



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:18 PM 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 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

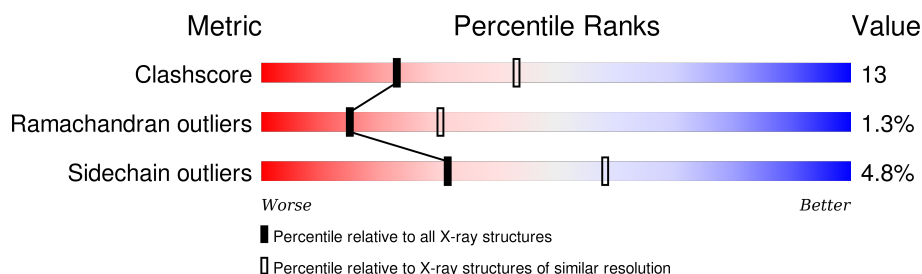
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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. 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.

Note EDS was not executed.

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

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6296 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.

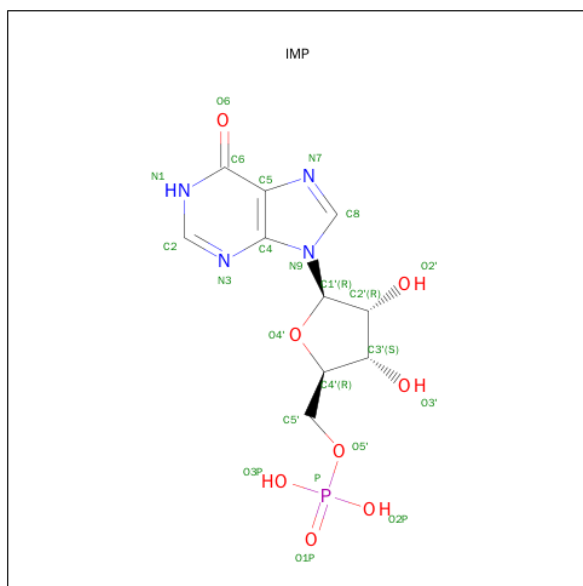
- Molecule 1 is a protein called Inosine-5'-Monophosphate Dehydrogenase 2.

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).

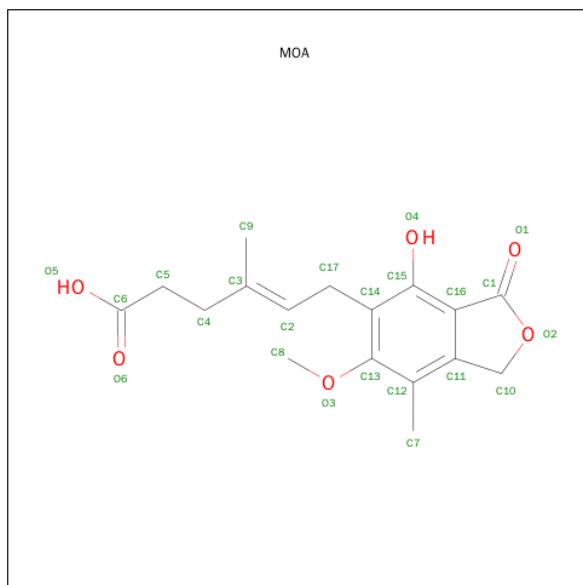
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- 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:  $C_{17}H_{20}O_6$ ).



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		



A440	S444	Y447	Q448	S452	R455	P456	Y457	P458	Y459	L460	I461	I464	Q465	C468	Q469	A473	P483	R493	T494	S495	Y499	G502	V503	H504	L513	F514
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 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, $\alpha$ , $\beta$ , $\gamma$	110.60 Å   110.60 Å   111.00 Å 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 [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	0.37	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 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	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
4	A	23	0	19	0	0
4	B	23	0	19	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	122	0	0	1	0
5	B	80	0	0	3	0
All	All	6296	0	6087	164	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 13.

