



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:00 PM BST

PDB ID : 4IXH  
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Cryptosporidium parvum*  
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 : 2013-01-25  
Resolution : 2.10 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

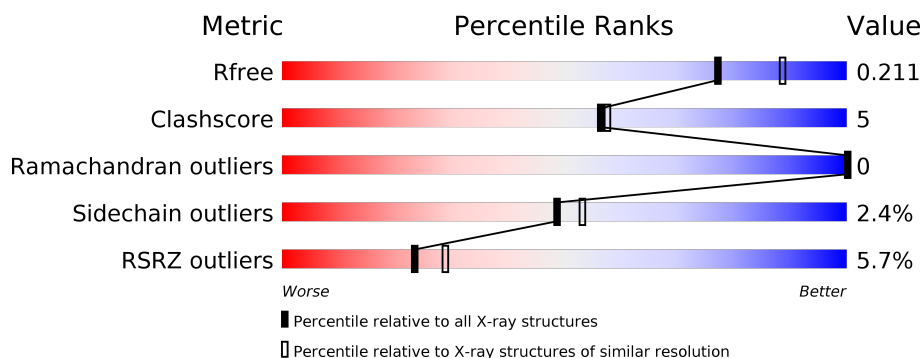
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>
1	B	361	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	361	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	D	361	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10776 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	336	Total	C	N	O	S	0	6	0
			2532	1588	434	494	16			
1	B	334	Total	C	N	O	S	0	6	0
			2520	1583	431	491	15			
1	C	336	Total	C	N	O	S	0	4	0
			2516	1581	431	488	16			
1	D	334	Total	C	N	O	S	0	2	0
			2486	1563	424	484	15			

There are 24 discrepancies between the modelled and reference sequences:

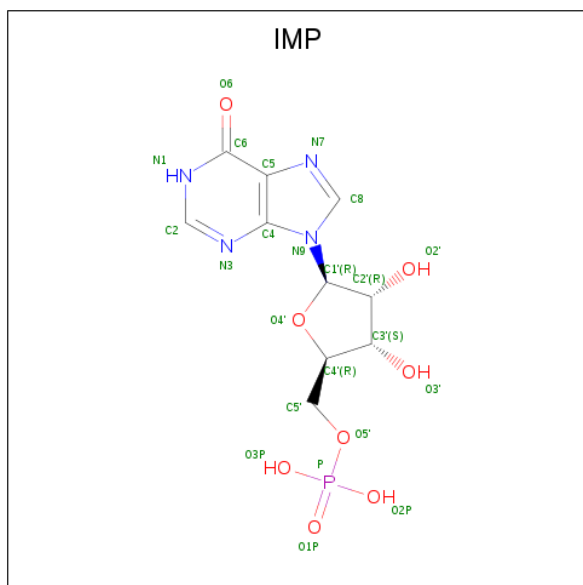
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
A	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
A	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
A	90	SER	-	LINKER	UNP Q8T6T2
A	91	GLY	-	LINKER	UNP Q8T6T2
A	92	GLY	-	LINKER	UNP Q8T6T2
B	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
B	-1	ASN	-	EXPRESSION 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:  $C_{10}H_{13}N_4O_8P$ ).



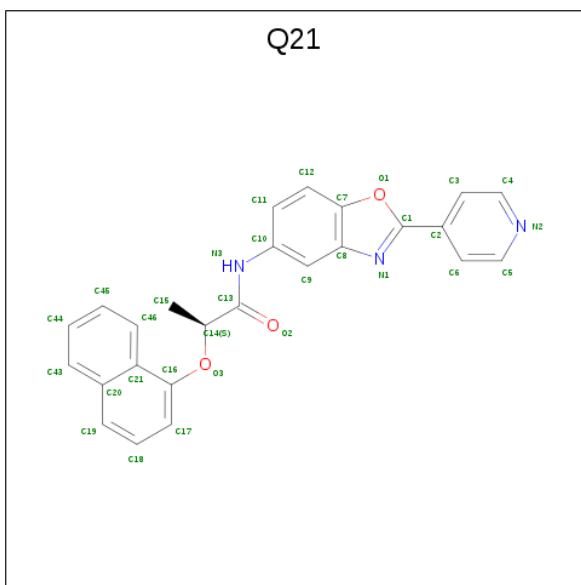
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 4 is (2S)-2-(naphthalen-1-yloxy)-N-[2-(pyridin-4-yl)-1,3-benzoxazol-5-yl]propanamide (three-letter code: Q21) (formula: C<sub>25</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	25	3	3		
4	B	1	Total	C	N	O	0	0
			31	25	3	3		
4	B	1	Total	C	N	O	0	0
			31	25	3	3		
4	C	1	Total	C	N	O	0	0
			31	25	3	3		

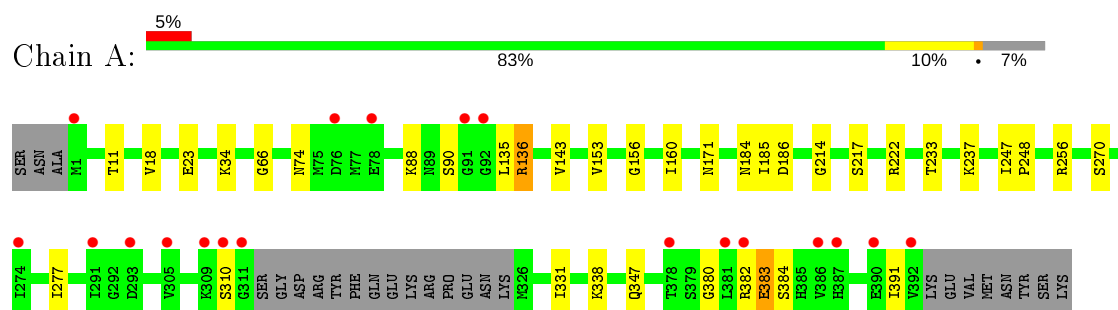
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	114	Total	O	0	0
			114	114		
5	C	114	Total	O	0	0
			114	114		
5	D	131	Total	O	0	0
			131	131		

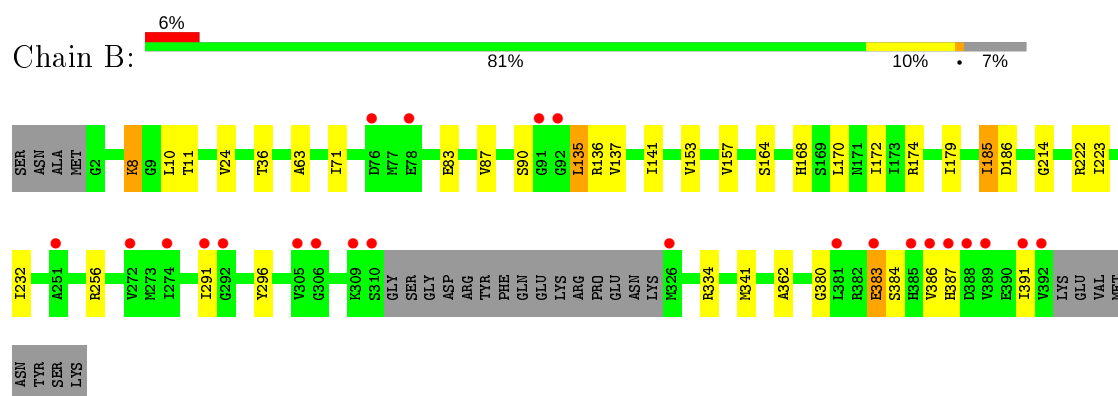
### 3 Residue-property plots [i](#)

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.

