Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:52 PM GMT

PDB ID	:	4MYX
Title	:	Crystal Structure of the Inosine 5'-monophosphate Dehydrogenase, with a Internal Deletion of CBS Domain from Bacillus anthracis str. Ame complexed with P32
Authors	:	Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Csgid; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-09-28
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:

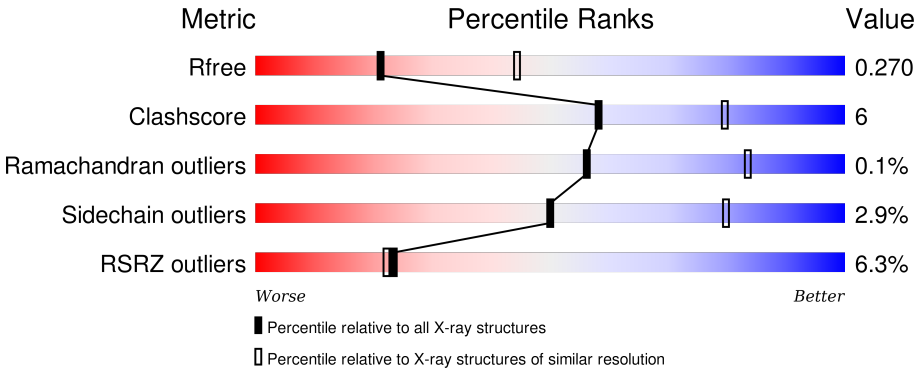
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	384	8% 79% 13% 9%
1	B	384	3% 77% 14% • 8%
1	C	384	2% 76% 15% 9%
1	D	384	7% 78% 13% 8%
1	E	384	6% 77% 13% • 8%

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Mol	Chain	Length	Quality of chain
1	F	384	8% 79% 11% • 9%
1	G	384	6% 80% 13% 7%
1	H	384	7% 73% 17% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2F0	A	502	-	-	-	X
3	2F0	C	503	-	-	-	X
4	FMT	A	503	-	-	-	X
4	FMT	D	507	-	-	-	X
4	FMT	H	502	-	-	-	X
7	EDO	B	502	-	-	-	X
7	EDO	C	506	-	-	-	X
7	EDO	F	504	-	-	-	X
8	SO4	G	502	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21740 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	351	Total	C	N	O	S	0	7	0
			2637	1656	465	498	18			
1	B	355	Total	C	N	O	S	0	1	0
			2614	1641	458	499	16			
1	C	348	Total	C	N	O	S	0	4	0
			2587	1623	451	496	17			
1	D	352	Total	C	N	O	S	0	4	0
			2615	1639	459	501	16			
1	E	352	Total	C	N	O	S	0	2	0
			2597	1629	455	496	17			
1	F	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			
1	G	356	Total	C	N	O	S	0	2	0
			2627	1647	462	502	16			
1	H	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			

There are 208 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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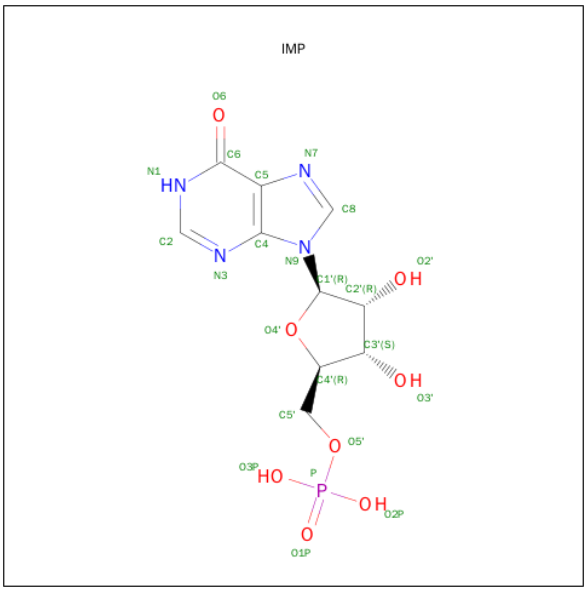
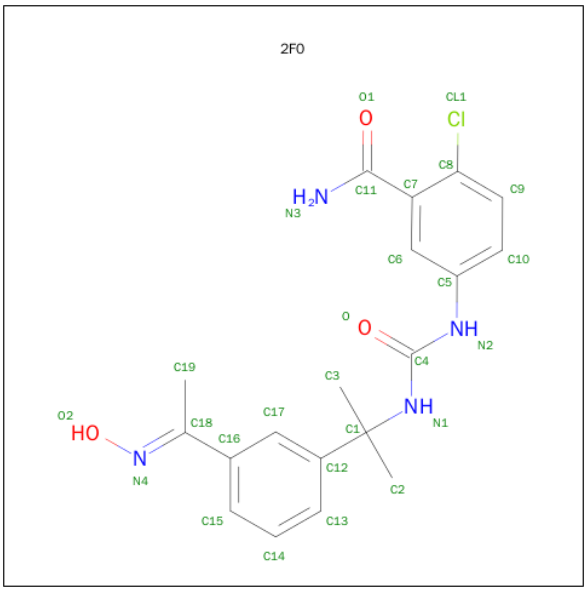
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	LINKER	UNP Q81W29
H	-23	MET	-	EXPRESSION TAG	UNP Q81W29
H	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-18	HIS	-	EXPRESSION TAG	UNP Q81W29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

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



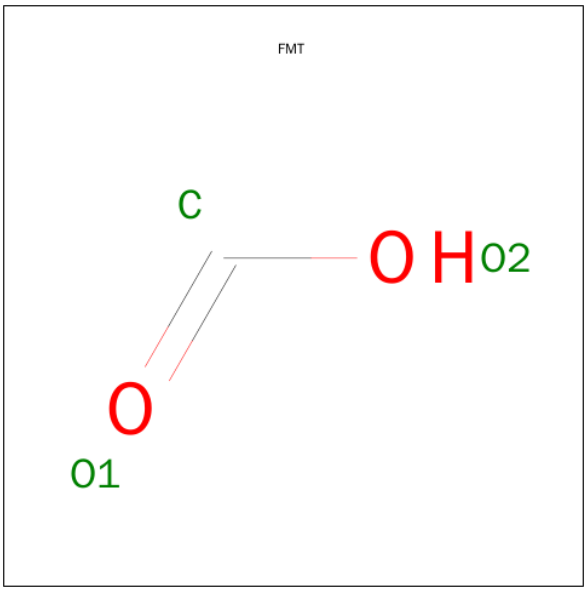
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	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 2-CHLORO-5-{[(2-{3-[(1E)-N-HYDROXYETHANIMIDOYL]PHENYL}PROPAN-2-YL)CARBAMOYL]AMINO}BENZAMIDE (three-letter code: 2F0) (formula: $C_{19}H_{21}ClN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	C	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	D	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	F	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	H	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0

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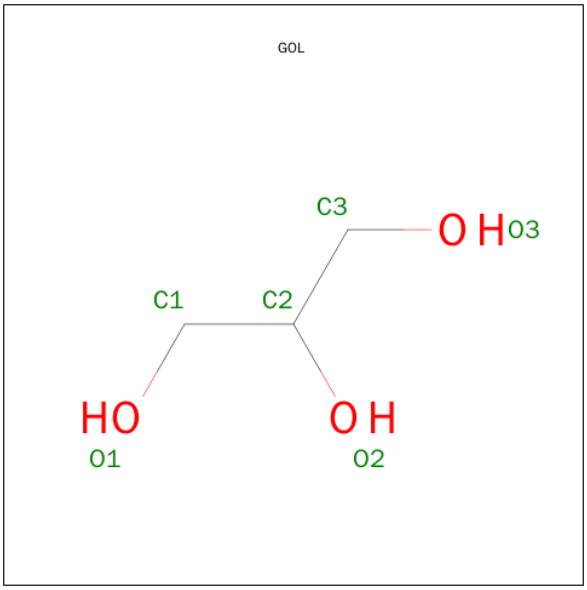
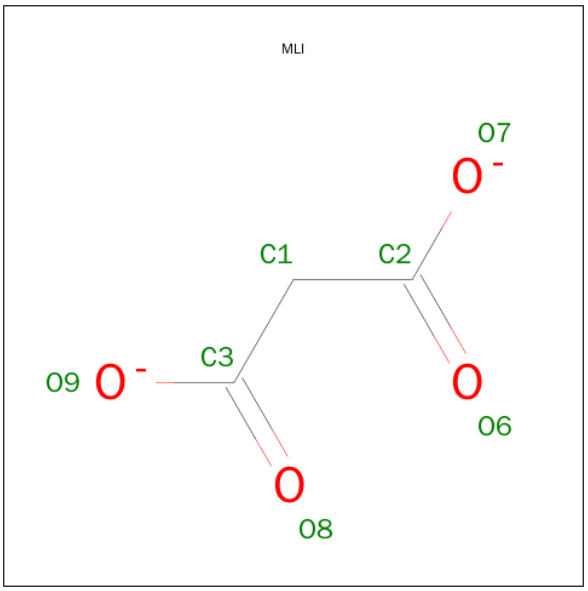
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 3 1 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



