



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 4QJ1 / pdb_00004qj1
Title : Co-crystal structure of the catalytic domain of the inosine monophosphate dehydrogenase from *Cryptosporidium parvum* with inhibitor N109
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2014-06-03
Resolution : 2.42 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

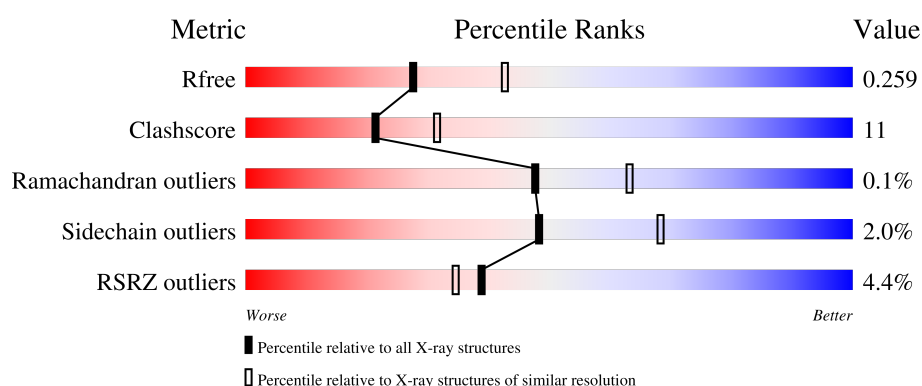
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	5% 71% 23% • 5%
1	B	361	3% 78% 16% • •
1	C	361	4% 71% 23% • •
1	D	361	4% 71% 24% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10616 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.

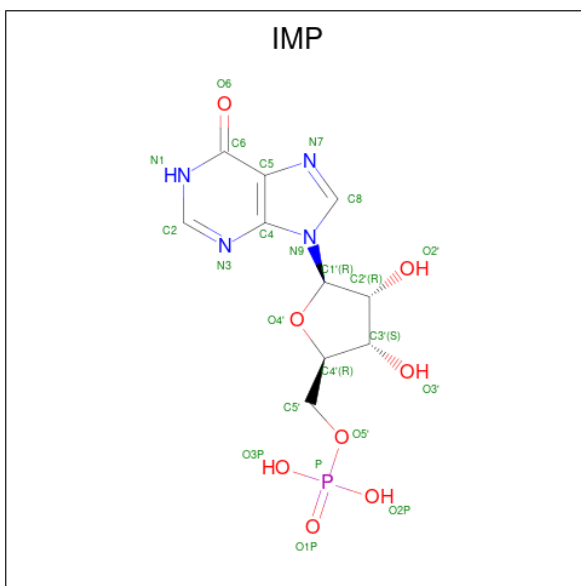
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	2	0
			2554	1606	435	497	16			
1	B	345	Total	C	N	O	S	0	2	0
			2570	1616	437	500	17			
1	C	345	Total	C	N	O	S	0	1	0
			2566	1613	437	499	17			
1	D	346	Total	C	N	O	S	0	1	0
			2574	1617	439	501	17			

There are 20 discrepancies between the modelled and reference sequences:

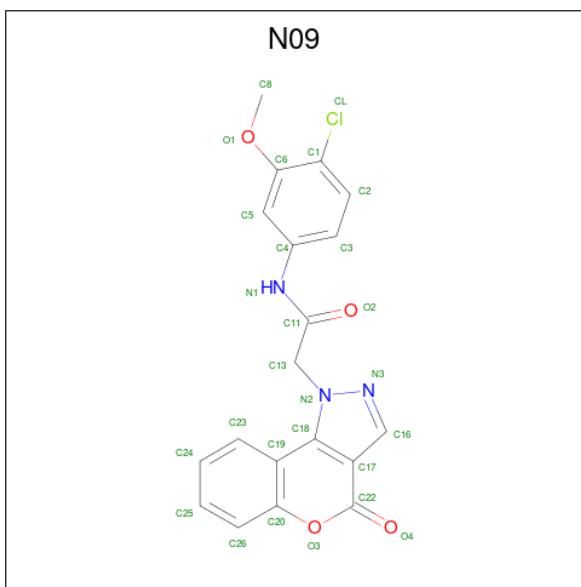
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8T6T2
A	-1	ASN	-	expression tag	UNP Q8T6T2
A	0	ALA	-	expression tag	UNP Q8T6T2
A	90	SER	LYS	engineered mutation	UNP Q8T6T2
A	92	GLY	ARG	engineered mutation	UNP Q8T6T2
B	-2	SER	-	expression tag	UNP Q8T6T2
B	-1	ASN	-	expression tag	UNP Q8T6T2
B	0	ALA	-	expression tag	UNP Q8T6T2
B	90	SER	LYS	engineered mutation	UNP Q8T6T2
B	92	GLY	ARG	engineered mutation	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	LYS	engineered mutation	UNP Q8T6T2
C	92	GLY	ARG	engineered mutation	UNP Q8T6T2
D	-2	SER	-	expression tag	UNP Q8T6T2
D	-1	ASN	-	expression tag	UNP Q8T6T2
D	0	ALA	-	expression tag	UNP Q8T6T2
D	90	SER	LYS	engineered mutation	UNP Q8T6T2
D	92	GLY	ARG	engineered mutation	UNP Q8T6T2