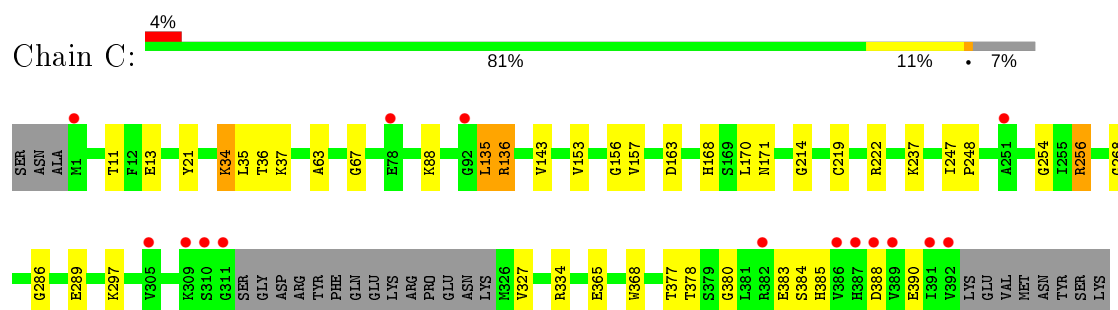
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



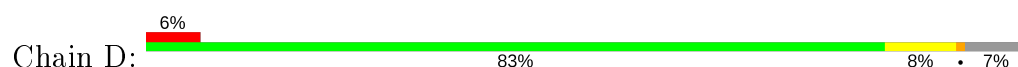
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

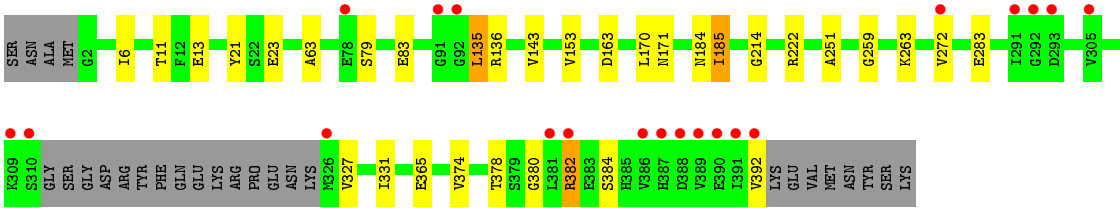


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- 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, $\alpha$ , $\beta$ , $\gamma$	89.19 Å 92.02 Å 92.14 Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	35.52 – 2.10 35.52 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.52-2.10) 99.0 (35.52-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.10 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, $R_{free}$	0.162 , 0.210 0.163 , 0.211	Depositor DCC
$R_{free}$ test set	4142 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	1.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: IMP, EDO, Q21

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	0.36	0/2557	0.51	0/3440
1	B	0.36	0/2545	0.53	0/3426
1	C	0.34	0/2541	0.53	0/3419
1	D	0.35	0/2511	0.53	0/3380
All	All	0.35	0/10154	0.53	0/13665

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	2532	0	2625	36	0
1	B	2520	0	2615	31	0
1	C	2516	0	2619	35	0
1	D	2486	0	2584	25	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	1	0
2	D	23	0	11	0	0
3	A	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	12	3	0
4	A	31	0	19	1	0
4	B	62	0	38	2	0
4	C	31	0	19	1	0
5	A	127	0	0	6	0
5	B	114	0	0	2	0
5	C	114	0	0	3	0
5	D	131	0	0	2	0
All	All	10776	0	10593	104	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 5.

All (104) 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:C:222:ARG:HD2	1:D:384:SER:HA	1.67	0.76
1:A:66:GLY:HA2	1:A:136[B]:ARG:HH21	1.57	0.68
1:B:222:ARG:HD2	1:C:384:SER:HA	1.73	0.67
1:A:222:ARG:HD2	1:B:384:SER:HA	1.75	0.67
1:C:286:GLY:O	1:C:297:LYS:NZ	2.30	0.65
1:B:256[A]:ARG:NE	1:C:388:ASP:OD2	2.21	0.64
1:D:143:VAL:HG21	1:D:171:ASN:HB3	1.81	0.62
1:A:380:GLY:HA2	1:D:11:THR:HG21	1.83	0.61
1:B:223:ILE:HD11	1:C:385:HIS:HA	1.82	0.61
1:A:153:VAL:HG22	1:A:185:ILE:HD12	1.83	0.60
1:A:384:SER:HA	1:D:222:ARG:HD2	1.83	0.60
1:A:256:ARG:NH1	5:A:710:HOH:O	2.35	0.59
1:A:160:ILE:HG12	1:A:185:ILE:HD13	1.85	0.58
1:B:11[A]:THR:HG21	1:C:380:GLY:HA2	1.86	0.58
1:A:331:ILE:HD13	1:B:391:ILE:HG12	1.86	0.58
1:C:143[A]:VAL:HG21	1:C:171:ASN:HB3	1.87	0.56
1:A:23:GLU:HG2	1:D:170:LEU:HB2	1.88	0.56
1:C:237:LYS:NZ	5:C:655:HOH:O	2.29	0.55
1:B:24:VAL:HG11	1:B:362:ALA:HB2	1.88	0.54
1:A:391:ILE:HG12	1:D:331:ILE:HD13	1.90	0.54
1:A:382:ARG:NH2	1:D:13:GLU:OE1	2.40	0.54
1:A:214:GLY:HA3	1:A:222:ARG:HE	1.72	0.54
1:A:237:LYS:HE3	5:A:707:HOH:O	2.07	0.54
1:A:11:THR:HG21	1:B:380:GLY:HA2	1.90	0.53
5:B:701:HOH:O	1:C:383:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG21	1:A:171[A]:ASN:HB3	1.92	0.52
1:D:365:GLU:HG2	5:D:712:HOH:O	2.09	0.51
1:A:171[A]:ASN:ND2	5:A:680:HOH:O	2.42	0.51
1:B:87:VAL:HG11	1:B:137:VAL:HB	1.92	0.51
1:B:214:GLY:HA3	1:B:222:ARG:HE	1.76	0.51
1:C:334:ARG:HE	1:D:392:VAL:HG22	1.76	0.51
1:A:347[B]:GLN:HG2	1:D:327:VAL:HG21	1.93	0.51
1:C:63:ALA:HB1	1:C:135:LEU:HG	1.92	0.51
1:C:170:LEU:HB2	1:D:23:GLU:HG2	1.94	0.50
1:A:136[A]:ARG:NH1	5:A:667:HOH:O	2.45	0.50
1:D:153:VAL:HG22	1:D:185:ILE:HD12	1.94	0.49
1:C:88:LYS:HE3	1:C:156:GLY:O	2.12	0.49
1:C:254:GLY:O	1:C:256[A]:ARG:HD3	2.13	0.49
1:D:63:ALA:CB	1:D:135:LEU:HG	2.43	0.48
1:A:214:GLY:HA3	1:A:222:ARG:NE	2.29	0.48
1:B:214:GLY:HA3	1:B:222:ARG:NE	2.29	0.48
1:C:63:ALA:CB	1:C:135:LEU:HG	2.44	0.48
1:D:63:ALA:HB1	1:D:135:LEU:HG	1.95	0.48
1:A:18:VAL:HG21	1:D:6:ILE:HD11	1.96	0.47
1:C:378:THR:HG23	1:D:382:ARG:HH12	1.78	0.47
1:A:88:LYS:HE3	1:A:156:GLY:O	2.14	0.47
1:B:291:ILE:HB	1:B:296:TYR:CE1	2.50	0.47
1:C:13:GLU:HG3	1:C:256[A]:ARG:NH2	2.30	0.46
1:A:383:GLU:HG2	5:D:719:HOH:O	2.16	0.46
1:C:219:CYS:SG	2:C:501:IMP:H2	2.56	0.46
1:C:35:LEU:HG	1:C:36:THR:HG23	1.98	0.45
1:B:136[B]:ARG:H	1:B:136[B]:ARG:HG3	1.49	0.45
1:B:334:ARG:HE	1:B:334:ARG:HB2	1.54	0.45
1:C:168:HIS:CE1	1:D:21:TYR:HB2	2.51	0.45
1:D:214:GLY:HA3	1:D:222:ARG:HE	1.81	0.45
1:C:34:LYS:H	3:C:504:EDO:H12	1.82	0.45
1:D:214:GLY:HA3	1:D:222:ARG:NE	2.31	0.45
1:C:11:THR:HG21	1:D:380:GLY:HA2	1.98	0.45
1:B:256[B]:ARG:NH1	5:B:693:HOH:O	2.34	0.45
1:C:13:GLU:OE1	1:C:256[B]:ARG:NH1	2.50	0.45
1:C:67:GLY:O	1:C:136[B]:ARG:NH1	2.50	0.44
1:B:90:SER:O	1:B:135:LEU:HD22	2.17	0.44
1:A:233:THR:HG22	1:A:237:LYS:HD3	1.99	0.44
1:C:368:TRP:CH2	3:C:504:EDO:H21	2.53	0.44
1:A:270:SER:OG	3:A:502:EDO:H11	2.17	0.44
1:B:8:LYS:HE2	1:C:377:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:NH2	1:B:383:GLU:OE1	2.52	0.43
1:D:79:SER:O	1:D:83:GLU:HG2	2.18	0.43
1:A:74:ASN:HD21	1:A:310:SER:HB2	1.84	0.43
1:D:251:ALA:HB3	1:D:272:VAL:HG12	2.00	0.43
1:A:88:LYS:HA	1:A:88:LYS:HD3	1.80	0.43
1:A:34:LYS:HB3	1:A:34:LYS:HE2	1.89	0.42
1:B:141:ILE:HD11	1:B:179:ILE:HD11	2.01	0.42
4:A:504:Q21:H15	4:A:504:Q21:O2	2.19	0.42
1:C:143[B]:VAL:HG23	5:C:650:HOH:O	2.19	0.42
1:B:153:VAL:CG2	1:B:185:ILE:HG12	2.49	0.42
1:B:10:LEU:O	1:B:232:ILE:HB	2.20	0.42
1:D:259:GLY:O	1:D:263:LYS:HG3	2.20	0.42
1:C:268:GLY:HA2	3:C:503:EDO:H22	2.01	0.42
1:A:277:ILE:HG23	5:A:664:HOH:O	2.19	0.42
1:B:170:LEU:O	1:B:174:ARG:HG3	2.20	0.42
1:A:171[B]:ASN:ND2	4:B:501:Q21:H17	2.35	0.42
1:B:63:ALA:HB3	1:B:135:LEU:HG	2.02	0.42
1:C:256[A]:ARG:HE	1:C:256[A]:ARG:HB2	1.68	0.42
1:A:185:ILE:HG12	1:A:186:ASP:N	2.34	0.41
1:A:90:SER:O	1:A:135:LEU:HD22	2.20	0.41
1:A:247:ILE:HA	1:A:248:PRO:HD3	1.85	0.41
1:C:153:VAL:HA	1:C:157:VAL:HG12	2.03	0.41
1:C:256[A]:ARG:NH1	5:C:684:HOH:O	2.50	0.41
1:A:338:LYS:NZ	5:A:664:HOH:O	2.37	0.41
1:C:214:GLY:HA3	1:C:222:ARG:HE	1.84	0.41
1:D:283:GLU:N	1:D:283:GLU:OE2	2.53	0.41
1:B:168:HIS:CE1	1:C:21:TYR:HB2	2.56	0.41
1:A:331:ILE:HG12	1:B:386:VAL:HG21	2.02	0.41
4:C:502:Q21:H15	4:C:502:Q21:O2	2.19	0.41
1:A:217:SER:HA	1:B:387:HIS:CE1	2.56	0.41
1:B:164:SER:HB2	1:B:172:ILE:HD11	2.02	0.41
1:B:71:ILE:HD13	1:B:83:GLU:HB3	2.02	0.41
1:C:247:ILE:HA	1:C:248:PRO:HD3	1.91	0.41
1:D:136[B]:ARG:HB2	1:D:136[B]:ARG:HE	1.75	0.41
1:B:63:ALA:CB	1:B:135:LEU:HG	2.50	0.41
1:B:8:LYS:HE2	1:C:377:THR:CG2	2.52	0.40
1:B:36:THR:OG1	1:B:186:ASP:OD1	2.20	0.40
4:B:503:Q21:O2	4:B:503:Q21:H15	2.21	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	338/361 (94%)	327 (97%)	11 (3%)	0	100	100
1	B	336/361 (93%)	324 (96%)	12 (4%)	0	100	100
1	C	336/361 (93%)	328 (98%)	8 (2%)	0	100	100
1	D	332/361 (92%)	324 (98%)	8 (2%)	0	100	100
All	All	1342/1444 (93%)	1303 (97%)	39 (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	278/295 (94%)	274 (99%)	4 (1%)	67	73
1	B	277/295 (94%)	271 (98%)	6 (2%)	52	57
1	C	276/295 (94%)	264 (96%)	12 (4%)	29	29
1	D	273/295 (92%)	266 (97%)	7 (3%)	46	50
All	All	1104/1180 (94%)	1075 (97%)	29 (3%)	49	50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136[A]	ARG
1	A	136[B]	ARG

