



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 1ZFJ / pdb_00001zfq
Title : INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH; EC 1.1.1.205) FROM STREPTOCOCCUS PYOGENES
Authors : Zhang, R.; Evans, G.; Rotella, F.J.; Westbrook, E.M.; Beno, D.; Huberman, E.; Joachimiak, A.; Collart, F.R.
Deposited on : 1999-03-29
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

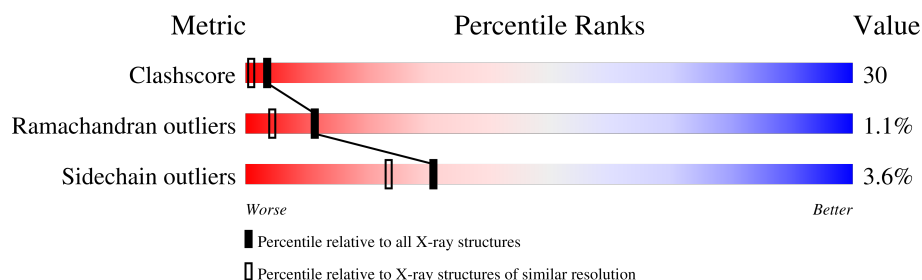
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4066 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.

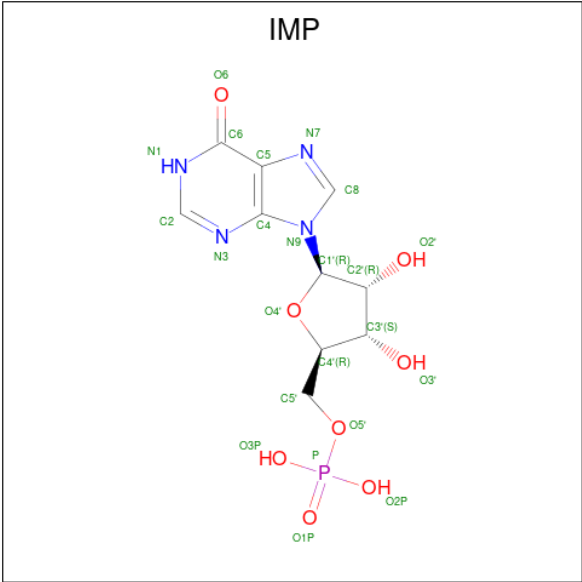
- Molecule 1 is a protein called INOSINE MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	477	3544	2230	615	685	1	13	0	0	1

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	TYR	PHE	conflict	UNP P0C0H6
A	53	MSE	MET	modified residue	UNP P0C0H6
A	61	MSE	MET	modified residue	UNP P0C0H6
A	78	MSE	MET	modified residue	UNP P0C0H6
A	117	MSE	MET	modified residue	UNP P0C0H6
A	145	MSE	MET	modified residue	UNP P0C0H6
A	159	MSE	MET	modified residue	UNP P0C0H6
A	364	MSE	MET	modified residue	UNP P0C0H6
A	368	MSE	MET	modified residue	UNP P0C0H6
A	393	MSE	MET	modified residue	UNP P0C0H6
A	399	MSE	MET	modified residue	UNP P0C0H6
A	440	MSE	MET	modified residue	UNP P0C0H6
A	448	MSE	MET	modified residue	UNP P0C0H6
A	468	MSE	MET	modified residue	UNP P0C0H6

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is water.

