Full wwPDB X-ray Structure Validation Report (i)

Feb 23, 2017 – 12:27 PM EST

PDB ID	:	5URQ
Title	:	Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Campylobacter jejuni in the complex with 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	:	2.70 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:

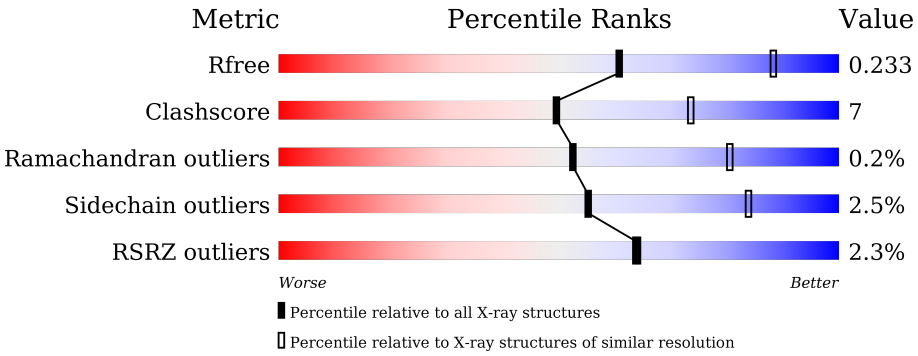
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	406	73% 14% 13%
1	B	406	68% 19% 12%
1	C	406	72% 14% 13%
1	D	406	75% 13% 12%
1	E	406	73% 15% 12%
1	F	406	70% 17% 12%

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Mol	Chain	Length	Quality of chain
1	G	406	2% 70% 17% 13%
1	H	406	4% 74% 13% 13%

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	8L7	G	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21625 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	355	Total	C	N	O	S	0	0	0
			2636	1658	464	500	14			
1	B	356	Total	C	N	O	S	0	0	0
			2649	1666	468	501	14			
1	C	354	Total	C	N	O	S	0	0	0
			2634	1656	466	498	14			
1	D	359	Total	C	N	O	S	0	0	0
			2669	1678	473	504	14			
1	E	357	Total	C	N	O	S	0	0	0
			2647	1663	467	503	14			
1	F	356	Total	C	N	O	S	0	0	0
			2642	1661	466	501	14			
1	H	355	Total	C	N	O	S	0	0	0
			2639	1661	465	499	14			
1	G	355	Total	C	N	O	S	0	0	0
			2636	1658	465	499	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
A	-11	LEU	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-9	THR	-	expression tag	UNP A0A1B3XFT6
B	-8	GLU	-	expression tag	UNP A0A1B3XFT6
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	195	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
C	-19	HIS	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	-2	SER	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
F	-10	GLY	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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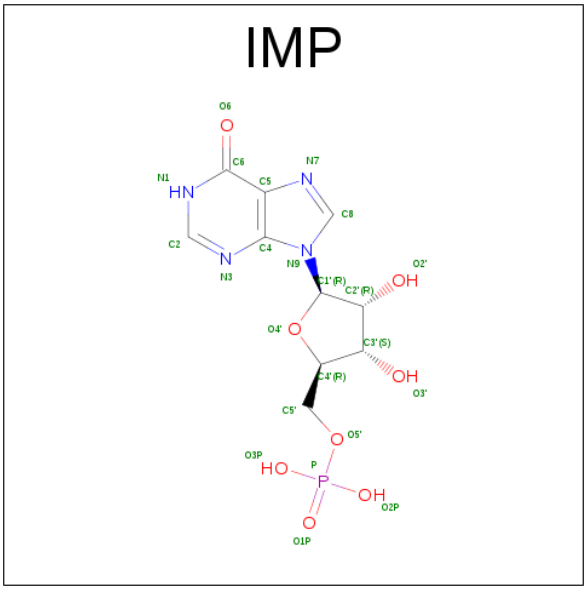
Chain	Residue	Modelled	Actual	Comment	Reference
G	-17	HIS	-	expression tag	UNP A0A1B3XFT6
G	-16	SER	-	expression tag	UNP A0A1B3XFT6
G	-15	SER	-	expression tag	UNP A0A1B3XFT6
G	-14	GLY	-	expression tag	UNP A0A1B3XFT6
G	-13	VAL	-	expression tag	UNP A0A1B3XFT6
G	-12	ASP	-	expression tag	UNP A0A1B3XFT6
G	-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

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



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		

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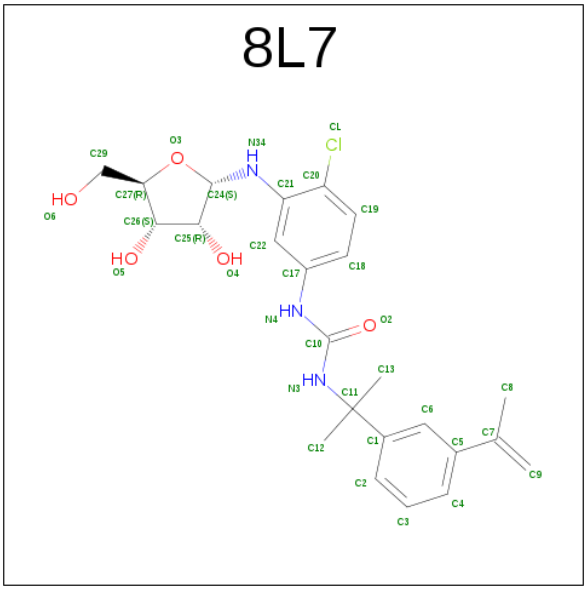
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- 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: $C_{24}H_{30}ClN_3O_5$).



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	E	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	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		
3	G	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	2	Total	K	0	0
			2	2		
4	B	1	Total	K	0	0
			1	1		
4	A	2	Total	K	0	0
			2	2		
4	F	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

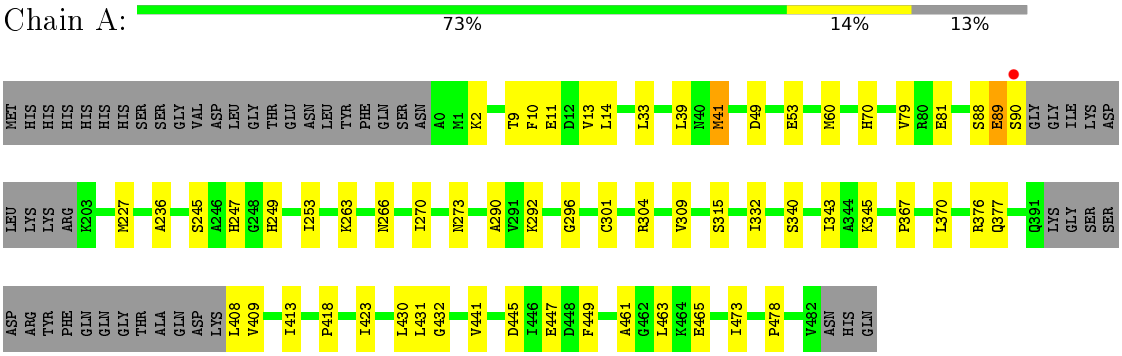
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	2	Total	O	0	0
			2	2		
5	D	3	Total	O	0	0
			3	3		
5	E	3	Total	O	0	0
			3	3		
5	F	4	Total	O	0	0
			4	4		
5	G	2	Total	O	0	0
			2	2		

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.

