Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2026 – 06:31 PM EST

PDB ID	:	5UZC / pdb_00005uzc
Title	:	Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from Clostridium perfringens Complexed with IMP and P221
Authors	:	Maltseva, N.; Kim, Y.; Mulligan, R.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.R.; Hedstrom, L.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2017-02-26
Resolution	:	1.85 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 (1)) were used in the production of this report:

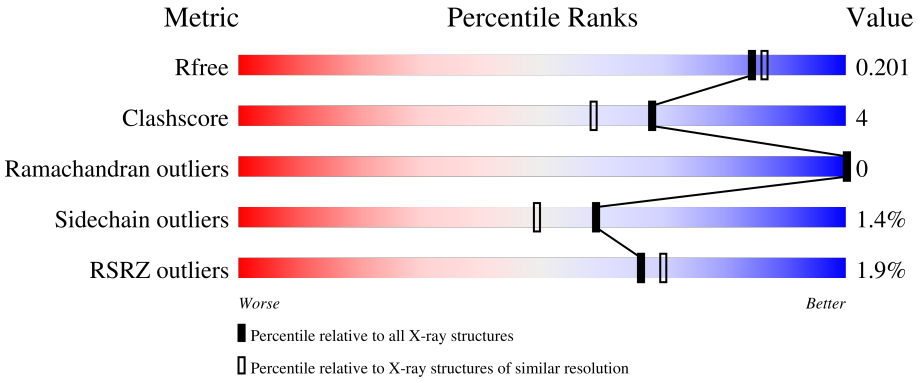
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 <=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	363	2% 86% 8% 5%
1	B	363	2% 84% 11%
1	C	363	% 84% 10% 6%
1	D	363	% 88% 7% 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11053 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
1	A	344	Total	C	N	O	S	0	5	0
			2577	1619	446	492	20			
1	B	347	Total	C	N	O	S	0	5	0
			2595	1627	447	501	20			
1	C	342	Total	C	N	O	S	0	3	0
			2546	1598	438	491	19			
1	D	345	Total	C	N	O	S	0	6	0
			2586	1619	449	498	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0H2YRZ7
A	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
A	0	ALA	-	expression tag	UNP A0A0H2YRZ7
A	89	SER	LYS	linker	UNP A0A0H2YRZ7
A	90	GLY	GLY	linker	UNP A0A0H2YRZ7
A	91	GLY	ARG	linker	UNP A0A0H2YRZ7
B	-2	SER	-	expression tag	UNP A0A0H2YRZ7
B	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
B	0	ALA	-	expression tag	UNP A0A0H2YRZ7
B	89	SER	LYS	linker	UNP A0A0H2YRZ7
B	90	GLY	GLY	linker	UNP A0A0H2YRZ7
B	91	GLY	ARG	linker	UNP A0A0H2YRZ7
C	-2	SER	-	expression tag	UNP A0A0H2YRZ7
C	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
C	0	ALA	-	expression tag	UNP A0A0H2YRZ7
C	89	SER	LYS	linker	UNP A0A0H2YRZ7
C	90	GLY	GLY	linker	UNP A0A0H2YRZ7
C	91	GLY	ARG	linker	UNP A0A0H2YRZ7
D	-2	SER	-	expression tag	UNP A0A0H2YRZ7
D	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
D	0	ALA	-	expression tag	UNP A0A0H2YRZ7

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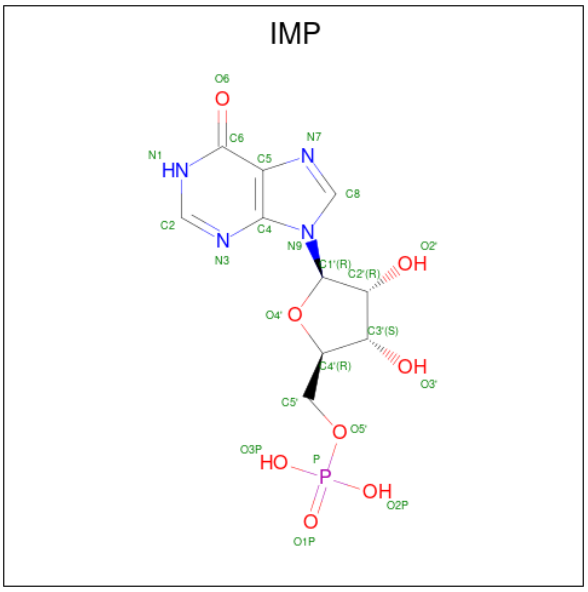
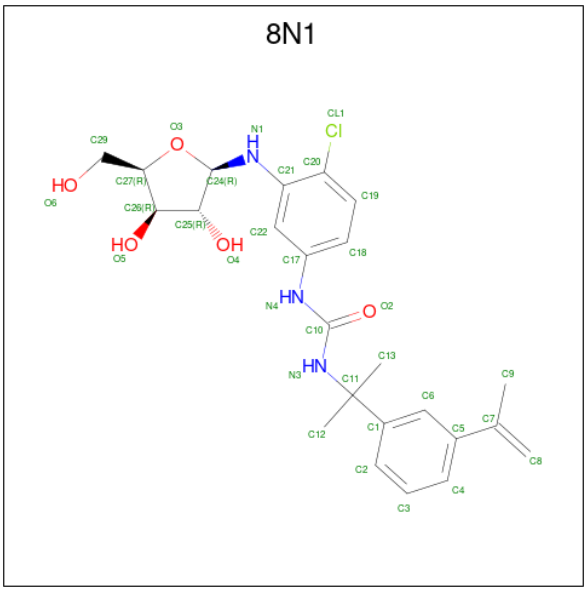
Chain	Residue	Modelled	Actual	Comment	Reference
D	89	SER	LYS	linker	UNP A0A0H2YRZ7
D	90	GLY	GLY	linker	UNP A0A0H2YRZ7
D	91	GLY	ARG	linker	UNP A0A0H2YRZ7

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



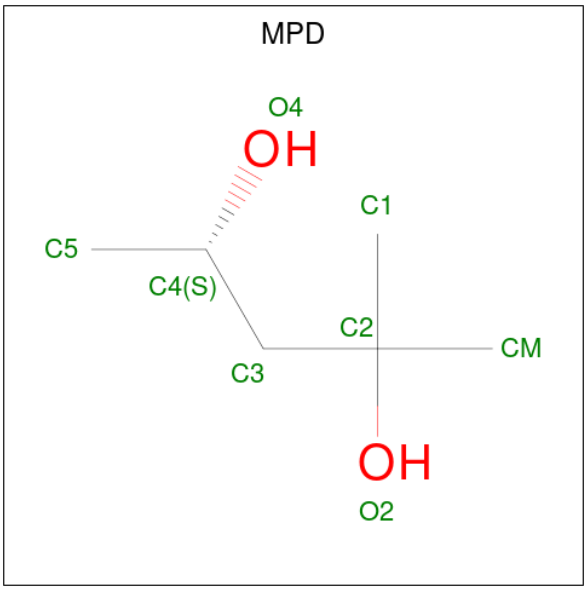
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-{2-chloro-5-[({2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}carbamoyl)amino]phenyl}-beta-D-xylofuranosylamine (CCD ID: 8N1) (formula: $C_{24}H_{30}ClN_3O_5$).



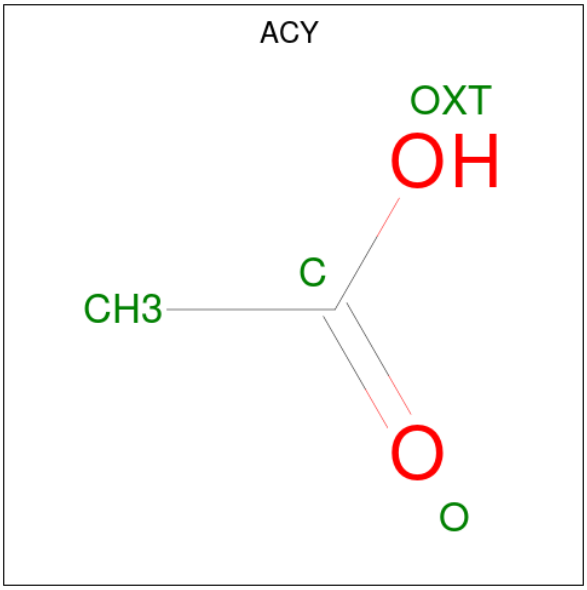
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
3	B	1	Total	C	Cl	N	O	0	1
			66	48	2	6	10		
3	C	1	Total	C	Cl	N	O	0	1
			66	48	2	6	10		
3	D	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



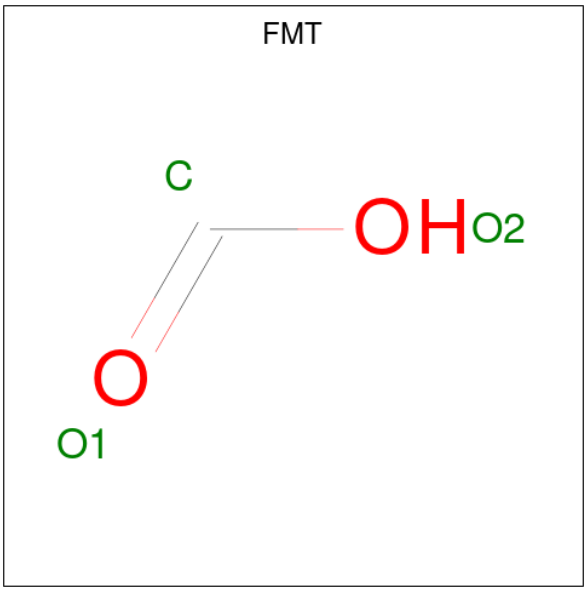
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



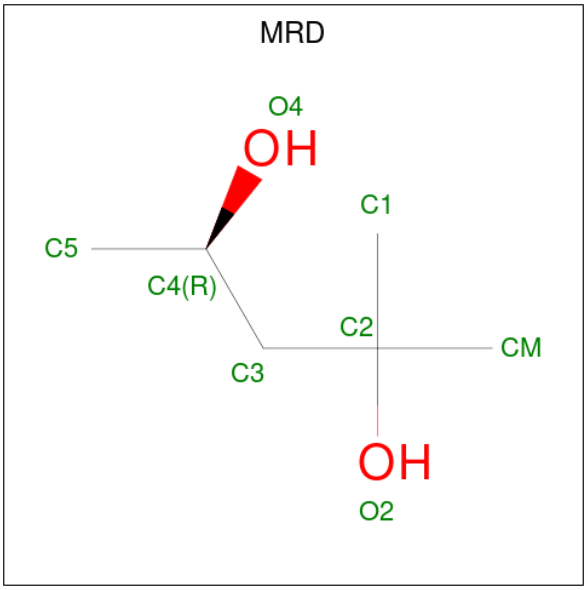
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

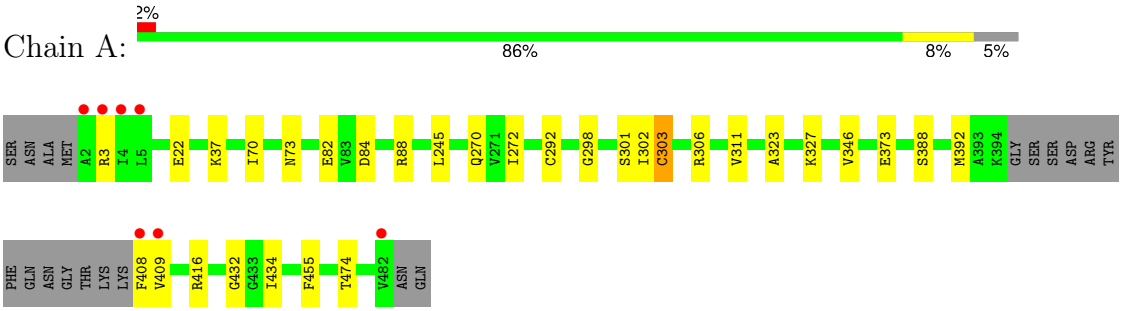
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	125	Total O 125 125	0	0
8	B	114	Total O 114 114	0	0
8	C	75	Total O 75 75	0	0
8	D	95	Total O 95 95	0	0

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.