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	383	GLU
1	B	8	LYS
1	B	135	LEU
1	B	157	VAL
1	B	185	ILE
1	B	341	MET
1	B	383	GLU
1	C	34	LYS
1	C	37	LYS
1	C	135	LEU
1	C	136[A]	ARG
1	C	136[B]	ARG
1	C	163	ASP
1	C	256[A]	ARG
1	C	256[B]	ARG
1	C	289	GLU
1	C	327	VAL
1	C	365	GLU
1	C	390	GLU
1	D	135	LEU
1	D	163	ASP
1	D	184	ASN
1	D	185	ILE
1	D	374	VAL
1	D	378	THR
1	D	382	ARG

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	387	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

13 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	B	502	-	21,25,25	1.21	3 (14%)	23,38,38	1.55	3 (13%)
4	Q21	A	504	-	31,35,35	1.02	1 (3%)	43,49,49	1.29	2 (4%)
4	Q21	B	501	-	31,35,35	1.00	1 (3%)	43,49,49	1.34	4 (9%)
2	IMP	C	501	-	21,25,25	1.10	2 (9%)	23,38,38	1.57	2 (8%)
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.37	0
2	IMP	A	501	-	21,25,25	1.13	3 (14%)	23,38,38	1.72	4 (17%)
2	IMP	D	501	-	21,25,25	1.23	3 (14%)	23,38,38	1.50	3 (13%)
3	EDO	C	503	-	3,3,3	0.55	0	2,2,2	0.09	0
4	Q21	C	502	-	31,35,35	1.00	1 (3%)	43,49,49	1.27	3 (6%)
3	EDO	A	503	-	3,3,3	0.36	0	2,2,2	0.37	0
3	EDO	C	504	-	3,3,3	0.45	0	2,2,2	0.35	0
4	Q21	B	503	-	31,35,35	0.99	1 (3%)	43,49,49	1.38	6 (13%)
3	EDO	A	505	-	3,3,3	0.58	0	2,2,2	0.07	0

