



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2022 – 10:05 AM EDT

PDB ID : 8EBC
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Listeria monocytogenes* in the complex with IMP
Authors : Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Osipiuk, J.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2022-08-31
Resolution : 2.50 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

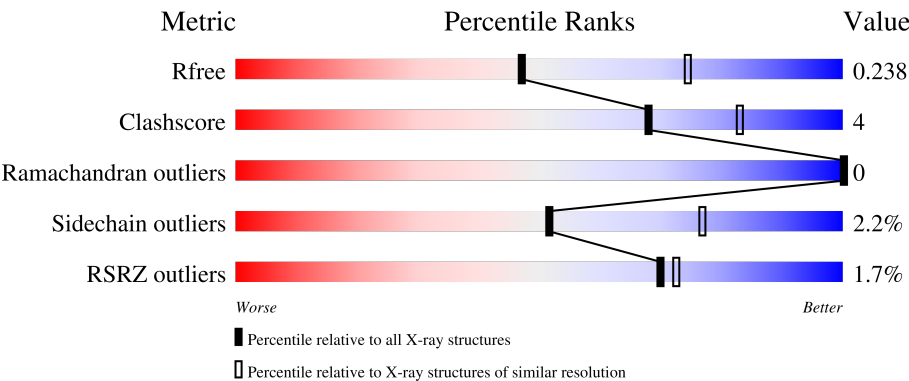
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	395	<div><div></div><div>78%7%15%</div></div>
1	B	395	<div><div>%</div><div>78%7%15%</div></div>
1	C	395	<div><div>2%</div><div>76%13%10%</div></div>
1	D	395	<div><div>4%</div><div>74%12%13%</div></div>
1	E	395	<div><div>%</div><div>80%8%11%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	395	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>77%9%14%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16120 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 Lmo0132 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2589	1633	437	502	17			
1	B	336	Total	C	N	O	S	0	1	0
			2581	1629	432	504	16			
1	C	355	Total	C	N	O	S	0	1	0
			2735	1726	460	534	15			
1	D	344	Total	C	N	O	S	0	0	0
			2631	1661	447	509	14			
1	F	338	Total	C	N	O	S	0	0	0
			2588	1633	434	506	15			
1	E	350	Total	C	N	O	S	0	2	0
			2696	1700	455	526	15			

There are 24 discrepancies between the modelled and reference sequences:

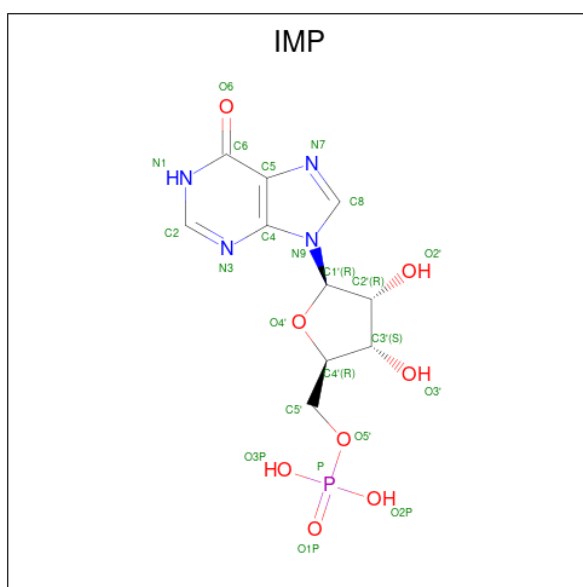
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q8YAJ3
A	100	SER	-	linker	UNP Q8YAJ3
A	101	GLY	-	linker	UNP Q8YAJ3
A	102	GLY	-	linker	UNP Q8YAJ3
B	-1	ALA	-	expression tag	UNP Q8YAJ3
B	100	SER	-	linker	UNP Q8YAJ3
B	101	GLY	-	linker	UNP Q8YAJ3
B	102	GLY	-	linker	UNP Q8YAJ3
C	-1	ALA	-	expression tag	UNP Q8YAJ3
C	100	SER	-	linker	UNP Q8YAJ3
C	101	GLY	-	linker	UNP Q8YAJ3
C	102	GLY	-	linker	UNP Q8YAJ3
D	-1	ALA	-	expression tag	UNP Q8YAJ3
D	100	SER	-	linker	UNP Q8YAJ3
D	101	GLY	-	linker	UNP Q8YAJ3
D	102	GLY	-	linker	UNP Q8YAJ3
F	-1	ALA	-	expression tag	UNP Q8YAJ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	100	SER	-	linker	UNP Q8YAJ3
F	101	GLY	-	linker	UNP Q8YAJ3
F	102	GLY	-	linker	UNP Q8YAJ3
E	-1	ALA	-	expression tag	UNP Q8YAJ3
E	100	SER	-	linker	UNP Q8YAJ3
E	101	GLY	-	linker	UNP Q8YAJ3
E	102	GLY	-	linker	UNP Q8YAJ3

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		

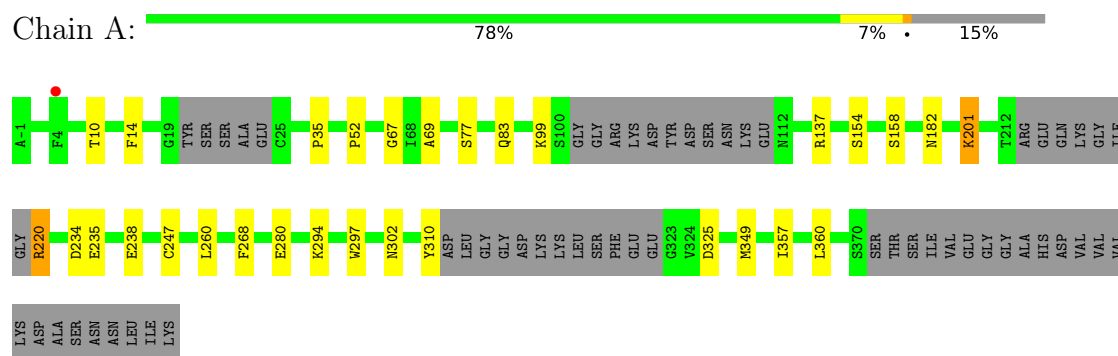
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total 51	O 51	0	0
5	B	34	Total 34	O 34	0	0
5	C	15	Total 15	O 15	0	0
5	D	1	Total 1	O 1	0	0
5	F	26	Total 26	O 26	0	0
5	E	23	Total 23	O 23	0	0

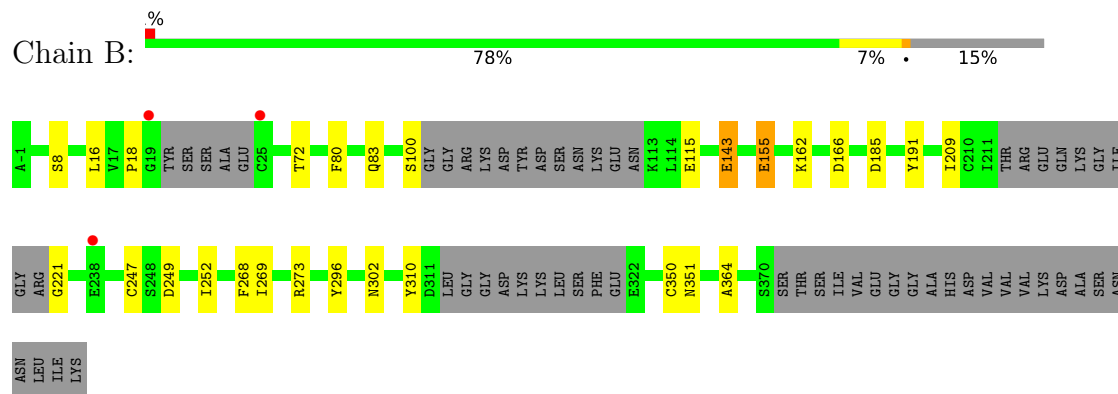
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

