



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2017 – 11:04 AM EST

PDB ID : 5UQH
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Campylobacter jejuni* in the complex with inhibitor p182
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 : 2017-02-08
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

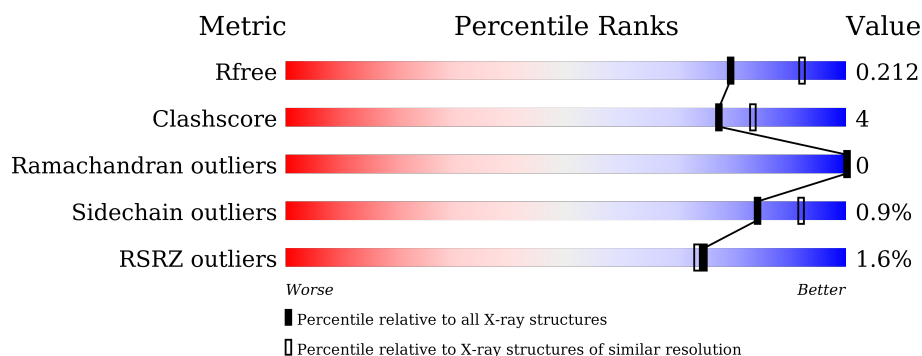
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	406	<div> <div>2%</div> <div>83% 8% 9%</div> </div>
1	B	406	<div> <div>%</div> <div>79% 9% 12%</div> </div>
1	C	406	<div> <div>%</div> <div>81% 7% 12%</div> </div>
1	D	406	<div> <div>83% 5% 13%</div> </div>
1	E	406	<div> <div>%</div> <div>81% 7% 12%</div> </div>
1	F	406	<div> <div>2%</div> <div>78% 11% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	406	
1	H	406	

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
3	K	A	502	-	-	-	X
4	8L1	C	501	-	-	-	X
4	8L1	E	502	-	-	-	X
4	8L1	F	503	-	-	-	X
4	8L1	G	503	-	-	-	X
4	8L1	H	503	-	-	-	X
5	EDO	D	505	-	-	-	X
5	EDO	E	503	-	-	-	X
5	EDO	E	504	-	-	-	X
5	EDO	F	505	-	-	-	X
6	IPA	G	504	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22377 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, Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2735	1718	482	521	14			
1	B	358	Total	C	N	O	S	0	0	0
			2654	1669	468	503	14			
1	C	356	Total	C	N	O	S	0	0	0
			2642	1662	467	499	14			
1	D	355	Total	C	N	O	S	0	0	0
			2643	1662	468	499	14			
1	E	357	Total	C	N	O	S	0	0	0
			2659	1673	471	501	14			
1	F	361	Total	C	N	O	S	0	0	0
			2687	1689	476	508	14			
1	G	354	Total	C	N	O	S	0	0	0
			2632	1656	464	498	14			
1	H	356	Total	C	N	O	S	0	0	0
			2652	1668	470	500	14			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
A	-22	HIS	-	expression tag	UNP A0A1B3XFT6
A	-21	HIS	-	expression tag	UNP A0A1B3XFT6
A	-20	HIS	-	expression tag	UNP A0A1B3XFT6
A	-19	HIS	-	expression tag	UNP A0A1B3XFT6
A	-18	HIS	-	expression tag	UNP A0A1B3XFT6
A	-17	HIS	-	expression tag	UNP A0A1B3XFT6
A	-16	SER	-	expression tag	UNP A0A1B3XFT6
A	-15	SER	-	expression tag	UNP A0A1B3XFT6
A	-14	GLY	-	expression tag	UNP A0A1B3XFT6
A	-13	VAL	-	expression tag	UNP A0A1B3XFT6
A	-12	ASP	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	LEU	-	expression tag	UNP A0A1B3XFT6
A	-10	GLY	-	expression tag	UNP A0A1B3XFT6
A	-9	THR	-	expression tag	UNP A0A1B3XFT6
A	-8	GLU	-	expression tag	UNP A0A1B3XFT6
A	-7	ASN	-	expression tag	UNP A0A1B3XFT6
A	-6	LEU	-	expression tag	UNP A0A1B3XFT6
A	-5	TYR	-	expression tag	UNP A0A1B3XFT6
A	-4	PHE	-	expression tag	UNP A0A1B3XFT6
A	-3	GLN	-	expression tag	UNP A0A1B3XFT6
A	-2	SER	-	expression tag	UNP A0A1B3XFT6
A	-1	ASN	-	expression tag	UNP A0A1B3XFT6
A	0	ALA	-	expression tag	UNP A0A1B3XFT6
A	195	GLY	-	linker	UNP A0A1B3XFT6
B	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
B	-22	HIS	-	expression tag	UNP A0A1B3XFT6
B	-21	HIS	-	expression tag	UNP A0A1B3XFT6
B	-20	HIS	-	expression tag	UNP A0A1B3XFT6
B	-19	HIS	-	expression tag	UNP A0A1B3XFT6
B	-18	HIS	-	expression tag	UNP A0A1B3XFT6
B	-17	HIS	-	expression tag	UNP A0A1B3XFT6
B	-16	SER	-	expression tag	UNP A0A1B3XFT6
B	-15	SER	-	expression tag	UNP A0A1B3XFT6
B	-14	GLY	-	expression tag	UNP A0A1B3XFT6
B	-13	VAL	-	expression tag	UNP A0A1B3XFT6
B	-12	ASP	-	expression tag	UNP A0A1B3XFT6
B	-11	LEU	-	expression tag	UNP A0A1B3XFT6
B	-10	GLY	-	expression tag	UNP A0A1B3XFT6
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B	-7	ASN	-	expression tag	UNP A0A1B3XFT6
B	-6	LEU	-	expression tag	UNP A0A1B3XFT6
B	-5	TYR	-	expression tag	UNP A0A1B3XFT6
B	-4	PHE	-	expression tag	UNP A0A1B3XFT6
B	-3	GLN	-	expression tag	UNP A0A1B3XFT6
B	-2	SER	-	expression tag	UNP A0A1B3XFT6
B	-1	ASN	-	expression tag	UNP A0A1B3XFT6
B	0	ALA	-	expression tag	UNP A0A1B3XFT6
B	92	GLY	-	linker	UNP A0A1B3XFT6
C	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
C	-22	HIS	-	expression tag	UNP A0A1B3XFT6
C	-21	HIS	-	expression tag	UNP A0A1B3XFT6
C	-20	HIS	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	HIS	-	expression tag	UNP A0A1B3XFT6
C	-18	HIS	-	expression tag	UNP A0A1B3XFT6
C	-17	HIS	-	expression tag	UNP A0A1B3XFT6
C	-16	SER	-	expression tag	UNP A0A1B3XFT6
C	-15	SER	-	expression tag	UNP A0A1B3XFT6
C	-14	GLY	-	expression tag	UNP A0A1B3XFT6
C	-13	VAL	-	expression tag	UNP A0A1B3XFT6
C	-12	ASP	-	expression tag	UNP A0A1B3XFT6
C	-11	LEU	-	expression tag	UNP A0A1B3XFT6
C	-10	GLY	-	expression tag	UNP A0A1B3XFT6
C	-9	THR	-	expression tag	UNP A0A1B3XFT6
C	-8	GLU	-	expression tag	UNP A0A1B3XFT6
C	-7	ASN	-	expression tag	UNP A0A1B3XFT6
C	-6	LEU	-	expression tag	UNP A0A1B3XFT6
C	-5	TYR	-	expression tag	UNP A0A1B3XFT6
C	-4	PHE	-	expression tag	UNP A0A1B3XFT6
C	-3	GLN	-	expression tag	UNP A0A1B3XFT6
C	-2	SER	-	expression tag	UNP A0A1B3XFT6
C	-1	ASN	-	expression tag	UNP A0A1B3XFT6
C	0	ALA	-	expression tag	UNP A0A1B3XFT6
C	195	GLY	-	linker	UNP A0A1B3XFT6
D	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
D	-22	HIS	-	expression tag	UNP A0A1B3XFT6
D	-21	HIS	-	expression tag	UNP A0A1B3XFT6
D	-20	HIS	-	expression tag	UNP A0A1B3XFT6
D	-19	HIS	-	expression tag	UNP A0A1B3XFT6
D	-18	HIS	-	expression tag	UNP A0A1B3XFT6
D	-17	HIS	-	expression tag	UNP A0A1B3XFT6
D	-16	SER	-	expression tag	UNP A0A1B3XFT6
D	-15	SER	-	expression tag	UNP A0A1B3XFT6
D	-14	GLY	-	expression tag	UNP A0A1B3XFT6
D	-13	VAL	-	expression tag	UNP A0A1B3XFT6
D	-12	ASP	-	expression tag	UNP A0A1B3XFT6
D	-11	LEU	-	expression tag	UNP A0A1B3XFT6
D	-10	GLY	-	expression tag	UNP A0A1B3XFT6
D	-9	THR	-	expression tag	UNP A0A1B3XFT6
D	-8	GLU	-	expression tag	UNP A0A1B3XFT6
D	-7	ASN	-	expression tag	UNP A0A1B3XFT6
D	-6	LEU	-	expression tag	UNP A0A1B3XFT6
D	-5	TYR	-	expression tag	UNP A0A1B3XFT6
D	-4	PHE	-	expression tag	UNP A0A1B3XFT6
D	-3	GLN	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP A0A1B3XFT6
D	-1	ASN	-	expression tag	UNP A0A1B3XFT6
D	0	ALA	-	expression tag	UNP A0A1B3XFT6
D	195	GLY	-	linker	UNP A0A1B3XFT6
E	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
E	-22	HIS	-	expression tag	UNP A0A1B3XFT6
E	-21	HIS	-	expression tag	UNP A0A1B3XFT6
E	-20	HIS	-	expression tag	UNP A0A1B3XFT6
E	-19	HIS	-	expression tag	UNP A0A1B3XFT6
E	-18	HIS	-	expression tag	UNP A0A1B3XFT6
E	-17	HIS	-	expression tag	UNP A0A1B3XFT6
E	-16	SER	-	expression tag	UNP A0A1B3XFT6
E	-15	SER	-	expression tag	UNP A0A1B3XFT6
E	-14	GLY	-	expression tag	UNP A0A1B3XFT6
E	-13	VAL	-	expression tag	UNP A0A1B3XFT6
E	-12	ASP	-	expression tag	UNP A0A1B3XFT6
E	-11	LEU	-	expression tag	UNP A0A1B3XFT6
E	-10	GLY	-	expression tag	UNP A0A1B3XFT6
E	-9	THR	-	expression tag	UNP A0A1B3XFT6
E	-8	GLU	-	expression tag	UNP A0A1B3XFT6
E	-7	ASN	-	expression tag	UNP A0A1B3XFT6
E	-6	LEU	-	expression tag	UNP A0A1B3XFT6
E	-5	TYR	-	expression tag	UNP A0A1B3XFT6
E	-4	PHE	-	expression tag	UNP A0A1B3XFT6
E	-3	GLN	-	expression tag	UNP A0A1B3XFT6
E	-2	SER	-	expression tag	UNP A0A1B3XFT6
E	-1	ASN	-	expression tag	UNP A0A1B3XFT6
E	0	ALA	-	expression tag	UNP A0A1B3XFT6
E	195	GLY	-	linker	UNP A0A1B3XFT6
F	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
F	-22	HIS	-	expression tag	UNP A0A1B3XFT6
F	-21	HIS	-	expression tag	UNP A0A1B3XFT6
F	-20	HIS	-	expression tag	UNP A0A1B3XFT6
F	-19	HIS	-	expression tag	UNP A0A1B3XFT6
F	-18	HIS	-	expression tag	UNP A0A1B3XFT6
F	-17	HIS	-	expression tag	UNP A0A1B3XFT6
F	-16	SER	-	expression tag	UNP A0A1B3XFT6
F	-15	SER	-	expression tag	UNP A0A1B3XFT6
F	-14	GLY	-	expression tag	UNP A0A1B3XFT6
F	-13	VAL	-	expression tag	UNP A0A1B3XFT6
F	-12	ASP	-	expression tag	UNP A0A1B3XFT6
F	-11	LEU	-	expression tag	UNP A0A1B3XFT6

