



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2017 – 06:38 PM EDT

PDB ID : 4Q33  
Title : Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from *Clostridium perfringens* Complexed with IMP and A110  
Authors : Maltseva, N.; Kim, Y.; Makowska-Grzyska, M.; Mulligan, R.; Gu, M.; Zhang, M.; Mandapati, K.; Gollapalli, D.R.; Gorla, S.K.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : unknown  
Resolution : 2.88 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

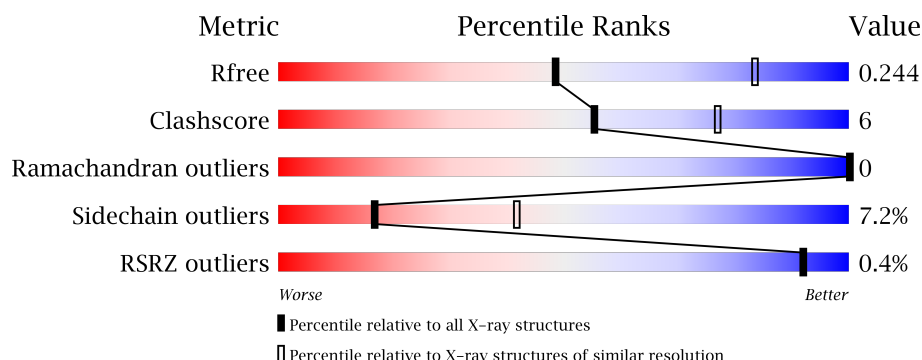
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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))
$R_{free}$	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 77%, yellow 18%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>77%</span> <span>18%</span> <span>5%</span> </div> </div>
1	B	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 80%, yellow 13%, orange 6%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>80%</span> <span>13%</span> <span>6%</span> </div> </div>
1	C	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 15%, orange 6%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>78%</span> <span>15%</span> <span>6%</span> </div> </div>
1	D	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 76%, yellow 17%, orange 6%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>76%</span> <span>17%</span> <span>6%</span> </div> </div>
1	E	363	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 72%, yellow 21%, orange 6%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>72%</span> <span>21%</span> <span>6%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	363	 74%20%5%
1	G	363	 76%17%5%
1	H	363	 80%13%5%

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	2YA	C	501	-	-	-	X
3	2YA	H	501	-	-	-	X
5	FMT	F	502	-	-	X	-
7	GOL	F	506	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20930 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	344	Total	C	N	O	S	0	4	0
			2574	1615	446	493	20			
1	B	342	Total	C	N	O	S	0	2	0
			2539	1594	441	485	19			
1	C	343	Total	C	N	O	S	0	1	0
			2536	1593	438	486	19			
1	D	342	Total	C	N	O	S	0	2	0
			2534	1591	437	486	20			
1	E	343	Total	C	N	O	S	0	3	0
			2552	1603	443	487	19			
1	F	344	Total	C	N	O	S	0	1	0
			2545	1601	440	485	19			
1	G	344	Total	C	N	O	S	0	0	0
			2535	1594	438	484	19			
1	H	344	Total	C	N	O	S	0	1	0
			2544	1599	439	487	19			

There are 48 discrepancies between the modelled and reference sequences:

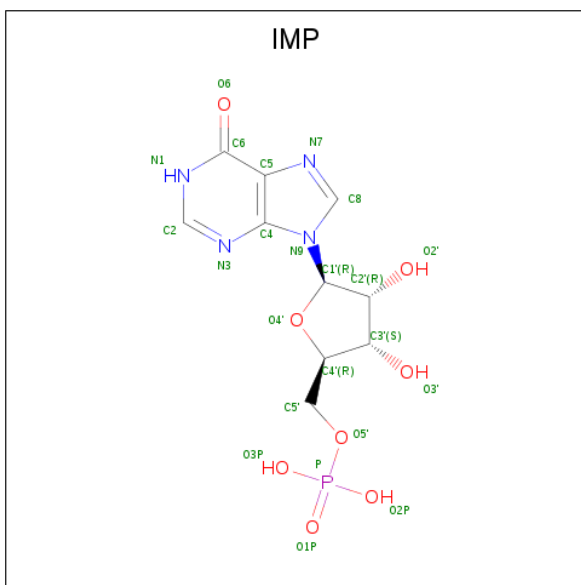
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
A	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
A	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
A	89	SER	-	LINKER	UNP Q0TN42
A	90	GLY	-	LINKER	UNP Q0TN42
A	91	GLY	-	LINKER	UNP Q0TN42
B	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
B	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
B	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
B	89	SER	-	LINKER	UNP Q0TN42
B	90	GLY	-	LINKER	UNP Q0TN42
B	91	GLY	-	LINKER	UNP Q0TN42
C	-2	SER	-	EXPRESSION TAG	UNP Q0TN42

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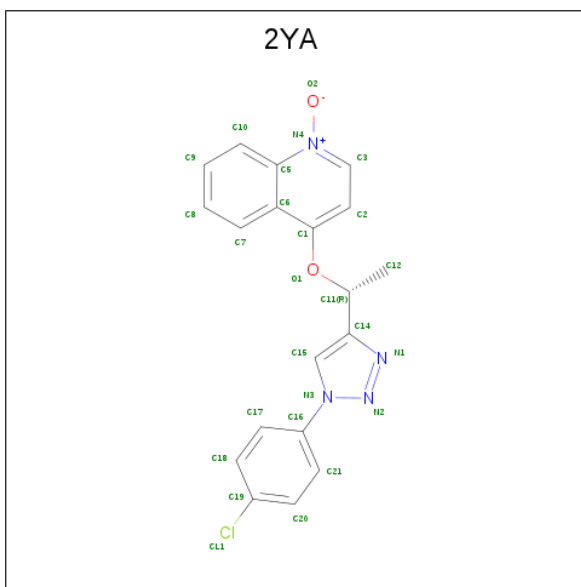
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
C	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
C	89	SER	-	LINKER	UNP Q0TN42
C	90	GLY	-	LINKER	UNP Q0TN42
C	91	GLY	-	LINKER	UNP Q0TN42
D	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
D	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
D	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
D	89	SER	-	LINKER	UNP Q0TN42
D	90	GLY	-	LINKER	UNP Q0TN42
D	91	GLY	-	LINKER	UNP Q0TN42
E	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
E	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
E	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
E	89	SER	-	LINKER	UNP Q0TN42
E	90	GLY	-	LINKER	UNP Q0TN42
E	91	GLY	-	LINKER	UNP Q0TN42
F	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
F	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
F	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
F	89	SER	-	LINKER	UNP Q0TN42
F	90	GLY	-	LINKER	UNP Q0TN42
F	91	GLY	-	LINKER	UNP Q0TN42
G	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
G	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
G	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
G	89	SER	-	LINKER	UNP Q0TN42
G	90	GLY	-	LINKER	UNP Q0TN42
G	91	GLY	-	LINKER	UNP Q0TN42
H	-2	SER	-	EXPRESSION TAG	UNP Q0TN42
H	-1	ASN	-	EXPRESSION TAG	UNP Q0TN42
H	0	ALA	-	EXPRESSION TAG	UNP Q0TN42
H	89	SER	-	LINKER	UNP Q0TN42
H	90	GLY	-	LINKER	UNP Q0TN42
H	91	GLY	-	LINKER	UNP Q0TN42

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



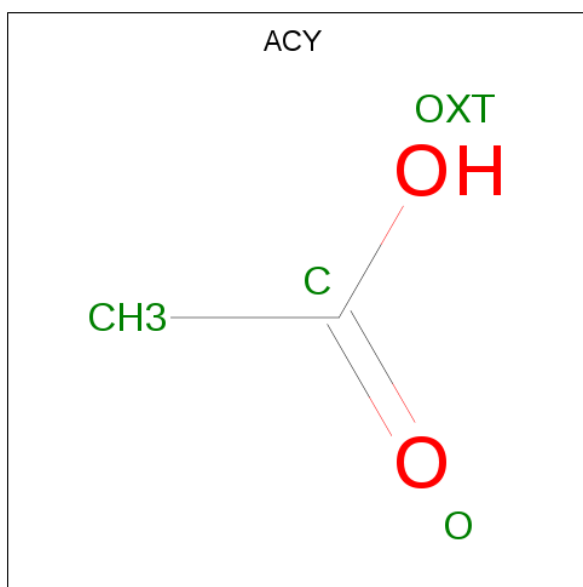
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total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

- Molecule 3 is 4-[(1R)-1-[1-(4-chlorophenyl)-1,2,3-triazol-4-yl]ethoxy]-1-oxidanyl-quinoline (three-letter code: 2YA) (formula: C<sub>19</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>2</sub>).