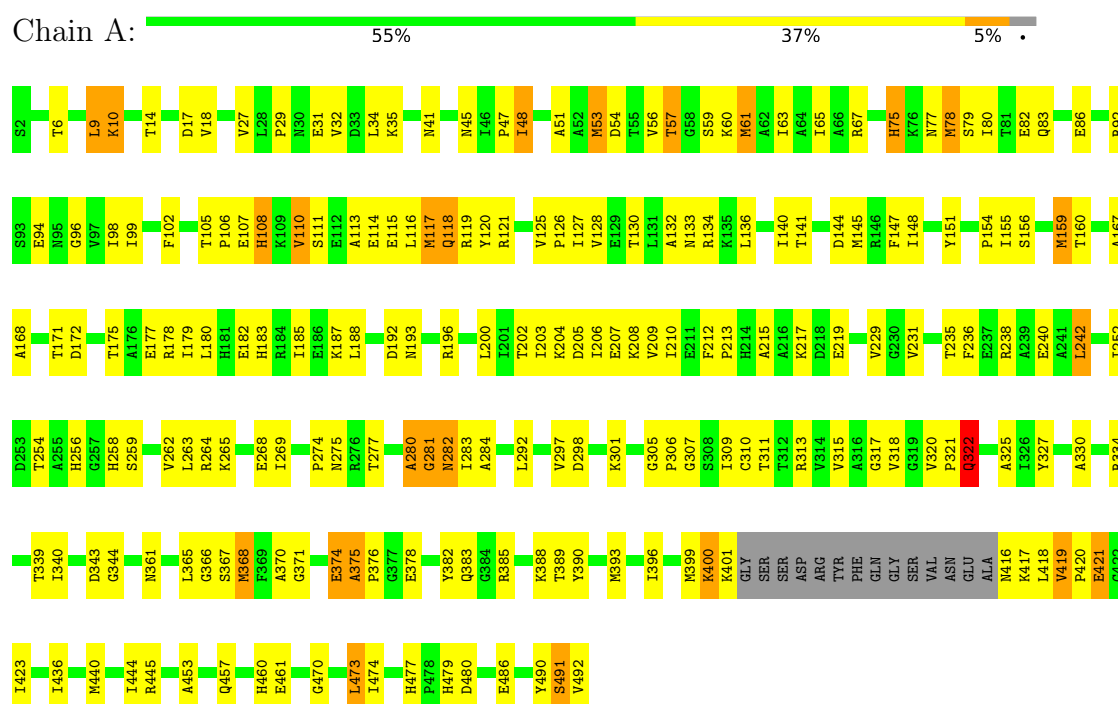
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	499	Total	O	0	0
			499	499		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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 MONOPHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.48Å 151.48Å 101.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	88.2 (6.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4066	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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

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	0.62	7/3587 (0.2%)	1.01	20/4840 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	MSE	SE-CE	-7.94	1.71	1.95
1	A	53	MSE	SE-CE	-7.13	1.74	1.95
1	A	61	MSE	SE-CE	-6.59	1.75	1.95
1	A	159	MSE	SE-CE	-6.01	1.77	1.95
1	A	491	SER	C-N	-5.50	1.25	1.33
1	A	78	MSE	SE-CE	-5.47	1.79	1.95
1	A	117	MSE	SE-CE	-5.24	1.79	1.95

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	MSE	N-CA-C	10.95	122.69	108.34
1	A	344	GLY	N-CA-C	8.67	122.00	112.29
1	A	322	GLN	N-CA-C	7.67	120.61	111.33
1	A	461	GLU	N-CA-C	6.79	118.76	111.36
1	A	57	THR	N-CA-C	6.77	121.31	107.69
1	A	339	THR	N-CA-C	6.72	120.02	110.14
1	A	419	VAL	CA-C-N	6.17	126.08	119.85
1	A	419	VAL	C-N-CA	6.17	126.08	119.85
1	A	280	ALA	N-CA-C	5.99	118.96	109.50
1	A	48	ILE	N-CA-C	5.47	115.76	108.11
1	A	370	ALA	N-CA-C	5.40	122.31	110.80
1	A	86	GLU	N-CA-C	-5.38	105.41	111.28
1	A	375	ALA	CA-C-N	5.32	125.03	119.82
1	A	375	ALA	C-N-CA	5.32	125.03	119.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	GLU	N-CA-C	5.16	117.80	111.82
1	A	9	LEU	N-CA-C	5.11	116.71	111.03
1	A	343	ASP	N-CA-C	5.08	116.98	107.99
1	A	18	VAL	N-CA-C	5.07	117.31	108.95
1	A	282	ASN	N-CA-C	5.06	118.06	109.76
1	A	421	GLU	N-CA-C	-5.01	105.88	112.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3544	0	3530	210	0
2	A	23	0	11	1	0
3	A	499	0	0	22	1
All	All	4066	0	3541	210	1

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 30.