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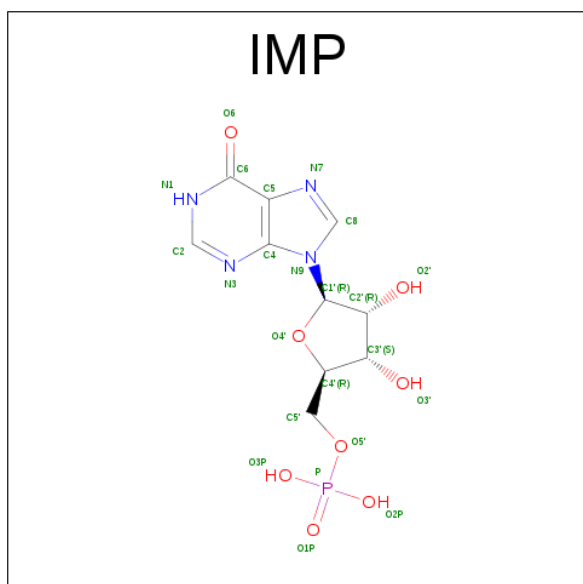
Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	GLY	-	expression tag	UNP A0A1B3XFT6
F	-9	THR	-	expression tag	UNP A0A1B3XFT6
F	-8	GLU	-	expression tag	UNP A0A1B3XFT6
F	-7	ASN	-	expression tag	UNP A0A1B3XFT6
F	-6	LEU	-	expression tag	UNP A0A1B3XFT6
F	-5	TYR	-	expression tag	UNP A0A1B3XFT6
F	-4	PHE	-	expression tag	UNP A0A1B3XFT6
F	-3	GLN	-	expression tag	UNP A0A1B3XFT6
F	-2	SER	-	expression tag	UNP A0A1B3XFT6
F	-1	ASN	-	expression tag	UNP A0A1B3XFT6
F	0	ALA	-	expression tag	UNP A0A1B3XFT6
F	195	GLY	-	linker	UNP A0A1B3XFT6
G	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
G	-22	HIS	-	expression tag	UNP A0A1B3XFT6
G	-21	HIS	-	expression tag	UNP A0A1B3XFT6
G	-20	HIS	-	expression tag	UNP A0A1B3XFT6
G	-19	HIS	-	expression tag	UNP A0A1B3XFT6
G	-18	HIS	-	expression tag	UNP A0A1B3XFT6
G	-17	HIS	-	expression tag	UNP A0A1B3XFT6
G	-16	SER	-	expression tag	UNP A0A1B3XFT6
G	-15	SER	-	expression tag	UNP A0A1B3XFT6
G	-14	GLY	-	expression tag	UNP A0A1B3XFT6
G	-13	VAL	-	expression tag	UNP A0A1B3XFT6
G	-12	ASP	-	expression tag	UNP A0A1B3XFT6
G	-11	LEU	-	expression tag	UNP A0A1B3XFT6
G	-10	GLY	-	expression tag	UNP A0A1B3XFT6
G	-9	THR	-	expression tag	UNP A0A1B3XFT6
G	-8	GLU	-	expression tag	UNP A0A1B3XFT6
G	-7	ASN	-	expression tag	UNP A0A1B3XFT6
G	-6	LEU	-	expression tag	UNP A0A1B3XFT6
G	-5	TYR	-	expression tag	UNP A0A1B3XFT6
G	-4	PHE	-	expression tag	UNP A0A1B3XFT6
G	-3	GLN	-	expression tag	UNP A0A1B3XFT6
G	-2	SER	-	expression tag	UNP A0A1B3XFT6
G	-1	ASN	-	expression tag	UNP A0A1B3XFT6
G	0	ALA	-	expression tag	UNP A0A1B3XFT6
G	195	GLY	-	linker	UNP A0A1B3XFT6
H	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
H	-22	HIS	-	expression tag	UNP A0A1B3XFT6
H	-21	HIS	-	expression tag	UNP A0A1B3XFT6
H	-20	HIS	-	expression tag	UNP A0A1B3XFT6
H	-19	HIS	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-18	HIS	-	expression tag	UNP A0A1B3XFT6
H	-17	HIS	-	expression tag	UNP A0A1B3XFT6
H	-16	SER	-	expression tag	UNP A0A1B3XFT6
H	-15	SER	-	expression tag	UNP A0A1B3XFT6
H	-14	GLY	-	expression tag	UNP A0A1B3XFT6
H	-13	VAL	-	expression tag	UNP A0A1B3XFT6
H	-12	ASP	-	expression tag	UNP A0A1B3XFT6
H	-11	LEU	-	expression tag	UNP A0A1B3XFT6
H	-10	GLY	-	expression tag	UNP A0A1B3XFT6
H	-9	THR	-	expression tag	UNP A0A1B3XFT6
H	-8	GLU	-	expression tag	UNP A0A1B3XFT6
H	-7	ASN	-	expression tag	UNP A0A1B3XFT6
H	-6	LEU	-	expression tag	UNP A0A1B3XFT6
H	-5	TYR	-	expression tag	UNP A0A1B3XFT6
H	-4	PHE	-	expression tag	UNP A0A1B3XFT6
H	-3	GLN	-	expression tag	UNP A0A1B3XFT6
H	-2	SER	-	expression tag	UNP A0A1B3XFT6
H	-1	ASN	-	expression tag	UNP A0A1B3XFT6
H	0	ALA	-	expression tag	UNP A0A1B3XFT6
H	195	GLY	-	linker	UNP A0A1B3XFT6