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



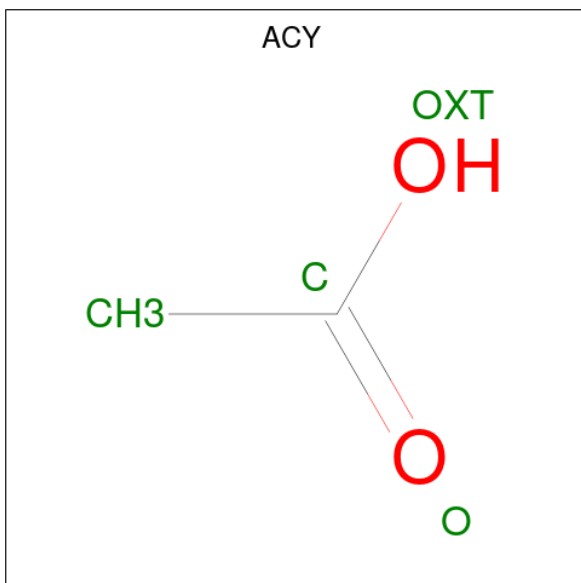
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-(4-chloro-3-methoxyphenyl)-2-(4-oxochromeno[4,3-c]pyrazol-1(4H)-yl)acetamide (CCD ID: N09) (formula: $C_{19}H_{14}ClN_3O_4$).



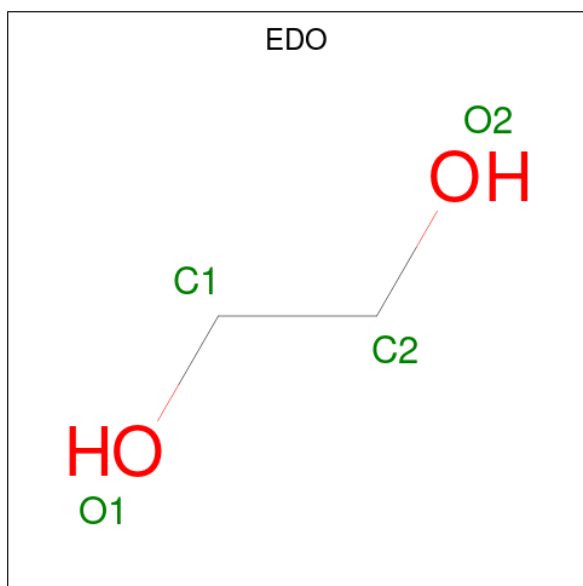
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	D	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



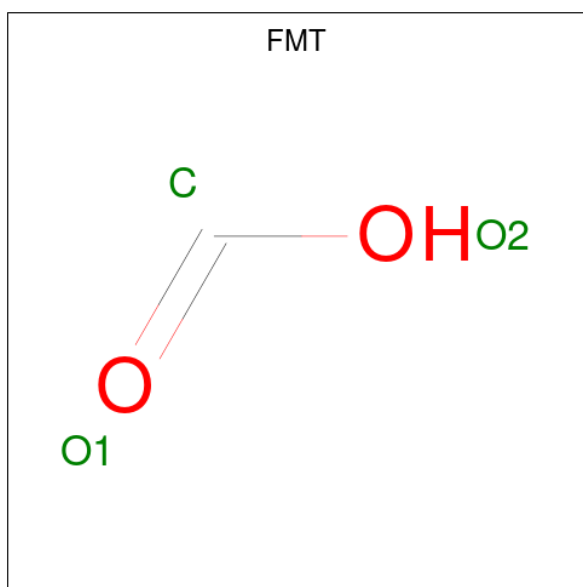
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

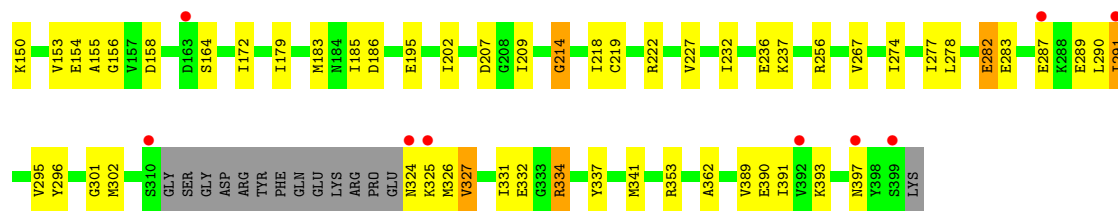
- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	34	Total	O	0	0
			34	34		
7	B	31	Total	O	0	0
			31	31		
7	C	26	Total	O	0	0
			26	26		
7	D	42	Total	O	0	0
			42	42		