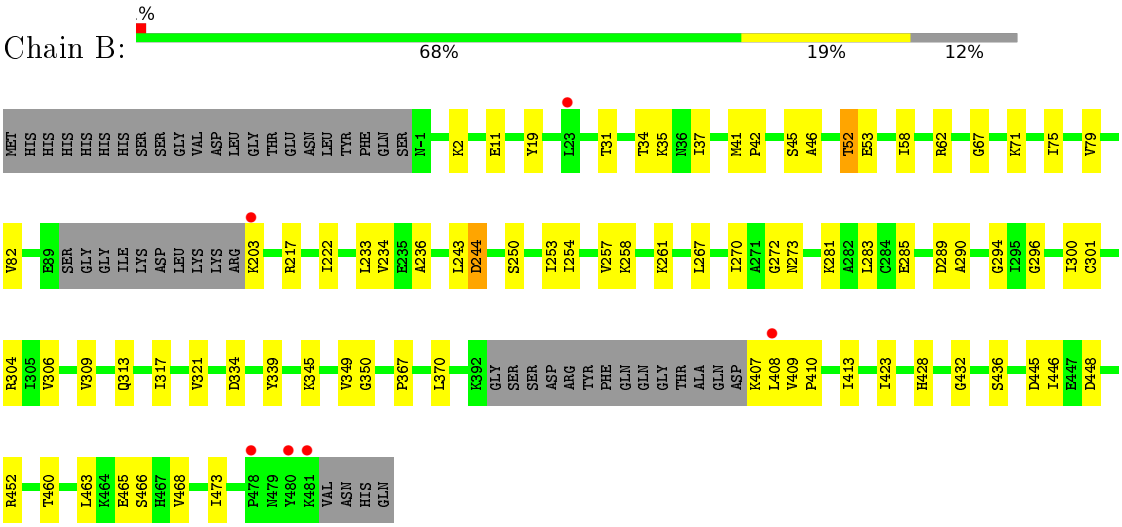
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



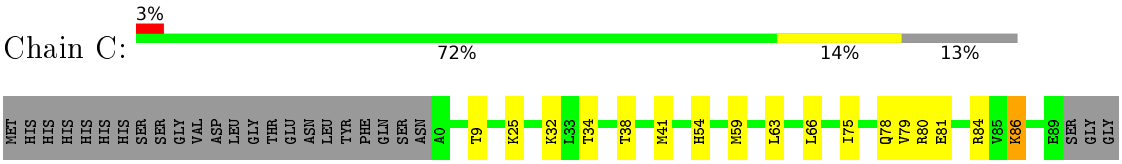
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

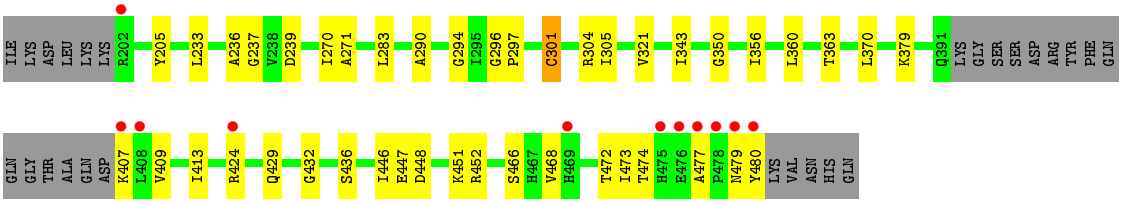
Chain B:



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

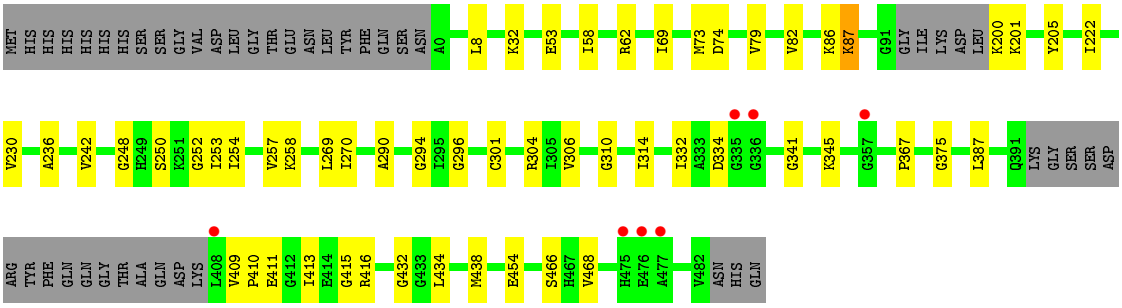
Chain C:





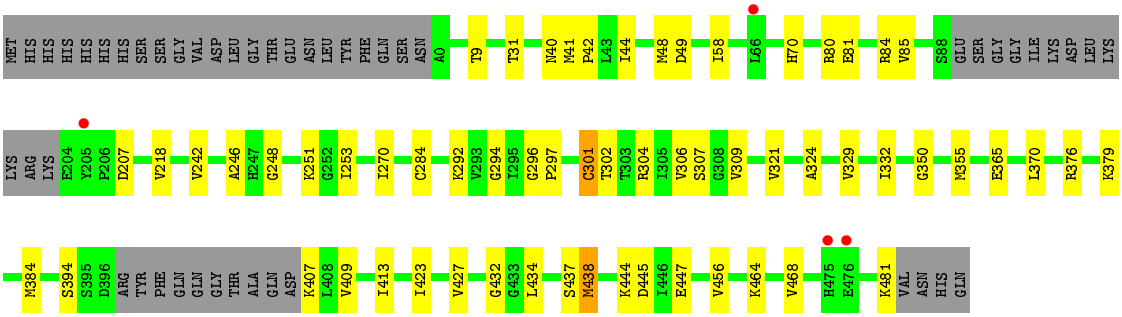
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:



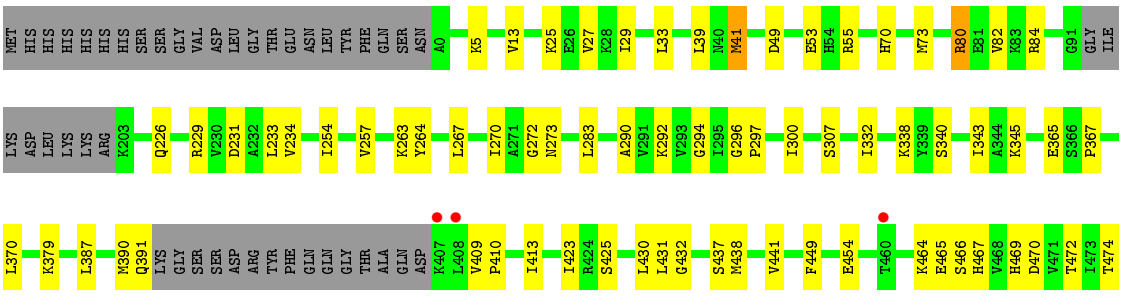
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

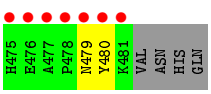
Chain E:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

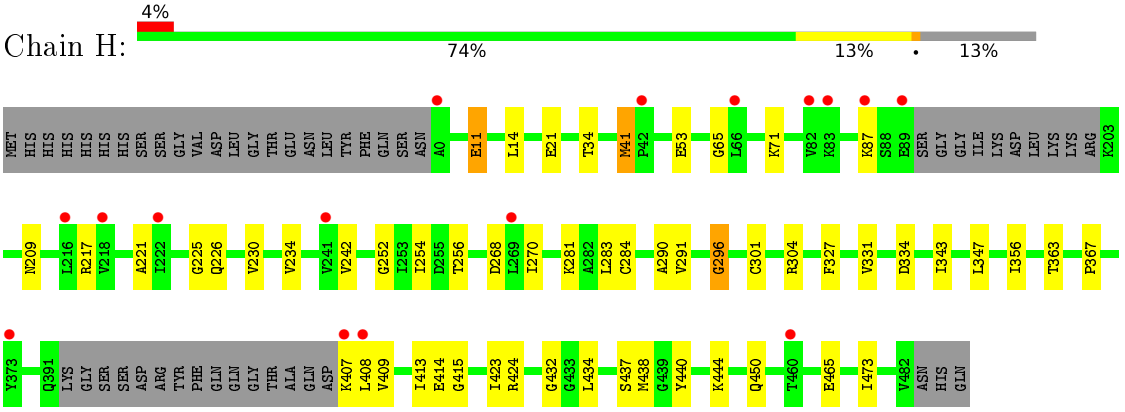
Chain F:





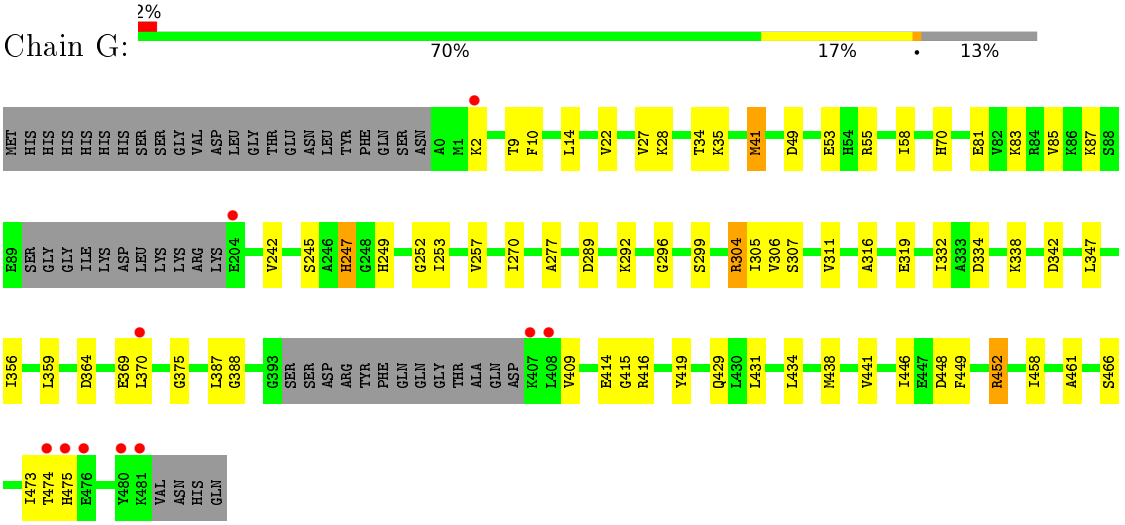
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain H:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.49Å 141.79Å 121.64Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	40.80 – 2.70 49.09 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.80-2.70) 97.8 (49.09-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.180 , 0.235 0.178 , 0.233	Depositor DCC
R_{free} test set	4461 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21625	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.44	0/2670	0.63	0/3600
1	B	0.46	0/2683	0.62	0/3615
1	C	0.42	0/2668	0.59	0/3596
1	D	0.44	0/2703	0.61	0/3641
1	E	0.42	0/2681	0.61	0/3613
1	F	0.43	0/2676	0.60	0/3606
1	G	0.40	0/2670	0.58	0/3598
1	H	0.41	0/2673	0.60	1/3603 (0.0%)
All	All	0.43	0/21424	0.61	1/28872 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	296	GLY	C-N-CD	5.06	139.03	128.40

There are no chirality outliers.

There are no planarity outliers.

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	2636	0	2720	41	0
1	B	2649	0	2738	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2634	0	2719	43	0
1	D	2669	0	2762	44	0
1	E	2647	0	2730	37	0
1	F	2642	0	2727	51	0
1	G	2636	0	2722	54	0
1	H	2639	0	2728	40	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	0	0
2	D	23	0	11	1	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	2	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	1	0
3	E	33	0	0	0	0
3	F	33	0	0	0	0
3	G	33	0	0	1	0
3	H	33	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	1	0
5	D	3	0	0	1	0
5	E	3	0	0	0	0
5	F	4	0	0	0	0
5	G	2	0	0	0	0
All	All	21625	0	21934	308	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 7.