All (210) 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:127:ILE:HG13	1:A:159:MSE:HE1	1.26	1.10
1:A:51:ALA:HB3	1:A:53:MSE:HE2	1.49	0.95
1:A:365:LEU:HD22	1:A:368:MSE:HE2	1.51	0.91
1:A:105:THR:H	1:A:108:HIS:HD2	1.14	0.91
1:A:168:ALA:O	1:A:171:THR:HG23	1.73	0.88
1:A:54:ASP:HA	1:A:75:HIS:CD2	2.11	0.85
1:A:396:ILE:HD11	1:A:420:PRO:HD3	1.58	0.84
1:A:340:ILE:H	1:A:361:ASN:HD22	1.20	0.84
1:A:53:MSE:O	1:A:75:HIS:HD2	1.61	0.83
1:A:172:ASP:OD2	1:A:175:THR:HG22	1.79	0.83
1:A:284:ALA:HB1	1:A:320:VAL:CG1	2.09	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:MSE:HB3	3:A:501:HOH:O	1.81	0.80
1:A:365:LEU:HD13	1:A:368:MSE:HE3	1.65	0.79
1:A:53:MSE:HE3	1:A:56:VAL:HG21	1.66	0.77
1:A:322:GLN:HE21	1:A:322:GLN:HA	1.50	0.76
1:A:127:ILE:HG13	1:A:159:MSE:CE	2.12	0.76
1:A:134:ARG:HD3	1:A:196:ARG:HH12	1.51	0.74
1:A:77:ASN:HD22	1:A:393:MSE:HE1	1.52	0.74
1:A:396:ILE:HD12	1:A:418:LEU:H	1.53	0.74
1:A:118:GLN:HE21	1:A:118:GLN:N	1.85	0.73
1:A:127:ILE:CG1	1:A:159:MSE:HE1	2.12	0.73
1:A:203:ILE:HG23	1:A:204:LYS:HD2	1.72	0.71
1:A:130:THR:HG22	1:A:132:ALA:H	1.54	0.71
1:A:457:GLN:HG3	3:A:1195:HOH:O	1.91	0.70
1:A:453:ALA:HB2	3:A:990:HOH:O	1.91	0.69
1:A:178:ARG:HD2	3:A:1054:HOH:O	1.90	0.69
1:A:60:LYS:HE3	1:A:374:GLU:HA	1.74	0.69
1:A:396:ILE:HD12	1:A:417:LYS:HA	1.75	0.69
1:A:436:ILE:HG22	1:A:440:MSE:HE3	1.73	0.69
1:A:440:MSE:HE2	3:A:501:HOH:O	1.92	0.69
1:A:236:PHE:O	1:A:240:GLU:HG2	1.92	0.68
1:A:275:ASN:OD1	3:A:641:HOH:O	2.10	0.68
1:A:53:MSE:HE3	1:A:56:VAL:CG2	2.23	0.68
1:A:254:THR:HG21	1:A:262:VAL:HG21	1.74	0.68
1:A:144:ASP:O	1:A:148:ILE:HG13	1.94	0.67
1:A:280:ALA:O	1:A:281:GLY:O	2.12	0.67
1:A:256:HIS:HD2	3:A:522:HOH:O	1.79	0.66
1:A:53:MSE:HE1	1:A:366:GLY:HA3	1.77	0.65
1:A:383:GLN:HB3	1:A:385:ARG:HH11	1.61	0.65
1:A:311:THR:O	1:A:315:VAL:HG22	1.96	0.65
1:A:105:THR:H	1:A:108:HIS:CD2	2.06	0.65
1:A:365:LEU:HD22	1:A:368:MSE:CE	2.23	0.65
1:A:53:MSE:CE	1:A:56:VAL:HG21	2.27	0.64
1:A:51:ALA:CB	1:A:53:MSE:HE2	2.26	0.64
1:A:155:ILE:O	1:A:159:MSE:HG2	1.97	0.64
1:A:167:ALA:HB1	1:A:171:THR:HG21	1.79	0.63
1:A:229:VAL:HG12	1:A:238:ARG:HD3	1.80	0.63
1:A:83:GLN:HE22	1:A:238:ARG:HE	1.45	0.63