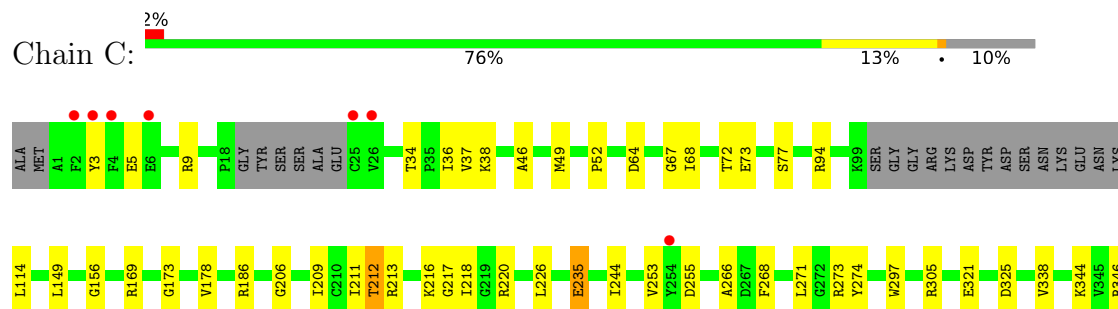
• Molecule 1: Lmo0132 protein

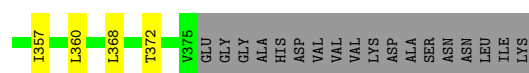


• Molecule 1: Lmo0132 protein

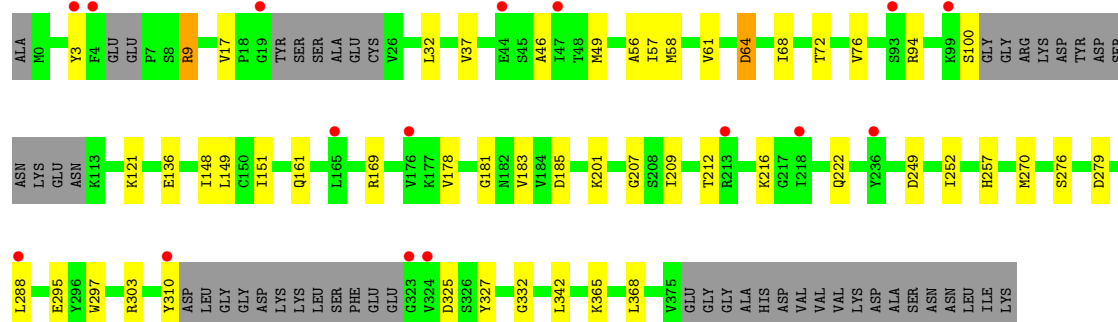
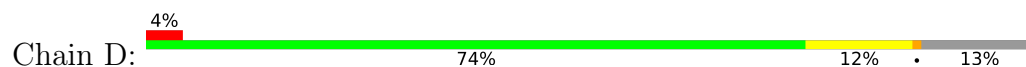


• Molecule 1: Lmo0132 protein

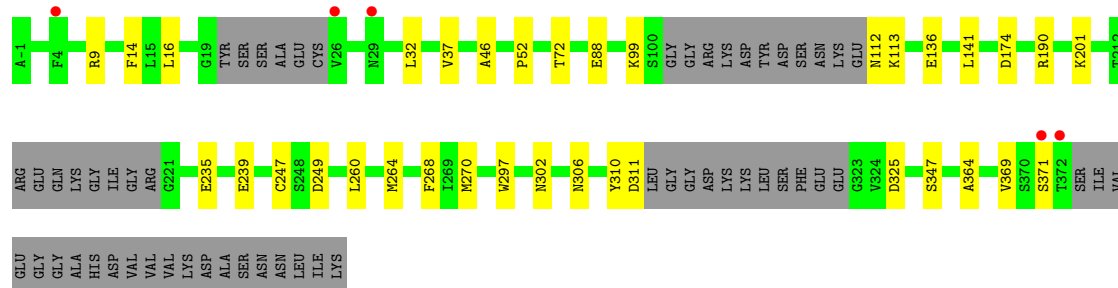
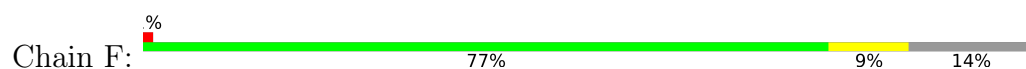




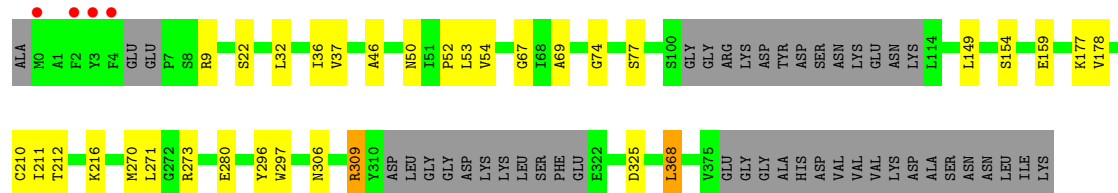
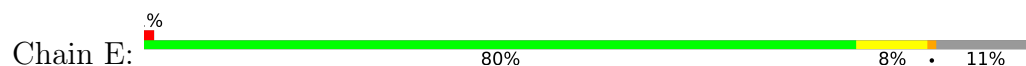
• Molecule 1: Lmo0132 protein



• Molecule 1: Lmo0132 protein



• Molecule 1: Lmo0132 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.98Å 95.70Å 97.60Å 111.36° 105.17° 107.61°	Depositor
Resolution (Å)	39.88 – 2.50 47.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	83.5 (39.88-2.50) 83.5 (47.07-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.239 0.194 , 0.238	Depositor DCC
R_{free} test set	3345 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-h-k-l,k 0.004 for h,l,-h-k-l 0.008 for -h,h+k+l,-l 0.008 for -h,-k,h+k+l 0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16120	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, 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	0.25	0/2632	0.47	0/3549
1	B	0.25	0/2624	0.46	0/3539
1	C	0.25	0/2782	0.47	0/3753
1	D	0.25	0/2674	0.47	0/3604
1	E	0.25	0/2742	0.47	0/3699
1	F	0.25	0/2631	0.47	0/3550
All	All	0.25	0/16085	0.47	0/21694

There are no bond length outliers.

There are no bond angle outliers.

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	2589	0	2548	16	0
1	B	2581	0	2535	17	0
1	C	2735	0	2691	28	0
1	D	2631	0	2605	28	0
1	E	2696	0	2646	17	0
1	F	2588	0	2547	17	0
2	A	23	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	11	2	0
2	C	23	0	11	2	0
2	D	23	0	11	1	0
2	E	23	0	11	2	0
2	F	23	0	11	1	0
3	A	6	0	8	1	0
4	A	3	0	1	0	0
4	F	3	0	1	0	0
5	A	51	0	0	0	0
5	B	34	0	0	0	0
5	C	15	0	0	1	0
5	D	1	0	0	0	0
5	E	23	0	0	0	0
5	F	26	0	0	0	0
All	All	16120	0	15648	121	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 4.

