



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 06:59 am BST

PDB ID : 4RV8
Title : Co-Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Cryptosporidium parvum* and the inhibitor p131
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Kavitha, M.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-11-25
Resolution : 2.05 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 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 : 2.11
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) : 2.11

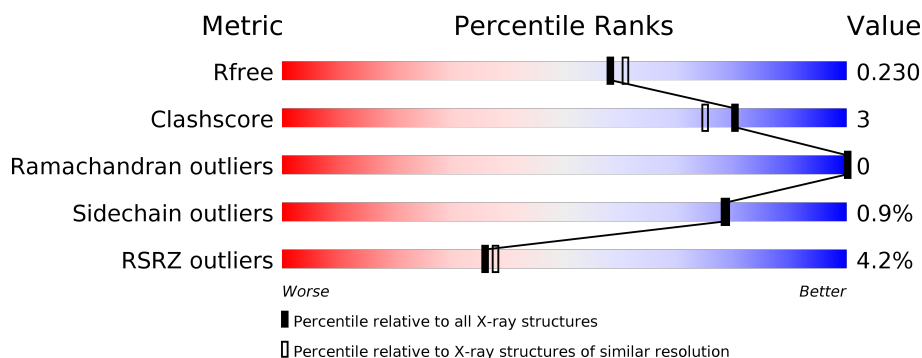
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	361	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	361	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	C	361	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>10%</div> </div> </div>
1	D	361	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10414 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	327	Total	C	N	O	S	0	5	0
			2459	1546	417	480	16			
1	B	327	Total	C	N	O	S	0	6	0
			2469	1552	418	482	17			
1	C	326	Total	C	N	O	S	0	3	0
			2436	1532	413	475	16			
1	D	327	Total	C	N	O	S	0	5	0
			2461	1546	417	482	16			

There are 24 discrepancies between the modelled and reference sequences:

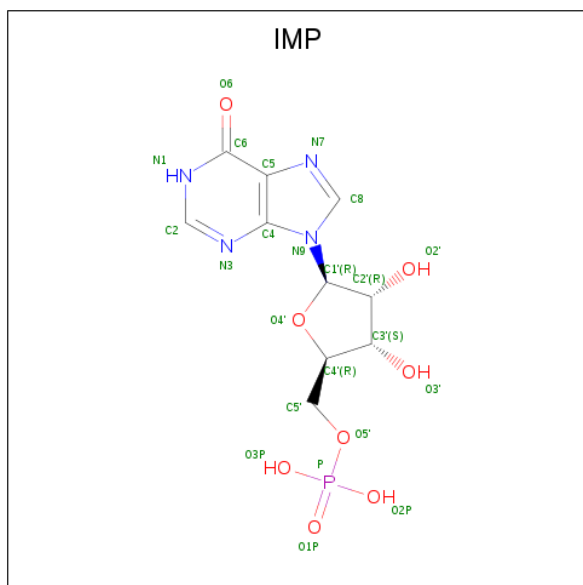
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
A	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
A	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
A	90	SER	-	LINKER	UNP Q8T6T2
A	91	GLY	-	LINKER	UNP Q8T6T2
A	92	GLY	-	LINKER	UNP Q8T6T2
B	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
B	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
B	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
B	90	SER	-	LINKER	UNP Q8T6T2
B	91	GLY	-	LINKER	UNP Q8T6T2
B	92	GLY	-	LINKER	UNP Q8T6T2
C	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
C	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
C	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
C	90	SER	-	LINKER	UNP Q8T6T2
C	91	GLY	-	LINKER	UNP Q8T6T2
C	92	GLY	-	LINKER	UNP Q8T6T2
D	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
D	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
D	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2

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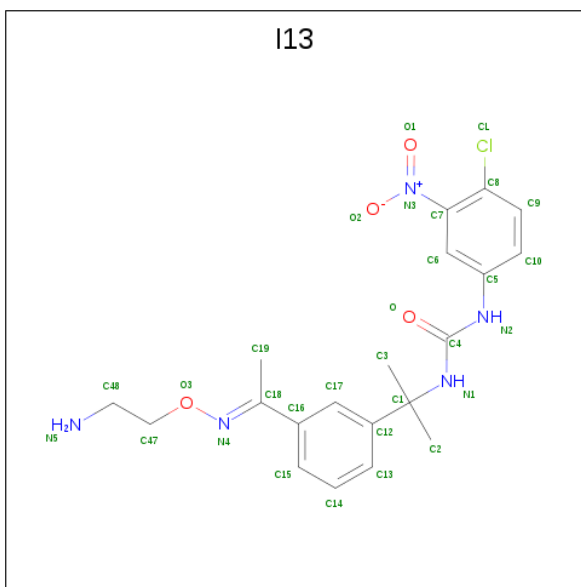
Chain	Residue	Modelled	Actual	Comment	Reference
D	90	SER	-	LINKER	UNP Q8T6T2
D	91	GLY	-	LINKER	UNP Q8T6T2
D	92	GLY	-	LINKER	UNP Q8T6T2

- Molecule 2 is INOSINIC ACID (three-letter code: 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 1-(2-{3-[(1E)-N-(2-aminoethoxy)ethanimidoyl]phenyl}propan-2-yl)-3-(4-chloro-3-nitrophenyl)urea (three-letter code: I13) (formula: $C_{20}H_{24}ClN_5O_4$).



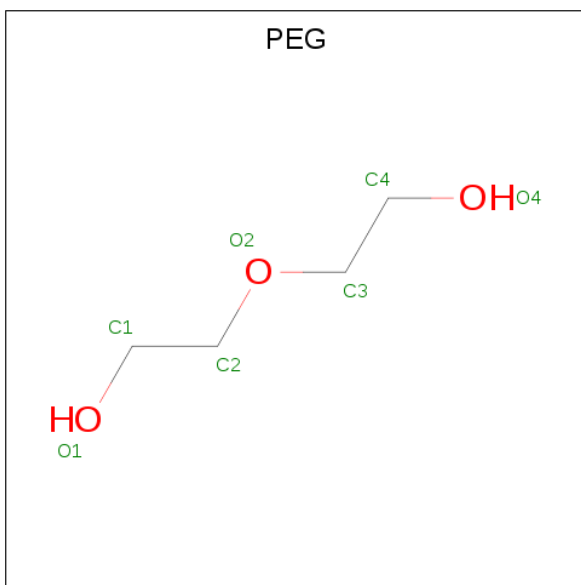
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			30	20	1	5	4		
3	B	1	Total	C	Cl	N	O	0	0
			30	20	1	5	4		
3	B	1	Total	C	Cl	N	O	0	0
			30	20	1	5	4		
3	C	1	Total	C	Cl	N	O	0	0
			30	20	1	5	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

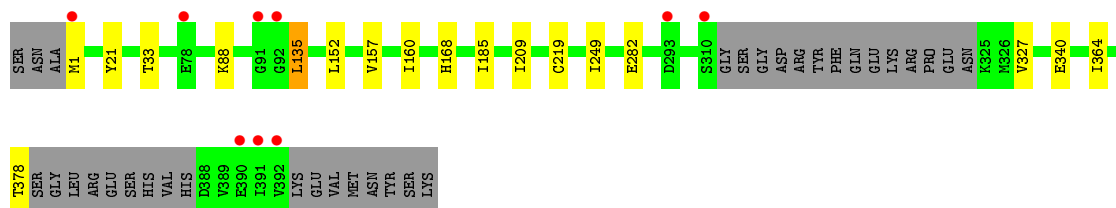
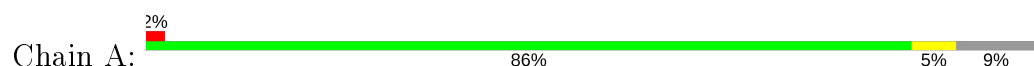
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total	O	0	0
			95	95		
6	B	81	Total	O	0	0
			81	81		
6	C	84	Total	O	0	0
			84	84		
6	D	79	Total	O	0	0
			79	79		