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	B	502	-	-	0/6/26/26	0/3/3/3
4	Q21	A	504	-	-	0/14/16/16	0/5/5/5
4	Q21	B	501	-	-	0/14/16/16	0/5/5/5
2	IMP	C	501	-	-	0/6/26/26	0/3/3/3
3	EDO	A	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
3	EDO	C	503	-	-	1/1/1/1	-
4	Q21	C	502	-	-	0/14/16/16	0/5/5/5
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
4	Q21	B	503	-	-	0/14/16/16	0/5/5/5
3	EDO	A	505	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	IMP	C2-N3	3.71	1.38	1.32
2	B	502	IMP	C2-N3	3.60	1.37	1.32
2	C	501	IMP	C2-N3	3.16	1.37	1.32
2	A	501	IMP	C2-N3	3.11	1.37	1.32
2	D	501	IMP	C6-N1	3.06	1.38	1.33
2	B	502	IMP	C6-N1	2.96	1.38	1.33
2	A	501	IMP	C6-N1	2.82	1.37	1.33
2	C	501	IMP	C6-N1	2.59	1.37	1.33
4	B	501	Q21	C10-N3	-2.56	1.36	1.41
4	A	504	Q21	C10-N3	-2.45	1.36	1.41
4	C	502	Q21	C10-N3	-2.38	1.36	1.41
4	B	503	Q21	C10-N3	-2.27	1.37	1.41
2	D	501	IMP	C2-N1	2.23	1.38	1.33
2	B	502	IMP	C2-N1	2.20	1.38	1.33
2	A	501	IMP	C2-N1	2.13	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IMP	N3-C2-N1	-5.29	120.41	128.68
2	B	502	IMP	N3-C2-N1	-5.29	120.41	128.68
2	C	501	IMP	N3-C2-N1	-5.20	120.55	128.68
2	D	501	IMP	N3-C2-N1	-5.05	120.78	128.68
4	B	503	Q21	O3-C16-C21	4.30	119.88	114.22
4	B	501	Q21	O3-C16-C21	4.01	119.50	114.22
4	A	504	Q21	O3-C16-C21	3.72	119.11	114.22
4	C	502	Q21	O3-C16-C21	3.70	119.09	114.22
4	B	501	Q21	C1-N1-C8	3.37	110.46	103.78
2	A	501	IMP	C2-N1-C6	3.30	121.41	115.88
4	A	504	Q21	C1-N1-C8	3.26	110.25	103.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	Q21	C1-N1-C8	3.04	109.80	103.78
2	C	501	IMP	C2-N1-C6	2.98	120.87	115.88
4	B	503	Q21	C1-N1-C8	2.92	109.57	103.78
2	A	501	IMP	C1'-N9-C4	-2.89	121.56	126.64
2	B	502	IMP	C2-N1-C6	2.77	120.52	115.88
2	D	501	IMP	C2-N1-C6	2.63	120.29	115.88
4	B	503	Q21	C2-C1-N1	2.31	126.66	123.56
4	B	503	Q21	O3-C16-C17	-2.30	120.42	124.59
2	B	502	IMP	C4-C5-N7	-2.21	107.09	109.40
4	B	503	Q21	C16-O3-C14	2.20	122.00	118.17
4	B	501	Q21	O3-C16-C17	-2.17	120.65	124.59
2	D	501	IMP	C4-C5-N7	-2.14	107.16	109.40
4	B	501	Q21	C5-N2-C4	2.13	121.85	116.85
2	A	501	IMP	C4-C5-N7	-2.12	107.19	109.40
4	C	502	Q21	C16-O3-C14	2.04	121.73	118.17
4	B	503	Q21	C5-N2-C4	2.01	121.58	116.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2

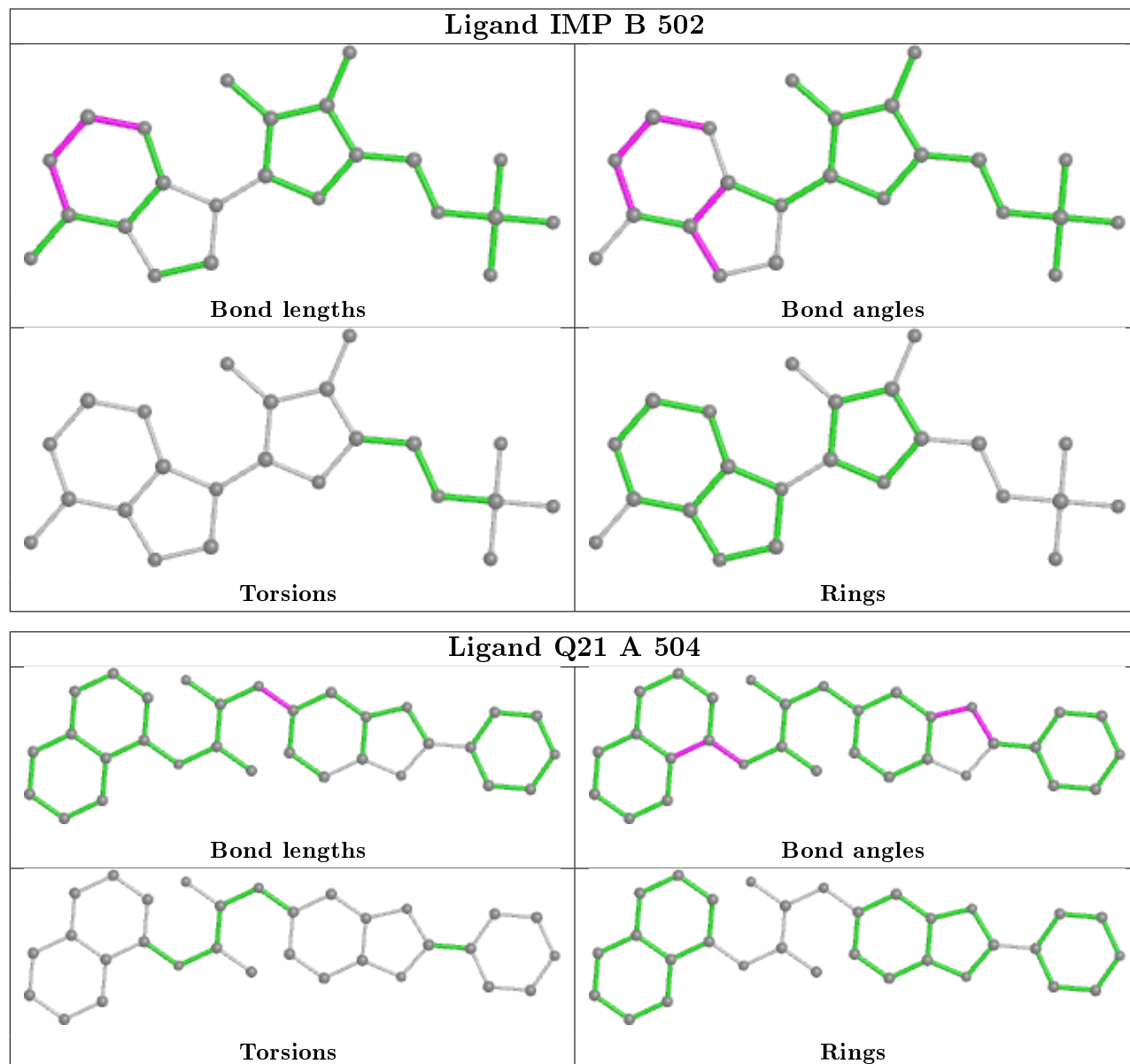
There are no ring outliers.

8 monomers are involved in 9 short contacts:

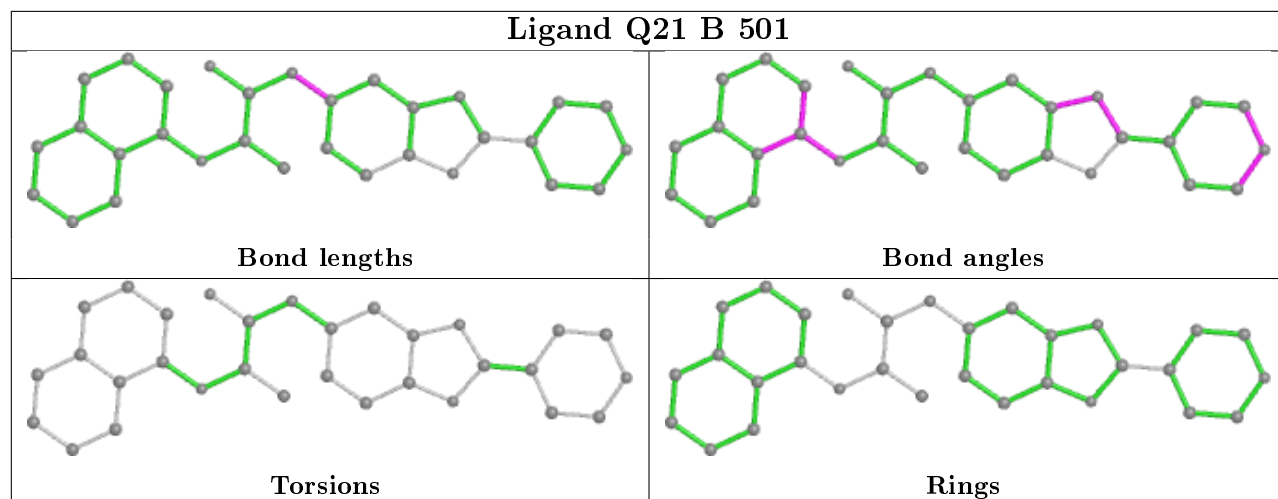
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	Q21	1	0
4	B	501	Q21	1	0
2	C	501	IMP	1	0
3	A	502	EDO	1	0
3	C	503	EDO	1	0
4	C	502	Q21	1	0
3	C	504	EDO	2	0
4	B	503	Q21	1	0

