



# Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 04:20 AM GMT

PDB ID : 1JR1  
Title : Crystal structure of Inosine Monophosphate Dehydrogenase in complex with Mycophenolic Acid  
Authors : Sintchak, M.D.; Fleming, M.A.; Futer, O.; Raybuck, S.A.; Chambers, S.P.; Caron, P.R.; Murcko, M.A.; Wilson, K.P.  
Deposited on : 2001-08-09  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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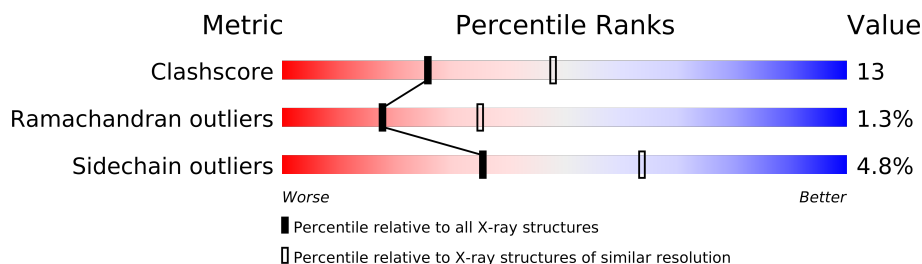
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6296 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

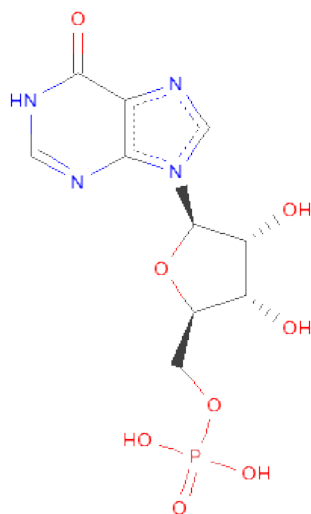
- Molecule 1 is a protein called Inosine-5'-MonophosphateDehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3236	2041	560	616	19			
1	B	368	Total	C	N	O	S	0	0	0
			2764	1750	471	525	18			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

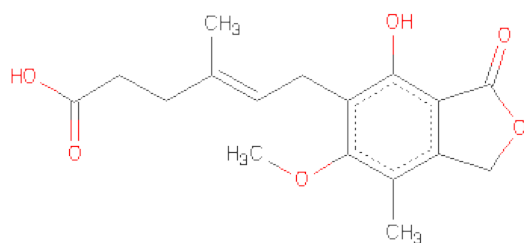
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 4 is MYCOPHENOLIC ACID (three-letter code: MOA) (formula: C<sub>17</sub>H<sub>20</sub>O<sub>6</sub>).



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

- Molecule 5 is water.

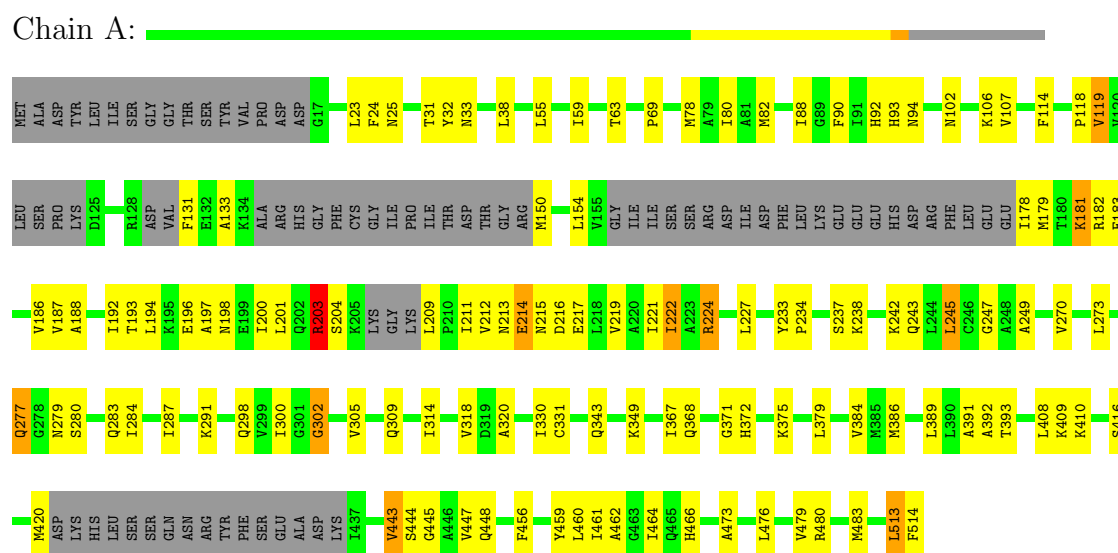
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	80	Total	O	0	0
			80	80		