All (121) 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:E:273:ARG:HG3	1:E:296:TYR:CZ	2.31	0.65
1:F:16:LEU:HD11	1:F:364:ALA:HB1	1.83	0.60
1:E:149:LEU:HB2	1:E:178:VAL:HG22	1.84	0.58
1:D:303:ARG:HA	1:D:310:TYR:HE2	1.70	0.56
1:A:83:GLN:O	1:A:137:ARG:NH2	2.27	0.56
1:C:149:LEU:HB2	1:C:178:VAL:HG22	1.88	0.56
1:C:37:VAL:HG21	1:C:46:ALA:HB3	1.89	0.55
1:C:218:ILE:HG12	1:C:273:ARG:HD2	1.89	0.54
1:D:58:MET:HB2	1:D:61:VAL:HG22	1.89	0.54
1:F:302:ASN:OD1	1:F:310:TYR:OH	2.24	0.54
1:D:295:GLU:HG2	1:D:327:TYR:HE1	1.73	0.53
1:C:212:THR:O	2:C:401:IMP:N1	2.42	0.53
1:E:212:THR:O	2:E:401:IMP:N1	2.41	0.53
1:C:169:ARG:NH1	1:C:173:GLY:O	2.42	0.52
1:C:64:ASP:N	1:C:64:ASP:OD1	2.41	0.52
1:E:9:ARG:HD2	1:E:368:LEU:HD21	1.92	0.52
1:B:16:LEU:HD21	1:B:364:ALA:HB1	1.92	0.52
1:C:211:ILE:HG23	2:C:401:IMP:C4	2.41	0.51
1:A:10:THR:HG22	1:A:220:ARG:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HG12	1:D:276:SER:HB2	1.93	0.51
1:B:209:ILE:O	2:B:401:IMP:N1	2.40	0.51
1:D:249:ASP:HA	1:D:270:MET:HB3	1.93	0.50
1:D:37:VAL:HG21	1:D:46:ALA:HB3	1.93	0.50
1:B:72:THR:HA	1:B:115:GLU:HG2	1.94	0.50
1:B:155:GLU:HG3	1:C:213:ARG:HH21	1.78	0.49
1:D:100:SER:OG	1:D:121:LYS:O	2.30	0.49
1:B:162:LYS:NZ	1:B:166:ASP:OD2	2.44	0.49
1:D:64:ASP:OD1	1:D:94:ARG:NH1	2.46	0.49
1:B:185:ASP:OD1	1:B:185:ASP:N	2.45	0.48
1:B:18:PRO:HB3	1:B:351:ASN:HB3	1.95	0.48
1:D:212:THR:O	2:D:401:IMP:N1	2.47	0.48
1:E:211:ILE:HG23	2:E:401:IMP:C4	2.43	0.48
1:C:206:GLY:HA2	1:C:216:LYS:HG3	1.95	0.48
1:E:32:LEU:HB3	1:E:52:PRO:HD3	1.96	0.47
1:A:302:ASN:ND2	1:A:310:TYR:OH	2.48	0.47
1:F:37:VAL:HG21	1:F:46:ALA:HB3	1.97	0.47
1:D:161:GLN:NE2	1:D:181:GLY:H	2.12	0.47
1:F:32:LEU:HB3	1:F:52:PRO:HD3	1.97	0.47
1:A:234:ASP:O	1:A:238:GLU:HG2	2.15	0.46
1:C:68:ILE:O	1:C:72:THR:HG23	2.15	0.46
1:C:255:ASP:OD2	1:C:344:LYS:HD2	2.15	0.46
1:A:297:TRP:HA	1:A:325:ASP:HB2	1.98	0.46
1:E:37:VAL:HG21	1:E:46:ALA:HB3	1.97	0.46
1:E:53:LEU:HD22	1:E:271:LEU:HD11	1.98	0.46
1:C:156:GLY:HA3	1:C:209:ILE:HD12	1.97	0.46
1:C:346:ARG:NH2	5:C:502:HOH:O	2.48	0.46
1:F:247:CYS:HB2	1:F:268:PHE:CZ	2.51	0.46
1:B:162:LYS:HD2	1:B:191:TYR:CZ	2.51	0.46
1:C:186:ARG:NE	1:C:235:GLU:OE2	2.47	0.45
1:E:306:ASN:HB3	1:E:309:ARG:HD3	1.98	0.45
1:C:34:THR:HB	1:C:357:ILE:HD12	1.97	0.45
1:E:37:VAL:HG11	1:E:177:LYS:HG2	1.98	0.45
1:F:260:LEU:O	1:F:264:MET:HG3	2.15	0.45
1:F:297:TRP:HA	1:F:325:ASP:HB2	1.98	0.45
1:D:297:TRP:HA	1:D:325:ASP:HB2	1.98	0.45
1:D:207:GLY:HA3	1:D:222:GLN:HG3	1.99	0.45
1:E:67:GLY:HA2	1:E:77:SER:HB2	1.99	0.45
1:A:67:GLY:HA2	1:A:77:SER:HB2	1.98	0.45
1:C:271:LEU:HB3	1:C:274:TYR:HB3	1.99	0.44
1:C:67:GLY:HA2	1:C:77:SER:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ARG:HA	1:C:305:ARG:HD2	1.72	0.44
1:E:297:TRP:HA	1:E:325:ASP:HB2	1.99	0.44
1:B:302:ASN:ND2	1:B:310:TYR:OH	2.50	0.44
1:C:297:TRP:HA	1:C:325:ASP:HB2	2.00	0.44
1:C:52:PRO:HG3	1:C:357:ILE:HD11	2.00	0.44
1:C:217:GLY:HA3	1:C:220:ARG:NH1	2.32	0.44
1:F:302:ASN:ND2	1:F:306:ASN:HD22	2.16	0.44
1:A:182:ASN:OD1	1:A:201:LYS:HB3	2.18	0.44
1:A:69:ALA:HB2	1:A:280:GLU:HG2	2.00	0.43
1:D:201:LYS:HG2	1:D:249:ASP:HB2	2.00	0.43
1:A:235:GLU:HG3	1:B:143:GLU:HG2	2.00	0.43
1:B:273:ARG:HG3	1:B:296:TYR:CZ	2.52	0.43
1:A:52:PRO:HG3	1:A:357:ILE:HD11	1.99	0.43
1:D:151:ILE:HG21	1:D:161:GLN:HG3	2.00	0.43
1:D:279:ASP:N	1:D:332:GLY:O	2.46	0.43
1:E:154:SER:O	1:E:210:CYS:HB3	2.18	0.43
1:D:32:LEU:HD13	1:D:342:LEU:HD22	2.00	0.43
1:D:56:ALA:HA	1:D:270:MET:HE3	1.99	0.43
1:F:201:LYS:HG3	1:F:247:CYS:HB3	1.99	0.43
1:D:183:VAL:HA	1:D:209:ILE:HD11	2.01	0.43
1:B:247:CYS:HB2	1:B:268:PHE:CZ	2.53	0.43
1:C:73:GLU:HG2	1:C:338:VAL:HG11	2.00	0.43
1:E:69:ALA:HB2	1:E:280:GLU:HG2	2.01	0.43
1:F:88:GLU:HB3	1:F:141:LEU:HD21	2.01	0.42
1:C:38:LYS:HB3	1:C:244:ILE:HD13	2.01	0.42
1:A:14:PHE:HB2	1:A:260:LEU:HD21	2.01	0.42
1:E:216:LYS:HA	1:E:216:LYS:HD3	1.76	0.42
1:D:149:LEU:HB2	1:D:178:VAL:HG22	2.00	0.42
1:D:57:ILE:HG13	1:D:270:MET:HE1	2.01	0.42
1:E:50:ASN:HB2	1:E:74:GLY:HA3	2.01	0.42
1:D:185:ASP:N	1:D:185:ASP:OD1	2.53	0.42
1:C:226:LEU:HD11	1:C:266:ALA:HB2	2.02	0.42
1:D:49:MET:SD	1:D:76:VAL:HG12	2.60	0.42
1:F:249:ASP:OD2	2:F:401:IMP:O2'	2.37	0.41
1:B:252:ILE:HG13	1:B:269:ILE:HG21	2.01	0.41
1:D:17:VAL:HB	1:D:365:LYS:HB2	2.00	0.41
1:A:35:PRO:HG3	3:A:402:GOL:H31	2.03	0.41
1:A:247:CYS:HB2	1:A:268:PHE:CZ	2.56	0.41
1:D:9:ARG:HD3	1:D:368:LEU:HD21	2.02	0.41
1:D:68:ILE:O	1:D:72:THR:HG23	2.20	0.41
1:D:216:LYS:HD2	1:D:216:LYS:HA	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ARG:HA	1:D:310:TYR:CE2	2.55	0.41
1:B:80:PHE:O	1:B:83:GLN:NE2	2.47	0.41
1:B:249:ASP:OD2	2:B:401:IMP:O2'	2.38	0.41
1:C:9:ARG:HD3	1:C:368:LEU:HD11	2.03	0.41
1:D:252:ILE:HG23	1:D:257:HIS:HB2	2.02	0.41
1:F:136:GLU:OE1	1:F:136:GLU:N	2.54	0.41
1:A:294:LYS:HE2	1:A:294:LYS:HB3	1.94	0.41
1:C:64:ASP:OD2	1:C:94:ARG:NE	2.43	0.41
1:F:9:ARG:HD3	1:F:14:PHE:CZ	2.54	0.41
1:F:16:LEU:HD12	1:F:16:LEU:HA	1.84	0.41
1:F:99:LYS:HE2	1:F:99:LYS:HB3	1.93	0.41
1:A:99:LYS:HD3	1:A:99:LYS:HA	1.89	0.41
1:F:190:ARG:NH2	1:F:239:GLU:OE1	2.53	0.40
1:B:8:SER:HB2	1:B:221:GLY:HA2	2.04	0.40
1:C:3:TYR:CE2	1:C:5:GLU:HB2	2.56	0.40
1:C:36:ILE:HG22	1:C:268:PHE:CD1	2.57	0.40
1:A:349:MET:HG2	1:A:360:LEU:HD22	2.04	0.40
1:B:16:LEU:HD23	1:B:16:LEU:HA	1.78	0.40
1:F:247:CYS:SG	1:F:270:MET:HB2	2.62	0.40
1:E:54:VAL:HG23	1:E:270:MET:HA	2.04	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	328/395 (83%)	319 (97%)	9 (3%)	0	100	100
1	B	327/395 (83%)	312 (95%)	15 (5%)	0	100	100
1	C	350/395 (89%)	331 (95%)	19 (5%)	0	100	100
1	D	334/395 (85%)	318 (95%)	16 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	344/395 (87%)	334 (97%)	10 (3%)	0	100	100
1	F	328/395 (83%)	315 (96%)	13 (4%)	0	100	100
All	All	2011/2370 (85%)	1929 (96%)	82 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	276/322 (86%)	272 (99%)	4 (1%)	67	86
1	B	275/322 (85%)	271 (98%)	4 (2%)	65	85
1	C	291/322 (90%)	283 (97%)	8 (3%)	44	71
1	D	280/322 (87%)	273 (98%)	7 (2%)	47	73
1	E	287/322 (89%)	282 (98%)	5 (2%)	60	82
1	F	276/322 (86%)	267 (97%)	9 (3%)	38	64
All	All	1685/1932 (87%)	1648 (98%)	37 (2%)	52	77