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

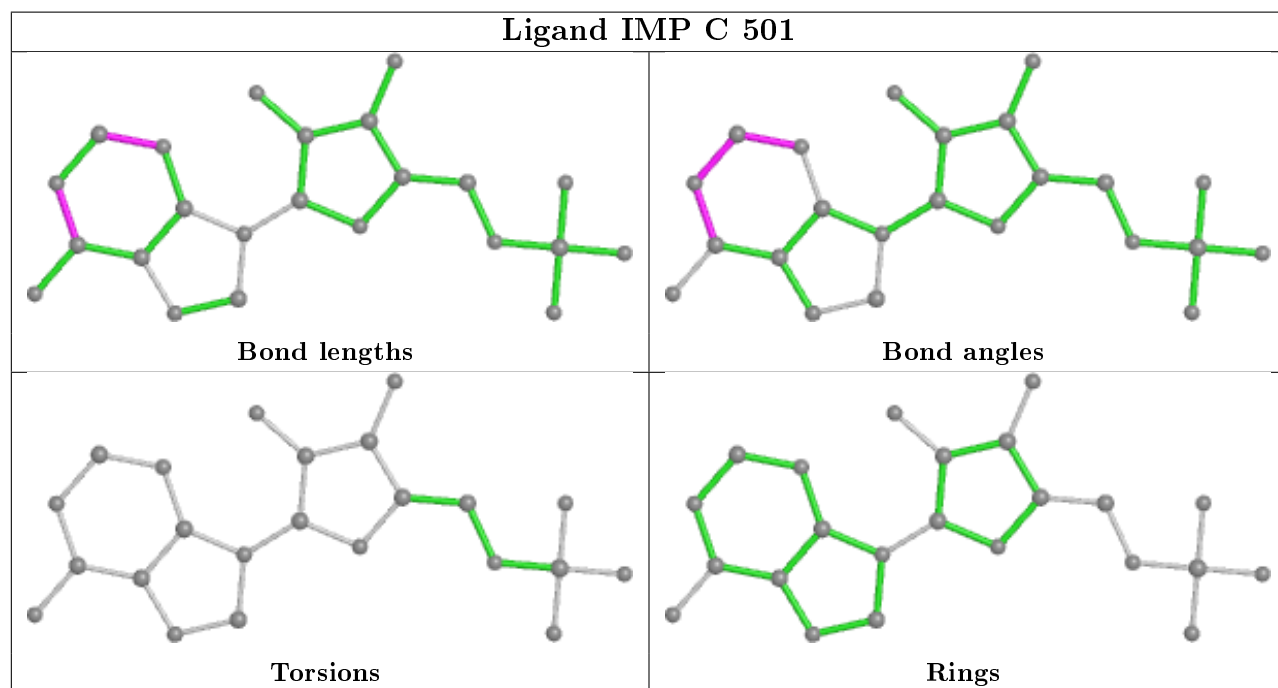
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