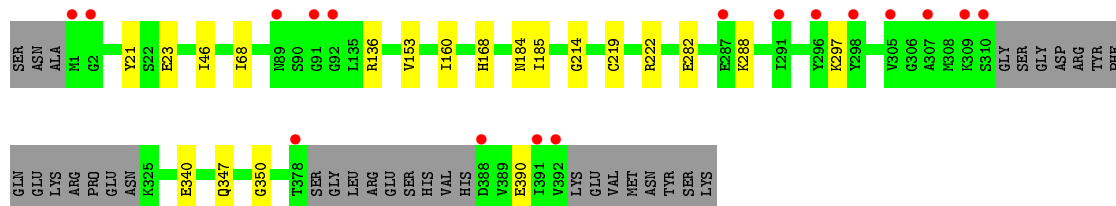
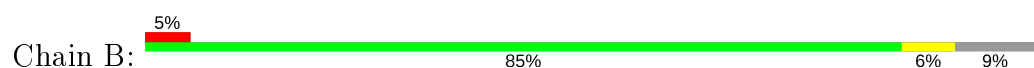
3 Residue-property plots [i](#)

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

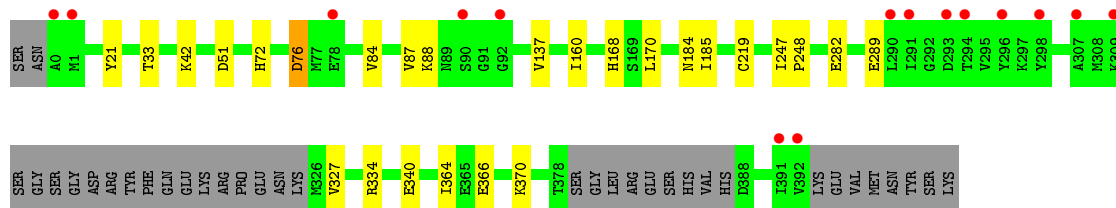
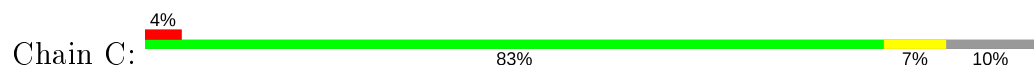
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



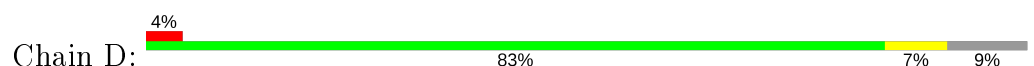
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

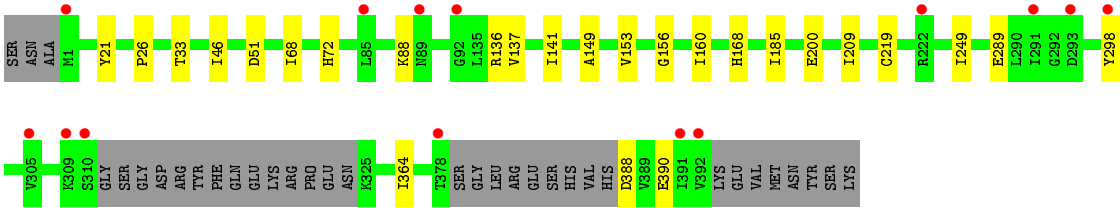


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.19Å 91.83Å 92.02Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	40.84 – 2.05 40.84 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.84-2.05) 99.6 (40.84-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, R_{free}	0.187 , 0.229 0.188 , 0.230	Depositor DCC
R_{free} test set	4501 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10414	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.41% 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, OCS, PEG, I13, 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	0/2471	0.45	0/3321
1	B	0.25	0/2481	0.45	0/3332
1	C	0.25	0/2448	0.45	0/3291
1	D	0.25	0/2473	0.45	0/3323
All	All	0.25	0/9873	0.45	0/13267

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	2459	0	2566	11	0
1	B	2469	0	2575	13	0
1	C	2436	0	2541	15	0
1	D	2461	0	2563	17	0
2	A	23	0	11	1	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	30	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	60	0	48	3	0
3	C	30	0	24	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	7	0	10	2	0
5	B	7	0	10	0	0
6	A	95	0	0	0	0
6	B	81	0	0	1	0
6	C	84	0	0	0	0
6	D	79	0	0	1	0
All	All	10414	0	10437	56	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 (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HG12	1:B:185:ILE:HD13	1.72	0.71
1:D:160:ILE:HG12	1:D:185:ILE:HD13	1.74	0.69
3:C:503:I13:CL	3:C:503:I13:O2	2.49	0.68
3:B:505:I13:CL	3:B:505:I13:O2	2.51	0.66
1:B:219:OCS:OD3	2:B:501:IMP:H2	1.99	0.63
1:D:219:OCS:OD1	2:D:501:IMP:H2	2.00	0.61
1:C:289:GLU:OE2	1:C:334:ARG:NH1	2.33	0.61
3:A:501:I13:O2	3:A:501:I13:CL	2.56	0.60
1:B:153:VAL:HG22	1:B:185:ILE:HD12	1.84	0.59
1:C:366:GLU:HG2	1:C:370:LYS:HD2	1.85	0.58
1:D:209:ILE:HB	1:D:249:ILE:HD13	1.87	0.57
5:A:503:PEG:H11	1:D:26:PRO:HG2	1.87	0.56
1:D:289:GLU:HB2	1:D:298:TYR:HE1	1.71	0.56
1:B:23:GLU:HG2	1:C:170:LEU:HB2	1.88	0.56
1:A:219:OCS:OD1	2:A:500:IMP:H2	2.05	0.55
1:D:388:ASP:OD2	1:D:388:ASP:N	2.41	0.54
1:B:282[A]:GLU:HG2	1:B:340:GLU:HA	1.89	0.53
1:B:136:ARG:NH2	6:B:643:HOH:O	2.42	0.52
1:A:152:LEU:O	1:A:157[B]:VAL:HG23	2.12	0.49
1:C:87:VAL:HG11	1:C:137:VAL:HB	1.94	0.49
1:C:282:GLU:HG2	1:C:340:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:VAL:HG22	1:D:185:ILE:HD12	1.95	0.48
1:C:219:OCS:OD2	2:C:501:IMP:H2	2.14	0.48
1:D:168:HIS:NE2	1:D:200:GLU:OE2	2.46	0.47
1:B:350:GLY:HA3	1:C:327:VAL:HG21	1.96	0.47
1:D:141:ILE:HD13	1:D:149:ALA:HB2	1.96	0.46
1:A:327:VAL:HB	5:A:503:PEG:H31	1.97	0.46
1:C:160:ILE:HG12	1:C:185:ILE:HG12	1.97	0.46
1:B:214:GLY:CA	1:B:222[B]:ARG:HE	2.29	0.46
1:D:88:LYS:HE3	1:D:156:GLY:O	2.16	0.46
1:D:88:LYS:HE2	1:D:137:VAL:HG12	1.97	0.45
1:A:88:LYS:HA	1:A:88:LYS:HD3	1.82	0.45
1:D:51:ASP:HA	1:D:72:HIS:CD2	2.51	0.45
3:B:502:I13:O	3:B:502:I13:H7	2.17	0.45
1:A:21:TYR:HB2	1:B:168:HIS:CE1	2.52	0.44
1:C:84:VAL:O	1:C:88:LYS:HG2	2.17	0.44
1:B:214:GLY:HA3	1:B:222[B]:ARG:HE	1.83	0.44
1:B:288:LYS:HG3	1:B:297:LYS:HG2	2.00	0.44
1:D:136:ARG:NH2	6:D:634:HOH:O	2.50	0.44
1:C:76:ASP:OD2	1:C:76:ASP:N	2.42	0.43
1:A:168:HIS:CE1	1:D:21:TYR:HB2	2.54	0.43
3:A:501:I13:O	3:A:501:I13:H7	2.18	0.43
1:A:282:GLU:HG2	1:A:340:GLU:HA	2.00	0.43
1:C:21:TYR:HB2	1:D:168:HIS:CE1	2.54	0.42
1:C:247:ILE:HA	1:C:248:PRO:HD3	1.91	0.42
1:C:51:ASP:HA	1:C:72:HIS:CD2	2.55	0.41
1:B:46:ILE:HG23	1:B:68:ILE:HG23	2.02	0.41
1:A:160:ILE:HG12	1:A:185:ILE:HG12	2.03	0.41
1:D:46:ILE:HG23	1:D:68:ILE:HG23	2.03	0.41
1:A:209:ILE:HB	1:A:249:ILE:HD13	2.02	0.41
1:A:33:THR:HB	1:A:364:ILE:HD12	2.02	0.41
1:C:33:THR:HB	1:C:364:ILE:HD12	2.02	0.40
1:D:33:THR:HB	1:D:364:ILE:HD12	2.02	0.40
1:A:135:LEU:HA	1:A:135:LEU:HD12	1.94	0.40
3:B:505:I13:O	3:B:505:I13:H7	2.22	0.40
1:B:21:TYR:HB2	1:C:168:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/361 (90%)	317 (98%)	8 (2%)	0	100	100
1	B	326/361 (90%)	317 (97%)	9 (3%)	0	100	100
1	C	322/361 (89%)	314 (98%)	8 (2%)	0	100	100
1	D	325/361 (90%)	315 (97%)	10 (3%)	0	100	100
All	All	1298/1444 (90%)	1263 (97%)	35 (3%)	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	269/294 (92%)	266 (99%)	3 (1%)	73	72
1	B	270/294 (92%)	267 (99%)	3 (1%)	73	72
1	C	265/294 (90%)	262 (99%)	3 (1%)	73	72
1	D	269/294 (92%)	268 (100%)	1 (0%)	91	91
All	All	1073/1176 (91%)	1063 (99%)	10 (1%)	78	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	378	THR
1	B	184	ASN
1	B	347	GLN
1	B	390	GLU
1	C	42	LYS
1	C	76	ASP
1	C	184	ASN
1	D	390	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	B	219	1	7,8,9	0.86	0	6,11,13	2.52	2 (33%)
1	OCS	A	219	1	7,8,9	0.78	0	6,11,13	2.78	3 (50%)
1	OCS	D	219	1	7,8,9	0.79	0	6,11,13	1.90	1 (16%)
1	OCS	C	219	1	7,8,9	0.85	0	6,11,13	2.21	1 (16%)