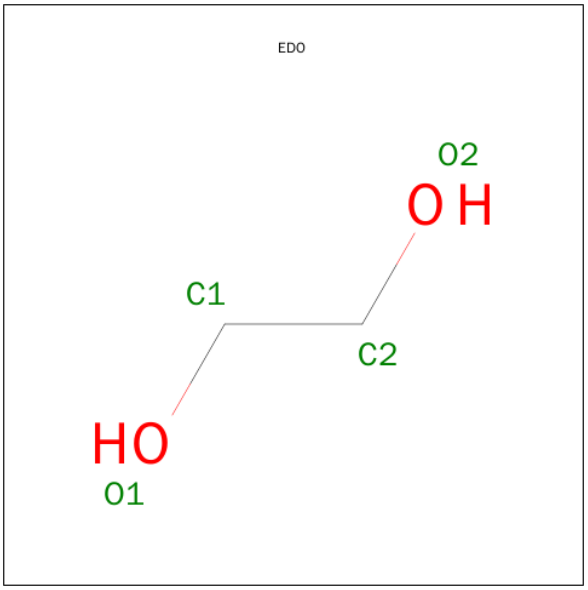
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	E	1	Total C O 7 3 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

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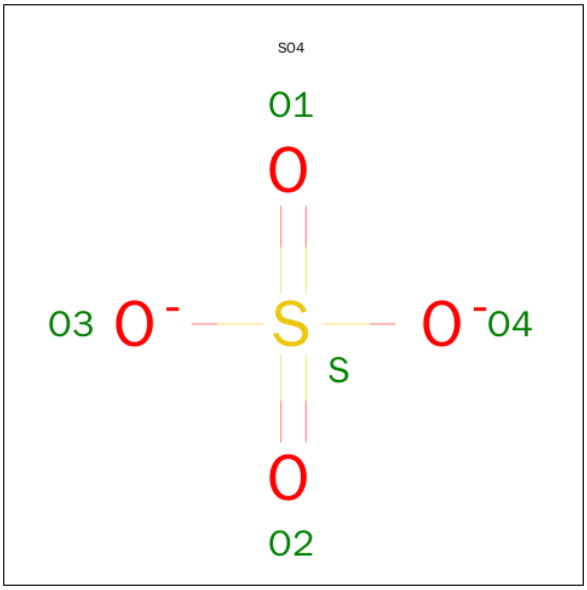
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

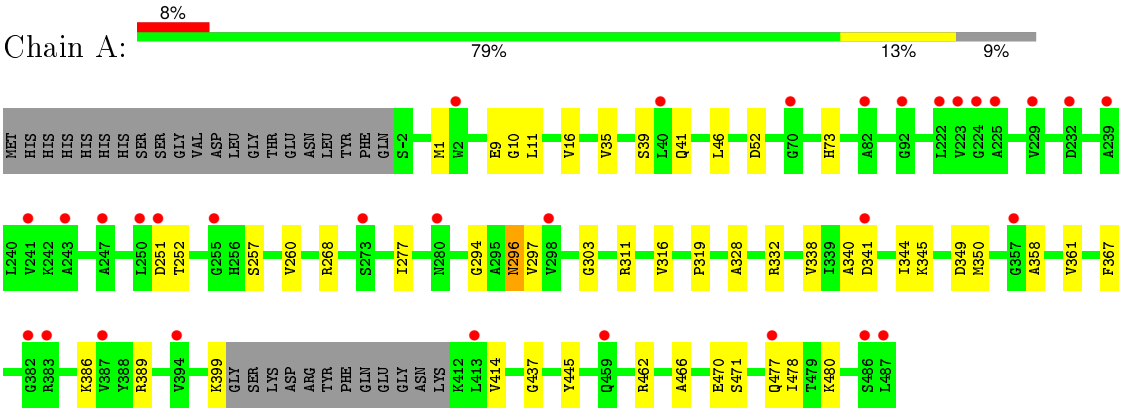
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	53	Total O 53 53	0	0
9	B	62	Total O 62 62	0	0
9	C	52	Total O 52 52	0	0
9	D	49	Total O 49 49	0	0
9	E	48	Total O 48 48	0	0
9	F	37	Total O 37 37	0	0
9	G	48	Total O 48 48	0	0
9	H	54	Total O 54 54	0	0

3 Residue-property plots

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

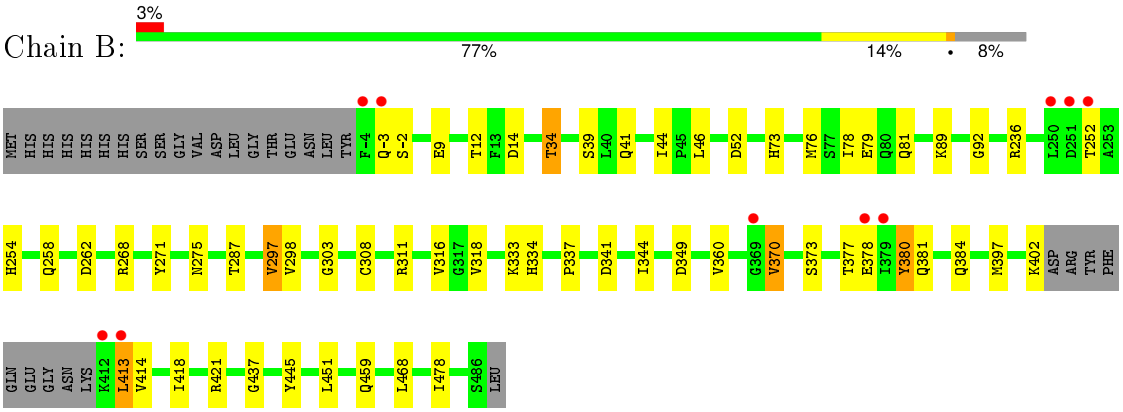
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



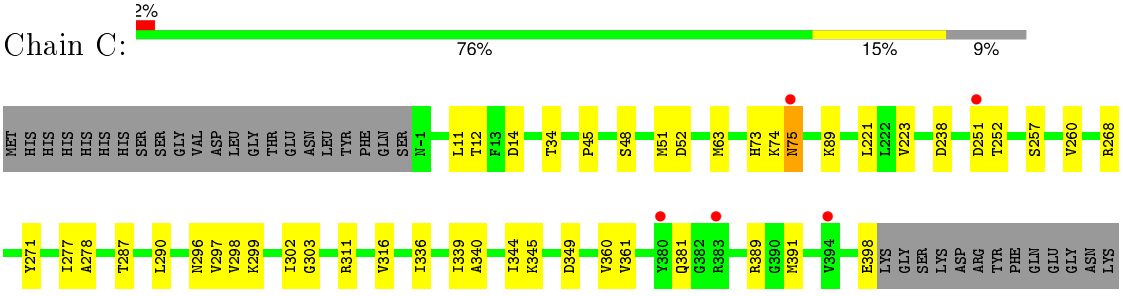
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:



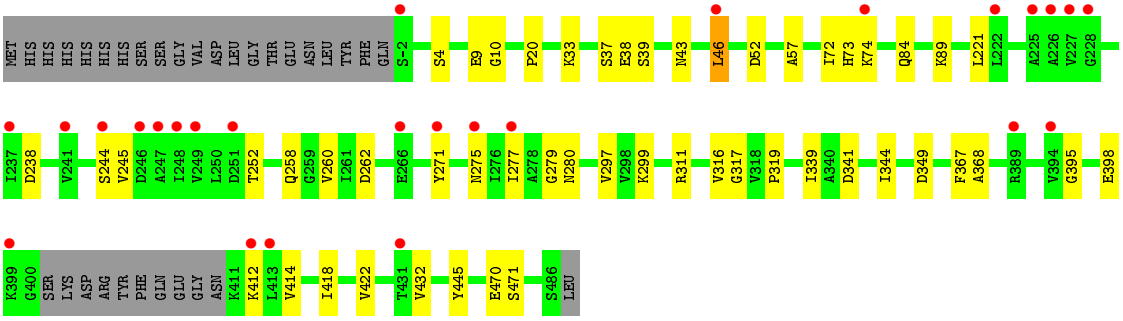
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain C:



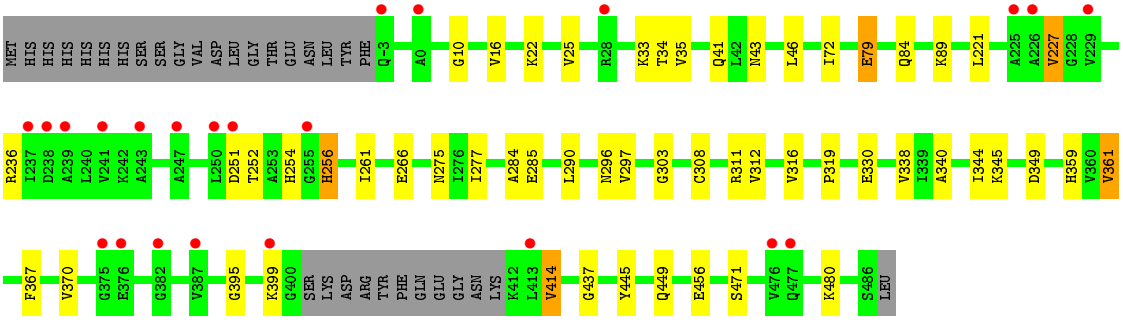
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:



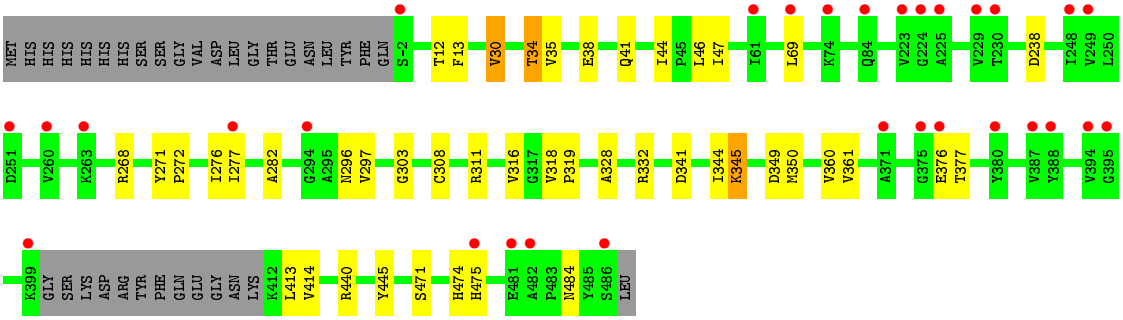
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain E:



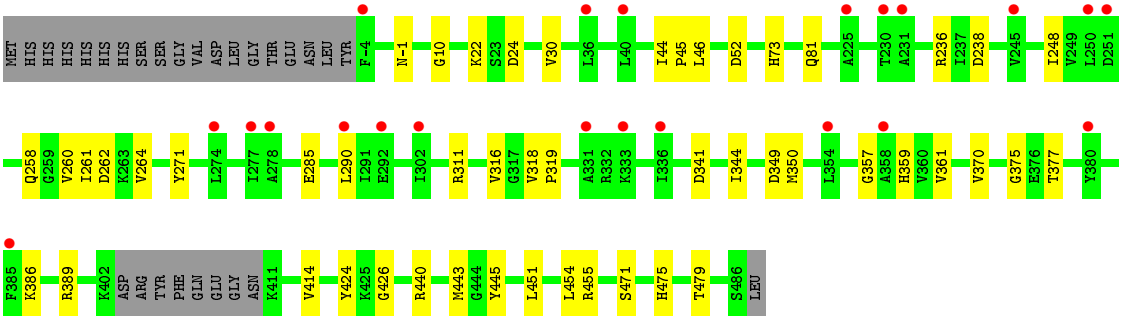
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F:

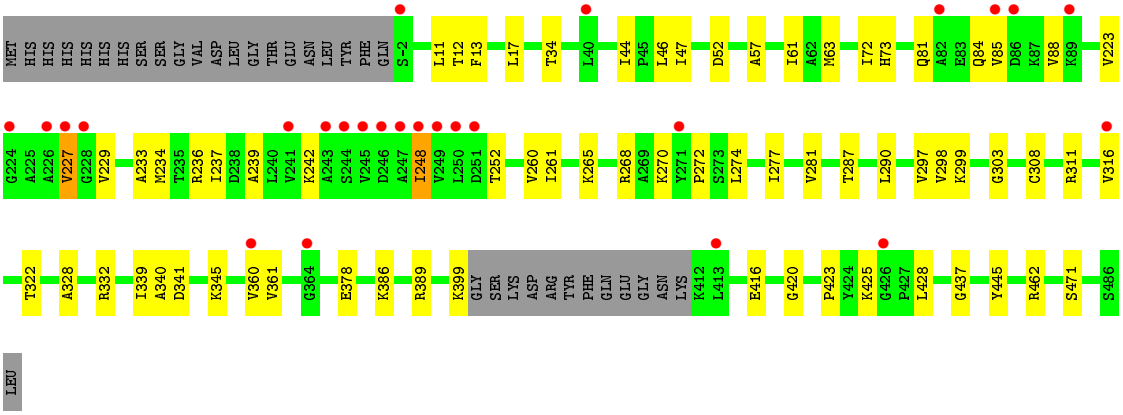


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain G:



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.36Å 89.82Å 104.50Å 81.41° 90.42° 83.50°	Depositor
Resolution (Å)	41.90 – 2.70 48.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.90-2.70) 93.4 (48.17-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.218 , 0.260 0.231 , 0.270	Depositor DCC
R_{free} test set	4101 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 82046 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21740	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 2F0, FMT, MLI, EDO, IMP, SO4