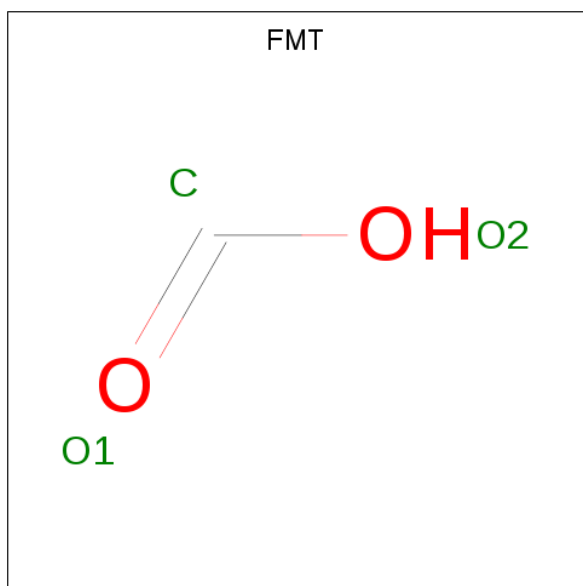
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	E	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	F	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	G	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		
3	H	1	Total	C	Cl	N	O	0	0
			26	19	1	4	2		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			3	1	2		
5	F	1	Total	C	O	0	0
			3	1	2		
5	F	1	Total	C	O	0	0
			3	1	2		

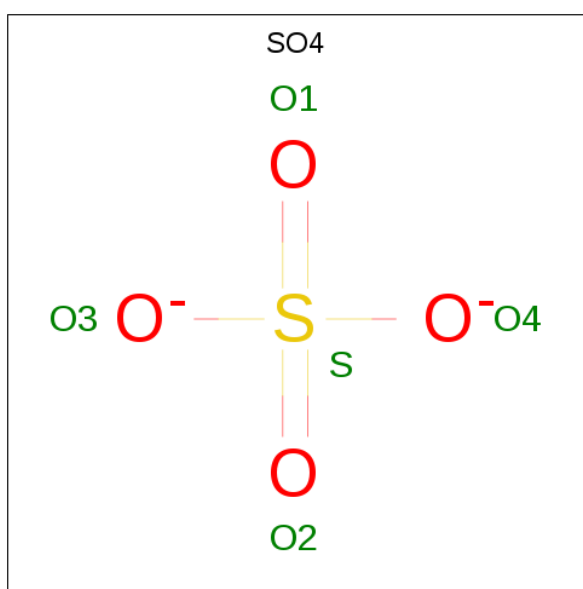
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			3	1	2		
5	G	1	Total	C	O	0	0
			3	1	2		
5	H	1	Total	C	O	0	0
			3	1	2		
5	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

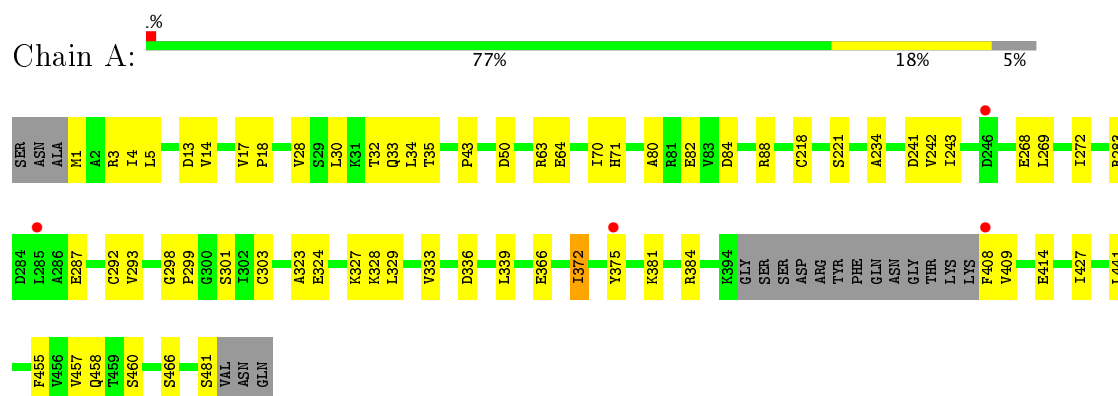
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	B	15	Total	O	0	0
			15	15		
8	C	16	Total	O	0	0
			16	16		
8	D	17	Total	O	0	0
			17	17		
8	E	22	Total	O	0	0
			22	22		
8	F	23	Total	O	0	0
			23	23		
8	G	11	Total	O	0	0
			11	11		
8	H	17	Total	O	0	0
			17	17		

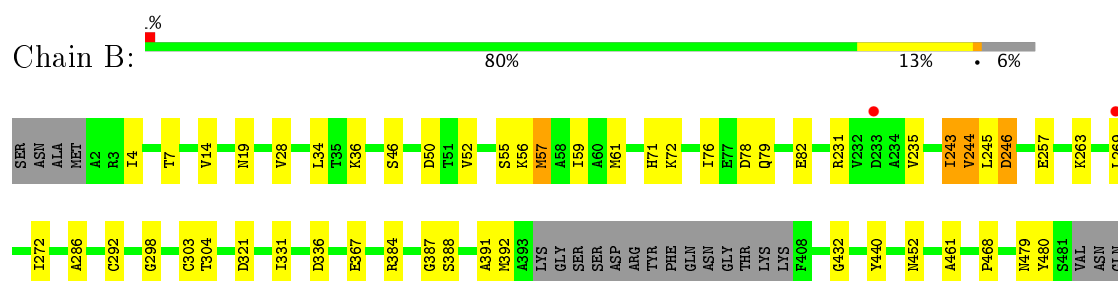
### 3 Residue-property plots [i](#)

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

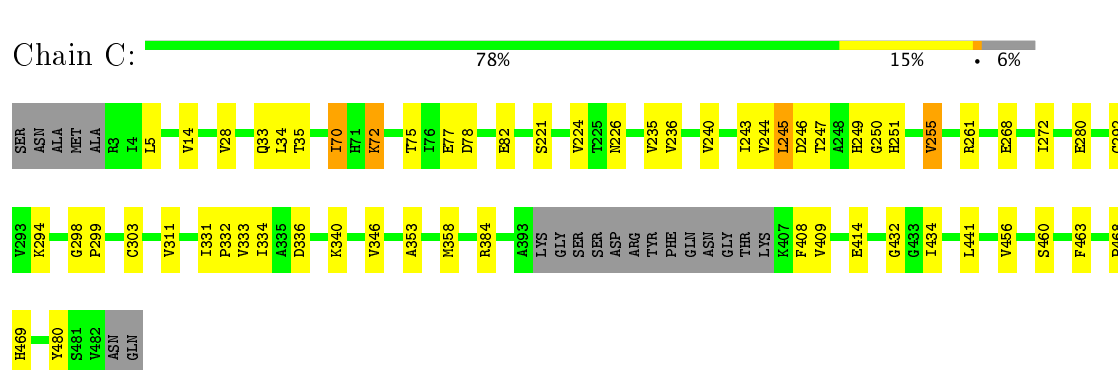
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



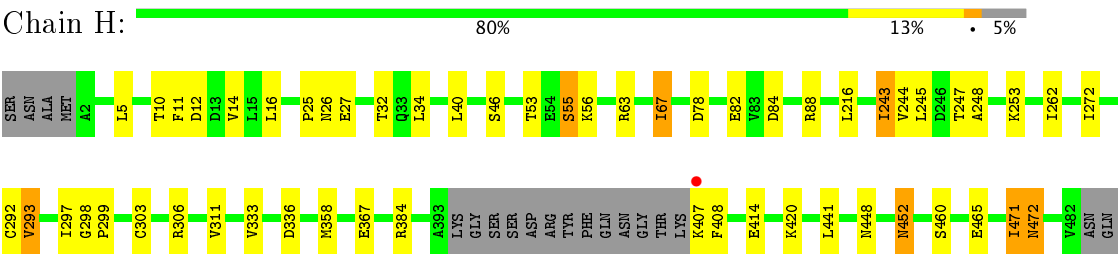
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