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	SER
1	A	158	SER
1	A	201	LYS
1	A	220	ARG
1	B	100	SER
1	B	143	GLU
1	B	155	GLU
1	B	350	CYS
1	C	49	MET
1	C	114	LEU
1	C	212	THR
1	C	235	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	253	VAL
1	C	321	GLU
1	C	360	LEU
1	C	372	THR
1	D	3	TYR
1	D	9	ARG
1	D	64	ASP
1	D	136	GLU
1	D	148	ILE
1	D	169	ARG
1	D	288	LEU
1	F	72	THR
1	F	112	ASN
1	F	113	LYS
1	F	174	ASP
1	F	235	GLU
1	F	311	ASP
1	F	347	SER
1	F	369	VAL
1	F	371	SER
1	E	22	SER
1	E	36	ILE
1	E	159	GLU
1	E	309	ARG
1	E	368	LEU

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

Mol	Chain	Res	Type
1	B	302	ASN
1	B	306	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
2	IMP	A	401	-	21,25,25	1.46	2 (9%)	24,38,38	1.21	4 (16%)
2	IMP	C	401	-	21,25,25	1.47	2 (9%)	24,38,38	1.24	4 (16%)
2	IMP	B	401	-	21,25,25	1.47	2 (9%)	24,38,38	1.26	5 (20%)
2	IMP	E	401	-	21,25,25	1.46	2 (9%)	24,38,38	1.32	5 (20%)
2	IMP	F	401	-	21,25,25	1.47	2 (9%)	24,38,38	1.26	5 (20%)
4	FMT	F	402	-	2,2,2	0.72	0	1,1,1	0.23	0
4	FMT	A	403	-	2,2,2	0.71	0	1,1,1	0.23	0
3	GOL	A	402	-	5,5,5	0.95	0	5,5,5	0.91	0
2	IMP	D	401	-	21,25,25	1.48	2 (9%)	24,38,38	1.36	5 (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
2	IMP	A	401	-	-	5/6/26/26	0/3/3/3
2	IMP	C	401	-	-	4/6/26/26	0/3/3/3
2	IMP	B	401	-	-	0/6/26/26	0/3/3/3
2	IMP	E	401	-	-	5/6/26/26	0/3/3/3
2	IMP	F	401	-	-	5/6/26/26	0/3/3/3
3	GOL	A	402	-	-	4/4/4/4	-
2	IMP	D	401	-	-	5/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	IMP	C2-N3	4.76	1.38	1.29
2	C	401	IMP	C2-N3	4.72	1.38	1.29
2	B	401	IMP	C2-N3	4.55	1.38	1.29
2	A	401	IMP	C2-N3	4.53	1.38	1.29
2	F	401	IMP	C2-N3	4.51	1.38	1.29
2	E	401	IMP	C2-N3	4.48	1.37	1.29
2	F	401	IMP	C5-C6	-4.04	1.39	1.47
2	E	401	IMP	C5-C6	-4.00	1.39	1.47
2	B	401	IMP	C5-C6	-3.99	1.39	1.47
2	A	401	IMP	C5-C6	-3.95	1.39	1.47
2	C	401	IMP	C5-C6	-3.95	1.39	1.47
2	D	401	IMP	C5-C6	-3.91	1.39	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	IMP	C5-C6-N1	3.06	119.36	113.95
2	B	401	IMP	C8-N7-C5	3.04	108.78	102.99
2	A	401	IMP	C8-N7-C5	3.03	108.76	102.99
2	B	401	IMP	C5-C6-N1	3.02	119.29	113.95
2	D	401	IMP	C8-N7-C5	3.01	108.72	102.99
2	F	401	IMP	C8-N7-C5	2.98	108.67	102.99
2	C	401	IMP	C5-C6-N1	2.98	119.21	113.95
2	F	401	IMP	C5-C6-N1	2.96	119.18	113.95
2	A	401	IMP	C5-C6-N1	2.96	119.17	113.95
2	E	401	IMP	C8-N7-C5	2.94	108.58	102.99
2	C	401	IMP	C8-N7-C5	2.94	108.58	102.99
2	D	401	IMP	O3P-P-O2P	2.93	118.84	107.64
2	E	401	IMP	C5-C6-N1	2.79	118.88	113.95
2	F	401	IMP	O3P-P-O2P	2.70	117.96	107.64
2	E	401	IMP	O6-C6-C5	-2.66	119.17	124.37
2	E	401	IMP	O3P-P-O2P	2.60	117.56	107.64
2	C	401	IMP	O6-C6-C5	-2.42	119.65	124.37
2	D	401	IMP	O6-C6-C5	-2.30	119.87	124.37
2	B	401	IMP	N1-C2-N3	-2.25	120.01	125.87
2	B	401	IMP	O6-C6-C5	-2.20	120.07	124.37
2	C	401	IMP	N1-C2-N3	-2.20	120.14	125.87
2	D	401	IMP	N1-C2-N3	-2.18	120.18	125.87
2	A	401	IMP	N1-C2-N3	-2.15	120.27	125.87
2	E	401	IMP	N1-C2-N3	-2.14	120.29	125.87
2	F	401	IMP	N1-C2-N3	-2.12	120.33	125.87
2	A	401	IMP	O6-C6-C5	-2.10	120.28	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	IMP	O6-C6-C5	-2.07	120.34	124.37
2	B	401	IMP	O2P-P-O1P	2.07	118.77	110.68

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	IMP	C5'-O5'-P-O1P
2	A	401	IMP	C5'-O5'-P-O2P
2	A	401	IMP	C5'-O5'-P-O3P
2	C	401	IMP	C5'-O5'-P-O1P
2	C	401	IMP	C5'-O5'-P-O2P
2	C	401	IMP	C5'-O5'-P-O3P
2	D	401	IMP	C5'-O5'-P-O1P
2	D	401	IMP	C5'-O5'-P-O2P
2	D	401	IMP	C5'-O5'-P-O3P
2	D	401	IMP	C3'-C4'-C5'-O5'
2	F	401	IMP	C5'-O5'-P-O1P
2	F	401	IMP	C5'-O5'-P-O2P
2	F	401	IMP	C5'-O5'-P-O3P
2	F	401	IMP	C3'-C4'-C5'-O5'
2	E	401	IMP	C5'-O5'-P-O1P
2	E	401	IMP	C5'-O5'-P-O2P
2	E	401	IMP	C5'-O5'-P-O3P
3	A	402	GOL	O1-C1-C2-C3
2	A	401	IMP	C3'-C4'-C5'-O5'
2	D	401	IMP	O4'-C4'-C5'-O5'
3	A	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O1-C1-C2-O2
2	A	401	IMP	O4'-C4'-C5'-O5'
2	F	401	IMP	O4'-C4'-C5'-O5'
2	E	401	IMP	C3'-C4'-C5'-O5'
2	C	401	IMP	C3'-C4'-C5'-O5'
3	A	402	GOL	O2-C2-C3-O3
2	E	401	IMP	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 9 short contacts:

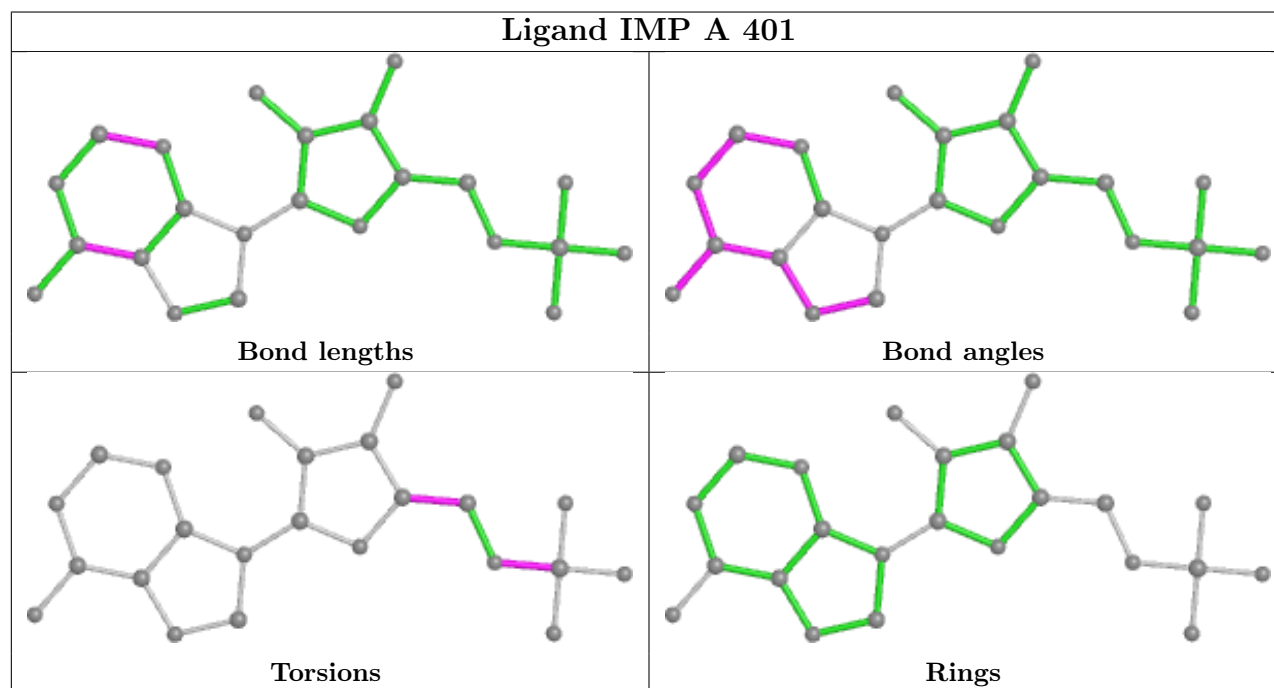
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	IMP	2	0

Continued on next page...

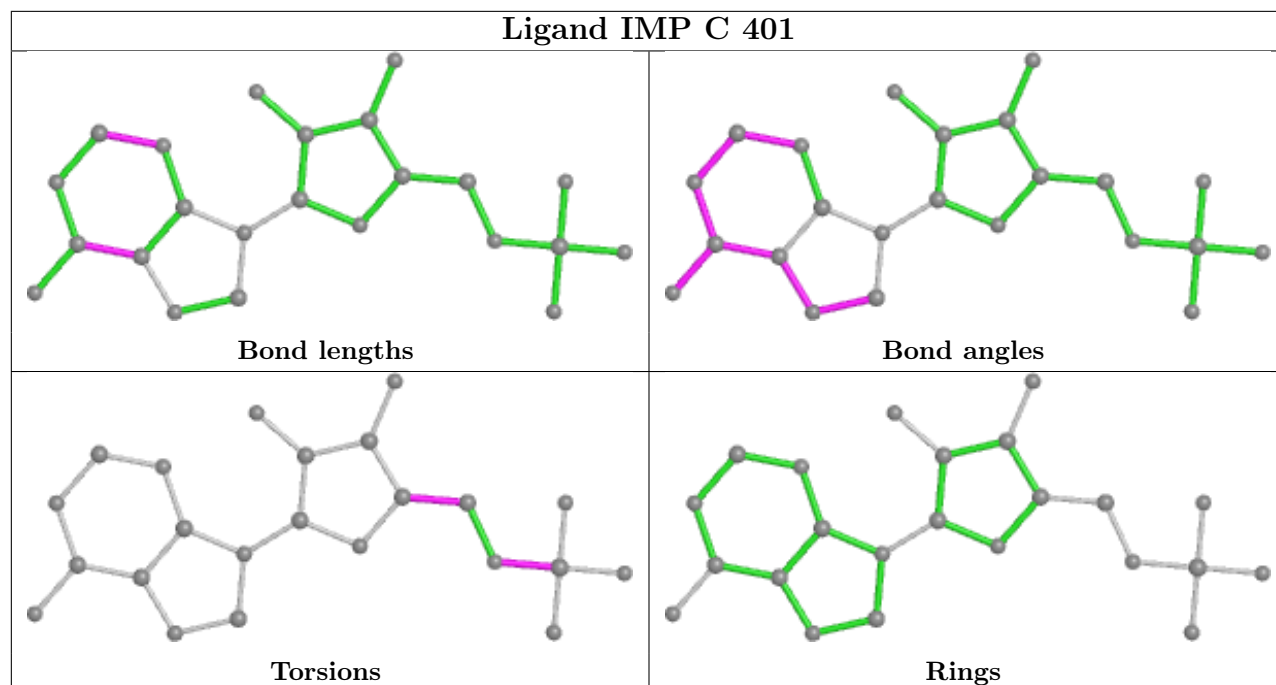
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	IMP	2	0
2	E	401	IMP	2	0
2	F	401	IMP	1	0
3	A	402	GOL	1	0
2	D	401	IMP	1	0

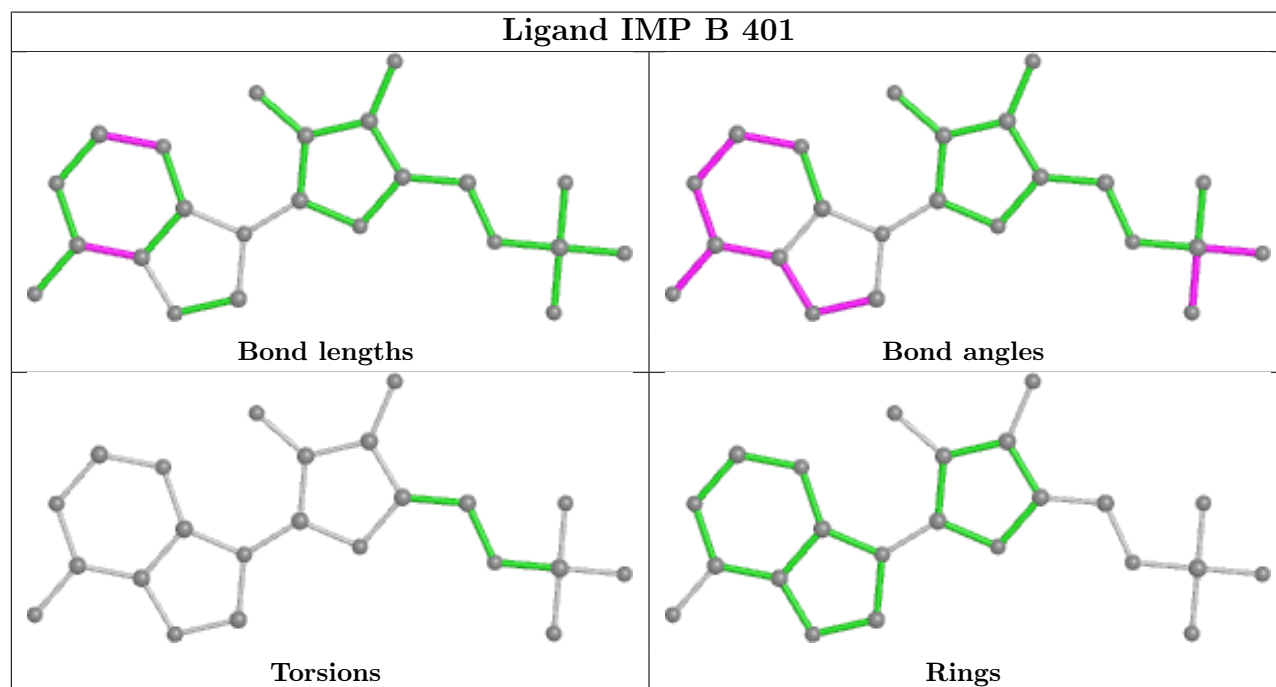
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