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
1	OCS	B	219	1	-	1/4/7/9	-
1	OCS	A	219	1	-	1/4/7/9	-
1	OCS	D	219	1	-	2/4/7/9	-
1	OCS	C	219	1	-	1/4/7/9	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	OCS	OD2-SG-CB	5.42	114.38	105.74
1	C	219	OCS	OD1-SG-CB	4.95	112.82	106.94
1	B	219	OCS	OD1-SG-CB	4.61	112.41	106.94
1	D	219	OCS	OD2-SG-CB	3.74	111.71	105.74
1	A	219	OCS	OD1-SG-CB	-3.38	102.92	106.94
1	B	219	OCS	OD2-SG-OD3	-2.77	104.52	111.27
1	A	219	OCS	OD3-SG-OD1	-2.06	106.81	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	219	OCS	N-CA-CB-SG
1	A	219	OCS	N-CA-CB-SG
1	D	219	OCS	N-CA-CB-SG
1	C	219	OCS	N-CA-CB-SG
1	D	219	OCS	CA-CB-SG-OD3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	219	OCS	1	0
1	A	219	OCS	1	0
1	D	219	OCS	1	0
1	C	219	OCS	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

14 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	PEG	A	503	-	6,6,6	0.36	0	5,5,5	0.30	0
3	I13	A	501	-	30,31,31	2.69	6 (20%)	39,43,43	2.64	4 (10%)
2	IMP	C	501	-	21,25,25	1.24	3 (14%)	23,38,38	1.58	4 (17%)
2	IMP	D	501	-	21,25,25	1.21	3 (14%)	23,38,38	1.56	5 (21%)
2	IMP	B	501	-	21,25,25	1.27	3 (14%)	23,38,38	1.47	2 (8%)
4	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.35	0
4	GOL	A	502	-	5,5,5	0.38	0	5,5,5	0.22	0
2	IMP	A	500	-	21,25,25	1.28	3 (14%)	23,38,38	1.62	3 (13%)
5	PEG	B	504	-	6,6,6	0.43	0	5,5,5	0.31	0
4	GOL	C	502	-	5,5,5	0.39	0	5,5,5	0.26	0
3	I13	C	503	-	30,31,31	2.71	7 (23%)	39,43,43	2.50	4 (10%)
3	I13	B	505	-	30,31,31	2.71	7 (23%)	39,43,43	2.53	4 (10%)
4	GOL	D	502	-	5,5,5	0.35	0	5,5,5	0.35	0
3	I13	B	502	-	30,31,31	2.73	7 (23%)	39,43,43	2.52	4 (10%)

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
5	PEG	A	503	-	-	1/4/4/4	-
3	I13	A	501	-	-	1/26/28/28	0/2/2/2
2	IMP	C	501	-	-	0/6/26/26	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
4	GOL	B	503	-	-	4/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-
2	IMP	A	500	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	504	-	-	1/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
3	I13	C	503	-	-	1/26/28/28	0/2/2/2
3	I13	B	505	-	-	1/26/28/28	0/2/2/2
4	GOL	D	502	-	-	0/4/4/4	-
3	I13	B	502	-	-	3/26/28/28	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	I13	O1-N3	10.10	1.39	1.22
3	B	505	I13	O1-N3	10.01	1.39	1.22
3	C	503	I13	O1-N3	9.99	1.39	1.22
3	A	501	I13	O1-N3	9.99	1.39	1.22
3	B	505	I13	O3-N4	-8.99	1.25	1.42
3	B	502	I13	O3-N4	-8.97	1.26	1.42
3	A	501	I13	O3-N4	-8.91	1.26	1.42
3	C	503	I13	O3-N4	-8.87	1.26	1.42
2	B	501	IMP	C2-N3	3.85	1.38	1.32
2	A	500	IMP	C2-N3	3.82	1.38	1.32
2	C	501	IMP	C2-N3	3.71	1.38	1.32
2	D	501	IMP	C2-N3	3.56	1.37	1.32
2	A	500	IMP	C6-N1	3.12	1.38	1.33
2	B	501	IMP	C6-N1	3.03	1.38	1.33
2	C	501	IMP	C6-N1	2.98	1.38	1.33
3	A	501	I13	C7-N3	-2.94	1.40	1.45
3	B	502	I13	C7-N3	-2.92	1.40	1.45
2	D	501	IMP	C6-N1	2.90	1.38	1.33
3	C	503	I13	C7-N3	-2.81	1.40	1.45
3	B	505	I13	C7-N3	-2.71	1.40	1.45
3	B	502	I13	C5-N2	-2.70	1.36	1.41
3	B	505	I13	C8-CL	2.70	1.80	1.73
3	C	503	I13	C5-N2	-2.63	1.36	1.41
3	A	501	I13	C8-CL	2.60	1.79	1.73
3	C	503	I13	C8-CL	2.60	1.79	1.73
3	B	505	I13	C5-N2	-2.58	1.36	1.41
3	B	505	I13	C1-C12	-2.57	1.50	1.53
3	B	502	I13	C8-CL	2.52	1.79	1.73
3	A	501	I13	C5-N2	-2.49	1.36	1.41
3	C	503	I13	C1-C12	-2.43	1.50	1.53
2	D	501	IMP	C2-N1	2.43	1.38	1.33
2	B	501	IMP	C2-N1	2.39	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	IMP	C2-N1	2.39	1.38	1.33
2	C	501	IMP	C2-N1	2.38	1.38	1.33
3	B	502	I13	C1-C12	-2.35	1.50	1.53
3	C	503	I13	C18-N4	-2.25	1.26	1.28
3	A	501	I13	C1-C12	-2.20	1.51	1.53
3	B	502	I13	C18-N4	-2.12	1.26	1.28
3	B	505	I13	C18-N4	-2.11	1.26	1.28