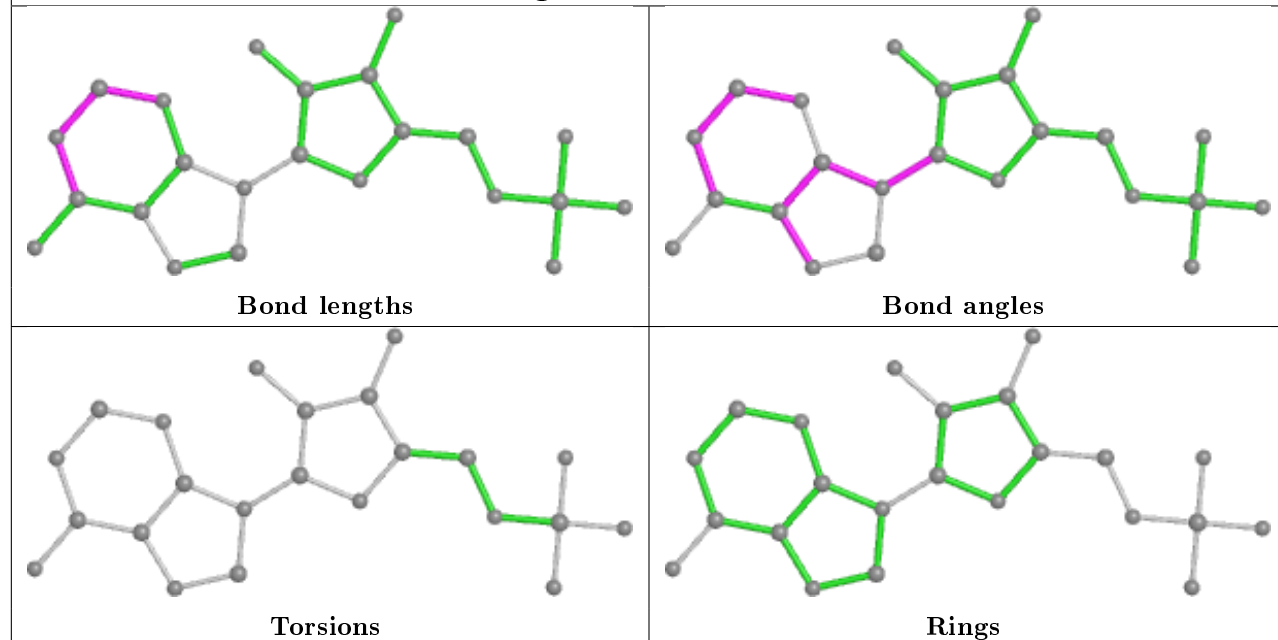
## Ligand Q21 B 501



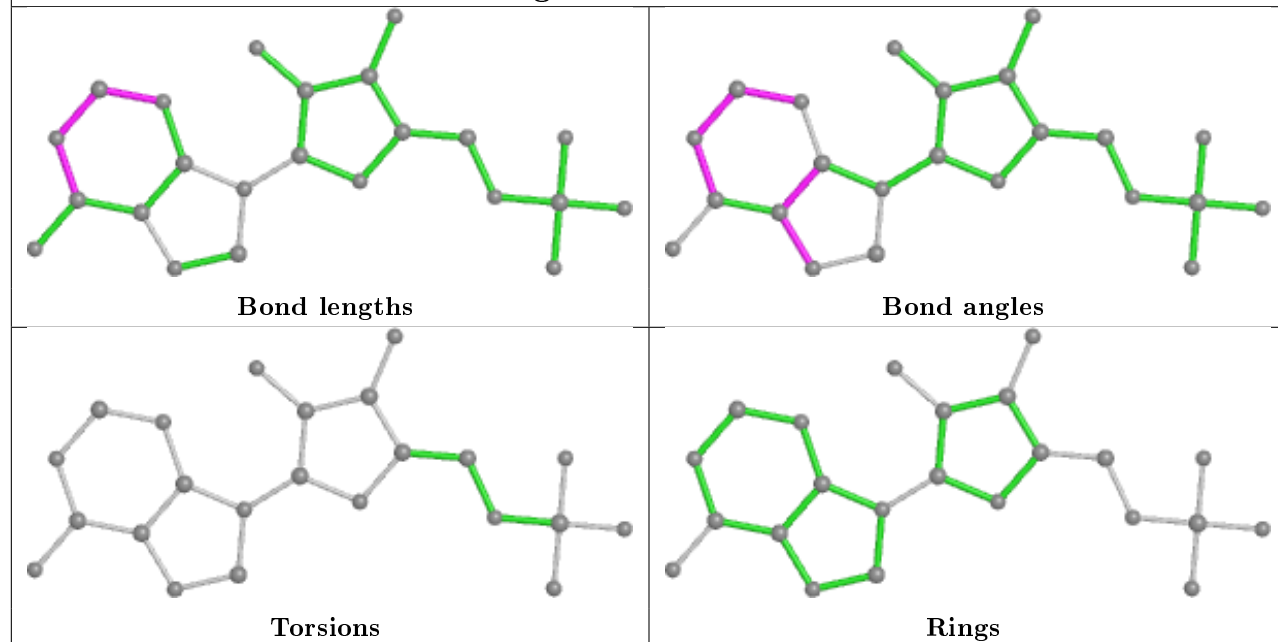
## Ligand IMP C 501

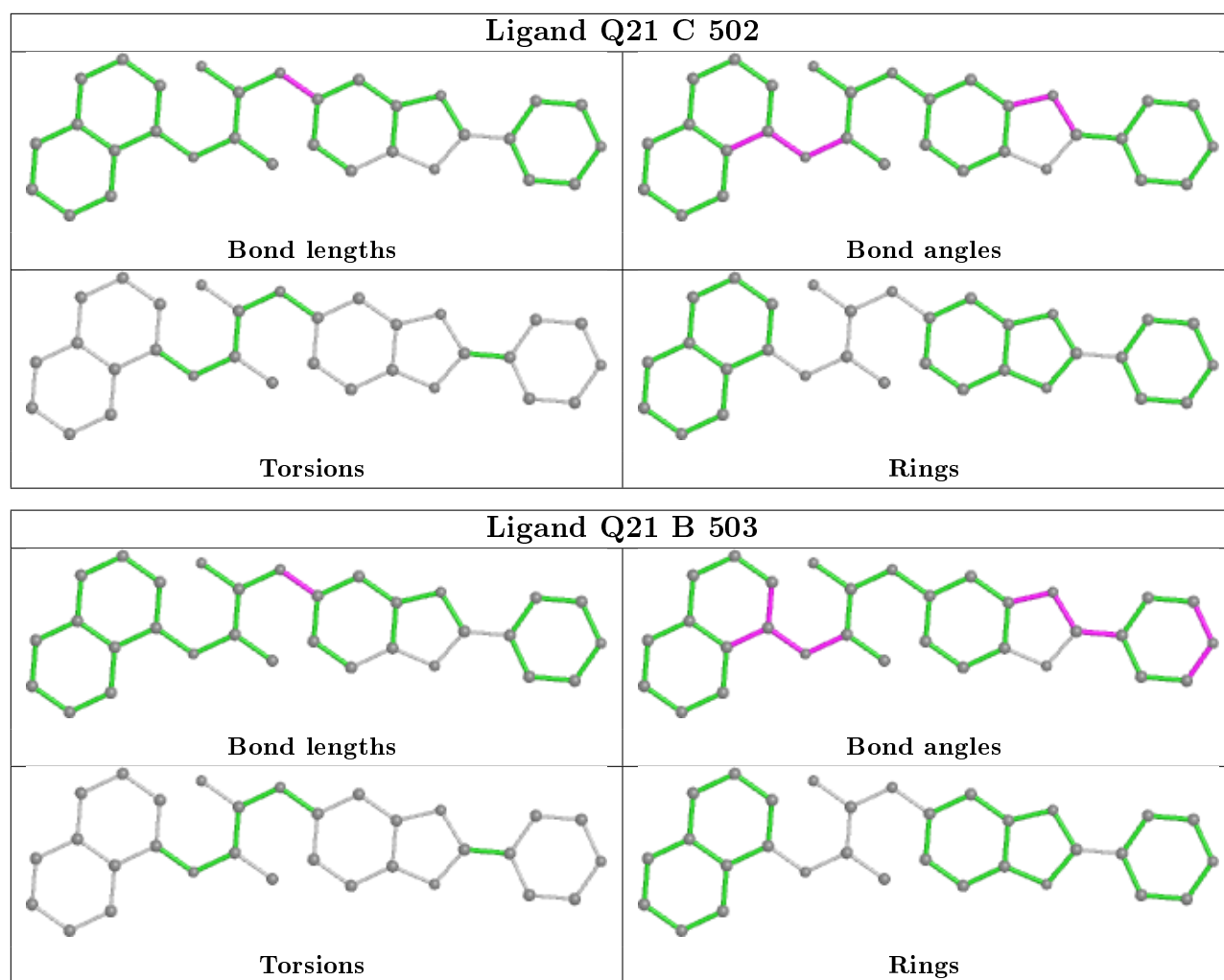


## Ligand IMP A 501



## Ligand IMP D 501





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	336/361 (93%)	0.03	19 (5%)	23 29	11, 31, 69, 100	3 (0%)
1	B	334/361 (92%)	0.19	23 (6%)	16 21	14, 33, 66, 96	6 (1%)
1	C	336/361 (93%)	0.04	15 (4%)	33 38	14, 33, 67, 103	7 (2%)
1	D	334/361 (92%)	0.06	20 (5%)	21 27	14, 33, 69, 94	7 (2%)
All	All	1340/1444 (92%)	0.08	77 (5%)	23 29	11, 33, 68, 103	23 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	311	GLY	7.2
1	A	311	GLY	5.8
1	D	386	VAL	5.8
1	B	305	VAL	5.7
1	A	386	VAL	5.4
1	C	386	VAL	5.4
1	D	92	GLY	5.3
1	A	305	VAL	5.0
1	B	386	VAL	4.7
1	B	91	GLY	4.7
1	C	391	ILE	4.4
1	B	92	GLY	4.3
1	C	310	SER	4.3
1	C	392	VAL	4.3
1	B	391	ILE	4.1
1	A	1	MET	3.9
1	D	381	LEU	3.9
1	C	388	ASP	3.8
1	B	387	HIS	3.6
1	B	392	VAL	3.6
1	B	381	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.5
1	C	309	LYS	3.5
1	D	310	SER	3.5
1	B	388	ASP	3.5
1	C	305	VAL	3.5
1	A	381	LEU	3.4
1	B	309	LYS	3.4
1	D	291	ILE	3.4
1	A	92	GLY	3.4
1	D	293	ASP	3.3
1	A	309	LYS	3.2
1	D	392	VAL	3.2
1	D	391	ILE	3.1
1	D	78	GLU	3.1
1	A	291	ILE	3.0
1	D	387	HIS	3.0
1	B	292	GLY	3.0
1	D	388	ASP	3.0
1	C	92	GLY	2.9
1	C	387	HIS	2.9
1	B	383	GLU	2.8
1	A	382	ARG	2.8
1	B	310	SER	2.8
1	B	291	ILE	2.7
1	A	387	HIS	2.7
1	B	389	VAL	2.6
1	D	309	LYS	2.6
1	C	382	ARG	2.6
1	B	78	GLU	2.6
1	B	326	MET	2.6
1	A	392	VAL	2.5
1	D	389	VAL	2.5
1	B	272	VAL	2.5
1	C	78	GLU	2.5
1	A	91	GLY	2.5
1	D	326	MET	2.5
1	D	91	GLY	2.5
1	D	305	VAL	2.4
1	A	293	ASP	2.4
1	B	76	ASP	2.4
1	B	274	ILE	2.3
1	D	272	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLY	2.3
1	D	382	ARG	2.3
1	B	306	GLY	2.2
1	A	274	ILE	2.2
1	A	390	GLU	2.2
1	C	251	ALA	2.2
1	D	390	GLU	2.1
1	B	385	HIS	2.1
1	A	310	SER	2.1
1	A	76	ASP	2.0
1	A	378	THR	2.0
1	B	251	ALA	2.0
1	C	389	VAL	2.0
1	A	78	GLU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	503	4/4	0.67	0.30	45,49,50,52	0
3	EDO	A	502	4/4	0.68	0.29	33,38,40,44	0
3	EDO	A	505	4/4	0.71	0.22	43,44,55,58	0
3	EDO	C	504	4/4	0.87	0.29	40,40,45,48	0
3	EDO	A	503	4/4	0.88	0.29	40,47,54,61	0
4	Q21	C	502	31/31	0.96	0.08	24,35,41,48	0
4	Q21	B	503	31/31	0.96	0.09	22,34,50,56	0
4	Q21	B	501	31/31	0.96	0.08	18,26,42,45	0
2	IMP	C	501	23/23	0.97	0.15	14,26,30,32	0