1:A:284:ALA:HB1	1:A:320:VAL:HG12	1.80	0.63
1:A:320:VAL:HG13	1:A:325:ALA:HB2	1.80	0.63
1:A:383:GLN:HB3	1:A:385:ARG:NH1	2.13	0.63
1:A:215:ALA:HB3	1:A:217:LYS:HE3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MSE:O	1:A:238:ARG:NH2	2.33	0.62
1:A:94:GLU:HG2	1:A:208:LYS:HD3	1.82	0.61
1:A:79:SER:OG	1:A:82:GLU:HG3	2.00	0.60
1:A:110:VAL:HG13	1:A:151:TYR:HA	1.83	0.60
1:A:118:GLN:N	1:A:118:GLN:NE2	2.48	0.60
1:A:110:VAL:CG1	1:A:151:TYR:HA	2.31	0.60
1:A:117:MSE:CE	1:A:140:ILE:HG23	2.31	0.60
1:A:77:ASN:HB2	1:A:393:MSE:HE1	1.84	0.60
1:A:113:ALA:O	1:A:116:LEU:HD12	2.01	0.60
1:A:202:THR:HG22	1:A:203:ILE:N	2.17	0.60
1:A:27:VAL:HG23	1:A:31:GLU:HG3	1.82	0.59
1:A:111:SER:O	1:A:115:GLU:HG3	2.02	0.59
1:A:203:ILE:O	1:A:207:GLU:HG3	2.03	0.59
1:A:264:ARG:O	1:A:268:GLU:HG3	2.00	0.59
1:A:330:ALA:O	1:A:334:ARG:HG2	2.03	0.59
1:A:119:ARG:HD2	1:A:120:TYR:CE1	2.38	0.58
1:A:53:MSE:C	1:A:75:HIS:HD2	2.11	0.58
1:A:322:GLN:HE21	1:A:322:GLN:CA	2.17	0.58
1:A:365:LEU:HD13	1:A:368:MSE:CE	2.34	0.58
1:A:284:ALA:HB1	1:A:320:VAL:HG11	1.84	0.57
1:A:179:ILE:O	1:A:183:HIS:HD2	1.87	0.57
1:A:292:LEU:O	1:A:297:VAL:HG12	2.04	0.57
1:A:265:LYS:O	1:A:269:ILE:HG13	2.05	0.56
1:A:282:ASN:OD1	1:A:301:LYS:HG3	2.05	0.56
1:A:252:ILE:O	1:A:281:GLY:N	2.38	0.56
1:A:140:ILE:HD12	1:A:155:ILE:HG13	1.87	0.56
1:A:6:THR:HG22	1:A:6:THR:O	2.07	0.55
1:A:113:ALA:O	1:A:117:MSE:HG3	2.05	0.55
1:A:125:VAL:HB	1:A:140:ILE:HG22	1.89	0.55
1:A:423:ILE:C	1:A:423:ILE:HD12	2.31	0.55
1:A:77:ASN:HD22	1:A:393:MSE:CE	2.20	0.55
1:A:479:HIS:HD2	1:A:480:ASP:OD2	1.89	0.55
1:A:486:GLU:OE2	1:A:492:VAL:N	2.41	0.54
1:A:14:THR:HG22	1:A:17:ASP:OD2	2.07	0.54
1:A:32:VAL:CG2	1:A:445:ARG:HG2	2.37	0.54
1:A:283:ILE:C	1:A:283:ILE:HD12	2.33	0.54
1:A:313:ARG:O	1:A:317:GLY:HA2	2.07	0.54
1:A:203:ILE:CG2	1:A:204:LYS:HD2	2.37	0.54
1:A:231:VAL:O	1:A:231:VAL:HG23	2.08	0.54
1:A:396:ILE:HD12	1:A:418:LEU:N	2.23	0.54
1:A:155:ILE:HG12	1:A:159:MSE:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HD2	1:A:204:LYS:N	2.23	0.53
1:A:117:MSE:HE3	1:A:140:ILE:HG23	1.89	0.53
1:A:419:VAL:HG12	1:A:419:VAL:O	2.09	0.53
1:A:127:ILE:HG21	1:A:159:MSE:HE3	1.91	0.53
