



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2017 – 01:29 PM EDT

PDB ID : 3KHJ  
Title : C. parvum inosine monophosphate dehydrogenase bound by inhibitor C64  
Authors : MacPherson, I.S.; Hedstrom, L.K.  
Deposited on : unknown  
Resolution : 2.80 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

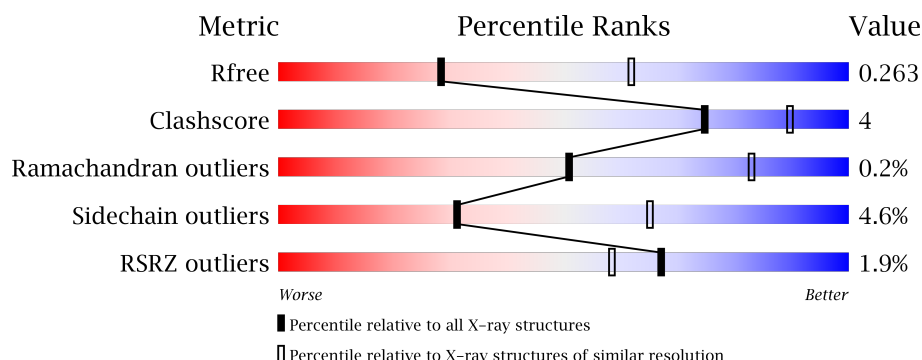
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	361	<div> <div>2%</div> <div>74% 10% 16%</div> </div>
1	B	361	<div> <div>78% 9% 12%</div> </div>
1	C	361	<div> <div>2%</div> <div>73% 10% 15%</div> </div>
1	D	361	<div> <div>79% 9% 11%</div> </div>
1	E	361	<div> <div>2%</div> <div>77% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	361	 .% 71% 11% • 17%
1	G	361	 4% 70% 12% • 17%
1	H	361	 2% 80% 10% • 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	C64	D	902	-	-	-	X
3	C64	H	903	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18502 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	302	Total	C	N	O	S	0	0	0
			2221	1404	374	431	12			
1	B	318	Total	C	N	O	S	0	1	0
			2330	1471	390	454	15			
1	C	306	Total	C	N	O	S	0	1	0
			2255	1422	383	438	12			
1	D	321	Total	C	N	O	S	0	0	0
			2322	1463	390	454	15			
1	E	298	Total	C	N	O	S	0	0	0
			2162	1369	365	416	12			
1	F	300	Total	C	N	O	S	0	1	0
			2198	1390	363	433	12			
1	G	300	Total	C	N	O	S	0	0	0
			2188	1379	370	428	11			
1	H	328	Total	C	N	O	S	0	0	0
			2355	1484	397	460	14			

There are 48 discrepancies between the modelled and reference sequences:

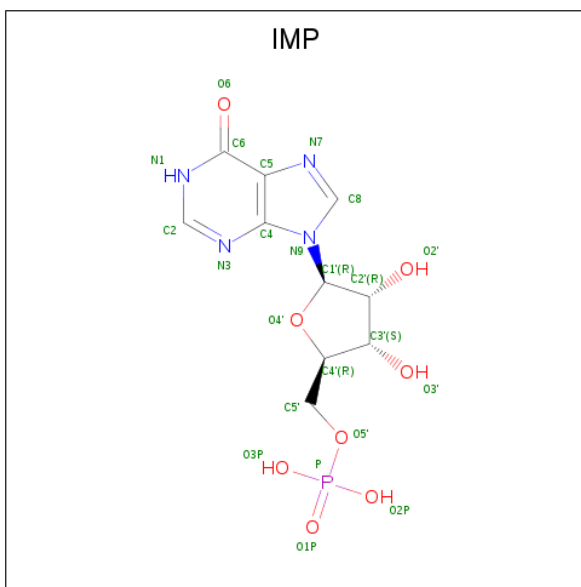
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
A	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
A	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
A	90	SER	-	LINKER	UNP Q5CPK7
A	91	GLY	-	LINKER	UNP Q5CPK7
A	92	GLY	-	LINKER	UNP Q5CPK7
B	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
B	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
B	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
B	90	SER	-	LINKER	UNP Q5CPK7
B	91	GLY	-	LINKER	UNP Q5CPK7
B	92	GLY	-	LINKER	UNP Q5CPK7
C	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7