● Molecule 1: Inosine-5'-monophosphate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.12Å 89.25Å 99.19Å 70.82° 72.66° 79.30°	Depositor
Resolution (Å)	37.21 – 2.88 48.50 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (37.21-2.88) 88.4 (48.50-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, $R_{free}$	0.185 , 0.243 0.185 , 0.244	Depositor DCC
$R_{free}$ test set	3012 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.21	0/2607	0.41	0/3515
1	B	0.22	0/2572	0.40	0/3470
1	C	0.22	0/2571	0.41	0/3469
1	D	0.22	0/2567	0.41	0/3464
1	E	0.21	0/2585	0.41	0/3489
1	F	0.22	0/2578	0.42	0/3477
1	G	0.23	0/2568	0.42	0/3465
1	H	0.23	0/2577	0.41	0/3477
All	All	0.22	0/20625	0.41	0/27826

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2637	25	0
1	B	2539	0	2602	29	0
1	C	2536	0	2604	28	0
1	D	2534	0	2592	33	0
1	E	2552	0	2617	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2545	0	2619	43	0
1	G	2535	0	2605	41	0
1	H	2544	0	2610	30	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	2	0
2	D	23	0	11	2	0
2	E	23	0	11	3	0
2	F	23	0	11	2	0
2	G	23	0	11	2	0
2	H	23	0	11	1	0
3	A	26	0	15	0	0
3	B	52	0	30	0	0
3	C	26	0	15	0	0
3	E	26	0	15	0	0
3	F	26	0	15	0	0
3	G	26	0	15	0	0
3	H	26	0	15	0	0
4	D	4	0	3	0	0
5	E	3	0	1	0	0
5	F	9	0	3	2	0
5	G	3	0	1	1	0
5	H	6	0	2	0	0
6	E	5	0	0	0	0
7	F	12	0	16	0	0
8	A	16	0	0	0	0
8	B	15	0	0	0	0
8	C	16	0	0	0	0
8	D	17	0	0	0	0
8	E	22	0	0	0	0
8	F	23	0	0	0	0
8	G	11	0	0	0	0
8	H	17	0	0	0	0
All	All	20930	0	21120	248	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 (248) 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:D:279:PRO:HB3	1:D:325[B]:GLU:HG3	1.66	0.78
1:E:444:PRO:HD2	1:E:448:ASN:HD22	1.49	0.77
1:E:83:VAL:O	1:E:87:LYS:HG2	1.86	0.76
1:D:283:ARG:NH1	1:D:325[A]:GLU:OE2	2.21	0.72
1:B:272:ILE:HG12	1:B:292:CYS:HB3	1.74	0.68
1:E:247:THR:OG1	1:E:248:ALA:N	2.26	0.67
1:A:243:ILE:HG13	1:A:269:LEU:HD21	1.75	0.67
1:D:226:ASN:OD1	1:D:226:ASN:N	2.29	0.65
1:E:358:MET:HG2	1:E:361:ILE:HD12	1.79	0.65
1:B:263:LYS:NZ	1:B:269:LEU:O	2.27	0.65
1:B:56:LYS:HD2	1:B:367:GLU:HA	1.78	0.65
1:C:298:GLY:HA2	1:C:303:CYS:SG	2.38	0.64
1:A:409:VAL:HG21	1:C:432:GLY:HA3	1.80	0.64
1:D:244:VAL:HG12	1:D:272:ILE:HB	1.79	0.63
1:F:358:MET:HG2	1:F:361:ILE:HD12	1.79	0.63
1:E:87:LYS:HA	1:E:87:LYS:HE3	1.82	0.62
1:G:221:SER:HA	1:G:244:VAL:HG22	1.82	0.62
1:E:349:LEU:HD13	1:E:446:LEU:HD11	1.82	0.62
1:H:272:ILE:HG12	1:H:292:CYS:HB3	1.82	0.61
1:C:75:THR:HG22	1:C:77:GLU:H	1.65	0.61
1:G:249:HIS:HB3	5:G:502:FMT:H	1.82	0.61
1:E:384:ARG:HB3	1:E:414:GLU:HG3	1.82	0.60
1:H:298:GLY:N	1:H:299:PRO:HD3	2.16	0.60
1:A:272:ILE:HG12	1:A:292:CYS:HB3	1.82	0.60
1:E:432:GLY:HA3	1:F:409:VAL:HG21	1.82	0.60
1:A:283:ARG:HG2	1:A:329:LEU:HD11	1.84	0.59
1:C:336:ASP:OD2	2:C:500:IMP:O2'	2.20	0.59
1:E:461:ALA:HB2	5:F:502:FMT:H	1.83	0.59
1:G:272:ILE:HG12	1:G:292:CYS:HB3	1.85	0.58
1:A:70:ILE:HD13	1:A:82:GLU:HB3	1.85	0.58
1:A:64:GLU:HG2	1:A:427:ILE:HG21	1.85	0.58
1:B:244:VAL:HB	1:B:272:ILE:HB	1.84	0.58
1:E:298:GLY:HA2	1:E:303:CYS:SG	2.43	0.58
1:D:74:MET:O	1:D:231:ARG:NH1	2.35	0.58
1:E:389:LEU:HD13	1:E:410:PRO:HG3	1.86	0.58
1:G:336:ASP:OD2	2:G:500:IMP:O2'	2.21	0.58
1:C:384:ARG:HB3	1:C:414:GLU:HG3	1.86	0.57
1:B:246:ASP:OD1	1:B:246:ASP:N	2.36	0.57
1:D:298:GLY:HA2	1:D:303:CYS:SG	2.44	0.57
1:G:257:GLU:HA	1:G:260:LYS:HE2	1.86	0.57
1:G:302:ILE:HG22	1:H:471:ILE:HD12	1.87	0.57
1:F:64:GLU:HG2	1:F:427:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:ASP:HA	1:G:236:VAL:HB	1.88	0.56
1:H:384:ARG:HB3	1:H:414:GLU:HG3	1.86	0.56
1:F:298:GLY:HA2	1:F:303:CYS:SG	2.45	0.56
1:C:272:ILE:HG12	1:C:292:CYS:HB3	1.86	0.56
1:E:32:THR:HG23	1:E:446:LEU:HD23	1.88	0.56
1:D:387:GLY:N	2:D:501:IMP:O6	2.36	0.56
1:A:372:ILE:HD13	1:A:381:LYS:HE2	1.88	0.56
1:G:59:ILE:HD11	1:G:86:VAL:HA	1.88	0.56
1:C:463:PHE:HZ	1:D:464:ARG:HH22	1.54	0.56
1:F:18:PRO:HG2	1:H:297:ILE:HD12	1.88	0.55
1:G:34:LEU:HD11	1:G:272:ILE:HD11	1.88	0.55
1:G:298:GLY:HA2	1:G:303:CYS:SG	2.47	0.55
1:C:235:VAL:HG21	1:C:243:ILE:HD11	1.89	0.54
1:E:455:PHE:HB2	1:F:4:ILE:HD13	1.88	0.54
1:D:57:MET:HE2	1:D:423:LEU:HD22	1.90	0.54
1:F:22:GLU:HG2	1:H:253:LYS:HB2	1.88	0.54
1:G:46:SER:HB2	1:G:61:MET:HG3	1.90	0.54
1:D:438:MET:HG2	1:D:449:LEU:HD13	1.88	0.54
1:F:461:ALA:HB1	1:H:12:ASP:HB2	1.90	0.54
1:C:346:VAL:HG22	1:C:434:ILE:HA	1.90	0.53
1:G:33:GLN:HG3	1:G:35:THR:O	2.09	0.53
1:D:225:THR:OG1	1:D:226:ASN:N	2.41	0.53
1:F:50:ASP:OD2	1:F:384:ARG:NH2	2.39	0.53
