



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 23, 2017 – 12:28 PM EST

PDB ID : 5URR  
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Bacillus anthracis in the complex with IMP and the inhibitor P176  
Authors : Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-02-12  
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

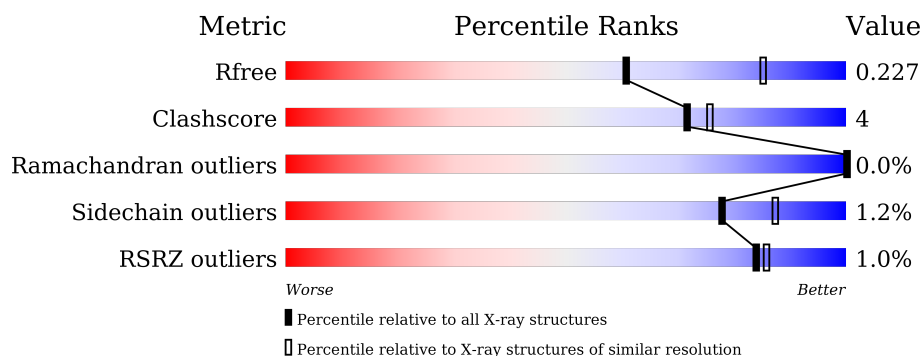
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	<div> <div>2%</div> <div>81% 10% 9%</div> </div>
1	B	384	<div> <div>%</div> <div>81% 10% 9%</div> </div>
1	C	384	<div> <div>%</div> <div>78% 13% 8%</div> </div>
1	D	384	<div> <div>81% 10% 9%</div> </div>
1	E	384	<div> <div>%</div> <div>82% 9% 9%</div> </div>
1	F	384	<div> <div>%</div> <div>84% 8% 8%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	384	 % 80% 11% 9%
1	H	384	 % 78% 13% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IMP	H	502	-	-	-	X
3	8L7	A	501	-	-	-	X
3	8L7	D	503	-	-	-	X
3	8L7	H	503	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21361 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2570	1615	451	488	16			
1	B	350	Total	C	N	O	S	0	0	0
			2570	1615	451	488	16			
1	C	352	Total	C	N	O	S	0	0	0
			2577	1616	452	493	16			
1	D	351	Total	C	N	O	S	0	0	0
			2571	1614	451	490	16			
1	E	350	Total	C	N	O	S	0	0	0
			2567	1611	450	490	16			
1	F	355	Total	C	N	O	S	0	0	0
			2606	1637	457	496	16			
1	G	349	Total	C	N	O	S	0	1	0
			2572	1615	453	488	16			
1	H	348	Total	C	N	O	S	0	0	0
			2552	1603	447	486	16			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q81W29
A	-22	HIS	-	expression tag	UNP Q81W29
A	-21	HIS	-	expression tag	UNP Q81W29
A	-20	HIS	-	expression tag	UNP Q81W29
A	-19	HIS	-	expression tag	UNP Q81W29
A	-18	HIS	-	expression tag	UNP Q81W29
A	-17	HIS	-	expression tag	UNP Q81W29
A	-16	SER	-	expression tag	UNP Q81W29
A	-15	SER	-	expression tag	UNP Q81W29
A	-14	GLY	-	expression tag	UNP Q81W29
A	-13	VAL	-	expression tag	UNP Q81W29
A	-12	ASP	-	expression tag	UNP Q81W29
A	-11	LEU	-	expression tag	UNP Q81W29

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q81W29
A	-9	THR	-	expression tag	UNP Q81W29
A	-8	GLU	-	expression tag	UNP Q81W29
A	-7	ASN	-	expression tag	UNP Q81W29
A	-6	LEU	-	expression tag	UNP Q81W29
A	-5	TYR	-	expression tag	UNP Q81W29
A	-4	PHE	-	expression tag	UNP Q81W29
A	-3	GLN	-	expression tag	UNP Q81W29
A	-2	SER	-	expression tag	UNP Q81W29
A	-1	ASN	-	expression tag	UNP Q81W29
A	0	ALA	-	expression tag	UNP Q81W29
A	92	GLY	-	linker	UNP Q81W29
A	220	GLY	-	linker	UNP Q81W29
B	-23	MET	-	initiating methionine	UNP Q81W29
B	-22	HIS	-	expression tag	UNP Q81W29
B	-21	HIS	-	expression tag	UNP Q81W29
B	-20	HIS	-	expression tag	UNP Q81W29
B	-19	HIS	-	expression tag	UNP Q81W29
B	-18	HIS	-	expression tag	UNP Q81W29
B	-17	HIS	-	expression tag	UNP Q81W29
B	-16	SER	-	expression tag	UNP Q81W29
B	-15	SER	-	expression tag	UNP Q81W29
B	-14	GLY	-	expression tag	UNP Q81W29
B	-13	VAL	-	expression tag	UNP Q81W29
B	-12	ASP	-	expression tag	UNP Q81W29
B	-11	LEU	-	expression tag	UNP Q81W29
B	-10	GLY	-	expression tag	UNP Q81W29
B	-9	THR	-	expression tag	UNP Q81W29
B	-8	GLU	-	expression tag	UNP Q81W29
B	-7	ASN	-	expression tag	UNP Q81W29
B	-6	LEU	-	expression tag	UNP Q81W29
B	-5	TYR	-	expression tag	UNP Q81W29
B	-4	PHE	-	expression tag	UNP Q81W29
B	-3	GLN	-	expression tag	UNP Q81W29
B	-2	SER	-	expression tag	UNP Q81W29
B	-1	ASN	-	expression tag	UNP Q81W29
B	0	ALA	-	expression tag	UNP Q81W29
B	92	GLY	-	linker	UNP Q81W29
B	220	GLY	-	linker	UNP Q81W29
C	-23	MET	-	initiating methionine	UNP Q81W29
C	-22	HIS	-	expression tag	UNP Q81W29
C	-21	HIS	-	expression tag	UNP Q81W29