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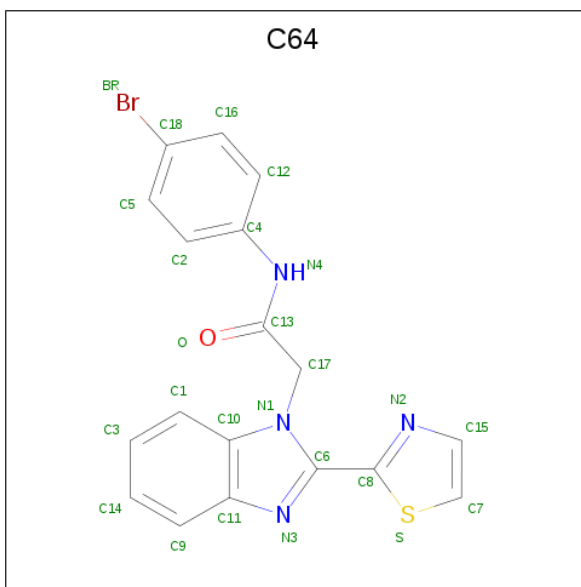
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
C	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
C	90	SER	-	LINKER	UNP Q5CPK7
C	91	GLY	-	LINKER	UNP Q5CPK7
C	92	GLY	-	LINKER	UNP Q5CPK7
D	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
D	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
D	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
D	90	SER	-	LINKER	UNP Q5CPK7
D	91	GLY	-	LINKER	UNP Q5CPK7
D	92	GLY	-	LINKER	UNP Q5CPK7
E	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
E	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
E	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
E	90	SER	-	LINKER	UNP Q5CPK7
E	91	GLY	-	LINKER	UNP Q5CPK7
E	92	GLY	-	LINKER	UNP Q5CPK7
F	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
F	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
F	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
F	90	SER	-	LINKER	UNP Q5CPK7
F	91	GLY	-	LINKER	UNP Q5CPK7
F	92	GLY	-	LINKER	UNP Q5CPK7
G	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
G	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
G	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
G	90	SER	-	LINKER	UNP Q5CPK7
G	91	GLY	-	LINKER	UNP Q5CPK7
G	92	GLY	-	LINKER	UNP Q5CPK7
H	-2	GLY	-	EXPRESSION TAG	UNP Q5CPK7
H	-1	SER	-	EXPRESSION TAG	UNP Q5CPK7
H	0	HIS	-	EXPRESSION TAG	UNP Q5CPK7
H	90	SER	-	LINKER	UNP Q5CPK7
H	91	GLY	-	LINKER	UNP Q5CPK7
H	92	GLY	-	LINKER	UNP Q5CPK7

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



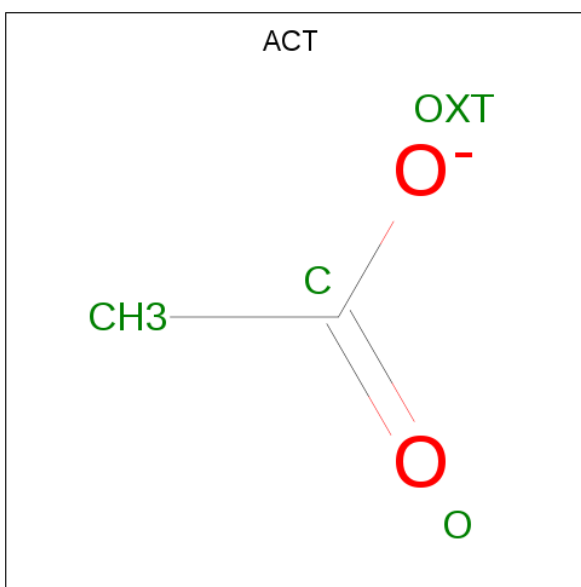
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total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

- Molecule 3 is N-(4-bromophenyl)-2-[2-(1,3-thiazol-2-yl)-1H-benzimidazol-1-yl]acetamide (three-letter code: C64) (formula: C<sub>18</sub>H<sub>13</sub>BrN<sub>4</sub>OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		
3	D	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		
3	H	1	Total	Br	C	N	O	S	0	0
			25	1	18	4	1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

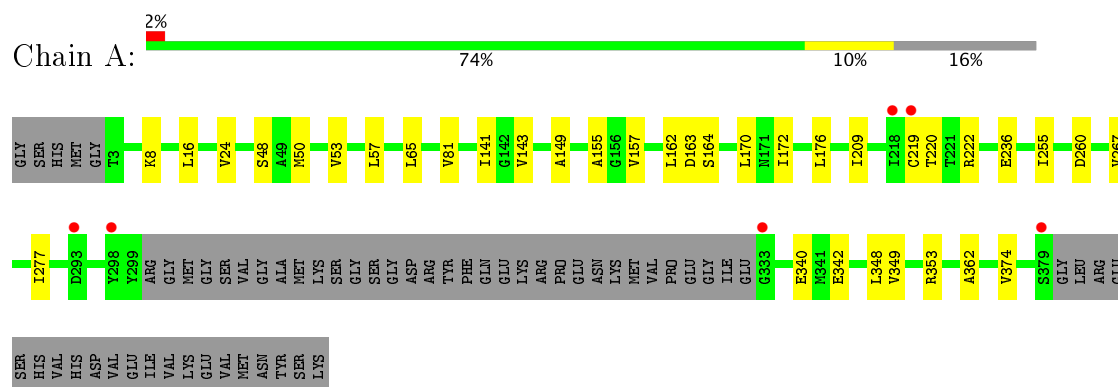
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total 37	O 37	0	0
5	B	38	Total 38	O 38	0	0
5	C	41	Total 41	O 41	0	0
5	D	40	Total 40	O 40	0	0
5	E	13	Total 13	O 13	0	0
5	F	17	Total 17	O 17	0	0
5	G	9	Total 9	O 9	0	0
5	H	13	Total 13	O 13	0	0

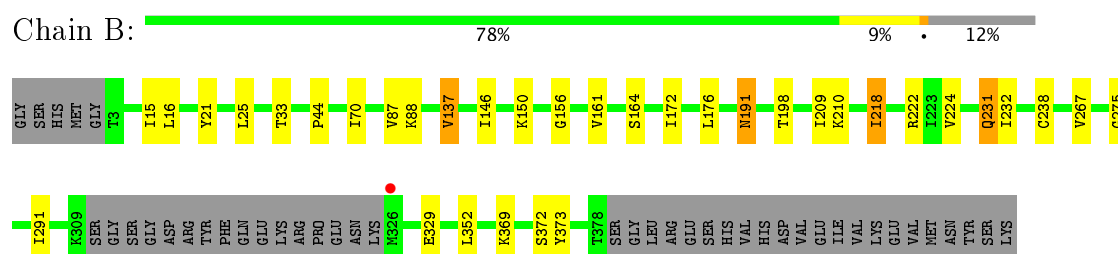
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