1:B:76:ILE:HG12	1:B:231[A]:ARG:HG2	1.89	0.53
1:E:340:LYS:HE2	1:G:469:HIS:CE1	2.43	0.53
1:E:315:GLN:NE2	1:E:336:ASP:O	2.42	0.53
1:G:233:ASP:HB3	1:G:266:TYR:OH	2.09	0.53
1:F:249:HIS:O	1:F:252:SER:OG	2.26	0.53
1:E:366:GLU:N	1:E:421:GLY:O	2.41	0.53
1:C:33:GLN:HG3	1:C:35:THR:O	2.09	0.52
1:H:10:THR:HG22	1:H:11:PHE:H	1.75	0.52
1:H:298:GLY:HA2	1:H:303:CYS:SG	2.50	0.52
1:E:478:PRO:HD2	1:F:410:PRO:HG2	1.92	0.52
1:A:336:ASP:OD2	2:A:500:IMP:O2'	2.28	0.52
1:B:286:ALA:HB2	1:B:331:ILE:HD13	1.92	0.52
1:D:250:GLY:HA2	1:D:255:VAL:HG21	1.91	0.52
1:E:440:TYR:HB3	1:F:311:VAL:HG11	1.92	0.52
1:F:329:LEU:HB2	1:F:331:ILE:HG22	1.91	0.52
1:E:23:VAL:HG23	1:E:27:GLU:HB2	1.91	0.51
1:E:466:SER:HA	1:F:306:ARG:HD2	1.93	0.51
1:B:432:GLY:HA3	1:D:409:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ALA:O	1:G:381:LYS:NZ	2.43	0.51
1:A:218:CYS:N	1:A:241:ASP:OD2	2.43	0.51
1:G:56:LYS:HD3	1:G:367:GLU:HA	1.93	0.51
1:F:336:ASP:OD2	2:F:500:IMP:O2'	2.29	0.50
1:G:235:VAL:HG13	1:G:240:VAL:HG21	1.93	0.50
1:G:83:VAL:HG11	1:G:240:VAL:HG23	1.93	0.50
1:C:294:LYS:HG3	1:C:334:ILE:HB	1.93	0.50
1:B:79[B]:GLN:HG3	1:B:231[B]:ARG:HH12	1.76	0.50
1:D:333:VAL:HG23	1:D:353:ALA:HA	1.93	0.50
1:H:243:ILE:HD11	1:H:262:ILE:HD13	1.94	0.49
1:A:33:GLN:NE2	1:A:35:THR:O	2.44	0.49
1:C:226:ASN:N	1:C:226:ASN:OD1	2.46	0.49
1:F:283:ARG:NH1	1:F:325:GLU:OE2	2.45	0.49
1:H:63:ARG:HG3	1:H:216:LEU:HD11	1.93	0.49
1:H:78:ASP:O	1:H:82:GLU:HG2	2.12	0.49
1:F:443:ALA:HA	1:F:448:ASN:HD22	1.78	0.49
1:D:419:TYR:CZ	1:D:421:GLY:HA2	2.48	0.49
1:H:472:ASN:OD1	1:H:472:ASN:N	2.46	0.49
1:C:221:SER:HB2	1:C:246:ASP:OD2	2.13	0.49
1:G:50:ASP:HA	1:G:71:HIS:CD2	2.48	0.49
1:A:323:ALA:O	1:A:327:LYS:HG2	2.13	0.48
1:B:440:TYR:HB3	1:D:311:VAL:HG11	1.95	0.48
1:H:55:SER:HB3	1:H:82:GLU:OE1	2.12	0.48
1:B:387:GLY:N	2:B:501:IMP:O6	2.37	0.48
1:F:466:SER:HA	1:H:306:ARG:HD2	1.95	0.48
1:A:384:ARG:HB3	1:A:414:GLU:HG3	1.94	0.48
1:F:56:LYS:HE2	1:F:367:GLU:HA	1.93	0.48
1:A:298:GLY:HA2	1:A:303:CYS:SG	2.53	0.48
1:F:384:ARG:HB3	1:F:414:GLU:HG3	1.96	0.48
1:C:250:GLY:HA2	1:C:255:VAL:HG21	1.95	0.48
1:F:12:ASP:OD2	1:F:340:LYS:NZ	2.34	0.48
1:B:243:ILE:HD13	1:B:269:LEU:HD21	1.96	0.48
1:D:389:LEU:HD13	1:D:410:PRO:HG3	1.95	0.48
1:C:298:GLY:N	1:C:299:PRO:HD3	2.29	0.47
1:G:283:ARG:HG2	1:G:329:LEU:HD11	1.95	0.47
1:C:408:PHE:HE2	1:D:25:PRO:HG2	1.78	0.47
1:C:224:VAL:HG22	1:C:245:LEU:HD22	1.95	0.47
1:D:361:ILE:HG21	1:D:430:LEU:HD11	1.96	0.47
1:F:6:LYS:HG2	1:F:7:THR:N	2.28	0.47
1:B:52:VAL:O	1:B:57:MET:HG3	2.15	0.47
1:C:34:LEU:HD11	1:C:272:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:CYS:SG	2:E:500:IMP:H2	2.54	0.47
1:F:232:VAL:O	1:F:236:VAL:HG12	2.13	0.47
1:E:336:ASP:OD1	2:E:500:IMP:O3'	2.33	0.47
1:E:298:GLY:HA3	1:E:306:ARG:HG3	1.96	0.47
1:H:16:LEU:HD22	1:H:441:LEU:HD21	1.96	0.47
1:C:78:ASP:O	1:C:82:GLU:HG2	2.14	0.46
1:D:283:ARG:HG2	1:D:329:LEU:HD11	1.98	0.46
1:F:87:LYS:HA	1:F:87:LYS:HD2	1.76	0.46
1:E:16:LEU:HD13	1:E:441:LEU:HD21	1.98	0.46
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.49	0.46
1:G:51:THR:OG1	1:G:51:THR:O	2.33	0.46
1:B:479:ASN:ND2	1:D:410:PRO:HD2	2.30	0.46
1:C:468:PRO:HD2	1:C:480:TYR:CZ	2.51	0.46
1:E:298:GLY:N	1:E:299:PRO:HD3	2.31	0.46
1:E:22:GLU:HG2	1:F:253:LYS:HB2	1.98	0.46
1:F:55:SER:N	1:F:82:GLU:OE1	2.44	0.46
1:A:84:ASP:O	1:A:88:ARG:HG2	2.16	0.45
1:E:59:ILE:HG13	1:E:86:VAL:HG22	1.98	0.45
1:G:48:SER:OG	1:G:246:ASP:OD1	2.34	0.45
1:F:32:THR:HB	1:F:446:LEU:HD12	1.97	0.45
1:F:469:HIS:ND1	1:F:470:ASP:OD2	2.31	0.45
1:E:441:LEU:HD23	1:E:449:LEU:HD11	1.97	0.45
1:G:303:CYS:SG	2:G:500:IMP:H2	2.56	0.45
1:G:263:LYS:NZ	1:G:269:LEU:O	2.33	0.45
1:A:455:PHE:HB2	1:B:4:ILE:HG12	1.99	0.45
1:A:458[B]:GLN:OE1	1:A:466:SER:OG	2.34	0.45
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.52	0.45
1:E:245:LEU:HD12	1:E:255:VAL:HG13	1.98	0.45
1:E:387:GLY:N	2:E:500:IMP:O6	2.33	0.45
1:B:461:ALA:HB1	1:D:12:ASP:HB2	1.99	0.44
1:G:232:VAL:O	1:G:236:VAL:N	2.47	0.44
1:B:298:GLY:HA2	1:B:303:CYS:SG	2.58	0.44
1:D:263:LYS:HA	1:D:263:LYS:HD2	1.78	0.44
1:C:72:LYS:HB3	1:C:221:SER:O	2.17	0.44
1:D:384:ARG:HB3	1:D:414:GLU:HG3	2.00	0.44
1:E:19:ASN:ND2	1:E:452:ASN:O	2.48	0.44
1:B:19:ASN:ND2	1:B:452:ASN:O	2.51	0.44
1:B:55:SER:O	1:B:59:ILE:HG13	2.18	0.44
1:E:380:TYR:CG	1:E:416:ARG:HD3	2.52	0.44
1:H:336:ASP:OD2	2:H:500:IMP:O2'	2.32	0.44
1:F:30:LEU:HB3	1:F:43:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HD13	1:G:219:GLY:HA3	1.99	0.44
1:E:306:ARG:NH2	1:G:465:GLU:OE1	2.48	0.44