● 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	90.41Å 92.34Å 91.91Å 90.00° 104.24° 90.00°	Depositor
Resolution (Å)	39.59 – 2.42 39.59 – 2.42	Depositor EDS
% Data completeness (in resolution range)	88.6 (39.59-2.42) 88.6 (39.59-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, R_{free}	0.202 , 0.258 0.207 , 0.259	Depositor DCC
R_{free} test set	2555 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10616	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, IMP, N09, FMT, ACY

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	0.62	0/2580	1.04	10/3472 (0.3%)
1	B	0.59	0/2599	1.02	3/3497 (0.1%)
1	C	0.63	0/2592	1.04	9/3487 (0.3%)
1	D	0.64	2/2600 (0.1%)	1.07	8/3498 (0.2%)
All	All	0.62	2/10371 (0.0%)	1.05	30/13954 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	214	GLY	C-N	5.45	1.40	1.34
1	D	215	PRO	N-CD	5.25	1.55	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	327	VAL	N-CA-C	9.20	117.44	107.60
1	B	214	GLY	CA-C-N	-8.51	110.85	120.04
1	B	214	GLY	C-N-CA	-8.51	110.85	120.04
1	D	0	ALA	N-CA-C	-7.02	104.03	112.59
1	C	214	GLY	CA-C-N	-6.09	113.49	119.64
1	C	214	GLY	C-N-CA	-6.09	113.49	119.64
1	C	334	ARG	CA-CB-CG	-5.97	102.16	114.10
1	A	327	VAL	CA-C-N	5.96	125.89	119.76
1	A	327	VAL	C-N-CA	5.96	125.89	119.76
1	D	214	GLY	CA-C-N	-5.95	113.55	119.56
1	D	214	GLY	C-N-CA	-5.95	113.55	119.56
1	D	293	ASP	N-CA-C	-5.80	105.39	112.88
1	C	18	VAL	N-CA-C	5.47	113.29	107.76
1	D	216	GLY	N-CA-C	5.44	118.18	111.93
1	A	214	GLY	CA-C-N	-5.30	113.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	GLY	C-N-CA	-5.30	113.22	119.84
1	C	327	VAL	CA-C-N	5.28	125.74	120.14
1	C	327	VAL	C-N-CA	5.28	125.74	120.14
1	A	60	VAL	N-CA-C	-5.26	104.52	111.09
1	D	43	ILE	CA-C-N	5.21	126.36	119.84
1	D	43	ILE	C-N-CA	5.21	126.36	119.84
1	A	18	VAL	CA-C-N	5.16	125.07	119.76
1	A	18	VAL	C-N-CA	5.16	125.07	119.76
1	C	54	THR	N-CA-C	5.11	117.03	107.99
1	B	286	GLY	CA-C-O	-5.08	118.73	122.23
1	A	365	GLU	N-CA-C	-5.07	105.75	111.28
1	A	15	ILE	N-CA-C	5.06	116.88	108.99
1	C	214	GLY	N-CA-C	5.03	122.61	112.34
1	A	158	ASP	N-CA-C	5.03	116.84	111.36
1	C	282	GLU	N-CA-C	-5.03	105.98	111.82

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	2554	0	2654	73	0
1	B	2570	0	2677	54	0
1	C	2566	0	2670	63	0
1	D	2574	0	2676	68	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	27	0	14	0	0
3	B	54	0	28	1	0
3	D	27	0	14	2	0
4	B	4	0	3	0	0
5	C	4	0	6	2	0
5	D	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	3	0	1	0	0
7	A	34	0	0	1	0
7	B	31	0	0	2	0
7	C	26	0	0	0	0
7	D	42	0	0	4	0
All	All	10616	0	10799	232	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 11.

