



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:07 AM UTC

PDB ID : 4AF0 / pdb_00004af0
Title : Crystal structure of cryptococcal inosine monophosphate dehydrogenase
Authors : Valkov, E.; Stamp, A.; Morrow, C.A.; Kobe, B.; Fraser, J.A.
Deposited on : 2012-01-15
Resolution : 2.20 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

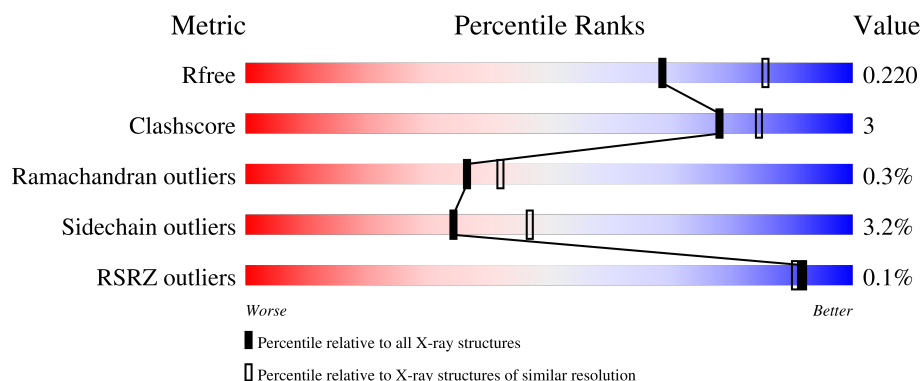
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	556	 63% 8% 29%
2	B	556	 63% 8% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6526 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			
1	A	395	2955	1853	519	568	15	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP E3P6S0
A	-10	ARG	-	expression tag	UNP E3P6S0
A	-9	GLY	-	expression tag	UNP E3P6S0
A	-8	SER	-	expression tag	UNP E3P6S0
A	-7	HIS	-	expression tag	UNP E3P6S0
A	-6	HIS	-	expression tag	UNP E3P6S0
A	-5	HIS	-	expression tag	UNP E3P6S0
A	-4	HIS	-	expression tag	UNP E3P6S0
A	-3	HIS	-	expression tag	UNP E3P6S0
A	-2	HIS	-	expression tag	UNP E3P6S0
A	-1	GLY	-	expression tag	UNP E3P6S0
A	0	SER	-	expression tag	UNP E3P6S0
A	501	ALA	GLY	conflict	UNP E3P6S0

- Molecule 2 is a protein called INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	395	2954	1852	519	568	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

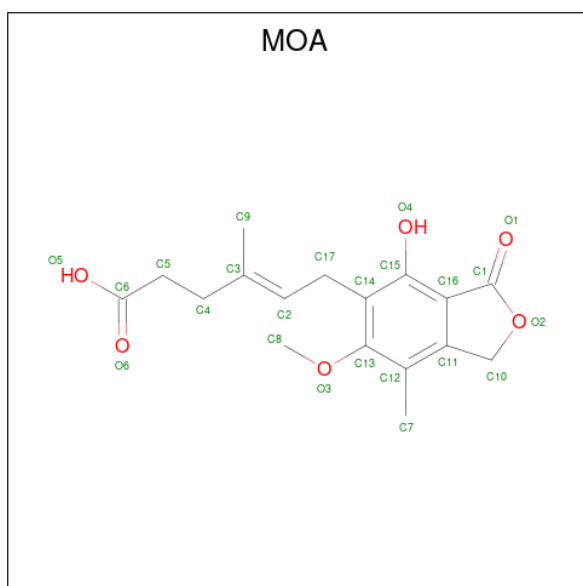
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP E3P6S0
B	-10	ARG	-	expression tag	UNP E3P6S0
B	-9	GLY	-	expression tag	UNP E3P6S0

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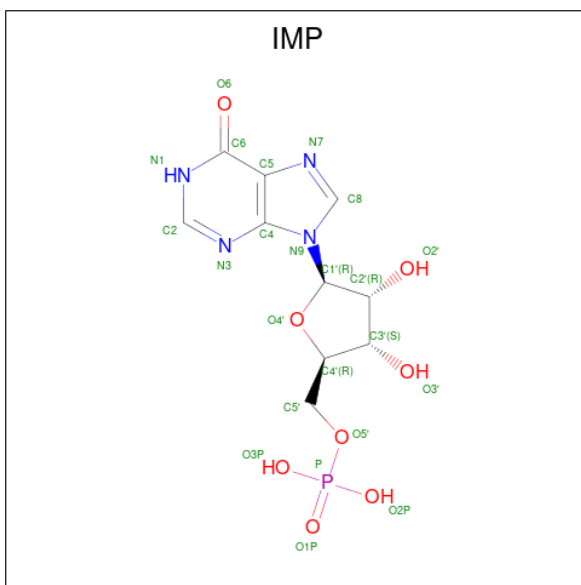
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP E3P6S0
B	-7	HIS	-	expression tag	UNP E3P6S0
B	-6	HIS	-	expression tag	UNP E3P6S0
B	-5	HIS	-	expression tag	UNP E3P6S0
B	-4	HIS	-	expression tag	UNP E3P6S0
B	-3	HIS	-	expression tag	UNP E3P6S0
B	-2	HIS	-	expression tag	UNP E3P6S0
B	-1	GLY	-	expression tag	UNP E3P6S0
B	0	SER	-	expression tag	UNP E3P6S0

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



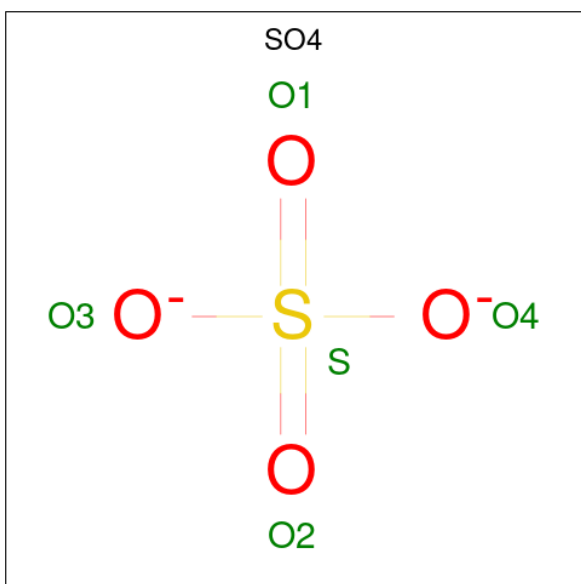
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	17	6		
3	B	1	Total	C	O	0	0
			23	17	6		