### 3 Residue-property plots

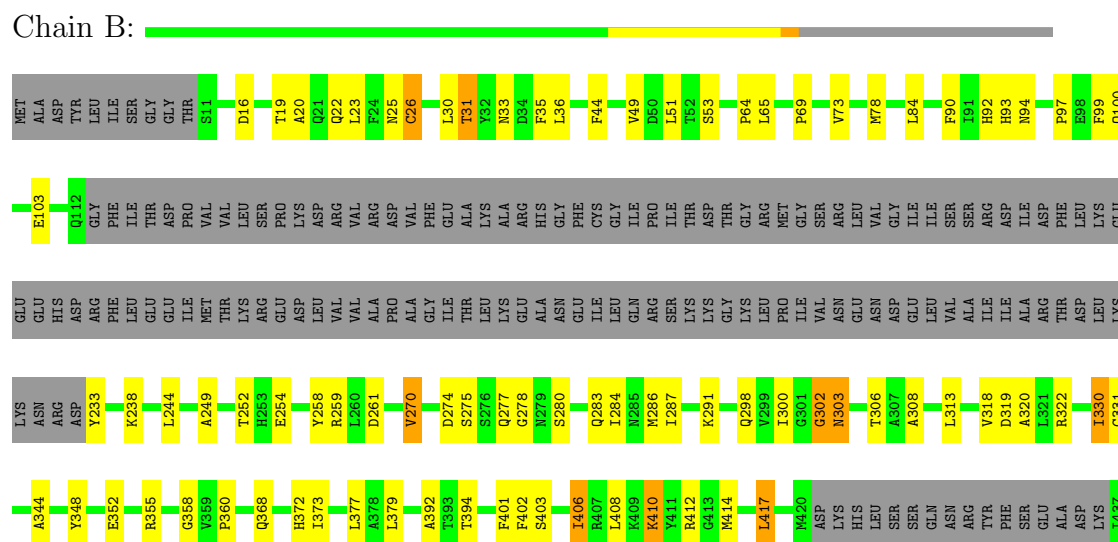
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: Inosine-5'-MonophosphateDehydrogenase 2