1:A:83:GLN:NE2	1:A:238:ARG:HE	2.07	0.53
1:A:305:GLY:HA2	1:A:310:CYS:SG	2.49	0.53
1:A:393:MSE:HE3	3:A:753:HOH:O	2.09	0.52
1:A:180:LEU:HD23	1:A:185:ILE:HG13	1.92	0.52
1:A:205:ASP:O	1:A:209:VAL:HG23	2.08	0.52
1:A:280:ALA:O	1:A:301:LYS:HG2	2.09	0.52
1:A:383:GLN:CB	1:A:385:ARG:HH11	2.22	0.52
1:A:440:MSE:O	1:A:444:ILE:HG13	2.10	0.52
1:A:396:ILE:CD1	1:A:418:LEU:H	2.22	0.51
1:A:202:THR:HG22	1:A:204:LYS:H	1.73	0.51
1:A:94:GLU:HG2	1:A:208:LYS:CD	2.40	0.51
1:A:53:MSE:O	1:A:75:HIS:CD2	2.53	0.51
1:A:292:LEU:C	1:A:297:VAL:HG12	2.36	0.50
1:A:134:ARG:HD3	1:A:196:ARG:NH1	2.23	0.50
1:A:80:ILE:HG12	1:A:238:ARG:HG3	1.93	0.50
1:A:258:HIS:HD2	3:A:685:HOH:O	1.94	0.50
1:A:305:GLY:N	1:A:306:PRO:HD2	2.25	0.50
1:A:110:VAL:HG23	1:A:145:MSE:SE	2.62	0.50
1:A:117:MSE:HB2	1:A:118:GLN:HE22	1.76	0.50
1:A:154:PRO:C	1:A:156:SER:H	2.19	0.50
1:A:147:PHE:C	1:A:147:PHE:CD1	2.89	0.50
1:A:53:MSE:HE1	1:A:366:GLY:CA	2.42	0.49
1:A:27:VAL:CG2	1:A:31:GLU:HG3	2.43	0.49
1:A:77:ASN:ND2	1:A:393:MSE:HE1	2.23	0.49
1:A:29:PRO:O	1:A:32:VAL:HG22	2.12	0.48
1:A:327:TYR:C	1:A:327:TYR:CD1	2.91	0.48
1:A:473:LEU:CD1	3:A:1280:HOH:O	2.62	0.48
1:A:371:GLY:HA2	1:A:388:LYS:HG3	1.95	0.47
1:A:57:THR:O	1:A:75:HIS:NE2	2.47	0.47
1:A:177:GLU:HB2	1:A:206:ILE:HD13	1.97	0.47
1:A:61:MSE:O	1:A:65:ILE:HG22	2.14	0.47
1:A:141:THR:O	1:A:144:ASP:HB2	2.15	0.47
1:A:182:GLU:HG3	3:A:794:HOH:O	2.13	0.47
1:A:202:THR:CG2	1:A:203:ILE:N	2.78	0.47
1:A:460:HIS:HD2	3:A:1051:HOH:O	1.98	0.47
1:A:59:SER:O	1:A:63:ILE:HG13	2.14	0.47
1:A:204:LYS:HD2	1:A:204:LYS:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:TYR:CD1	1:A:383:GLN:HG2	2.50	0.47
1:A:480:ASP:HB2	3:A:921:HOH:O	2.14	0.47
1:A:110:VAL:HG13	1:A:151:TYR:O	2.14	0.46
1:A:374:GLU:H	1:A:374:GLU:CD	2.23	0.46
1:A:110:VAL:HG13	1:A:151:TYR:CA	2.44	0.46
1:A:382:TYR:CE1	1:A:383:GLN:HG2	2.50	0.46
1:A:48:ILE:HD13	1:A:440:MSE:SE	2.64	0.46
1:A:238:ARG:O	1:A:242:LEU:HD13	2.16	0.46
1:A:53:MSE:HE1	1:A:390:TYR:OH	2.16	0.46
1:A:180:LEU:HD21	1:A:188:LEU:HB2	1.98	0.46
1:A:6:THR:HG21	3:A:1110:HOH:O	2.16	0.46
1:A:473:LEU:HD12	3:A:1280:HOH:O	2.15	0.46
1:A:374:GLU:CD	1:A:374:GLU:N	2.74	0.46
1:A:396:ILE:HD12	1:A:417:LYS:CA	2.45	0.45