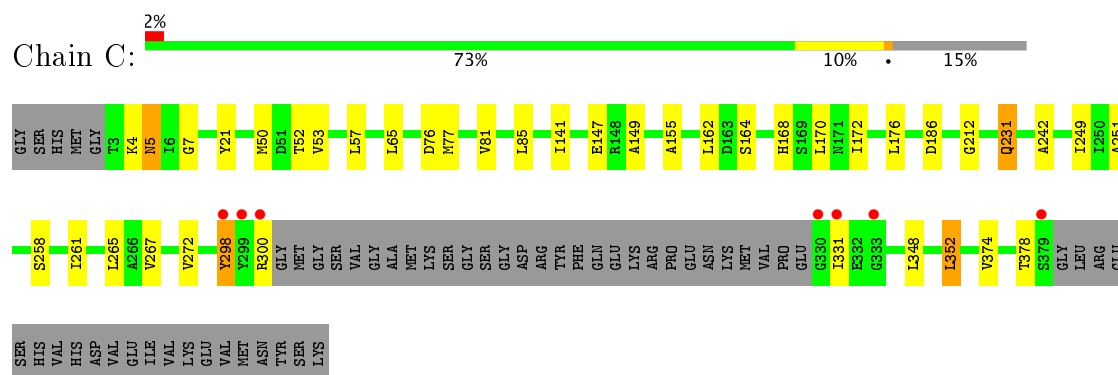
- Molecule 1: Inosine-5-monophosphate dehydrogenase




- Molecule 1: Inosine-5-monophosphate dehydrogenase

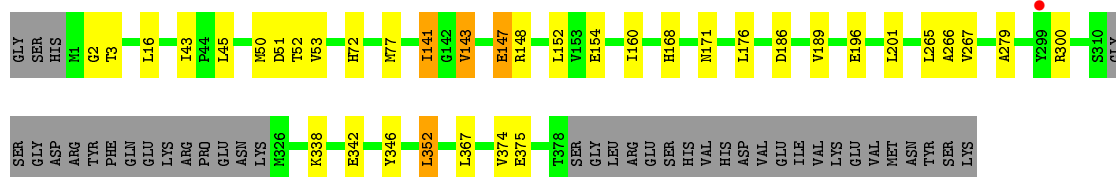


- Molecule 1: Inosine-5-monophosphate dehydrogenase




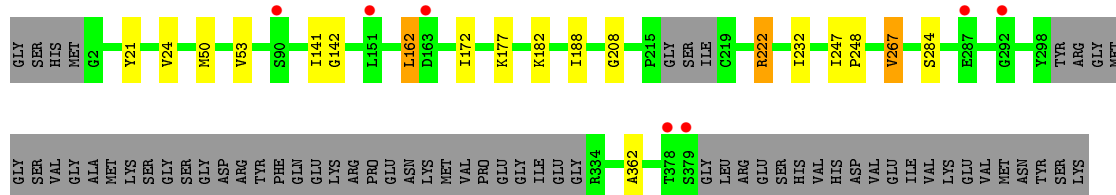
- Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain D:  79% 9% 11%



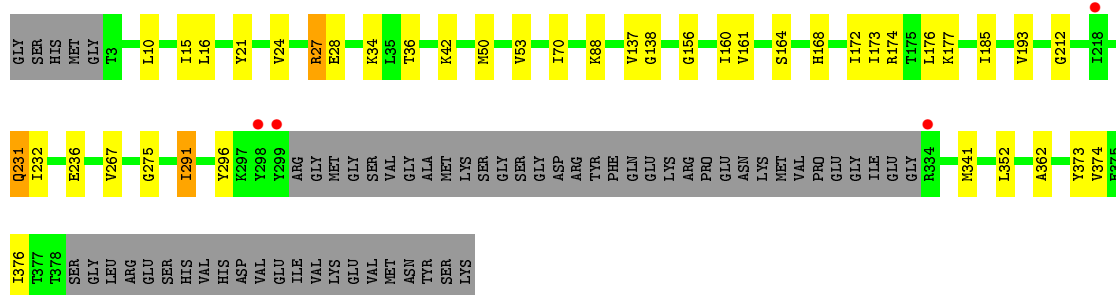
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain E:  77% 17% 2%



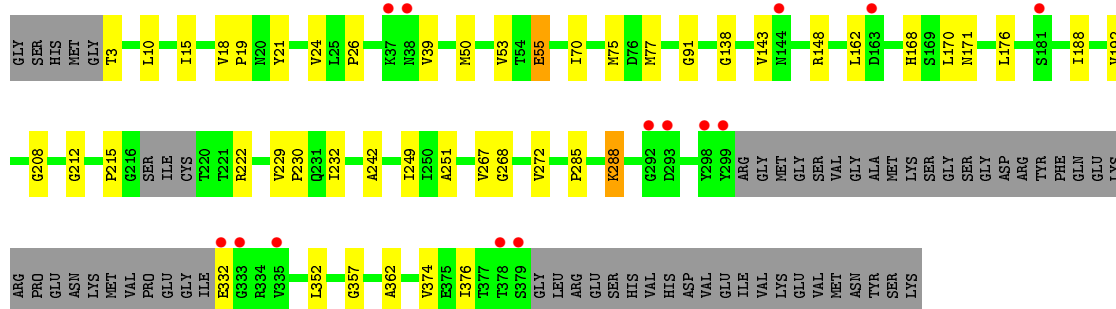
• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain F:  71% 17% 11%



