



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 PM GMT

PDB ID : 4FXS  
Title : Inosine 5'-monophosphate dehydrogenase from *Vibrio cholerae* complexed with IMP and mycophenolic acid  
Authors : Osipiuk, J.; Maltseva, N.; Makowska-Grzyska, M.; Jedrzejczak, R.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-07-03  
Resolution : 2.24 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 (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

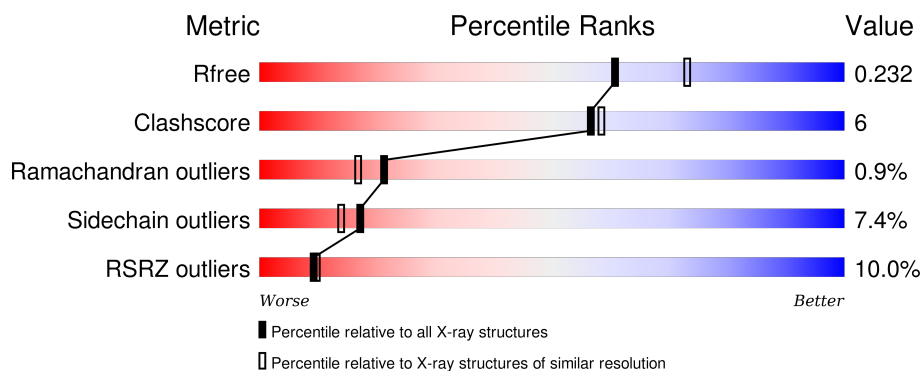
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	496	<div> <div>9%</div> <div>79%</div> <div>13%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3667 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.

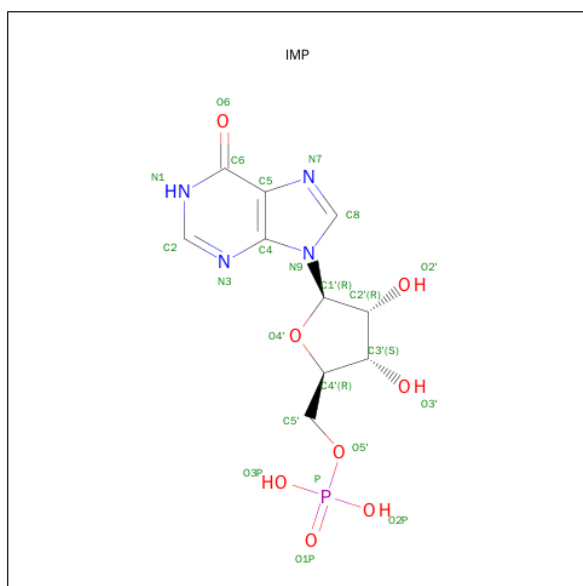
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	467	3533	2214	626	674	4	15	0	10	0

There are 7 discrepancies between the modelled and reference sequences:

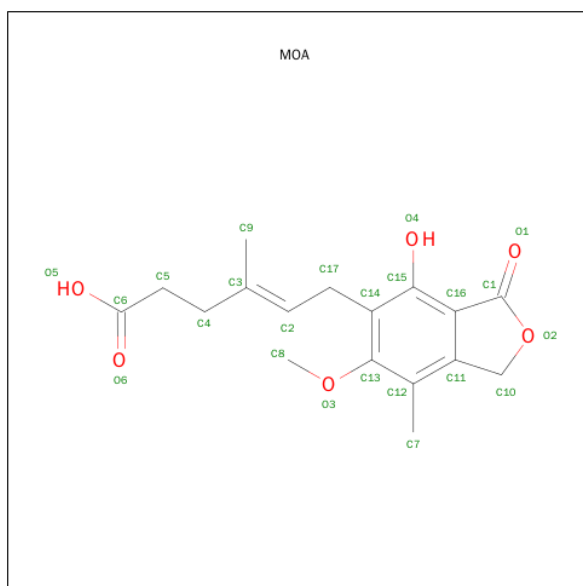
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	GLY	-	EXPRESSION TAG	UNP Q9KTW3
A	491	GLU	-	EXPRESSION TAG	UNP Q9KTW3
A	492	ASN	-	EXPRESSION TAG	UNP Q9KTW3
A	493	LEU	-	EXPRESSION TAG	UNP Q9KTW3
A	494	TYR	-	EXPRESSION TAG	UNP Q9KTW3
A	495	PHE	-	EXPRESSION TAG	UNP Q9KTW3
A	496	GLN	-	EXPRESSION TAG	UNP Q9KTW3