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

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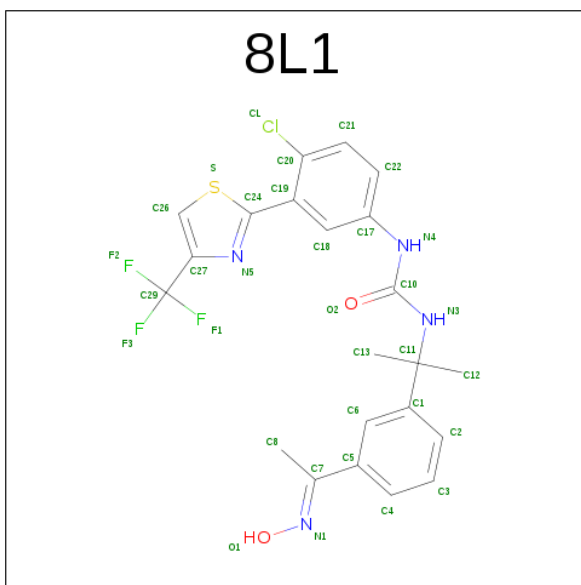
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
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 POTASSIUM ION (three-letter code: K) (formula: K).

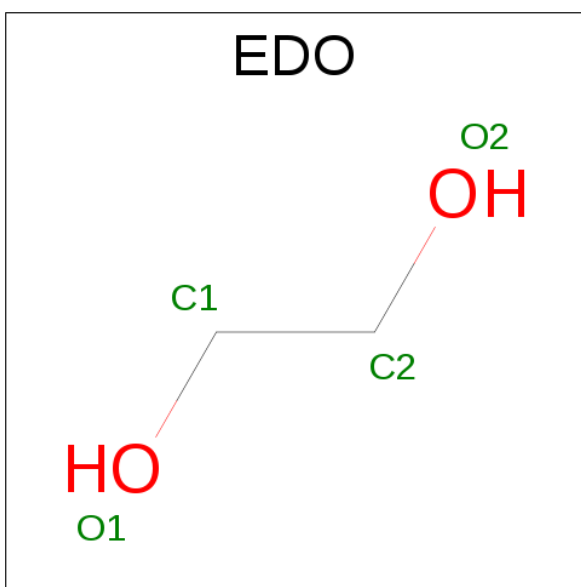
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		

- Molecule 4 is N-{4-chloro-3-[4-(trifluoromethyl)-1,3-thiazol-2-yl]phenyl}-N'-(2-{3-[(1E)-N-hydroxyethanimidoyl]phenyl}propan-2-yl)urea (three-letter code: 8L1) (formula: C₂₂H₂₀ClF₃N₄O₂S).



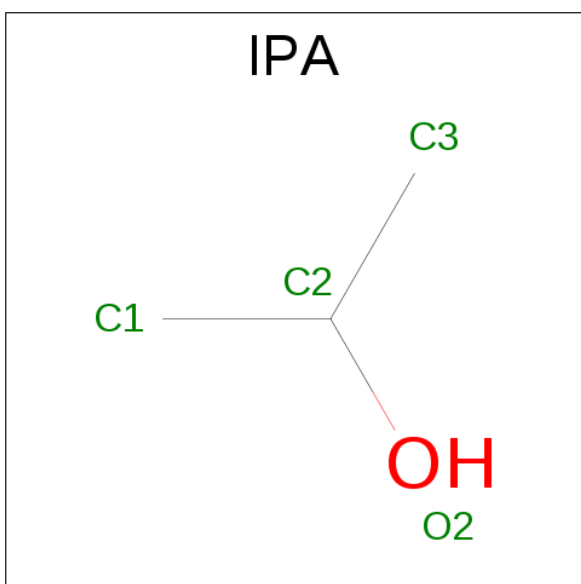
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	C	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	D	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	D	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	E	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	F	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	G	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
4	H	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			4	3	1		

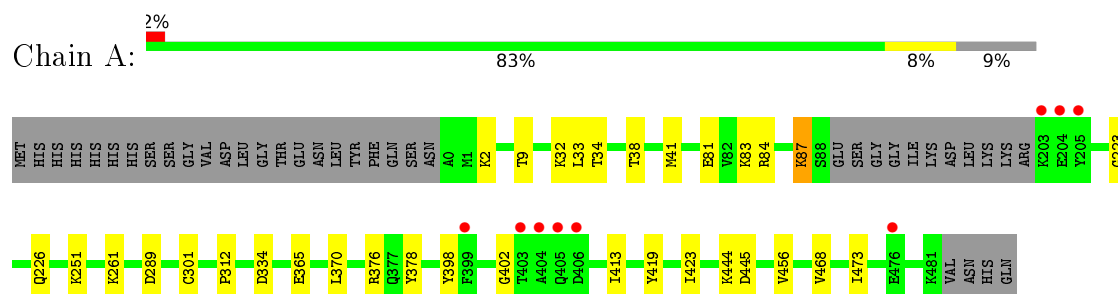
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	68	Total	O	0	0
			68	68		
7	C	63	Total	O	0	0
			63	63		
7	D	68	Total	O	0	0
			68	68		
7	E	119	Total	O	0	0
			119	119		
7	F	54	Total	O	0	0
			54	54		
7	G	50	Total	O	0	0
			50	50		
7	H	88	Total	O	0	0
			88	88		

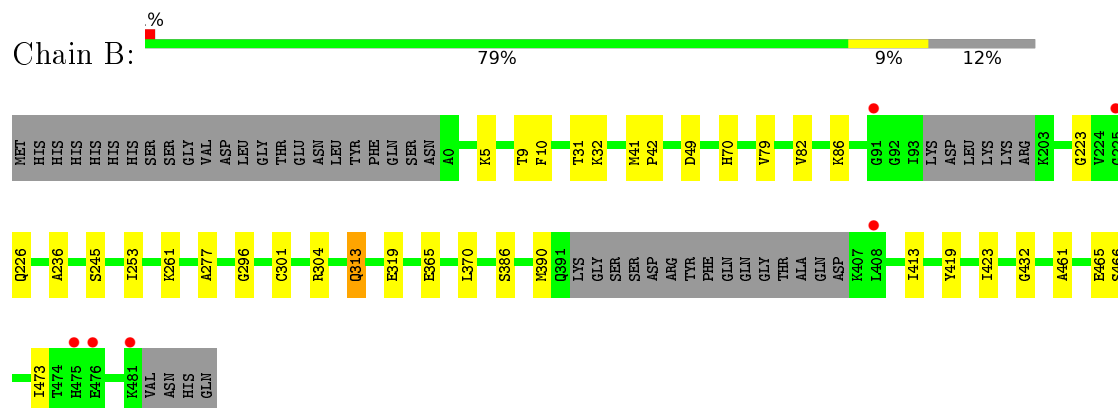
3 Residue-property plots [i](#)

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.