All (232) 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:304:SER:O	1:B:308:MET:HG3	1.82	0.80
1:A:331:ILE:HD13	1:D:391:ILE:HG12	1.63	0.78
1:A:391:ILE:HG12	1:B:331:ILE:HD13	1.65	0.76
1:D:291:ILE:HD12	1:D:334:ARG:NH1	1.99	0.76
1:A:347:GLN:HG3	1:A:396:MET:HG2	1.68	0.75
1:A:141:ILE:HG12	1:A:160:ILE:HD11	1.69	0.74
1:C:11:THR:HG22	1:C:12:PHE:H	1.52	0.74
1:D:291:ILE:HD12	1:D:334:ARG:HH11	1.51	0.73
1:D:13:GLU:OE2	1:D:256:ARG:NH1	2.21	0.73
1:B:74:ASN:HB2	1:B:302:MET:HE1	1.71	0.72
1:B:287:GLU:HG3	1:B:288:LYS:N	2.06	0.70
1:D:295:VAL:HG23	1:D:337:TYR:HB3	1.75	0.69
1:C:391:ILE:HG12	1:D:331:ILE:HD13	1.76	0.68
1:B:65:LEU:HD12	1:B:341:MET:HE2	1.74	0.67
1:B:291:ILE:HG13	1:B:334:ARG:NH1	2.09	0.67
1:B:391:ILE:HG12	1:C:331:ILE:HD13	1.75	0.67
1:A:309:LYS:HE2	1:A:324:ASN:OD1	1.94	0.66
1:C:13:GLU:OE2	1:C:256:ARG:NH1	2.28	0.66
1:D:74:ASN:HB2	1:D:302:MET:HE1	1.77	0.66
1:A:219:CYS:SG	2:A:501:IMP:H2	2.35	0.66
1:A:186:ASP:HA	1:A:207:ASP:OD2	1.96	0.65
1:A:56:HIS:O	1:A:60:VAL:HG23	1.96	0.64
1:D:219:CYS:SG	2:D:501:IMP:H2	2.37	0.64
1:B:350:GLY:HA3	1:C:327:VAL:HG21	1.79	0.64
1:C:218:ILE:HD13	1:C:301:GLY:HA2	1.79	0.64
1:D:218:ILE:HD13	1:D:301:GLY:HA2	1.80	0.63
1:B:219:CYS:SG	2:B:501:IMP:H2	2.39	0.63
1:D:306:GLY:HA2	1:D:309:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HA	1:B:157:VAL:HG12	1.81	0.63
1:A:13:GLU:OE1	1:D:382:ARG:NH2	2.32	0.62
1:A:143:VAL:HG21	1:A:171:ASN:HB3	1.80	0.62
1:D:71:ILE:HD13	1:D:84:VAL:HG12	1.82	0.62
1:B:193:VAL:HG13	1:B:213:ILE:HG12	1.80	0.62
1:C:274:ILE:HD11	1:C:278:LEU:HG	1.80	0.62
1:D:27[A]:ARG:HG3	7:D:603:HOH:O	1.98	0.62
5:C:502:EDO:H21	1:D:14:ASP:OD1	1.99	0.62
1:C:219:CYS:SG	2:C:501:IMP:H2	2.40	0.62
1:C:295:VAL:HG13	1:C:337:TYR:HB3	1.82	0.61
1:D:214:GLY:HA2	1:D:219:CYS:SG	2.40	0.61
1:B:218:ILE:HD13	1:B:301:GLY:CA	2.32	0.60
1:C:11:THR:HG22	1:C:12:PHE:N	2.16	0.59
1:C:39:VAL:HG13	1:C:136:ARG:HD3	1.84	0.59
1:A:328:PRO:O	1:D:397:ASN:ND2	2.36	0.59
1:D:72:HIS:CE1	1:D:75:MET:HE2	2.38	0.59
1:A:222:ARG:HG2	1:A:227:VAL:O	2.03	0.59
1:D:338:LYS:NZ	5:D:503:EDO:H21	2.19	0.58
1:D:186:ASP:HA	1:D:207:ASP:OD2	2.03	0.58
1:C:202:ILE:HG13	1:C:209:ILE:HD11	1.87	0.57
1:D:27[B]:ARG:HD3	1:D:28:GLU:HG3	1.88	0.56
1:D:51:ASP:HA	1:D:72:HIS:CD2	2.40	0.56
1:C:218:ILE:HD13	1:C:301:GLY:CA	2.36	0.56
1:A:324:ASN:HA	1:A:326:MET:HG2	1.88	0.56
1:B:390:GLU:OE1	1:C:334:ARG:HD2	2.06	0.55
1:A:179:ILE:HA	1:A:183:MET:HE3	1.89	0.55
1:A:74:ASN:HB2	1:A:302:MET:HE1	1.88	0.55
1:A:283:GLU:N	1:A:283:GLU:OE1	2.40	0.55
1:A:150:LYS:HB3	1:A:183:MET:SD	2.46	0.55
1:B:218:ILE:HD13	1:B:301:GLY:HA2	1.88	0.55