- 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		

- Molecule 3 is MYCOPHENOLIC ACID (three-letter code: MOA) (formula:  $C_{17}H_{20}O_6$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			23	17 6		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

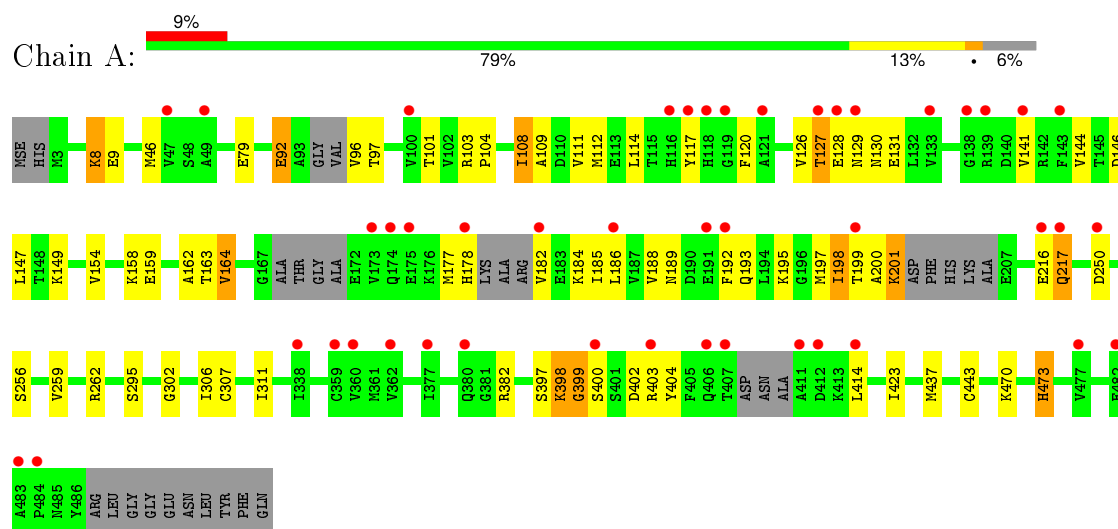
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		