#### • Molecule 1: Inosine-5'-MonophosphateDehydrogenase 2



A440	S444	V447 Q448	S452	K455	F456	V457	P458	Y459	L460	I461	T464	Q465	C468	Q469	A473	M483	R493	T494	S495	V499	G502	V503	H504	L513	F514
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.60Å 110.60Å 111.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	5.20	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.37	0/3276	0.62	1/4417 (0.0%)
1	B	0.38	0/2807	0.62	0/3787
All	All	0.37	0/6083	0.62	1/8204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	PRO	N-CA-CB	5.75	110.20	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3234	89	0
1	B	2764	0	2794	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	23	0	10	0	0
3	B	23	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	19	0	0
4	B	23	0	19	0	0
5	A	122	0	0	1	0
5	B	80	0	0	3	0
All	All	6296	0	6087	164	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (164) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:417:LEU:HD23	1:B:440:ALA:HB2	1.47	0.96
1:A:392:ALA:HB2	1:A:447:VAL:HG23	1.51	0.92
1:A:283:GLN:HE22	1:A:302:GLY:HA3	1.43	0.84
1:B:100:GLN:OE1	1:B:259:ARG:HD2	1.80	0.82
1:A:368:GLN:H	1:A:372:HIS:HD2	1.27	0.80
1:A:386:MET:HE3	1:A:389:LEU:HD23	1.70	0.74
1:A:197:ALA:HB1	1:A:222:ILE:HD12	1.68	0.73
1:A:201:LEU:HB3	1:A:224:ARG:NH1	2.05	0.71
1:B:330:ILE:H	1:B:330:ILE:HD13	1.55	0.70
1:A:80:ILE:HG13	1:A:107:VAL:HG22	1.74	0.70
1:B:392:ALA:HB2	1:B:447:VAL:HG23	1.74	0.70
1:B:459:TYR:CE1	1:B:513:LEU:HD12	2.29	0.68
1:B:410:LYS:H	1:B:410:LYS:HD3	1.60	0.66
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.77	0.66
1:A:212:VAL:HG13	1:A:216:ASP:HA	1.79	0.65
1:B:252:THR:HG23	1:B:286:MET:HB2	1.78	0.64
1:A:393:THR:O	1:A:409:LYS:HE3	1.97	0.64
1:A:93:HIS:HB3	1:A:249:ALA:O	1.99	0.63
1:B:306:THR:HG22	1:B:308:ALA:H	1.62	0.63
1:A:460:LEU:O	1:A:464:ILE:HG13	2.00	0.62
1:A:213:ASN:HB3	1:A:217:GLU:HG3	1.82	0.61
1:A:133:ALA:HB3	1:A:181:LYS:HA	1.81	0.61
1:B:417:LEU:CD2	1:B:440:ALA:HB2	2.26	0.61
1:A:31:THR:HG22	1:A:32:TYR:H	1.66	0.60
1:B:368:GLN:H	1:B:372:HIS:HD2	1.50	0.60
1:A:237:SER:HB3	1:A:245:LEU:HD11	1.83	0.60
1:A:92:HIS:HD2	1:A:94:ASN:H	1.49	0.60
1:B:274:ASP:HA	5:B:726:HOH:O	2.00	0.60
1:B:459:TYR:HE1	1:B:513:LEU:HD12	1.66	0.60
1:A:462:ALA:O	1:A:466:HIS:HD2	1.83	0.60
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:ILE:HA	1:A:318:VAL:HG22	1.83	0.59
1:B:93:HIS:HB3	1:B:249:ALA:O	2.03	0.59
1:B:452:SER:HB3	1:B:455:LYS:HE2	1.85	0.59
1:B:402:PHE:HA	1:B:406:ILE:O	2.03	0.59
1:A:31:THR:HG22	1:A:32:TYR:N	2.18	0.58
1:A:330:ILE:HG22	1:A:443:VAL:HG12	1.85	0.58
1:B:331:CYS:CB	3:B:1332:IMP:C2	2.81	0.58
1:A:459:TYR:OH	1:A:513:LEU:HD22	2.04	0.58
1:A:194:LEU:HD11	1:A:242:LYS:HG3	1.84	0.58
1:B:275:SER:O	1:B:303:ASN:HB2	2.03	0.58
1:B:330:ILE:H	1:B:330:ILE:CD1	2.18	0.57
1:A:23:LEU:HD23	1:A:24:PHE:CE2	2.40	0.56