• Molecule 1: Inosine-5-monophosphate dehydrogenase

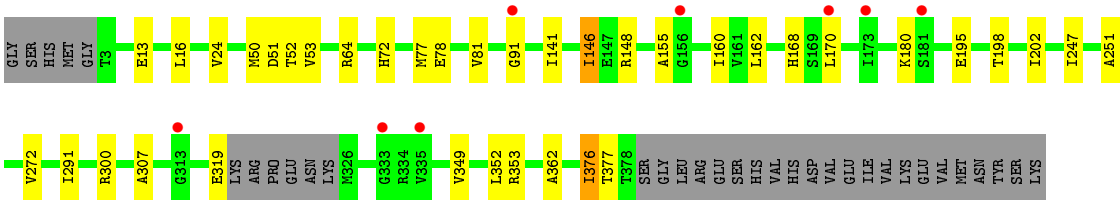
Chain G:  70% 12% 4%



• Molecule 1: Inosine-5-monophosphate dehydrogenase

Chain H:  80% 10% 2%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.48Å 166.14Å 101.29Å 90.00° 105.14° 90.00°	Depositor
Resolution (Å)	42.13 – 2.80 42.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.13-2.80) 99.2 (42.13-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.266 0.222 , 0.263	Depositor DCC
$R_{free}$ test set	3301 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18502	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 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, C64, ACT

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	0.31	0/2243	0.49	0/3025
1	B	0.31	0/2356	0.48	0/3176
1	C	0.31	0/2279	0.50	0/3072
1	D	0.30	0/2345	0.48	0/3165
1	E	0.31	0/2181	0.46	0/2941
1	F	0.31	0/2223	0.47	0/3004
1	G	0.30	0/2209	0.46	0/2980
1	H	0.30	0/2380	0.46	0/3216
All	All	0.31	0/18216	0.48	0/24579