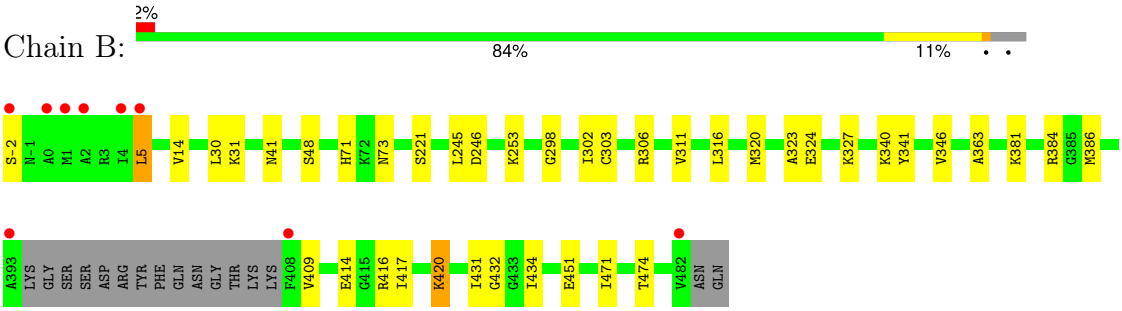
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



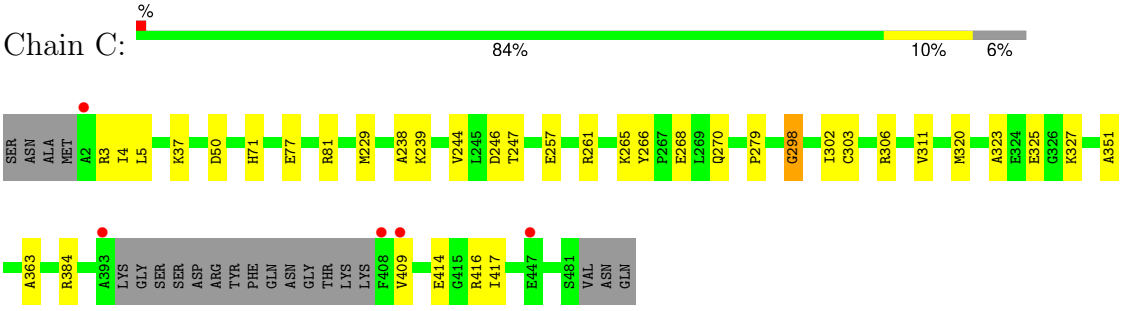
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:



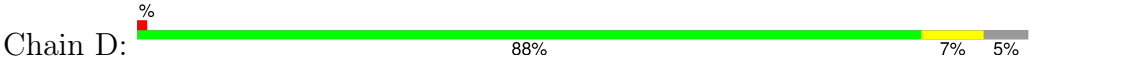
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

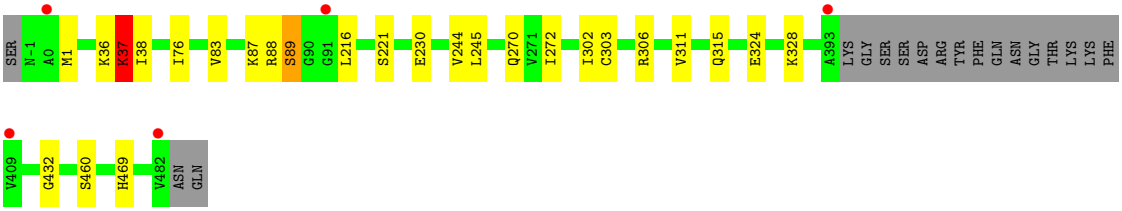
Chain C:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:




SER
N-1
A0
M1
K36
K37
I38
I76
V83
K87
R88
S89
G90
G91
L216
S221
E230
V244
L245
Q270
V271
I272
I302
C303
R306
V311
Q315
E324
K328
A393
LYS
GLY
SER
SER
ASP
ARG
TYR
PHE
GLN
ASN
GLY
THR
LYS
LYS
PHE

V409
G432
S460
H469
V482
ASN
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.02Å 119.31Å 97.20Å 90.00° 102.83° 90.00°	Depositor
Resolution (Å)	44.51 – 1.85 44.51 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.51-1.85) 99.3 (44.51-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.171 , 0.201 0.172 , 0.201	Depositor DCC
R_{free} test set	5935 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11053	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 8N1, ACY, FMT, MRD, IMP, MPD

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	0.53	0/2610	0.71	2/3521 (0.1%)
1	B	0.48	0/2628	0.65	2/3545 (0.1%)
1	C	0.43	1/2579 (0.0%)	0.63	4/3480 (0.1%)
1	D	0.50	0/2618	0.72	3/3531 (0.1%)
All	All	0.49	1/10435 (0.0%)	0.68	11/14077 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	GLY	C-N	6.14	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	GLN	N-CA-C	10.16	122.36	111.28
1	D	38	ILE	N-CA-C	7.52	118.71	107.80
1	C	5	LEU	N-CA-C	7.23	118.95	111.14
1	A	245	LEU	N-CA-C	-5.91	97.59	107.99
1	D	37	LYS	N-CA-C	5.66	117.53	111.36
1	C	298	GLY	CA-C-N	-5.56	114.16	120.89
1	C	298	GLY	C-N-CA	-5.56	114.16	120.89
1	B	245	LEU	N-CA-C	-5.53	98.72	108.23
1	B	246	ASP	N-CA-C	5.16	117.03	108.20
1	A	303	CYS	N-CA-C	5.10	118.53	109.96
1	C	298	GLY	N-CA-C	5.06	122.67	112.34

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	2577	0	2645	18	0
1	B	2595	0	2651	28	0
1	C	2546	0	2598	25	0
1	D	2586	0	2648	12	0
2	A	23	0	11	2	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	33	0	0	1	0
3	B	66	0	0	0	0
3	C	66	0	0	1	0
3	D	33	0	0	0	0
4	A	8	0	14	1	0
4	B	8	0	14	0	0
4	D	8	0	14	1	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	3	0	1	1	0
6	B	3	0	1	0	0
7	C	8	0	14	0	0
8	A	125	0	0	0	0
8	B	114	0	0	3	0
8	C	75	0	0	0	0
8	D	95	0	0	0	0
All	All	11053	0	10653	76	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 (76) 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:D:303:CYS:SG	2:D:500:IMP:H2	2.36	0.66
1:A:409:VAL:HG21	1:D:432:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:CYS:SG	2:A:501:IMP:H2	2.39	0.62
1:C:303:CYS:SG	2:C:500:IMP:H2	2.43	0.59
1:C:298:GLY:HA2	1:C:303:CYS:SG	2.43	0.58
1:B:303:CYS:SG	2:B:501:IMP:H2	2.44	0.58
1:A:432:GLY:HA3	1:B:409:VAL:HG21	1.86	0.57
1:C:320:MET:HG3	1:C:351:ALA:HB1	1.86	0.57
1:C:37:LYS:NZ	1:C:268:GLU:OE1	2.39	0.56
1:A:298:GLY:HA2	1:A:303:CYS:SG	2.46	0.56
1:B:73:ASN:HB2	1:B:386:MET:HE1	1.88	0.56
1:C:265:LYS:HD3	1:C:266:TYR:CE2	2.41	0.55
1:A:323:ALA:O	1:A:327:LYS:HG2	2.05	0.55
1:C:3:ARG:HG3	1:C:4:ILE:N	2.22	0.55
1:C:323:ALA:O	1:C:327:LYS:HG2	2.07	0.54
1:B:420[B]:LYS:HD2	8:B:629:HOH:O	2.06	0.54
1:B:451:GLU:HG3	8:B:708:HOH:O	2.10	0.52
1:A:84:ASP:O	1:A:88:ARG:HG3	2.10	0.51
1:A:474:THR:HG21	1:B:416:ARG:HD2	1.92	0.51
3:A:502:8N1:O6	3:A:502:8N1:O5	2.24	0.51
1:C:244:VAL:HG12	1:C:246:ASP:HB3	1.93	0.50
1:A:346:VAL:HG22	1:A:434:ILE:HA	1.93	0.50
1:A:306:ARG:HG2	1:A:311:VAL:O	2.11	0.50
1:B:320:MET:HE1	1:C:4:ILE:HD11	1.94	0.50
1:B:14:VAL:HG21	1:B:316:LEU:HD22	1.95	0.49
1:B:346:VAL:HG22	1:B:434:ILE:HA	1.95	0.49
1:B:340:LYS:HE2	1:B:341:TYR:CZ	2.48	0.49
1:B:381:LYS:NZ	8:B:601:HOH:O	2.45	0.49
1:C:77[A]:GLU:OE1	1:C:81:ARG:NH2	2.36	0.48
1:A:22:GLU:HG2	1:B:253:LYS:HB2	1.96	0.47
1:A:303:CYS:HB2	2:A:501:IMP:C2	2.44	0.47
1:B:302:ILE:C	1:B:302:ILE:HD12	2.39	0.47
1:B:31:LYS:NZ	1:B:41:ASN:OD1	2.47	0.47
1:B:298:GLY:HA2	1:B:303:CYS:SG	2.54	0.47
1:B:471:ILE:HD13	1:C:302:ILE:HG22	1.97	0.47
1:D:37:LYS:HD2	1:D:270:GLN:NE2	2.30	0.47
1:A:272:ILE:HG12	1:A:292:CYS:HB3	1.97	0.46
1:B:48[B]:SER:OG	1:B:71:HIS:HA	2.15	0.46
1:C:37:LYS:HE3	1:C:270:GLN:NE2	2.31	0.46
1:C:384:ARG:HB3	1:C:414[A]:GLU:HG3	1.97	0.46
1:B:432:GLY:HA3	1:C:409:VAL:HG21	1.98	0.46
1:C:3:ARG:NH2	1:C:4:ILE:H	2.13	0.46
1:A:455:PHE:HB2	1:B:5:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ARG:HB3	1:B:414[A]:GLU:HG3	1.98	0.45
1:B:306:ARG:HG2	1:B:311:VAL:O	2.16	0.45
1:A:301:SER:HB2	1:D:469:HIS:O	2.16	0.45
1:A:388:SER:O	1:A:392[A]:MET:HG3	2.16	0.45
1:B:474:THR:HG21	1:C:416:ARG:HD2	1.98	0.45
1:B:48[B]:SER:OG	1:B:221:SER:HB2	2.17	0.44
1:C:298:GLY:HA3	1:C:306:ARG:HG3	2.00	0.44
1:B:323:ALA:O	1:B:327:LYS:HG2	2.18	0.43
6:A:505:FMT:H	1:D:460[B]:SER:OG	2.17	0.43
1:D:244:VAL:HG22	1:D:272:ILE:HB	1.99	0.43
1:D:76:ILE:HD13	1:D:230[B]:GLU:HG2	2.01	0.43
4:A:503:MPD:O2	4:A:503:MPD:H52	2.19	0.43
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.86	0.42
1:B:302:ILE:C	1:B:302:ILE:CD1	2.92	0.42
1:B:363:ALA:HB3	1:B:417:ILE:HD11	2.02	0.42
1:C:247:THR:HB	3:C:501[A]:8N1:O4	2.19	0.42
1:D:89:SER:O	1:D:216:LEU:HG	2.20	0.42
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.54	0.42
1:C:238:ALA:C	1:C:239:LYS:HG2	2.45	0.42
1:D:83:VAL:O	1:D:87:LYS:HG2	2.20	0.42
4:D:502:MPD:O2	4:D:502:MPD:H52	2.20	0.42
1:C:306:ARG:HG2	1:C:311:VAL:O	2.21	0.41
1:A:70:ILE:HD12	1:A:82:GLU:HB3	2.02	0.41
1:B:30:LEU:HD13	1:B:431:ILE:HD12	2.01	0.41
1:A:373:GLU:OE2	1:A:416:ARG:NH1	2.52	0.41
1:C:229:MET:HE2	1:C:265:LYS:HD3	2.02	0.41
1:C:279:PRO:HB3	1:C:325:GLU:HB2	2.02	0.41
1:D:306:ARG:HG2	1:D:311:VAL:O	2.21	0.41
1:A:37:LYS:HD2	1:A:270:GLN:NE2	2.36	0.40
1:B:346:VAL:CG2	1:B:434:ILE:HA	2.51	0.40
1:C:257:GLU:O	1:C:261:ARG:HG3	2.22	0.40
1:C:363:ALA:HB3	1:C:417:ILE:HD11	2.04	0.40
1:D:324:GLU:O	1:D:328:LYS:HG3	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	345/363 (95%)	337 (98%)	8 (2%)	0	100	100
1	B	348/363 (96%)	339 (97%)	9 (3%)	0	100	100
1	C	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	D	347/363 (96%)	340 (98%)	7 (2%)	0	100	100
All	All	1381/1452 (95%)	1348 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/282 (96%)	267 (98%)	4 (2%)	57	47
1	B	273/282 (97%)	267 (98%)	6 (2%)	45	32
1	C	267/282 (95%)	267 (100%)	0	100	100
1	D	272/282 (96%)	265 (97%)	7 (3%)	40	25
All	All	1083/1128 (96%)	1066 (98%)	17 (2%)	59	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	73	ASN