1:B:368:GLN:N	1:B:372:HIS:HD2	2.04	0.56
1:B:278:GLY:HA3	1:B:302:GLY:HA3	1.87	0.56
1:A:213:ASN:HB2	1:A:219:VAL:HB	1.87	0.56
1:B:283:GLN:OE1	1:B:302:GLY:N	2.38	0.56
1:A:131:PHE:N	1:A:154:LEU:O	2.40	0.55
1:A:78:MET:SD	1:A:82:MET:CE	2.94	0.55
1:B:92:HIS:HD2	1:B:94:ASN:H	1.55	0.55
1:A:102:ASN:ND2	1:A:106:LYS:HE3	2.22	0.55
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.37	0.54
1:B:270:VAL:HG13	1:B:298:GLN:HB2	1.89	0.54
1:A:212:VAL:CG1	1:A:216:ASP:HA	2.37	0.54
1:B:20:ALA:HB3	1:B:483:MET:HE3	1.91	0.53
1:A:198:ASN:HA	1:A:227:LEU:HD23	1.91	0.53
1:A:201:LEU:HD12	1:A:203:ARG:HD2	1.89	0.53
1:B:31:THR:HA	1:B:344:ALA:HB3	1.90	0.52
1:A:59:ILE:HG13	1:A:270:VAL:CG1	2.39	0.52
1:A:193:THR:HG22	1:A:196:GLU:HG3	1.92	0.52
1:A:133:ALA:HA	1:A:178:ILE:N	2.25	0.52
1:A:88:ILE:HD12	1:A:245:LEU:HD13	1.92	0.52
1:B:373:ILE:O	1:B:377:LEU:HG	2.10	0.51
1:A:247:GLY:HA3	1:A:270:VAL:HG23	1.91	0.51
1:B:408:LEU:HD23	1:B:448:GLN:HA	1.92	0.51
1:A:198:ASN:HD22	1:A:227:LEU:HB3	1.76	0.51
1:B:414:MET:HE3	5:B:716:HOH:O	2.11	0.51
1:A:63:THR:HG21	1:A:461:ILE:HD11	1.93	0.51
1:B:331:CYS:CB	3:B:1332:IMP:H2	2.41	0.50
1:B:31:THR:HG22	1:B:344:ALA:H	1.77	0.50
1:A:410:LYS:NZ	1:A:444:SER:HB3	2.26	0.50
1:A:211:ILE:HD11	1:A:222:ILE:HD11	1.94	0.50
1:A:201:LEU:O	1:A:224:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:408:LEU:HD23	1:A:448:GLN:HA	1.94	0.50
1:B:287:ILE:O	1:B:291:LYS:HG2	2.12	0.50
1:A:214:GLU:C	1:A:216:ASP:H	2.16	0.50
1:A:300:ILE:HG12	1:A:320:ALA:HB3	1.94	0.50
1:A:456:PHE:CE2	1:A:460:LEU:HD11	2.47	0.49
1:A:114:PHE:HE1	1:A:211:ILE:HG13	1.77	0.49
1:B:303:ASN:HA	1:B:322:ARG:O	2.12	0.49
1:A:410:LYS:HD2	1:A:445:GLY:O	2.13	0.49
1:B:457:VAL:HB	1:B:458:PRO:HD3	1.94	0.49
1:A:204:SER:HA	1:A:224:ARG:HG2	1.94	0.49
1:A:221:ILE:HG22	1:A:222:ILE:N	2.28	0.49
1:B:84:LEU:HD13	1:B:233:TYR:CE2	2.48	0.49
1:A:368:GLN:H	1:A:372:HIS:CD2	2.18	0.48
1:B:358:GLY:O	1:B:360:PRO:HD3	2.14	0.48
1:B:99:PHE:O	1:B:103:GLU:HG2	2.13	0.48
1:B:238:LYS:HB3	1:B:244:LEU:HA	1.94	0.47
1:A:25:ASN:OD1	1:A:349:LYS:HE2	2.14	0.47
1:A:69:PRO:HG3	1:A:90:PHE:HB3	1.96	0.47
1:B:403:SER:OG	1:B:408:LEU:HD12	2.14	0.47
1:B:319:ASP:O	1:B:360:PRO:HD2	2.13	0.47
1:A:92:HIS:HD2	1:A:94:ASN:N	2.12	0.47
1:A:133:ALA:CB	1:A:181:LYS:HA	2.45	0.47
1:B:73:VAL:O	1:B:78:MET:HE2	2.15	0.47
1:B:412:ARG:HB3	1:B:444:SER:OG	2.14	0.47
1:A:238:LYS:HA	1:A:243:GLN:O	2.15	0.47
1:B:406:ILE:H	1:B:406:ILE:HD13	1.80	0.46
1:A:459:TYR:CD1	1:A:514:PHE:HB3	2.49	0.46
1:B:19:THR:OG1	1:B:22:GLN:HG3	2.15	0.46
1:A:33:ASN:OD1	1:A:372:HIS:HE1	1.97	0.46
1:B:280:SER:O	1:B:284:ILE:HG13	2.15	0.46
1:B:502:GLY:O	1:B:504:HIS:HD2	1.99	0.46
1:A:476:LEU:HB3	1:A:480:ARG:NH2	2.30	0.46
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.97	0.46
1:A:277:GLN:HE22	1:A:279:ASN:HB3	1.81	0.46
1:A:201:LEU:HB3	1:A:224:ARG:HH12	1.81	0.46