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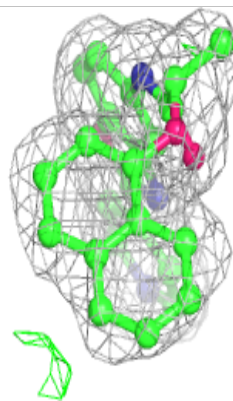
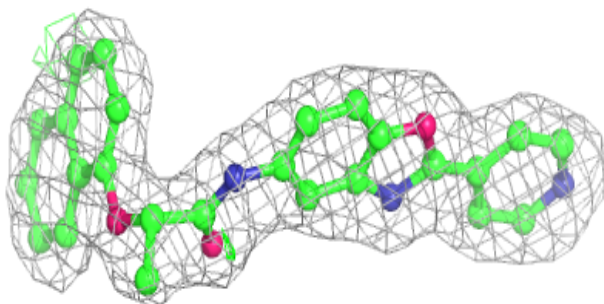
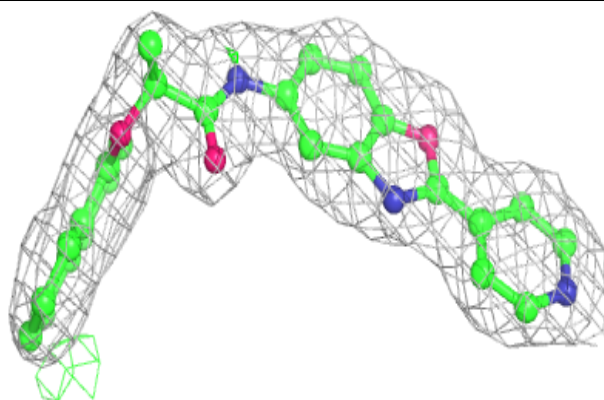
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	Q21	A	504	31/31	0.97	0.08	16,29,49,52	0
2	IMP	D	501	23/23	0.97	0.17	20,27,31,32	0
2	IMP	A	501	23/23	0.98	0.13	14,22,32,34	0
2	IMP	B	502	23/23	0.98	0.12	16,23,28,33	0

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.

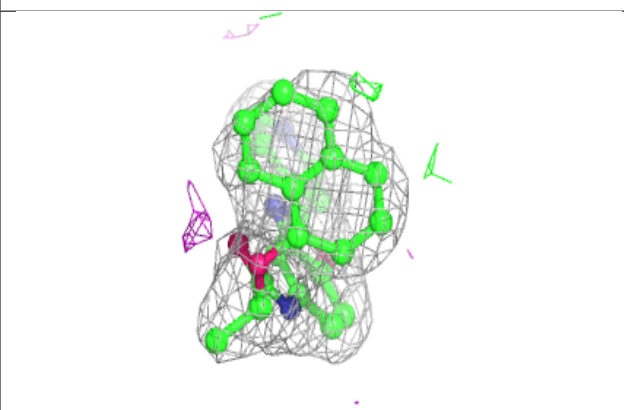
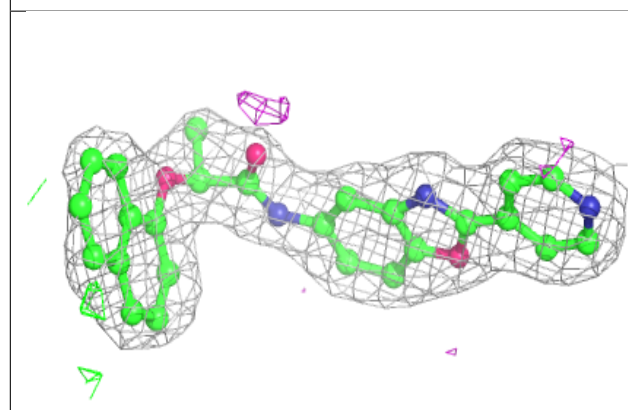
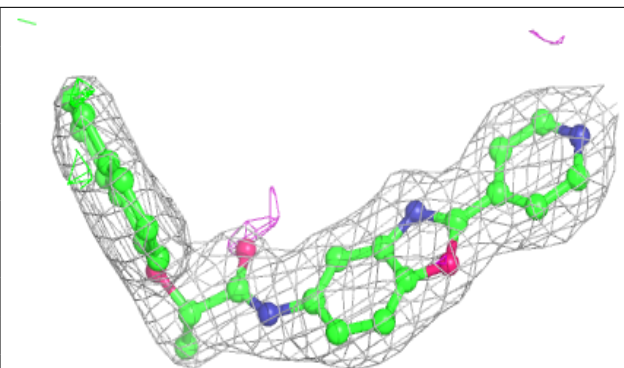
**Electron density around Q21 C 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

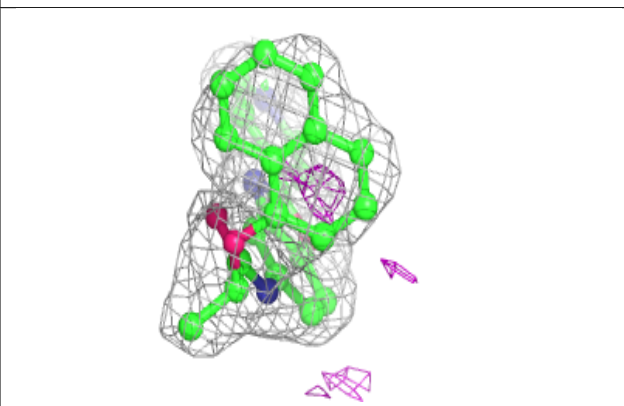
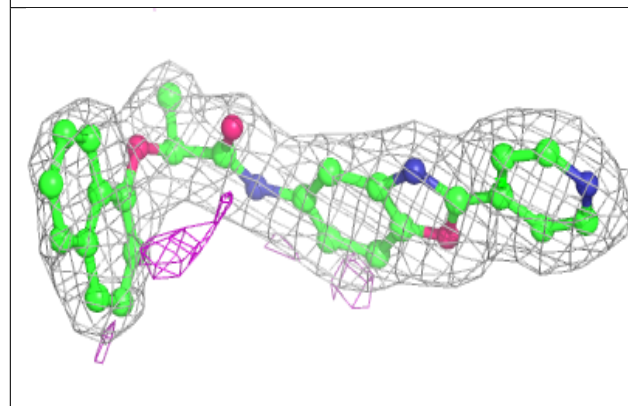
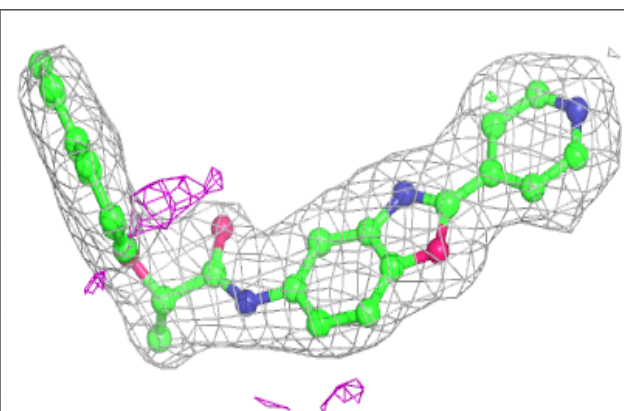


**Electron density around Q21 B 503:**

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

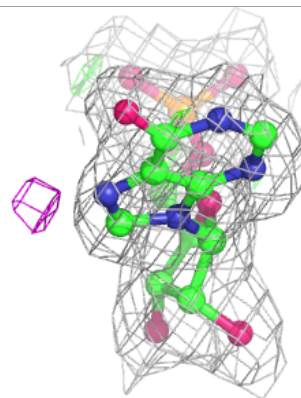
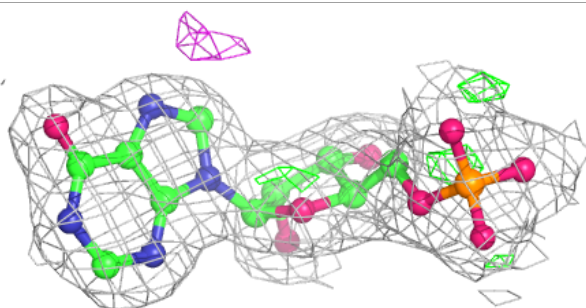
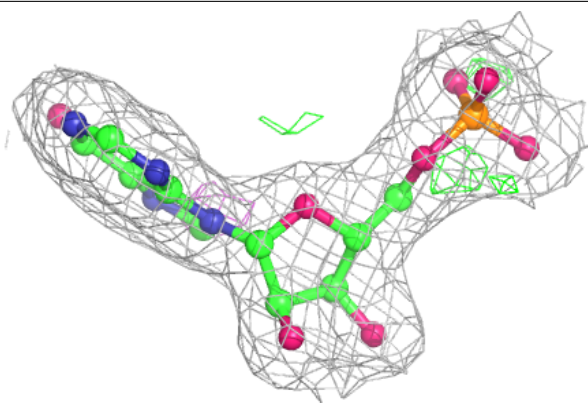
**Electron density around Q21 B 501:**