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q81W29
C	-19	HIS	-	expression tag	UNP Q81W29
C	-18	HIS	-	expression tag	UNP Q81W29
C	-17	HIS	-	expression tag	UNP Q81W29
C	-16	SER	-	expression tag	UNP Q81W29
C	-15	SER	-	expression tag	UNP Q81W29
C	-14	GLY	-	expression tag	UNP Q81W29
C	-13	VAL	-	expression tag	UNP Q81W29
C	-12	ASP	-	expression tag	UNP Q81W29
C	-11	LEU	-	expression tag	UNP Q81W29
C	-10	GLY	-	expression tag	UNP Q81W29
C	-9	THR	-	expression tag	UNP Q81W29
C	-8	GLU	-	expression tag	UNP Q81W29
C	-7	ASN	-	expression tag	UNP Q81W29
C	-6	LEU	-	expression tag	UNP Q81W29
C	-5	TYR	-	expression tag	UNP Q81W29
C	-4	PHE	-	expression tag	UNP Q81W29
C	-3	GLN	-	expression tag	UNP Q81W29
C	-2	SER	-	expression tag	UNP Q81W29
C	-1	ASN	-	expression tag	UNP Q81W29
C	0	ALA	-	expression tag	UNP Q81W29
C	92	GLY	-	linker	UNP Q81W29
C	220	GLY	-	linker	UNP Q81W29
D	-23	MET	-	initiating methionine	UNP Q81W29
D	-22	HIS	-	expression tag	UNP Q81W29
D	-21	HIS	-	expression tag	UNP Q81W29
D	-20	HIS	-	expression tag	UNP Q81W29
D	-19	HIS	-	expression tag	UNP Q81W29
D	-18	HIS	-	expression tag	UNP Q81W29
D	-17	HIS	-	expression tag	UNP Q81W29
D	-16	SER	-	expression tag	UNP Q81W29
D	-15	SER	-	expression tag	UNP Q81W29
D	-14	GLY	-	expression tag	UNP Q81W29
D	-13	VAL	-	expression tag	UNP Q81W29
D	-12	ASP	-	expression tag	UNP Q81W29
D	-11	LEU	-	expression tag	UNP Q81W29
D	-10	GLY	-	expression tag	UNP Q81W29
D	-9	THR	-	expression tag	UNP Q81W29
D	-8	GLU	-	expression tag	UNP Q81W29
D	-7	ASN	-	expression tag	UNP Q81W29
D	-6	LEU	-	expression tag	UNP Q81W29
D	-5	TYR	-	expression tag	UNP Q81W29