All (308) 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:473:ILE:HG12	1:C:413:ILE:HD13	1.75	0.68
1:B:432:GLY:HA3	1:C:409:VAL:HG21	1.75	0.67
1:H:296:GLY:HA2	1:H:301:CYS:SG	2.35	0.67
1:G:83:LYS:HB3	1:G:87:LYS:HE3	1.77	0.66
1:F:465:GLU:OE1	1:G:304:ARG:NH1	2.27	0.65
1:B:19:TYR:O	1:B:452:ARG:NH2	2.29	0.65
1:B:281:LYS:O	1:B:285:GLU:HG3	1.96	0.65
1:H:343:ILE:HD11	1:H:356:ILE:HD11	1.77	0.65
1:H:270:ILE:HG12	1:H:290:ALA:HB3	1.77	0.65
1:C:432:GLY:HA3	1:D:409:VAL:HG21	1.77	0.65
1:H:87:LYS:HG3	1:H:87:LYS:O	1.97	0.64
1:G:58:ILE:HG13	1:G:85:VAL:HG22	1.80	0.64
1:D:301:CYS:SG	5:D:602:HOH:O	2.55	0.64
1:C:296:GLY:HA2	1:C:301:CYS:SG	2.38	0.63
1:B:313:GLN:O	1:B:317:ILE:HG13	1.98	0.63
1:B:370:LEU:HD12	1:B:370:LEU:N	2.15	0.62
1:B:79:VAL:HG13	1:B:236:ALA:HB2	1.82	0.62
1:E:365:GLU:HB2	1:E:423:ILE:HD12	1.81	0.62
1:B:407:LYS:HD3	1:B:408:LEU:H	1.65	0.61
1:F:479:ASN:ND2	1:G:306:VAL:HB	2.15	0.61
1:A:432:GLY:HA3	1:B:409:VAL:HG21	1.81	0.61
1:F:343:ILE:HD11	1:F:430:LEU:HD22	1.83	0.61
1:F:474:THR:HG22	1:G:416:ARG:HH11	1.65	0.60
1:E:302:THR:O	1:E:306:VAL:HG22	2.02	0.60
1:C:86:LYS:NZ	1:C:239:ASP:OD2	2.35	0.60
1:C:86:LYS:HE2	1:C:237:GLY:O	2.02	0.60
1:A:301:CYS:SG	2:A:501:IMP:H2	2.42	0.60
1:E:432:GLY:HA3	1:F:409:VAL:HG21	1.82	0.60
1:C:466:SER:OG	1:D:304:ARG:NH1	2.27	0.59
1:G:252:GLY:HA3	3:G:503:8L7:O6	2.03	0.59
1:H:34:THR:OG1	1:H:268:ASP:OD1	2.20	0.59
1:G:448:ASP:O	1:G:452:ARG:HG2	2.03	0.59
1:H:252:GLY:O	1:H:256:THR:HG23	2.04	0.58
1:F:80:ARG:O	1:F:84:ARG:HG3	2.02	0.58
1:B:58:ILE:O	1:B:62:ARG:HG3	2.04	0.58
1:B:301:CYS:SG	2:B:500:IMP:H2	2.44	0.58
1:C:80:ARG:O	1:C:84:ARG:HG3	2.04	0.57
1:E:468:VAL:HG21	1:F:413:ILE:HG12	1.85	0.57
1:C:305:ILE:N	1:C:305:ILE:HD12	2.18	0.57
1:B:34:THR:HG22	1:B:37:ILE:HB	1.85	0.57
1:C:343:ILE:HD11	1:C:356:ILE:HD11	1.85	0.57
1:B:339:TYR:CG	1:C:305:ILE:HG23	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:HIS:ND1	1:C:81:GLU:OE1	2.26	0.57
1:G:334:ASP:OD2	2:G:502:IMP:O2'	2.22	0.57
1:H:434:LEU:HG	1:H:438:MET:HE1	1.86	0.57
1:F:454:GLU:HG2	1:G:2:LYS:HE2	1.86	0.57
1:A:2:LYS:HD2	1:D:454:GLU:HG2	1.87	0.57
1:E:248:GLY:HA2	1:E:253:ILE:HG13	1.87	0.57
1:D:375:GLY:HA3	1:G:375:GLY:HA2	1.88	0.56
1:F:432:GLY:HA3	1:G:409:VAL:HG21	1.87	0.56
1:B:296:GLY:HA2	1:B:301:CYS:SG	2.45	0.56
1:F:390:MET:O	1:F:391:GLN:HB2	2.04	0.56
1:D:296:GLY:HA3	1:D:304:ARG:HE	1.70	0.56
1:E:85:VAL:HB	1:E:218:VAL:HG21	1.87	0.56
1:A:88:SER:O	1:A:89:GLU:HB2	2.07	0.55
1:G:434:LEU:O	1:G:438:MET:HG3	2.06	0.55
1:D:62:ARG:HD3	1:D:205:TYR:CE1	2.41	0.55
1:E:58:ILE:HG12	1:E:85:VAL:HG13	1.89	0.55
1:G:34:THR:OG1	1:G:289:ASP:HB3	2.07	0.55
1:E:284:CYS:SG	1:E:329:VAL:HG11	2.47	0.55
1:H:407:LYS:HG3	1:H:408:LEU:N	2.22	0.54
1:C:205:TYR:HE1	1:C:424:ARG:HH12	1.55	0.54
1:B:71:LYS:HE2	1:B:244:ASP:OD1	2.08	0.54
1:D:257:VAL:HG22	1:D:269:LEU:HD21	1.88	0.54
1:F:263:LYS:HE3	1:F:264:TYR:OH	2.08	0.54
1:E:292:LYS:HG2	1:E:332:ILE:HB	1.90	0.54
1:F:49:ASP:HA	1:F:70:HIS:CD2	2.43	0.53
1:G:370:LEU:HD21	1:G:419:TYR:CD1	2.43	0.53
1:B:428:HIS:CE1	1:C:407:LYS:HB2	2.43	0.53
1:F:343:ILE:CD1	1:F:430:LEU:HD22	2.38	0.53
1:C:270:ILE:HG12	1:C:290:ALA:HB3	1.90	0.53
1:F:263:LYS:HE3	1:F:264:TYR:CZ	2.43	0.53
1:H:284:CYS:HB2	1:H:327:PHE:CD1	2.44	0.53
1:B:270:ILE:HG12	1:B:290:ALA:HB3	1.90	0.53
1:C:59:MET:O	1:C:63:LEU:HD12	2.08	0.53
1:F:254:ILE:HD13	1:F:283:LEU:HD23	1.90	0.53
1:G:34:THR:OG1	1:G:35:LYS:N	2.42	0.53
1:E:423:ILE:O	1:E:427:VAL:HG23	2.09	0.52
1:B:45:SER:HB3	1:B:52:THR:OG1	2.10	0.52
1:H:53:GLU:HG3	1:H:367:PRO:HG3	1.91	0.52
1:A:9:THR:OG1	1:A:10:PHE:N	2.42	0.52
1:B:334:ASP:OD1	2:B:500:IMP:O3'	2.22	0.52
1:A:409:VAL:HG21	1:D:432:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:414:GLU:HB2	1:G:475:HIS:HB2	1.92	0.51
1:G:292:LYS:HG2	1:G:332:ILE:HB	1.92	0.51
1:D:334:ASP:OD1	2:D:500:IMP:O3'	2.18	0.51
1:E:40:ASN:ND2	1:E:207:ASP:O	2.43	0.51
1:D:53:GLU:HB2	1:D:367:PRO:HG3	1.93	0.51
1:D:8:LEU:O	1:D:314:ILE:HB	2.11	0.51
1:F:80:ARG:HE	1:F:84:ARG:HG2	1.76	0.51
1:B:53:GLU:HG3	1:B:367:PRO:HG3	1.91	0.51
1:B:45:SER:HB2	1:B:67:GLY:HA2	1.92	0.51
1:E:49:ASP:HA	1:E:70:HIS:CD2	2.46	0.51
1:A:53:GLU:HG2	1:A:81:GLU:OE1	2.10	0.50
1:C:448:ASP:HA	1:C:451:LYS:HE2	1.93	0.50
1:E:434:LEU:O	1:E:438:MET:HG3	2.10	0.50
1:A:41:MET:SD	1:A:431:LEU:HD11	2.52	0.50
1:B:250:SER:O	1:B:254:ILE:HG12	2.11	0.50
1:G:55:ARG:NH1	1:G:364:ASP:O	2.45	0.50
1:B:468:VAL:HG21	1:C:413:ILE:HG12	1.93	0.50
1:C:32:LYS:NZ	1:C:38:THR:HG22	2.26	0.50
1:E:456:VAL:HG12	1:F:5:LYS:HG2	1.94	0.50
1:F:469:HIS:CE1	1:G:299:SER:HA	2.47	0.50
1:A:296:GLY:HA3	1:A:304:ARG:NE	2.27	0.49
1:E:9:THR:OG1	1:H:465:GLU:OE2	2.29	0.49
1:D:242:VAL:HG12	1:D:270:ILE:HD12	1.93	0.49
1:F:226:GLN:NE2	1:F:229:ARG:HE	2.11	0.49
1:F:231:ASP:OD1	1:F:263:LYS:HE2	2.12	0.49
1:G:247:HIS:CE1	1:G:249:HIS:HB3	2.48	0.49
1:A:473:ILE:HG12	1:B:413:ILE:HD13	1.95	0.49
1:E:246:ALA:HB1	1:H:440:TYR:OH	2.13	0.49
1:A:88:SER:O	1:A:89:GLU:CB	2.61	0.49
1:B:345:LYS:O	1:B:349:VAL:HG23	2.12	0.49
1:C:468:VAL:HG21	1:D:413:ILE:HG12	1.94	0.48
1:A:370:LEU:HD13	1:A:377:GLN:NE2	2.28	0.48
1:E:445:ASP:OD1	1:E:447:GLU:HG3	2.13	0.48
1:F:231:ASP:OD1	1:F:263:LYS:CE	2.61	0.48
1:H:407:LYS:HG2	1:G:429:GLN:NE2	2.28	0.48
1:A:343:ILE:HD11	1:A:430:LEU:HD22	1.95	0.48
1:A:441:VAL:HG21	1:A:449:PHE:HE1	1.77	0.48
1:C:79:VAL:HG13	1:C:236:ALA:HB2	1.96	0.48
1:A:304:ARG:HD2	1:D:466:SER:HA	1.95	0.48
1:E:307:SER:O	1:H:437:SER:HB2	2.14	0.48
1:G:277:ALA:HB2	1:G:319:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ILE:CG1	1:E:85:VAL:HG13	2.43	0.48
1:E:304:ARG:HG2	1:E:309:VAL:O	2.14	0.48
1:G:253:ILE:O	1:G:257:VAL:HG23	2.13	0.48
1:A:376:ARG:HE	1:A:418:PRO:HB3	1.79	0.48
1:B:222:ILE:HG13	1:B:243:LEU:HA	1.96	0.48
1:H:413:ILE:HD13	1:G:473:ILE:HG12	1.96	0.48
1:E:321:VAL:HG11	1:E:350:GLY:HA3	1.96	0.47
1:D:248:GLY:HA2	1:D:253:ILE:HG13	1.95	0.47
1:D:304:ARG:HD3	1:D:310:GLY:HA3	1.96	0.47
1:B:370:LEU:N	1:B:370:LEU:CD1	2.77	0.47
1:D:250:SER:O	1:D:254:ILE:HG13	2.14	0.47
1:H:363:THR:HG21	1:H:423:ILE:HG12	1.97	0.47
1:F:466:SER:HB3	1:G:304:ARG:HB2	1.95	0.47
1:B:304:ARG:HG2	1:B:309:VAL:O	2.14	0.47
1:F:340:SER:HA	1:F:343:ILE:HD12	1.97	0.47
1:G:9:THR:OG1	1:G:10:PHE:N	2.46	0.47
1:B:370:LEU:CD1	1:B:370:LEU:H	2.28	0.47
1:C:75:ILE:O	1:C:79:VAL:HG23	2.14	0.47
1:A:413:ILE:HG12	1:D:468:VAL:HG21	1.96	0.47
1:B:53:GLU:HG3	1:B:367:PRO:CG	2.45	0.46
1:D:200:LYS:NZ	1:D:201:LYS:HG3	2.30	0.46
1:A:273:ASN:OD1	1:A:292:LYS:HE3	2.15	0.46
1:C:370:LEU:HD12	1:C:370:LEU:H	1.80	0.46
1:C:363:THR:O	1:C:379:LYS:HE3	2.16	0.46
1:D:306:VAL:HG21	1:D:411:GLU:HG2	1.97	0.46
1:F:229:ARG:O	1:F:233:LEU:HD22	2.16	0.46
1:G:14:LEU:HD12	1:G:458:ILE:HG21	1.97	0.46
1:A:292:LYS:HG2	1:A:332:ILE:HB	1.96	0.46
1:D:252:GLY:HA3	3:D:501:8L7:O6	2.15	0.46
1:B:234:VAL:HG22	1:B:267:LEU:HD22	1.97	0.46
1:E:296:GLY:HA2	1:E:301:CYS:SG	2.55	0.46
1:F:292:LYS:HG2	1:F:332:ILE:HB	1.98	0.46
1:C:466:SER:HB3	1:D:304:ARG:HB2	1.98	0.46
1:F:467:HIS:O	1:F:469:HIS:HD2	1.98	0.46
1:C:343:ILE:CD1	1:C:356:ILE:HD11	2.44	0.46
1:C:474:THR:HG23	1:D:415:GLY:HA2	1.96	0.46
1:H:291:VAL:HG22	1:H:331:VAL:HG12	1.98	0.46