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	I13	C47-O3-N4	13.80	120.15	108.36
3	B	505	I13	C47-O3-N4	12.93	119.40	108.36
3	B	502	I13	C47-O3-N4	12.93	119.40	108.36
3	C	503	I13	C47-O3-N4	12.77	119.27	108.36
3	B	502	I13	O3-N4-C18	6.32	121.57	111.91
3	B	505	I13	O3-N4-C18	6.32	121.56	111.91
3	C	503	I13	O3-N4-C18	6.10	121.22	111.91
3	A	501	I13	O3-N4-C18	5.64	120.53	111.91
2	A	500	IMP	N3-C2-N1	-5.49	120.09	128.68
2	C	501	IMP	N3-C2-N1	-5.35	120.31	128.68
2	B	501	IMP	N3-C2-N1	-5.07	120.75	128.68
2	D	501	IMP	N3-C2-N1	-5.00	120.87	128.68
3	A	501	I13	C19-C18-N4	-3.76	118.12	123.88
3	C	503	I13	C19-C18-N4	-3.63	118.32	123.88
3	B	502	I13	C19-C18-N4	-3.48	118.56	123.88
3	B	505	I13	C19-C18-N4	-3.40	118.68	123.88
3	A	501	I13	C16-C18-N4	2.88	120.46	115.28
3	C	503	I13	C16-C18-N4	2.88	120.45	115.28
2	C	501	IMP	C2-N1-C6	2.81	120.58	115.88
2	D	501	IMP	O3P-P-O2P	2.66	117.82	107.64
2	A	500	IMP	C2-N1-C6	2.66	120.34	115.88
2	D	501	IMP	C2-N1-C6	2.59	120.22	115.88
3	B	505	I13	C16-C18-N4	2.56	119.89	115.28
3	B	502	I13	C16-C18-N4	2.56	119.88	115.28
2	B	501	IMP	C2-N1-C6	2.45	119.98	115.88
2	A	500	IMP	O3P-P-O2P	2.44	116.98	107.64
2	D	501	IMP	C4-C5-N7	-2.22	107.08	109.40
2	C	501	IMP	C1'-N9-C4	-2.12	122.91	126.64
2	D	501	IMP	C1'-N9-C4	-2.09	122.97	126.64
2	C	501	IMP	C4-C5-N7	-2.04	107.28	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
3	B	502	I13	C6-C7-N3-O1
3	B	502	I13	C8-C7-N3-O1
5	B	504	PEG	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
3	A	501	I13	C48-C47-O3-N4
3	C	503	I13	C48-C47-O3-N4
3	B	502	I13	C48-C47-O3-N4
4	B	503	GOL	O1-C1-C2-O2
5	A	503	PEG	C1-C2-O2-C3
3	B	505	I13	C48-C47-O3-N4

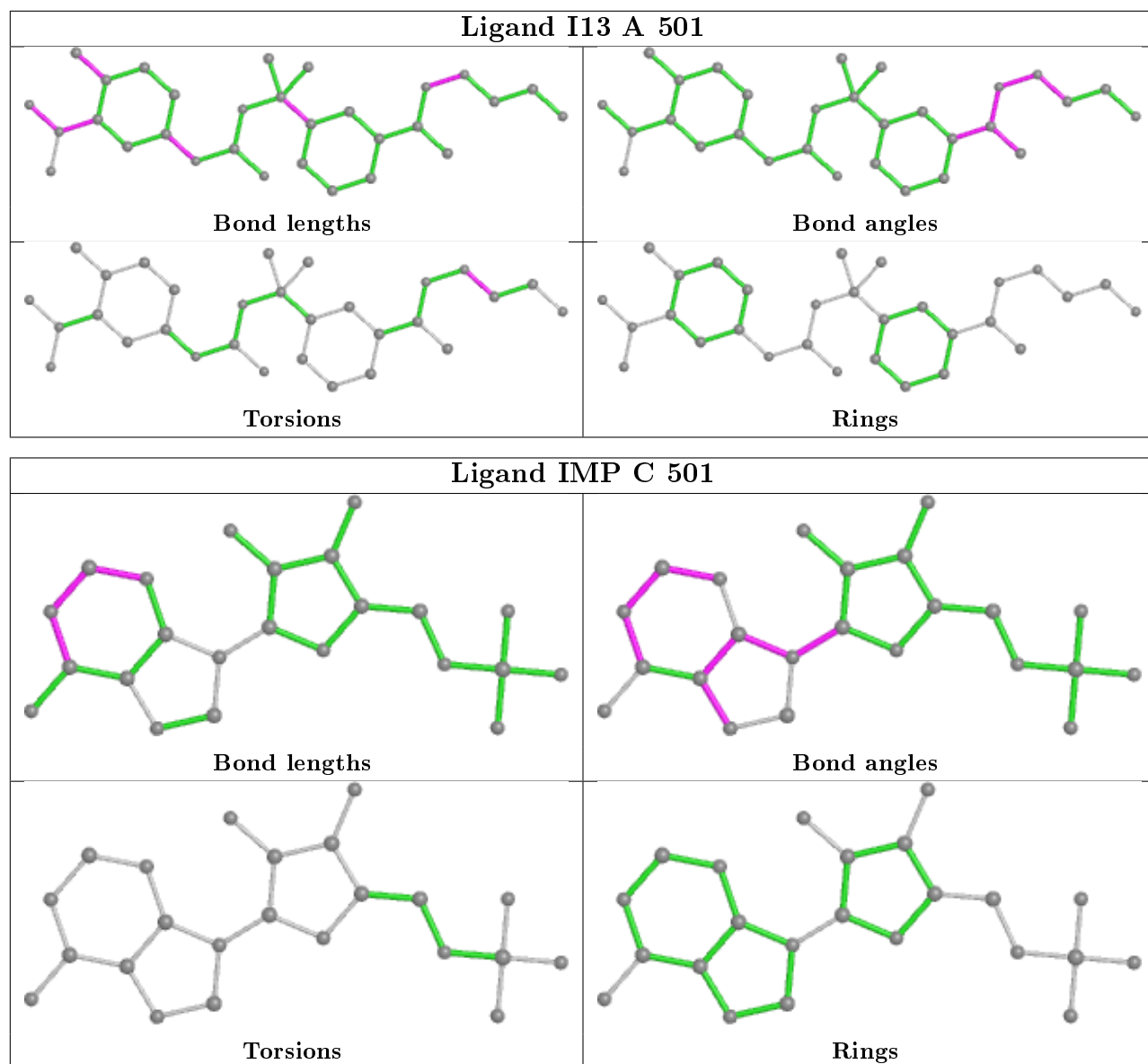
There are no ring outliers.

9 monomers are involved in 12 short contacts:

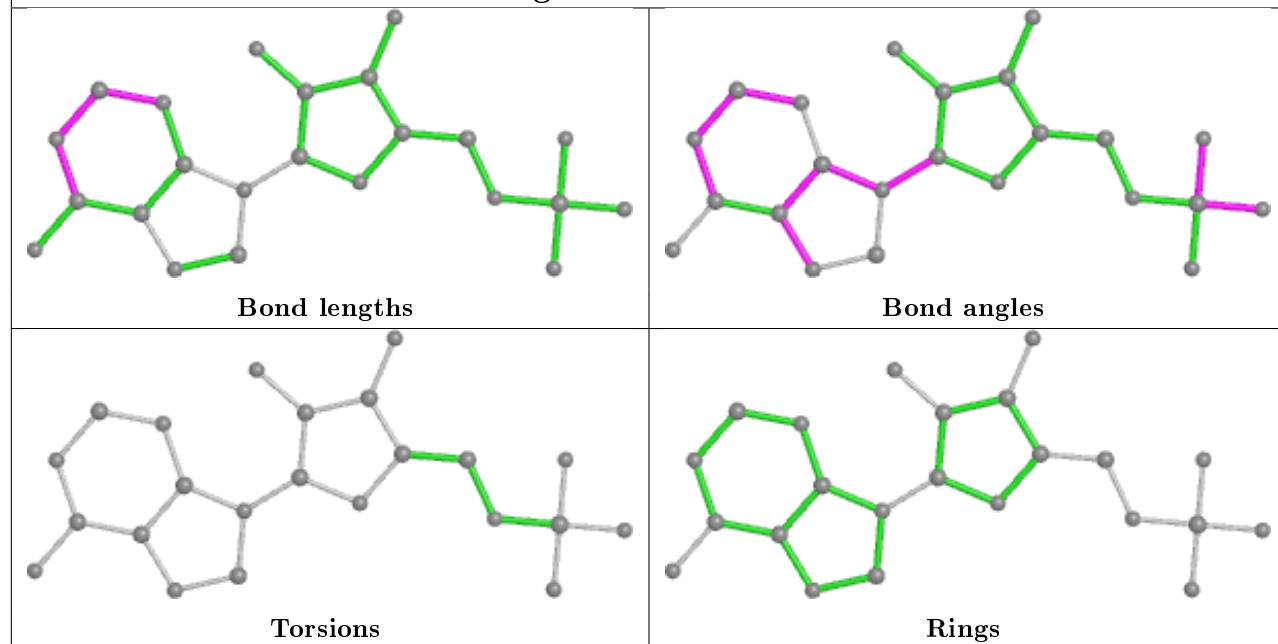
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	PEG	2	0
3	A	501	I13	2	0
2	C	501	IMP	1	0
2	D	501	IMP	1	0
2	B	501	IMP	1	0
2	A	500	IMP	1	0
3	C	503	I13	1	0
3	B	505	I13	2	0
3	B	502	I13	1	0