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PHE	-	expression tag	UNP Q81W29
D	-3	GLN	-	expression tag	UNP Q81W29
D	-2	SER	-	expression tag	UNP Q81W29
D	-1	ASN	-	expression tag	UNP Q81W29
D	0	ALA	-	expression tag	UNP Q81W29
D	92	GLY	-	linker	UNP Q81W29
D	220	GLY	-	linker	UNP Q81W29
E	-23	MET	-	initiating methionine	UNP Q81W29
E	-22	HIS	-	expression tag	UNP Q81W29
E	-21	HIS	-	expression tag	UNP Q81W29
E	-20	HIS	-	expression tag	UNP Q81W29
E	-19	HIS	-	expression tag	UNP Q81W29
E	-18	HIS	-	expression tag	UNP Q81W29
E	-17	HIS	-	expression tag	UNP Q81W29
E	-16	SER	-	expression tag	UNP Q81W29
E	-15	SER	-	expression tag	UNP Q81W29
E	-14	GLY	-	expression tag	UNP Q81W29
E	-13	VAL	-	expression tag	UNP Q81W29
E	-12	ASP	-	expression tag	UNP Q81W29
E	-11	LEU	-	expression tag	UNP Q81W29
E	-10	GLY	-	expression tag	UNP Q81W29
E	-9	THR	-	expression tag	UNP Q81W29
E	-8	GLU	-	expression tag	UNP Q81W29
E	-7	ASN	-	expression tag	UNP Q81W29
E	-6	LEU	-	expression tag	UNP Q81W29
E	-5	TYR	-	expression tag	UNP Q81W29
E	-4	PHE	-	expression tag	UNP Q81W29
E	-3	GLN	-	expression tag	UNP Q81W29
E	-2	SER	-	expression tag	UNP Q81W29
E	-1	ASN	-	expression tag	UNP Q81W29
E	0	ALA	-	expression tag	UNP Q81W29
E	92	GLY	-	linker	UNP Q81W29
E	220	GLY	-	linker	UNP Q81W29
F	-23	MET	-	initiating methionine	UNP Q81W29
F	-22	HIS	-	expression tag	UNP Q81W29
F	-21	HIS	-	expression tag	UNP Q81W29
F	-20	HIS	-	expression tag	UNP Q81W29
F	-19	HIS	-	expression tag	UNP Q81W29
F	-18	HIS	-	expression tag	UNP Q81W29
F	-17	HIS	-	expression tag	UNP Q81W29
F	-16	SER	-	expression tag	UNP Q81W29
F	-15	SER	-	expression tag	UNP Q81W29

*Continued on next page...*

*Continued from previous page...*

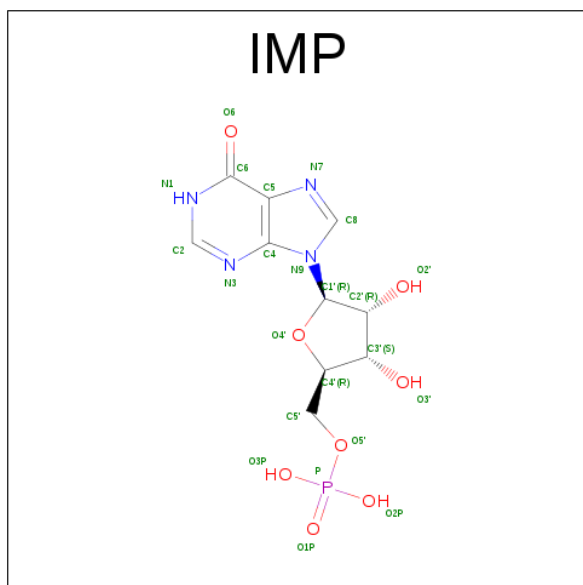
Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	expression tag	UNP Q81W29
F	-13	VAL	-	expression tag	UNP Q81W29
F	-12	ASP	-	expression tag	UNP Q81W29
F	-11	LEU	-	expression tag	UNP Q81W29
F	-10	GLY	-	expression tag	UNP Q81W29
F	-9	THR	-	expression tag	UNP Q81W29
F	-8	GLU	-	expression tag	UNP Q81W29
F	-7	ASN	-	expression tag	UNP Q81W29
F	-6	LEU	-	expression tag	UNP Q81W29
F	-5	TYR	-	expression tag	UNP Q81W29
F	-4	PHE	-	expression tag	UNP Q81W29
F	-3	GLN	-	expression tag	UNP Q81W29
F	-2	SER	-	expression tag	UNP Q81W29
F	-1	ASN	-	expression tag	UNP Q81W29
F	0	ALA	-	expression tag	UNP Q81W29
F	92	GLY	-	linker	UNP Q81W29
F	220	GLY	-	linker	UNP Q81W29
G	-23	MET	-	initiating methionine	UNP Q81W29
G	-22	HIS	-	expression tag	UNP Q81W29
G	-21	HIS	-	expression tag	UNP Q81W29
G	-20	HIS	-	expression tag	UNP Q81W29
G	-19	HIS	-	expression tag	UNP Q81W29
G	-18	HIS	-	expression tag	UNP Q81W29
G	-17	HIS	-	expression tag	UNP Q81W29
G	-16	SER	-	expression tag	UNP Q81W29
G	-15	SER	-	expression tag	UNP Q81W29
G	-14	GLY	-	expression tag	UNP Q81W29
G	-13	VAL	-	expression tag	UNP Q81W29
G	-12	ASP	-	expression tag	UNP Q81W29
G	-11	LEU	-	expression tag	UNP Q81W29
G	-10	GLY	-	expression tag	UNP Q81W29
G	-9	THR	-	expression tag	UNP Q81W29
G	-8	GLU	-	expression tag	UNP Q81W29
G	-7	ASN	-	expression tag	UNP Q81W29
G	-6	LEU	-	expression tag	UNP Q81W29
G	-5	TYR	-	expression tag	UNP Q81W29
G	-4	PHE	-	expression tag	UNP Q81W29
G	-3	GLN	-	expression tag	UNP Q81W29
G	-2	SER	-	expression tag	UNP Q81W29
G	-1	ASN	-	expression tag	UNP Q81W29
G	0	ALA	-	expression tag	UNP Q81W29
G	92	GLY	-	linker	UNP Q81W29