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Mol	Chain	Res	Type
1	A	302	ILE
1	A	408	PHE
1	B	-2	SER
1	B	5	LEU
1	B	324[A]	GLU
1	B	324[B]	GLU
1	B	420[A]	LYS
1	B	420[B]	LYS
1	D	1	MET
1	D	36	LYS
1	D	37	LYS
1	D	88	ARG
1	D	89	SER
1	D	221	SER
1	D	302	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	B	39	GLN
1	B	452	ASN
1	C	33	GLN
1	C	39	GLN
1	C	454	ASN
1	D	33	GLN
1	D	39	GLN
1	D	448	ASN
1	D	452	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	ACY	D	503	-	3,3,3	0.87	0	3,3,3	0.71	0
2	IMP	A	501	-	25,25,25	0.99	1 (4%)	37,38,38	1.81	9 (24%)
3	8N1	B	502[A]	-	35,35,35	1.14	5 (14%)	51,51,51	1.57	2 (3%)
7	MRD	C	502	-	7,7,7	0.42	0	9,10,10	0.48	0
2	IMP	C	500	-	25,25,25	1.02	1 (4%)	37,38,38	2.15	9 (24%)
5	ACY	C	503	-	3,3,3	0.83	0	3,3,3	0.80	0
2	IMP	B	501	-	25,25,25	1.03	1 (4%)	37,38,38	1.98	11 (29%)
4	MPD	D	502	-	7,7,7	0.37	0	9,10,10	0.85	0
4	MPD	A	503	-	7,7,7	0.40	0	9,10,10	0.61	0
3	8N1	C	501[A]	-	35,35,35	1.14	5 (14%)	51,51,51	1.58	2 (3%)
3	8N1	B	502[B]	-	35,35,35	1.31	5 (14%)	51,51,51	1.58	5 (9%)
6	FMT	B	504	-	2,2,2	0.68	0	1,1,1	0.24	0
6	FMT	A	505	-	2,2,2	0.71	0	1,1,1	0.10	0
3	8N1	A	502	-	35,35,35	1.38	5 (14%)	51,51,51	2.04	9 (17%)
4	MPD	B	503	-	7,7,7	0.38	0	9,10,10	0.53	0
3	8N1	D	501	-	35,35,35	1.32	5 (14%)	51,51,51	1.79	9 (17%)
3	8N1	C	501[B]	-	35,35,35	1.16	5 (14%)	51,51,51	1.50	3 (5%)
5	ACY	A	504	-	3,3,3	0.78	0	3,3,3	0.87	0
2	IMP	D	500	-	25,25,25	1.08	1 (4%)	37,38,38	2.17	10 (27%)

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
7	MRD	C	502	-	-	5/5/5/5	-
3	8N1	C	501[B]	-	-	1/25/41/41	0/3/3/3
2	IMP	C	500	-	-	0/10/26/26	0/3/3/3
4	MPD	B	503	-	-	4/5/5/5	-
3	8N1	A	502	-	-	3/25/41/41	0/3/3/3
4	MPD	D	502	-	-	3/5/5/5	-
2	IMP	B	501	-	-	0/10/26/26	0/3/3/3
2	IMP	A	501	-	-	0/10/26/26	0/3/3/3
2	IMP	D	500	-	-	0/10/26/26	0/3/3/3
4	MPD	A	503	-	-	1/5/5/5	-
3	8N1	C	501[A]	-	-	2/25/41/41	0/3/3/3
3	8N1	B	502[A]	-	-	2/25/41/41	0/3/3/3
3	8N1	B	502[B]	-	-	2/25/41/41	0/3/3/3
3	8N1	D	501	-	-	2/25/41/41	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	8N1	C11-C1	-5.63	1.47	1.53
3	D	501	8N1	C11-C1	-4.77	1.48	1.53
3	B	502[B]	8N1	C11-C1	-4.60	1.48	1.53
2	B	501	IMP	C2-N3	4.42	1.38	1.30
2	C	500	IMP	C2-N3	4.30	1.38	1.30
2	D	500	IMP	C2-N3	3.96	1.37	1.30
3	C	501[B]	8N1	C11-C1	-3.89	1.49	1.53
2	A	501	IMP	C2-N3	3.73	1.37	1.30
3	C	501[A]	8N1	C11-C1	-3.68	1.49	1.53
3	B	502[A]	8N1	C11-C1	-3.49	1.49	1.53
3	A	502	8N1	C24-N1	2.94	1.47	1.42
3	B	502[B]	8N1	C24-N1	2.89	1.47	1.42
3	D	501	8N1	C20-CL1	2.86	1.80	1.73
3	C	501[A]	8N1	C9-C7	-2.82	1.32	1.46
3	C	501[B]	8N1	C9-C7	-2.81	1.32	1.46
3	D	501	8N1	C9-C7	-2.78	1.32	1.46
3	B	502[A]	8N1	C9-C7	-2.74	1.33	1.46
3	C	501[A]	8N1	C20-CL1	2.70	1.80	1.73
3	C	501[B]	8N1	C20-CL1	2.61	1.79	1.73
3	B	502[B]	8N1	C9-C7	-2.61	1.33	1.46
3	B	502[A]	8N1	C20-CL1	2.60	1.79	1.73
3	B	502[B]	8N1	C20-CL1	2.58	1.79	1.73
3	D	501	8N1	C24-N1	2.53	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	8N1	C24-N1	2.44	1.46	1.42
3	B	502[B]	8N1	C17-N4	-2.36	1.36	1.41
3	A	502	8N1	C9-C7	-2.35	1.34	1.46
3	A	502	8N1	C20-CL1	2.32	1.79	1.73
3	B	502[A]	8N1	C17-N4	-2.30	1.37	1.41
3	D	501	8N1	C17-N4	-2.21	1.37	1.41
3	C	501[A]	8N1	C17-N4	-2.19	1.37	1.41
3	A	502	8N1	C17-N4	-2.16	1.37	1.41
3	C	501[B]	8N1	C17-N4	-2.15	1.37	1.41
3	C	501[A]	8N1	C24-N1	2.03	1.45	1.42
3	C	501[B]	8N1	C24-N1	2.02	1.45	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	8N1	C25-C24-N1	-8.84	100.91	112.02
3	D	501	8N1	C25-C24-N1	-8.73	101.05	112.02
3	C	501[A]	8N1	C25-C24-N1	-8.66	101.14	112.02
3	B	502[A]	8N1	C25-C24-N1	-7.86	102.15	112.02
3	C	501[B]	8N1	C25-C24-N1	-7.56	102.52	112.02
3	B	502[B]	8N1	C25-C24-N1	-7.36	102.77	112.02
2	C	500	IMP	C5-C6-N1	6.27	119.79	110.78
3	A	502	8N1	C21-N1-C24	-6.09	117.14	123.18
2	B	501	IMP	C5-C6-N1	5.80	119.11	110.78
2	D	500	IMP	C5-C6-N1	5.56	118.78	110.78
2	A	501	IMP	C5-C6-N1	5.16	118.19	110.78
3	B	502[A]	8N1	C21-N1-C24	-4.92	118.30	123.18
2	D	500	IMP	C5-C4-N3	-4.87	120.10	127.27
2	C	500	IMP	C2-N1-C6	-4.79	118.52	125.09
2	C	500	IMP	C5-C4-N3	-4.71	120.34	127.27
2	D	500	IMP	C2-N1-C6	-4.63	118.75	125.09
2	A	501	IMP	N1-C2-N3	-4.37	120.47	125.50
2	D	500	IMP	C2-N3-C4	4.31	119.12	111.53
2	C	500	IMP	C2-N3-C4	4.30	119.09	111.53
3	B	502[B]	8N1	C21-N1-C24	-4.01	119.20	123.18
3	C	501[A]	8N1	C21-N1-C24	-3.99	119.22	123.18
2	B	501	IMP	C2-N3-C4	3.96	118.49	111.53
3	A	502	8N1	C29-C27-C26	-3.94	105.79	115.10
2	A	501	IMP	C2-N3-C4	3.90	118.39	111.53
2	B	501	IMP	C2-N1-C6	-3.73	119.97	125.09
2	D	500	IMP	C8-N7-C5	3.70	110.85	104.26
2	D	500	IMP	N9-C8-N7	-3.66	106.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	IMP	C5-C4-N3	-3.43	122.23	127.27
2	B	501	IMP	N1-C2-N3	-3.39	121.59	125.50
3	A	502	8N1	O3-C24-N1	3.36	114.04	110.22
3	D	501	8N1	C29-C27-C26	-3.26	107.41	115.10
2	D	500	IMP	C4-C5-N7	-3.25	105.51	110.67
2	C	500	IMP	N9-C8-N7	-3.22	107.42	113.40
3	C	501[B]	8N1	C21-N1-C24	-3.17	120.04	123.18
3	A	502	8N1	C13-C11-C12	-3.09	106.04	109.50
2	C	500	IMP	C8-N7-C5	3.02	109.64	104.26
2	A	501	IMP	C5-C4-N3	-2.95	122.93	127.27
2	B	501	IMP	N9-C8-N7	-2.94	107.96	113.40
3	C	501[B]	8N1	C29-C27-C26	-2.74	108.63	115.10
3	D	501	8N1	O2-C10-N3	-2.72	119.08	123.79
2	A	501	IMP	N9-C8-N7	-2.71	108.37	113.40
2	C	500	IMP	N1-C2-N3	-2.67	122.42	125.50
2	B	501	IMP	C8-N7-C5	2.61	108.91	104.26
2	C	500	IMP	C4-C5-N7	-2.60	106.55	110.67
3	D	501	8N1	C21-N1-C24	-2.55	120.65	123.18
2	A	501	IMP	C6-C5-N7	2.50	134.84	130.29
2	A	501	IMP	C2-N1-C6	-2.50	121.66	125.09
3	D	501	8N1	C11-N3-C10	2.42	129.04	124.01
2	A	501	IMP	C4-C5-N7	-2.41	106.85	110.67
2	D	500	IMP	O6-C6-N1	-2.41	116.14	120.75
3	B	502[B]	8N1	C13-C11-C12	-2.39	106.83	109.50
2	B	501	IMP	C6-C5-N7	2.38	134.63	130.29
2	B	501	IMP	C4-C5-N7	-2.37	106.92	110.67
2	A	501	IMP	C8-N7-C5	2.36	108.46	104.26
2	B	501	IMP	C1'-N9-C4	-2.33	119.61	126.49
3	A	502	8N1	C2-C1-C6	2.31	122.31	117.86
2	D	500	IMP	N1-C2-N3	-2.29	122.86	125.50
3	D	501	8N1	C20-C21-N1	-2.27	119.27	120.43
3	A	502	8N1	O2-C10-N3	-2.23	119.93	123.79
3	D	501	8N1	C6-C1-C11	-2.21	117.18	120.63
3	A	502	8N1	C3-C2-C1	-2.20	118.52	120.75
2	C	500	IMP	O6-C6-N1	-2.20	116.54	120.75
3	B	502[B]	8N1	C3-C2-C1	-2.18	118.54	120.75
3	D	501	8N1	C1-C11-N3	2.14	113.70	110.81
3	A	502	8N1	O6-C29-C27	-2.12	104.11	111.33
3	B	502[B]	8N1	C29-C27-C26	-2.11	110.10	115.10
2	D	500	IMP	C6-C5-N7	2.10	134.11	130.29
2	B	501	IMP	O6-C6-C5	-2.05	121.11	126.53
3	D	501	8N1	C6-C5-C7	-2.00	116.91	120.27