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	2221	0	2315	17	0
1	B	2330	0	2417	21	0
1	C	2255	0	2349	20	0
1	D	2322	0	2382	19	0
1	E	2162	0	2252	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2198	0	2262	24	0
1	G	2188	0	2241	19	0
1	H	2355	0	2380	16	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
3	B	25	0	13	2	0
3	D	25	0	13	1	0
3	H	25	0	13	2	0
4	D	4	0	3	0	0
5	A	37	0	0	1	0
5	B	38	0	0	0	0
5	C	41	0	0	0	0
5	D	40	0	0	0	0
5	E	13	0	0	0	0
5	F	17	0	0	0	0
5	G	9	0	0	0	0
5	H	13	0	0	0	0
All	All	18502	0	18728	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLN:HA	1:C:231:GLN:HE21	1.45	0.82
1:C:50:MET:HB2	1:C:53:VAL:HG12	1.64	0.79
1:D:143:VAL:HG11	1:D:171:ASN:HB3	1.66	0.77
1:C:242:ALA:HB3	1:C:249:ILE:HD11	1.67	0.75
1:E:50:MET:HB2	1:E:53:VAL:HG22	1.71	0.73
1:F:16:LEU:HD21	1:G:222:ARG:HG2	1.71	0.72
1:H:141:ILE:HD13	1:H:160:ILE:HG23	1.70	0.72
1:A:50:MET:HB2	1:A:53:VAL:HG12	1.70	0.72
1:D:50:MET:HB2	1:D:53:VAL:HG22	1.74	0.69
1:C:52:THR:HG21	1:C:300:ARG:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:SER:HB2	1:C:172:ILE:HD11	1.75	0.68
1:B:218:ILE:HD13	1:B:218:ILE:H	1.60	0.67
1:F:50:MET:HB2	1:F:53:VAL:HG12	1.77	0.67
1:B:231:GLN:HE21	1:B:231:GLN:HA	1.60	0.66
1:B:70:ILE:HD13	1:B:161:VAL:HG21	1.78	0.66
1:H:50:MET:HB2	1:H:53:VAL:HG12	1.78	0.65
1:F:376:ILE:HD11	1:G:230:PRO:HD3	1.79	0.65
1:A:236:GLU:HG3	1:A:267:VAL:HG13	1.79	0.64
1:H:77:MET:HG2	1:H:148:ARG:HD3	1.79	0.64
1:B:198:THR:HG22	1:B:209:ILE:HG21	1.78	0.64
1:G:143:VAL:HG21	1:G:171:ASN:HB3	1.81	0.63
1:D:52:THR:HG21	1:D:300:ARG:H	1.64	0.62
1:H:52:THR:HG21	1:H:300:ARG:H	1.65	0.61
1:G:288:LYS:HE3	1:G:288:LYS:H	1.66	0.61
1:C:298:TYR:OH	1:C:331:ILE:HG12	2.01	0.60
1:F:231:GLN:HE21	1:F:231:GLN:HA	1.68	0.59
1:D:279:ALA:O	1:D:338:LYS:HE2	2.02	0.59
1:D:141:ILE:HD12	1:D:160:ILE:HD12	1.87	0.57
1:G:242:ALA:HB3	1:G:249:ILE:HD11	1.87	0.56
1:G:50:MET:HB2	1:G:53:VAL:HG12	1.88	0.56
1:C:50:MET:HB2	1:C:53:VAL:CG1	2.34	0.55
1:H:300:ARG:HD3	1:H:307:ALA:HB2	1.89	0.55
1:B:164:SER:HB2	1:B:172:ILE:HD11	1.88	0.54
1:A:16:LEU:HD21	1:B:222:ARG:HB2	1.88	0.54
1:C:77:MET:HE3	1:C:147:GLU:HG3	1.90	0.54
1:F:236:GLU:HG3	1:F:267:VAL:HG13	1.90	0.54
1:A:24:VAL:HG11	1:A:362:ALA:HB2	1.90	0.54
1:A:141:ILE:HD13	1:A:149:ALA:HB2	1.91	0.52
3:B:901:C64:O	3:B:901:C64:H2	2.08	0.52
1:A:8:LYS:HD2	1:D:375:GLU:HB3	1.91	0.52
1:A:164:SER:HB3	1:A:172:ILE:HD11	1.91	0.52
1:F:70:ILE:HG13	1:F:138:GLY:HA3	1.92	0.52
1:G:188:ILE:HG12	1:G:208:GLY:HA3	1.92	0.52
3:H:903:C64:O	3:H:903:C64:H2	2.09	0.52
3:D:902:C64:H2	3:D:902:C64:O	2.08	0.52
1:B:15:ILE:HD13	1:B:232:ILE:HG21	1.91	0.51
1:F:160:ILE:HD12	1:F:185:ILE:HG21	1.91	0.51
1:F:88:LYS:HE3	1:F:156:GLY:O	2.11	0.51
1:B:231:GLN:NE2	1:B:231:GLN:HA	2.25	0.51
1:D:51:ASP:HA	1:D:72:HIS:CD2	2.46	0.51
1:C:261:ILE:HG12	1:C:272:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ILE:HA	1:E:208:GLY:O	2.11	0.50
1:B:88:LYS:HE3	1:B:156:GLY:O	2.12	0.50
1:F:291:ILE:HG13	1:F:291:ILE:O	2.12	0.50
1:G:70:ILE:HG13	1:G:138:GLY:HA3	1.94	0.50
1:E:21:TYR:HB2	1:F:168:HIS:CE1	2.48	0.49
1:C:251:ALA:HB3	1:C:272:VAL:HG12	1.93	0.49
1:C:258:SER:HB3	1:C:348:LEU:HA	1.94	0.49
1:G:77:MET:HG2	1:G:148:ARG:HG3	1.94	0.49
1:H:195:GLU:HA	1:H:198:THR:HG22	1.95	0.48
1:B:146:ILE:HG22	1:B:150:LYS:HE2	1.94	0.48
1:C:81:VAL:HG13	1:C:155:ALA:HB2	1.94	0.47
1:B:291:ILE:O	1:B:291:ILE:HG13	2.14	0.47
1:C:21:TYR:HB2	1:D:168:HIS:CE1	2.49	0.47
1:C:212:GLY:HA2	1:C:231:GLN:HE22	1.79	0.47
1:F:212:GLY:HA2	1:F:231:GLN:HE22	1.80	0.47
1:H:24:VAL:HG21	1:H:362:ALA:HB2	1.96	0.47
1:A:349:VAL:O	1:A:353:ARG:HG3	2.14	0.46
1:G:251:ALA:HB3	1:G:272:VAL:HG12	1.97	0.46
1:A:16:LEU:CD2	1:B:222:ARG:HB2	2.45	0.46
1:B:15:ILE:HG12	1:B:373:TYR:CD2	2.50	0.46
1:B:218:ILE:CD1	1:B:218:ILE:H	2.28	0.46
1:D:143:VAL:CG1	1:D:171:ASN:HB3	2.39	0.46
1:D:2:GLY:HA3	1:D:3:THR:HA	1.61	0.46
1:D:342:GLU:O	1:D:346:TYR:HD1	1.99	0.46
1:D:43:ILE:HD12	1:D:45:LEU:HD12	1.98	0.46
1:G:21:TYR:HB2	1:H:168:HIS:CE1	2.51	0.45
1:F:173:ILE:HG22	1:F:177:LYS:HE2	1.97	0.45
1:G:215:PRO:HD3	1:G:222:ARG:HH11	1.80	0.45
1:G:24:VAL:HG11	1:G:362:ALA:HB2	1.99	0.45
1:C:141:ILE:HD13	1:C:149:ALA:HB2	1.99	0.45
1:E:24:VAL:HG21	1:E:362:ALA:HB2	1.98	0.45
1:A:222:ARG:HG3	1:D:16:LEU:HD21	1.98	0.45
1:A:236:GLU:HG3	1:A:267:VAL:CG1	2.46	0.45
3:B:901:C64:N2	3:B:901:C64:H17A	2.32	0.45
1:B:21:TYR:HB2	1:C:168:HIS:CE1	2.52	0.45
1:C:265:LEU:HD12	1:C:352:LEU:HD21	1.98	0.45
1:A:81:VAL:HG13	1:A:155:ALA:HB2	1.98	0.44
1:B:372:SER:HA	1:C:4:LYS:HB3	1.99	0.44
1:F:15:ILE:HG23	1:F:373:TYR:HB2	1.98	0.44
1:D:265:LEU:HD12	1:D:352:LEU:HD21	2.00	0.44
1:F:10:LEU:HD13	1:F:15:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ILE:HG13	1:H:146:ILE:H	1.57	0.44
1:D:77:MET:HG2	1:D:148:ARG:HG3	2.00	0.44
1:G:55:GLU:HB2	1:G:285:PRO:HG3	1.99	0.43
1:H:349:VAL:O	1:H:353:ARG:HG3	2.19	0.43
1:F:15:ILE:HD13	1:F:232:ILE:HG21	2.00	0.43
1:D:196:GLU:H	1:D:196:GLU:CD	2.21	0.43
1:C:5:ASN:HD22	1:C:7:GLY:H	1.66	0.43
1:E:222:ARG:HG3	1:H:16:LEU:HD21	1.99	0.43
1:E:247:ILE:HA	1:E:248:PRO:HD3	1.86	0.43
1:H:202:ILE:HG12	1:H:247:ILE:HG13	2.01	0.43
1:D:77:MET:SD	1:D:147:GLU:HG2	2.58	0.43
1:G:232:ILE:HG23	1:G:267:VAL:HG21	2.00	0.43
1:F:236:GLU:HG3	1:F:267:VAL:CG1	2.49	0.42
1:G:26:PRO:HG3	1:G:357:GLY:HA3	2.01	0.42
1:H:51:ASP:HA	1:H:72:HIS:CD2	2.54	0.42
1:F:164:SER:HB2	1:F:172:ILE:HD11	2.00	0.42
1:H:376:ILE:HD13	1:H:377:THR:H	1.84	0.42
1:G:229:VAL:HA	1:G:230:PRO:HD2	1.90	0.42
1:B:87:VAL:HG11	1:B:137:VAL:HG13	2.00	0.42
1:B:224:VAL:HG21	1:B:329:GLU:HG2	2.02	0.42
1:F:236:GLU:CG	1:F:267:VAL:HG13	2.50	0.42
1:F:24:VAL:HG11	1:F:362:ALA:HB2	2.01	0.42
1:F:27:ARG:HD3	1:F:28:GLU:HG3	2.01	0.41
1:G:18:VAL:HA	1:G:19:PRO:HD3	1.93	0.41
1:A:65:LEU:HD21	1:A:342:GLU:HG3	2.01	0.41
1:F:21:TYR:HB2	1:G:168:HIS:CE1	2.55	0.41
1:B:198:THR:HG21	1:B:238:CYS:HB3	2.02	0.41
1:D:266:ALA:HA	1:D:367:LEU:HG	2.02	0.41
1:F:291:ILE:HG12	1:F:296:TYR:CE1	2.55	0.41
1:C:77:MET:CE	1:C:147:GLU:HG3	2.50	0.41
1:A:48:SER:HB2	1:A:53:VAL:HG11	2.02	0.41
1:A:277:ILE:HG21	1:A:348:LEU:HD11	2.03	0.41
3:H:903:C64:N2	3:H:903:C64:H17A	2.35	0.41
1:A:255:ILE:HG23	1:A:260:ASP:HB2	2.03	0.41
1:E:232:ILE:HG23	1:E:267:VAL:HG21	2.03	0.41
1:A:219:CYS:HA	5:A:434:HOH:O	2.22	0.40
1:D:189:VAL:HG11	1:D:201:LEU:HD22	2.03	0.40
1:F:70:ILE:HG12	1:F:161:VAL:HG21	2.02	0.40
1:H:251:ALA:HB3	1:H:272:VAL:HG23	2.04	0.40
1:E:162:LEU:HD22	1:E:172:ILE:HG23	2.02	0.40
1:B:33:THR:HG21	1:B:44:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASN:HD21	1:B:210:LYS:NZ	2.18	0.40
1:E:141:ILE:HG13	1:E:142:GLY:N	2.37	0.40
1:F:34:LYS:HG2	1:F:36:THR:O	2.22	0.40
1:H:81:VAL:HG13	1:H:155:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/361 (82%)	288 (97%)	10 (3%)	0	100	100
1	B	315/361 (87%)	304 (96%)	10 (3%)	1 (0%)	44	77
1	C	303/361 (84%)	290 (96%)	13 (4%)	0	100	100
1	D	317/361 (88%)	307 (97%)	10 (3%)	0	100	100
1	E	292/361 (81%)	278 (95%)	14 (5%)	0	100	100
1	F	297/361 (82%)	285 (96%)	11 (4%)	1 (0%)	44	77
1	G	294/361 (81%)	279 (95%)	12 (4%)	3 (1%)	18	50
1	H	324/361 (90%)	300 (93%)	23 (7%)	1 (0%)	44	77
All	All	2440/2888 (84%)	2331 (96%)	103 (4%)	6 (0%)	51	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	91	GLY
1	H	91	GLY
1	G	212	GLY
1	G	268	GLY
1	B	275	GLY
1	F	275	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/295 (82%)	232 (96%)	11 (4%)	32	66
1	B	253/295 (86%)	243 (96%)	10 (4%)	36	70
1	C	246/295 (83%)	231 (94%)	15 (6%)	22	53
1	D	248/295 (84%)	238 (96%)	10 (4%)	36	70
1	E	233/295 (79%)	227 (97%)	6 (3%)	51	83
1	F	239/295 (81%)	228 (95%)	11 (5%)	31	65
1	G	234/295 (79%)	219 (94%)	15 (6%)	20	50
1	H	247/295 (84%)	236 (96%)	11 (4%)	32	66
All	All	1943/2360 (82%)	1854 (95%)	89 (5%)	31	65