1:B:46:SER:OG	1:B:61:MET:HG3	2.18	0.44
1:G:243:ILE:HG13	1:G:269:LEU:HD21	1.99	0.44
1:C:249:HIS:CE1	1:C:251:HIS:HB3	2.53	0.43
1:G:30:LEU:HB3	1:G:43:PRO:HD3	2.00	0.43
1:E:306:ARG:HD2	1:G:466:SER:HA	1.99	0.43
1:G:408:PHE:CZ	1:H:25:PRO:HG2	2.53	0.43
1:E:62:ALA:HB1	1:E:216:LEU:HB3	1.99	0.43
1:G:285:LEU:HD12	1:G:285:LEU:HA	1.83	0.43
1:F:440:TYR:HB3	1:H:311:VAL:HG11	1.99	0.43
1:H:293:VAL:HG23	1:H:333:VAL:HG12	1.99	0.43
1:C:331:ILE:HA	1:C:332:PRO:HD3	1.84	0.43
1:D:409:VAL:HA	1:D:410:PRO:HD3	1.69	0.43
1:G:407:LYS:HE2	1:G:407:LYS:HB2	1.67	0.43
1:E:286:ALA:HB2	1:E:331:ILE:HD13	1.99	0.43
1:F:19:ASN:ND2	1:F:452:ASN:O	2.48	0.43
1:D:79:GLN:NE2	1:D:221:SER:H	2.17	0.43
1:F:87:LYS:HG2	1:F:239:LYS:HB3	2.01	0.43
1:B:78:ASP:O	1:B:82:GLU:HG2	2.19	0.42
1:A:301:SER:HB2	1:C:469:HIS:O	2.19	0.42
1:G:10:THR:OG1	1:H:465:GLU:OE2	2.32	0.42
1:E:72:LYS:HB3	1:E:221:SER:O	2.19	0.42
1:E:323:ALA:O	1:E:327:LYS:HG2	2.18	0.42
1:E:32:THR:HG21	1:E:354:CYS:O	2.19	0.42
1:H:46:SER:HB3	1:H:53:THR:OG1	2.19	0.42
1:B:336:ASP:OD2	2:B:501:IMP:O2'	2.28	0.42
1:F:438:MET:HG2	1:F:449:LEU:HD22	2.00	0.42
1:G:243:ILE:HG12	1:G:269:LEU:HD11	2.01	0.42
1:D:303:CYS:SG	2:D:501:IMP:H2	2.59	0.42
1:G:59:ILE:HD13	1:G:86:VAL:HG13	2.01	0.42
1:A:298:GLY:N	1:A:299:PRO:HD3	2.34	0.42
1:A:293:VAL:HG23	1:A:333:VAL:HG12	2.01	0.42
1:E:388:SER:O	1:E:392:MET:HG2	2.20	0.42
1:F:331:ILE:HA	1:F:332:PRO:HD3	1.82	0.42
1:F:46:SER:OG	1:F:53:THR:OG1	2.20	0.42
1:H:26:ASN:ND2	1:H:27:GLU:HG3	2.34	0.42
1:A:324:GLU:HG2	1:A:328:LYS:HE3	2.00	0.42
1:E:444:PRO:HD2	1:E:448:ASN:ND2	2.27	0.42
1:D:220:ALA:O	1:D:244:VAL:HG22	2.20	0.42
1:E:389:LEU:HD22	1:G:478:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:VAL:HG23	1:C:353:ALA:HA	2.01	0.42
1:E:459:THR:OG1	1:F:13:ASP:OD1	2.28	0.42
1:F:303:CYS:SG	2:F:500:IMP:H2	2.59	0.42
1:H:84:ASP:O	1:H:88:ARG:HG2	2.20	0.42
1:G:43:PRO:HG3	1:G:446:LEU:HD11	2.02	0.41
1:A:17:VAL:HA	1:A:18:PRO:HD3	1.92	0.41
1:H:40:LEU:HD21	1:H:67:ILE:HB	2.02	0.41
1:A:80:ALA:HB2	1:A:234:ALA:HB1	2.01	0.41
1:C:311:VAL:HG21	1:D:440:TYR:HB2	2.02	0.41
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.55	0.41
1:G:32:THR:HG21	1:G:354:CYS:O	2.19	0.41
1:G:79:GLN:OE1	1:G:231:ARG:NH1	2.45	0.41
1:F:440:TYR:OH	1:H:248:ALA:HB1	2.19	0.41
1:E:461:ALA:HB2	5:F:502:FMT:C	2.47	0.41
1:E:389:LEU:HD12	1:E:389:LEU:HA	1.82	0.41
1:C:70:ILE:HG12	1:C:70:ILE:H	1.70	0.41
1:F:247:THR:OG1	1:F:248:ALA:N	2.54	0.41
1:G:34:LEU:HD13	1:G:35:THR:HG23	2.02	0.41
1:C:303:CYS:SG	2:C:500:IMP:H2	2.61	0.41
1:D:42:ILE:HA	1:D:43:PRO:HD3	1.85	0.41
1:E:272:ILE:HG12	1:E:292:CYS:HB3	2.02	0.41
1:B:388:SER:O	1:B:392:MET:HG3	2.21	0.41
1:F:361:ILE:HG21	1:F:430:LEU:HD11	2.03	0.41
1:H:10:THR:HG22	1:H:11:PHE:N	2.35	0.41
1:B:384:ARG:HD2	1:B:391:ALA:HB2	2.02	0.41
1:E:245:LEU:HA	1:E:245:LEU:HD22	1.85	0.41
1:B:468:PRO:HD2	1:B:480:TYR:CZ	2.56	0.41
1:H:56:LYS:HD2	1:H:367:GLU:HA	2.02	0.41
1:A:457:VAL:HB	1:B:7:THR:HA	2.03	0.40
1:E:364:GLY:HA3	1:E:420:LYS:HE2	2.03	0.40
1:F:11:PHE:O	1:F:347:LYS:NZ	2.41	0.40
1:F:394:LYS:HB2	1:F:394:LYS:NZ	2.36	0.40
1:B:231[B]:ARG:O	1:B:235:VAL:HG22	2.20	0.40
1:D:479:ASN:OD1	1:D:479:ASN:N	2.54	0.40
1:E:48:SER:HB3	1:E:69:ILE:HB	2.03	0.40
1:H:298:GLY:N	1:H:299:PRO:CD	2.81	0.40
1:A:30:LEU:HB3	1:A:43:PRO:HD3	2.04	0.40
1:B:36:LYS:HE2	1:B:36:LYS:HB3	1.97	0.40
1:D:43:PRO:HG3	1:D:446:LEU:HD11	2.03	0.40
1:E:46:SER:HB3	1:E:53:THR:OG1	2.21	0.40
1:F:365:CYS:O	1:F:381:LYS:NZ	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:448:ASN:O	1:H:452:ASN:ND2	2.55	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	344/363 (95%)	333 (97%)	11 (3%)	0	100	100
1	B	340/363 (94%)	328 (96%)	12 (4%)	0	100	100
1	C	340/363 (94%)	325 (96%)	15 (4%)	0	100	100
1	D	340/363 (94%)	324 (95%)	16 (5%)	0	100	100
1	E	342/363 (94%)	331 (97%)	11 (3%)	0	100	100
1	F	341/363 (94%)	325 (95%)	16 (5%)	0	100	100
1	G	340/363 (94%)	326 (96%)	14 (4%)	0	100	100
1	H	341/363 (94%)	329 (96%)	12 (4%)	0	100	100
All	All	2728/2904 (94%)	2621 (96%)	107 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/282 (96%)	248 (92%)	22 (8%)	14	36
1	B	266/282 (94%)	254 (96%)	12 (4%)	32	65
1	C	267/282 (95%)	247 (92%)	20 (8%)	16	40
1	D	266/282 (94%)	238 (90%)	28 (10%)	8	22
1	E	268/282 (95%)	247 (92%)	21 (8%)	15	37
1	F	267/282 (95%)	255 (96%)	12 (4%)	32	65
1	G	266/282 (94%)	247 (93%)	19 (7%)	17	43
1	H	267/282 (95%)	248 (93%)	19 (7%)	17	43
All	All	2137/2256 (95%)	1984 (93%)	153 (7%)	17	42