1:D:58:ILE:O	1:D:62:ARG:HG3	2.16	0.46
1:E:437:SER:HB2	1:F:307:SER:HB2	1.98	0.46
1:G:296:GLY:HA3	1:G:304:ARG:HD3	1.97	0.46
1:G:22:VAL:HG11	1:G:27:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:THR:HG23	1:G:415:GLY:HA2	1.98	0.45
1:E:31:THR:HG21	1:E:42:PRO:HB3	1.97	0.45
1:G:347:LEU:HD13	1:G:446:ILE:HD13	1.97	0.45
1:H:230:VAL:O	1:H:234:VAL:HG13	2.15	0.45
1:B:300:ILE:HG22	1:B:413:ILE:HD11	1.98	0.45
1:C:305:ILE:N	1:C:305:ILE:CD1	2.79	0.45
1:F:29:ILE:HG22	1:F:438:MET:HE1	1.97	0.45
1:B:370:LEU:HD12	1:B:370:LEU:H	1.81	0.45
1:D:296:GLY:HA3	1:D:304:ARG:NE	2.30	0.45
1:E:242:VAL:HG22	1:E:270:ILE:HD12	1.99	0.45
1:E:324:ALA:HB1	1:E:329:VAL:HG13	1.98	0.45
1:E:296:GLY:N	1:E:297:PRO:CD	2.80	0.45
1:F:365:GLU:HB2	1:F:423:ILE:HD12	1.98	0.45
1:A:79:VAL:HG13	1:A:236:ALA:HB2	1.98	0.45
1:A:14:LEU:HD13	1:B:304:ARG:HD3	1.98	0.45
1:D:254:ILE:HG22	1:D:258:LYS:HZ3	1.80	0.45
1:D:200:LYS:HB3	1:D:200:LYS:HE3	1.77	0.45
1:G:242:VAL:HG22	1:G:270:ILE:HD12	1.98	0.45
1:A:247:HIS:CE1	1:A:249:HIS:HB3	2.52	0.44
1:B:321:VAL:HG11	1:B:350:GLY:HA3	1.99	0.44
1:F:441:VAL:HG21	1:F:449:PHE:HE1	1.82	0.44
1:B:11:GLU:HB3	1:B:463:LEU:HD22	1.98	0.44
1:H:71:LYS:HB3	1:H:221:ALA:O	2.18	0.44
1:A:270:ILE:HG12	1:A:290:ALA:HB3	1.99	0.44
1:B:253:ILE:O	1:B:257:VAL:HG23	2.18	0.44
1:D:341:GLY:O	1:D:345:LYS:HG3	2.18	0.44
1:E:409:VAL:HG21	1:H:432:GLY:HA3	1.99	0.44
1:A:340:SER:OG	1:B:306:VAL:O	2.30	0.44
1:B:466:SER:CB	1:C:304:ARG:HD2	2.48	0.44
1:E:44:ILE:O	1:E:355:MET:HA	2.18	0.44
1:F:229:ARG:HG2	1:F:233:LEU:CD2	2.48	0.44
1:C:321:VAL:HG11	1:C:350:GLY:HA3	1.99	0.44
1:F:13:VAL:O	1:F:345:LYS:HE2	2.18	0.44
1:F:272:GLY:HA3	1:F:273:ASN:HA	1.88	0.44
1:F:340:SER:OG	1:G:306:VAL:O	2.26	0.44
1:G:311:VAL:HG12	1:G:316:ALA:HB2	1.99	0.44
1:A:245:SER:HB2	1:A:253:ILE:HD11	2.00	0.43
1:F:82:VAL:HG21	1:F:233:LEU:HD12	2.00	0.43
1:F:387:LEU:HD23	1:F:410:PRO:HG3	2.00	0.43
1:H:409:VAL:O	1:H:409:VAL:HG13	2.18	0.43
1:C:477:ALA:HB3	1:C:480:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ILE:HG12	1:F:290:ALA:HB3	1.99	0.43
1:G:441:VAL:O	1:G:452:ARG:HD3	2.18	0.43
1:A:11:GLU:HB3	1:A:463:LEU:HD22	1.99	0.43
1:D:62:ARG:NH2	1:D:201:LYS:HE3	2.32	0.43
1:G:22:VAL:CG1	1:G:27:VAL:HG12	2.47	0.43
1:H:407:LYS:HG2	1:G:429:GLN:HE22	1.83	0.43
1:H:11:GLU:HB2	1:G:461:ALA:HB1	2.00	0.43
1:H:347:LEU:O	1:H:450:GLN:HG2	2.18	0.43
1:H:304:ARG:HD2	1:G:466:SER:OG	2.19	0.43
1:A:465:GLU:HG2	1:B:304:ARG:HH12	1.82	0.43
1:A:53:GLU:HB2	1:A:367:PRO:HG3	2.00	0.43
1:A:49:ASP:HA	1:A:70:HIS:CD2	2.54	0.43
1:B:82:VAL:HG21	1:B:233:LEU:HD22	2.00	0.43
1:B:294:GLY:HA2	5:B:601:HOH:O	2.17	0.43
1:E:413:ILE:HD13	1:H:473:ILE:HG12	2.01	0.43
1:G:338:LYS:HE2	1:G:342:ASP:OD2	2.18	0.43
1:F:300:ILE:HD12	1:F:300:ILE:C	2.39	0.43
1:D:87:LYS:HB3	1:D:87:LYS:HE3	1.72	0.43
1:H:254:ILE:HD13	1:H:283:LEU:HD23	2.00	0.43
1:D:254:ILE:HG22	1:D:258:LYS:NZ	2.34	0.43
1:D:387:LEU:HA	1:D:387:LEU:HD23	1.91	0.43
1:E:370:LEU:HD12	1:E:379:LYS:HE2	2.00	0.43
1:F:254:ILE:O	1:F:257:VAL:HG22	2.18	0.43
1:G:41:MET:SD	1:G:431:LEU:HD11	2.58	0.43
1:B:75:ILE:O	1:B:79:VAL:HG23	2.18	0.43
1:C:271:ALA:HB3	1:C:283:LEU:HD13	2.01	0.43
1:A:296:GLY:HA3	1:A:304:ARG:HE	1.84	0.42
1:A:2:LYS:HB2	1:A:2:LYS:HE3	1.84	0.42
1:D:200:LYS:HG2	1:D:201:LYS:N	2.33	0.42
1:F:480:TYR:CD1	1:G:305:ILE:HG21	2.54	0.42
1:F:27:VAL:HG11	1:F:438:MET:SD	2.58	0.42
1:F:33:LEU:HB2	1:F:39:LEU:HG	2.01	0.42
1:D:222:ILE:HD13	1:D:230:VAL:HG22	2.02	0.42
1:D:79:VAL:HG13	1:D:236:ALA:HB2	2.01	0.42
1:F:480:TYR:CE1	1:G:305:ILE:HG21	2.54	0.42
1:C:360:LEU:O	1:C:363:THR:HG23	2.19	0.42
1:C:473:ILE:HG12	1:D:413:ILE:HD13	2.01	0.42
1:G:441:VAL:HG21	1:G:449:PHE:CE1	2.54	0.42
1:D:69:ILE:HG22	1:D:73:MET:HE3	2.02	0.42
1:A:33:LEU:HB2	1:A:39:LEU:HG	2.01	0.42
1:A:13:VAL:O	1:A:345:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LEU:O	1:D:438:MET:HG3	2.19	0.42
1:H:209:ASN:O	1:H:217:ARG:HG3	2.19	0.42
1:C:54:HIS:HD1	1:C:81:GLU:CD	2.19	0.42
1:F:234:VAL:HG22	1:F:267:LEU:HD22	2.01	0.42
1:G:53:GLU:HG2	1:G:81:GLU:OE1	2.20	0.42
1:B:423:ILE:HG21	1:B:423:ILE:HD13	1.79	0.42
1:B:445:ASP:OD1	1:B:448:ASP:HB2	2.20	0.42
1:F:53:GLU:HB2	1:F:367:PRO:HG3	2.02	0.42
1:A:304:ARG:HG2	1:A:309:VAL:O	2.20	0.42
1:B:31:THR:HG21	1:B:42:PRO:HB3	2.01	0.42
1:B:465:GLU:OE2	1:C:9:THR:OG1	2.35	0.42
1:C:429:GLN:HB3	1:C:479:ASN:HB3	2.01	0.42
1:D:200:LYS:HG2	1:D:201:LYS:HG2	2.01	0.42
1:G:356:ILE:HG21	1:G:359:LEU:HB2	2.00	0.42
1:G:49:ASP:HA	1:G:70:HIS:CD2	2.55	0.41
1:A:478:PRO:HD2	1:B:410:PRO:HG2	2.02	0.41
1:G:247:HIS:HE1	1:G:249:HIS:HB3	1.85	0.41
1:G:388:GLY:HA3	1:G:414:GLU:OE1	2.20	0.41
1:E:251:LYS:HD2	1:H:21:GLU:HG2	2.01	0.41
1:H:41:MET:HG2	1:H:65:GLY:N	2.35	0.41
1:H:434:LEU:O	1:H:438:MET:HE2	2.19	0.41
1:A:413:ILE:HG13	1:A:413:ILE:H	1.78	0.41
1:E:464:LYS:HB2	1:E:464:LYS:HE3	1.79	0.41
1:E:48:MET:HA	1:E:384:MET:SD	2.59	0.41
1:G:388:GLY:N	1:G:414:GLU:OE1	2.53	0.41
1:G:409:VAL:HG12	1:G:409:VAL:O	2.19	0.41
1:B:46:ALA:O	1:B:52:THR:OG1	2.24	0.41
1:C:472:THR:HG21	1:D:416:ARG:NH2	2.36	0.41
1:F:370:LEU:HD23	1:F:379:LYS:HD3	2.02	0.41
1:A:266:ASN:HA	1:A:266:ASN:HD22	1.71	0.41
1:D:270:ILE:HG21	1:D:332:ILE:HD12	2.01	0.41
1:D:270:ILE:HG12	1:D:290:ALA:HB3	2.03	0.41
1:F:437:SER:HB2	1:G:307:SER:O	2.19	0.41
1:A:60:MET:HE2	1:A:423:ILE:HG21	2.03	0.41
1:B:254:ILE:HD13	1:B:283:LEU:HD23	2.03	0.41
1:H:334:ASP:OD2	2:H:500:IMP:O2'	2.32	0.41
1:H:301:CYS:SG	2:H:500:IMP:H2	2.61	0.41
1:A:461:ALA:HB1	1:B:11:GLU:HB2	2.03	0.41
1:B:261:LYS:HA	1:B:261:LYS:HD3	1.93	0.41
1:C:78:GLN:HG2	1:C:233:LEU:HD21	2.01	0.41
1:H:225:GLY:H	1:H:256:THR:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LYS:NZ	1:C:239:ASP:CG	2.74	0.41
1:E:80:ARG:O	1:E:84:ARG:HG3	2.21	0.41
1:A:445:ASP:OD1	1:A:447:GLU:HG2	2.21	0.40
1:B:35:LYS:HD2	1:B:289:ASP:HA	2.02	0.40
1:G:245:SER:HB2	1:G:253:ILE:HD11	2.03	0.40
1:H:415:GLY:HA2	1:G:474:THR:H	1.86	0.40
1:H:226:GLN:O	1:H:230:VAL:HG23	2.21	0.40
1:C:32:LYS:HE3	1:C:34:THR:O	2.21	0.40
1:C:447:GLU:O	1:C:451:LYS:HG3	2.21	0.40
1:D:82:VAL:O	1:D:86:LYS:HG2	2.21	0.40
1:E:81:GLU:O	1:E:85:VAL:HG23	2.21	0.40
1:F:263:LYS:HG2	1:F:264:TYR:CE2	2.56	0.40
1:A:227:MET:HE2	1:A:263:LYS:HD3	2.03	0.40
1:B:272:GLY:HA3	1:B:273:ASN:HA	1.95	0.40
1:H:221:ALA:HA	1:H:242:VAL:O	2.21	0.40
1:E:304:ARG:HD3	1:H:14:LEU:HD13	2.02	0.40
1:H:281:LYS:HA	1:H:327:PHE:HE1	1.86	0.40
1:C:296:GLY:N	1:C:297:PRO:CD	2.85	0.40
1:F:296:GLY:N	1:F:297:PRO:CD	2.85	0.40
1:F:41:MET:SD	1:F:431:LEU:HD11	2.61	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	349/406 (86%)	341 (98%)	7 (2%)	1 (0%)	46 75
1	B	350/406 (86%)	337 (96%)	13 (4%)	0	100 100
1	C	348/406 (86%)	339 (97%)	8 (2%)	1 (0%)	46 75
1	D	353/406 (87%)	338 (96%)	14 (4%)	1 (0%)	46 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	351/406 (86%)	341 (97%)	9 (3%)	1 (0%)	46 75
1	F	350/406 (86%)	338 (97%)	11 (3%)	1 (0%)	46 75
1	G	349/406 (86%)	338 (97%)	11 (3%)	0	100 100
1	H	349/406 (86%)	340 (97%)	9 (3%)	0	100 100
All	All	2799/3248 (86%)	2712 (97%)	82 (3%)	5 (0%)	52 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	D	294	GLY
1	E	294	GLY
1	F	294	GLY
1	C	294	GLY