1:D:26:PRO:O	1:D:29:VAL:HG12	2.06	0.55
1:B:393:LYS:HE2	1:C:332:GLU:CD	2.33	0.54
1:C:214:GLY:HA2	1:C:219:CYS:SG	2.47	0.54
1:C:186:ASP:HA	1:C:207:ASP:OD2	2.07	0.54
1:A:80:GLN:OE1	1:A:148:ARG:NH2	2.38	0.54
1:A:60:VAL:HG22	1:A:87:VAL:HG13	1.90	0.54
1:C:51:ASP:HA	1:C:72:HIS:CD2	2.43	0.54
1:C:397:ASN:ND2	1:D:328:PRO:O	2.41	0.54
1:C:142:GLY:H	1:C:145:GLU:CD	2.15	0.54
1:A:61:GLY:HA2	1:A:64:ARG:NE	2.23	0.54
1:A:218:ILE:HD13	1:A:301:GLY:HA2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:CD1	1:C:296:TYR:CD2	2.92	0.53
1:B:56:HIS:O	1:B:60:VAL:HG22	2.09	0.53
1:D:261:ILE:HD12	1:D:272:VAL:HG21	1.91	0.53
1:D:289:GLU:OE1	1:D:298:TYR:OH	2.25	0.53
1:D:364:ILE:HG12	7:D:629:HOH:O	2.08	0.53
1:C:76:ASP:OD1	1:C:79:SER:HB3	2.08	0.53
1:C:393:LYS:HD3	1:D:332:GLU:OE1	2.09	0.53
1:A:11[B]:THR:O	1:A:14:ASP:HB2	2.09	0.53
1:A:79:SER:O	1:A:83:GLU:HG2	2.08	0.53
1:B:309:LYS:O	1:B:310:SER:CB	2.57	0.53
1:A:141:ILE:HD12	1:A:142:GLY:O	2.08	0.53
1:C:195:GLU:OE2	1:C:237:LYS:HD2	2.08	0.53
1:B:51:ASP:HA	1:B:72:HIS:CD2	2.44	0.52
1:D:87:VAL:HG11	1:D:137:VAL:HB	1.92	0.52
1:D:37:LYS:HE2	7:D:616:HOH:O	2.08	0.52
1:C:72:HIS:CE1	1:C:75:MET:HE2	2.45	0.52
1:A:383:GLU:OE2	1:B:215:PRO:HB3	2.08	0.52
1:C:164:SER:HB2	1:C:172:ILE:HD11	1.92	0.52
1:B:186:ASP:HA	1:B:207:ASP:OD2	2.09	0.51
1:C:82:ASN:O	1:C:86:LYS:HG3	2.10	0.51
1:A:51:ASP:HA	1:A:72:HIS:CD2	2.45	0.51
1:B:179:ILE:HG23	1:B:183:MET:HE3	1.93	0.51
1:A:61:GLY:HA2	1:A:64:ARG:HE	1.77	0.50
1:C:153:VAL:HG22	1:C:185:ILE:HD13	1.93	0.50
1:C:274:ILE:CD1	1:C:278:LEU:HG	2.40	0.50
1:C:81:VAL:HG13	1:C:155:ALA:HB2	1.93	0.50
1:D:236:GLU:OE2	1:D:373:TYR:OH	2.24	0.50
1:A:346:TYR:CZ	1:B:325:LYS:HG2	2.47	0.50
1:C:40:SER:H	1:C:136:ARG:NH2	2.09	0.50
1:B:11[B]:THR:HG22	1:B:12:PHE:N	2.27	0.50
1:D:218:ILE:HD13	1:D:301:GLY:CA	2.40	0.50
1:C:29:VAL:O	1:C:353:ARG:NH1	2.41	0.49
1:A:168:HIS:CE1	1:D:21:TYR:HB2	2.47	0.49
1:A:214:GLY:HA2	1:A:219:CYS:SG	2.52	0.49
1:C:10:LEU:O	1:C:232:ILE:HB	2.12	0.49
1:C:74:ASN:HB2	1:C:302:MET:HE1	1.94	0.49
1:C:179:ILE:HG23	1:C:183:MET:HE3	1.93	0.49
1:A:149:ALA:O	1:A:153:VAL:HG23	2.12	0.49
1:B:143:VAL:HG12	1:B:172:ILE:HG13	1.94	0.49
1:C:26:PRO:O	1:C:353:ARG:HD3	2.13	0.49
1:D:282:GLU:HG2	1:D:337:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLU:OE1	1:D:283:GLU:N	2.43	0.49
1:A:189:VAL:HG11	1:A:201:LEU:HD22	1.93	0.49
1:D:76:ASP:OD1	1:D:79:SER:HB3	2.12	0.49
1:C:397:ASN:ND2	1:D:328:PRO:HD2	2.28	0.49
1:D:141:ILE:HG22	1:D:148:ARG:HD2	1.95	0.49
1:D:56:HIS:ND1	1:D:83:GLU:OE2	2.42	0.49
1:D:76:ASP:OD1	1:D:76:ASP:N	2.43	0.49
1:B:65:LEU:CD1	1:B:341:MET:HE2	2.41	0.48