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ARG
1	A	4	ILE
1	A	5	LEU
1	A	13	ASP
1	A	14	VAL
1	A	28	VAL
1	A	32	THR
1	A	34	LEU
1	A	63	ARG
1	A	221	SER
1	A	242	VAL
1	A	268	GLU
1	A	287	GLU
1	A	339	LEU
1	A	366	GLU
1	A	372	ILE
1	A	375	TYR
1	A	408	PHE
1	A	441	LEU
1	A	460	SER
1	A	481	SER
1	B	14	VAL
1	B	28	VAL
1	B	34	LEU
1	B	57	MET
1	B	72	LYS

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Mol	Chain	Res	Type
1	B	243	ILE
1	B	244	VAL
1	B	245	LEU
1	B	246	ASP
1	B	257	GLU
1	B	304	THR
1	B	321	ASP
1	C	5	LEU
1	C	14	VAL
1	C	28	VAL
1	C	70	ILE
1	C	72	LYS
1	C	236	VAL
1	C	240	VAL
1	C	244	VAL
1	C	245	LEU
1	C	247	THR
1	C	255	VAL
1	C	261	ARG
1	C	268	GLU
1	C	280	GLU
1	C	340	LYS
1	C	358	MET
1	C	409	VAL
1	C	441	LEU
1	C	456	VAL
1	C	460	SER
1	D	4	ILE
1	D	5	LEU
1	D	6	LYS
1	D	24	LEU
1	D	32	THR
1	D	34	LEU
1	D	39	GLN
1	D	52	VAL
1	D	57	MET
1	D	63	ARG
1	D	73	ASN
1	D	85	ARG
1	D	225	THR
1	D	226	ASN
1	D	229	MET

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Mol	Chain	Res	Type
1	D	237	LYS
1	D	245	LEU
1	D	263	LYS
1	D	285	LEU
1	D	287	GLU
1	D	354[A]	CYS
1	D	354[B]	CYS
1	D	374	ILE
1	D	389	LEU
1	D	392	MET
1	D	420	LYS
1	D	456	VAL
1	D	464	ARG
1	E	14	VAL
1	E	32	THR
1	E	34	LEU
1	E	36	LYS
1	E	39	GLN
1	E	50	ASP
1	E	55	SER
1	E	63	ARG
1	E	87	LYS
1	E	217	LEU
1	E	237	LYS
1	E	245	LEU
1	E	247	THR
1	E	249	HIS
1	E	321	ASP
1	E	373	GLU
1	E	378	ARG
1	E	408	PHE
1	E	441	LEU
1	E	456	VAL
1	E	471	ILE
1	F	10	THR
1	F	14	VAL
1	F	34	LEU
1	F	37	LYS
1	F	77	GLU
1	F	86	VAL
1	F	88	ARG
1	F	285	LEU

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Mol	Chain	Res	Type
1	F	366	GLU
1	F	394	LYS
1	F	441	LEU
1	F	475	LYS
1	G	4	ILE
1	G	14	VAL
1	G	26	ASN
1	G	32	THR
1	G	39	GLN
1	G	51	THR
1	G	77	GLU
1	G	233	ASP
1	G	235	VAL
1	G	244	VAL
1	G	246	ASP
1	G	247	THR
1	G	276	ILE
1	G	285	LEU
1	G	294	LYS
1	G	324	GLU
1	G	382	VAL
1	G	426	THR
1	G	441	LEU
1	H	5	LEU
1	H	14	VAL
1	H	32	THR
1	H	34	LEU
1	H	55	SER
1	H	67	ILE
1	H	243	ILE
1	H	244	VAL
1	H	245	LEU
1	H	247	THR
1	H	293	VAL
1	H	358	MET
1	H	407	LYS
1	H	408	PHE
1	H	420	LYS
1	H	452	ASN
1	H	460	SER
1	H	471	ILE
1	H	472	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	452	ASN
1	C	454	ASN
1	D	422	HIS
1	E	448	ASN
1	F	448	ASN
1	F	452	ASN
1	G	39	GLN
1	G	452	ASN
1	G	458	GLN
1	H	33	GLN
1	H	39	GLN
1	H	452	ASN

### 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](#)

27 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	500	-	21,25,25	1.98	2 (9%)	22,38,38	2.17	4 (18%)
3	2YA	A	501	-	26,29,29	1.83	6 (23%)	29,41,41	2.66	8 (27%)
2	IMP	B	501	-	21,25,25	1.96	2 (9%)	22,38,38	2.23	4 (18%)
3	2YA	B	502	-	26,29,29	1.85	6 (23%)	29,41,41	2.77	9 (31%)
3	2YA	B	503	-	26,29,29	1.84	6 (23%)	29,41,41	2.72	7 (24%)
2	IMP	C	500	-	21,25,25	1.96	2 (9%)	22,38,38	2.30	4 (18%)
3	2YA	C	501	-	26,29,29	1.85	6 (23%)	29,41,41	2.71	9 (31%)
2	IMP	D	501	-	21,25,25	2.46	3 (14%)	22,38,38	2.98	4 (18%)
4	ACY	D	502	-	1,3,3	1.36	0	0,3,3	0.00	-
2	IMP	E	500	-	21,25,25	1.97	2 (9%)	22,38,38	2.11	4 (18%)
3	2YA	E	501	-	26,29,29	1.85	6 (23%)	29,41,41	2.76	9 (31%)
5	FMT	E	502	-	0,2,2	0.00	-	0,1,1	0.00	-
6	SO4	E	503	-	4,4,4	0.16	0	6,6,6	0.07	0
2	IMP	F	500	-	21,25,25	1.98	2 (9%)	22,38,38	2.30	5 (22%)
3	2YA	F	501	-	26,29,29	1.83	6 (23%)	29,41,41	2.65	8 (27%)
5	FMT	F	502	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	F	503	-	5,5,5	0.36	0	5,5,5	0.25	0
5	FMT	F	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	505	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	F	506	-	5,5,5	0.32	0	5,5,5	0.33	0
2	IMP	G	500	-	21,25,25	1.96	2 (9%)	22,38,38	2.23	4 (18%)
3	2YA	G	501	-	26,29,29	1.83	6 (23%)	29,41,41	2.66	9 (31%)
5	FMT	G	502	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	H	500	-	21,25,25	1.98	2 (9%)	22,38,38	2.25	4 (18%)
3	2YA	H	501	-	26,29,29	1.87	6 (23%)	29,41,41	2.81	8 (27%)
5	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	H	503	-	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	500	-	-	0/6/26/26	0/3/3/3
3	2YA	A	501	-	-	0/10/12/12	0/4/4/4
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
3	2YA	B	502	-	-	0/10/12/12	0/4/4/4
3	2YA	B	503	-	-	0/10/12/12	0/4/4/4

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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	2YA	C	501	-	-	0/10/12/12	0/4/4/4
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
4	ACY	D	502	-	-	0/0/0/0	0/0/0/0
2	IMP	E	500	-	-	0/6/26/26	0/3/3/3
3	2YA	E	501	-	-	0/10/12/12	0/4/4/4
5	FMT	E	502	-	-	0/0/0/0	0/0/0/0
6	SO4	E	503	-	-	0/0/0/0	0/0/0/0
2	IMP	F	500	-	-	0/6/26/26	0/3/3/3
3	2YA	F	501	-	-	0/10/12/12	0/4/4/4
5	FMT	F	502	-	-	0/0/0/0	0/0/0/0
7	GOL	F	503	-	-	0/4/4/4	0/0/0/0
5	FMT	F	504	-	-	0/0/0/0	0/0/0/0
5	FMT	F	505	-	-	0/0/0/0	0/0/0/0
7	GOL	F	506	-	-	0/4/4/4	0/0/0/0
2	IMP	G	500	-	-	0/6/26/26	0/3/3/3
3	2YA	G	501	-	-	0/10/12/12	0/4/4/4
5	FMT	G	502	-	-	0/0/0/0	0/0/0/0
2	IMP	H	500	-	-	0/6/26/26	0/3/3/3
3	2YA	H	501	-	-	0/10/12/12	0/4/4/4
5	FMT	H	502	-	-	0/0/0/0	0/0/0/0
5	FMT	H	503	-	-	0/0/0/0	0/0/0/0