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	254	Total 254	O 254	0	0
6	B	261	Total 261	O 261	0	0

• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

LEU	ASN	E436	LYS	ALA	LEU	MET
	SER	H436		ASN	ILE	ARG
	TYR	T437		SER	LYS	GLY
	THR	GLN		LEU	ALA	HIS
	LYS	ARG		LEU	LYS	HIS
	ARG	GLY		ARG	PHE	HIS
	LEU	SER		GLU	PHE	HIS
	LEU	ALA		THR	CYS	HIS
	PHE	SER		LYS	GLY	GLY
	ALA	LYS		GLY	VAL	SER
LEU	ARG	LYS	LYS	PRO	MET	
	SER	ILE	PRO	THR	PRO	
	ILE	LEU	ILE	GLU	GLU	
	LEU	G450	VAL	THR	T4	
	LEU	L451	ASP	GLY	L36	
	LEU	A454	SER	GLU	L36	
	LEU	A455	ASN	PRO	R43	
	LEU	F460	HIS	ASP	L54	
	LEU	S461	LEU	LYS	H59	
	LEU	E462	VAL	LEU	L69	
LEU	LEU	A463	VAL	ILE	F83	
	LEU	D464	ALA	VAL	L84	
	LEU	K467	ARG	THR	L84	
	LEU	V476	SER	GLY	P87	
	LEU	L482	ASP	ARG	M88	
	LEU	N483	LEU	VAL	D89	
	LEU	K484	LYS	GLN	T92	
	LEU	F486	ASN	PHE	T92	
	LEU	G492	GLN	ASP	L106	
	LEU	L493	GLY	ALA	G107	
LEU	LEU	A500	THR	THR	I108	
	LEU	A501	PRO	PRO	E129	
	LEU	T502	ILE	ILE	ASN	
	LEU	K503	VAL	LYS	GLY	
	LEU	A512	VAL	VAL	PHE	
	LEU	R522	THR	THR	ILE	
	LEU	S525	THR	THR	THR	
	LEU	GLN	GLY	GLY	ASP	
	LEU	LEU	SER	SER	PRO	
	LEU	GLU	SER	SER	LEU	
LEU	GLY	L393	PRO	PRO	CYS	
	VAL	L403	THR	THR	GLY	
	HIS	H417	LEU	LEU	THR	
	GLY		GLU	GLU	VAL	
	ASN		ASN	ASN	ASN	
	THR		THR	THR	THR	
	LYS		LYS	LYS	LYS	
	ARG		ARG	ARG	ARG	
	LEU		LEU	LEU	LEU	
	ALA		ALA	ALA	ALA	

- Molecule 2: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

LEU	G427	SER	LYS	MET
ASN	M428	LEU	ALA	ARG
SER		LEU	LYS	GLY
TYR	I431	ARG	PHE	HIS
THR		GLU	PHE	HIS
LYS	I437	THR	CYS	HIS
ARG	GLN	LYS	GLY	HIS
LEU	ARG	LYS	VAL	HIS
PHE	GLY	LYS	PRO	HIS
ALA	SER	LEU	ILE	GLY
	ALA	PRO	THR	SER
	GLY	ILE	GLU	MET
	LYS	VAL	GLY	PRO
	ARG	ASP	GLU	GLU
	ILE	ASN	PRO	T4
	LEU	GLY	ASP	S35
	G450	HIS	SER	L36
	L451	LEU	LYS	
	L452	VAL	LEU	R43
	N453	SER	LEU	
		LEU	GLY	L54
	T456	VAL	ILE	
	A457	ALA	VAL	F83
	R458	ARG	THR	L84
	Y459	SER	GLY	
	F460	ASP	ARG	P87
	S461	LEU	ASP	M88
	E462	LEU	VAL	D89
	A463	LYS	GLN	
	D464	ASN	GLN	T92
	A465		ALA	L106
	V466	G1245	ASP	G107
	K467		GLU	I108
		V286	THR	E129
	V472		PRO	ASN
	F485	I314	ILE	GLY
	V486	I337	SER	PHE
			VAL	ILE
	G492	G340	VAL	THR
	K503	I344	THR	ASP
		C345	GLU	PRO
	A512		VAL	CYS
	R522	O348	VAL	LEU
	T523	F349	THR	GLY
	A524	V350	GLY	PRO
	S525	M351	SER	ASP
			SER	ALA
	ALA	Q357	SER	THR
	GLN		PRO	VAL
	LEU	C375	ILE	GLY
	GLU		THR	ASP
	GLY	I384	LEU	VAL
	GLY		GLU	LEU
	VAL	L403	LYS	GLU
	HIS		ALA	TYR
	GLY	R406	ASN	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	149.63Å 149.63Å 122.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 2.20 47.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.44-2.20) 99.1 (47.44-2.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.173 , 0.208 0.185 , 0.220	Depositor DCC
R_{free} test set	3429 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.469 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6526	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, SO4, 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	0.86	0/3007	1.29	10/4066 (0.2%)
2	B	0.85	0/3006	1.32	15/4064 (0.4%)
All	All	0.86	0/6013	1.31	25/8130 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	PHE	CA-CB-CG	11.52	125.32	113.80
1	A	460	PHE	CA-CB-CG	7.73	121.53	113.80
1	A	92	THR	N-CA-C	7.41	121.00	108.02
2	B	92	THR	N-CA-C	7.38	120.94	108.02
2	B	463	ALA	N-CA-C	-7.29	106.31	114.62
2	B	83	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	83	PHE	CA-CB-CG	6.38	120.18	113.80
2	B	524	ALA	CA-C-N	5.84	132.21	121.70
2	B	524	ALA	C-N-CA	5.84	132.21	121.70
1	A	485	PHE	CA-C-N	5.81	123.90	120.24
1	A	485	PHE	C-N-CA	5.81	123.90	120.24
2	B	349	GLU	N-CA-C	-5.73	105.02	112.23
2	B	485	PHE	CA-C-N	5.72	123.84	120.24
2	B	485	PHE	C-N-CA	5.72	123.84	120.24
2	B	453	ASN	N-CA-C	5.62	117.09	110.97
2	B	357	GLN	N-CA-C	5.61	118.11	111.33
1	A	357	GLN	N-CA-C	5.45	117.92	111.33
2	B	459	TYR	N-CA-C	5.19	116.98	108.52
1	A	486	VAL	N-CA-CB	5.14	113.74	110.50
2	B	35	SER	N-CA-C	-5.13	103.62	110.55
2	B	486	VAL	N-CA-CB	5.11	113.72	110.50
1	A	484	LYS	CA-C-N	5.09	127.36	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	LYS	C-N-CA	5.09	127.36	120.44
1	A	89	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	89	ASP	CA-CB-CG	5.00	117.60	112.60