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

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

- Molecule 1: Inosine-5'-monophosphate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.96Å 111.96Å 188.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.70 – 2.24 30.64 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.70-2.24) 99.9 (30.64-2.24)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.190 , 0.232 0.189 , 0.232	Depositor DCC
$R_{free}$ test set	1540 reflections (5.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29244 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.75	0/3594	0.81	1/4825 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	250	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3533	0	3610	44	0
2	A	23	0	11	1	0
3	A	23	0	19	0	0
4	A	1	0	0	0	0
5	A	87	0	0	1	0
All	All	3667	0	3640	44	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 (44) 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:A:216[B]:GLU:HG2	1:A:217:GLN:HE21	1.14	1.07
1:A:216[B]:GLU:HG2	1:A:217:GLN:NE2	1.92	0.84
1:A:307:CYS:SG	2:A:701:IMP:H2	2.25	0.77
1:A:216[B]:GLU:CG	1:A:217:GLN:HE21	1.98	0.72
1:A:112:MSE:HG2	1:A:117:TYR:CZ	2.27	0.70
1:A:112:MSE:HG2	1:A:117:TYR:CE2	2.34	0.63
1:A:397:SER:C	1:A:399:GLY:H	2.04	0.60
1:A:127:THR:HG23	1:A:128:GLU:N	2.16	0.60
1:A:8:LYS:HG2	1:A:9:GLU:H	1.67	0.58
1:A:199:THR:O	1:A:201:LYS:HG3	2.07	0.55
1:A:256[B]:SER:OG	1:A:259:VAL:HG23	2.07	0.54
1:A:79:GLU:CD	1:A:79:GLU:H	2.10	0.54
1:A:163:THR:HG22	1:A:186:LEU:HB2	1.89	0.54
1:A:127:THR:HG23	1:A:128:GLU:H	1.73	0.53
1:A:92[A]:GLU:HA	1:A:92[A]:GLU:OE1	2.08	0.53
1:A:96:VAL:HA	1:A:198:ILE:HG23	1.91	0.53
1:A:120:PHE:CZ	1:A:141:VAL:HG21	2.45	0.52
1:A:189:ASN:HD22	1:A:195:LYS:HE3	1.74	0.52
1:A:127:THR:CG2	1:A:128:GLU:N	2.74	0.51
1:A:104:PRO:HD3	1:A:126:VAL:O	2.09	0.51
1:A:414:LEU:HD12	1:A:414:LEU:H	1.76	0.51
1:A:397:SER:C	1:A:399:GLY:N	2.64	0.51
1:A:402:ASP:C	1:A:404:TYR:H	2.15	0.50
1:A:164:VAL:HG22	1:A:185:ILE:HG12	1.96	0.47
1:A:184:LYS:HG2	1:A:199:THR:HG23	1.96	0.47
1:A:109:ALA:HB2	1:A:147:LEU:HB3	1.97	0.46
1:A:46:MSE:SE	1:A:437:MSE:HE3	2.65	0.46
1:A:108:ILE:HG12	1:A:149:LYS:O	2.17	0.45
1:A:120:PHE:HZ	1:A:141:VAL:HG21	1.82	0.44
1:A:177:MSE:HE1	1:A:200:ALA:HA	2.00	0.43
1:A:108:ILE:HA	1:A:111:VAL:HG23	1.99	0.43
1:A:158:LYS:HE3	1:A:192:PHE:CZ	2.54	0.43
1:A:473:HIS:HB2	5:A:824:HOH:O	2.19	0.42
1:A:144:VAL:HG21	1:A:154:VAL:HG21	2.01	0.42
1:A:108:ILE:HB	1:A:147:LEU:HA	2.02	0.41
1:A:109:ALA:HA	1:A:147:LEU:HD22	2.03	0.41
1:A:127:THR:HB	1:A:131:GLU:HB3	2.02	0.41
1:A:162:ALA:O	1:A:185:ILE:HG13	2.21	0.41
1:A:130:ASN:HB3	1:A:193:GLN:HG2	2.03	0.41
1:A:8:LYS:HG2	1:A:9:GLU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MSE:HE3	1:A:199:THR:OG1	2.20	0.41
1:A:302:GLY:HA2	1:A:307:CYS:SG	2.61	0.40
1:A:108:ILE:H	1:A:108:ILE:HG12	1.70	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	465/496 (94%)	435 (94%)	26 (6%)	4 (1%)	21 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	473	HIS
1	A	398	LYS
1	A	399	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/369 (101%)	346 (92%)	28 (8%)	17 14

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	92[A]	GLU
1	A	92[B]	GLU
1	A	97	THR
1	A	101	THR
1	A	103	ARG
1	A	108	ILE
1	A	114	LEU
1	A	127	THR
1	A	129	ASN
1	A	159	GLU
1	A	164	VAL
1	A	178	HIS
1	A	182	VAL
1	A	188	VAL
1	A	198	ILE
1	A	201	LYS
1	A	217	GLN
1	A	262	ARG
1	A	295	SER
1	A	306	ILE
1	A	382	ARG
1	A	398	LYS
1	A	400	SER
1	A	403	ARG
1	A	423	ILE
1	A	443	CYS
1	A	470	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	130	ASN
1	A	217	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	IMP	A	701	-	20,25,25	1.23	2 (10%)	22,38,38	2.36	6 (27%)
3	MOA	A	702	-	21,24,24	3.23	7 (33%)	30,34,34	1.48	5 (16%)