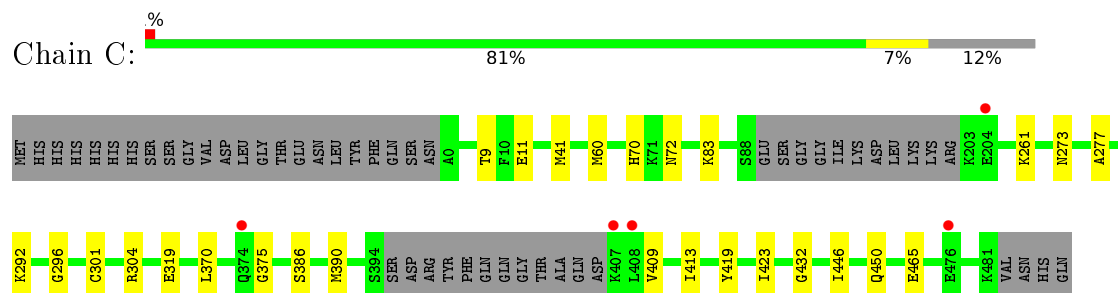
- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase



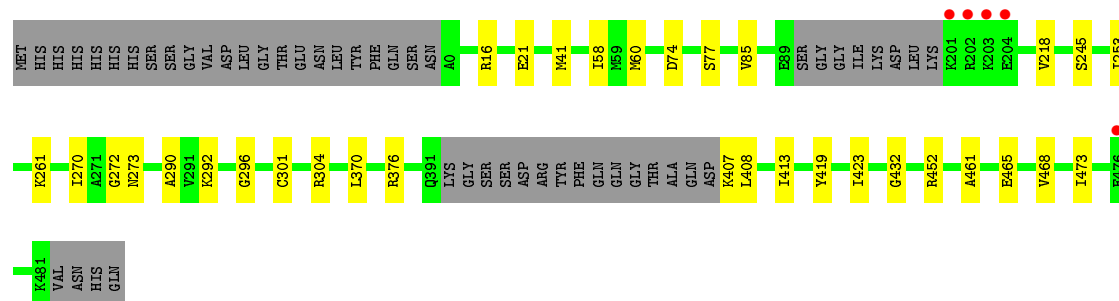
- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase



- [illegible]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.44Å 141.28Å 121.06Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	46.72 – 2.20 49.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (46.72-2.20) 90.4 (49.83-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.172 , 0.213 0.171 , 0.212	Depositor DCC
R_{free} test set	7429 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22377	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: IMP, K, IPA, EDO, 8L1

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	0.26	0/2772	0.47	0/3737
1	B	0.25	0/2688	0.46	0/3622
1	C	0.25	0/2676	0.46	0/3605
1	D	0.26	0/2677	0.46	0/3607
1	E	0.26	0/2693	0.48	0/3628
1	F	0.25	0/2721	0.45	0/3664
1	G	0.26	0/2666	0.47	0/3593
1	H	0.26	0/2686	0.49	1/3618 (0.0%)
All	All	0.26	0/21579	0.47	1/29074 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	376	ARG	NE-CZ-NH1	-8.72	115.94	120.30

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	2735	0	2807	23	0
1	B	2654	0	2741	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2642	0	2734	20	0
1	D	2643	0	2732	16	0
1	E	2659	0	2754	18	0
1	F	2687	0	2781	31	0
1	G	2632	0	2719	25	0
1	H	2652	0	2745	25	0
2	A	23	0	11	2	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	0	0
2	E	23	0	11	1	0
2	F	23	0	11	2	0
2	G	23	0	11	2	0
2	H	23	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	33	0	0	1	0
4	C	33	0	0	1	0
4	D	66	0	0	2	0
4	E	33	0	0	1	0
4	F	33	0	0	1	0
4	G	33	0	0	1	0
4	H	33	0	0	1	0
5	D	4	0	6	2	0
5	E	8	0	12	1	0
5	F	8	0	12	1	0
6	G	4	0	8	1	0
7	A	83	0	0	0	0
7	B	68	0	0	0	0
7	C	63	0	0	0	0
7	D	68	0	0	1	0
7	E	119	0	0	1	0
7	F	54	0	0	3	0
7	G	50	0	0	0	0
7	H	88	0	0	1	0
All	All	22377	0	22139	161	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.