1:D:136:ARG:HA	1:D:158:ASP:OD2	2.13	0.48
1:D:191:ASN:OD1	1:D:210:LYS:HD2	2.14	0.48
1:B:289:GLU:OE1	1:B:298:TYR:OH	2.24	0.48
1:D:366:GLU:CG	1:D:370:LYS:HE2	2.44	0.48
1:A:7:GLY:HA3	1:B:0:ALA:H1	1.79	0.48
1:A:77:MET:O	1:A:81:VAL:HG23	2.14	0.48
1:A:150:LYS:O	1:A:154:GLU:HG3	2.14	0.48
1:A:397:ASN:HB3	1:B:224:VAL:HG22	1.96	0.47
1:C:282:GLU:HG2	1:C:283:GLU:CD	2.38	0.47
1:A:38:ASN:HB2	1:A:186:ASP:OD2	2.14	0.47
1:A:346:TYR:OH	1:B:325:LYS:HG2	2.13	0.47
1:B:202:ILE:HG13	1:B:209:ILE:HD11	1.95	0.47
1:B:11[A]:THR:OG1	1:B:12:PHE:N	2.46	0.47
1:D:81:VAL:O	1:D:84:VAL:HG22	2.14	0.47
1:A:347:GLN:HG3	1:A:396:MET:CG	2.42	0.47
1:B:32:GLU:HA	1:B:42:LYS:HA	1.97	0.47
1:C:218:ILE:H	1:C:218:ILE:HG13	1.56	0.47
1:D:82:ASN:HA	1:D:85:LEU:HD12	1.96	0.47
1:D:164:SER:HB2	1:D:172:ILE:HD11	1.97	0.47
1:A:217:SER:HB2	1:D:387:HIS:O	2.15	0.47
1:A:218:ILE:H	1:A:218:ILE:HG13	1.46	0.47
1:A:309:LYS:HE2	1:A:324:ASN:CG	2.38	0.47
1:A:153:VAL:HA	1:A:157:VAL:HG12	1.97	0.46
1:C:214:GLY:HA3	1:C:222:ARG:NE	2.29	0.46
1:C:291:ILE:HD13	1:C:334:ARG:NH2	2.30	0.46
1:A:60:VAL:O	1:A:64:ARG:HG3	2.16	0.46
1:A:282:GLU:C	1:A:284:SER:H	2.23	0.46
1:A:388:ASP:OD2	1:B:256:ARG:NE	2.46	0.46
1:C:21:TYR:HB2	1:D:168:HIS:CE1	2.51	0.46
1:C:24:VAL:HG21	1:C:362:ALA:HB2	1.98	0.46
1:A:7:GLY:HA3	1:B:0:ALA:N	2.32	0.45
1:A:81:VAL:HG13	1:A:155:ALA:HB2	1.97	0.45
1:A:383:GLU:CD	1:B:222:ARG:HH12	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:HG2	7:B:624:HOH:O	2.16	0.45
1:D:338:LYS:HZ1	5:D:503:EDO:H21	1.80	0.45
1:A:61:GLY:O	1:A:64:ARG:HB2	2.17	0.45
1:A:72:HIS:CE1	1:A:75:MET:HE2	2.52	0.45
1:B:252:ASP:OD2	2:B:501:IMP:O2'	2.33	0.45
1:A:31:LEU:CD1	1:A:349:VAL:HG13	2.47	0.45
1:A:61:GLY:HA2	1:A:64:ARG:NH2	2.32	0.45
1:A:11[A]:THR:O	1:A:14:ASP:HB2	2.17	0.44
1:A:324:ASN:C	1:A:326:MET:H	2.25	0.44
1:D:72:HIS:O	1:D:75:MET:HE3	2.18	0.44
1:A:150:LYS:HB2	1:A:150:LYS:HE3	1.66	0.44
1:D:397:ASN:OD1	7:D:631:HOH:O	2.20	0.44
1:A:191:ASN:OD1	1:A:210:LYS:HE2	2.17	0.44
1:B:177:LYS:HD3	1:B:204:ASN:OD1	2.17	0.44
1:B:392:VAL:HG22	1:C:332:GLU:O	2.17	0.44
1:A:218:ILE:HD13	1:A:301:GLY:CA	2.48	0.44
1:D:210:LYS:HD3	1:D:252:ASP:OD2	2.18	0.44
1:D:32:GLU:OE2	1:D:42:LYS:NZ	2.40	0.44
1:A:11[A]:THR:HG21	1:D:380:GLY:HA2	2.00	0.44
1:B:214:GLY:HA3	1:B:222:ARG:HE	1.83	0.43
1:A:136:ARG:HA	1:A:158:ASP:OD2	2.17	0.43
1:A:382:ARG:NH1	1:B:13:GLU:OE1	2.38	0.43
1:C:76:ASP:OD1	1:C:76:ASP:N	2.50	0.43
1:C:88:LYS:HE3	1:C:156:GLY:O	2.18	0.43
1:A:164:SER:HB2	1:A:172:ILE:HD11	2.00	0.43
1:C:390:GLU:CD	1:D:334:ARG:HH21	2.27	0.43
1:A:341:MET:HE2	1:A:341:MET:HB3	1.95	0.43
1:B:56:HIS:HB3	1:B:83:GLU:OE1	2.19	0.43