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	501	2YA	C16-N3	-5.14	1.33	1.44
3	C	501	2YA	C16-N3	-5.12	1.33	1.44
3	E	501	2YA	C16-N3	-5.08	1.34	1.44
3	B	503	2YA	C16-N3	-5.04	1.34	1.44
3	B	502	2YA	C16-N3	-5.02	1.34	1.44
3	A	501	2YA	C16-N3	-5.02	1.34	1.44
3	F	501	2YA	C16-N3	-5.00	1.34	1.44
3	H	501	2YA	C16-N3	-4.98	1.34	1.44
3	E	501	2YA	C14-C11	-2.74	1.48	1.52
3	H	501	2YA	C14-C11	-2.74	1.48	1.52
3	G	501	2YA	C14-C11	-2.71	1.48	1.52
3	C	501	2YA	C14-C11	-2.71	1.48	1.52
3	B	502	2YA	C14-C11	-2.71	1.48	1.52
3	B	503	2YA	C14-C11	-2.57	1.48	1.52
3	A	501	2YA	C14-C11	-2.54	1.48	1.52
3	H	501	2YA	C5-N4	-2.53	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	2YA	C14-C11	-2.52	1.48	1.52
3	B	502	2YA	C5-N4	-2.48	1.34	1.39
3	A	501	2YA	C5-N4	-2.43	1.34	1.39
3	E	501	2YA	C5-N4	-2.41	1.34	1.39
3	G	501	2YA	C5-N4	-2.40	1.34	1.39
3	C	501	2YA	C5-N4	-2.40	1.34	1.39
3	B	503	2YA	C5-N4	-2.40	1.34	1.39
3	F	501	2YA	C5-N4	-2.39	1.34	1.39
3	H	501	2YA	C15-C14	2.06	1.39	1.36
3	C	501	2YA	C15-C14	2.09	1.39	1.36
3	B	502	2YA	C15-C14	2.09	1.39	1.36
3	B	503	2YA	C15-C14	2.12	1.39	1.36
3	E	501	2YA	C15-C14	2.16	1.39	1.36
2	D	501	IMP	O4'-C1'	2.20	1.44	1.41
3	A	501	2YA	C15-C14	2.27	1.39	1.36
3	F	501	2YA	C15-C14	2.27	1.39	1.36
3	G	501	2YA	C15-C14	2.28	1.39	1.36
3	G	501	2YA	C19-CL1	2.29	1.79	1.74
2	G	500	IMP	C6-N1	2.35	1.37	1.33
3	C	501	2YA	C19-CL1	2.41	1.79	1.74
3	B	502	2YA	C19-CL1	2.41	1.79	1.74
2	C	500	IMP	C6-N1	2.43	1.37	1.33
2	A	500	IMP	C6-N1	2.44	1.37	1.33
2	H	500	IMP	C6-N1	2.45	1.37	1.33
3	E	501	2YA	C19-CL1	2.45	1.79	1.74
3	B	503	2YA	C19-CL1	2.46	1.79	1.74
3	F	501	2YA	C19-CL1	2.46	1.79	1.74
3	A	501	2YA	C19-CL1	2.49	1.80	1.74
2	F	500	IMP	C6-N1	2.50	1.37	1.33
2	E	500	IMP	C6-N1	2.50	1.37	1.33
2	B	501	IMP	C6-N1	2.53	1.37	1.33
3	H	501	2YA	C19-CL1	2.61	1.80	1.74
2	D	501	IMP	C6-N1	3.86	1.40	1.33
3	G	501	2YA	N1-N2	4.59	1.40	1.34
3	F	501	2YA	N1-N2	4.65	1.40	1.34
3	A	501	2YA	N1-N2	4.69	1.40	1.34
3	E	501	2YA	N1-N2	4.77	1.40	1.34
3	B	503	2YA	N1-N2	4.81	1.41	1.34
3	C	501	2YA	N1-N2	4.82	1.41	1.34
3	B	502	2YA	N1-N2	4.91	1.41	1.34
3	H	501	2YA	N1-N2	4.94	1.41	1.34
2	E	500	IMP	O6-C6	8.21	1.45	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	IMP	O6-C6	8.26	1.45	1.24
2	B	501	IMP	O6-C6	8.27	1.45	1.24
2	C	500	IMP	O6-C6	8.32	1.45	1.24
2	F	500	IMP	O6-C6	8.33	1.45	1.24
2	H	500	IMP	O6-C6	8.33	1.45	1.24
2	A	500	IMP	O6-C6	8.34	1.45	1.24
2	D	501	IMP	O6-C6	9.63	1.48	1.24