*Continued on next page...*

*Continued from previous page...*

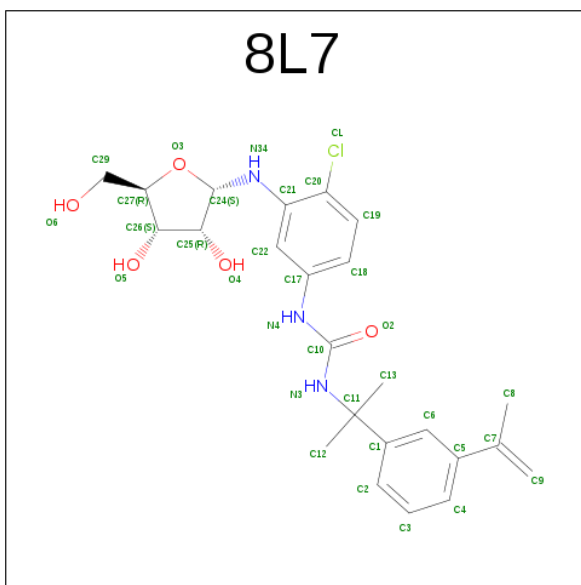
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	linker	UNP Q81W29
H	-23	MET	-	initiating methionine	UNP Q81W29
H	-22	HIS	-	expression tag	UNP Q81W29
H	-21	HIS	-	expression tag	UNP Q81W29
H	-20	HIS	-	expression tag	UNP Q81W29
H	-19	HIS	-	expression tag	UNP Q81W29
H	-18	HIS	-	expression tag	UNP Q81W29
H	-17	HIS	-	expression tag	UNP Q81W29
H	-16	SER	-	expression tag	UNP Q81W29
H	-15	SER	-	expression tag	UNP Q81W29
H	-14	GLY	-	expression tag	UNP Q81W29
H	-13	VAL	-	expression tag	UNP Q81W29
H	-12	ASP	-	expression tag	UNP Q81W29
H	-11	LEU	-	expression tag	UNP Q81W29
H	-10	GLY	-	expression tag	UNP Q81W29
H	-9	THR	-	expression tag	UNP Q81W29
H	-8	GLU	-	expression tag	UNP Q81W29
H	-7	ASN	-	expression tag	UNP Q81W29
H	-6	LEU	-	expression tag	UNP Q81W29
H	-5	TYR	-	expression tag	UNP Q81W29
H	-4	PHE	-	expression tag	UNP Q81W29
H	-3	GLN	-	expression tag	UNP Q81W29
H	-2	SER	-	expression tag	UNP Q81W29
H	-1	ASN	-	expression tag	UNP Q81W29
H	0	ALA	-	expression tag	UNP Q81W29
H	92	GLY	-	linker	UNP Q81W29
H	220	GLY	-	linker	UNP Q81W29

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-{2-chloro-5-[(2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}carbamoyl)amino]phenyl}-alpha-D-ribofuranosylamine (three-letter code: 8L7) (formula: C<sub>24</sub>H<sub>30</sub>ClN<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	B	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	C	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	D	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	F	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	G	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	G	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	H	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	H	1	Total	K	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0
4	F	1	Total 1	K 1	0	0

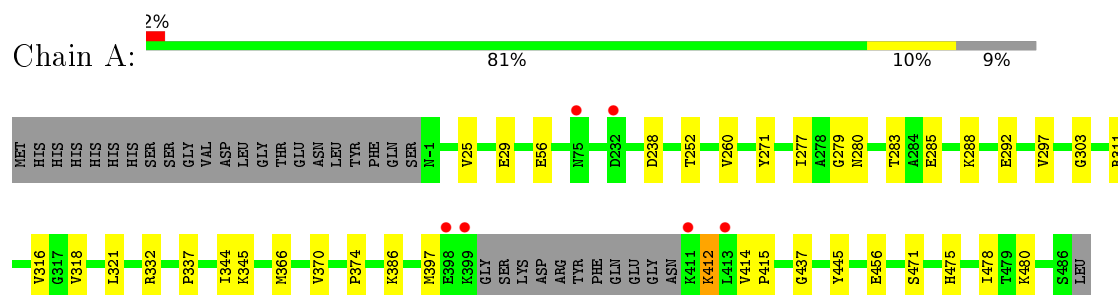
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total 44	O 44	0	0
5	B	52	Total 52	O 52	0	0
5	C	51	Total 51	O 51	0	0
5	D	42	Total 42	O 42	0	0
5	E	37	Total 37	O 37	0	0
5	F	32	Total 32	O 32	0	0
5	G	34	Total 34	O 34	0	0
5	H	28	Total 28	O 28	0	0