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	2955	0	2945	18	0
2	B	2954	0	2943	16	0
3	A	23	0	19	0	0
3	B	23	0	19	1	0
4	A	23	0	11	0	0
4	B	23	0	11	1	0
5	B	10	0	0	0	0
6	A	254	0	0	0	0
6	B	261	0	0	0	0
All	All	6526	0	5948	34	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 3.

All (34) 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:59:HIS:N	1:A:501:ALA:HB2	2.03	0.73
2:B:451:LEU:HD21	2:B:472:VAL:HG21	1.73	0.71
1:A:59:HIS:H	1:A:501:ALA:HB2	1.63	0.64
1:A:454:ALA:HB3	1:A:476:VAL:HG12	1.79	0.64
2:B:384:ILE:HD13	2:B:492:GLY:HA3	1.85	0.58
2:B:345:CYS:SG	4:B:1527:IMP:H2	2.44	0.57
1:A:384:ILE:HD13	1:A:492:GLY:HA3	1.85	0.57
2:B:340:GLY:HA2	2:B:345:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HG	1:A:522:ARG:HD2	1.88	0.55
1:A:464:ASP:HB3	1:A:467:LYS:HB2	1.90	0.54
2:B:54:LEU:HG	2:B:522:ARG:HD2	1.89	0.54
1:A:340:GLY:HA2	1:A:345:CYS:SG	2.48	0.53
2:B:428:MET:HB2	3:B:1526:MOA:H83	1.91	0.52
2:B:337:ILE:HD11	2:B:375:CYS:HB3	1.93	0.51
1:A:337:ILE:HD11	1:A:375:CYS:HB3	1.93	0.50
2:B:426:ARG:HH12	2:B:437:THR:HG23	1.77	0.50
1:A:347:THR:HG22	1:A:451:LEU:HG	1.94	0.50
2:B:337:ILE:CD1	2:B:375:CYS:HB3	2.42	0.49
1:A:337:ILE:CD1	1:A:375:CYS:HB3	2.43	0.49
2:B:464:ASP:HB3	2:B:467:LYS:HB2	1.94	0.48
1:A:84:LEU:HA	1:A:106:LEU:O	2.15	0.46
1:A:500:ALA:O	1:A:501:ALA:HB3	2.16	0.46
1:A:59:HIS:H	1:A:501:ALA:CB	2.28	0.46
2:B:84:LEU:HA	2:B:106:LEU:O	2.16	0.45
2:B:431:ILE:HG21	2:B:463:ALA:HB2	1.99	0.45
1:A:36:LEU:HD22	1:A:512:ALA:HB1	1.99	0.44
2:B:36:LEU:HD22	2:B:512:ALA:HB1	1.99	0.43
1:A:69:LEU:HD13	1:A:493:LEU:HD23	2.00	0.42
2:B:87:PRO:HB3	2:B:108:ILE:HG22	2.01	0.41
1:A:87:PRO:HB3	1:A:108:ILE:HG22	2.02	0.41
2:B:286:VAL:HG22	2:B:314:ILE:HB	2.02	0.41
2:B:403:LEU:HD22	2:B:485:PHE:HZ	1.86	0.41
1:A:403:LEU:HD22	1:A:485:PHE:HZ	1.85	0.40
1:A:389:LYS:O	1:A:393:LEU:HG	2.22	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	389/556 (70%)	371 (95%)	16 (4%)	2 (0%)	24	27
2	B	389/556 (70%)	375 (96%)	14 (4%)	0	100	100
All	All	778/1112 (70%)	746 (96%)	30 (4%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	GLU
1	A	455	ALA

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	310/445 (70%)	302 (97%)	8 (3%)	40	55
2	B	310/445 (70%)	298 (96%)	12 (4%)	28	39
All	All	620/890 (70%)	600 (97%)	20 (3%)	34	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	344	ILE
1	A	346	ILE
1	A	417	HIS
1	A	460	PHE
1	A	462	GLU
1	A	482	ILE
1	A	503	LYS
2	B	43	ARG
2	B	344	ILE
2	B	348	GLN
2	B	351	MET
2	B	451	LEU
2	B	453	ASN

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Mol	Chain	Res	Type
2	B	456	THR
2	B	458	ARG
2	B	460	PHE
2	B	462	GLU
2	B	466	VAL
2	B	503	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
2	B	59	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	SO4	B	1529	-	4,4,4	0.25	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1528	-	4,4,4	0.25	0	6,6,6	0.08	0
4	IMP	A	1527	-	25,25,25	2.34	6 (24%)	37,38,38	2.53	10 (27%)
4	IMP	B	1527	-	25,25,25	2.31	7 (28%)	37,38,38	2.37	10 (27%)
3	MOA	A	1526	-	24,24,24	2.42	5 (20%)	34,34,34	3.04	11 (32%)
3	MOA	B	1526	-	24,24,24	2.46	5 (20%)	34,34,34	3.22	16 (47%)