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	MPD	C2-C3-C4-C5
7	C	502	MRD	C2-C3-C4-O4
7	C	502	MRD	C2-C3-C4-C5
3	B	502[B]	8N1	O3-C24-N1-C21
3	C	501[B]	8N1	O3-C24-N1-C21
3	D	501	8N1	O3-C24-N1-C21
4	D	502	MPD	CM-C2-C3-C4
3	B	502[A]	8N1	C25-C24-N1-C21
4	B	503	MPD	C2-C3-C4-C5
4	D	502	MPD	C2-C3-C4-C5
3	A	502	8N1	O3-C24-N1-C21
3	B	502[A]	8N1	O3-C24-N1-C21
3	C	501[A]	8N1	O3-C24-N1-C21
3	C	501[A]	8N1	O3-C27-C29-O6
3	A	502	8N1	O3-C27-C29-O6
3	D	501	8N1	O3-C27-C29-O6
4	B	503	MPD	O2-C2-C3-C4
7	C	502	MRD	O2-C2-C3-C4
4	B	503	MPD	C1-C2-C3-C4
4	B	503	MPD	CM-C2-C3-C4
4	D	502	MPD	C1-C2-C3-C4
7	C	502	MRD	C1-C2-C3-C4
7	C	502	MRD	CM-C2-C3-C4
3	A	502	8N1	C25-C24-N1-C21
3	B	502[B]	8N1	C25-C24-N1-C21

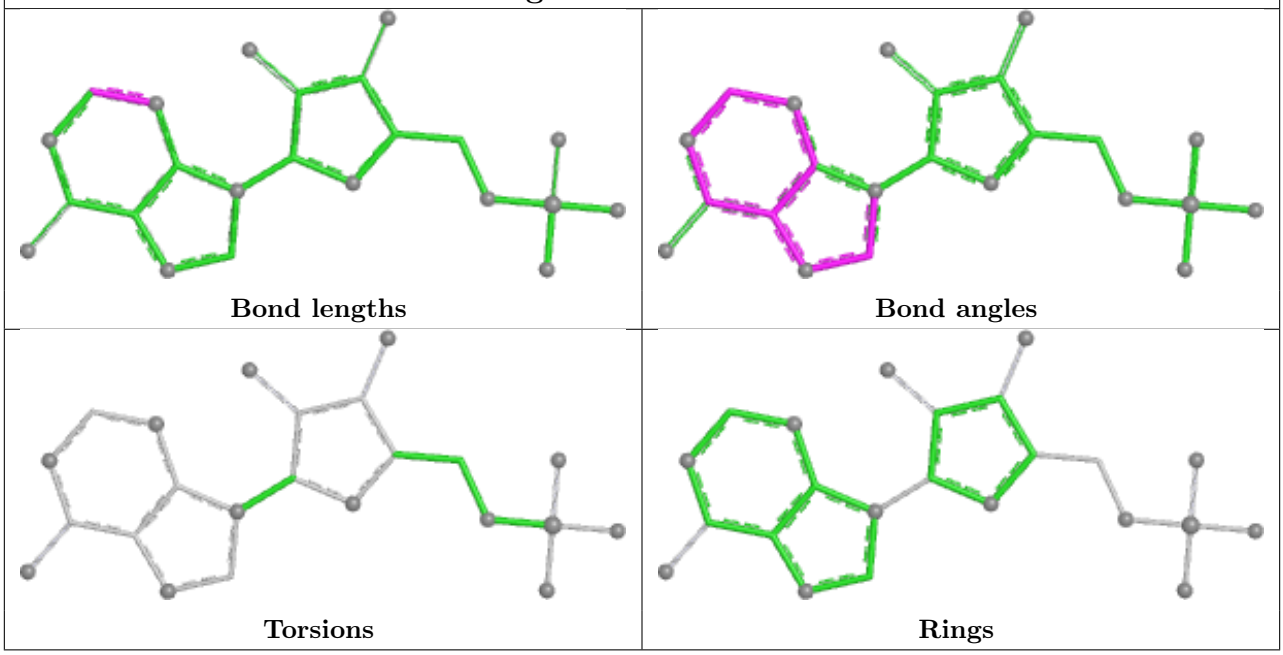
There are no ring outliers.

9 monomers are involved in 10 short contacts:

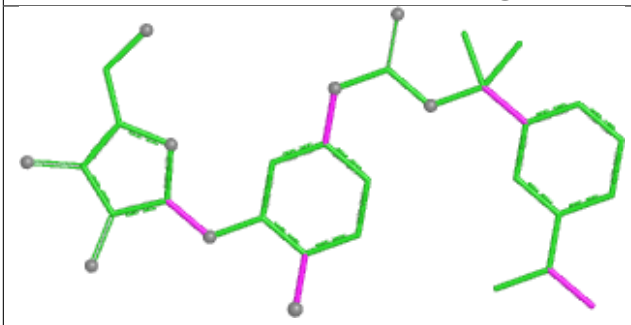
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	2	0
2	C	500	IMP	1	0
2	B	501	IMP	1	0
4	D	502	MPD	1	0
4	A	503	MPD	1	0
3	C	501[A]	8N1	1	0
6	A	505	FMT	1	0
3	A	502	8N1	1	0
2	D	500	IMP	1	0

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 then 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.

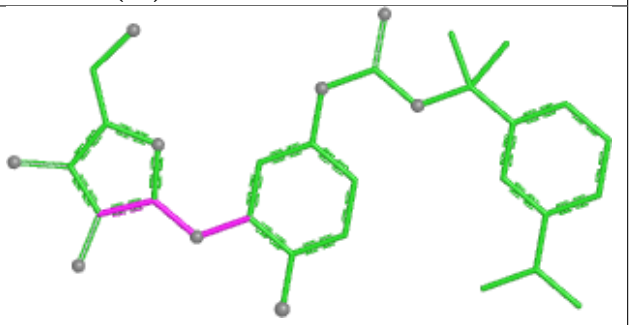
Ligand IMP A 501



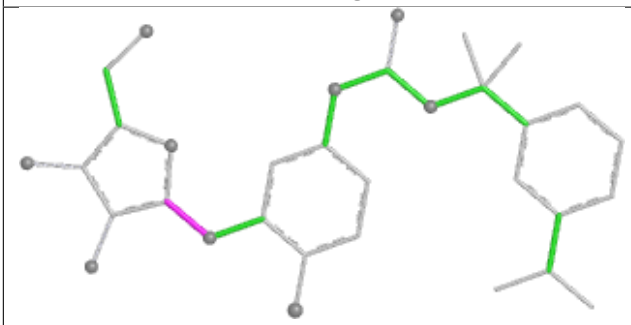
Ligand 8N1 B 502 (A)



