1 (0%) 93 95	13, 25, 50, 62	0
1	B	256/282 (90%)	0.10	3 (1%) 81 87	14, 25, 46, 57	0
1	C	262/282 (92%)	0.16	4 (1%) 76 84	13, 27, 50, 62	0
1	D	256/282 (90%)	0.03	4 (1%) 74 83	14, 26, 52, 67	0
1	E	256/282 (90%)	0.10	7 (2%) 58 68	13, 25, 51, 64	0
1	F	262/282 (92%)	0.08	1 (0%) 93 95	13, 26, 49, 59	0
1	G	257/282 (91%)	0.24	11 (4%) 39 50	17, 29, 56, 79	0
1	H	263/282 (93%)	0.18	4 (1%) 76 84	16, 29, 57, 78	0
All	All	2074/2256 (91%)	0.11	35 (1%) 73 81	13, 27, 52, 79	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	44	SER	3.8
1	C	-5	LEU	3.6
1	H	46	LYS	3.4
1	E	103[A]	ARG	3.3
1	C	103	ARG	3.2
1	E	104	GLY	3.1
1	B	58	PRO	3.0
1	B	202[A]	GLY	3.0
1	G	60	ALA	2.9
1	E	206[A]	THR	2.9
1	G	52	LEU	2.8
1	D	52	LEU	2.8
1	D	104	GLY	2.7
1	G	6	ASN	2.7
1	G	43	ARG	2.7
1	E	6	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	58	PRO	2.7
1	G	48	LEU	2.6
1	C	46	LYS	2.6
1	A	46	LYS	2.5
1	G	45	ARG	2.4
1	H	52	LEU	2.4
1	B	196	LEU	2.3
1	D	6	ASN	2.2
1	E	46	LYS	2.2
1	H	59	GLU	2.1
1	D	196[A]	LEU	2.1
1	G	53	GLU	2.1
1	H	-6	ASN	2.1
1	E	196	LEU	2.1
1	F	52	LEU	2.1
1	G	46	LYS	2.1
1	E	199[A]	LYS	2.1
1	C	52	LEU	2.0
1	G	203	GLY	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^{th} 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
5	EDO	H	1257	4/4	0.88	0.15	6.66	40,42,44,45	0
5	EDO	G	1358	4/4	0.90	0.18	1.56	45,47,51,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	B	1258	4/4	0.90	0.14	1.00	43,45,51,52	0
5	EDO	C	1270	4/4	0.87	0.12	0.92	36,37,39,40	0
2	SO4	A	1257	5/5	0.98	0.14	0.86	47,50,53,54	0
5	EDO	A	1270	4/4	0.86	0.14	0.83	49,49,51,53	0
2	SO4	H	1358	5/5	0.93	0.14	0.75	52,52,55,57	0
4	PT6	F	1259	24/24	0.97	0.11	0.65	17,22,26,29	0
4	PT6	A	1261	24/24	0.96	0.10	-0.04	23,26,29,30	0
4	PT6	H	1259	24/24	0.95	0.10	-0.09	23,28,31,33	0
5	EDO	G	1257	4/4	0.87	0.14	-0.09	43,44,45,46	0
2	SO4	A	1259	5/5	0.96	0.13	-0.26	51,51,54,54	0
3	NDP	F	1258	48/48	0.97	0.09	-0.34	19,27,44,50	0
3	NDP	B	1259	48/48	0.97	0.10	-0.38	17,26,38,40	0
4	PT6	G	1260	24/24	0.97	0.10	-0.42	21,28,34,35	0
4	PT6	D	1258	24/24	0.98	0.10	-0.44	19,25,29,32	0
3	NDP	H	1258	48/48	0.96	0.10	-0.44	22,31,46,54	0
3	NDP	G	1259	48/48	0.96	0.10	-0.46	20,28,47,56	0
3	NDP	C	1258	48/48	0.96	0.09	-0.51	21,27,42,47	0
3	NDP	D	1257	48/48	0.97	0.09	-0.54	17,26,41,50	0
3	NDP	A	1260	48/48	0.97	0.08	-0.59	20,27,43,48	0
4	PT6	E	1260	24/24	0.97	0.10	-0.71	20,24,27,30	0
4	PT6	C	1259	24/24	0.97	0.09	-0.73	21,29,31,32	0
3	NDP	E	1259	48/48	0.97	0.09	-0.74	18,25,43,44	0
4	PT6	B	1260	24/24	0.97	0.09	-0.92	18,23,27,31	0
2	SO4	E	1257	5/5	0.96	0.08	-2.13	45,45,45,46	5
2	SO4	B	1257	5/5	0.96	0.10	-2.61	33,34,36,36	5
6	CL	F	1357	1/1	0.96	0.06	-	60,60,60,60	0
5	EDO	E	1261	4/4	0.70	0.20	-	61,62,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.