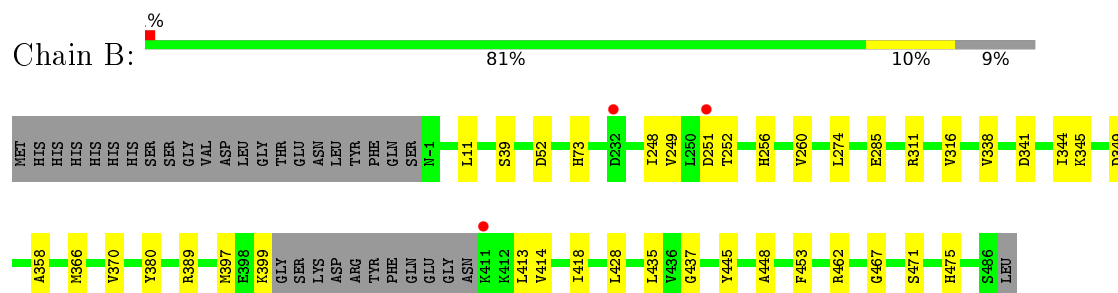
### 3 Residue-property plots [i](#)

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.

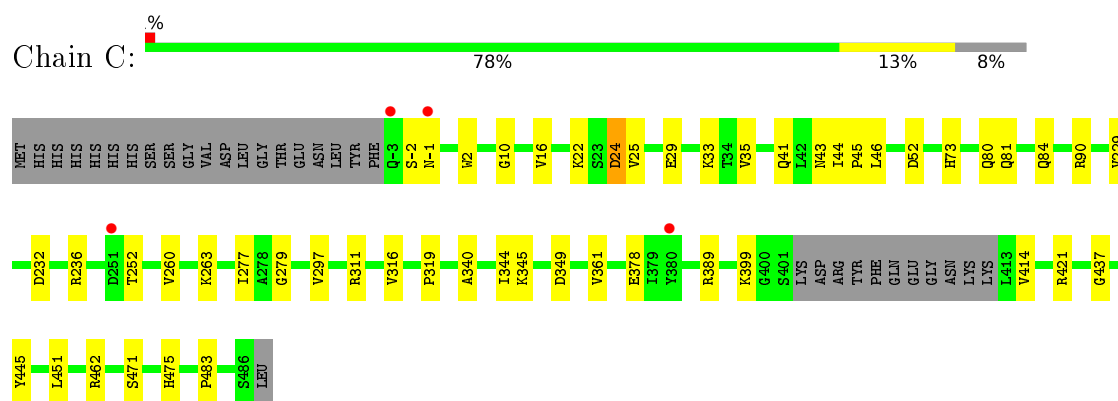
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



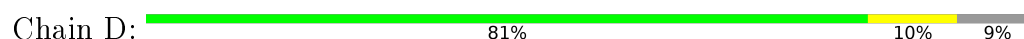
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

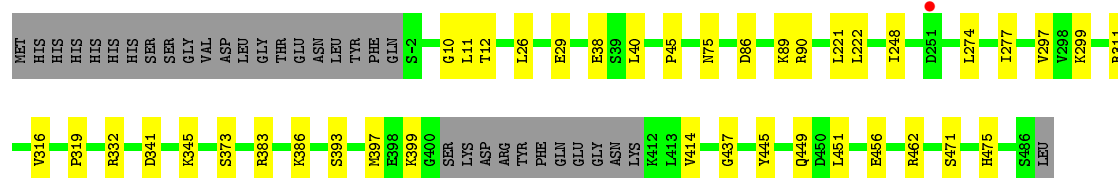


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

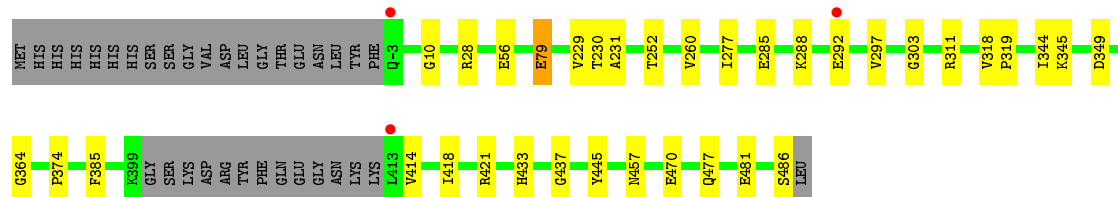
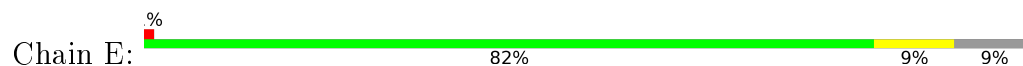