1:C:236:GLU:HG3	1:C:267:VAL:HG13	2.01	0.43
3:D:502:N09:H11	3:D:502:N09:O2	2.19	0.43
1:C:62:MET:N	1:C:341:MET:HE1	2.34	0.42
1:D:306:GLY:HA2	1:D:309:LYS:CE	2.49	0.42
1:D:43:ILE:HA	1:D:44:PRO:HD3	1.76	0.42
1:A:61:GLY:CA	1:A:64:ARG:NH2	2.83	0.42
1:B:214:GLY:HA3	1:B:222:ARG:NE	2.35	0.42
1:C:195:GLU:H	1:C:195:GLU:CD	2.28	0.42
1:C:149:ALA:O	1:C:153:VAL:HG23	2.20	0.42
1:A:251:ALA:HB3	1:A:272:VAL:HG12	2.02	0.42
1:A:160:ILE:CG2	1:A:187:VAL:HG22	2.50	0.42
1:D:78:GLU:HA	1:D:81:VAL:HB	2.01	0.42
1:D:218:ILE:H	1:D:218:ILE:HG13	1.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:GLU:HG2	1:D:370:LYS:HE2	2.02	0.42
1:C:137:VAL:HG22	1:C:138:GLY:N	2.35	0.42
1:C:150:LYS:O	1:C:154:GLU:HG3	2.20	0.42
1:A:84:VAL:HG23	1:A:137:VAL:HG11	2.00	0.41
1:C:274:ILE:HD13	1:C:277:ILE:HB	2.01	0.41
1:D:305:VAL:O	1:D:309:LYS:HG3	2.20	0.41
1:B:222:ARG:HG2	1:B:227:VAL:O	2.20	0.41
1:C:136:ARG:HA	1:C:158:ASP:OD2	2.20	0.41
1:B:79:SER:O	1:B:83:GLU:HG2	2.20	0.41
3:D:502:N09:H7	3:D:502:N09:H5	2.01	0.41
1:D:150:LYS:O	1:D:154:GLU:HG3	2.20	0.41
1:D:283:GLU:OE1	1:D:341:MET:HB2	2.21	0.41
1:C:389:VAL:HG12	1:D:335:VAL:HG22	2.02	0.41
1:A:81:VAL:HA	1:A:84:VAL:HG12	2.01	0.41
1:A:282:GLU:OE1	1:A:337:TYR:OH	2.36	0.41
1:B:214:GLY:HA2	1:B:219:CYS:SG	2.60	0.41
1:B:293:ASP:N	7:B:623:HOH:O	2.53	0.41
1:C:141:ILE:HD12	1:C:142:GLY:O	2.20	0.41
1:B:309:LYS:O	1:B:310:SER:OG	2.37	0.41
1:C:81:VAL:HA	1:C:84:VAL:HG12	2.03	0.41
1:C:214:GLY:HA3	1:C:222:ARG:HG3	2.02	0.41
1:C:222:ARG:HG2	1:C:227:VAL:O	2.21	0.41
1:D:277:ILE:HG23	1:D:338:LYS:HZ1	1.86	0.41
1:A:83:GLU:O	1:A:87:VAL:HG23	2.21	0.41
1:B:393:LYS:HE2	1:C:332:GLU:OE1	2.20	0.41
1:D:222:ARG:HG2	1:D:227:VAL:O	2.20	0.41
1:A:61:GLY:CA	1:A:64:ARG:HH21	2.34	0.40
1:A:146:ILE:HD13	1:A:178:GLU:OE1	2.21	0.40
1:B:309:LYS:C	1:B:310:SER:HG	2.29	0.40
3:B:503:N09:O2	3:B:503:N09:H11	2.20	0.40
1:D:82:ASN:HD22	1:D:85:LEU:HD12	1.86	0.40
1:B:76:ASP:N	1:B:76:ASP:OD1	2.52	0.40
1:B:288:LYS:H	1:B:288:LYS:HG3	1.73	0.40
5:C:502:EDO:H12	1:D:378:THR:N	2.36	0.40
1:C:38:ASN:HB2	1:C:186:ASP:OD2	2.22	0.40
1:B:194:THR:O	1:B:198:THR:HG23	2.21	0.40
1:D:179:ILE:HG23	1:D:183:MET:HE3	2.03	0.40
1:A:180:LYS:NZ	7:A:612:HOH:O	2.53	0.40
1:C:179:ILE:HA	1:C:183:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/361 (94%)	323 (95%)	17 (5%)	0	100	100
1	B	343/361 (95%)	330 (96%)	12 (4%)	1 (0%)	36	49
1	C	342/361 (95%)	327 (96%)	15 (4%)	0	100	100
1	D	343/361 (95%)	330 (96%)	12 (4%)	1 (0%)	36	49
All	All	1368/1444 (95%)	1310 (96%)	56 (4%)	2 (0%)	48	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	VAL
1	D	193	VAL