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
4	IMP	A	1527	-	-	0/10/26/26	0/3/3/3
4	IMP	B	1527	-	-	0/10/26/26	0/3/3/3
3	MOA	A	1526	-	-	0/12/21/21	0/2/2/2
3	MOA	B	1526	-	-	2/12/21/21	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1526	MOA	C10-C11	8.27	1.58	1.50
3	A	1526	MOA	C10-C11	8.15	1.58	1.50
4	A	1527	IMP	C2-N3	7.19	1.43	1.30
4	B	1527	IMP	C2-N3	6.75	1.42	1.30
3	B	1526	MOA	C17-C14	5.50	1.57	1.51
3	A	1526	MOA	C17-C14	4.74	1.56	1.51
4	B	1527	IMP	C4-N3	4.60	1.45	1.35
4	A	1527	IMP	C4-N3	4.50	1.44	1.35
4	A	1527	IMP	C2-N1	4.21	1.42	1.35
3	A	1526	MOA	C16-C1	-4.07	1.40	1.47
4	B	1527	IMP	C2-N1	4.00	1.42	1.35
3	B	1526	MOA	C16-C1	-3.67	1.41	1.47
3	A	1526	MOA	O2-C1	-3.51	1.32	1.36
3	B	1526	MOA	O2-C1	-3.20	1.32	1.36
4	A	1527	IMP	C2'-C3'	-2.85	1.45	1.53
4	B	1527	IMP	C2'-C3'	-2.78	1.45	1.53
4	B	1527	IMP	O4'-C4'	-2.77	1.38	1.45
4	A	1527	IMP	O4'-C1'	2.62	1.48	1.42
4	A	1527	IMP	O4'-C4'	-2.62	1.39	1.45
4	B	1527	IMP	O4'-C1'	2.44	1.47	1.42
3	B	1526	MOA	C2-C3	2.26	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1526	MOA	C2-C3	2.13	1.38	1.33
4	B	1527	IMP	C4-N9	-2.10	1.32	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1526	MOA	O2-C1-C16	10.95	116.84	108.28
3	B	1526	MOA	O2-C1-C16	10.38	116.39	108.28
3	B	1526	MOA	C10-O2-C1	-9.97	104.12	110.64
3	A	1526	MOA	C10-O2-C1	-8.08	105.36	110.64
4	A	1527	IMP	N1-C2-N3	-7.80	116.52	125.50
4	B	1527	IMP	N1-C2-N3	-6.98	117.46	125.50
4	A	1527	IMP	C2-N3-C4	6.61	123.16	111.53
4	B	1527	IMP	C2-N3-C4	6.06	122.19	111.53
4	A	1527	IMP	C5-C6-N1	6.00	119.41	110.78
4	B	1527	IMP	C5-C6-N1	5.72	119.00	110.78
4	A	1527	IMP	C5-C4-N3	-5.21	119.59	127.27
3	A	1526	MOA	O1-C1-C16	-5.02	122.05	130.99
4	B	1527	IMP	C5-C4-N3	-4.79	120.21	127.27
3	B	1526	MOA	O1-C1-C16	-4.52	122.93	130.99
3	B	1526	MOA	C15-C16-C1	4.41	135.29	129.35
3	A	1526	MOA	C15-C16-C1	4.17	134.97	129.35
3	B	1526	MOA	C8-O3-C13	3.65	124.65	114.74
3	B	1526	MOA	C10-C11-C12	3.20	134.26	129.81
3	B	1526	MOA	C15-C16-C11	-2.99	119.42	121.87
3	A	1526	MOA	C4-C3-C2	-2.95	114.54	121.17
3	B	1526	MOA	C11-C16-C1	-2.87	105.19	108.39
4	B	1527	IMP	C4-C5-N7	-2.86	106.13	110.67
4	A	1527	IMP	O5'-P-O1P	2.77	113.92	106.44
4	A	1527	IMP	C4-C5-N7	-2.77	106.29	110.67
3	A	1526	MOA	C15-C16-C11	-2.76	119.60	121.87
3	A	1526	MOA	C11-C16-C1	-2.67	105.40	108.39
3	A	1526	MOA	C10-C11-C12	2.64	133.48	129.81
4	B	1527	IMP	C6-C5-N7	2.62	135.05	130.29
4	B	1527	IMP	O3P-P-O5'	2.60	113.45	106.67
3	B	1526	MOA	C14-C13-C12	-2.59	119.43	122.79
3	B	1526	MOA	C5-C4-C3	2.54	119.97	112.86
4	A	1527	IMP	C6-C5-N7	2.53	134.90	130.29
3	A	1526	MOA	C14-C13-C12	-2.44	119.63	122.79
3	B	1526	MOA	C4-C3-C2	-2.35	115.89	121.17
3	B	1526	MOA	C9-C3-C4	2.30	119.23	115.23
4	A	1527	IMP	O4'-C1'-N9	2.26	113.48	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1526	MOA	C16-C11-C12	-2.26	120.72	122.68
4	B	1527	IMP	C2'-C1'-N9	2.25	119.52	113.25
3	B	1526	MOA	C10-C11-C16	-2.25	105.02	107.90
3	A	1526	MOA	C5-C4-C3	2.25	119.14	112.86
4	B	1527	IMP	C8-N7-C5	2.22	108.21	104.26
4	A	1527	IMP	C8-N7-C5	2.16	108.12	104.26
3	A	1526	MOA	C17-C2-C3	-2.16	124.33	127.42
4	B	1527	IMP	N9-C8-N7	-2.12	109.47	113.40
3	B	1526	MOA	C7-C12-C11	-2.04	117.49	120.43
4	A	1527	IMP	C2'-C1'-N9	2.03	118.91	113.25
3	B	1526	MOA	O5-C6-C5	2.02	120.39	114.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1526	MOA	C4-C5-C6-O5
3	B	1526	MOA	C4-C5-C6-O6