1:A:470:GLY:O	1:A:474:ILE:HG12	2.15	0.45
1:A:57:THR:O	1:A:75:HIS:CD2	2.69	0.45
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.80	0.45
1:A:307:GLY:HA2	2:A:500:IMP:H5'2	1.99	0.45
1:A:92:ARG:HA	1:A:96:GLY:HA2	1.98	0.45
1:A:125:VAL:HB	1:A:140:ILE:CG2	2.47	0.45
1:A:140:ILE:HD11	1:A:145:MSE:SE	2.67	0.45
1:A:159:MSE:SE	1:A:160:THR:H	2.49	0.45
1:A:231:VAL:HG23	3:A:865:HOH:O	2.15	0.45
1:A:473:LEU:HD12	3:A:609:HOH:O	2.17	0.45
1:A:171:THR:CG2	3:A:605:HOH:O	2.65	0.44
1:A:53:MSE:CE	1:A:366:GLY:HA3	2.45	0.44
1:A:215:ALA:CB	1:A:217:LYS:HE3	2.47	0.44
1:A:259:SER:O	1:A:263:LEU:HG	2.18	0.44
1:A:311:THR:CG2	1:A:423:ILE:HG23	2.47	0.44
1:A:154:PRO:C	1:A:156:SER:N	2.73	0.44
1:A:284:ALA:CB	1:A:320:VAL:HG12	2.47	0.44
1:A:264:ARG:HD2	3:A:1053:HOH:O	2.17	0.44
1:A:399:MSE:O	1:A:400:LYS:O	2.35	0.44
1:A:61:MSE:HA	1:A:61:MSE:HE3	2.00	0.44
1:A:254:THR:HG21	1:A:262:VAL:CG2	2.46	0.44
1:A:102:PHE:O	1:A:126:PRO:HD2	2.18	0.43
1:A:140:ILE:HB	1:A:155:ILE:HD11	2.00	0.43
1:A:160:THR:HG22	1:A:160:THR:O	2.18	0.43
1:A:210:ILE:O	1:A:213:PRO:HD3	2.18	0.43
1:A:306:PRO:HD3	1:A:313:ARG:HH21	1.83	0.43
1:A:53:MSE:C	1:A:75:HIS:CD2	2.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HB	1:A:133:ASN:OD1	2.18	0.43
1:A:34:LEU:O	1:A:47:PRO:HD3	2.19	0.43
1:A:371:GLY:HA2	1:A:388:LYS:CB	2.48	0.43
1:A:9:LEU:HG	1:A:10:LYS:HG3	2.00	0.43
1:A:309:ILE:C	1:A:309:ILE:HD12	2.43	0.43
1:A:311:THR:OG1	1:A:421:GLU:C	2.62	0.42
1:A:375:ALA:HA	1:A:376:PRO:HD3	1.80	0.42
1:A:192:ASP:OD2	1:A:196:ARG:HB3	2.19	0.42
1:A:313:ARG:HG2	1:A:318:VAL:O	2.19	0.42
1:A:114:GLU:CB	1:A:145:MSE:HE2	2.50	0.42
1:A:367:SER:HA	1:A:390:TYR:CE1	2.54	0.42
1:A:117:MSE:HB2	1:A:118:GLN:NE2	2.35	0.42
1:A:106:PRO:HD3	1:A:128:VAL:O	2.19	0.42
1:A:400:LYS:O	1:A:401:LYS:O	2.38	0.42
1:A:67:ARG:HD3	1:A:212:PHE:CZ	2.54	0.42
1:A:378:GLU:O	1:A:389:THR:HG23	2.19	0.42
1:A:396:ILE:CG2	1:A:416:ASN:O	2.67	0.42
1:A:32:VAL:HG22	1:A:445:ARG:HH11	1.84	0.41
1:A:219:GLU:HG2	3:A:1032:HOH:O	2.19	0.41
1:A:140:ILE:HG21	1:A:155:ILE:HD11	2.01	0.41
1:A:35:LYS:HG2	1:A:45:ASN:HA	2.02	0.41
1:A:179:ILE:O	1:A:183:HIS:CD2	2.72	0.41