All (161) 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:C:375:GLY:HA2	1:F:375:GLY:HA3	1.75	0.68
1:D:41:MET:HB3	5:D:505:EDO:H11	1.77	0.66
1:F:413:ILE:HD13	1:G:473:ILE:HG12	1.77	0.65
1:B:365:GLU:HB2	1:B:423:ILE:HD12	1.78	0.65
1:B:473:ILE:HG12	1:C:413:ILE:HD13	1.80	0.63
1:A:251:LYS:HB2	1:D:21:GLU:HG2	1.81	0.63
1:F:338:LYS:NZ	7:F:602:HOH:O	2.31	0.63
1:D:270:ILE:HG12	1:D:290:ALA:HB3	1.79	0.62
1:F:258:LYS:NZ	7:F:601:HOH:O	2.29	0.62
1:A:473:ILE:HG12	1:B:413:ILE:HD13	1.80	0.61
1:A:444:LYS:NZ	1:A:445:ASP:OD2	2.35	0.59
1:B:245:SER:HB2	1:B:253:ILE:HD11	1.84	0.59
1:C:465:GLU:OE2	1:D:9:THR:OG1	2.20	0.58
1:C:70:HIS:HD2	1:C:72:ASN:H	1.50	0.58
1:F:454:GLU:HB2	5:F:505:EDO:H12	1.85	0.58
1:G:365:GLU:HB2	1:G:423:ILE:HD12	1.85	0.57
1:G:413:ILE:HD13	1:H:473:ILE:HG12	1.87	0.57
1:E:473:ILE:HG12	1:H:413:ILE:HD13	1.86	0.57
1:C:446:ILE:O	1:C:450:GLN:HG3	2.05	0.56
1:F:365:GLU:OE1	1:F:365:GLU:N	2.37	0.56
1:B:79:VAL:HG13	1:B:236:ALA:HB2	1.86	0.56
1:H:273:ASN:HD21	1:H:292:LYS:NZ	2.04	0.56
4:D:504:8L1:S	4:D:504:8L1:CL	3.01	0.55
1:F:83:LYS:HD2	1:F:87:LYS:HE3	1.88	0.55
1:G:386:SER:O	1:G:390:MET:HG3	2.05	0.55
1:A:81:GLU:OE2	1:A:84:ARG:NH1	2.39	0.55
1:H:58:ILE:HG13	1:H:85:VAL:HG22	1.88	0.55
4:C:501:8L1:S	4:C:501:8L1:CL	3.03	0.54
1:F:251:LYS:HB2	1:G:21:GLU:HG2	1.90	0.54
1:G:85:VAL:HG11	1:G:218:VAL:HB	1.89	0.54
1:A:223:GLY:H	1:A:226:GLN:NE2	2.07	0.53
1:A:32:LYS:HD2	1:A:38:THR:HG22	1.90	0.53
1:D:370:LEU:HD13	7:D:606:HOH:O	2.08	0.53
1:F:409:VAL:HG21	1:G:432:GLY:HA3	1.90	0.53
1:G:245:SER:HB2	1:G:253:ILE:HD11	1.91	0.53
1:G:4:VAL:HG21	1:H:16:ARG:HD2	1.91	0.53
1:G:29:ILE:HD11	6:G:504:IPA:H2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD21	1:B:419:TYR:CD1	2.46	0.51
1:E:300:ILE:HD13	1:E:383:GLY:CA	2.40	0.51
1:B:386:SER:O	1:B:390:MET:HG3	2.11	0.51
1:B:313:GLN:HE21	1:B:313:GLN:HA	1.75	0.50
1:G:409:VAL:HG21	1:H:432:GLY:HA3	1.93	0.50
1:A:365:GLU:HB2	1:A:423:ILE:HD12	1.92	0.50
1:E:245:SER:HB2	1:E:253:ILE:HD11	1.94	0.50
1:E:377:GLN:NE2	7:E:602:HOH:O	2.45	0.50
1:H:270:ILE:HG12	1:H:290:ALA:HB3	1.92	0.50
1:C:60:MET:HE2	1:C:423:ILE:CG2	2.42	0.49
1:H:370:LEU:HD21	1:H:419:TYR:CD1	2.47	0.49
1:E:300:ILE:HD13	1:E:383:GLY:HA2	1.94	0.49
1:C:273:ASN:OD1	1:C:292:LYS:HE3	2.13	0.49
1:A:334:ASP:OD2	2:A:501:IMP:O2'	2.31	0.49
1:B:277:ALA:HB2	1:B:319:GLU:HG2	1.93	0.49
1:E:270:ILE:HG12	1:E:290:ALA:HB3	1.95	0.49
1:F:34:THR:HB	1:F:289:ASP:HB3	1.95	0.49
1:E:222:ILE:HG12	1:E:241:VAL:HG13	1.93	0.49
1:E:365:GLU:HB2	1:E:423:ILE:HD12	1.93	0.48
4:E:502:8L1:S	4:E:502:8L1:CL	3.09	0.48
1:F:296:GLY:HA3	1:F:304:ARG:HE	1.78	0.48
1:F:476:GLU:OE2	1:F:481:LYS:HE2	2.13	0.48
4:H:503:8L1:CL	4:H:503:8L1:S	3.08	0.48
1:F:334:ASP:OD2	2:F:502:IMP:O2'	2.30	0.48
1:G:413:ILE:HG12	1:H:468:VAL:HG21	1.95	0.48
1:C:301:CYS:SG	2:C:500:IMP:H2	2.54	0.48
1:G:334:ASP:OD2	2:G:502:IMP:O2'	2.31	0.48
4:G:503:8L1:S	4:G:503:8L1:CL	3.08	0.48
1:G:9:THR:OG1	1:H:465:GLU:OE2	2.30	0.47
1:B:466:SER:HA	1:C:304:ARG:HD2	1.97	0.47
1:A:9:THR:CG2	1:A:312:PRO:HB3	2.44	0.47
1:H:301:CYS:SG	2:H:502:IMP:H2	2.54	0.47
1:A:301:CYS:SG	2:A:501:IMP:H2	2.55	0.47
1:G:11:GLU:HB2	1:H:461:ALA:HB1	1.97	0.47
1:E:413:ILE:HD13	1:F:473:ILE:HG12	1.97	0.46
1:C:386:SER:O	1:C:390:MET:HG3	2.15	0.46
1:B:223:GLY:H	1:B:226:GLN:NE2	2.14	0.46
1:B:465:GLU:OE2	1:C:9:THR:OG1	2.32	0.46
1:B:9:THR:OG1	1:B:10:PHE:N	2.47	0.46
1:H:273:ASN:HD21	1:H:292:LYS:HZ1	1.61	0.46
1:A:398:TYR:O	1:A:402:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ALA:HB2	1:F:319:GLU:HG2	1.98	0.46
1:A:456:VAL:HG12	1:B:5:LYS:HG2	1.98	0.45
1:H:85:VAL:HG11	1:H:218:VAL:HB	1.97	0.45
1:C:432:GLY:HA3	1:D:409:VAL:HG21	1.98	0.45
1:F:296:GLY:HA3	1:F:304:ARG:NE	2.31	0.45
1:A:2:LYS:HB2	1:A:2:LYS:HE3	1.64	0.45
1:A:468:VAL:HG21	1:B:413:ILE:HG12	1.98	0.45
1:H:74:ASP:OD1	1:H:77:SER:N	2.39	0.45
1:B:461:ALA:HB1	1:C:11:GLU:HB2	1.99	0.45
1:B:296:GLY:HA3	1:B:304:ARG:NE	2.32	0.45
1:F:386:SER:O	1:F:390:MET:HG3	2.17	0.45
1:H:296:GLY:HA3	1:H:304:ARG:HG3	1.99	0.45
1:G:301:CYS:SG	2:G:502:IMP:H2	2.57	0.45
1:B:49:ASP:HA	1:B:70:HIS:CD2	2.52	0.44
1:E:301:CYS:SG	2:E:501:IMP:H2	2.57	0.44
1:B:31:THR:HG21	1:B:42:PRO:HB3	2.00	0.44
1:A:34:THR:HB	1:A:289:ASP:HB3	1.99	0.44
1:D:11:GLU:OE2	1:D:338:LYS:NZ	2.27	0.44
1:C:277:ALA:HB2	1:C:319:GLU:HG2	2.00	0.44
1:D:254:ILE:HD13	1:D:283:LEU:HD23	2.00	0.44
1:E:49:ASP:HA	1:E:70:HIS:CD2	2.53	0.44
1:B:296:GLY:HA3	1:B:304:ARG:HE	1.82	0.43
4:B:501:8L1:CL	4:B:501:8L1:S	3.12	0.43
1:B:432:GLY:HA3	1:C:409:VAL:HG21	1.99	0.43
1:C:70:HIS:CD2	1:C:72:ASN:H	2.33	0.43
1:E:409:VAL:HG21	1:F:432:GLY:HA3	2.00	0.43
1:B:301:CYS:SG	2:B:500:IMP:H2	2.59	0.43
1:F:204:GLU:HG2	1:F:205:TYR:CE2	2.53	0.43
1:H:60:MET:HE2	1:H:423:ILE:CG2	2.49	0.43
4:F:503:8L1:CL	4:F:503:8L1:S	3.13	0.43
1:H:60:MET:HE2	1:H:423:ILE:HG23	2.00	0.43
1:C:296:GLY:HA3	1:C:304:ARG:HE	1.82	0.43
1:H:245:SER:HB2	1:H:253:ILE:HD11	2.01	0.43
1:E:454:GLU:HB2	5:E:504:EDO:H22	2.01	0.43