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

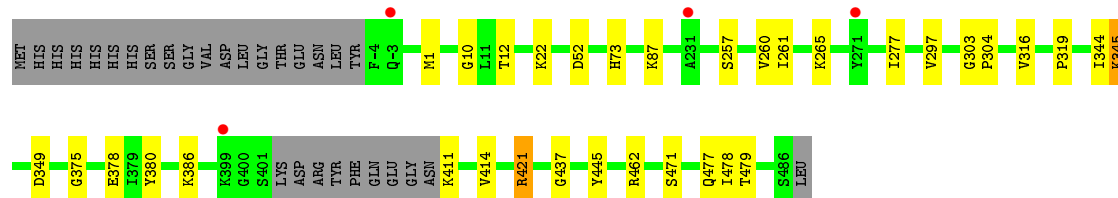
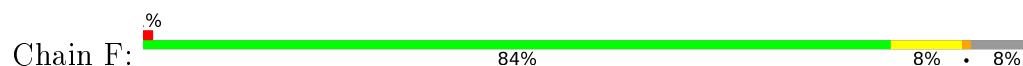




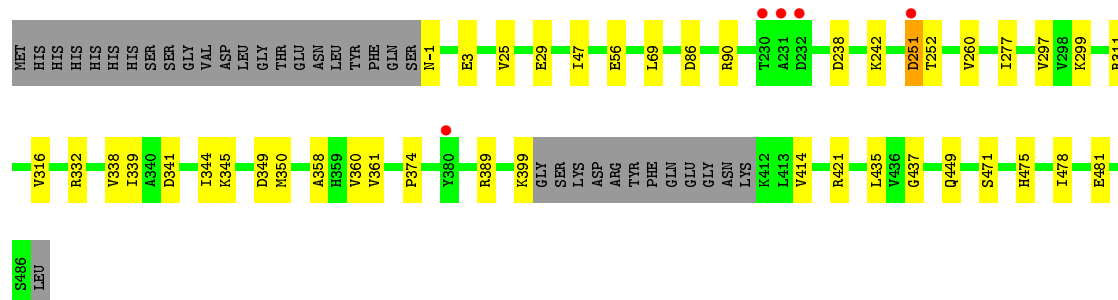
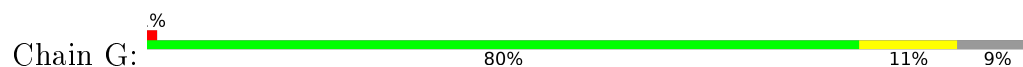
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



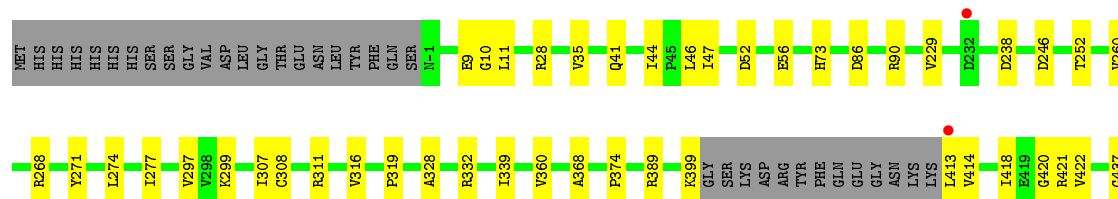
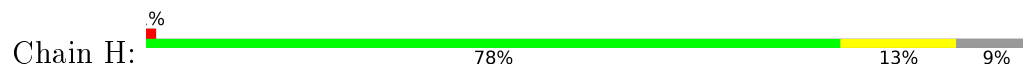
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



Y445	R462	S471	H476	Q477	S486	LEU
------	------	------	------	------	------	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.39Å 89.92Å 104.86Å 81.41° 90.03° 83.44°	Depositor
Resolution (Å)	40.08 – 2.45 48.33 – 2.44	Depositor EDS
% Data completeness (in resolution range)	91.2 (40.08-2.45) 87.7 (48.33-2.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.182 , 0.228 0.179 , 0.227	Depositor DCC
$R_{free}$ test set	5138 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8L7, IMP, K

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	0.28	0/2606	0.42	0/3521
1	B	0.31	0/2606	0.44	0/3521
1	C	0.27	0/2613	0.43	0/3532
1	D	0.29	0/2607	0.43	0/3523
1	E	0.27	0/2603	0.41	0/3519
1	F	0.26	0/2643	0.42	0/3570
1	G	0.24	0/2608	0.41	0/3524
1	H	0.28	0/2588	0.44	0/3499
All	All	0.28	0/20874	0.42	0/28209

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2570	0	2634	30	0
1	B	2570	0	2634	27	0
1	C	2577	0	2629	32	0
1	D	2571	0	2629	25	0
1	E	2567	0	2621	25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2606	0	2664	27	0
1	G	2572	0	2633	28	0
1	H	2552	0	2608	32	0
2	A	23	0	11	0	0
2	B	23	0	11	1	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
2	G	23	0	11	1	0
2	H	23	0	11	0	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
3	C	33	0	0	0	0
3	D	33	0	0	0	0
3	F	33	0	0	0	0
3	G	66	0	0	0	0
3	H	33	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	44	0	0	0	0
5	B	52	0	0	1	0
5	C	51	0	0	0	0
5	D	42	0	0	1	0
5	E	37	0	0	1	0
5	F	32	0	0	0	0
5	G	34	0	0	0	0
5	H	28	0	0	0	0
All	All	21361	0	21140	182	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 4.