1:A:182:GLU:O	1:A:182:GLU:HG2	2.19	0.41
1:A:200:LEU:C	1:A:200:LEU:HD23	2.45	0.41
1:A:330:ALA:HA	1:A:340:ILE:HD12	2.02	0.41
1:A:477:HIS:ND1	1:A:490:TYR:OH	2.53	0.41
1:A:140:ILE:CG2	1:A:155:ILE:HD11	2.51	0.41
1:A:274:PRO:HB3	3:A:647:HOH:O	2.19	0.41
1:A:127:ILE:HG21	1:A:159:MSE:CE	2.50	0.41
1:A:258:HIS:HE1	3:A:618:HOH:O	2.03	0.41
1:A:98:ILE:HG23	1:A:99:ILE:HG23	2.01	0.40
1:A:235:THR:HG21	1:A:269:ILE:HD11	2.04	0.40
1:A:83:GLN:HE22	1:A:238:ARG:NE	2.15	0.40
1:A:277:THR:HA	1:A:298:ASP:OD2	2.21	0.40
1:A:105:THR:HA	1:A:128:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:866:HOH:O	3:A:866:HOH:O[6_565]	2.10	0.10

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	473/491 (96%)	447 (94%)	21 (4%)	5 (1%)	11 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	GLY
1	A	400	LYS
1	A	121	ARG
1	A	491	SER
1	A	108	HIS

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	363/371 (98%)	350 (96%)	13 (4%)	31 23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	41	ASN
1	A	75	HIS
1	A	107	GLU
1	A	110	VAL
1	A	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	136	LEU
1	A	187	LYS
1	A	193	ASN
1	A	242	LEU
1	A	321	PRO
1	A	322	GLN
1	A	473	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	75	HIS
1	A	77	ASN
1	A	83	GLN
1	A	95	ASN
1	A	108	HIS
1	A	118	GLN
1	A	142	ASN
1	A	152	ASN
1	A	183	HIS
1	A	256	HIS
1	A	258	HIS
1	A	322	GLN
1	A	361	ASN
1	A	460	HIS
1	A	462	ASN
1	A	479	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	IMP	A	500	-	25,25,25	1.61	3 (12%)	37,38,38	1.65	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	A	500	-	-	0/10/26/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	IMP	C8-N7	4.63	1.45	1.32
2	A	500	IMP	C2-N1	3.82	1.42	1.35
2	A	500	IMP	C1'-N9	2.30	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	IMP	N1-C2-N3	-4.37	120.46	125.50
2	A	500	IMP	N9-C8-N7	-2.98	107.87	113.40
2	A	500	IMP	O4'-C1'-N9	2.93	115.00	108.36
2	A	500	IMP	C2-N3-C4	2.92	116.66	111.53
2	A	500	IMP	O3'-C3'-C2'	-2.41	104.09	111.82
2	A	500	IMP	C1'-N9-C4	-2.35	119.55	126.49
2	A	500	IMP	O5'-P-O1P	2.02	111.91	106.44
2	A	500	IMP	O3'-C3'-C4'	2.01	116.85	111.08

There are no chirality outliers.