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	0.20	0/2673	0.39	0/3610
1	B	0.21	0/2651	0.41	0/3581
1	C	0.20	0/2623	0.40	0/3545
1	D	0.21	0/2651	0.40	0/3581
1	E	0.21	0/2633	0.39	0/3557
1	F	0.21	0/2603	0.39	0/3518
1	G	0.20	0/2663	0.38	0/3596
1	H	0.20	0/2603	0.39	0/3518
All	All	0.21	0/21100	0.39	0/28506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2637	0	2702	35	0
1	B	2614	0	2667	41	0
1	C	2587	0	2631	36	0
1	D	2615	0	2664	29	0
1	E	2597	0	2651	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2567	0	2626	26	0
1	G	2627	0	2682	32	0
1	H	2567	0	2626	44	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
2	E	23	0	11	0	0
2	F	23	0	11	1	0
2	G	23	0	11	1	0
2	H	23	0	11	1	0
3	A	27	0	21	3	0
3	B	27	0	21	2	0
3	C	27	0	21	1	0
3	D	27	0	21	3	0
3	E	54	0	42	6	0
3	F	27	0	21	2	0
3	H	27	0	21	4	0
4	A	6	0	2	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	6	0	2	0	0
4	E	9	0	3	0	0
4	F	6	0	2	0	0
4	H	12	0	4	0	0
5	A	6	0	8	0	0
5	E	6	0	8	0	0
6	A	7	0	2	0	0
6	E	7	0	2	0	0
7	B	4	0	6	0	0
7	C	8	0	12	4	0
7	D	12	0	18	0	0
7	E	4	0	6	0	0
7	F	12	0	18	2	0
8	C	5	0	0	0	0
8	G	10	0	0	0	0
9	A	53	0	0	0	0
9	B	62	0	0	1	0
9	C	52	0	0	0	0
9	D	49	0	0	0	0
9	E	48	0	0	0	0
9	F	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	48	0	0	1	0
9	H	54	0	0	1	0
All	All	21740	0	21600	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (253) 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)
3:H:505:2F0:H3	3:H:505:2F0:O	1.89	0.72
3:F:502:2F0:H3	3:F:502:2F0:O	1.89	0.72
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.72	0.71
3:A:502:2F0:H13	3:A:502:2F0:O	1.93	0.68
1:E:344:ILE:HG23	1:E:349:ASP:HB2	1.75	0.68
1:A:340:ALA:HB3	1:A:361:VAL:HG12	1.76	0.68
1:A:268[A]:ARG:NH2	1:A:296:ASN:OD1	2.28	0.67
1:B:297:VAL:HG13	1:B:337:PRO:HG2	1.77	0.66
1:A:389:ARG:HH22	1:A:399:LYS:HD2	1.60	0.66
3:E:502:2F0:O	3:E:502:2F0:H13	1.95	0.66
1:D:57:ALA:HB2	1:D:84:GLN:HB2	1.78	0.65
1:C:278:ALA:HB3	1:C:290:LEU:HD21	1.79	0.65
1:A:344[A]:ILE:HG23	1:A:349:ASP:HB2	1.79	0.63
1:H:389:ARG:HH22	1:H:399:LYS:HD2	1.63	0.63
1:B:459:GLN:NE2	1:D:4:SER:O	2.31	0.62
1:E:72:ILE:HD13	1:E:84:GLN:HB3	1.80	0.62
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.82	0.62
1:A:462:ARG:NH1	1:B:9:GLU:OE1	2.33	0.61
1:D:258:GLN:NE2	1:D:262:ASP:OD2	2.32	0.61
1:H:227:VAL:HG12	1:H:236:ARG:HD2	1.81	0.61
1:E:456:GLU:OE1	1:G:-1:ASN:ND2	2.33	0.61
1:H:239:ALA:HA	1:H:242:LYS:HE3	1.82	0.61
1:B:258:GLN:NE2	1:B:262:ASP:OD1	2.31	0.60
1:C:299:LYS:HG3	1:C:339:ILE:HB	1.82	0.60
1:A:277:ILE:HG13	1:A:297:VAL:HB	1.83	0.60
1:A:341:ASP:OD2	2:A:501:IMP:O2'	2.20	0.58
1:D:311:ARG:HD3	1:D:317:GLY:HA3	1.84	0.58
1:C:51:MET:SD	2:C:502:IMP:H8	2.43	0.58
1:G:359:HIS:ND1	9:G:628:HOH:O	2.32	0.58
1:E:437:GLY:HA3	1:G:414:VAL:HG21	1.86	0.58
1:E:46:LEU:HD23	1:E:367:PHE:HZ	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:501:2F0:O	3:D:501:2F0:H13	2.04	0.57
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.87	0.57
1:H:340:ALA:HB3	1:H:361:VAL:HG12	1.86	0.57
1:C:455:ARG:HH12	7:C:504:EDO:H22	1.69	0.57
1:B:380:TYR:HD2	1:B:381:GLN:H	1.52	0.56
1:H:11:LEU:HD11	1:H:462:ARG:HD3	1.88	0.56
1:F:34:THR:HG21	1:F:360:VAL:HG23	1.87	0.56
1:A:471:SER:HA	1:B:311:ARG:HD2	1.85	0.56
1:H:281:VAL:HG11	1:H:290:LEU:HD11	1.86	0.56
1:E:312:VAL:HG22	7:F:506:EDO:H12	1.87	0.56
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.87	0.55
1:F:35:VAL:HG13	1:F:41:GLN:HG2	1.88	0.55
1:H:341:ASP:OD2	2:H:504:IMP:O2'	2.25	0.55
1:G:30:VAL:O	1:G:440:ARG:NH1	2.40	0.55
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.87	0.55
3:A:502:2F0:H3	3:A:502:2F0:O	2.06	0.55
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.88	0.55
1:G:375:GLY:O	1:G:386:LYS:NZ	2.31	0.55
1:E:10:GLY:HA3	1:E:319:PRO:HG2	1.89	0.55
1:H:423:PRO:HB2	1:H:425:LYS:HE3	1.89	0.55
1:C:316:VAL:HG11	1:D:445:TYR:HB3	1.89	0.55
1:D:277:ILE:HG12	1:D:297:VAL:HB	1.89	0.54
1:B:341:ASP:OD2	2:B:500:IMP:O2'	2.24	0.54
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.89	0.54
1:G:81:GLN:OE1	1:G:236:ARG:NH1	2.35	0.54
1:D:39:SER:HB2	1:D:275:ASN:HD21	1.71	0.54
1:B:380:TYR:CD2	1:B:381:GLN:N	2.76	0.54
1:E:311:ARG:HD2	1:F:471:SER:HA	1.89	0.54
1:F:47:ILE:HG12	1:F:69:LEU:HB3	1.90	0.54
1:H:299:LYS:HG3	1:H:339:ILE:HB	1.89	0.54
1:G:238:ASP:OD1	1:G:271:TYR:OH	2.25	0.53
1:C:431:THR:HG23	7:C:506:EDO:H22	1.91	0.53
1:A:11:LEU:HD11	1:A:462:ARG:HD3	1.91	0.53
1:E:22:LYS:NZ	1:G:285:GLU:OE1	2.41	0.53
1:D:72:ILE:HG23	1:D:84:GLN:HE21	1.74	0.53
1:F:341:ASP:OD2	2:F:501:IMP:O2'	2.26	0.53
1:H:44:ILE:HD12	1:H:46:LEU:HD12	1.91	0.53
1:B:397:MET:SD	3:B:501:2F0:H21	2.49	0.53
1:G:341:ASP:OD2	2:G:501:IMP:O2'	2.25	0.53
1:E:277:ILE:HG12	1:E:297:VAL:HB	1.91	0.53
1:A:46[B]:LEU:HD23	1:A:367:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:NH2	1:C:296:ASN:OD1	2.42	0.52
1:H:72:ILE:HD13	1:H:84:GLN:HB3	1.92	0.52
1:E:227:VAL:HG13	1:E:236:ARG:HD2	1.92	0.52
1:G:445:TYR:HB3	1:H:316:VAL:HG11	1.91	0.52
1:C:252:THR:HG21	1:C:260:VAL:HG22	1.92	0.52
3:C:503:2F0:H3	3:C:503:2F0:O	2.09	0.52
1:F:311:ARG:HD2	1:H:471:SER:HA	1.92	0.51
1:E:445:TYR:HB2	1:G:316:VAL:HG21	1.92	0.51
1:B:76:MET:O	1:B:236:ARG:NH1	2.42	0.51
1:A:296:ASN:OD1	1:A:296:ASN:N	2.42	0.51
1:F:44:ILE:HD12	1:F:46:LEU:HD12	1.93	0.51
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.26	0.51
1:A:9:GLU:OE2	1:C:462:ARG:NH1	2.45	0.50
1:F:12:THR:OG1	1:F:13:PHE:N	2.41	0.50
1:D:252:THR:HG21	1:D:260:VAL:HG21	1.93	0.50
1:G:10:GLY:HA3	1:G:319:PRO:HG2	1.92	0.50
3:E:502:2F0:O1	3:E:502:2F0:CL1	2.66	0.50
3:E:502:2F0:O	3:E:502:2F0:H3	2.10	0.50
3:E:509:2F0:H13	3:E:509:2F0:O	2.11	0.50
1:G:443:MET:HG2	1:G:454:LEU:HD22	1.94	0.50
1:B:333:LYS:HB2	1:B:334:HIS:HD2	1.76	0.50
3:B:501:2F0:H3	3:B:501:2F0:O	2.11	0.50
1:C:277:ILE:HG12	1:C:297:VAL:HB	1.94	0.50
1:B:478:ILE:HG12	1:D:418:ILE:HD13	1.94	0.50
1:C:302:ILE:HD12	1:D:20:PRO:HG3	1.93	0.50
1:G:311:ARG:NH2	1:G:318:VAL:O	2.44	0.50
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.94	0.50
3:H:505:2F0:H13	3:H:505:2F0:O	2.11	0.50
3:E:502:2F0:C3	3:E:502:2F0:O	2.59	0.50
1:E:35:VAL:HG13	1:E:41:GLN:HG2	1.94	0.50
1:F:350:MET:HG3	1:F:361:VAL:HG21	1.94	0.50
1:H:61:ILE:HD11	1:H:88:VAL:HA	1.93	0.49
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.94	0.49
1:D:341:ASP:OD2	2:D:504:IMP:O2'	2.30	0.49
1:C:381:GLN:HG2	1:E:25:VAL:HG12	1.94	0.49
1:A:478:ILE:HG12	1:B:418:ILE:HD12	1.94	0.49
1:E:252:THR:HG22	1:E:254:HIS:H	1.77	0.49
1:E:25:VAL:HG11	1:E:449:GLN:HG2	1.95	0.49
1:G:475:HIS:NE2	1:H:345:LYS:HD2	2.27	0.49
1:B:377:THR:CG2	1:B:384:GLN:HB3	2.43	0.49
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:VAL:HG11	1:H:445:TYR:HB3	1.95	0.48
1:D:46:LEU:HD12	1:D:367:PHE:HZ	1.78	0.48
1:G:471:SER:HA	1:H:311:ARG:HD2	1.95	0.48