1:A:459:TYR:OH	1:A:513:LEU:HD13	2.16	0.45
1:A:181:LYS:H	1:A:181:LYS:HD2	1.81	0.45
1:A:188:ALA:HB1	1:A:192:ILE:HD13	1.97	0.45
1:B:455:LYS:HE3	1:B:455:LYS:HB2	1.83	0.45
1:A:24:PHE:CE2	1:A:379:LEU:HD21	2.51	0.45
1:A:270:VAL:HG12	1:A:298:GLN:CB	2.44	0.45
1:A:55:LEU:HB3	1:A:59:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:322:ARG:NH1	5:B:726:HOH:O	2.49	0.45
1:B:401:PHE:CE1	1:B:408:LEU:HB2	2.52	0.45
1:A:280:SER:O	1:A:284:ILE:HG13	2.17	0.45
1:B:368:GLN:H	1:B:372:HIS:CD2	2.33	0.45
1:B:495:SER:O	1:B:499:VAL:HG23	2.16	0.45
1:A:213:ASN:O	1:A:215:ASN:N	2.51	0.44
1:A:59:ILE:HG13	1:A:270:VAL:HG11	1.98	0.44
1:A:150:MET:N	1:A:216:ASP:O	2.50	0.44
1:A:69:PRO:HG3	1:A:90:PHE:HB2	1.99	0.44
1:B:373:ILE:HG21	1:B:464:ILE:HD11	2.00	0.44
1:B:352:GLU:O	1:B:355:ARG:HG2	2.17	0.44
1:B:258:TYR:O	1:B:261:ASP:HB2	2.18	0.44
1:B:44:PHE:CZ	1:B:469:GLN:HA	2.52	0.44
1:B:20:ALA:HB3	1:B:483:MET:CE	2.46	0.44
1:A:305:VAL:H	1:A:309:GLN:NE2	2.15	0.43
1:A:367:ILE:HG13	1:A:384:VAL:CG1	2.48	0.43
1:A:88:ILE:CD1	1:A:245:LEU:HD13	2.48	0.43
1:B:69:PRO:HA	1:B:90:PHE:O	2.18	0.43
1:B:44:PHE:N	1:B:44:PHE:CD1	2.87	0.43
1:A:114:PHE:CE1	1:A:211:ILE:HG13	2.54	0.43
1:B:313:LEU:HB3	1:B:318:VAL:HG11	2.01	0.43
1:B:65:LEU:HD12	1:B:457:VAL:HG13	1.99	0.43
1:A:187:VAL:CG1	1:A:188:ALA:N	2.81	0.43
1:B:468:CYS:HB3	1:B:473:ALA:O	2.19	0.43
1:B:44:PHE:HE2	1:B:49:VAL:HG22	1.84	0.43
1:B:36:LEU:HG	1:B:493:ARG:HD3	2.01	0.43
1:A:392:ALA:HB2	1:A:447:VAL:CG2	2.37	0.43
1:A:119:VAL:CB	1:A:221:ILE:HG13	2.49	0.43
1:A:343:GLN:HA	1:A:343:GLN:NE2	2.34	0.43
1:B:461:ILE:O	1:B:465:GLN:HG3	2.18	0.42
1:A:213:ASN:O	1:A:216:ASP:N	2.52	0.42
1:A:343:GLN:NE2	5:A:662:HOH:O	2.53	0.42
1:A:416:SER:O	1:A:420:MET:HG3	2.20	0.42
1:B:53:SER:OG	1:B:64:PRO:HB3	2.20	0.42
1:A:273:LEU:HD12	1:A:287:ILE:HD11	2.02	0.42
1:A:473:ALA:CB	1:A:479:VAL:HG22	2.49	0.42
1:A:233:TYR:HA	1:A:234:PRO:HD2	1.89	0.42
1:B:283:GLN:HE22	1:B:302:GLY:CA	2.32	0.42
1:B:35:PHE:CZ	1:B:379:LEU:HD11	2.54	0.42
1:A:82:MET:HG2	1:A:88:ILE:O	2.20	0.41
1:B:455:LYS:C	1:B:458:PRO:HD2	2.40	0.41
1:B:25:ASN:HD21	1:B:348:TYR:HE2	1.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:97:PRO:HA	1:B:259:ARG:HD3	2.01	0.41
1:A:201:LEU:CD1	1:A:203:ARG:HD2	2.51	0.41
1:A:371:GLY:O	1:A:375:LYS:HG3	2.20	0.41
1:B:252:THR:HG23	1:B:286:MET:CB	2.49	0.41
1:B:283:GLN:HE22	1:B:302:GLY:HA2	1.86	0.41
1:B:33:ASN:OD1	1:B:372:HIS:HE1	2.03	0.40
1:B:23:LEU:O	1:B:26:CYS:HB2	2.20	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	422/514 (82%)	386 (92%)	28 (7%)	8 (2%)	12	23
1	B	362/514 (70%)	338 (93%)	22 (6%)	2 (1%)	33	63
All	All	784/1028 (76%)	724 (92%)	50 (6%)	10 (1%)	18	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL
1	A	179	MET
1	A	214	GLU
1	B	254	GLU
1	A	183	GLU
1	A	203	ARG
1	A	302	GLY
1	A	391	ALA
1	B	302	GLY
1	A	200	ILE