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

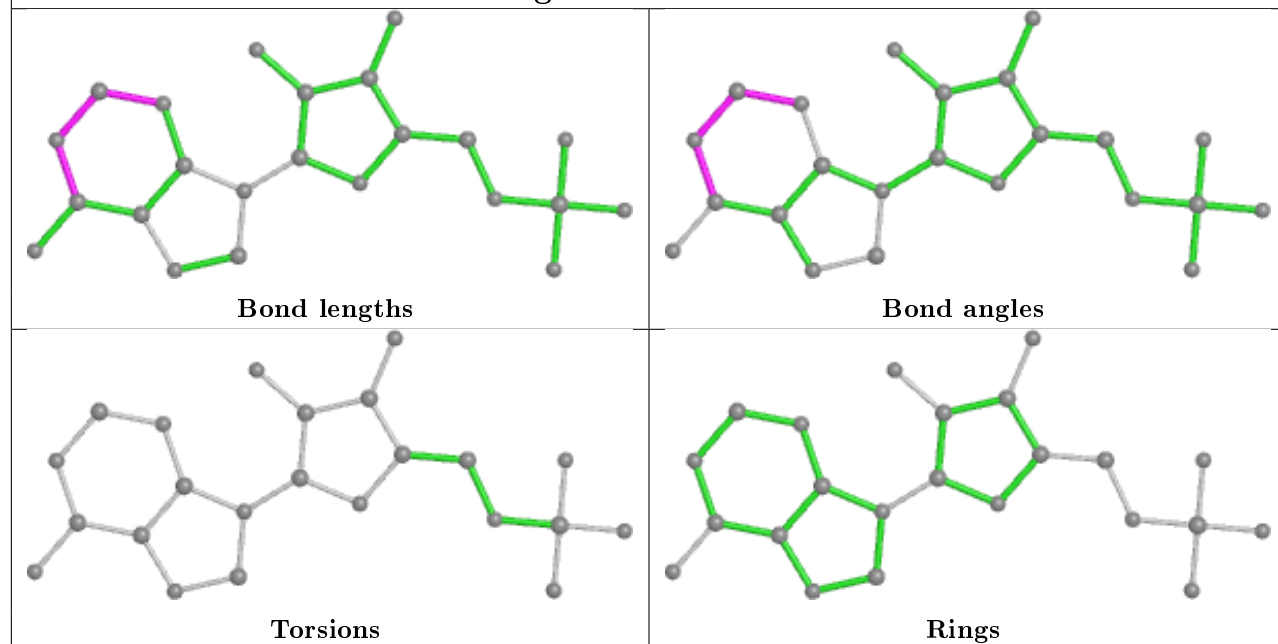
equivalents in the CSD to analyse the geometry.