1:F:9:THR:OG1	1:G:465:GLU:OE2	2.37	0.43
1:G:464:LYS:HB2	1:G:464:LYS:HE3	1.79	0.43
1:A:413:ILE:HD13	1:D:473:ILE:HG12	2.01	0.42
1:C:60:MET:HE2	1:C:423:ILE:HG23	2.00	0.42
1:F:270:ILE:HG12	1:F:290:ALA:HB3	2.01	0.42
1:D:332:ILE:HG12	1:D:353:SER:OG	2.19	0.42
1:E:9:THR:OG1	1:F:465:GLU:OE2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:GLU:HB2	1:F:423:ILE:HD12	2.00	0.42
1:B:296:GLY:HA2	1:B:301:CYS:SG	2.60	0.42
1:D:292:LYS:HB2	1:D:292:LYS:HE3	1.80	0.42
4:D:501:8L1:CL	4:D:501:8L1:S	3.15	0.42
1:F:304:ARG:HG2	1:F:309:VAL:O	2.18	0.42
1:F:301:CYS:SG	2:F:502:IMP:H2	2.60	0.42
1:H:272:GLY:HA3	1:H:273:ASN:HD22	1.84	0.42
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.81	0.42
1:A:376:ARG:NH2	1:A:378:TYR:OH	2.52	0.42
1:A:83:LYS:O	1:A:87:LYS:HB2	2.20	0.42
1:D:368:GLY:O	1:D:379:LYS:HE2	2.19	0.42
1:E:365:GLU:OE1	1:E:365:GLU:N	2.53	0.42
1:F:407:LYS:O	1:G:428:HIS:HE1	2.02	0.42
1:H:296:GLY:HA2	1:H:301:CYS:SG	2.60	0.42
1:D:413:ILE:C	1:D:413:ILE:HD12	2.40	0.42
1:F:82:VAL:O	1:F:86:LYS:HG2	2.20	0.42
1:A:9:THR:HG23	1:A:312:PRO:HB3	2.03	0.41
1:G:304:ARG:HG2	1:G:309:VAL:O	2.19	0.41
1:B:82:VAL:O	1:B:86:LYS:HG2	2.20	0.41
1:A:370:LEU:HD21	1:A:419:TYR:CD1	2.55	0.41
1:C:261:LYS:HA	1:C:261:LYS:HD3	1.81	0.41
1:D:29:ILE:HD11	5:D:505:EDO:H12	2.02	0.41
1:F:247:HIS:HD2	7:F:610:HOH:O	2.03	0.41
1:G:448:ASP:O	1:G:451:LYS:HG2	2.21	0.41
1:E:227:MET:CE	1:E:263:LYS:HD3	2.51	0.41
1:H:407:LYS:HE2	1:H:408:LEU:O	2.19	0.41
1:E:296:GLY:HA3	1:E:304:ARG:NE	2.36	0.41
1:F:83:LYS:HA	1:F:83:LYS:HD3	1.87	0.41
1:H:261:LYS:HA	1:H:261:LYS:HD3	1.88	0.41
1:A:33:LEU:HG	1:A:34:THR:HG23	2.03	0.41
1:B:261:LYS:HD2	1:B:261:LYS:HA	1.89	0.41
1:E:227:MET:HE3	1:E:263:LYS:HD3	2.03	0.41
1:F:321:VAL:HG11	1:F:350:GLY:HA3	2.02	0.41
1:H:452:ARG:NH1	7:H:606:HOH:O	2.53	0.40
1:C:370:LEU:HD21	1:C:419:TYR:CD1	2.55	0.40
1:D:338:LYS:HB2	1:D:338:LYS:HE2	1.83	0.40
1:G:370:LEU:HD23	1:G:379:LYS:HG2	2.03	0.40
1:G:251:LYS:HB2	1:H:21:GLU:HG2	2.03	0.40
1:G:86:LYS:HE3	1:G:86:LYS:HB3	1.76	0.40
1:A:413:ILE:HG12	1:D:468:VAL:HG21	2.02	0.40
1:F:296:GLY:N	1:F:297:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ALA:HB3	1:G:210:LYS:HE3	2.02	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	364/406 (90%)	357 (98%)	7 (2%)	0	100	100
1	B	352/406 (87%)	342 (97%)	10 (3%)	0	100	100
1	C	350/406 (86%)	343 (98%)	7 (2%)	0	100	100
1	D	349/406 (86%)	340 (97%)	9 (3%)	0	100	100
1	E	351/406 (86%)	343 (98%)	8 (2%)	0	100	100
1	F	355/406 (87%)	347 (98%)	8 (2%)	0	100	100
1	G	348/406 (86%)	341 (98%)	7 (2%)	0	100	100
1	H	350/406 (86%)	341 (97%)	9 (3%)	0	100	100
All	All	2819/3248 (87%)	2754 (98%)	65 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	288/323 (89%)	286 (99%)	2 (1%)	88	94
1	B	280/323 (87%)	277 (99%)	3 (1%)	80	89
1	C	279/323 (86%)	277 (99%)	2 (1%)	88	94
1	D	279/323 (86%)	278 (100%)	1 (0%)	93	97
1	E	281/323 (87%)	275 (98%)	6 (2%)	61	74
1	F	284/323 (88%)	279 (98%)	5 (2%)	66	79
1	G	278/323 (86%)	277 (100%)	1 (0%)	93	97
1	H	280/323 (87%)	279 (100%)	1 (0%)	93	97
All	All	2249/2584 (87%)	2228 (99%)	21 (1%)	84	92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	87	LYS
1	B	32	LYS
1	B	41	MET
1	B	313	GLN
1	C	41	MET
1	C	83	LYS
1	D	41	MET
1	E	28	LYS
1	E	41	MET
1	E	72	ASN
1	E	244	ASP
1	E	380	SER
1	E	407	LYS
1	F	41	MET
1	F	48	MET
1	F	80	ARG
1	F	200	LYS
1	F	376	ARG
1	G	41	MET
1	H	41	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	377	GLN
1	A	391	GLN
1	A	400	GLN
1	B	226	GLN
1	B	266	ASN
1	B	313	GLN
1	C	40	ASN
1	C	70	HIS
1	C	212	ASN
1	D	325	ASN
1	D	429	GLN
1	E	72	ASN
1	F	247	HIS
1	G	428	HIS
1	H	40	ASN
1	H	273	ASN
1	H	374	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	501	-	21,25,25	1.17	3 (14%)	22,38,38	2.47	3 (13%)
2	IMP	B	500	-	21,25,25	1.18	3 (14%)	22,38,38	2.45	3 (13%)
4	8L1	B	501	-	32,35,35	1.99	6 (18%)	44,52,52	2.07	9 (20%)
2	IMP	C	500	-	21,25,25	1.20	3 (14%)	22,38,38	2.55	4 (18%)
4	8L1	C	501	-	32,35,35	2.03	5 (15%)	44,52,52	2.22	10 (22%)
4	8L1	D	501	-	32,35,35	1.98	7 (21%)	44,52,52	1.96	9 (20%)
2	IMP	D	503	-	21,25,25	1.14	3 (14%)	22,38,38	2.40	4 (18%)
4	8L1	D	504	-	32,35,35	2.02	5 (15%)	44,52,52	2.22	9 (20%)
5	EDO	D	505	-	3,3,3	0.45	0	2,2,2	0.38	0
2	IMP	E	501	-	21,25,25	1.13	3 (14%)	22,38,38	2.46	4 (18%)
4	8L1	E	502	-	32,35,35	2.01	5 (15%)	44,52,52	2.12	8 (18%)
5	EDO	E	503	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	E	504	-	3,3,3	0.47	0	2,2,2	0.37	0
2	IMP	F	502	-	21,25,25	1.18	3 (14%)	22,38,38	2.61	4 (18%)
4	8L1	F	503	-	32,35,35	2.01	5 (15%)	44,52,52	2.12	9 (20%)
5	EDO	F	504	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	F	505	-	3,3,3	0.45	0	2,2,2	0.35	0
2	IMP	G	502	-	21,25,25	1.18	3 (14%)	22,38,38	2.43	3 (13%)
4	8L1	G	503	-	32,35,35	2.00	5 (15%)	44,52,52	2.18	9 (20%)
6	IPA	G	504	-	3,3,3	0.52	0	3,3,3	0.27	0
2	IMP	H	502	-	21,25,25	1.19	3 (14%)	22,38,38	2.43	4 (18%)
4	8L1	H	503	-	32,35,35	2.03	5 (15%)	44,52,52	2.19	10 (22%)