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	279/323 (86%)	275 (99%)	4 (1%)	74 92
1	B	280/323 (87%)	270 (96%)	10 (4%)	42 73
1	C	278/323 (86%)	270 (97%)	8 (3%)	50 80
1	D	282/323 (87%)	278 (99%)	4 (1%)	74 92
1	E	280/323 (87%)	272 (97%)	8 (3%)	50 80
1	F	279/323 (86%)	269 (96%)	10 (4%)	42 73
1	G	278/323 (86%)	271 (98%)	7 (2%)	55 84
1	H	279/323 (86%)	275 (99%)	4 (1%)	74 92
All	All	2235/2584 (86%)	2180 (98%)	55 (2%)	55 84

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	90	SER
1	A	315	SER
1	A	408	LEU
1	B	2	LYS
1	B	41	MET
1	B	52	THR
1	B	203	LYS
1	B	217	ARG
1	B	244	ASP
1	B	258	LYS
1	B	436	SER
1	B	446	ILE
1	B	460	THR
1	C	25	LYS
1	C	41	MET
1	C	66	LEU
1	C	86	LYS
1	C	301	CYS
1	C	436	SER
1	C	446	ILE
1	C	452	ARG
1	D	32	LYS
1	D	74	ASP
1	D	87	LYS
1	D	410	PRO
1	E	41	MET
1	E	301	CYS
1	E	376	ARG
1	E	394	SER
1	E	407	LYS
1	E	438	MET
1	E	444	LYS
1	E	481	LYS
1	F	25	LYS
1	F	41	MET
1	F	55	ARG
1	F	73	MET
1	F	80	ARG
1	F	338	LYS
1	F	425	SER
1	F	464	LYS
1	F	470	ASP

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Mol	Chain	Res	Type
1	F	472	THR
1	H	11	GLU
1	H	41	MET
1	H	424	ARG
1	H	444	LYS
1	G	28	LYS
1	G	41	MET
1	G	247	HIS
1	G	304	ARG
1	G	369	GLU
1	G	387	LEU
1	G	452	ARG