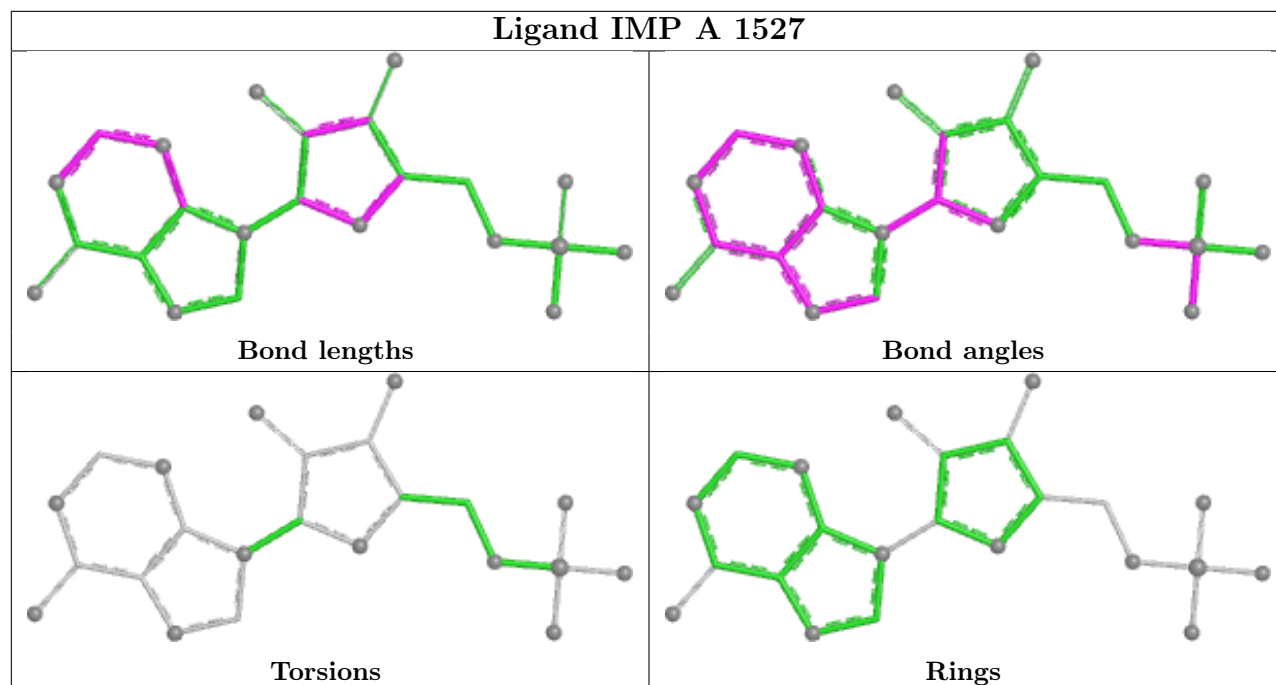
There are no ring outliers.

2 monomers are involved in 2 short contacts:

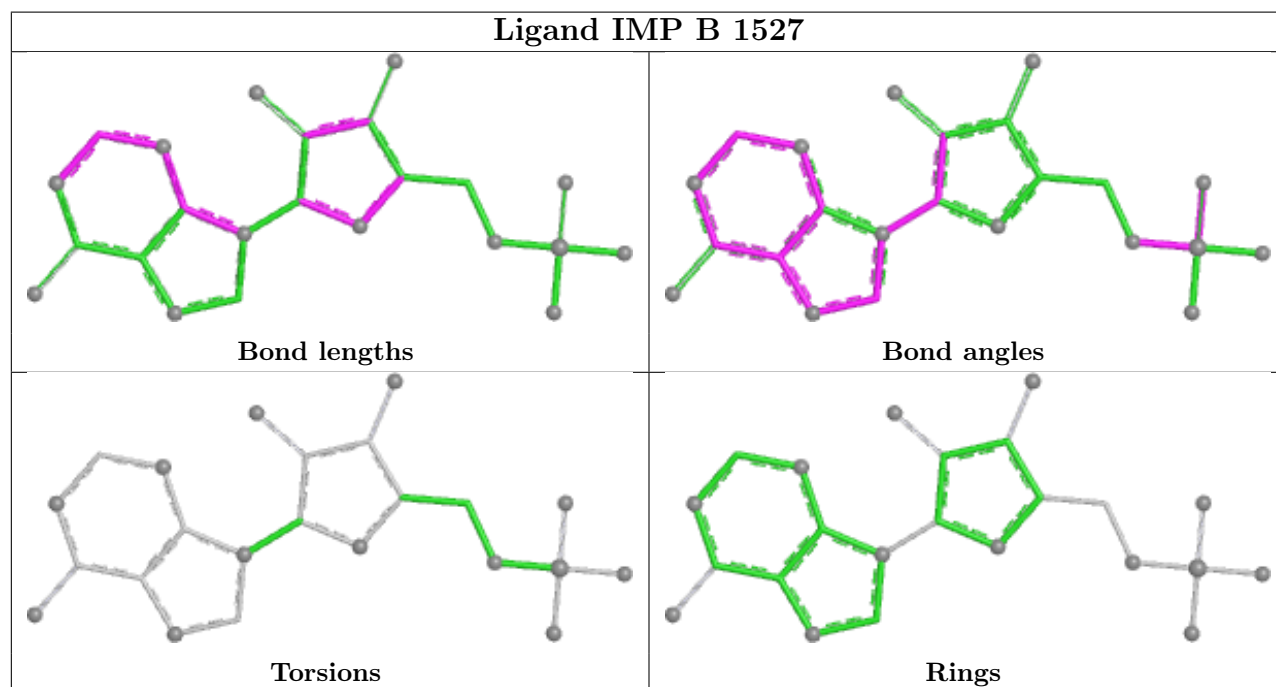
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1527	IMP	1	0
3	B	1526	MOA	1	0