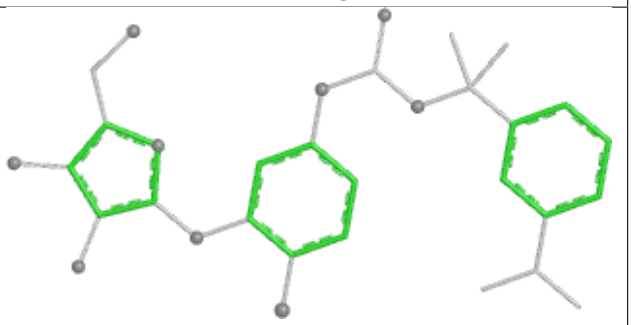
Bond lengths



Bond angles

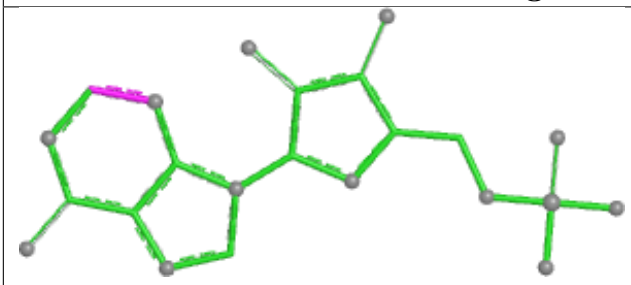


Torsions

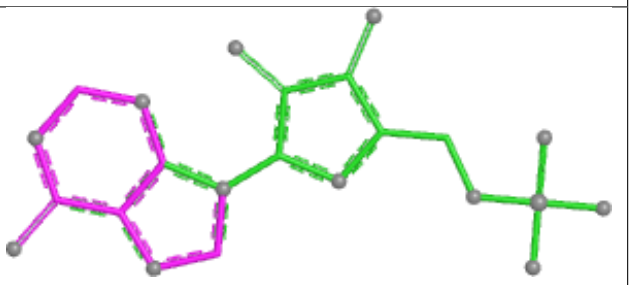


Rings

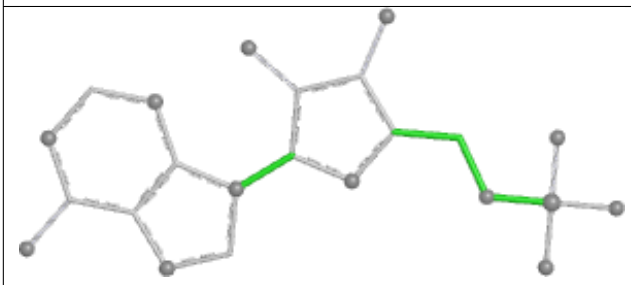
Ligand IMP C 500



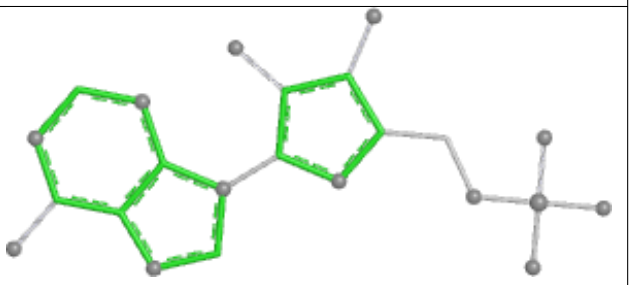
Bond lengths



Bond angles

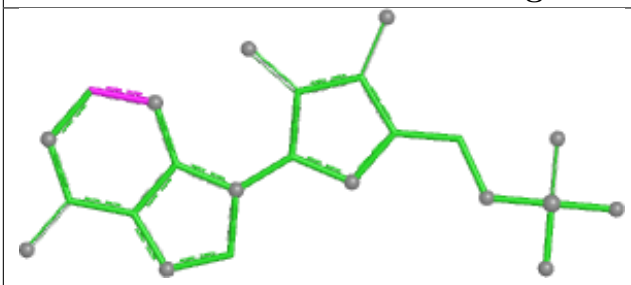


Torsions

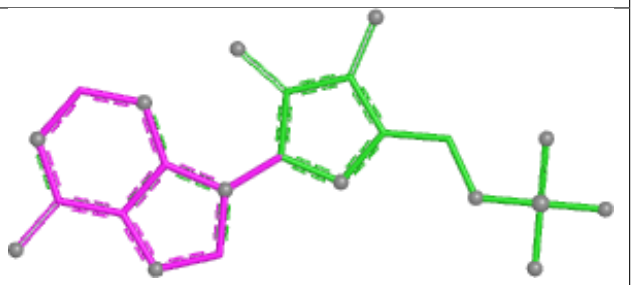


Rings

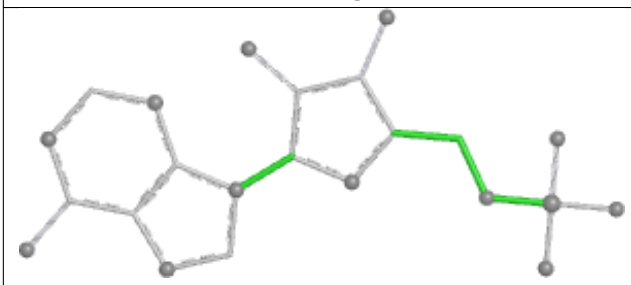
Ligand IMP B 501



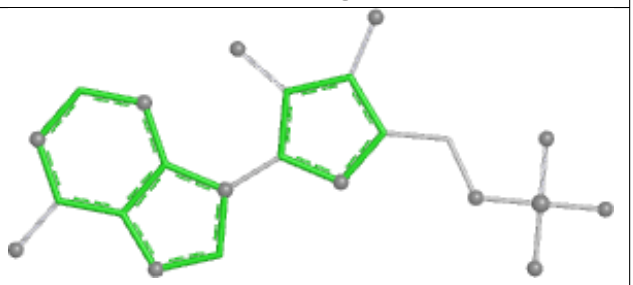
Bond lengths



Bond angles

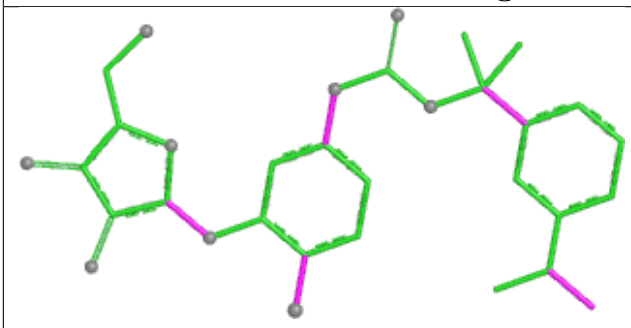


Torsions

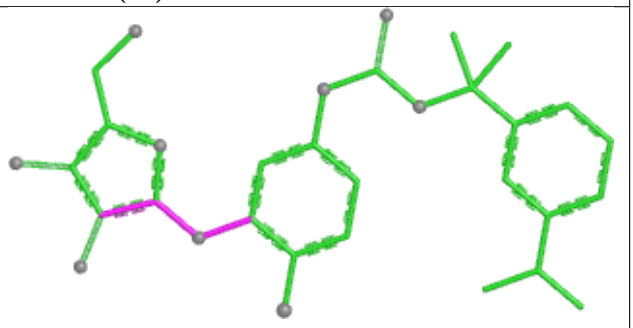


Rings

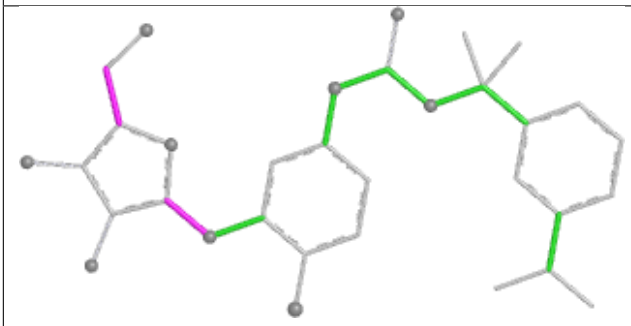
Ligand 8N1 C 501 (A)



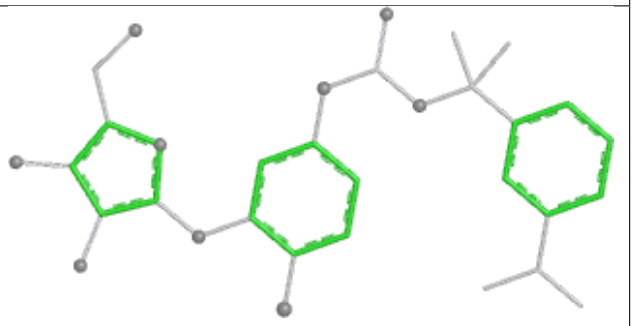
Bond lengths



Bond angles

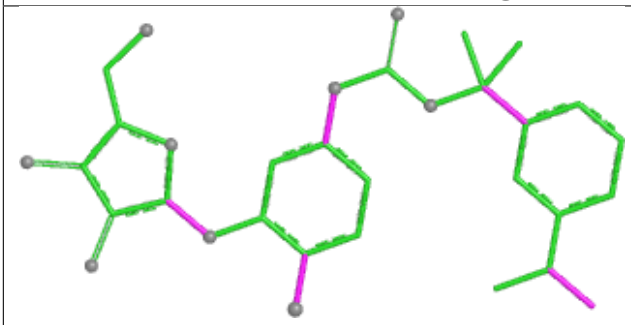


Torsions

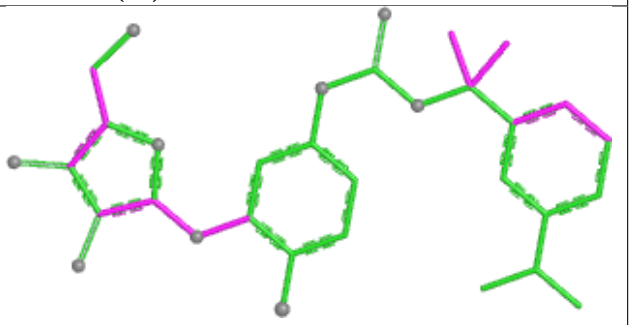


Rings

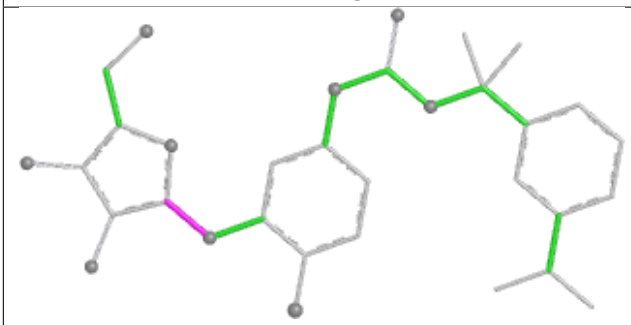
Ligand 8N1 B 502 (B)