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

Mol	Chain	Res	Type
1	A	266	ASN
1	A	374	GLN
1	B	450	GLN
1	D	266	ASN
1	E	266	ASN
1	E	391	GLN
1	F	212	ASN
1	F	469	HIS
1	H	212	ASN
1	G	450	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 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	501	-	21,25,25	1.07	3 (14%)	22,38,38	2.12	3 (13%)
3	8L7	A	502	-	34,35,35	1.17	4 (11%)	44,51,51	1.64	5 (11%)
2	IMP	B	500	-	21,25,25	1.21	3 (14%)	22,38,38	2.24	2 (9%)
3	8L7	B	501	-	34,35,35	1.34	6 (17%)	44,51,51	1.46	4 (9%)
2	IMP	C	500	-	21,25,25	1.29	3 (14%)	22,38,38	2.59	3 (13%)
3	8L7	C	501	-	34,35,35	1.20	5 (14%)	44,51,51	1.11	2 (4%)
2	IMP	D	500	-	21,25,25	1.13	3 (14%)	22,38,38	2.57	3 (13%)
3	8L7	D	501	-	34,35,35	1.23	5 (14%)	44,51,51	1.22	3 (6%)
2	IMP	E	501	-	21,25,25	1.14	3 (14%)	22,38,38	2.62	4 (18%)
3	8L7	E	502	-	34,35,35	1.12	6 (17%)	44,51,51	1.34	5 (11%)
2	IMP	F	500	-	21,25,25	1.10	3 (14%)	22,38,38	2.54	4 (18%)
3	8L7	F	501	-	34,35,35	1.11	4 (11%)	44,51,51	1.10	2 (4%)
2	IMP	G	502	-	21,25,25	1.24	3 (14%)	22,38,38	2.45	3 (13%)
3	8L7	G	503	-	34,35,35	1.21	5 (14%)	44,51,51	1.39	5 (11%)
2	IMP	H	500	-	21,25,25	1.14	3 (14%)	22,38,38	2.46	4 (18%)
3	8L7	H	501	-	34,35,35	1.25	5 (14%)	44,51,51	1.34	5 (11%)

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
3	8L7	A	502	-	-	2/25/41/41	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	C	500	-	-	0/6/26/26	0/3/3/3
3	8L7	C	501	-	-	0/25/41/41	0/3/3/3
2	IMP	D	500	-	-	0/6/26/26	0/3/3/3
3	8L7	D	501	-	-	2/25/41/41	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
3	8L7	E	502	-	-	0/25/41/41	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
2	IMP	G	502	-	-	0/6/26/26	0/3/3/3
3	8L7	G	503	-	-	2/25/41/41	0/3/3/3
2	IMP	H	500	-	-	0/6/26/26	0/3/3/3
3	8L7	H	501	-	-	2/25/41/41	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	8L7	C11-C1	-3.15	1.48	1.53
3	C	501	8L7	C17-N4	-2.82	1.36	1.41
3	B	501	8L7	C17-N4	-2.82	1.36	1.41
3	H	501	8L7	C17-N4	-2.81	1.36	1.41
3	G	503	8L7	C17-N4	-2.68	1.36	1.41
3	D	501	8L7	C8-C7	-2.67	1.32	1.46
3	G	503	8L7	C11-C1	-2.59	1.49	1.53
3	G	503	8L7	C8-C7	-2.57	1.32	1.46
3	H	501	8L7	C8-C7	-2.56	1.32	1.46
3	B	501	8L7	C8-C7	-2.49	1.33	1.46
3	C	501	8L7	C8-C7	-2.48	1.33	1.46
3	F	501	8L7	C8-C7	-2.48	1.33	1.46
3	A	502	8L7	C8-C7	-2.44	1.33	1.46
3	E	502	8L7	C8-C7	-2.38	1.33	1.46
3	D	501	8L7	C17-N4	-2.35	1.37	1.41
3	E	502	8L7	C11-C1	-2.28	1.50	1.53
3	C	501	8L7	C11-C1	-2.21	1.50	1.53
3	F	501	8L7	C17-N4	-2.15	1.37	1.41
3	A	502	8L7	C17-N4	-2.11	1.37	1.41
3	B	501	8L7	C10-N4	-2.05	1.33	1.37
3	D	501	8L7	C11-C1	-2.03	1.50	1.53
3	E	502	8L7	C17-N4	-2.00	1.37	1.41
3	E	502	8L7	C20-CL	2.02	1.78	1.73
2	A	501	IMP	C2-N1	2.06	1.37	1.33
2	B	500	IMP	C2-N1	2.09	1.37	1.33
2	D	500	IMP	C2-N1	2.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	IMP	C2-N1	2.20	1.38	1.33
2	F	500	IMP	C2-N1	2.20	1.38	1.33
3	E	502	8L7	C24-N34	2.23	1.46	1.43
2	H	500	IMP	C2-N1	2.26	1.38	1.33
2	G	502	IMP	C2-N1	2.31	1.38	1.33
3	H	501	8L7	C20-CL	2.33	1.79	1.73
3	G	503	8L7	C20-CL	2.33	1.79	1.73
2	A	501	IMP	C6-N1	2.46	1.37	1.33
2	C	500	IMP	C2-N1	2.50	1.38	1.33
3	B	501	8L7	C20-CL	2.56	1.80	1.73
3	F	501	8L7	C20-CL	2.57	1.80	1.73
3	D	501	8L7	C20-CL	2.61	1.80	1.73
3	C	501	8L7	C20-CL	2.62	1.80	1.73
3	H	501	8L7	C24-N34	2.66	1.47	1.43
2	H	500	IMP	C6-N1	2.66	1.37	1.33
2	E	501	IMP	C6-N1	2.70	1.37	1.33
2	D	500	IMP	C6-N1	2.73	1.38	1.33
2	F	500	IMP	C6-N1	2.76	1.38	1.33
3	G	503	8L7	C21-C20	2.79	1.47	1.39
3	A	502	8L7	C20-CL	2.84	1.81	1.73
2	E	501	IMP	C2-N3	3.00	1.37	1.32
2	A	501	IMP	C2-N3	3.06	1.37	1.32
3	B	501	8L7	C21-C20	3.06	1.48	1.39
3	E	502	8L7	C21-C20	3.07	1.48	1.39
2	B	500	IMP	C6-N1	3.10	1.38	1.33
2	G	502	IMP	C6-N1	3.12	1.38	1.33
2	C	500	IMP	C6-N1	3.12	1.38	1.33
2	D	500	IMP	C2-N3	3.16	1.37	1.32
2	H	500	IMP	C2-N3	3.16	1.37	1.32
2	F	500	IMP	C2-N3	3.22	1.37	1.32
3	C	501	8L7	C21-C20	3.23	1.48	1.39
3	F	501	8L7	C21-C20	3.30	1.48	1.39
3	D	501	8L7	C21-C20	3.36	1.48	1.39
2	G	502	IMP	C2-N3	3.51	1.38	1.32
2	B	500	IMP	C2-N3	3.56	1.38	1.32
3	A	502	8L7	C21-C20	3.64	1.49	1.39
2	C	500	IMP	C2-N3	3.68	1.38	1.32
3	H	501	8L7	C21-C20	3.75	1.50	1.39