1:A:257:SER:HB3	1:A:260:VAL:HG23	1.95	0.48
1:C:311:ARG:HD2	1:D:471:SER:HA	1.96	0.48
1:B:303:GLY:HA2	1:B:308:CYS:SG	2.53	0.48
1:B:268:ARG:NH1	1:B:271:TYR:O	2.47	0.47
1:H:229:VAL:HG11	1:H:260:VAL:HA	1.96	0.47
1:H:88:VAL:HG11	1:H:223:VAL:HB	1.96	0.47
1:A:303:GLY:HA3	1:A:311:ARG:HE	1.79	0.47
1:A:311:ARG:HD2	1:C:471:SER:HA	1.96	0.47
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.95	0.47
3:F:502:2F0:O	3:F:502:2F0:C6	2.54	0.47
1:H:328:ALA:O	1:H:332:ARG:HB2	2.14	0.47
1:G:260:VAL:O	1:G:264:VAL:HG12	2.14	0.47
1:E:33:LYS:HG2	1:E:43:ASN:HD22	1.80	0.47
1:C:11:LEU:HD11	1:C:462:ARG:HD3	1.96	0.47
1:C:340:ALA:HB3	1:C:361:VAL:HG12	1.96	0.47
1:G:424:TYR:CZ	1:G:426:GLY:HA2	2.49	0.47
1:H:47:ILE:HG13	1:H:360:VAL:HG11	1.97	0.47
1:E:275:ASN:HA	1:E:296:ASN:HD21	1.80	0.47
1:H:416:GLU:OE1	3:H:505:2F0:N2	2.32	0.47
1:C:339:ILE:HD13	1:C:360:VAL:HG13	1.96	0.47
1:E:471:SER:HA	1:G:311:ARG:HD2	1.96	0.46
1:F:238:ASP:OD1	1:F:271:TYR:OH	2.27	0.46
1:H:11:LEU:N	1:H:322:THR:OG1	2.39	0.46
1:F:30:VAL:O	1:F:440:ARG:NH1	2.48	0.46
1:A:345:LYS:HD2	1:C:475:HIS:CD2	2.50	0.46
1:F:328:ALA:O	1:F:332:ARG:HB2	2.15	0.46
1:D:299:LYS:HG3	1:D:339:ILE:HB	1.98	0.46
3:A:502:2F0:C3	3:A:502:2F0:O	2.56	0.46
1:A:303:GLY:HA3	1:A:311:ARG:NE	2.31	0.46
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.98	0.46
1:A:350:MET:HG3	1:A:361:VAL:HG21	1.98	0.46
1:C:12:THR:OG1	1:D:470:GLU:OE1	2.34	0.46
1:C:75:ASN:HB2	1:C:391:MET:HE1	1.98	0.46
1:C:34:THR:HA	7:C:504:EDO:H21	1.98	0.45
1:G:261:ILE:HD13	1:G:290:LEU:HD23	1.97	0.45
1:D:238:ASP:OD1	1:D:271:TYR:OH	2.27	0.45
1:G:52:ASP:HA	1:G:73:HIS:CD2	2.52	0.45
3:D:501:2F0:O	3:D:501:2F0:H3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ARG:O	7:F:506:EDO:O2	2.33	0.45
1:B:377:THR:HG21	1:B:384:GLN:HB3	1.98	0.45
1:B:252:THR:HG22	1:B:254:HIS:H	1.80	0.45
1:F:319:PRO:HD3	1:H:17:LEU:HD12	1.97	0.45
1:A:344[B]:ILE:HB	1:A:349:ASP:HB2	1.99	0.45
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.52	0.45
1:E:316:VAL:HG11	1:F:445:TYR:HB3	1.99	0.45
1:B:81:GLN:OE1	1:B:236:ARG:NE	2.48	0.45
1:H:265:LYS:NZ	9:H:633:HOH:O	2.50	0.45
1:F:303:GLY:HA2	1:F:308:CYS:SG	2.56	0.45
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.52	0.45
1:B:413:LEU:O	9:B:645:HOH:O	2.20	0.45
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.52	0.45
1:G:45:PRO:HG3	1:G:451:LEU:HD11	1.99	0.44
1:C:434:GLN:HB2	7:C:506:EDO:H12	2.00	0.44
1:C:52:ASP:HA	1:C:73:HIS:CD2	2.51	0.44
1:H:248:ILE:HD12	1:H:274:LEU:HD21	1.99	0.44
1:D:344:ILE:HG23	1:D:349:ASP:HB2	2.00	0.44
3:D:501:2F0:O	3:D:501:2F0:C3	2.66	0.44
1:E:303:GLY:HA2	1:E:308:CYS:SG	2.57	0.44
1:D:89:LYS:HD2	1:D:244:SER:O	2.17	0.44
1:A:328:ALA:O	1:A:332:ARG:N	2.46	0.44
1:H:81:GLN:O	1:H:85:VAL:HG12	2.17	0.44
1:F:414:VAL:HG21	1:H:437:GLY:HA3	1.98	0.44
3:H:505:2F0:CL1	3:H:505:2F0:O1	2.72	0.44
1:B:378:GLU:OE1	1:B:421:ARG:NH2	2.50	0.44
1:F:276:ILE:H	1:F:296:ASN:HB2	1.83	0.44
1:H:268:ARG:HD3	1:H:272:PRO:HA	1.99	0.43
1:H:57:ALA:O	1:H:61:ILE:HG12	2.17	0.43
1:E:395:GLY:O	1:E:399:LYS:HD3	2.18	0.43
1:E:285:GLU:N	1:E:285:GLU:OE1	2.47	0.43
1:F:38:GLU:H	1:F:38:GLU:CD	2.21	0.43
1:E:480:LYS:HE3	1:E:480:LYS:HB2	1.73	0.43
1:H:303:GLY:HA2	1:H:308:CYS:SG	2.58	0.43
1:G:258[B]:GLN:NE2	1:G:262:ASP:OD1	2.43	0.43
1:B:308:CYS:SG	2:B:500:IMP:H2	2.59	0.43
1:D:10:GLY:HA3	1:D:319:PRO:HG2	1.99	0.43
1:G:44:ILE:HD12	1:G:46:LEU:HD12	1.99	0.43
1:B:39:SER:OG	1:B:275:ASN:ND2	2.52	0.43
1:H:233:ALA:O	1:H:237:ILE:HG12	2.18	0.43
1:E:414:VAL:HG23	1:F:484:ASN:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ARG:NH1	1:F:272:PRO:O	2.52	0.43
1:E:284:ALA:HB1	1:E:330:GLU:HB2	2.01	0.43
1:C:48:SER:HB2	1:C:63:MET:HG3	2.01	0.42
1:E:79:GLU:H	1:E:79:GLU:CD	2.22	0.42
1:H:234:MET:HE1	1:H:270:LYS:HD3	2.01	0.42
1:G:344:ILE:HG23	1:G:349:ASP:HB2	2.00	0.42
1:C:344:ILE:HG23	1:C:349:ASP:HB2	2.01	0.42
1:B:34:THR:HG23	1:B:451:LEU:HD12	2.01	0.42
1:D:37:SER:OG	1:D:38:GLU:N	2.53	0.42
1:B:311:ARG:NH2	1:B:318:VAL:O	2.53	0.42
1:H:237:ILE:HG23	1:H:248:ILE:HD13	2.02	0.42
1:G:479:THR:HG23	1:H:420:GLY:HA2	2.01	0.42
1:E:340:ALA:HB3	1:E:361:VAL:HG22	2.01	0.42
1:H:287:THR:HG23	1:H:298:VAL:HG11	2.02	0.42
1:D:395:GLY:O	1:D:398[A]:GLU:HG2	2.20	0.42
1:H:12:THR:OG1	1:H:13:PHE:N	2.51	0.42
1:D:33:LYS:HG2	1:D:43:ASN:HA	2.02	0.42
1:E:445:TYR:HB3	1:G:316:VAL:HG11	2.00	0.42
1:G:357:GLY:HA2	1:G:455:ARG:HG2	2.01	0.42
1:G:445:TYR:HB2	1:H:316:VAL:HG21	2.02	0.42
1:H:61:ILE:HD13	1:H:88:VAL:HG13	2.01	0.42
1:A:345:LYS:HD2	1:C:475:HIS:NE2	2.34	0.42
1:E:89:LYS:HA	1:E:89:LYS:HD3	1.88	0.42
1:A:10:GLY:HA3	1:A:319:PRO:HG2	2.02	0.42
1:C:45:PRO:C	1:C:360:VAL:HG23	2.40	0.41
3:E:509:2F0:H3	3:E:509:2F0:O	2.20	0.41
1:A:466:ALA:HB1	1:B:14:ASP:HB2	2.02	0.41
1:A:470:GLU:OE1	1:B:12:THR:OG1	2.32	0.41
1:H:34:THR:HG21	1:H:360:VAL:HG22	2.01	0.41
1:C:14:ASP:HB3	1:C:468:LEU:HD22	2.02	0.41
1:F:282:ALA:HB1	1:F:318:VAL:HB	2.01	0.41
1:G:22:LYS:HE2	1:H:261:ILE:HD12	2.02	0.41
1:A:35:VAL:HG13	1:A:41:GLN:HG2	2.02	0.41
1:B:78:ILE:H	1:B:78:ILE:HD12	1.85	0.41
1:E:254:HIS:CE1	1:E:256:HIS:HB3	2.55	0.41
1:A:345:LYS:HB2	1:A:345:LYS:HE2	1.89	0.41
1:F:345:LYS:HG3	1:F:345:LYS:H	1.71	0.41
1:D:368:ALA:HB3	1:D:422:VAL:HG21	2.02	0.41
1:H:63:MET:SD	1:H:428:LEU:HD21	2.60	0.41
1:D:279:GLY:HA3	1:D:280:ASN:HA	1.92	0.41
1:G:24:ASP:OD1	1:G:24:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HE3	1:C:221:LEU:O	2.21	0.41
1:A:338:VAL:HG23	1:A:358:ALA:HA	2.01	0.41
1:E:345:LYS:HZ3	1:F:474:HIS:CD2	2.38	0.41
1:C:296:ASN:O	1:C:336:ILE:HG23	2.21	0.41
1:B:14:ASP:HB3	1:B:468:LEU:HD22	2.03	0.41
1:A:268[A]:ARG:NH2	1:A:294:GLY:O	2.54	0.41
1:A:316:VAL:HG11	1:C:445:TYR:HB3	2.03	0.40
1:C:287:THR:HG23	1:C:298:VAL:HG21	2.03	0.40
1:G:350:MET:HG3	1:G:361:VAL:HG21	2.03	0.40
1:C:303:GLY:HA3	1:C:311:ARG:HG3	2.03	0.40
1:B:370:VAL:O	1:B:373:SER:HB3	2.22	0.40
1:E:261:ILE:HD13	1:E:290:LEU:HD23	2.03	0.40
1:B:445:TYR:HB2	1:D:316:VAL:HG21	2.04	0.40
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.94	0.40
1:B:89:LYS:HA	1:B:89:LYS:HD2	1.76	0.40
1:C:257:SER:OG	1:C:260:VAL:HG23	2.22	0.40
1:B:287:THR:HG23	1:B:298:VAL:HG21	2.04	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	354/384 (92%)	342 (97%)	12 (3%)	0	100	100
1	B	352/384 (92%)	343 (97%)	8 (2%)	1 (0%)	46	75
1	C	348/384 (91%)	338 (97%)	10 (3%)	0	100	100
1	D	352/384 (92%)	340 (97%)	11 (3%)	1 (0%)	46	75
1	E	350/384 (91%)	342 (98%)	8 (2%)	0	100	100
1	F	346/384 (90%)	336 (97%)	10 (3%)	0	100	100
1	G	354/384 (92%)	350 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	346/384 (90%)	337 (97%)	9 (3%)	0	100 100
All	All	2802/3072 (91%)	2728 (97%)	72 (3%)	2 (0%)	56 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	GLY
1	D	412	LYS