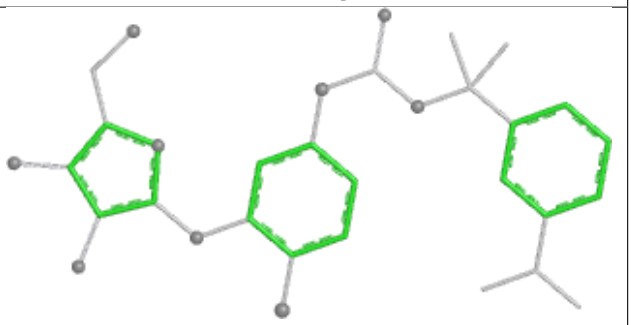
Bond lengths



Bond angles

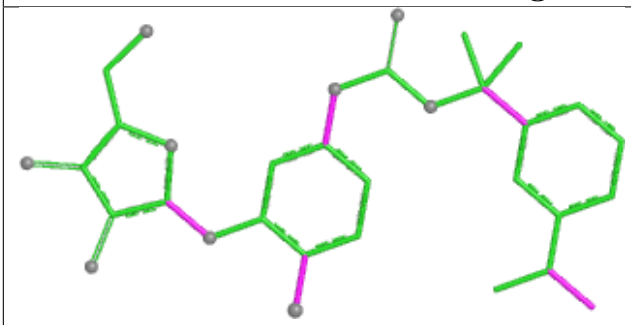


Torsions

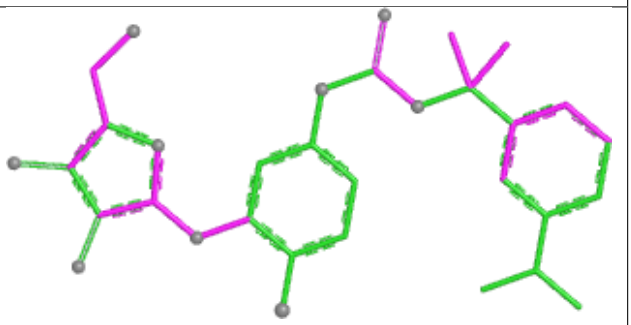


Rings

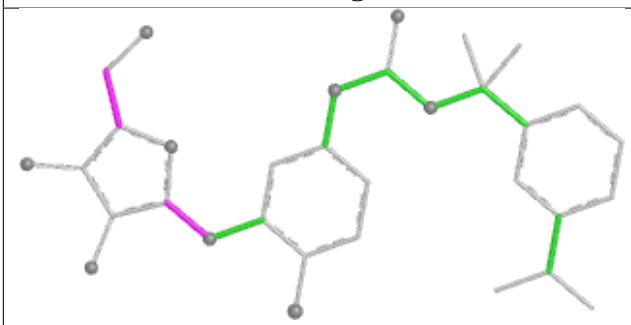
Ligand 8N1 A 502



Bond lengths



Bond angles



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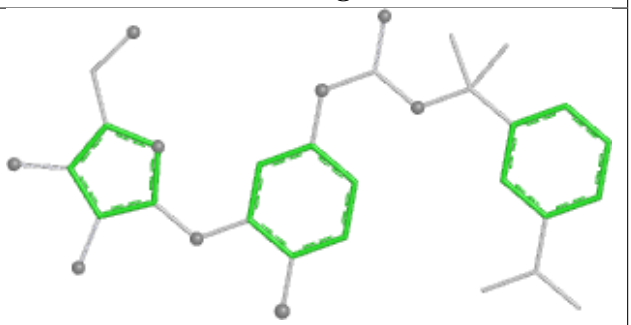
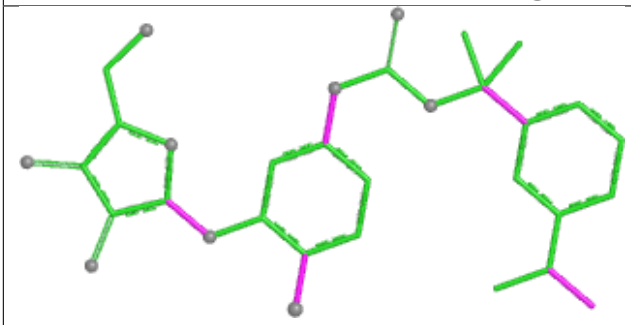
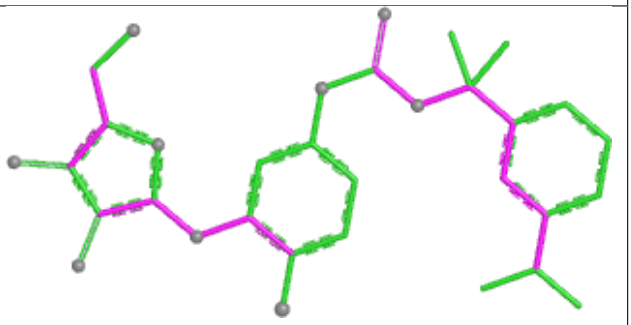


Rings

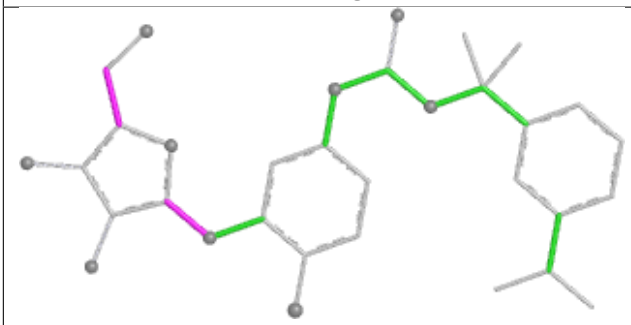
Ligand 8N1 D 501



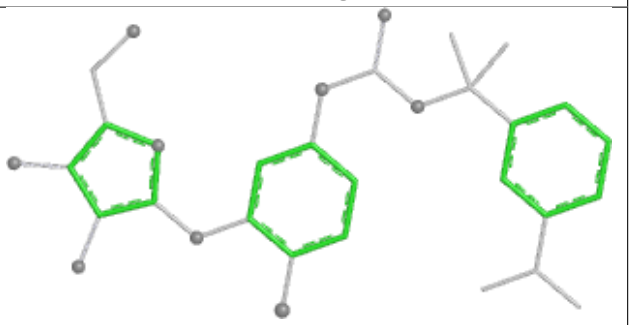
Bond lengths



Bond angles

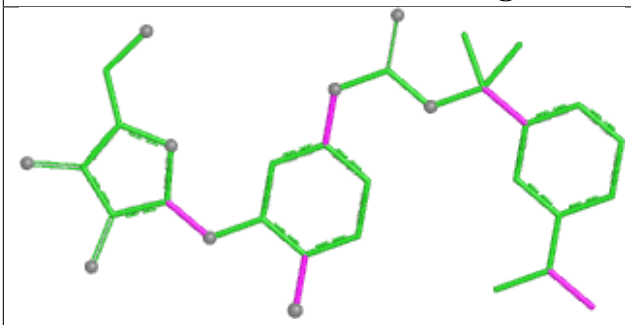


Torsions

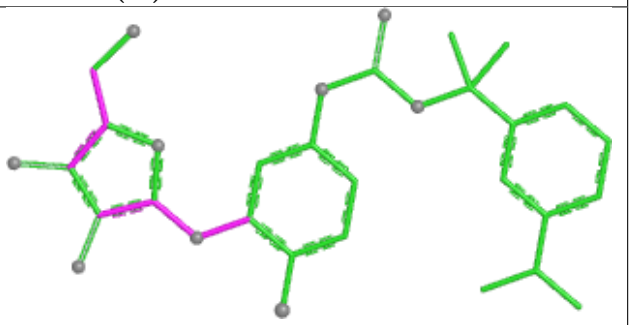


Rings

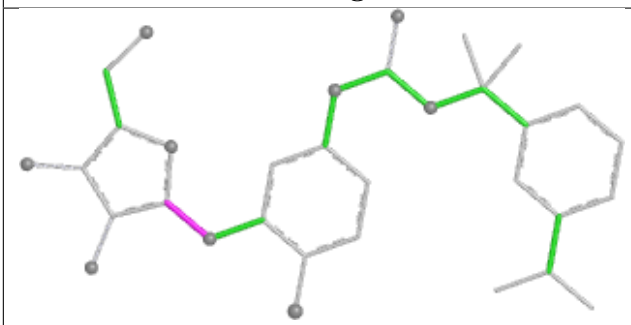
Ligand 8N1 C 501 (B)



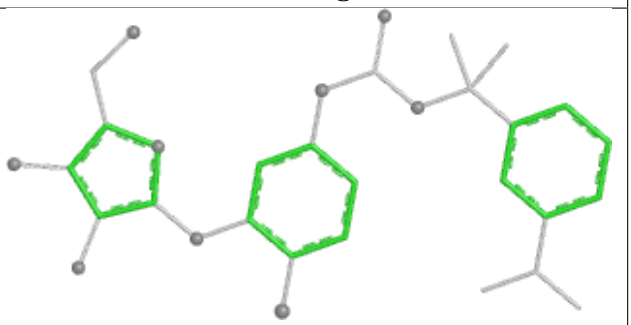
Bond lengths



Bond angles

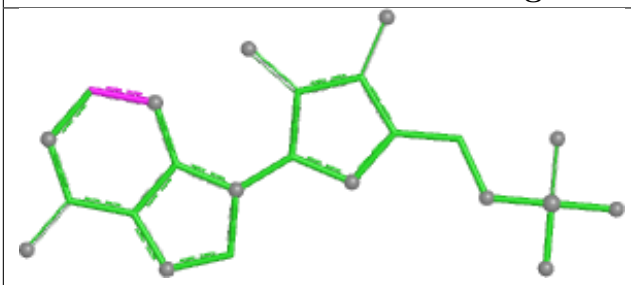


Torsions

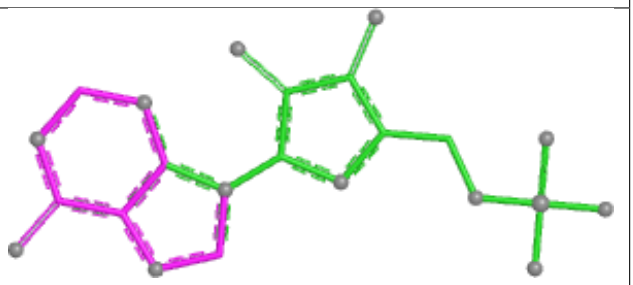


Rings

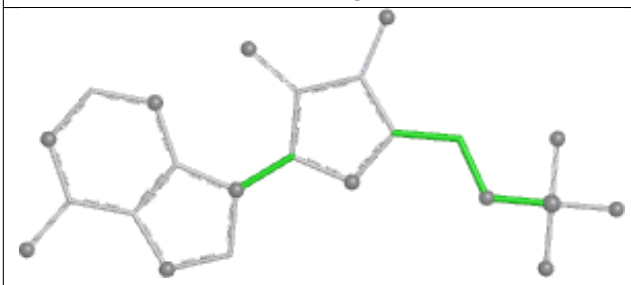
Ligand IMP D 500



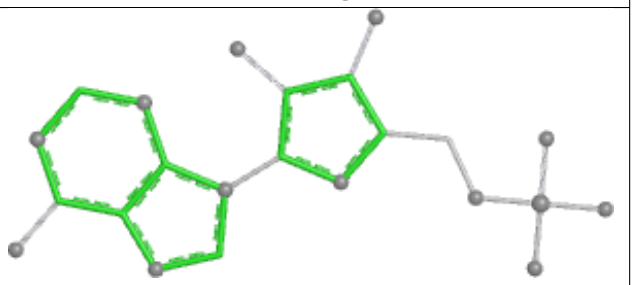
Bond lengths



Bond angles



Torsions



Rings

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	344/363 (94%)	-0.19	7 (2%)	65	68	17, 38, 61, 87	5 (1%)
1	B	347/363 (95%)	-0.16	9 (2%)	57	61	17, 38, 61, 89	5 (1%)
1	C	342/363 (94%)	-0.00	5 (1%)	72	76	20, 46, 69, 89	4 (1%)
1	D	345/363 (95%)	-0.13	5 (1%)	73	77	15, 41, 65, 81	7 (2%)
All	All	1378/1452 (94%)	-0.12	26 (1%)	66	70	15, 40, 65, 89	21 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	PHE	4.6
1	A	482	VAL	4.6
1	A	2	ALA	4.1
1	B	4	ILE	4.0
1	C	2	ALA	3.9
1	B	0	ALA	3.7
1	C	408	PHE	3.7
1	B	5	LEU	3.6
1	B	482	VAL	3.6
1	C	447[A]	GLU	3.5
1	B	408	PHE	3.5
1	B	2	ALA	3.2
1	D	482	VAL	3.0
1	C	393	ALA	3.0
1	D	91	GLY	2.8
1	C	409	VAL	2.8
1	D	0	ALA	2.7
1	A	409	VAL	2.7
1	A	5	LEU	2.6
1	B	-2	SER	2.6
1	D	393	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	409	VAL	2.2
1	A	4	ILE	2.1
1	B	1	MET	2.1
1	A	3	ARG	2.1
1	B	393	ALA	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	ACY	A	504	4/4	0.72	0.26	81,82,82,82	0
4	MPD	A	503	8/8	0.79	0.18	54,55,59,60	0
5	ACY	D	503	4/4	0.80	0.18	66,66,66,67	0
3	8N1	B	502[B]	33/33	0.83	0.12	37,42,57,62	33
3	8N1	B	502[A]	33/33	0.83	0.12	37,42,57,60	33
5	ACY	C	503	4/4	0.84	0.19	74,74,74,74	0
4	MPD	B	503	8/8	0.86	0.17	59,61,65,65	0
6	FMT	B	504	3/3	0.88	0.16	72,72,73,73	0
4	MPD	D	502	8/8	0.89	0.14	53,54,58,59	0
7	MRD	C	502	8/8	0.89	0.14	57,58,65,66	0
3	8N1	C	501[A]	33/33	0.90	0.11	45,49,64,65	33
3	8N1	C	501[B]	33/33	0.90	0.11	45,49,64,65	33
6	FMT	A	505	3/3	0.92	0.12	59,59,60,60	0
3	8N1	D	501	33/33	0.93	0.09	42,45,66,72	0
3	8N1	A	502	33/33	0.94	0.09	34,36,57,65	0
2	IMP	C	500	23/23	0.97	0.05	35,37,39,40	0
2	IMP	B	501	23/23	0.98	0.05	28,32,34,34	0
2	IMP	A	501	23/23	0.98	0.04	25,27,32,33	0