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	501	-	-	0/6/26/26	0/3/3/3
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3
4	8L1	B	501	-	-	0/29/31/31	0/3/3/3
2	IMP	C	500	-	-	0/6/26/26	0/3/3/3
4	8L1	C	501	-	-	0/29/31/31	0/3/3/3
4	8L1	D	501	-	-	0/29/31/31	0/3/3/3
2	IMP	D	503	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	8L1	D	504	-	-	0/29/31/31	0/3/3/3
5	EDO	D	505	-	-	0/1/1/1	0/0/0/0
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
4	8L1	E	502	-	-	0/29/31/31	0/3/3/3
5	EDO	E	503	-	-	0/1/1/1	0/0/0/0
5	EDO	E	504	-	-	0/1/1/1	0/0/0/0
2	IMP	F	502	-	-	0/6/26/26	0/3/3/3
4	8L1	F	503	-	-	0/29/31/31	0/3/3/3
5	EDO	F	504	-	-	0/1/1/1	0/0/0/0
5	EDO	F	505	-	-	0/1/1/1	0/0/0/0
2	IMP	G	502	-	-	0/6/26/26	0/3/3/3
4	8L1	G	503	-	-	0/29/31/31	0/3/3/3
6	IPA	G	504	-	-	0/0/0/0	0/0/0/0
2	IMP	H	502	-	-	0/6/26/26	0/3/3/3
4	8L1	H	503	-	-	0/29/31/31	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	8L1	C8-C7	-9.25	1.32	1.50
4	E	502	8L1	C8-C7	-9.23	1.32	1.50
4	F	503	8L1	C8-C7	-9.21	1.32	1.50
4	B	501	8L1	C8-C7	-9.20	1.32	1.50
4	H	503	8L1	C8-C7	-9.18	1.32	1.50
4	G	503	8L1	C8-C7	-9.17	1.32	1.50
4	D	504	8L1	C8-C7	-9.17	1.32	1.50
4	D	501	8L1	C8-C7	-9.17	1.32	1.50
4	D	504	8L1	C17-N4	-2.59	1.36	1.41
4	H	503	8L1	C17-N4	-2.59	1.36	1.41
4	E	502	8L1	C17-N4	-2.48	1.37	1.41
4	C	501	8L1	C17-N4	-2.47	1.37	1.41
4	F	503	8L1	C17-N4	-2.42	1.37	1.41
4	G	503	8L1	C17-N4	-2.41	1.37	1.41
4	B	501	8L1	C17-N4	-2.33	1.37	1.41
4	D	501	8L1	C17-N4	-2.22	1.37	1.41
4	D	501	8L1	C11-C1	-2.08	1.50	1.53
2	E	501	IMP	C2-N1	2.03	1.37	1.33
2	D	503	IMP	C2-N1	2.04	1.37	1.33
4	D	501	8L1	C26-S	2.12	1.74	1.70
4	B	501	8L1	C26-S	2.16	1.74	1.70
2	A	501	IMP	C2-N1	2.16	1.38	1.33
2	F	502	IMP	C2-N1	2.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	502	IMP	C2-N1	2.21	1.38	1.33
2	G	502	IMP	C2-N1	2.24	1.38	1.33
2	B	500	IMP	C2-N1	2.27	1.38	1.33
2	C	500	IMP	C2-N1	2.29	1.38	1.33
4	G	503	8L1	C20-CL	2.43	1.79	1.73
4	E	502	8L1	C20-CL	2.44	1.80	1.73
4	D	504	8L1	C20-CL	2.45	1.80	1.73
4	D	501	8L1	C20-CL	2.46	1.80	1.73
4	H	503	8L1	C20-CL	2.47	1.80	1.73
4	B	501	8L1	C20-CL	2.50	1.80	1.73
4	C	501	8L1	C20-CL	2.52	1.80	1.73
4	F	503	8L1	C20-CL	2.55	1.80	1.73
2	E	501	IMP	C6-N1	2.68	1.37	1.33
2	D	503	IMP	C6-N1	2.73	1.38	1.33
2	C	500	IMP	C6-N1	2.76	1.38	1.33
2	A	501	IMP	C6-N1	2.78	1.38	1.33
4	D	501	8L1	C24-N5	2.79	1.35	1.31
2	B	500	IMP	C6-N1	2.83	1.38	1.33
2	G	502	IMP	C6-N1	2.84	1.38	1.33
4	D	501	8L1	C7-N1	2.86	1.33	1.28
2	F	502	IMP	C6-N1	2.87	1.38	1.33
2	H	502	IMP	C6-N1	2.94	1.38	1.33
4	D	504	8L1	C7-N1	2.97	1.34	1.28
4	B	501	8L1	C24-N5	2.97	1.35	1.31
4	B	501	8L1	C7-N1	2.99	1.34	1.28
4	F	503	8L1	C24-N5	3.00	1.35	1.31
4	F	503	8L1	C7-N1	3.04	1.34	1.28
4	E	502	8L1	C7-N1	3.05	1.34	1.28
4	G	503	8L1	C7-N1	3.05	1.34	1.28
4	H	503	8L1	C24-N5	3.09	1.35	1.31
4	E	502	8L1	C24-N5	3.09	1.35	1.31
4	H	503	8L1	C7-N1	3.11	1.34	1.28
4	C	501	8L1	C7-N1	3.12	1.34	1.28
4	G	503	8L1	C24-N5	3.16	1.36	1.31
2	E	501	IMP	C2-N3	3.34	1.38	1.32
4	D	504	8L1	C24-N5	3.35	1.36	1.31
4	C	501	8L1	C24-N5	3.36	1.36	1.31
2	D	503	IMP	C2-N3	3.41	1.38	1.32
2	F	502	IMP	C2-N3	3.45	1.38	1.32
2	A	501	IMP	C2-N3	3.46	1.38	1.32
2	G	502	IMP	C2-N3	3.49	1.38	1.32
2	B	500	IMP	C2-N3	3.51	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	502	IMP	C2-N3	3.52	1.38	1.32
2	C	500	IMP	C2-N3	3.55	1.38	1.32