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	701	-	-	0/6/26/26	0/3/3/3
3	MOA	A	702	-	-	0/10/21/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	IMP	C2-N3	2.11	1.35	1.32
3	A	702	MOA	C16-C11	3.48	1.46	1.39
3	A	702	MOA	C16-C15	3.70	1.49	1.41
2	A	701	IMP	O4'-C1'	3.76	1.46	1.41
3	A	702	MOA	C11-C12	4.43	1.48	1.40
3	A	702	MOA	C13-C12	5.47	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	MOA	C13-C14	6.39	1.50	1.39
3	A	702	MOA	O2-C1	6.70	1.44	1.36
3	A	702	MOA	C15-C14	6.83	1.50	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	IMP	N3-C2-N1	-7.62	123.06	128.89
2	A	701	IMP	C4-C5-N7	-3.45	106.30	109.48
2	A	701	IMP	C1'-N9-C4	-3.20	122.11	126.94
3	A	702	MOA	C17-C2-C3	-2.98	122.02	127.29
2	A	701	IMP	O3P-P-O1P	-2.51	102.51	110.58
3	A	702	MOA	C11-C16-C1	-2.30	105.23	108.28
3	A	702	MOA	C8-O3-C13	2.49	121.38	114.82
2	A	701	IMP	O3P-P-O2P	2.67	117.54	107.38
2	A	701	IMP	O5'-P-O1P	2.70	114.02	107.14
3	A	702	MOA	C9-C3-C4	2.99	119.97	115.41
3	A	702	MOA	C15-C16-C1	3.29	133.73	129.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	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	452/496 (91%)	0.34	45 (9%) 9 10	30, 53, 128, 172	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	GLU	6.6
1	A	173	VAL	5.0
1	A	128	GLU	4.6
1	A	406	GLN	4.4
1	A	129	ASN	4.2
1	A	119	GLY	4.1
1	A	360	VAL	4.0
1	A	250	ASP	3.8
1	A	216[A]	GLU	3.7
1	A	191	GLU	3.6
1	A	47	VAL	3.6
1	A	117	TYR	3.4
1	A	484	PRO	3.4
1	A	412	ASP	3.3
1	A	182	VAL	3.3
1	A	178	HIS	3.3
1	A	483	ALA	3.3
1	A	143	PHE	3.1
1	A	121	ALA	3.0
1	A	174	GLN	3.0
1	A	217	GLN	2.9
1	A	192	PHE	2.9
1	A	141	VAL	2.9
1	A	118[A]	HIS	2.9
1	A	116	HIS	2.8
1	A	100	VAL	2.7
1	A	133	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	414	LEU	2.6
1	A	139[A]	ARG	2.5
1	A	199	THR	2.5
1	A	407	THR	2.5
1	A	403	ARG	2.4
1	A	338	ILE	2.4
1	A	49	ALA	2.3
1	A	127	THR	2.3
1	A	186	LEU	2.3
1	A	138	GLY	2.3
1	A	400	SER	2.3
1	A	482	GLU	2.2
1	A	411	ALA	2.2
1	A	362	VAL	2.1
1	A	359	CYS	2.1
1	A	477	VAL	2.1
1	A	380	GLN	2.0
1	A	377	ILE	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	MOA	A	702	23/23	0.93	0.17	0.02	57,71,88,93	0
2	IMP	A	701	23/23	0.97	0.15	-0.01	32,35,47,53	0
4	K	A	703	1/1	0.97	0.04	-2.84	47,47,47,47	1

## 6.5 Other polymers

There are no such residues in this entry.