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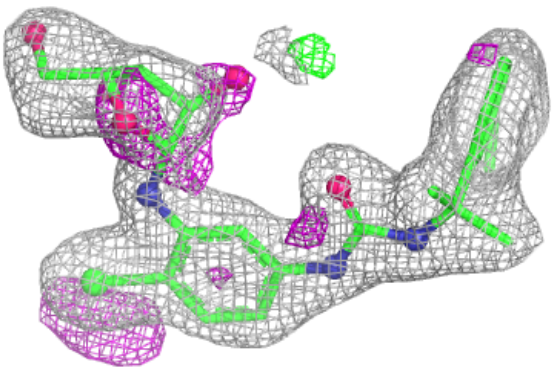
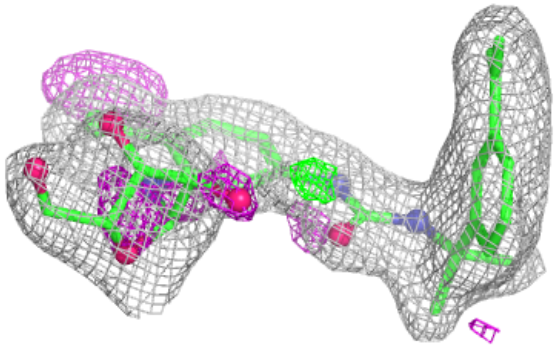
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IMP	D	500	23/23	0.98	0.05	30,33,36,37	0

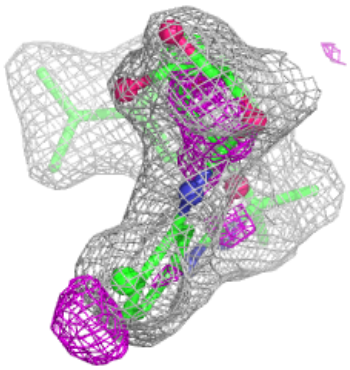
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8N1 B 502 (B):

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

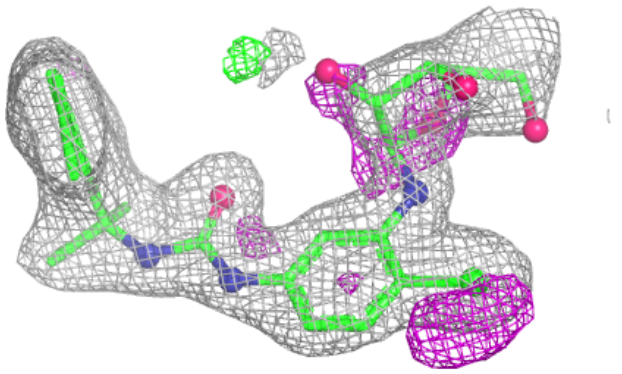


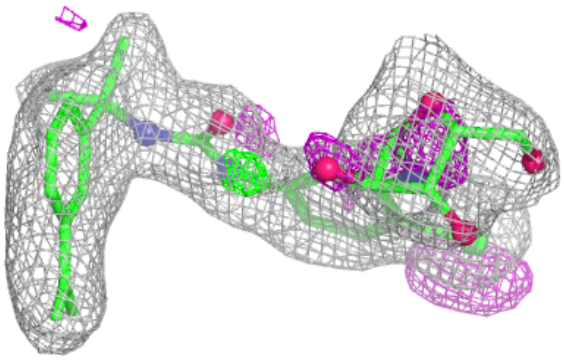


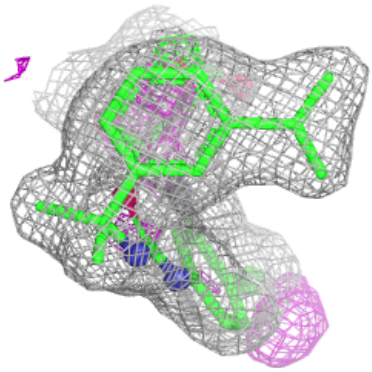


Electron density around 8N1 B 502 (A):

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

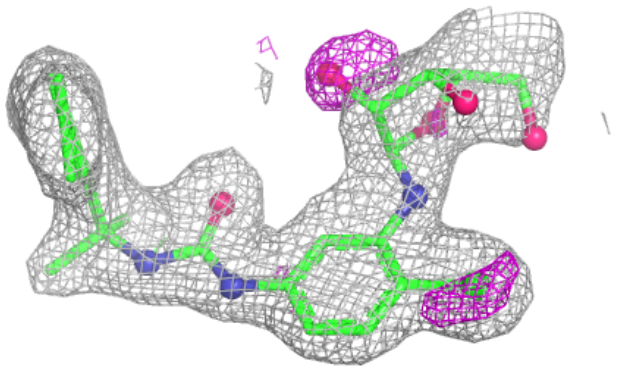


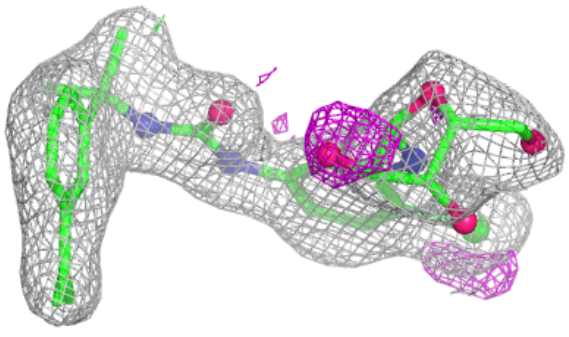


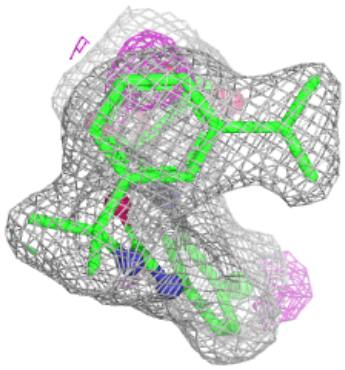


Electron density around 8N1 C 501 (A):

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

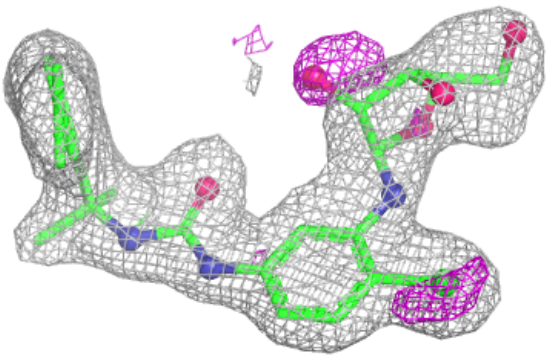


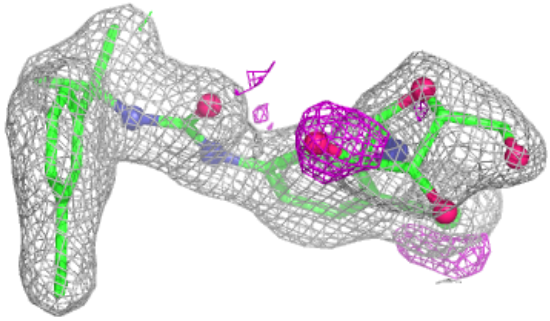


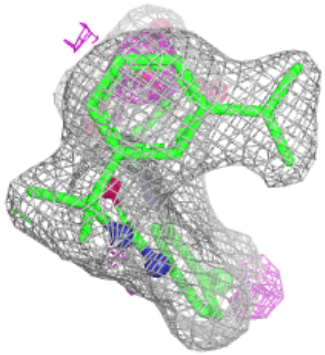


Electron density around 8N1 C 501 (B):

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

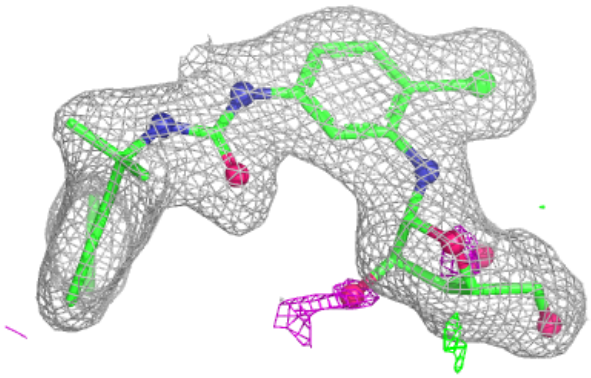


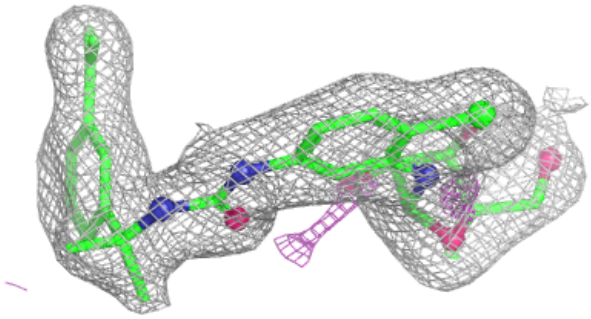


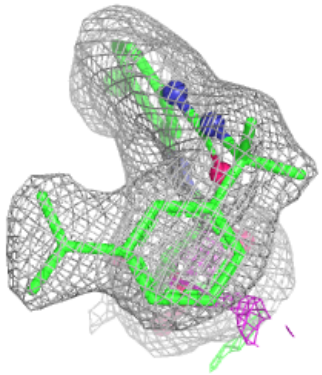


Electron density around 8N1 D 501:

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

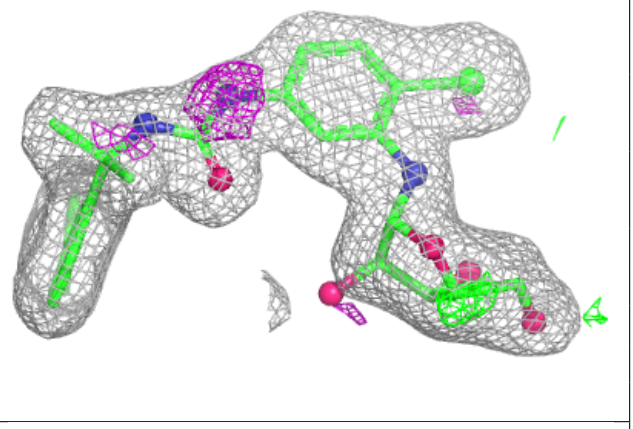


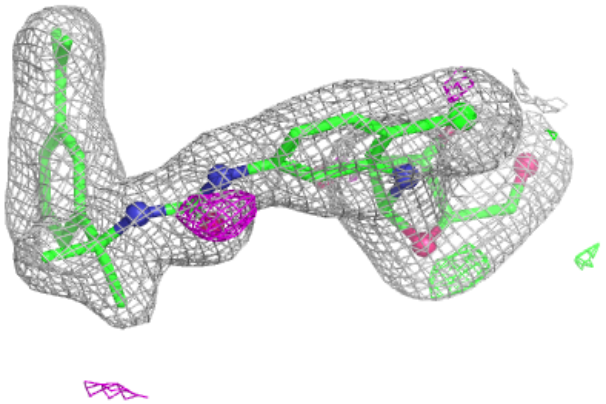


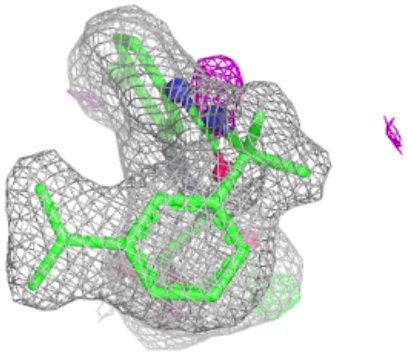


Electron density around 8N1 A 502:

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

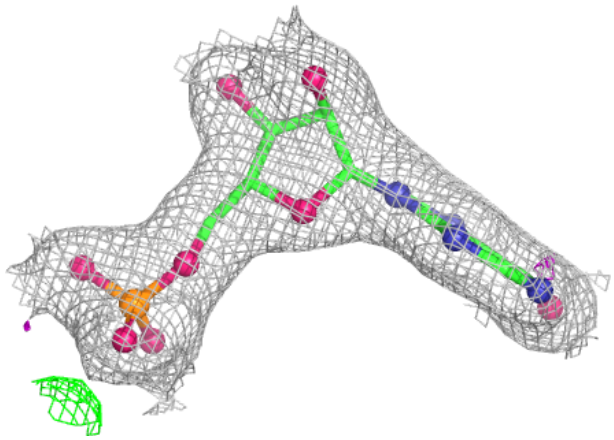


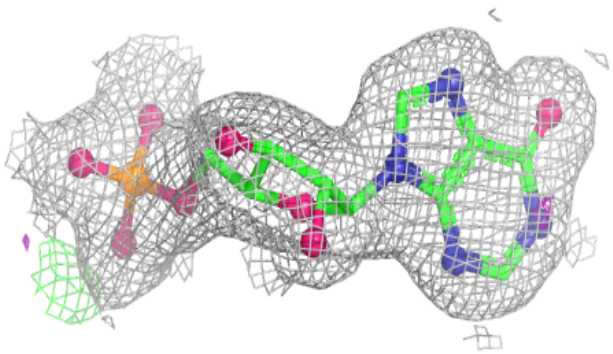


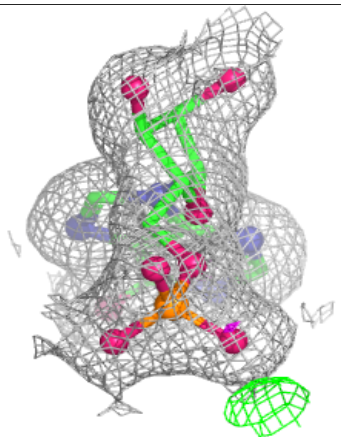


Electron density around IMP C 500:

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

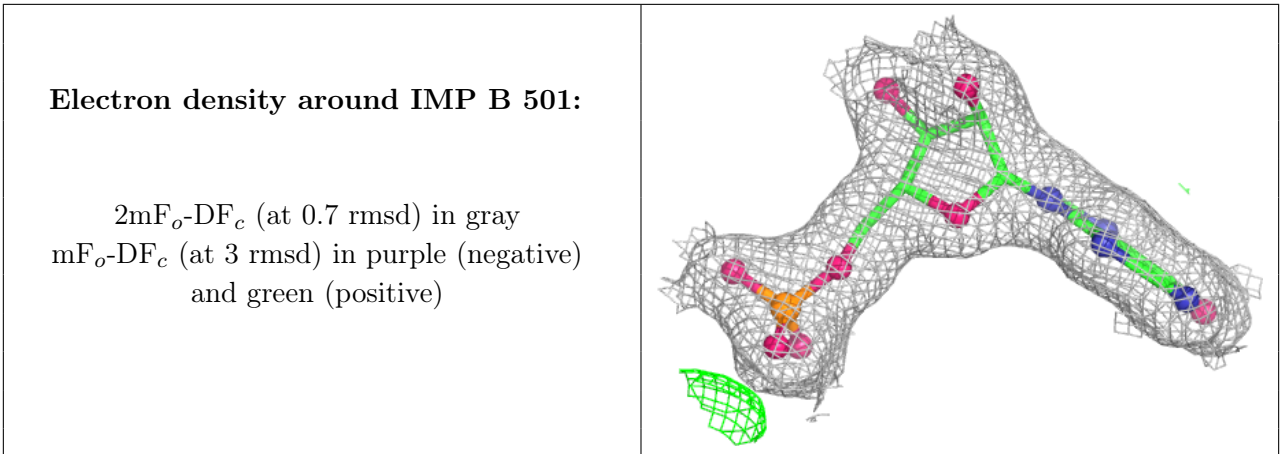






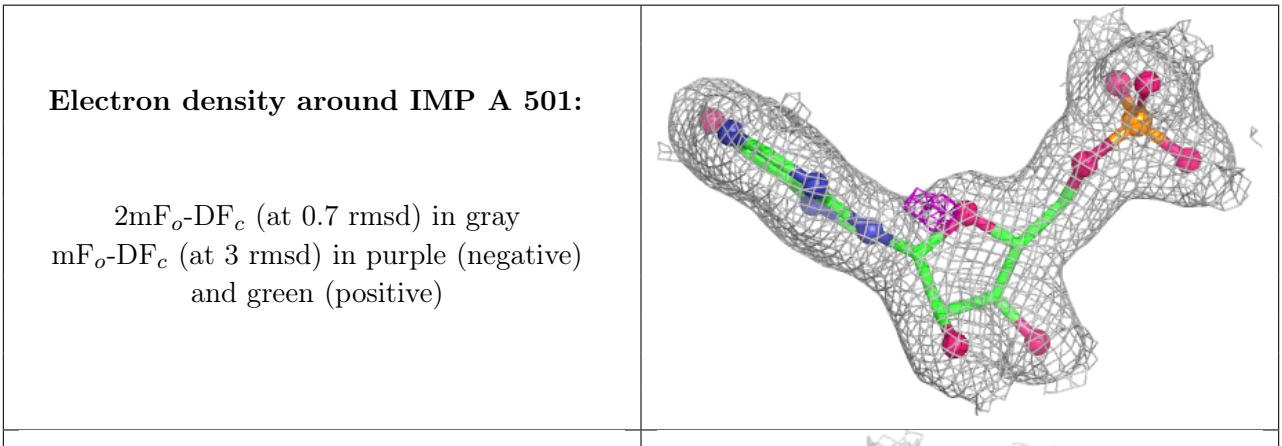
Electron density around IMP B 501:

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



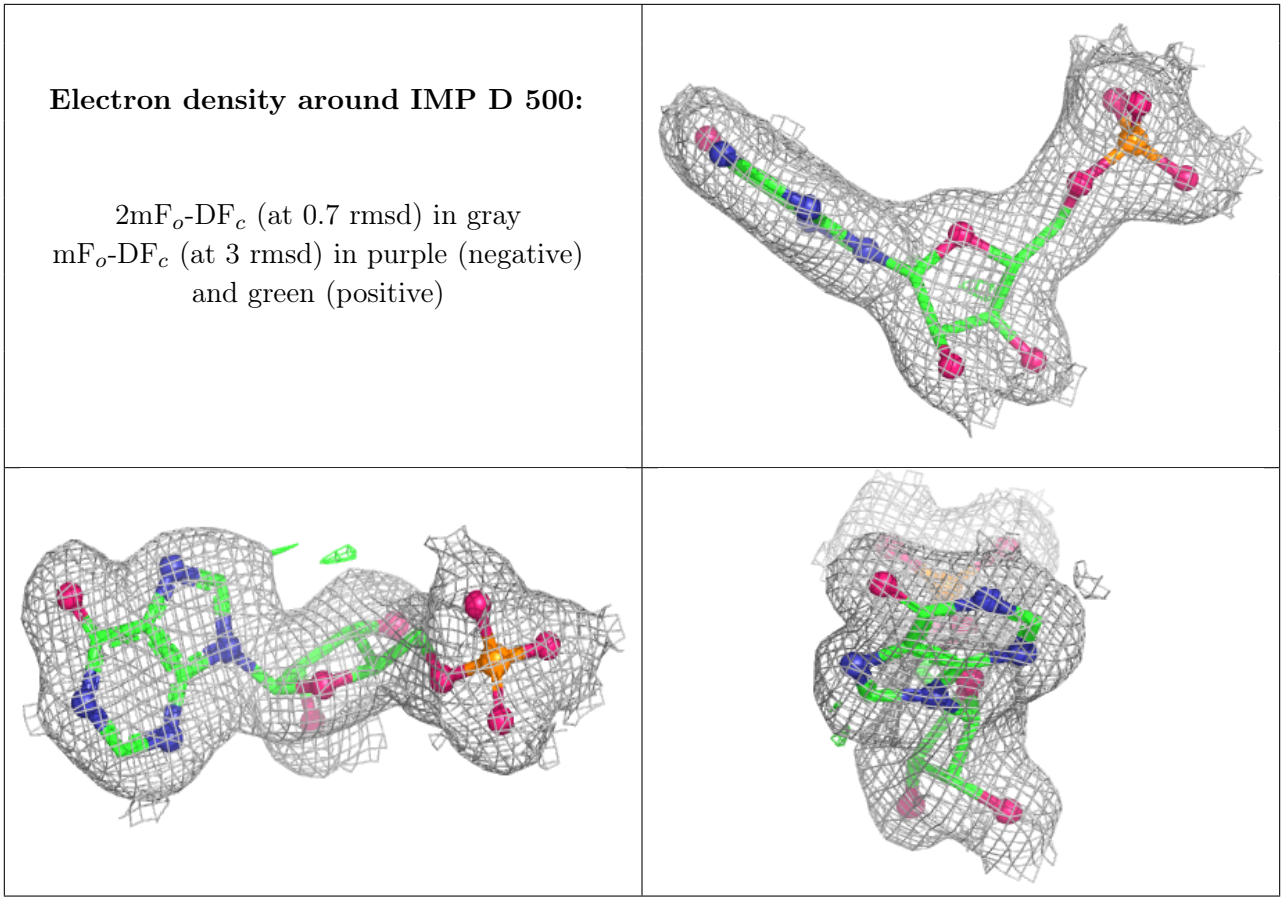
Electron density around IMP A 501:

$2mF_o$-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 500:

$2mF_o$-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.