The worst 5 of 182 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:285:GLU:HB2	5:B:636:HOH:O	1.83	0.78
1:C:414:VAL:HG21	1:D:437:GLY:HA3	1.75	0.67
1:D:12:THR:HG22	1:D:319:PRO:HB3	1.76	0.66
1:E:437:GLY:HA3	1:F:414:VAL:HG21	1.78	0.66
1:C:252:THR:HG21	1:C:260:VAL:HG21	1.79	0.64

There are no symmetry-related clashes.

## 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	346/384 (90%)	336 (97%)	10 (3%)	0	100	100
1	B	346/384 (90%)	339 (98%)	7 (2%)	0	100	100
1	C	348/384 (91%)	342 (98%)	6 (2%)	0	100	100
1	D	347/384 (90%)	338 (97%)	9 (3%)	0	100	100
1	E	346/384 (90%)	336 (97%)	9 (3%)	1 (0%)	46	57
1	F	351/384 (91%)	343 (98%)	8 (2%)	0	100	100
1	G	346/384 (90%)	337 (97%)	9 (3%)	0	100	100
1	H	344/384 (90%)	336 (98%)	8 (2%)	0	100	100
All	All	2774/3072 (90%)	2707 (98%)	66 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	364	GLY

### 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	268/298 (90%)	266 (99%)	2 (1%)	88	93
1	B	268/298 (90%)	265 (99%)	3 (1%)	80	88
1	C	269/298 (90%)	264 (98%)	5 (2%)	65	79
1	D	268/298 (90%)	264 (98%)	4 (2%)	72	84
1	E	268/298 (90%)	266 (99%)	2 (1%)	88	93
1	F	272/298 (91%)	269 (99%)	3 (1%)	80	88
1	G	268/298 (90%)	265 (99%)	3 (1%)	80	88
1	H	266/298 (89%)	263 (99%)	3 (1%)	80	88
All	All	2147/2384 (90%)	2122 (99%)	25 (1%)	78	87

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	383	ARG
1	D	449	GLN
1	H	246	ASP
1	D	386	LYS
1	E	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	381	GLN
1	D	449	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	IMP	A	500	-	21,25,25	1.21	3 (14%)	22,38,38	2.56	3 (13%)
3	8L7	A	501	-	34,35,35	1.13	5 (14%)	44,51,51	1.12	2 (4%)
2	IMP	B	500	-	21,25,25	1.22	3 (14%)	22,38,38	2.48	3 (13%)
3	8L7	B	501	-	34,35,35	1.79	8 (23%)	44,51,51	1.17	4 (9%)
2	IMP	C	502	-	21,25,25	1.20	3 (14%)	22,38,38	2.47	3 (13%)
3	8L7	C	503	-	34,35,35	1.16	5 (14%)	44,51,51	1.15	1 (2%)
2	IMP	D	502	-	21,25,25	1.21	3 (14%)	22,38,38	2.50	3 (13%)
3	8L7	D	503	-	34,35,35	1.13	5 (14%)	44,51,51	1.16	3 (6%)
2	IMP	E	501	-	21,25,25	1.22	3 (14%)	22,38,38	2.48	3 (13%)
2	IMP	F	500	-	21,25,25	1.22	3 (14%)	22,38,38	2.48	3 (13%)
3	8L7	F	501	-	34,35,35	1.15	5 (14%)	44,51,51	1.13	3 (6%)
3	8L7	G	501	-	34,35,35	1.13	4 (11%)	44,51,51	1.20	3 (6%)
2	IMP	G	503	-	21,25,25	1.22	3 (14%)	22,38,38	2.49	3 (13%)
3	8L7	G	504	-	34,35,35	1.14	4 (11%)	44,51,51	1.19	3 (6%)
2	IMP	H	502	-	21,25,25	1.21	3 (14%)	22,38,38	2.48	3 (13%)
3	8L7	H	503	-	34,35,35	1.16	5 (14%)	44,51,51	1.22	3 (6%)