### 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	333/420 (79%)	318 (96%)	15 (4%)	38	67
1	B	292/420 (70%)	277 (95%)	15 (5%)	33	60
All	All	625/840 (74%)	595 (95%)	30 (5%)	35	64

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	181	LYS
1	A	182	ARG
1	A	186	VAL
1	A	203	ARG
1	A	209	LEU
1	A	222	ILE
1	A	224	ARG
1	A	245	LEU
1	A	277	GLN
1	A	291	LYS
1	A	331	CYS
1	A	443	VAL
1	A	483	MET
1	A	513	LEU
1	B	16	ASP
1	B	26	CYS
1	B	30	LEU
1	B	31	THR
1	B	270	VAL
1	B	277	GLN
1	B	303	ASN
1	B	330	ILE
1	B	394	THR
1	B	406	ILE
1	B	410	LYS
1	B	417	LEU
1	B	483	MET
1	B	513	LEU

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Mol	Chain	Res	Type
1	B	514	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	198	ASN
1	A	230	ASN
1	A	277	GLN
1	A	303	ASN
1	A	309	GLN
1	A	312	ASN
1	A	343	GLN
1	A	372	HIS
1	A	448	GLN
1	A	466	HIS
1	B	22	GLN
1	B	92	HIS
1	B	243	GLN
1	B	279	ASN
1	B	285	ASN
1	B	312	ASN
1	B	372	HIS
1	B	498	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	IMP	A	1331	1	25,25,25	1.33	4 (16%)	35,38,38	4.25	7 (20%)
4	MOA	A	1332	-	24,24,24	1.01	0	34,34,34	1.81	7 (20%)
3	IMP	B	1332	-	25,25,25	1.26	3 (12%)	35,38,38	5.14	5 (14%)
4	MOA	B	1333	-	24,24,24	1.31	2 (8%)	34,34,34	1.68	5 (14%)

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
3	IMP	A	1331	1	-	0/10/26/26	0/1/3/3
4	MOA	A	1332	-	-	0/12/21/21	0/0/2/2
3	IMP	B	1332	-	-	0/10/26/26	0/1/3/3
4	MOA	B	1333	-	-	0/12/21/21	0/0/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	IMP	C5-C4	3.69	1.48	1.40
4	B	1333	MOA	O2-C10	3.13	1.49	1.45
3	A	1331	IMP	C2-N1	3.07	1.43	1.35
3	A	1331	IMP	C5-C4	2.82	1.46	1.40
4	B	1333	MOA	C16-C1	2.76	1.52	1.47
3	A	1331	IMP	C4-N9	-2.50	1.34	1.37
3	B	1332	IMP	P-O5'	-2.44	1.51	1.60
3	B	1332	IMP	C2-N1	2.11	1.40	1.35
3	A	1331	IMP	P-O5'	-2.08	1.52	1.60

All (24) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1331	IMP	O4'-C1'-N9	21.96	128.86	108.44
3	B	1332	IMP	C6-C5-N7	-20.73	131.35	134.14
3	B	1332	IMP	O4'-C1'-N9	20.63	127.63	108.44
3	A	1331	IMP	C6-C5-N7	-9.48	132.86	134.14
4	A	1332	MOA	C10-O2-C1	5.66	114.64	110.56
4	B	1333	MOA	C10-O2-C1	5.31	114.39	110.56
3	B	1332	IMP	N3-C4-N9	4.57	133.68	125.43
4	B	1333	MOA	O2-C1-C16	-3.85	104.99	108.36
4	B	1333	MOA	C17-C2-C3	-3.65	121.44	127.45
4	A	1332	MOA	O2-C1-C16	-3.47	105.32	108.36
4	A	1332	MOA	C17-C2-C3	-3.03	122.45	127.45
4	A	1332	MOA	O2-C1-O1	2.91	124.07	121.07
4	A	1332	MOA	C9-C3-C4	2.89	119.78	115.39
3	A	1331	IMP	N3-C4-N9	2.81	130.51	125.43
3	A	1331	IMP	O2'-C2'-C1'	-2.71	103.02	111.23
4	A	1332	MOA	O2-C10-C11	-2.66	101.85	104.71
4	B	1333	MOA	O2-C1-O1	2.65	123.79	121.07
4	B	1333	MOA	C16-C15-C14	-2.41	116.94	121.55
3	B	1332	IMP	N1-C2-N3	-2.30	120.33	125.75
3	A	1331	IMP	C3'-C2'-C1'	-2.27	97.36	100.91
4	A	1332	MOA	C4-C3-C2	-2.14	116.97	121.08
3	B	1332	IMP	C2-N1-C6	2.12	127.46	120.06
3	A	1331	IMP	O5'-P-O1P	2.10	112.86	106.71
3	A	1331	IMP	N1-C2-N3	-2.03	120.98	125.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.