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	276/298 (93%)	268 (97%)	8 (3%)	50 80
1	B	273/298 (92%)	262 (96%)	11 (4%)	38 69
1	C	270/298 (91%)	261 (97%)	9 (3%)	45 76
1	D	273/298 (92%)	267 (98%)	6 (2%)	60 86
1	E	271/298 (91%)	258 (95%)	13 (5%)	31 62
1	F	268/298 (90%)	261 (97%)	7 (3%)	54 83
1	G	274/298 (92%)	270 (98%)	4 (2%)	72 91
1	H	268/298 (90%)	263 (98%)	5 (2%)	65 88
All	All	2173/2384 (91%)	2110 (97%)	63 (3%)	50 80

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	VAL
1	A	39	SER
1	A	251	ASP
1	A	296	ASN
1	A	386	LYS

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Mol	Chain	Res	Type
1	A	477	GLN
1	A	480	LYS
1	B	-3	GLN
1	B	-2	SER
1	B	34	THR
1	B	41	GLN
1	B	79	GLU
1	B	297	VAL
1	B	360	VAL
1	B	370	VAL
1	B	380	TYR
1	B	402	LYS
1	B	413	LEU
1	C	74	LYS
1	C	75	ASN
1	C	223	VAL
1	C	251	ASP
1	C	345	LYS
1	C	389	ARG
1	C	398	GLU
1	C	414	VAL
1	C	469	LEU
1	D	9	GLU
1	D	46	LEU
1	D	74	LYS
1	D	221	LEU
1	D	245	VAL
1	D	432	VAL
1	E	16	VAL
1	E	34	THR
1	E	79	GLU
1	E	221	LEU
1	E	227	VAL
1	E	251	ASP
1	E	256	HIS
1	E	266	GLU
1	E	338	VAL
1	E	359	HIS
1	E	361	VAL
1	E	370	VAL
1	E	414	VAL
1	F	30	VAL

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Mol	Chain	Res	Type
1	F	34	THR
1	F	345	LYS
1	F	376	GLU
1	F	377	THR
1	F	413	LEU
1	F	475	HIS
1	G	248	ILE
1	G	370	VAL
1	G	377	THR
1	G	389	ARG
1	H	227	VAL
1	H	248	ILE
1	H	252	THR
1	H	378	GLU
1	H	386	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	B	275	ASN
1	B	334	HIS
1	C	75	ASN
1	C	475	HIS
1	D	84	GLN
1	E	43	ASN
1	E	474	HIS
1	E	475	HIS
1	E	477	GLN
1	F	474	HIS
1	G	459	GLN
1	G	474	HIS
1	H	434	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

48 ligands are modelled in this entry.