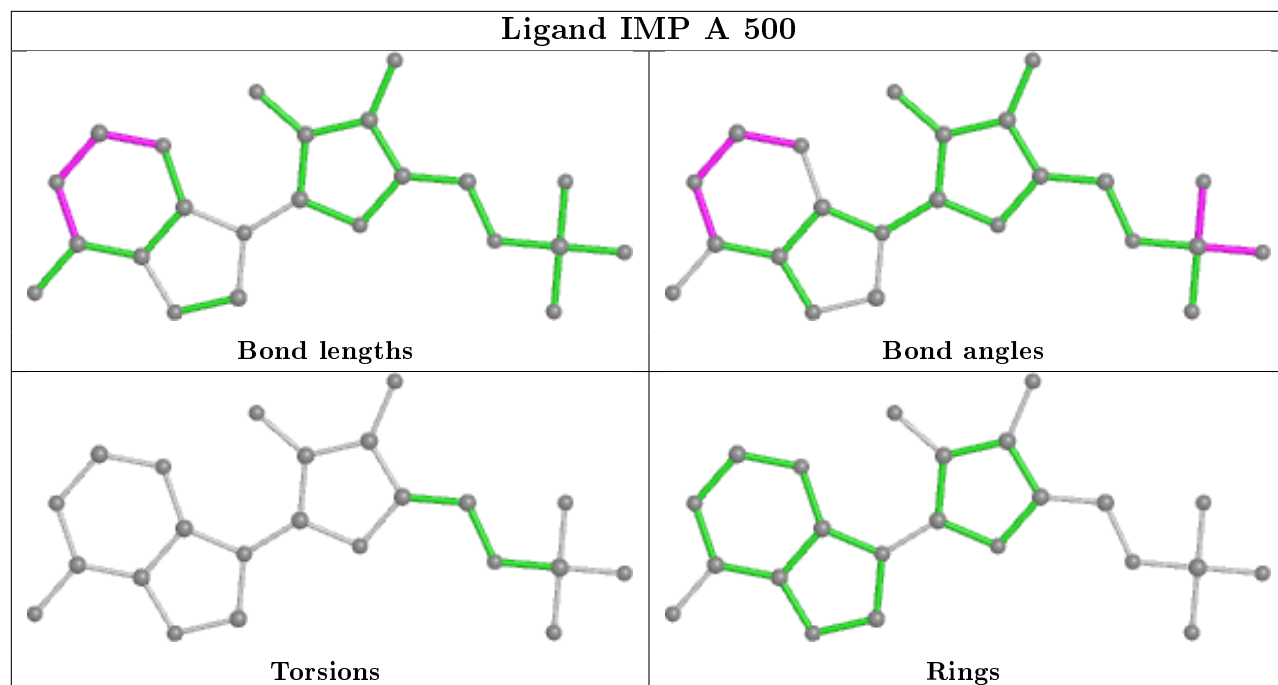
Ligand IMP D 501



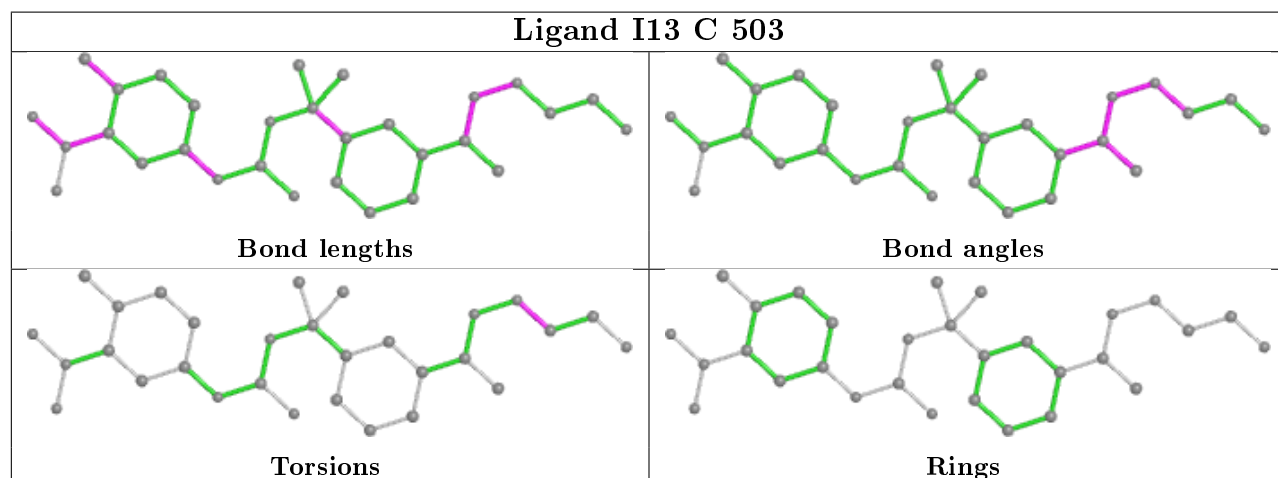
Ligand IMP B 501



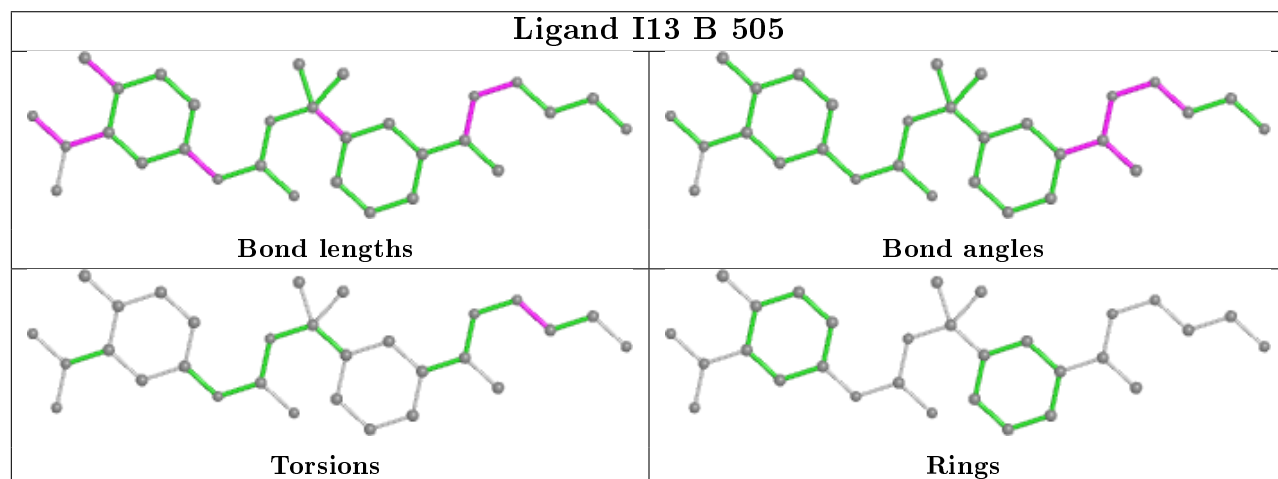
Ligand IMP A 500

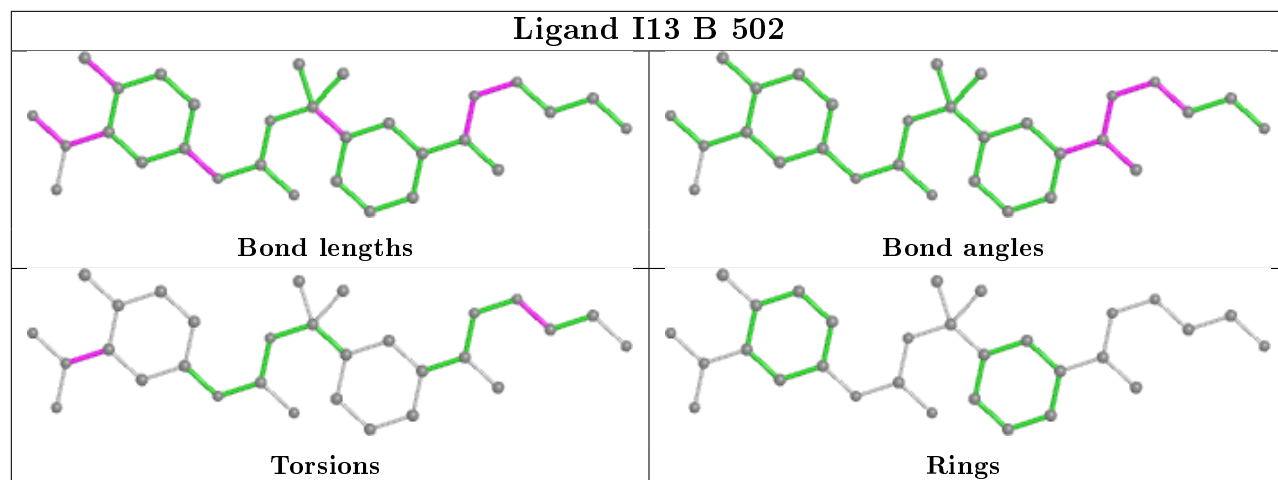


Ligand I13 C 503



Ligand I13 B 505





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	326/361 (90%)	-0.02	9 (2%) 53 56	18, 32, 59, 93	0
1	B	326/361 (90%)	0.05	17 (5%) 27 27	22, 32, 59, 82	0
1	C	325/361 (90%)	0.19	15 (4%) 32 33	20, 33, 60, 84	0
1	D	326/361 (90%)	-0.03	14 (4%) 35 36	18, 31, 58, 79	0
All	All	1303/1444 (90%)	0.05	55 (4%) 36 38	18, 32, 60, 93	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	ALA	9.3
1	D	1	MET	5.1
1	D	310	SER	4.7
1	C	391	ILE	4.5
1	C	291	ILE	4.1
1	D	291	ILE	4.0
1	D	92	GLY	3.8
1	B	310	SER	3.7
1	A	1	MET	3.5
1	A	391	ILE	3.4
1	A	92	GLY	3.4
1	C	92	GLY	3.2
1	B	92	GLY	3.2
1	B	91	GLY	3.1
1	D	293	ASP	3.1
1	D	309	LYS	3.1
1	B	89	ASN	3.0
1	B	309	LYS	2.9
1	B	298	TYR	2.9
1	A	310	SER	2.9
1	A	293	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	293	ASP	2.8
1	C	294	THR	2.8
1	D	85	LEU	2.7
1	B	388	ASP	2.7
1	B	2	GLY	2.7
1	C	296	TYR	2.7
1	D	392	VAL	2.7
1	B	378	THR	2.7
1	D	378	THR	2.6
1	C	1	MET	2.5
1	B	291	ILE	2.5
1	D	305	VAL	2.4
1	B	296	TYR	2.4
1	C	309	LYS	2.4
1	C	298	TYR	2.3
1	A	91	GLY	2.3
1	A	390	GLU	2.3
1	B	307	ALA	2.2
1	B	1	MET	2.2
1	A	78	GLU	2.2
1	D	89	ASN	2.2
1	B	287	GLU	2.2
1	C	78	GLU	2.2
1	C	307	ALA	2.1
1	B	391	ILE	2.1
1	A	392	VAL	2.1
1	C	392	VAL	2.1
1	C	90	SER	2.1
1	B	392	VAL	2.1
1	D	222[A]	ARG	2.0
1	B	305	VAL	2.0
1	D	298	TYR	2.0
1	C	290	LEU	2.0
1	D	391	ILE	2.0

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

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(\AA^2)	Q<0.9
1	OCS	B	219	9/10	0.93	0.13	25,31,45,50	0
1	OCS	D	219	9/10	0.93	0.15	31,34,54,59	0
1	OCS	A	219	9/10	0.95	0.10	30,35,47,53	0
1	OCS	C	219	9/10	0.96	0.10	31,33,50,51	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