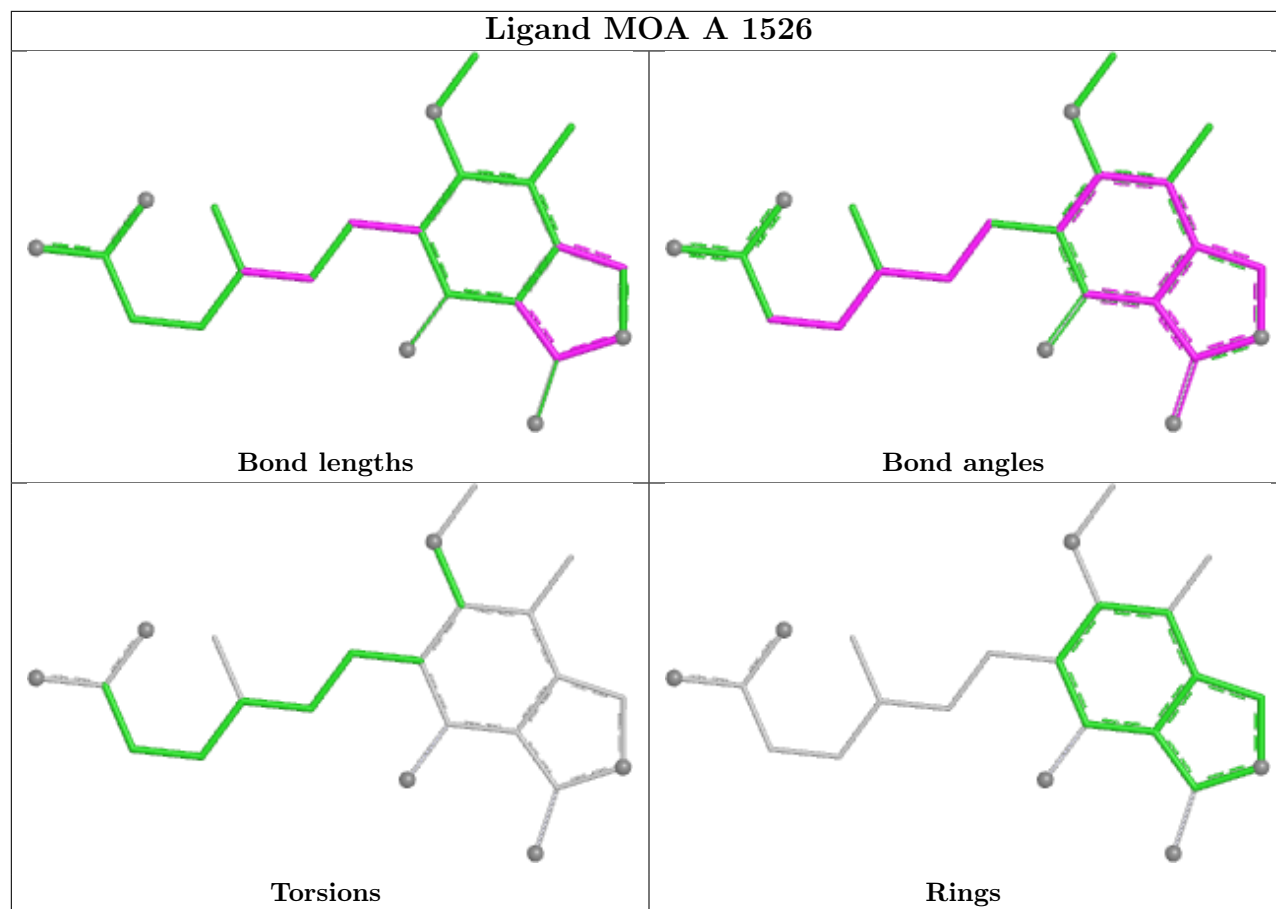
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