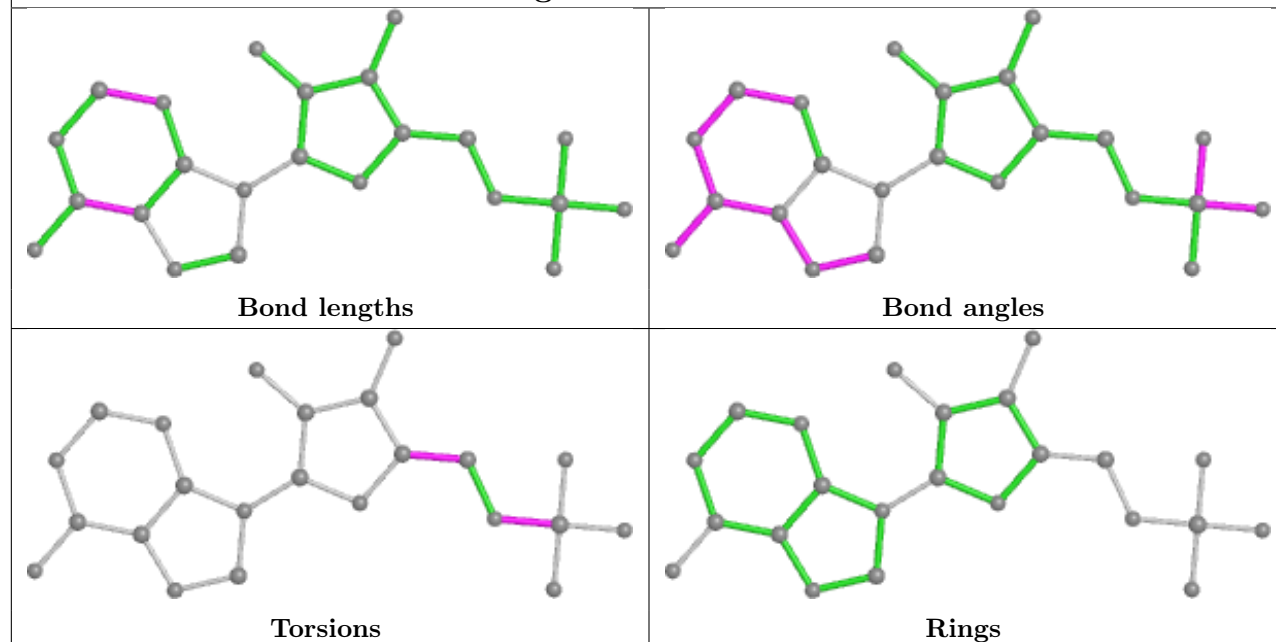
Ligand IMP C 401



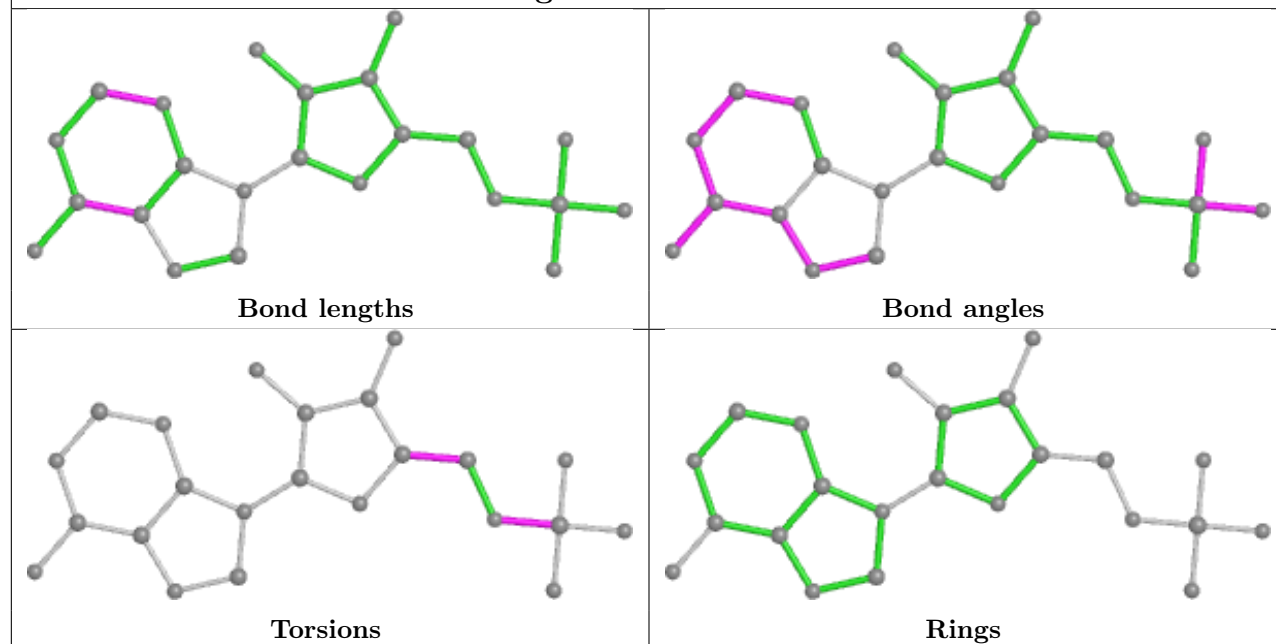
Ligand IMP B 401

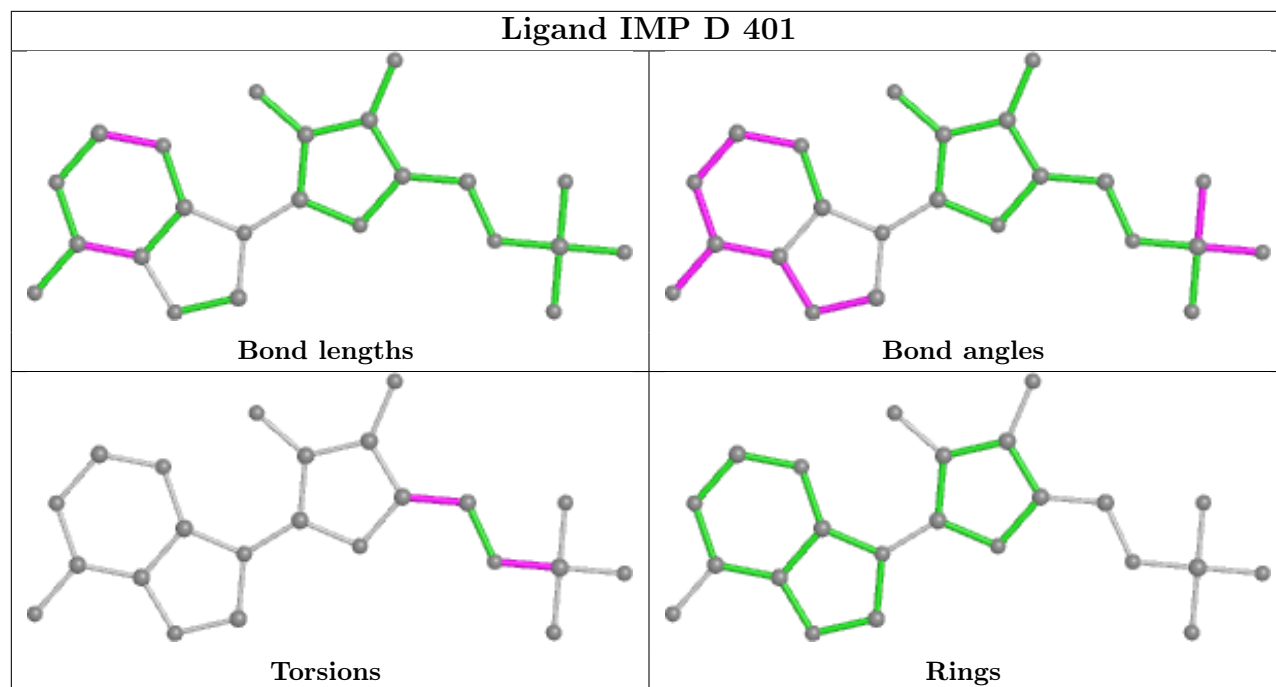


Ligand IMP E 401



Ligand IMP F 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	337/395 (85%)	-0.30	1 (0%) 94 94	13, 26, 53, 81	0
1	B	336/395 (85%)	-0.27	3 (0%) 84 86	18, 33, 61, 88	0
1	C	355/395 (89%)	-0.00	7 (1%) 65 68	28, 47, 73, 105	0
1	D	344/395 (87%)	0.18	16 (4%) 31 33	35, 55, 78, 90	0
1	E	350/395 (88%)	-0.15	4 (1%) 80 82	25, 39, 63, 81	0
1	F	338/395 (85%)	-0.04	5 (1%) 73 75	20, 38, 66, 101	0
All	All	2060/2370 (86%)	-0.10	36 (1%) 70 72	13, 41, 70, 105	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	0	MET	7.2
1	D	4	PHE	6.5
1	C	2	PHE	5.8
1	F	372	THR	5.4
1	C	3	TYR	5.0
1	D	213	ARG	4.7
1	E	3	TYR	3.9
1	C	6	GLU	3.9
1	D	47	ILE	3.2
1	C	25	CYS	3.0
1	D	3	TYR	3.0
1	D	99	LYS	2.9
1	D	218	ILE	2.8
1	C	26	VAL	2.7
1	D	324	VAL	2.7
1	E	2	PHE	2.6
1	B	25	CYS	2.6
1	F	26	VAL	2.6
1	C	4	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	19	GLY	2.5
1	F	29	ASN	2.5
1	D	176	VAL	2.5
1	F	371	SER	2.4
1	A	4	PHE	2.4