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	143	VAL
1	A	157	VAL
1	A	162	LEU
1	A	163	ASP
1	A	170	LEU
1	A	176	LEU
1	A	209	ILE
1	A	220	THR
1	A	340	GLU
1	A	374	VAL
1	B	16	LEU
1	B	25	LEU
1	B	137	VAL
1	B	176	LEU
1	B	191	ASN
1	B	218	ILE
1	B	231	GLN
1	B	267	VAL

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Mol	Chain	Res	Type
1	B	352	LEU
1	B	369	LYS
1	C	5	ASN
1	C	57	LEU
1	C	65	LEU
1	C	76	ASP
1	C	85	LEU
1	C	162	LEU
1	C	170	LEU
1	C	176	LEU
1	C	186	ASP
1	C	231	GLN
1	C	267	VAL
1	C	298	TYR
1	C	352	LEU
1	C	374	VAL
1	C	378	THR
1	D	141	ILE
1	D	143	VAL
1	D	147	GLU
1	D	152	LEU
1	D	154	GLU
1	D	176	LEU
1	D	186	ASP
1	D	267	VAL
1	D	352	LEU
1	D	374	VAL
1	E	162	LEU
1	E	177	LYS
1	E	182	LYS
1	E	222	ARG
1	E	267	VAL
1	E	284	SER
1	F	27	ARG
1	F	42	LYS
1	F	137	VAL
1	F	174	ARG
1	F	176	LEU
1	F	193	VAL
1	F	231	GLN
1	F	291	ILE
1	F	341	MET