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	-	20,25,25	1.29	3 (15%)	22,38,38	2.63	4 (18%)
3	2F0	A	502	-	28,28,28	1.72	4 (14%)	39,40,40	1.28	3 (7%)
4	FMT	A	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.28	0
6	MLI	A	506	-	0,6,6	0.00	-	0,7,7	0.00	-
2	IMP	B	500	-	20,25,25	1.20	3 (15%)	22,38,38	2.47	4 (18%)
3	2F0	B	501	-	28,28,28	1.79	4 (14%)	39,40,40	1.37	6 (15%)
7	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.45	0
4	FMT	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	C	502	-	20,25,25	1.23	3 (15%)	22,38,38	2.59	3 (13%)
3	2F0	C	503	-	28,28,28	1.64	4 (14%)	39,40,40	1.56	7 (17%)
7	EDO	C	504	-	3,3,3	0.47	0	2,2,2	0.42	0
8	SO4	C	505	-	4,4,4	0.23	0	6,6,6	0.08	0
7	EDO	C	506	-	3,3,3	0.47	0	2,2,2	0.35	0
3	2F0	D	501	-	28,28,28	1.43	3 (10%)	39,40,40	1.97	6 (15%)
7	EDO	D	502	-	3,3,3	0.47	0	2,2,2	0.41	0
7	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.40	0
2	IMP	D	504	-	20,25,25	1.22	3 (15%)	22,38,38	2.57	3 (13%)
7	EDO	D	505	-	3,3,3	0.48	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	E	501	-	20,25,25	1.22	3 (15%)	22,38,38	2.56	3 (13%)
3	2F0	E	502	-	28,28,28	1.62	4 (14%)	39,40,40	1.33	4 (10%)
4	FMT	E	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	504	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	E	505	-	3,3,3	0.48	0	2,2,2	0.41	0
5	GOL	E	506	-	5,5,5	0.37	0	5,5,5	0.21	0
4	FMT	E	507	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLI	E	508	-	0,6,6	0.00	-	0,7,7	0.00	-
3	2F0	E	509	-	28,28,28	1.78	4 (14%)	39,40,40	1.29	3 (7%)
2	IMP	F	501	-	20,25,25	1.23	3 (15%)	22,38,38	2.59	3 (13%)
3	2F0	F	502	-	28,28,28	1.62	3 (10%)	39,40,40	1.74	6 (15%)
4	FMT	F	503	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	F	504	-	3,3,3	0.48	0	2,2,2	0.42	0
7	EDO	F	505	-	3,3,3	0.47	0	2,2,2	0.41	0
7	EDO	F	506	-	3,3,3	0.46	0	2,2,2	0.40	0
4	FMT	F	507	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	G	501	-	20,25,25	1.24	3 (15%)	22,38,38	2.60	3 (13%)
8	SO4	G	502	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	G	503	-	4,4,4	0.23	0	6,6,6	0.08	0
4	FMT	H	501	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	H	503	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	H	504	-	20,25,25	1.24	3 (15%)	22,38,38	2.59	3 (13%)
3	2F0	H	505	-	28,28,28	1.52	3 (10%)	39,40,40	1.73	5 (12%)
4	FMT	H	506	-	0,2,2	0.00	-	0,1,1	0.00	-

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	2F0	A	502	-	-	0/25/25/25	0/2/2/2
4	FMT	A	503	-	-	0/0/0/0	0/0/0/0
4	FMT	A	504	-	-	0/0/0/0	0/0/0/0
5	GOL	A	505	-	-	0/4/4/4	0/0/0/0
6	MLI	A	506	-	-	0/0/4/4	0/0/0/0
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2F0	B	501	-	-	0/25/25/25	0/2/2/2
7	EDO	B	502	-	-	0/1/1/1	0/0/0/0
4	FMT	B	503	-	-	0/0/0/0	0/0/0/0
4	FMT	C	501	-	-	0/0/0/0	0/0/0/0
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3
3	2F0	C	503	-	-	0/25/25/25	0/2/2/2
7	EDO	C	504	-	-	0/1/1/1	0/0/0/0
8	SO4	C	505	-	-	0/0/0/0	0/0/0/0
7	EDO	C	506	-	-	0/1/1/1	0/0/0/0
3	2F0	D	501	-	-	0/25/25/25	0/2/2/2
7	EDO	D	502	-	-	0/1/1/1	0/0/0/0
7	EDO	D	503	-	-	0/1/1/1	0/0/0/0
2	IMP	D	504	-	-	0/6/26/26	0/3/3/3
7	EDO	D	505	-	-	0/1/1/1	0/0/0/0
4	FMT	D	506	-	-	0/0/0/0	0/0/0/0
4	FMT	D	507	-	-	0/0/0/0	0/0/0/0
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
3	2F0	E	502	-	-	0/25/25/25	0/2/2/2
4	FMT	E	503	-	-	0/0/0/0	0/0/0/0
4	FMT	E	504	-	-	0/0/0/0	0/0/0/0
7	EDO	E	505	-	-	0/1/1/1	0/0/0/0
5	GOL	E	506	-	-	0/4/4/4	0/0/0/0
4	FMT	E	507	-	-	0/0/0/0	0/0/0/0
6	MLI	E	508	-	-	0/0/4/4	0/0/0/0
3	2F0	E	509	-	-	0/25/25/25	0/2/2/2
2	IMP	F	501	-	-	0/6/26/26	0/3/3/3
3	2F0	F	502	-	-	0/25/25/25	0/2/2/2
4	FMT	F	503	-	-	0/0/0/0	0/0/0/0
7	EDO	F	504	-	-	0/1/1/1	0/0/0/0
7	EDO	F	505	-	-	0/1/1/1	0/0/0/0
7	EDO	F	506	-	-	0/1/1/1	0/0/0/0
4	FMT	F	507	-	-	0/0/0/0	0/0/0/0
2	IMP	G	501	-	-	0/6/26/26	0/3/3/3
8	SO4	G	502	-	-	0/0/0/0	0/0/0/0
8	SO4	G	503	-	-	0/0/0/0	0/0/0/0
4	FMT	H	501	-	-	0/0/0/0	0/0/0/0
4	FMT	H	502	-	-	0/0/0/0	0/0/0/0
4	FMT	H	503	-	-	0/0/0/0	0/0/0/0
2	IMP	H	504	-	-	0/6/26/26	0/3/3/3
3	2F0	H	505	-	-	0/25/25/25	0/2/2/2
4	FMT	H	506	-	-	0/0/0/0	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	2F0	C1-C12	-5.06	1.47	1.54
3	E	509	2F0	C1-C12	-5.03	1.47	1.54
3	C	503	2F0	C1-C12	-4.87	1.47	1.54
3	F	502	2F0	C1-C12	-4.87	1.47	1.54
3	A	502	2F0	C1-N1	-4.56	1.43	1.47
3	A	502	2F0	C1-C12	-4.55	1.48	1.54
3	E	509	2F0	C1-N1	-4.55	1.43	1.47
3	B	501	2F0	C1-N1	-4.33	1.43	1.47
3	E	502	2F0	C1-C12	-4.00	1.48	1.54
3	E	502	2F0	C1-N1	-4.00	1.43	1.47
3	H	505	2F0	C1-C12	-3.88	1.49	1.54
3	D	501	2F0	C1-C12	-3.88	1.49	1.54
3	C	503	2F0	C1-N1	-3.71	1.43	1.47
3	H	505	2F0	C1-N1	-3.70	1.44	1.47
3	F	502	2F0	C4-N2	-3.50	1.31	1.37
3	B	501	2F0	C4-N2	-3.20	1.31	1.37
3	F	502	2F0	C1-N1	-3.13	1.44	1.47
3	C	503	2F0	C4-N2	-3.07	1.32	1.37
3	E	509	2F0	C4-N2	-3.01	1.32	1.37
3	E	502	2F0	C4-N2	-2.96	1.32	1.37
3	H	505	2F0	C4-N2	-2.94	1.32	1.37
3	B	501	2F0	C18-N4	-2.94	1.23	1.28
3	A	502	2F0	C4-N2	-2.90	1.32	1.37
3	D	501	2F0	C1-N1	-2.80	1.44	1.47
3	D	501	2F0	C4-N2	-2.51	1.33	1.37
3	E	509	2F0	C18-N4	-2.37	1.24	1.28
3	A	502	2F0	C18-N4	-2.21	1.24	1.28
3	E	502	2F0	C18-N4	-2.14	1.24	1.28
3	C	503	2F0	C18-N4	-2.03	1.24	1.28
2	B	500	IMP	C2-N1	2.26	1.38	1.33
2	F	501	IMP	C2-N1	2.32	1.38	1.33
2	G	501	IMP	C2-N1	2.33	1.38	1.33
2	E	501	IMP	C2-N1	2.34	1.38	1.33
2	C	502	IMP	C2-N1	2.38	1.38	1.33
2	D	504	IMP	C2-N1	2.39	1.38	1.33
2	H	504	IMP	C2-N1	2.43	1.38	1.33
2	A	501	IMP	C2-N1	2.45	1.38	1.33
2	A	501	IMP	C6-N1	2.73	1.38	1.33
2	B	500	IMP	C6-N1	2.80	1.38	1.33
2	D	504	IMP	C6-N1	2.80	1.38	1.33
2	F	501	IMP	C6-N1	2.81	1.38	1.33
2	E	501	IMP	C6-N1	2.82	1.38	1.33
2	C	502	IMP	C6-N1	2.84	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	504	IMP	C6-N1	2.89	1.38	1.33
2	G	501	IMP	C6-N1	2.92	1.38	1.33
2	B	500	IMP	C2-N3	3.43	1.38	1.32
2	H	504	IMP	C2-N3	3.46	1.38	1.32
2	D	504	IMP	C2-N3	3.48	1.38	1.32
2	E	501	IMP	C2-N3	3.49	1.38	1.32
2	C	502	IMP	C2-N3	3.52	1.38	1.32
2	G	501	IMP	C2-N3	3.53	1.38	1.32
2	F	501	IMP	C2-N3	3.54	1.38	1.32
2	A	501	IMP	C2-N3	3.91	1.39	1.32