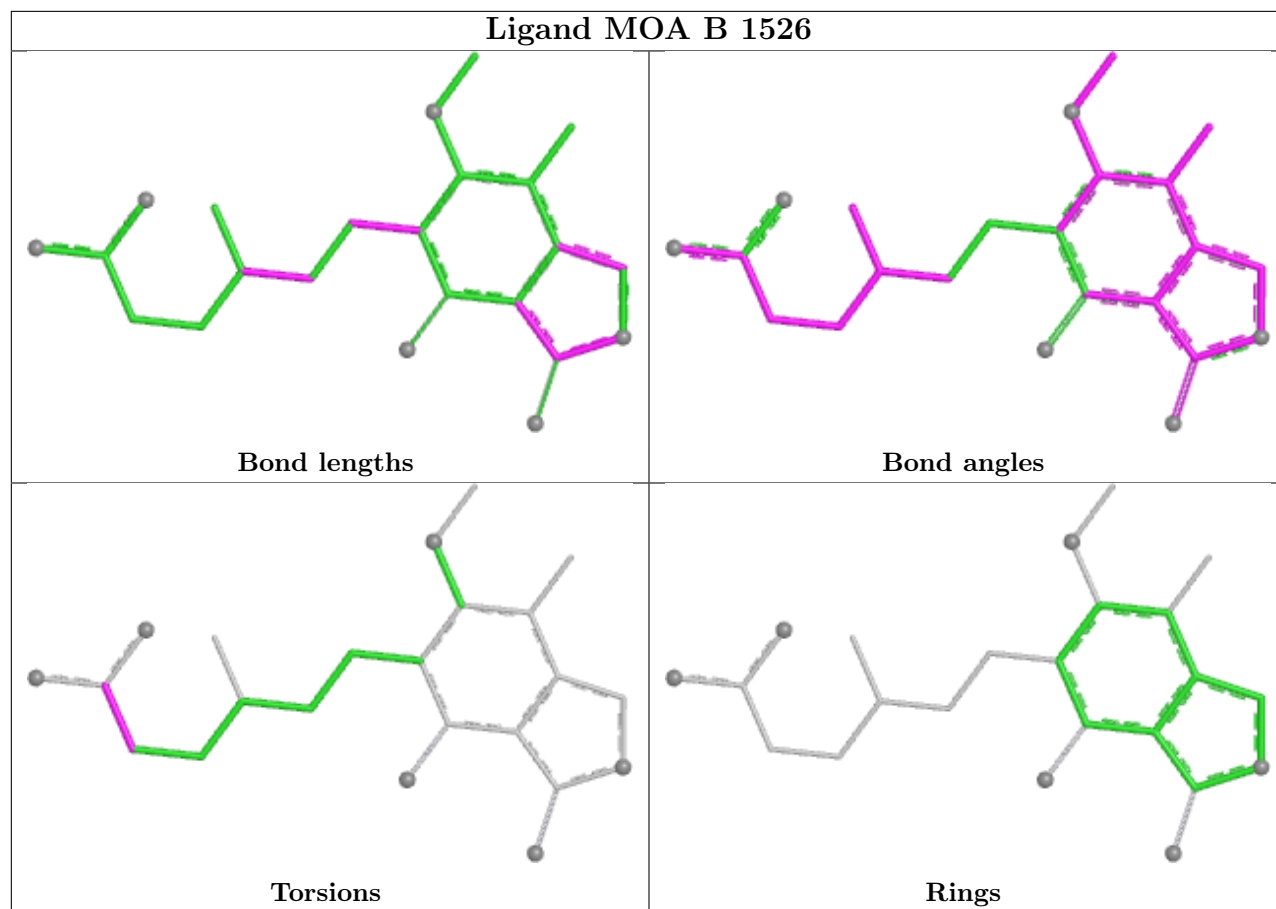
Ligand IMP A 1527



Ligand IMP B 1527







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	395/556 (71%)	-1.45	0 100 100	20, 33, 81, 102	0
2	B	395/556 (71%)	-1.44	1 (0%) 90 88	22, 33, 79, 124	0
All	All	790/1112 (71%)	-1.45	1 (0%) 92 90	20, 33, 81, 124	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	450	GLY	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
5	SO4	B	1528	5/5	0.98	0.07	134,134,135,135	0
3	MOA	B	1526	23/23	0.99	0.04	34,37,42,49	0
5	SO4	B	1529	5/5	0.99	0.04	114,114,115,116	0
4	IMP	B	1527	23/23	1.00	0.02	21,29,31,32	0

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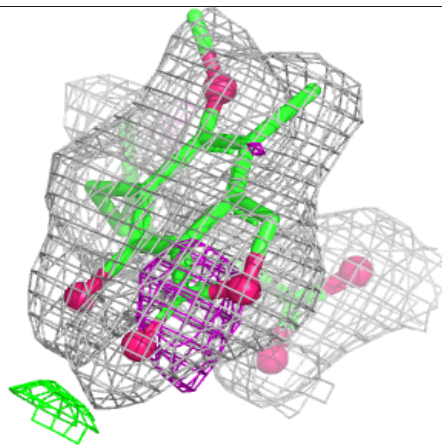
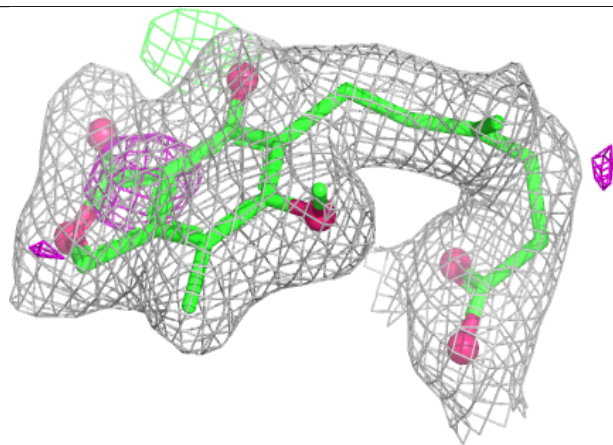
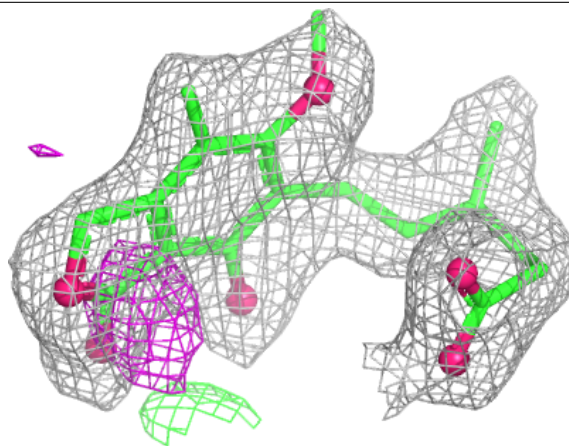
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MOA	A	1526	23/23	1.00	0.03	28,35,38,40	0
4	IMP	A	1527	23/23	1.00	0.02	21,29,33,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

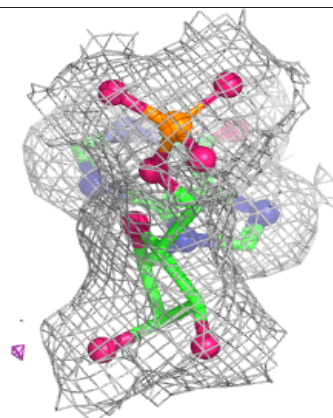
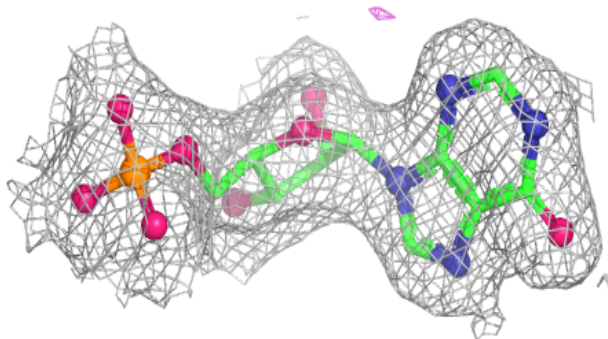
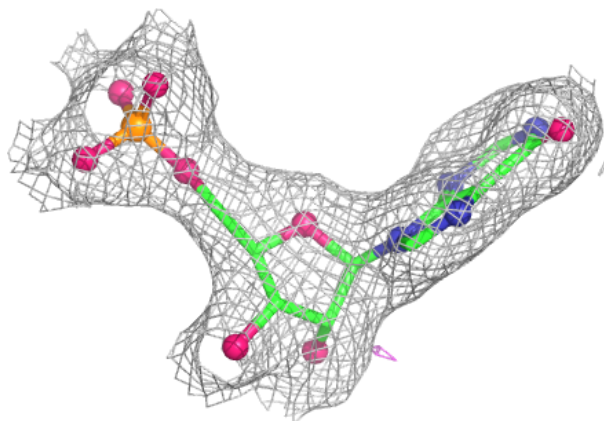
Electron density around MOA B 1526:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