1	D	93	SER	2.3
1	D	19	GLY	2.3
1	D	165	LEU	2.3
1	B	238	GLU	2.2
1	D	44	GLU	2.2
1	D	236	TYR	2.2
1	D	323	GLY	2.2
1	D	310	TYR	2.1
1	E	4	PHE	2.1
1	C	254[A]	TYR	2.1
1	D	288	LEU	2.1
1	F	4	PHE	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 monosaccharides 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
4	FMT	F	402	3/3	0.88	0.43	51,51,54,57	0
4	FMT	A	403	3/3	0.92	0.22	30,30,41,41	0
3	GOL	A	402	6/6	0.96	0.23	27,36,37,41	0
2	IMP	F	401	23/23	0.97	0.15	21,26,50,52	0
2	IMP	B	401	23/23	0.97	0.14	21,31,42,51	0
2	IMP	D	401	23/23	0.98	0.12	32,42,49,55	0

Continued on next page...

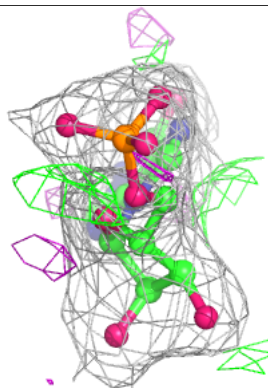
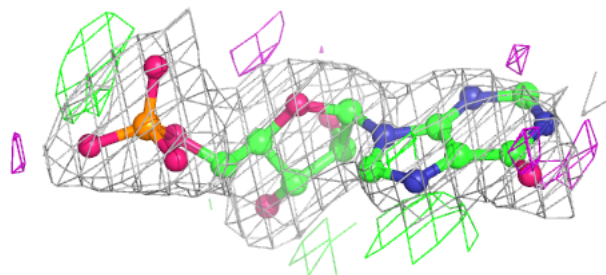
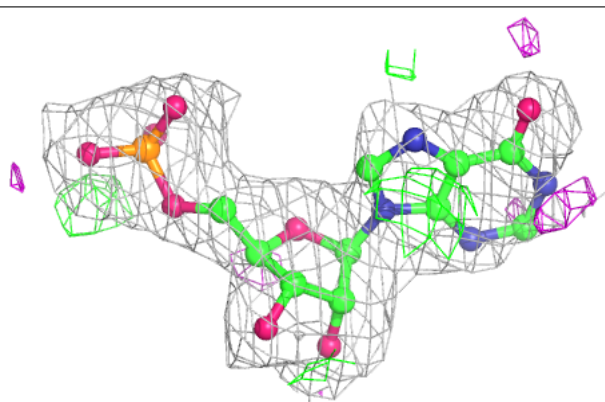
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IMP	A	401	23/23	0.98	0.13	14,25,31,37	0
2	IMP	E	401	23/23	0.98	0.13	19,31,41,43	0
2	IMP	C	401	23/23	0.99	0.15	24,34,42,56	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.

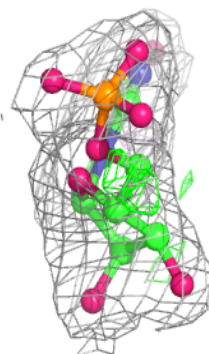
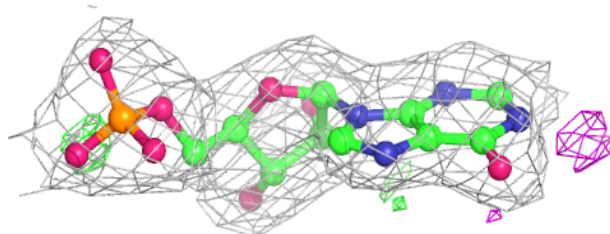
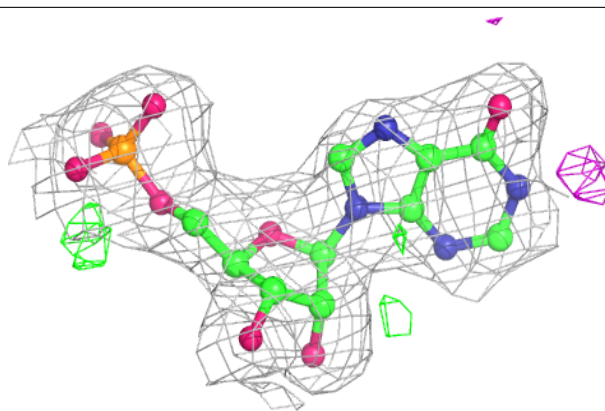
Electron density around IMP F 401:

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

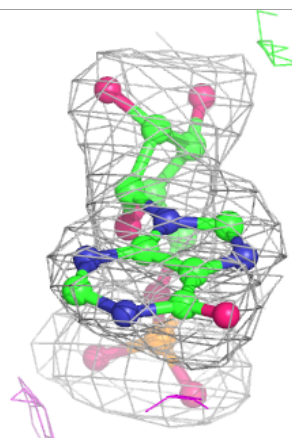
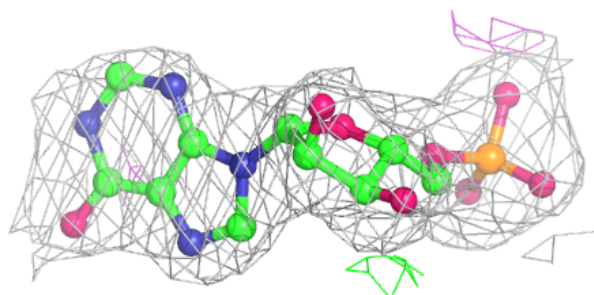
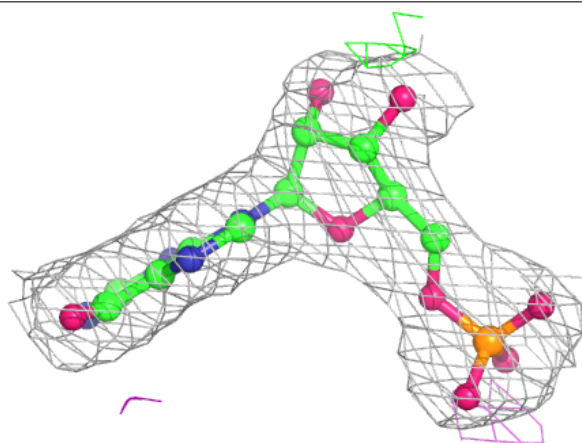


Electron density around IMP B 401:

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

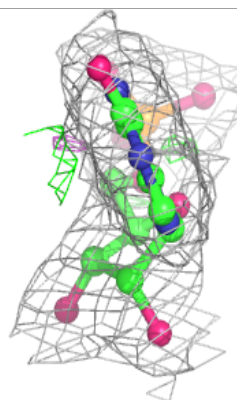
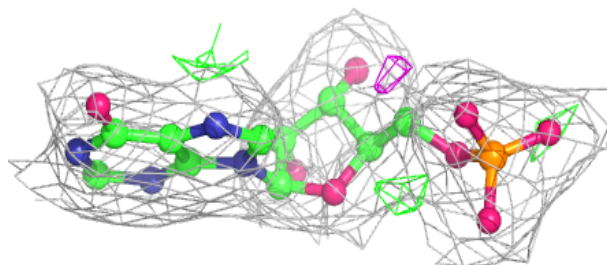
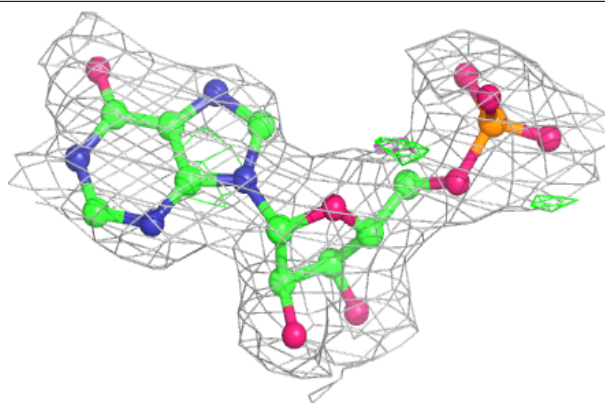
**Electron density around IMP D 401:**

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

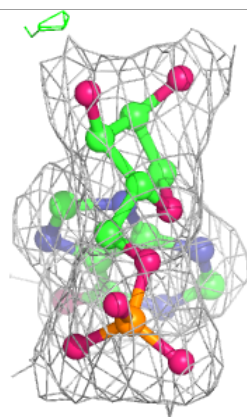
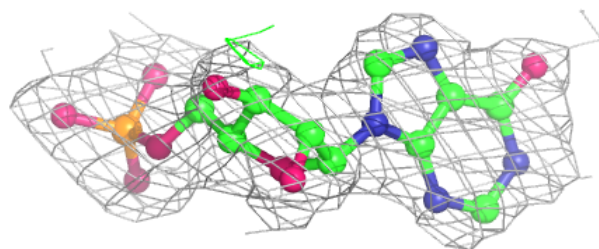
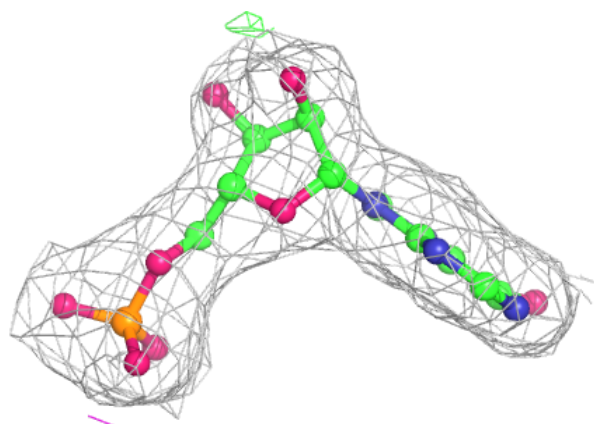


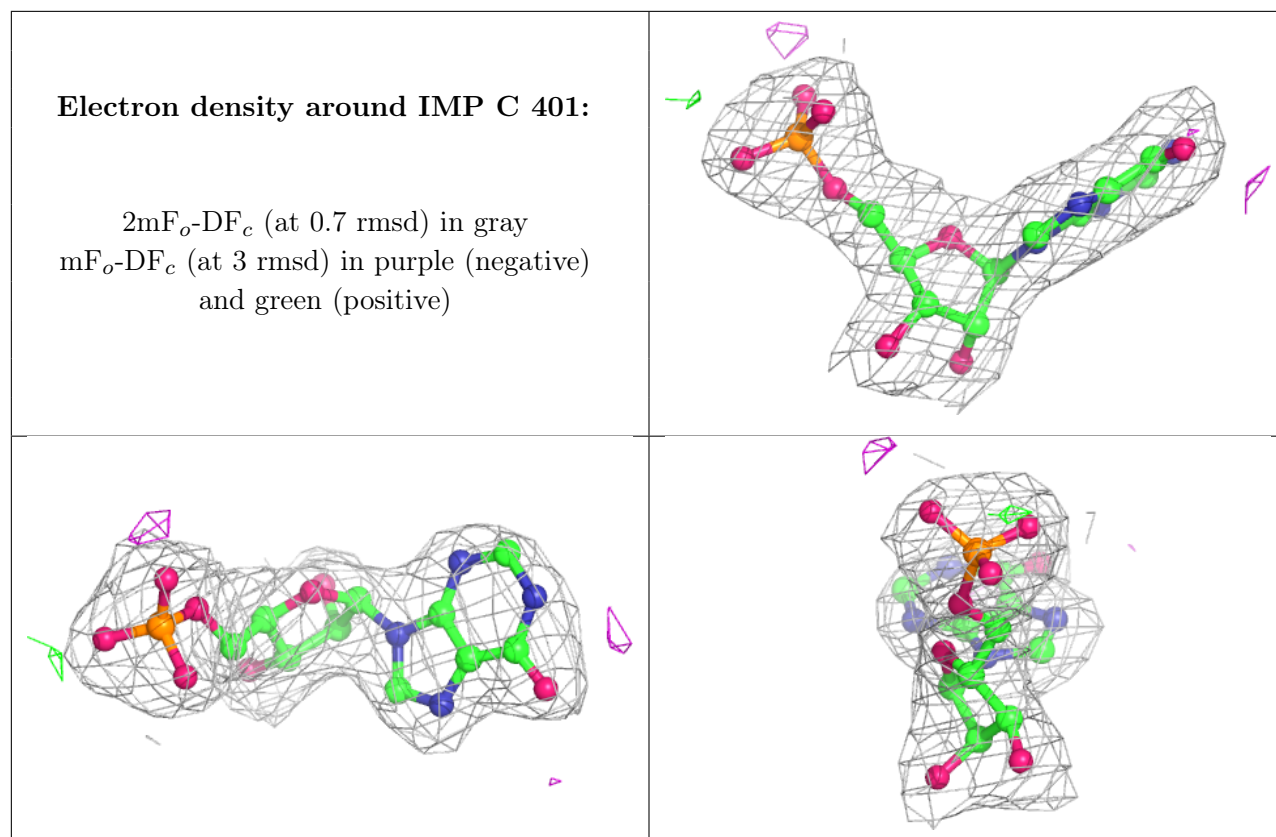
Electron density around IMP A 401:

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

**Electron density around IMP E 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.