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

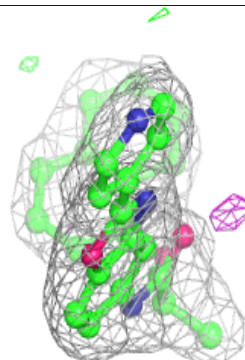
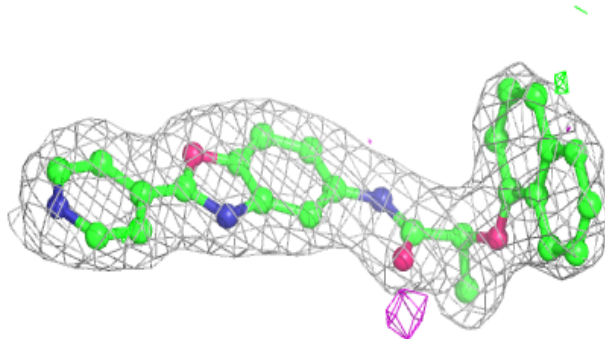
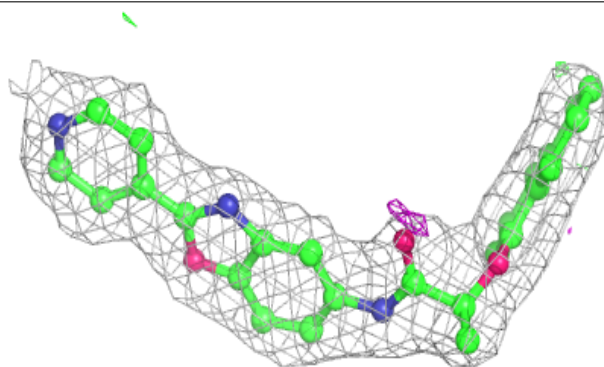


**Electron density around IMP C 501:**

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

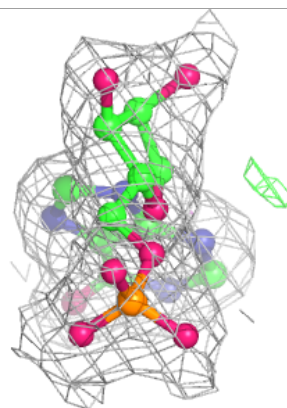
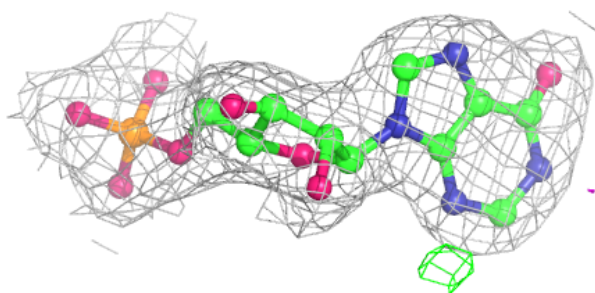
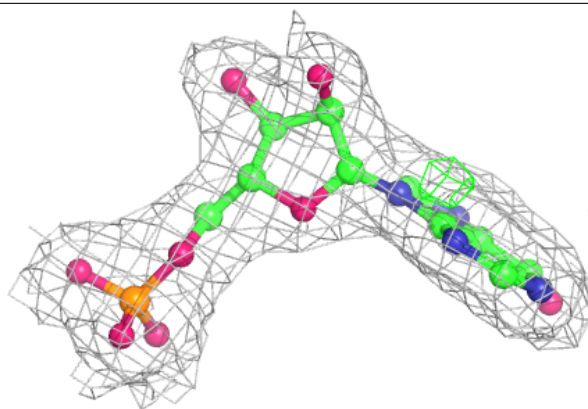
**Electron density around Q21 A 504:**

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

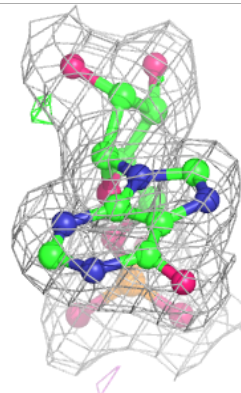
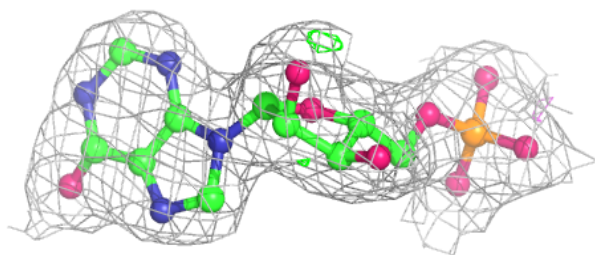
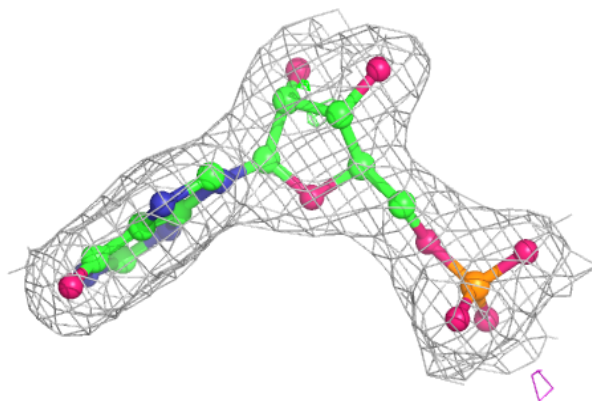


**Electron density around IMP D 501:**

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

**Electron density around IMP A 501:**

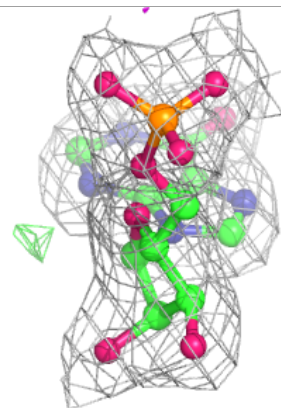
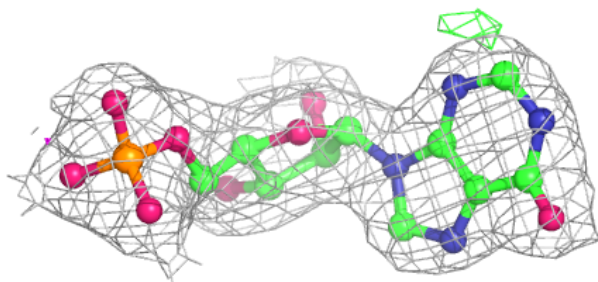
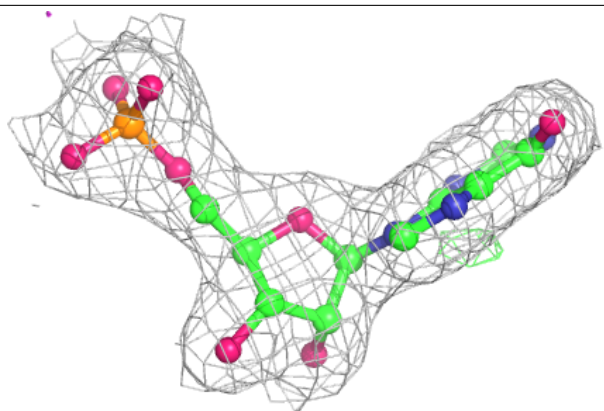
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around IMP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.