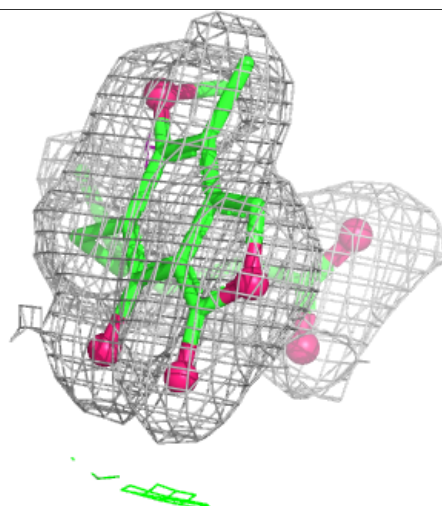
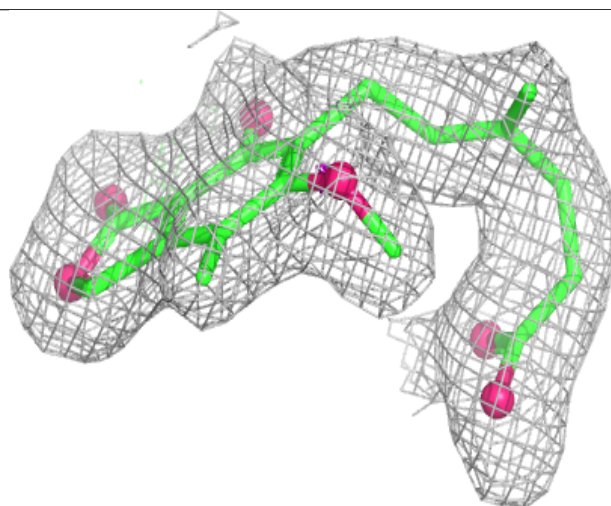
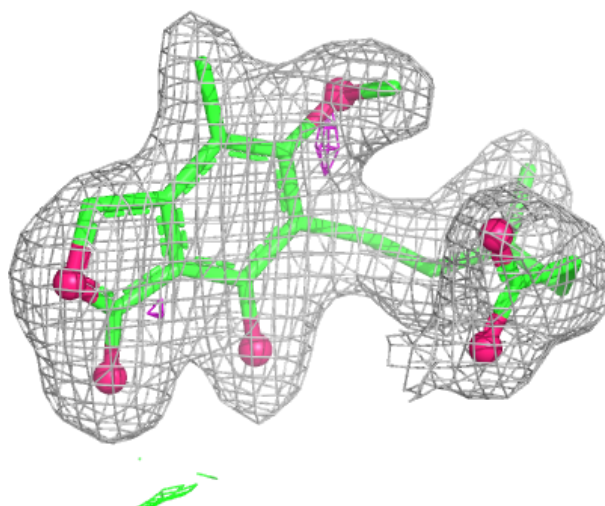
Electron density around IMP B 1527:

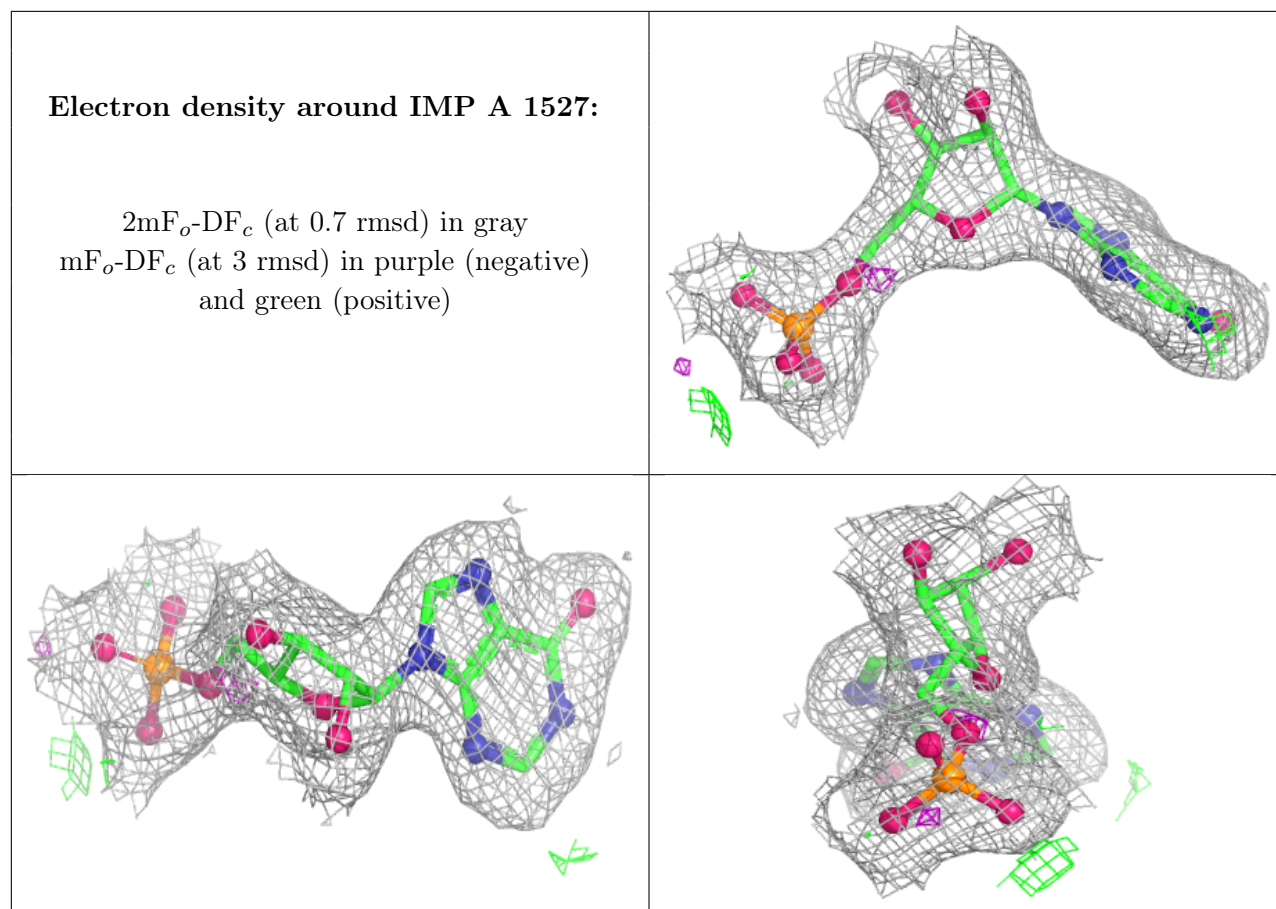
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MOA A 1526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.