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	IMP	A	500	-	-	0/6/26/26	0/3/3/3
3	8L7	A	501	-	-	0/25/41/41	0/3/3/3
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3
3	8L7	B	501	-	-	2/25/41/41	0/3/3/3
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3
3	8L7	C	503	-	-	0/25/41/41	0/3/3/3
2	IMP	D	502	-	-	0/6/26/26	0/3/3/3
3	8L7	D	503	-	-	0/25/41/41	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
2	IMP	F	500	-	-	0/6/26/26	0/3/3/3
3	8L7	F	501	-	-	0/25/41/41	0/3/3/3
3	8L7	G	501	-	-	0/25/41/41	0/3/3/3
2	IMP	G	503	-	-	0/6/26/26	0/3/3/3
3	8L7	G	504	-	-	0/25/41/41	0/3/3/3
2	IMP	H	502	-	-	0/6/26/26	0/3/3/3
3	8L7	H	503	-	-	0/25/41/41	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	8L7	C17-N4	-4.69	1.32	1.41
3	B	501	8L7	C10-N4	-4.26	1.29	1.37
3	B	501	8L7	C8-C7	-2.92	1.31	1.46
3	B	501	8L7	C11-N3	-2.88	1.43	1.48
3	G	504	8L7	C8-C7	-2.64	1.32	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	IMP	N3-C2-N1	-11.13	120.13	128.87
2	D	502	IMP	N3-C2-N1	-10.90	120.31	128.87
2	G	503	IMP	N3-C2-N1	-10.83	120.37	128.87
2	F	500	IMP	N3-C2-N1	-10.79	120.39	128.87
2	E	501	IMP	N3-C2-N1	-10.79	120.39	128.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	8L7	C22-C21-N34-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	501	8L7	C20-C21-N34-C24

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	IMP	1	0
2	G	503	IMP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	350/384 (91%)	-0.05	6 (1%) 73 75	21, 36, 63, 87	0
1	B	350/384 (91%)	-0.14	3 (0%) 85 87	17, 33, 62, 89	0
1	C	352/384 (91%)	-0.14	4 (1%) 82 84	20, 34, 63, 104	0
1	D	351/384 (91%)	-0.21	1 (0%) 94 95	21, 35, 63, 99	0
1	E	350/384 (91%)	-0.16	3 (0%) 85 87	22, 37, 63, 96	0
1	F	355/384 (92%)	-0.05	4 (1%) 82 84	23, 39, 66, 111	0
1	G	349/384 (90%)	0.06	5 (1%) 78 80	24, 41, 69, 86	0
1	H	348/384 (90%)	-0.08	2 (0%) 90 91	26, 42, 65, 88	0
All	All	2805/3072 (91%)	-0.10	28 (0%) 84 86	17, 37, 65, 111	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	LYS	5.4
1	A	232	ASP	4.0
1	A	413	LEU	3.7
1	G	232	ASP	3.3
1	G	230	THR	3.3

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	8L7	H	503	33/33	0.88	0.23	4.22	32,53,91,98	0
3	8L7	D	503	33/33	0.92	0.22	2.57	27,42,96,98	0
3	8L7	A	501	33/33	0.90	0.22	2.24	26,45,80,87	0
2	IMP	H	502	23/23	0.95	0.17	2.00	27,38,40,45	0
3	8L7	C	503	33/33	0.93	0.20	1.90	26,37,88,95	0
3	8L7	F	501	33/33	0.92	0.21	1.86	32,47,87,89	0
3	8L7	G	504	33/33	0.91	0.21	1.83	29,48,87,91	0
3	8L7	B	501	33/33	0.92	0.18	1.13	24,36,89,92	0
3	8L7	G	501	33/33	0.92	0.17	1.11	21,42,86,91	0
2	IMP	E	501	23/23	0.97	0.15	0.85	24,32,38,43	0
2	IMP	A	500	23/23	0.98	0.14	0.74	25,31,35,40	0
2	IMP	F	500	23/23	0.96	0.15	0.35	31,35,40,45	0
2	IMP	B	500	23/23	0.97	0.15	0.07	23,30,37,40	0
2	IMP	D	502	23/23	0.97	0.14	0.04	20,29,36,37	0
2	IMP	C	502	23/23	0.96	0.14	-0.11	21,27,33,40	0
2	IMP	G	503	23/23	0.95	0.13	-0.14	27,34,38,39	0
4	K	G	502	1/1	0.98	0.13	-0.52	31,31,31,31	0
4	K	D	501	1/1	0.99	0.12	-0.52	29,29,29,29	0
4	K	E	502	1/1	0.98	0.13	-0.99	34,34,34,34	0
4	K	A	502	1/1	0.99	0.12	-1.10	32,32,32,32	0
4	K	H	501	1/1	0.99	0.07	-3.88	30,30,30,30	0
4	K	F	502	1/1	0.99	0.06	-4.23	36,36,36,36	0
4	K	B	502	1/1	0.99	0.05	-4.73	32,32,32,32	0
4	K	C	501	1/1	0.99	0.05	-12.13	34,34,34,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.