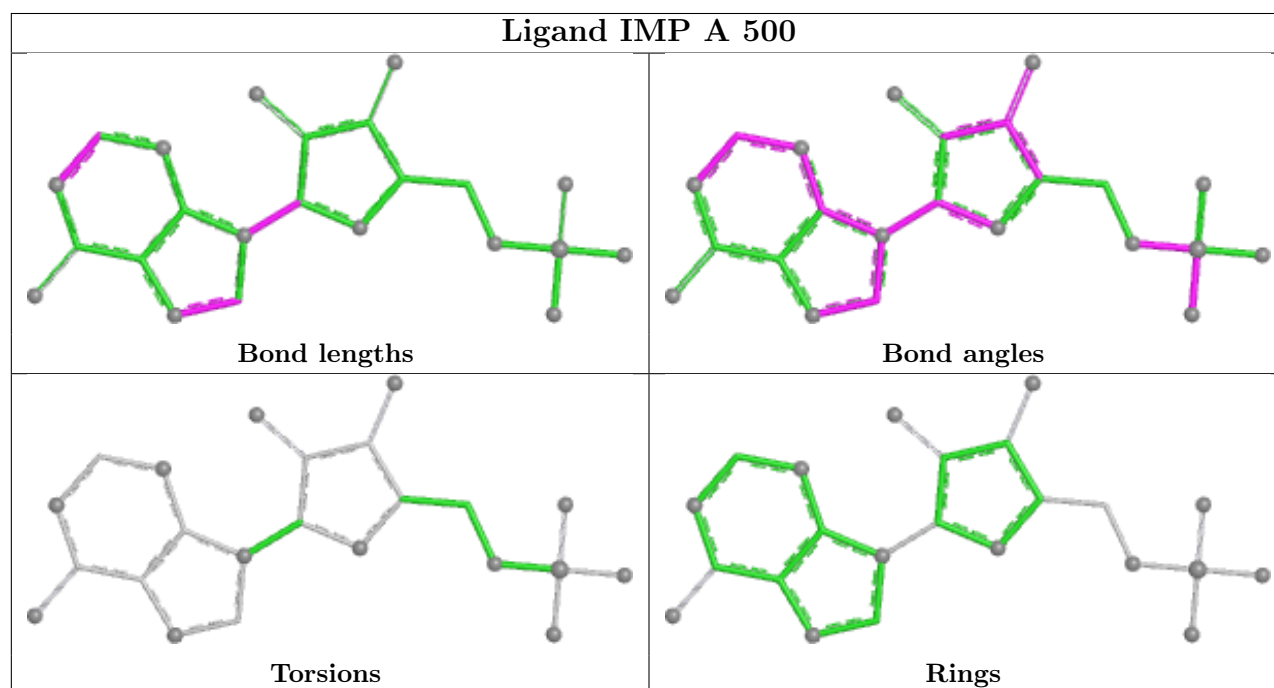
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.