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Mol	Chain	Res	Type
1	F	352	LEU
1	F	374	VAL
1	G	3	THR
1	G	10	LEU
1	G	15	ILE
1	G	39	VAL
1	G	55	GLU
1	G	75	MET
1	G	162	LEU
1	G	170	LEU
1	G	176	LEU
1	G	192	VAL
1	G	288	LYS
1	G	332	GLU
1	G	352	LEU
1	G	374	VAL
1	G	376	ILE
1	H	13	GLU
1	H	64	ARG
1	H	78	GLU
1	H	146	ILE
1	H	162	LEU
1	H	170	LEU
1	H	180	LYS
1	H	291	ILE
1	H	319	GLU
1	H	352	LEU
1	H	376	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	ASN
1	B	191	ASN
1	B	231	GLN
1	C	5	ASN
1	C	171	ASN
1	C	204	ASN
1	C	231	GLN
1	D	89	ASN
1	F	191	ASN
1	F	231	GLN

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Mol	Chain	Res	Type
1	G	5	ASN
1	G	204	ASN
1	H	168	HIS

### 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](#)

12 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	801	-	21,25,25	1.43	3 (14%)	22,38,38	2.39	2 (9%)
2	IMP	B	804	-	21,25,25	1.40	3 (14%)	22,38,38	2.31	2 (9%)
3	C64	B	901	-	25,28,28	1.38	3 (12%)	27,39,39	0.90	1 (3%)
2	IMP	C	803	-	21,25,25	1.38	3 (14%)	22,38,38	2.36	2 (9%)
4	ACT	D	401	-	1,3,3	1.36	0	0,3,3	0.00	-
2	IMP	D	802	-	21,25,25	1.41	3 (14%)	22,38,38	2.33	2 (9%)
3	C64	D	902	-	25,28,28	1.38	3 (12%)	27,39,39	0.94	2 (7%)
2	IMP	E	805	-	21,25,25	1.43	3 (14%)	22,38,38	2.43	2 (9%)
2	IMP	F	808	-	21,25,25	1.45	3 (14%)	22,38,38	2.41	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	IMP	G	807	-	21,25,25	1.41	3 (14%)	22,38,38	2.43	2 (9%)
2	IMP	H	806	-	21,25,25	1.37	3 (14%)	22,38,38	2.26	2 (9%)
3	C64	H	903	-	25,28,28	1.38	3 (12%)	27,39,39	0.91	1 (3%)