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	IMP	N3-C2-N1	-11.37	120.19	128.89
2	G	501	IMP	N3-C2-N1	-11.23	120.30	128.89
2	C	502	IMP	N3-C2-N1	-11.19	120.32	128.89
2	F	501	IMP	N3-C2-N1	-11.17	120.34	128.89
2	H	504	IMP	N3-C2-N1	-11.14	120.36	128.89
2	E	501	IMP	N3-C2-N1	-11.08	120.41	128.89
2	D	504	IMP	N3-C2-N1	-11.06	120.42	128.89
2	B	500	IMP	N3-C2-N1	-10.58	120.80	128.89
3	D	501	2F0	C17-C16-C18	-7.27	114.82	120.58
3	H	505	2F0	C17-C16-C18	-5.01	116.61	120.58
3	H	505	2F0	C8-C7-C11	-4.78	116.09	122.71
3	A	502	2F0	C17-C16-C18	-3.59	117.73	120.58
3	E	502	2F0	C8-C7-C11	-3.00	118.55	122.71
3	D	501	2F0	C8-C7-C11	-2.74	118.92	122.71
3	D	501	2F0	C17-C12-C1	-2.72	117.14	120.64
3	E	502	2F0	C17-C16-C18	-2.69	118.45	120.58
3	E	509	2F0	C17-C16-C18	-2.63	118.50	120.58
3	C	503	2F0	C8-C7-C11	-2.56	119.17	122.71
3	C	503	2F0	C17-C16-C18	-2.53	118.58	120.58
3	B	501	2F0	C17-C16-C18	-2.42	118.66	120.58
3	B	501	2F0	C19-C18-N4	-2.32	115.72	123.16
3	F	502	2F0	O-C4-N2	-2.16	120.30	123.58
3	F	502	2F0	O1-C11-N3	-2.13	119.59	122.59
3	B	501	2F0	C8-C7-C11	-2.05	119.87	122.71
2	A	501	IMP	C1'-N9-C4	-2.03	123.87	126.94
2	B	500	IMP	C4-C5-N7	-2.03	107.61	109.48
3	C	503	2F0	C13-C12-C1	-2.02	118.50	121.27
3	F	502	2F0	C12-C1-N1	-2.01	108.78	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	IMP	O2P-P-O1P	2.01	117.05	110.58
3	C	503	2F0	C3-C1-N1	2.03	112.37	108.02
3	H	505	2F0	C15-C16-C17	2.06	121.74	119.24
3	H	505	2F0	C6-C7-C8	2.18	120.65	117.86
3	A	502	2F0	C19-C18-C16	2.20	122.80	119.66
2	E	501	IMP	O2P-P-O1P	2.21	117.70	110.58
3	D	501	2F0	C15-C16-C18	2.25	123.94	121.21
2	G	501	IMP	O2P-P-O1P	2.31	118.00	110.58
2	H	504	IMP	O2P-P-O1P	2.34	118.11	110.58
2	D	504	IMP	O2P-P-O1P	2.34	118.11	110.58
3	E	502	2F0	C19-C18-C16	2.38	123.05	119.66
2	C	502	IMP	O2P-P-O1P	2.38	118.24	110.58
2	B	500	IMP	O2P-P-O1P	2.39	118.26	110.58
2	B	500	IMP	C2-N1-C6	2.39	119.66	116.04
3	F	502	2F0	C3-C1-N1	2.41	113.17	108.02
2	F	501	IMP	O2P-P-O1P	2.42	118.36	110.58
2	F	501	IMP	C2-N1-C6	2.45	119.75	116.04
2	A	501	IMP	C2-N1-C6	2.46	119.77	116.04
2	E	501	IMP	C2-N1-C6	2.49	119.81	116.04
2	C	502	IMP	C2-N1-C6	2.55	119.91	116.04
2	D	504	IMP	C2-N1-C6	2.59	119.97	116.04
3	C	503	2F0	C12-C1-N1	2.61	112.33	110.32
2	G	501	IMP	C2-N1-C6	2.62	120.00	116.04
3	E	509	2F0	C1-N1-C4	2.69	126.60	123.78
2	H	504	IMP	C2-N1-C6	2.72	120.16	116.04
3	B	501	2F0	C12-C1-N1	2.92	112.57	110.32
3	D	501	2F0	C19-C18-C16	2.96	123.88	119.66
3	B	501	2F0	C19-C18-C16	3.08	124.05	119.66
3	E	509	2F0	O2-N4-C18	3.65	117.99	112.83
3	C	503	2F0	O2-N4-C18	3.88	118.32	112.83
3	B	501	2F0	C1-N1-C4	3.89	127.86	123.78
3	E	502	2F0	O2-N4-C18	4.04	118.54	112.83
3	A	502	2F0	O2-N4-C18	4.47	119.15	112.83
3	C	503	2F0	C1-N1-C4	4.90	128.92	123.78
3	H	505	2F0	O2-N4-C18	4.91	119.77	112.83
3	F	502	2F0	C1-N1-C4	5.44	129.49	123.78
3	F	502	2F0	O2-N4-C18	5.82	121.06	112.83
3	D	501	2F0	O2-N4-C18	6.21	121.61	112.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	1	0
3	A	502	2F0	3	0
2	B	500	IMP	2	0
3	B	501	2F0	2	0
2	C	502	IMP	1	0
3	C	503	2F0	1	0
7	C	504	EDO	2	0
7	C	506	EDO	2	0
3	D	501	2F0	3	0
2	D	504	IMP	1	0
3	E	502	2F0	4	0
3	E	509	2F0	2	0
2	F	501	IMP	1	0
3	F	502	2F0	2	0
7	F	506	EDO	2	0
2	G	501	IMP	1	0
2	H	504	IMP	1	0
3	H	505	2F0	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	351/384 (91%)	0.53	32 (9%) 11 9	27, 47, 70, 84	1 (0%)
1	B	355/384 (92%)	0.39	10 (2%) 56 57	25, 45, 68, 102	2 (0%)
1	C	348/384 (90%)	0.30	7 (2%) 68 69	32, 45, 64, 74	0
1	D	352/384 (91%)	0.60	26 (7%) 17 15	30, 48, 68, 97	0
1	E	352/384 (91%)	0.50	23 (6%) 22 20	31, 46, 73, 89	1 (0%)
1	F	350/384 (91%)	0.62	30 (8%) 13 10	34, 50, 70, 85	1 (0%)
1	G	356/384 (92%)	0.54	22 (6%) 24 23	31, 49, 67, 87	1 (0%)
1	H	350/384 (91%)	0.61	26 (7%) 17 15	33, 51, 71, 80	1 (0%)
All	All	2814/3072 (91%)	0.51	176 (6%) 23 22	25, 48, 70, 102	7 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ALA	7.5
1	H	-2	SER	6.7
1	H	226	ALA	6.2
1	E	413	LEU	5.6
1	H	250	LEU	5.2
1	F	-2	SER	4.8
1	C	486	SER	4.6
1	F	229	VAL	4.6
1	H	271	TYR	4.5
1	H	228	GLY	4.5
1	D	249	VAL	4.5
1	H	249	VAL	4.4
1	D	227	VAL	4.4
1	A	225	ALA	4.4
1	B	-4	PHE	4.2
1	F	395	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	244	SER	4.1
1	A	224	GLY	4.1
1	E	382	GLY	4.1
1	H	246	ASP	4.0
1	G	278	ALA	4.0
1	A	477	GLN	3.9
1	D	246	ASP	3.9
1	A	223	VAL	3.9
1	D	248	ILE	3.8
1	F	248	ILE	3.8
1	F	251	ASP	3.8
1	D	241	VAL	3.7
1	F	482	ALA	3.7
1	D	228	GLY	3.6
1	A	251	ASP	3.6
1	H	243	ALA	3.6
1	A	298	VAL	3.6
1	A	413	LEU	3.5
1	G	36	LEU	3.5
1	G	251	ASP	3.5
1	F	394	VAL	3.5
1	F	475	HIS	3.4
1	H	227	VAL	3.4
1	F	481	GLU	3.4
1	G	250	LEU	3.4
1	F	230	THR	3.3
1	C	380	TYR	3.3
1	F	399	LYS	3.3
1	H	85	VAL	3.2
1	D	412	LYS	3.2
1	E	-3	GLN	3.2
1	E	250	LEU	3.2
1	D	237	ILE	3.2
1	B	251	ASP	3.2
1	F	380	TYR	3.2
1	A	357	GLY	3.2
1	G	277	ILE	3.1
1	H	316	VAL	3.1
1	A	250	LEU	3.1
1	H	241	VAL	3.1
1	B	412	LYS	3.1
1	F	223	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	271	TYR	3.0
1	E	255	GLY	3.0
1	A	280	ASN	3.0
1	D	413	LEU	3.0
1	E	0	ALA	3.0
1	G	245	VAL	3.0
1	F	376	GLU	2.9
1	E	225	ALA	2.9
1	G	380	TYR	2.9
1	E	477	GLN	2.9
1	A	383	ARG	2.9
1	E	237	ILE	2.9
1	F	249	VAL	2.9
1	G	-4	PHE	2.8
1	F	387	VAL	2.8
1	A	382	GLY	2.8
1	H	224	GLY	2.8
1	A	40	LEU	2.8
1	D	222	LEU	2.8
1	F	388	TYR	2.8
1	G	230	THR	2.8
1	A	92	GLY	2.8
1	F	375	GLY	2.8
1	D	394	VAL	2.8
1	H	247	ALA	2.8
1	F	74	LYS	2.7
1	G	292	GLU	2.7
1	A	459	GLN	2.7
1	E	239	ALA	2.7
1	D	277	ILE	2.7
1	B	413	LEU	2.7
1	D	431	THR	2.6
1	A	222	LEU	2.6
1	G	336	ILE	2.6
1	H	244	SER	2.6
1	A	387	VAL	2.6
1	E	476	VAL	2.6
1	A	486	SER	2.6
1	H	245	VAL	2.6
1	C	482	ALA	2.6
1	F	84	GLN	2.6
1	F	61	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	241	VAL	2.6
1	F	277	ILE	2.6
1	D	399	LYS	2.5
1	F	260	VAL	2.5
1	A	229	VAL	2.5
1	B	379	ILE	2.5
1	D	266	GLU	2.5
1	D	74	LYS	2.5
1	C	75	ASN	2.5
1	G	354	LEU	2.4
1	F	225	ALA	2.4
1	B	378	GLU	2.4
1	E	375	GLY	2.4
1	H	413	LEU	2.4
1	E	226	ALA	2.4
1	F	69	LEU	2.4
1	A	255	GLY	2.4
1	D	275	ASN	2.4
1	E	399	LYS	2.4
1	A	487	LEU	2.3
1	A	341	ASP	2.3
1	E	251	ASP	2.3
1	H	426	GLY	2.3
1	F	371	ALA	2.3
1	A	70	GLY	2.3
1	E	243	ALA	2.3
1	G	231	ALA	2.3
1	A	241	VAL	2.3
1	H	86	ASP	2.3
1	G	385	PHE	2.3
1	A	232	ASP	2.3
1	F	263	LYS	2.3
1	E	28	ARG	2.3
1	H	364	GLY	2.3
1	G	333	LYS	2.3
1	D	-2	SER	2.2
1	E	238	ASP	2.2
1	A	247	ALA	2.2
1	D	247	ALA	2.2
1	H	251	ASP	2.2
1	A	82	ALA	2.2
1	G	358	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	ASP	2.2
1	A	243	ALA	2.2
1	B	250	LEU	2.2
1	F	224	GLY	2.2
1	F	294	GLY	2.2
1	A	394	VAL	2.2
1	C	394	VAL	2.2
1	G	302	ILE	2.2
1	H	82	ALA	2.2
1	E	376	GLU	2.2
1	G	290	LEU	2.2
1	H	248	ILE	2.2
1	D	389	ARG	2.1
1	A	273	SER	2.1
1	B	369	GLY	2.1
1	H	89	LYS	2.1
1	D	225	ALA	2.1
1	G	225	ALA	2.1
1	G	274	LEU	2.1
1	A	239	ALA	2.1
1	C	383	ARG	2.1
1	G	331	ALA	2.1
1	F	486	SER	2.1
1	E	229	VAL	2.1
1	A	2	TRP	2.1
1	H	40	LEU	2.1
1	E	247	ALA	2.1
1	B	252	THR	2.0
1	H	360	VAL	2.0
1	D	251	ASP	2.0
1	B	-3	GLN	2.0
1	D	46	LEU	2.0
1	G	40	LEU	2.0
1	E	387	VAL	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
7	EDO	F	504	4/4	0.60	0.39	7.03	66,67,69,69	0
8	SO4	G	502	5/5	0.68	0.52	6.51	127,128,128,128	0
7	EDO	B	502	4/4	0.90	0.37	5.61	71,71,71,72	0
4	FMT	A	503	3/3	0.90	0.31	4.94	48,48,48,49	0
4	FMT	H	502	3/3	0.81	0.30	3.89	68,68,68,68	0
3	2F0	A	502	27/27	0.91	0.30	3.83	37,45,50,58	0
4	FMT	D	507	3/3	0.75	0.30	3.61	62,62,63,64	0
7	EDO	C	506	4/4	0.81	0.39	3.13	54,56,58,59	0
3	2F0	C	503	27/27	0.92	0.25	2.85	43,50,54,56	0
3	2F0	E	509	27/27	0.91	0.26	1.65	39,51,55,57	0
3	2F0	B	501	27/27	0.90	0.31	1.52	41,50,56,61	0
8	SO4	G	503	5/5	0.75	0.34	1.45	144,144,145,145	0
3	2F0	F	502	27/27	0.89	0.24	1.17	42,49,54,67	0
4	FMT	H	506	3/3	0.83	0.24	0.87	65,65,65,65	0
3	2F0	H	505	27/27	0.89	0.24	0.67	47,53,59,63	0
2	IMP	D	504	23/23	0.95	0.23	0.63	36,41,45,49	0
3	2F0	D	501	27/27	0.91	0.22	0.60	34,42,57,61	0
3	2F0	E	502	27/27	0.92	0.24	0.37	38,43,52,54	0
2	IMP	F	501	23/23	0.94	0.19	-0.07	37,44,47,48	0
7	EDO	F	506	4/4	0.96	0.20	-0.11	39,39,39,40	0
4	FMT	E	507	3/3	0.94	0.19	-0.18	37,37,37,37	0
7	EDO	C	504	4/4	0.86	0.18	-0.34	53,54,54,54	0
2	IMP	E	501	23/23	0.92	0.18	-0.34	31,35,43,44	0
2	IMP	H	504	23/23	0.95	0.18	-0.49	37,41,47,48	0
2	IMP	C	502	23/23	0.96	0.17	-0.58	32,41,44,46	0
2	IMP	B	500	23/23	0.96	0.16	-0.92	33,36,38,39	0
2	IMP	G	501	23/23	0.95	0.16	-1.01	36,39,41,42	0
2	IMP	A	501	23/23	0.95	0.15	-1.01	35,40,44,45	0
4	FMT	D	506	3/3	0.84	0.14	-1.23	43,43,46,47	0
4	FMT	E	503	3/3	0.85	0.23	-	74,74,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FMT	B	503	3/3	0.84	0.35	-	46,46,47,49	0
6	MLI	A	506	7/7	0.71	0.40	-	87,88,91,91	0
4	FMT	A	504	3/3	0.85	0.37	-	62,62,63,64	0
7	EDO	D	505	4/4	0.85	0.24	-	55,56,57,57	0
4	FMT	E	504	3/3	0.79	0.19	-	53,53,53,53	0
4	FMT	F	507	3/3	0.65	0.37	-	69,69,70,70	0
4	FMT	H	501	3/3	0.84	0.20	-	62,62,63,63	0
8	SO4	C	505	5/5	0.88	0.23	-	119,119,119,119	0
7	EDO	D	503	4/4	0.73	0.30	-	51,53,55,56	0
4	FMT	C	501	3/3	0.92	0.32	-	69,69,70,71	0
7	EDO	D	502	4/4	0.74	0.23	-	59,60,60,60	0
6	MLI	E	508	7/7	0.88	0.25	-	64,65,67,68	0
7	EDO	E	505	4/4	0.86	0.14	-	41,43,45,46	0
5	GOL	A	505	6/6	0.67	0.29	-	48,51,51,52	0
7	EDO	F	505	4/4	0.81	0.13	-	56,58,59,59	0
4	FMT	F	503	3/3	0.94	0.14	-	42,42,43,44	0
5	GOL	E	506	6/6	0.70	0.30	-	50,52,53,54	0
4	FMT	H	503	3/3	0.84	0.17	-	66,66,67,67	0

6.5 Other polymers

There are no such residues in this entry.