All (164) 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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:O	1:A:224:ARG:NH1	2.44	0.50
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	10	19
1	B	362/514 (70%)	338 (93%)	22 (6%)	2 (1%)	30	56
All	All	784/1028 (76%)	724 (92%)	50 (6%)	10 (1%)	15	30

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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%)	34	62
1	B	292/420 (70%)	277 (95%)	15 (5%)	29	55
All	All	625/840 (74%)	595 (95%)	30 (5%)	31	58

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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 molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	20,25,25	1.63	4 (20%)	22,38,38	3.56	4 (18%)
4	MOA	A	1332	-	21,24,24	1.04	1 (4%)	30,34,34	1.94	8 (26%)
3	IMP	B	1332	-	20,25,25	1.59	5 (25%)	22,38,38	3.60	3 (13%)
4	MOA	B	1333	-	21,24,24	1.40	3 (14%)	30,34,34	1.81	6 (20%)

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	-	0/6/26/26	0/3/3/3
4	MOA	A	1332	-	-	0/10/21/21	0/2/2/2
3	IMP	B	1332	-	-	0/6/26/26	0/3/3/3
4	MOA	B	1333	-	-	0/10/21/21	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	IMP	P-O5'	-2.57	1.51	1.60
3	A	1331	IMP	P-O5'	-2.20	1.52	1.60
4	A	1332	MOA	O2-C1	-2.05	1.34	1.36
3	A	1331	IMP	P-O3P	-2.02	1.47	1.54
3	B	1332	IMP	C4-N3	2.01	1.38	1.35
4	B	1333	MOA	C15-C14	2.03	1.43	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	IMP	C6-N1	2.37	1.37	1.33
3	A	1331	IMP	C5-C4	2.82	1.46	1.40
4	B	1333	MOA	C16-C1	2.88	1.52	1.47
4	B	1333	MOA	O2-C10	3.24	1.49	1.45
3	B	1332	IMP	C5-C4	3.69	1.48	1.40
3	B	1332	IMP	C2-N1	3.70	1.40	1.33
3	A	1331	IMP	C2-N1	5.00	1.43	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1332	IMP	N3-C2-N1	-11.18	120.33	128.89
3	A	1331	IMP	N3-C2-N1	-10.34	120.98	128.89
4	B	1333	MOA	O2-C1-C16	-3.88	104.99	108.31
4	A	1332	MOA	O2-C1-C16	-3.48	105.32	108.31
4	B	1333	MOA	C17-C2-C3	-3.32	121.44	127.29
4	A	1332	MOA	C17-C2-C3	-2.74	122.45	127.29
4	A	1332	MOA	O2-C10-C11	-2.72	101.85	104.69
4	B	1333	MOA	C16-C15-C14	-2.44	116.94	121.59
4	A	1332	MOA	C4-C3-C2	-2.15	116.97	121.05
3	A	1331	IMP	O5'-P-O1P	2.25	112.86	107.14
4	A	1332	MOA	C15-C14-C13	2.57	121.36	117.90
4	B	1333	MOA	C15-C14-C13	2.58	121.38	117.90
4	B	1333	MOA	O2-C1-O1	2.75	123.79	121.05
4	A	1332	MOA	C9-C3-C4	2.87	119.78	115.41
4	A	1332	MOA	O2-C1-O1	3.03	124.07	121.05
4	B	1333	MOA	C10-O2-C1	5.60	114.39	110.59
4	A	1332	MOA	C10-O2-C1	5.97	114.64	110.59
3	A	1331	IMP	C2-N1-C6	6.87	126.45	116.04
3	B	1332	IMP	C2-N1-C6	7.54	127.46	116.04
3	B	1332	IMP	O4'-C1'-N9	9.33	127.63	108.10
3	A	1331	IMP	O4'-C1'-N9	9.92	128.86	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1332	IMP	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.