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	801	-	-	0/6/26/26	0/3/3/3
2	IMP	B	804	-	-	0/6/26/26	0/3/3/3
3	C64	B	901	-	-	0/9/12/12	0/4/4/4
2	IMP	C	803	-	-	0/6/26/26	0/3/3/3
4	ACT	D	401	-	-	0/0/0/0	0/0/0/0
2	IMP	D	802	-	-	0/6/26/26	0/3/3/3
3	C64	D	902	-	-	0/9/12/12	0/4/4/4
2	IMP	E	805	-	-	0/6/26/26	0/3/3/3
2	IMP	F	808	-	-	0/6/26/26	0/3/3/3
2	IMP	G	807	-	-	0/6/26/26	0/3/3/3
2	IMP	H	806	-	-	0/6/26/26	0/3/3/3
3	C64	H	903	-	-	0/9/12/12	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	C64	C4-N4	-2.59	1.36	1.41
3	H	903	C64	C4-N4	-2.54	1.36	1.41
3	D	902	C64	C4-N4	-2.44	1.36	1.41
3	D	902	C64	C8-N2	2.44	1.35	1.31
3	H	903	C64	C8-N2	2.52	1.35	1.31
3	B	901	C64	C8-N2	2.53	1.35	1.31
2	H	806	IMP	C2-N1	2.55	1.38	1.33
2	C	803	IMP	C2-N1	2.58	1.38	1.33
2	B	804	IMP	C2-N1	2.59	1.38	1.33
2	G	807	IMP	C2-N1	2.61	1.38	1.33
2	D	802	IMP	C2-N1	2.64	1.38	1.33
2	E	805	IMP	C2-N1	2.71	1.39	1.33
2	F	808	IMP	C2-N1	2.73	1.39	1.33
2	A	801	IMP	C2-N1	2.74	1.39	1.33
2	H	806	IMP	C6-N1	3.06	1.38	1.33
2	C	803	IMP	C6-N1	3.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	IMP	C6-N1	3.10	1.38	1.33
2	G	807	IMP	C6-N1	3.24	1.38	1.33
2	D	802	IMP	C6-N1	3.26	1.39	1.33
2	A	801	IMP	C6-N1	3.26	1.39	1.33
2	E	805	IMP	C6-N1	3.27	1.39	1.33
2	F	808	IMP	C6-N1	3.40	1.39	1.33
2	H	806	IMP	C2-N3	3.91	1.38	1.32
2	C	803	IMP	C2-N3	3.98	1.38	1.32
2	D	802	IMP	C2-N3	3.99	1.38	1.32
2	B	804	IMP	C2-N3	4.02	1.38	1.32
2	G	807	IMP	C2-N3	4.03	1.38	1.32
2	E	805	IMP	C2-N3	4.05	1.38	1.32
2	F	808	IMP	C2-N3	4.07	1.39	1.32
2	A	801	IMP	C2-N3	4.08	1.39	1.32
3	B	901	C64	C10-C11	4.61	1.49	1.40
3	D	902	C64	C10-C11	4.67	1.49	1.40
3	H	903	C64	C10-C11	4.68	1.49	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	808	IMP	N3-C2-N1	-10.37	119.83	128.86
2	G	807	IMP	N3-C2-N1	-10.35	119.84	128.86
2	A	801	IMP	N3-C2-N1	-10.34	119.86	128.86
2	E	805	IMP	N3-C2-N1	-10.27	119.91	128.86
2	D	802	IMP	N3-C2-N1	-10.11	120.05	128.86
2	C	803	IMP	N3-C2-N1	-10.07	120.09	128.86
2	B	804	IMP	N3-C2-N1	-9.99	120.16	128.86
2	H	806	IMP	N3-C2-N1	-9.84	120.29	128.86
3	D	902	C64	C8-C6-N3	-2.07	119.77	124.89
3	H	903	C64	C15-N2-C8	2.26	110.23	104.39
3	D	902	C64	C15-N2-C8	2.31	110.34	104.39
3	B	901	C64	C15-N2-C8	2.31	110.36	104.39
2	C	803	IMP	C2-N1-C6	2.39	119.89	115.91
2	H	806	IMP	C2-N1-C6	2.47	120.03	115.91
2	G	807	IMP	C2-N1-C6	2.48	120.05	115.91
2	A	801	IMP	C2-N1-C6	2.51	120.10	115.91
2	D	802	IMP	C2-N1-C6	2.54	120.15	115.91
2	E	805	IMP	C2-N1-C6	2.56	120.18	115.91
2	F	808	IMP	C2-N1-C6	2.58	120.22	115.91
2	B	804	IMP	C2-N1-C6	2.59	120.22	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	C64	2	0
3	D	902	C64	1	0
3	H	903	C64	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	302/361 (83%)	-0.25	6 (1%) 65 56	28, 38, 55, 68	0
1	B	318/361 (88%)	-0.16	1 (0%) 93 92	31, 40, 59, 63	0
1	C	306/361 (84%)	-0.25	7 (2%) 61 51	23, 37, 55, 64	0
1	D	321/361 (88%)	-0.25	1 (0%) 93 92	28, 38, 58, 70	0
1	E	298/361 (82%)	0.04	7 (2%) 61 51	50, 64, 86, 88	0
1	F	300/361 (83%)	-0.00	4 (1%) 77 71	50, 62, 76, 77	0
1	G	300/361 (83%)	0.28	14 (4%) 32 22	57, 73, 93, 94	0
1	H	328/361 (90%)	0.17	8 (2%) 59 49	52, 66, 84, 85	0
All	All	2473/2888 (85%)	-0.05	48 (1%) 67 58	23, 54, 83, 94	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	218	ILE	6.1
1	C	331	ILE	5.4
1	F	299	TYR	4.4
1	F	298	TYR	4.0
1	A	379	SER	3.8
1	G	379	SER	3.6
1	H	181	SER	3.5
1	E	163	ASP	3.4
1	A	218	ILE	3.2
1	G	298	TYR	3.1
1	G	181	SER	3.1
1	A	298	TYR	3.1
1	A	293	ASP	3.0
1	E	379	SER	2.9
1	G	333	GLY	2.9
1	G	292	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	219	CYS	2.8
1	G	37	LYS	2.5
1	G	38	ASN	2.5
1	C	298	TYR	2.5
1	G	144	ASN	2.5
1	G	335	VAL	2.4
1	G	378	THR	2.4
1	H	313	GLY	2.4
1	G	293	ASP	2.4
1	H	335	VAL	2.4
1	H	91	GLY	2.4
1	A	333	GLY	2.3
1	G	332	GLU	2.3
1	C	299	TYR	2.3
1	F	334	ARG	2.3
1	C	333	GLY	2.3
1	E	292	GLY	2.2
1	B	326	MET	2.2
1	E	90	SER	2.2
1	E	151	LEU	2.2
1	H	333	GLY	2.2
1	C	300	ARG	2.1
1	D	299	TYR	2.1
1	H	173	ILE	2.1
1	G	299	TYR	2.1
1	E	378	THR	2.1
1	G	163	ASP	2.1
1	H	170	LEU	2.0
1	C	330	GLY	2.0
1	H	156	GLY	2.0
1	E	287	GLU	2.0
1	C	379	SER	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	C64	H	903	25/25	0.83	0.41	5.38	51,52,52,52	25
3	C64	D	902	25/25	0.80	0.37	3.16	50,50,50,51	25
3	C64	B	901	25/25	0.89	0.29	1.48	54,54,54,54	25
2	IMP	G	807	23/23	0.84	0.20	0.36	104,105,105,105	0
2	IMP	E	805	23/23	0.83	0.21	0.10	79,81,82,82	0
2	IMP	A	801	23/23	0.91	0.17	-0.04	57,61,62,62	0
2	IMP	F	808	23/23	0.87	0.19	-0.15	56,59,61,61	0
2	IMP	C	803	23/23	0.94	0.16	-0.36	44,49,50,50	0
2	IMP	H	806	23/23	0.96	0.14	-1.06	51,52,52,53	0
2	IMP	B	804	23/23	0.96	0.12	-1.07	46,48,49,49	0
2	IMP	D	802	23/23	0.96	0.13	-1.25	39,41,41,41	0
4	ACT	D	401	4/4	0.78	0.17	-1.46	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.