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	502	IMP	N3-C2-N1	-10.95	120.27	128.87
2	C	500	IMP	N3-C2-N1	-10.77	120.41	128.87
2	G	502	IMP	N3-C2-N1	-10.51	120.62	128.87
2	E	501	IMP	N3-C2-N1	-10.49	120.63	128.87
2	A	501	IMP	N3-C2-N1	-10.47	120.65	128.87
2	H	502	IMP	N3-C2-N1	-10.36	120.73	128.87
2	D	503	IMP	N3-C2-N1	-10.32	120.77	128.87
2	B	500	IMP	N3-C2-N1	-10.30	120.78	128.87
4	C	501	8L1	C26-C27-C29	-8.13	118.57	128.14
4	D	504	8L1	C26-C27-C29	-7.86	118.89	128.14
4	H	503	8L1	C26-C27-C29	-7.53	119.28	128.14
4	G	503	8L1	C26-C27-C29	-7.13	119.75	128.14
4	E	502	8L1	C26-C27-C29	-6.81	120.13	128.14
4	F	503	8L1	C26-C27-C29	-6.22	120.82	128.14
4	B	501	8L1	C26-C27-C29	-6.03	121.04	128.14
4	D	501	8L1	C26-C27-C29	-5.46	121.71	128.14
4	D	501	8L1	C6-C5-C7	-5.43	116.15	120.54
4	F	503	8L1	C4-C5-C7	-3.46	116.84	121.21
2	F	502	IMP	C1'-N9-C4	-3.30	123.12	126.81
4	H	503	8L1	C4-C5-C7	-3.15	117.23	121.21
4	D	504	8L1	C4-C5-C7	-3.09	117.31	121.21
4	G	503	8L1	C4-C5-C7	-2.98	117.44	121.21
4	E	502	8L1	C4-C5-C7	-2.95	117.48	121.21
2	C	500	IMP	C1'-N9-C4	-2.83	123.64	126.81
4	B	501	8L1	C4-C5-C7	-2.74	117.75	121.21
4	C	501	8L1	C4-C5-C7	-2.56	117.98	121.21
4	H	503	8L1	F3-C29-C27	-2.55	107.88	112.54
2	E	501	IMP	C1'-N9-C4	-2.53	123.98	126.81
4	H	503	8L1	C8-C7-N1	-2.36	115.53	123.11
4	B	501	8L1	C8-C7-N1	-2.34	115.59	123.11
4	F	503	8L1	C8-C7-N1	-2.33	115.60	123.11
2	H	502	IMP	C1'-N9-C4	-2.31	124.22	126.81
4	D	504	8L1	C8-C7-N1	-2.30	115.70	123.11
4	G	503	8L1	C8-C7-N1	-2.29	115.75	123.11
4	C	501	8L1	C8-C7-N1	-2.29	115.75	123.11
4	E	502	8L1	C8-C7-N1	-2.24	115.91	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	8L1	C29-C27-N5	-2.20	116.93	119.69
4	B	501	8L1	F1-C29-C27	-2.14	108.63	112.54
4	C	501	8L1	F3-C29-C27	-2.11	108.68	112.54
2	D	503	IMP	C1'-N9-C4	-2.05	124.51	126.81
4	D	501	8L1	C22-C17-C18	-2.05	117.24	119.68
4	G	503	8L1	C2-C1-C11	-2.04	118.56	121.17
4	F	503	8L1	F1-C29-C27	-2.03	108.83	112.54
4	D	501	8L1	F2-C29-C27	-2.02	108.86	112.54
4	C	501	8L1	C5-C7-N1	2.02	125.24	116.90
4	B	501	8L1	C5-C7-N1	2.03	125.30	116.90
4	E	502	8L1	C5-C7-N1	2.04	125.32	116.90
4	D	504	8L1	C5-C7-N1	2.04	125.32	116.90
4	D	504	8L1	C19-C18-C17	2.07	122.14	119.32
2	E	501	IMP	C2-N1-C6	2.08	119.71	116.13
2	G	502	IMP	C2-N1-C6	2.09	119.74	116.13
4	D	501	8L1	C8-C7-C5	2.11	122.84	119.64
2	A	501	IMP	C2-N1-C6	2.11	119.76	116.13
4	F	503	8L1	C19-C18-C17	2.12	122.20	119.32
4	E	502	8L1	C19-C18-C17	2.12	122.21	119.32
2	D	503	IMP	C2-N1-C6	2.13	119.81	116.13
4	F	503	8L1	C5-C7-N1	2.14	125.78	116.90
4	H	503	8L1	C5-C7-N1	2.17	125.88	116.90
4	H	503	8L1	C19-C20-CL	2.17	124.07	120.70
2	C	500	IMP	C2-N1-C6	2.20	119.91	116.13
2	H	502	IMP	C2-N1-C6	2.22	119.95	116.13
2	B	500	IMP	C2-N1-C6	2.26	120.02	116.13
4	H	503	8L1	C19-C18-C17	2.29	122.44	119.32
4	G	503	8L1	C19-C20-CL	2.33	124.31	120.70
4	C	501	8L1	C6-C5-C7	2.34	122.44	120.54
2	F	502	IMP	C2-N1-C6	2.35	120.18	116.13
4	C	501	8L1	C19-C18-C17	2.41	122.60	119.32
2	D	503	IMP	O2P-P-O1P	2.46	118.64	110.63
2	G	502	IMP	O2P-P-O1P	2.50	118.77	110.63
2	H	502	IMP	O2P-P-O1P	2.54	118.91	110.63
2	E	501	IMP	O2P-P-O1P	2.55	118.95	110.63
2	F	502	IMP	O2P-P-O1P	2.56	118.97	110.63
4	G	503	8L1	C19-C18-C17	2.57	122.82	119.32
4	C	501	8L1	C19-C20-CL	2.60	124.72	120.70
2	C	500	IMP	O2P-P-O1P	2.63	119.21	110.63
4	B	501	8L1	C19-C18-C17	2.64	122.92	119.32
4	B	501	8L1	C6-C5-C7	2.68	122.71	120.54
4	D	501	8L1	C19-C18-C17	2.74	123.05	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	8L1	C19-C24-N5	2.82	128.37	123.50
4	D	504	8L1	C19-C20-CL	2.87	125.15	120.70
4	G	503	8L1	C6-C5-C7	3.01	122.98	120.54
4	B	501	8L1	C19-C24-N5	3.05	128.76	123.50
4	E	502	8L1	C6-C5-C7	3.05	123.02	120.54
2	A	501	IMP	O3P-P-O2P	3.14	118.95	107.44
2	B	500	IMP	O3P-P-O2P	3.16	119.03	107.44
4	D	504	8L1	C6-C5-C7	3.19	123.13	120.54
4	H	503	8L1	C19-C24-N5	3.39	129.36	123.50
4	H	503	8L1	C6-C5-C7	3.52	123.39	120.54
4	F	503	8L1	C19-C24-N5	3.53	129.59	123.50
4	F	503	8L1	C6-C5-C7	3.86	123.67	120.54
4	G	503	8L1	C19-C24-N5	3.92	130.27	123.50
4	E	502	8L1	C19-C24-N5	3.99	130.39	123.50
4	C	501	8L1	C19-C24-N5	4.11	130.59	123.50
4	D	504	8L1	C19-C24-N5	4.18	130.72	123.50
4	D	501	8L1	O1-N1-C7	5.99	121.61	112.90
4	G	503	8L1	O1-N1-C7	7.65	124.03	112.90
4	D	504	8L1	O1-N1-C7	7.74	124.16	112.90
4	E	502	8L1	O1-N1-C7	7.84	124.31	112.90
4	F	503	8L1	O1-N1-C7	7.86	124.34	112.90
4	B	501	8L1	O1-N1-C7	7.92	124.42	112.90
4	C	501	8L1	O1-N1-C7	8.02	124.57	112.90
4	H	503	8L1	O1-N1-C7	8.11	124.69	112.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	2	0
2	B	500	IMP	1	0
4	B	501	8L1	1	0
2	C	500	IMP	1	0
4	C	501	8L1	1	0
4	D	501	8L1	1	0
4	D	504	8L1	1	0
5	D	505	EDO	2	0
2	E	501	IMP	1	0
4	E	502	8L1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	504	EDO	1	0
2	F	502	IMP	2	0
4	F	503	8L1	1	0
5	F	505	EDO	1	0
2	G	502	IMP	2	0
4	G	503	8L1	1	0
6	G	504	IPA	1	0
2	H	502	IMP	1	0
4	H	503	8L1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	368/406 (90%)	-0.23	9 (2%) 62 61	20, 33, 68, 108	0
1	B	358/406 (88%)	-0.35	6 (1%) 73 72	22, 36, 62, 92	0
1	C	356/406 (87%)	-0.40	5 (1%) 78 77	25, 37, 60, 91	0
1	D	355/406 (87%)	-0.39	2 (0%) 90 90	24, 38, 62, 107	0
1	E	357/406 (87%)	-0.48	5 (1%) 78 77	19, 29, 53, 120	0
1	F	361/406 (88%)	-0.20	7 (1%) 70 68	22, 40, 73, 113	0
1	G	354/406 (87%)	-0.33	8 (2%) 64 63	22, 37, 66, 109	0
1	H	356/406 (87%)	-0.40	5 (1%) 78 77	21, 34, 58, 111	0
All	All	2865/3248 (88%)	-0.35	47 (1%) 74 73	19, 35, 63, 120	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	202	ARG	6.6
1	E	202	ARG	5.5
1	A	406	ASP	5.1
1	B	476	GLU	5.0
1	A	203	LYS	5.0
1	F	476	GLU	4.9
1	D	202	ARG	4.5
1	F	199	LEU	4.0
1	A	399	PHE	4.0
1	H	201	LYS	3.8
1	G	476	GLU	3.7
1	H	203	LYS	3.5
1	F	408	LEU	3.4
1	E	392	LYS	3.2
1	B	481	LYS	3.2
1	A	404	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	3.2
1	F	475	HIS	3.0
1	C	476	GLU	2.9
1	E	408	LEU	2.9
1	B	408	LEU	2.7
1	H	204	GLU	2.7
1	C	204	GLU	2.6
1	C	408	LEU	2.6
1	F	477	ALA	2.6
1	F	407	LYS	2.5
1	G	203	LYS	2.5
1	B	475	HIS	2.5
1	G	213	PHE	2.5
1	G	89	GLU	2.4
1	F	373	TYR	2.4
1	D	213	PHE	2.3
1	C	407	LYS	2.3
1	E	203	LYS	2.2
1	A	205	TYR	2.2
1	G	481	LYS	2.2
1	G	477	ALA	2.2
1	A	476	GLU	2.2
1	A	405	GLN	2.1
1	B	91	GLY	2.1
1	A	403	THR	2.1
1	E	244	ASP	2.1
1	H	476	GLU	2.1
1	G	212	ASN	2.1
1	G	475	HIS	2.0
1	B	225	GLY	2.0
1	C	374	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	E	503	4/4	0.92	0.21	4.25	41,43,44,50	0
6	IPA	G	504	4/4	0.86	0.20	3.47	44,48,48,51	0
4	8L1	E	502	33/33	0.92	0.18	3.38	28,37,90,91	0
5	EDO	F	505	4/4	0.93	0.17	3.26	42,43,45,52	0
4	8L1	C	501	33/33	0.89	0.14	3.16	32,39,83,85	0
5	EDO	E	504	4/4	0.87	0.15	2.62	43,50,52,54	0
5	EDO	D	505	4/4	0.88	0.18	2.41	43,45,47,51	0
4	8L1	G	503	33/33	0.92	0.16	2.35	32,43,93,94	0
4	8L1	H	503	33/33	0.93	0.14	2.32	24,33,79,81	0
3	K	A	502	1/1	0.98	0.15	2.19	37,37,37,37	0
4	8L1	F	503	33/33	0.87	0.16	2.12	35,46,98,100	0
4	8L1	B	501	33/33	0.89	0.17	1.85	34,41,94,96	0
4	8L1	D	504	33/33	0.93	0.13	0.96	38,46,77,80	0
3	K	E	505	1/1	0.98	0.13	0.87	29,29,29,29	0
5	EDO	F	504	4/4	0.93	0.14	0.83	44,46,49,54	0
4	8L1	D	501	33/33	0.93	0.12	0.58	22,36,80,81	0
2	IMP	B	500	23/23	0.97	0.12	0.54	22,26,28,31	0
2	IMP	C	500	23/23	0.98	0.12	0.33	22,27,31,32	0
2	IMP	H	502	23/23	0.98	0.12	0.15	19,26,30,33	0
2	IMP	F	502	23/23	0.98	0.14	0.10	26,31,35,37	0
2	IMP	D	503	23/23	0.98	0.10	0.05	26,30,34,35	0
2	IMP	E	501	23/23	0.98	0.10	0.03	17,23,26,27	0
3	K	D	502	1/1	0.99	0.13	-0.12	28,28,28,28	0
2	IMP	A	501	23/23	0.98	0.12	-0.16	18,22,25,29	0
2	IMP	G	502	23/23	0.98	0.10	-0.30	22,30,33,34	0
3	K	F	501	1/1	0.99	0.08	-0.93	32,32,32,32	0
3	K	B	502	1/1	0.99	0.10	-1.19	47,47,47,47	0
3	K	C	502	1/1	0.99	0.07	-1.39	40,40,40,40	0
3	K	H	501	1/1	0.97	0.08	-1.40	39,39,39,39	0
3	K	G	501	1/1	0.97	0.07	-4.45	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.