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	IMP	N3-C2-N1	-11.44	118.89	128.86
3	H	501	2YA	C15-C14-C11	-8.97	114.86	129.21
3	B	502	2YA	C15-C14-C11	-8.81	115.11	129.21
3	E	501	2YA	C15-C14-C11	-8.79	115.14	129.21
3	C	501	2YA	C15-C14-C11	-8.67	115.33	129.21
3	B	503	2YA	C15-C14-C11	-8.51	115.60	129.21
2	C	500	IMP	N3-C2-N1	-8.45	121.50	128.86
2	F	500	IMP	N3-C2-N1	-8.35	121.58	128.86
2	H	500	IMP	N3-C2-N1	-8.35	121.58	128.86
3	G	501	2YA	C15-C14-C11	-8.34	115.86	129.21
2	B	501	IMP	N3-C2-N1	-8.32	121.62	128.86
3	F	501	2YA	C15-C14-C11	-8.24	116.03	129.21
2	G	500	IMP	N3-C2-N1	-8.19	121.72	128.86
3	A	501	2YA	C15-C14-C11	-8.17	116.13	129.21
2	A	500	IMP	N3-C2-N1	-7.94	121.94	128.86
2	E	500	IMP	N3-C2-N1	-7.81	122.06	128.86
2	D	501	IMP	C4-C5-N7	-4.40	105.16	109.41
3	A	501	2YA	C17-C16-C21	-4.02	115.11	121.28
3	H	501	2YA	C17-C16-C21	-3.98	115.17	121.28
3	B	502	2YA	C17-C16-C21	-3.92	115.27	121.28
3	F	501	2YA	C17-C16-C21	-3.89	115.31	121.28
3	E	501	2YA	C17-C16-C21	-3.85	115.37	121.28
3	B	503	2YA	C17-C16-C21	-3.85	115.38	121.28
3	G	501	2YA	C17-C16-C21	-3.79	115.46	121.28
3	C	501	2YA	C17-C16-C21	-3.79	115.46	121.28
2	C	500	IMP	C6-C5-C4	-3.73	117.14	120.84
2	F	500	IMP	C6-C5-C4	-3.51	117.35	120.84
2	B	501	IMP	C6-C5-C4	-3.42	117.44	120.84
2	H	500	IMP	C6-C5-C4	-3.41	117.45	120.84
2	G	500	IMP	C4-C5-N7	-3.39	106.13	109.41
2	G	500	IMP	C6-C5-C4	-3.38	117.49	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	IMP	C4-C5-N7	-3.28	106.24	109.41
2	A	500	IMP	C4-C5-N7	-3.28	106.24	109.41
2	H	500	IMP	C4-C5-N7	-3.25	106.27	109.41
3	G	501	2YA	C14-C15-N3	-3.21	101.74	106.42
2	C	500	IMP	C4-C5-N7	-3.18	106.34	109.41
2	E	500	IMP	C6-C5-C4	-3.16	117.70	120.84
3	E	501	2YA	C14-C15-N3	-3.15	101.82	106.42
2	E	500	IMP	C4-C5-N7	-3.11	106.41	109.41
3	A	501	2YA	C14-C15-N3	-3.10	101.89	106.42
3	C	501	2YA	C14-C15-N3	-3.10	101.90	106.42
2	B	501	IMP	C4-C5-N7	-3.09	106.42	109.41
3	F	501	2YA	C14-C15-N3	-3.09	101.91	106.42
2	A	500	IMP	C6-C5-C4	-3.08	117.78	120.84
3	B	502	2YA	C14-C15-N3	-3.05	101.97	106.42
3	B	503	2YA	C14-C15-N3	-3.02	102.02	106.42
3	H	501	2YA	C14-C15-N3	-2.93	102.14	106.42
3	G	501	2YA	C15-C14-N1	2.01	112.97	110.11
3	B	502	2YA	C15-C14-N1	2.01	112.97	110.11
3	A	501	2YA	C7-C6-C5	2.01	120.39	118.16
3	F	501	2YA	C7-C6-C5	2.03	120.42	118.16
3	E	501	2YA	C15-C14-N1	2.04	113.02	110.11
3	C	501	2YA	C15-C14-N1	2.05	113.03	110.11
3	G	501	2YA	C7-C6-C5	2.05	120.43	118.16
3	E	501	2YA	C16-N3-N2	2.06	121.45	117.38
3	C	501	2YA	C16-N3-N2	2.06	121.45	117.38
3	B	502	2YA	C16-N3-N2	2.17	121.67	117.38
3	H	501	2YA	C16-N3-N2	2.29	121.91	117.38
2	F	500	IMP	O3P-P-O2P	2.45	117.49	107.61
2	D	501	IMP	O3P-P-O5'	2.45	113.26	106.73
2	E	500	IMP	C2-N1-C6	2.98	120.88	115.91
3	G	501	2YA	C20-C21-C16	3.23	122.61	119.12
2	B	501	IMP	C2-N1-C6	3.27	121.37	115.91
2	G	500	IMP	C2-N1-C6	3.29	121.41	115.91
3	F	501	2YA	C20-C21-C16	3.31	122.69	119.12
2	A	500	IMP	C2-N1-C6	3.35	121.50	115.91
2	H	500	IMP	C2-N1-C6	3.38	121.55	115.91
2	F	500	IMP	C2-N1-C6	3.38	121.56	115.91
3	B	503	2YA	C20-C21-C16	3.41	122.80	119.12
3	A	501	2YA	C20-C21-C16	3.42	122.81	119.12
3	C	501	2YA	C20-C21-C16	3.44	122.83	119.12
3	E	501	2YA	C20-C21-C16	3.47	122.86	119.12
2	C	500	IMP	C2-N1-C6	3.47	121.70	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	2YA	C20-C21-C16	3.54	122.94	119.12
3	C	501	2YA	C18-C17-C16	3.58	122.98	119.12
3	H	501	2YA	C20-C21-C16	3.62	123.02	119.12
3	E	501	2YA	C18-C17-C16	3.63	123.04	119.12
3	H	501	2YA	C18-C17-C16	3.65	123.06	119.12
3	B	502	2YA	C18-C17-C16	3.66	123.07	119.12
3	B	503	2YA	C18-C17-C16	3.66	123.07	119.12
3	G	501	2YA	C18-C17-C16	3.76	123.17	119.12
3	F	501	2YA	C18-C17-C16	3.83	123.25	119.12
3	A	501	2YA	C18-C17-C16	3.90	123.33	119.12
3	C	501	2YA	O1-C1-C6	4.08	120.18	114.31
3	G	501	2YA	O1-C1-C6	4.21	120.38	114.31
3	F	501	2YA	O1-C1-C6	4.24	120.42	114.31
3	A	501	2YA	O1-C1-C6	4.30	120.50	114.31
3	H	501	2YA	O1-C1-C6	4.31	120.52	114.31
3	B	502	2YA	O1-C1-C6	4.38	120.61	114.31
3	E	501	2YA	O1-C1-C6	4.38	120.62	114.31
3	B	503	2YA	O1-C1-C6	4.53	120.83	114.31
2	D	501	IMP	C2-N1-C6	4.53	123.48	115.91
3	A	501	2YA	C11-C14-N1	6.53	131.00	120.27
3	F	501	2YA	C11-C14-N1	6.59	131.09	120.27
3	G	501	2YA	C11-C14-N1	6.64	131.17	120.27
3	B	503	2YA	C11-C14-N1	6.89	131.59	120.27
3	C	501	2YA	C11-C14-N1	6.92	131.64	120.27
3	E	501	2YA	C11-C14-N1	7.04	131.84	120.27
3	B	502	2YA	C11-C14-N1	7.09	131.91	120.27
3	H	501	2YA	C11-C14-N1	7.30	132.27	120.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IMP	1	0
2	B	501	IMP	2	0
2	C	500	IMP	2	0
2	D	501	IMP	2	0
2	E	500	IMP	3	0
2	F	500	IMP	2	0
5	F	502	FMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	500	IMP	2	0
5	G	502	FMT	1	0
2	H	500	IMP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	344/363 (94%)	-0.14	4 (1%) 79 78	36, 53, 73, 90	7 (2%)
1	B	342/363 (94%)	-0.16	2 (0%) 89 88	38, 59, 80, 97	12 (3%)
1	C	343/363 (94%)	-0.31	0 100 100	31, 48, 69, 83	4 (1%)
1	D	342/363 (94%)	-0.12	0 100 100	37, 58, 78, 95	15 (4%)
1	E	343/363 (94%)	-0.17	2 (0%) 89 88	30, 54, 78, 92	13 (3%)
1	F	344/363 (94%)	-0.33	0 100 100	31, 46, 64, 79	2 (0%)
1	G	344/363 (94%)	-0.22	1 (0%) 93 93	35, 54, 77, 85	6 (1%)
1	H	344/363 (94%)	-0.24	1 (0%) 93 93	30, 49, 71, 90	9 (2%)
All	All	2746/2904 (94%)	-0.21	10 (0%) 92 92	30, 53, 76, 97	68 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	407	LYS	3.5
1	A	375	TYR	3.5
1	B	233	ASP	3.1
1	A	246	ASP	2.5
1	E	89	SER	2.5
1	B	269	LEU	2.4
1	A	285	LEU	2.3
1	G	407	LYS	2.3
1	E	408	PHE	2.2
1	A	408	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	F	506	6/6	0.86	0.27	4.36	67,76,80,80	0
3	2YA	H	501	26/26	0.94	0.26	3.31	53,66,74,77	0
3	2YA	C	501	26/26	0.94	0.28	2.58	59,65,77,91	0
3	2YA	B	502	26/26	0.95	0.26	1.80	59,65,81,83	0
7	GOL	F	503	6/6	0.90	0.23	1.63	66,68,70,72	0
3	2YA	E	501	26/26	0.93	0.28	1.39	62,70,77,79	0
3	2YA	B	503	26/26	0.90	0.22	0.92	58,66,78,79	0
3	2YA	G	501	26/26	0.93	0.24	0.78	59,66,76,80	0
3	2YA	A	501	26/26	0.93	0.21	0.31	49,60,68,79	0
3	2YA	F	501	26/26	0.96	0.20	0.30	41,46,62,66	0
5	FMT	F	502	3/3	0.84	0.17	0.22	56,56,60,64	0
5	FMT	H	502	3/3	0.93	0.18	0.19	74,74,78,83	0
5	FMT	H	503	3/3	0.91	0.16	-0.00	58,58,59,60	0
2	IMP	G	500	23/23	0.96	0.16	-0.07	35,43,52,54	0
5	FMT	E	502	3/3	0.82	0.16	-0.37	53,53,53,54	0
2	IMP	H	500	23/23	0.97	0.14	-0.45	29,37,46,47	0
2	IMP	F	500	23/23	0.97	0.14	-0.55	24,36,44,46	0
2	IMP	B	501	23/23	0.96	0.14	-0.60	31,39,46,48	0
2	IMP	A	500	23/23	0.96	0.14	-0.77	24,40,49,52	0
2	IMP	E	500	23/23	0.97	0.11	-1.07	40,50,54,55	0
2	IMP	D	501	23/23	0.97	0.13	-1.20	32,42,47,50	0
2	IMP	C	500	23/23	0.96	0.13	-1.21	26,36,55,61	0
5	FMT	F	505	3/3	0.93	0.14	-1.31	57,57,61,63	0
6	SO4	E	503	5/5	0.79	0.40	-	30,34,35,35	5
4	ACY	D	502	4/4	0.89	0.23	-	69,70,72,72	0
5	FMT	G	502	3/3	0.94	0.17	-	36,36,44,49	0
5	FMT	F	504	3/3	0.79	0.23	-	71,71,72,73	0

## 6.5 Other polymers

There are no such residues in this entry.