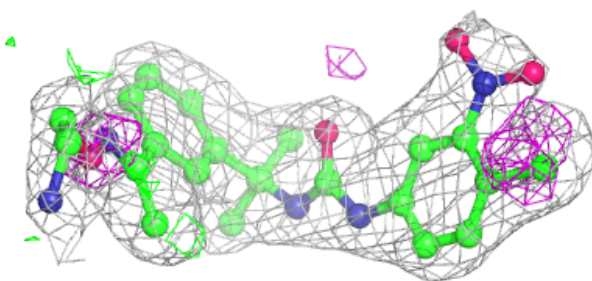
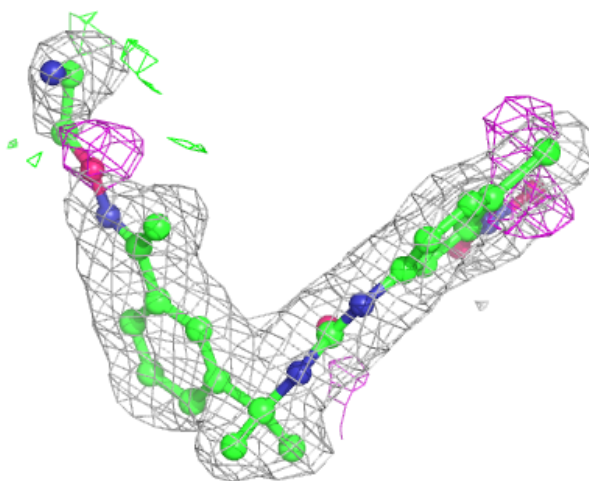
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	502	6/6	0.76	0.18	49,58,59,62	0
5	PEG	A	503	7/7	0.77	0.16	64,66,67,69	0
4	GOL	A	502	6/6	0.83	0.29	63,65,69,70	0
4	GOL	C	502	6/6	0.86	0.19	55,63,66,66	0
3	I13	B	505	30/30	0.88	0.15	25,34,58,64	0
5	PEG	B	504	7/7	0.88	0.18	57,63,66,67	0
4	GOL	B	503	6/6	0.89	0.23	52,65,70,72	0
3	I13	A	501	30/30	0.89	0.16	22,37,59,70	0
3	I13	B	502	30/30	0.92	0.13	26,34,56,61	0
3	I13	C	503	30/30	0.93	0.13	22,31,60,62	0
2	IMP	B	501	23/23	0.96	0.10	20,25,29,30	0
2	IMP	D	501	23/23	0.97	0.09	19,25,28,30	0
2	IMP	A	500	23/23	0.97	0.09	19,25,28,36	0
2	IMP	C	501	23/23	0.98	0.10	20,27,30,32	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.

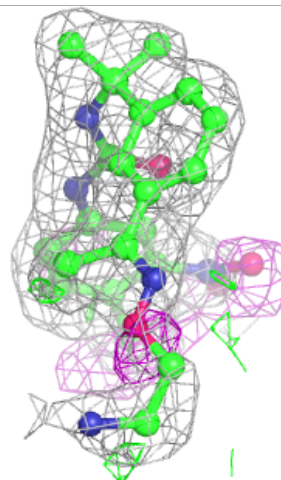
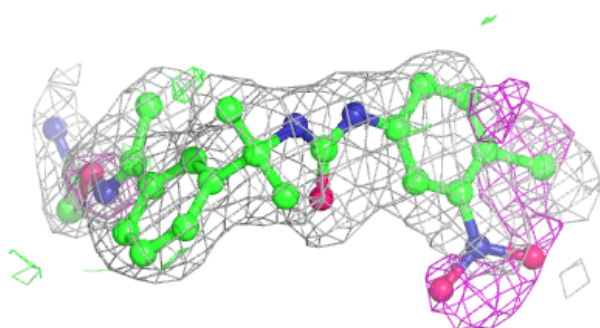
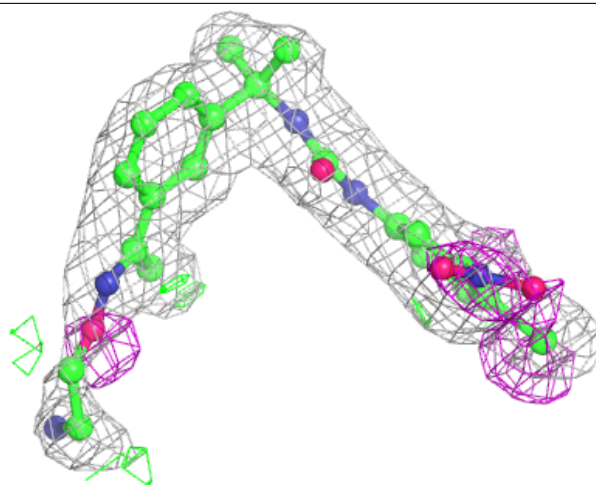
Electron density around I13 B 505:

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



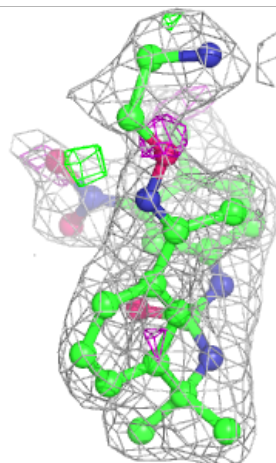
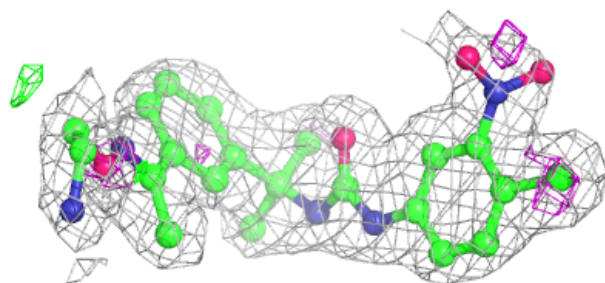
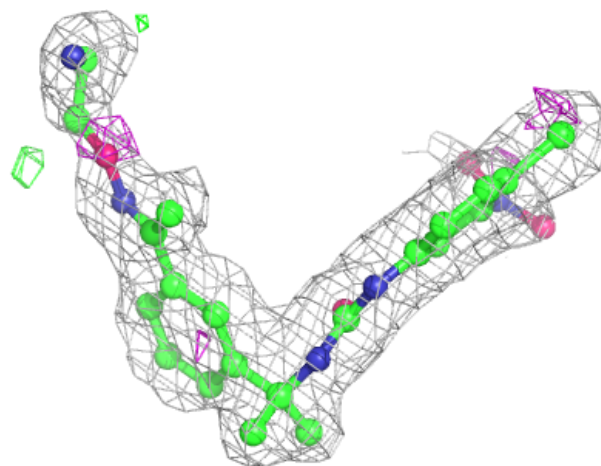
Electron density around I13 A 501:

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



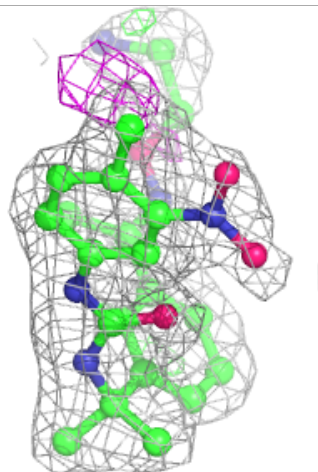
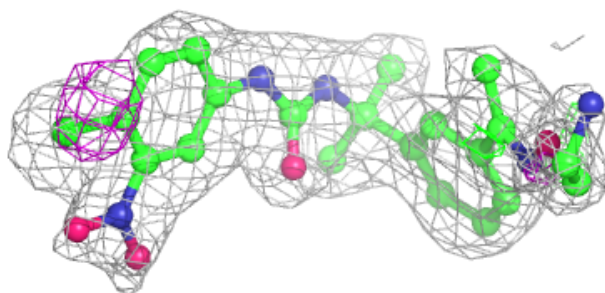
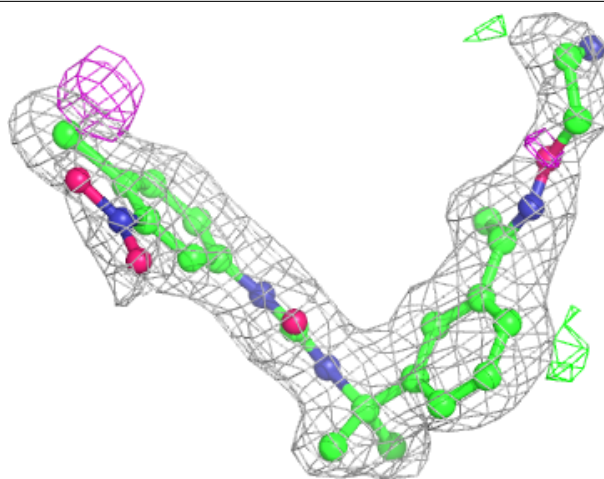
Electron density around I13 B 502:

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



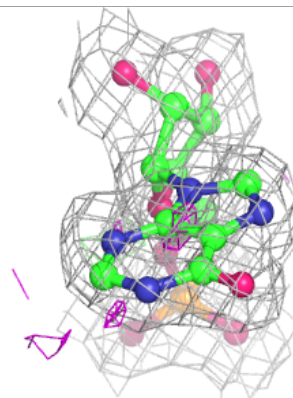
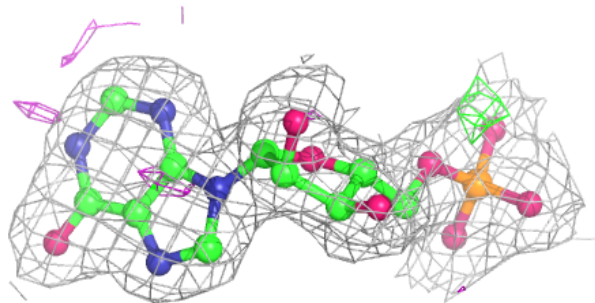
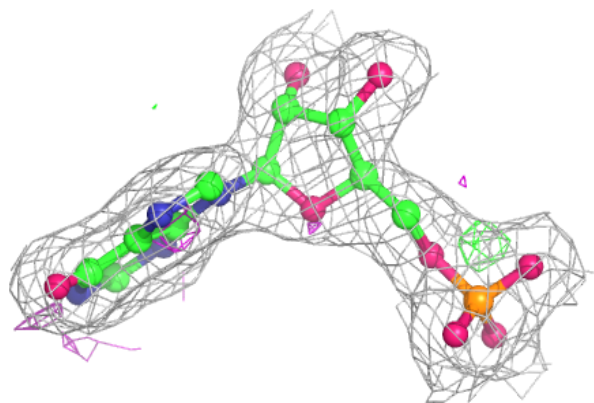
Electron density around I13 C 503:

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

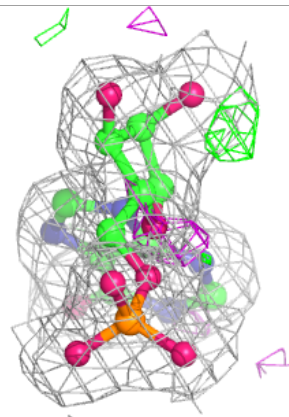
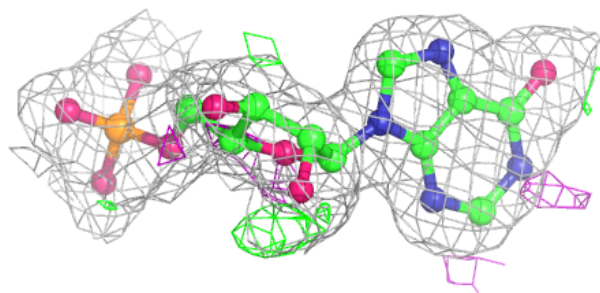
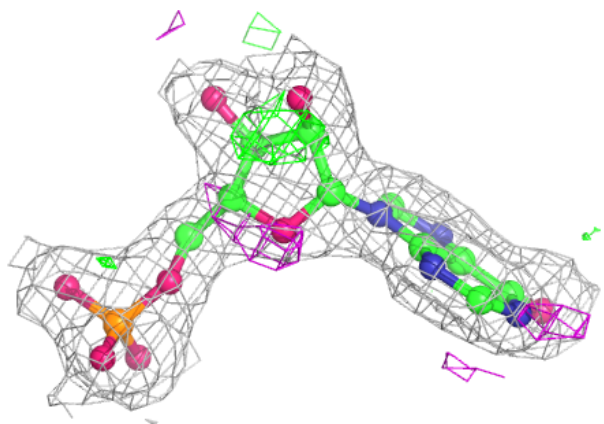


Electron density around IMP B 501:

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

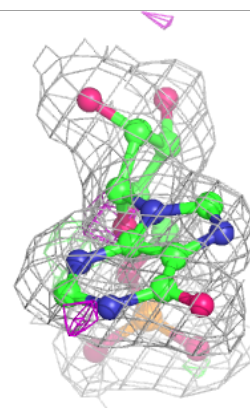
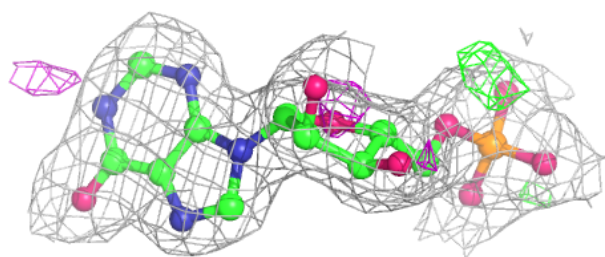
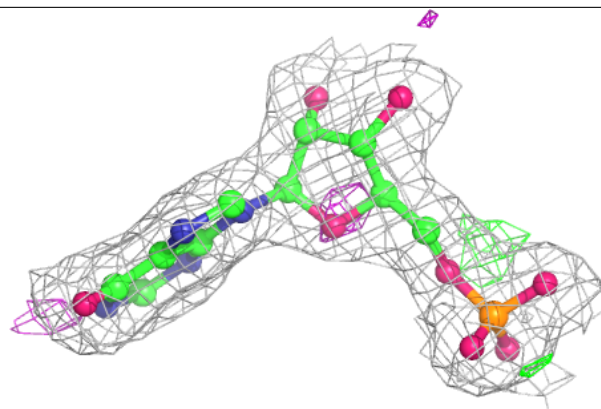
**Electron density around IMP D 501:**

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

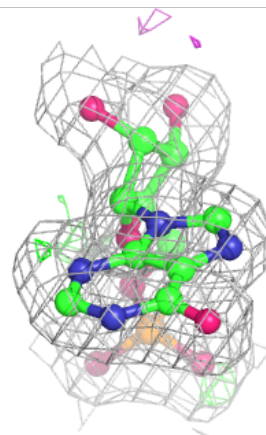
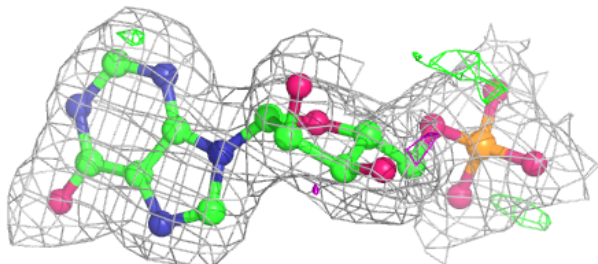
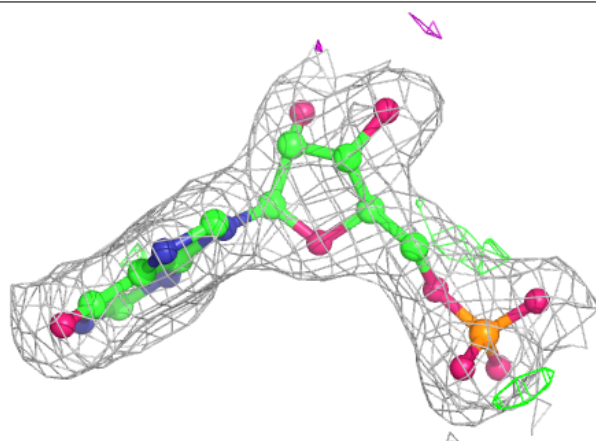


Electron density around IMP A 500:

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

**Electron density around IMP C 501:**

$2mF_o-DF_c$ (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.