All (57) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	IMP	N3-C2-N1	-11.39	119.92	128.87
2	E	501	IMP	N3-C2-N1	-11.07	120.17	128.87
2	D	500	IMP	N3-C2-N1	-11.06	120.19	128.87
2	G	502	IMP	N3-C2-N1	-10.54	120.59	128.87
2	H	500	IMP	N3-C2-N1	-10.36	120.73	128.87
2	F	500	IMP	N3-C2-N1	-10.32	120.76	128.87
2	B	500	IMP	N3-C2-N1	-9.82	121.16	128.87
2	A	501	IMP	N3-C2-N1	-9.09	121.73	128.87
3	A	502	8L7	C25-C24-N34	-7.18	99.39	112.25
3	B	501	8L7	C25-C24-N34	-5.51	102.39	112.25
3	H	501	8L7	C1-C11-N3	-4.63	105.49	110.49
3	D	501	8L7	C25-C24-N34	-4.27	104.61	112.25
3	G	503	8L7	C25-C24-N34	-4.23	104.68	112.25
3	C	501	8L7	C25-C24-N34	-3.71	105.61	112.25
2	F	500	IMP	C1'-N9-C4	-3.42	122.99	126.81
3	G	503	8L7	C1-C11-N3	-3.20	107.03	110.49
3	E	502	8L7	C12-C11-C13	-3.16	105.88	109.72
3	F	501	8L7	C25-C24-N34	-3.14	106.62	112.25
3	E	502	8L7	C6-C1-C11	-3.05	116.68	120.82
3	G	503	8L7	C12-C11-C13	-3.02	106.05	109.72
3	D	501	8L7	C12-C11-C13	-2.99	106.09	109.72
3	E	502	8L7	C25-C24-N34	-2.88	107.09	112.25
3	H	501	8L7	C22-C21-N34	-2.75	117.97	121.94
3	G	503	8L7	C6-C1-C11	-2.50	117.43	120.82
2	E	501	IMP	C1'-N9-C4	-2.40	124.13	126.81
3	B	501	8L7	O5-C26-C25	-2.39	104.14	111.86
3	C	501	8L7	C12-C11-C13	-2.37	106.84	109.72
3	B	501	8L7	C6-C1-C11	-2.20	117.84	120.82
3	A	502	8L7	C6-C1-C11	-2.19	117.85	120.82
3	E	502	8L7	C6-C5-C7	-2.12	116.41	120.17
2	H	500	IMP	C1'-N9-C4	-2.05	124.52	126.81
2	C	500	IMP	C2-N1-C6	2.03	119.63	116.13
3	D	501	8L7	C19-C18-C17	2.04	122.59	120.30
2	B	500	IMP	C2-N1-C6	2.06	119.68	116.13
3	F	501	8L7	C12-C11-N3	2.17	114.76	108.21
3	A	502	8L7	C17-N4-C10	2.23	131.04	126.65
3	A	502	8L7	C22-C21-C20	2.30	120.38	117.97
3	H	501	8L7	C26-C25-C24	2.30	106.05	101.43
2	G	502	IMP	C2-N1-C6	2.34	120.15	116.13
2	A	501	IMP	C2-N1-C6	2.39	120.25	116.13
3	E	502	8L7	C12-C11-N3	2.39	115.42	108.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	IMP	C2-N1-C6	2.43	120.31	116.13
3	H	501	8L7	C12-C11-N3	2.45	115.58	108.21
2	G	502	IMP	O2P-P-O1P	2.46	118.64	110.63
2	D	500	IMP	C2-N1-C6	2.47	120.39	116.13
2	A	501	IMP	O2P-P-O1P	2.50	118.80	110.63
2	C	500	IMP	O2P-P-O1P	2.53	118.88	110.63
2	E	501	IMP	O3P-P-O2P	2.54	116.76	107.44
2	H	500	IMP	O2P-P-O1P	2.54	118.93	110.63
2	E	501	IMP	C2-N1-C6	2.71	120.79	116.13
2	F	500	IMP	C2-N1-C6	2.74	120.84	116.13
3	A	502	8L7	C19-C18-C17	2.87	123.52	120.30
3	H	501	8L7	C21-C20-CL	2.97	123.38	119.46
3	B	501	8L7	C12-C11-N3	2.98	117.19	108.21
3	G	503	8L7	C12-C11-N3	3.03	117.33	108.21
2	F	500	IMP	O3P-P-O2P	3.06	118.68	107.44
2	D	500	IMP	O2P-P-O1P	3.07	120.66	110.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	503	8L7	C22-C21-N34-C24
3	D	501	8L7	C20-C21-N34-C24
3	G	503	8L7	C20-C21-N34-C24
3	D	501	8L7	C22-C21-N34-C24
3	B	501	8L7	C20-C21-N34-C24
3	B	501	8L7	C22-C21-N34-C24
3	A	502	8L7	C20-C21-N34-C24
3	A	502	8L7	C22-C21-N34-C24
3	H	501	8L7	C20-C21-N34-C24
3	H	501	8L7	C22-C21-N34-C24

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	1	0
2	B	500	IMP	2	0
2	D	500	IMP	1	0
3	D	501	8L7	1	0
2	G	502	IMP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	503	8L7	1	0
2	H	500	IMP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	355/406 (87%)	-0.25	1 (0%)	94	95	38, 52, 73, 119	0
1	B	356/406 (87%)	-0.22	6 (1%)	73	74	40, 55, 89, 112	0
1	C	354/406 (87%)	-0.01	11 (3%)	52	52	38, 58, 97, 132	0
1	D	359/406 (88%)	-0.01	7 (1%)	70	70	40, 64, 96, 122	0
1	E	357/406 (87%)	-0.01	4 (1%)	82	83	40, 61, 86, 144	0
1	F	356/406 (87%)	-0.03	10 (2%)	56	57	46, 61, 99, 149	0
1	G	355/406 (87%)	0.02	10 (2%)	56	57	46, 69, 96, 118	0
1	H	355/406 (87%)	0.16	16 (4%)	37	36	46, 66, 95, 122	0
All	All	2847/3248 (87%)	-0.04	65 (2%)	64	64	38, 60, 94, 149	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	481	LYS	7.1
1	F	476	GLU	6.5
1	C	480	TYR	6.3
1	F	477	ALA	5.6
1	F	407	LYS	5.1
1	F	478	PRO	4.6
1	F	479	ASN	4.6
1	C	407	LYS	4.4
1	C	408	LEU	4.3
1	F	408	LEU	4.3
1	G	408	LEU	4.2
1	D	476	GLU	4.1
1	C	202	ARG	4.1
1	G	475	HIS	4.0
1	B	203	LYS	4.0
1	C	477	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	241	VAL	3.9
1	C	478	PRO	3.9
1	E	205	TYR	3.8
1	E	475	HIS	3.8
1	H	0	ALA	3.8
1	G	476	GLU	3.6
1	D	475	HIS	3.6
1	A	90	SER	3.6
1	C	475	HIS	3.4
1	D	408	LEU	3.4
1	C	479	ASN	3.3
1	H	407	LYS	3.3
1	G	204	GLU	3.2
1	B	480	TYR	3.0
1	C	424	ARG	3.0
1	G	407	LYS	2.9
1	H	66	LEU	2.9
1	F	480	TYR	2.8
1	C	476	GLU	2.8
1	H	269	LEU	2.8
1	B	481	LYS	2.8
1	F	475	HIS	2.7
1	E	66	LEU	2.7
1	E	476	GLU	2.7
1	H	373	TYR	2.6
1	B	478	PRO	2.5
1	G	480	TYR	2.5
1	H	408	LEU	2.5
1	G	481	LYS	2.4
1	D	335	GLY	2.4
1	H	89	GLU	2.3
1	B	23	LEU	2.3
1	H	42	PRO	2.3
1	H	83	LYS	2.3
1	D	357	GLY	2.3
1	C	469	HIS	2.3
1	H	82	VAL	2.3
1	H	222	ILE	2.2
1	G	370	LEU	2.2
1	F	460	THR	2.2
1	G	474	THR	2.2
1	H	218	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	460	THR	2.2
1	D	336	GLY	2.1
1	D	477	ALA	2.1
1	B	408	LEU	2.1
1	H	87	LYS	2.1
1	G	2	LYS	2.1
1	H	216	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	8L7	G	503	33/33	0.92	0.21	2.14	63,67,87,88	0
3	8L7	B	501	33/33	0.94	0.18	1.33	47,53,71,73	0
3	8L7	D	501	33/33	0.90	0.19	0.83	64,70,88,89	0
2	IMP	F	500	23/23	0.97	0.17	0.74	40,49,50,50	0
3	8L7	F	501	33/33	0.94	0.20	0.66	45,60,85,86	0
3	8L7	A	502	33/33	0.95	0.20	0.55	40,49,78,79	0
3	8L7	C	501	33/33	0.91	0.17	0.37	48,58,71,73	0
2	IMP	G	502	23/23	0.95	0.15	0.34	46,50,53,53	0
2	IMP	D	500	23/23	0.94	0.24	0.28	42,47,51,52	0
2	IMP	B	500	23/23	0.98	0.14	0.05	44,47,51,51	0
2	IMP	C	500	23/23	0.96	0.16	0.01	38,43,45,46	0
4	K	D	502	1/1	0.96	0.26	-0.11	97,97,97,97	0
2	IMP	E	501	23/23	0.98	0.17	-0.19	40,42,45,46	0
4	K	A	504	1/1	0.97	0.13	-0.24	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	IMP	A	501	23/23	0.96	0.14	-0.35	39,44,50,50	0
2	IMP	H	500	23/23	0.96	0.13	-0.38	50,54,58,59	0
4	K	A	503	1/1	0.98	0.14	-0.52	75,75,75,75	0
4	K	E	503	1/1	0.98	0.19	-0.55	63,63,63,63	0
3	8L7	H	501	33/33	0.94	0.17	-0.60	68,75,91,93	0
3	8L7	E	502	33/33	0.94	0.13	-0.90	47,56,76,79	0
4	K	E	504	1/1	0.96	0.16	-1.06	74,74,74,74	0
4	K	F	502	1/1	0.90	0.12	-1.67	92,92,92,92	0
4	K	B	502	1/1	0.94	0.10	-1.79	81,81,81,81	0
4	K	G	501	1/1	0.97	0.05	-2.81	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.