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	281/295 (95%)	279 (99%)	2 (1%)	76	87
1	B	283/295 (96%)	274 (97%)	9 (3%)	34	54
1	C	282/295 (96%)	275 (98%)	7 (2%)	42	62
1	D	283/295 (96%)	278 (98%)	5 (2%)	51	71
All	All	1129/1180 (96%)	1106 (98%)	23 (2%)	48	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27[A]	ARG
1	A	27[B]	ARG
1	B	64	ARG
1	B	172	ILE
1	B	209	ILE
1	B	287	GLU
1	B	288	LYS
1	B	289	GLU
1	B	290	LEU
1	B	291	ILE
1	B	310	SER
1	C	287	GLU
1	C	289	GLU
1	C	290	LEU
1	C	291	ILE
1	C	324	ASN
1	C	325	LYS
1	C	326	MET
1	D	209	ILE
1	D	218	ILE
1	D	287	GLU
1	D	289	GLU
1	D	291	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	184	ASN
1	A	347	GLN
1	B	56	HIS
1	B	347	GLN
1	C	56	HIS
1	C	347	GLN
1	D	74	ASN
1	D	82	ASN
1	D	89	ASN
1	D	166	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	N09	A	502	-	30,30,30	1.75	7 (23%)	41,43,43	3.03	14 (34%)
2	IMP	D	501	-	25,25,25	1.09	1 (4%)	37,38,38	1.96	8 (21%)
2	IMP	B	501	-	25,25,25	1.13	1 (4%)	37,38,38	2.09	10 (27%)
5	EDO	D	503	-	3,3,3	0.59	0	2,2,2	0.10	0
6	FMT	D	504	-	2,2,2	0.70	0	1,1,1	0.14	0
2	IMP	A	501	-	25,25,25	1.23	1 (4%)	37,38,38	2.19	9 (24%)
4	ACY	B	504	-	3,3,3	0.84	0	3,3,3	0.76	0
3	N09	B	502	-	30,30,30	1.78	8 (26%)	41,43,43	2.79	10 (24%)
2	IMP	C	501	-	25,25,25	1.10	1 (4%)	37,38,38	2.25	11 (29%)
3	N09	D	502	-	30,30,30	1.75	8 (26%)	41,43,43	2.79	9 (21%)
3	N09	B	503	-	30,30,30	1.76	8 (26%)	41,43,43	3.00	11 (26%)
5	EDO	D	505	-	3,3,3	0.54	0	2,2,2	0.24	0
5	EDO	C	502	-	3,3,3	0.49	0	2,2,2	0.03	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
3	N09	A	502	-	-	2/10/10/10	0/4/4/4
2	IMP	D	501	-	-	2/10/26/26	0/3/3/3
2	IMP	B	501	-	-	1/10/26/26	0/3/3/3
5	EDO	D	503	-	-	0/1/1/1	-
2	IMP	A	501	-	-	2/10/26/26	0/3/3/3
3	N09	B	502	-	-	2/10/10/10	0/4/4/4
2	IMP	C	501	-	-	0/10/26/26	0/3/3/3
3	N09	D	502	-	-	2/10/10/10	0/4/4/4
3	N09	B	503	-	-	2/10/10/10	0/4/4/4
5	EDO	D	505	-	-	1/1/1/1	-
5	EDO	C	502	-	-	0/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	N09	C6-C1	5.44	1.49	1.39
3	B	503	N09	C6-C1	5.38	1.49	1.39
2	A	501	IMP	C2-N3	5.02	1.39	1.30
3	A	502	N09	C6-C1	4.99	1.48	1.39
3	D	502	N09	C6-C1	4.84	1.48	1.39
2	C	501	IMP	C2-N3	4.60	1.38	1.30
2	B	501	IMP	C2-N3	4.41	1.38	1.30
2	D	501	IMP	C2-N3	4.30	1.38	1.30
3	D	502	N09	N2-N3	3.97	1.42	1.37
3	A	502	N09	N2-N3	3.69	1.42	1.37
3	B	503	N09	N2-N3	3.55	1.41	1.37
3	B	502	N09	N2-N3	3.53	1.41	1.37
3	D	502	N09	C19-C18	-3.35	1.40	1.45
3	A	502	N09	C19-C18	-3.11	1.40	1.45
3	A	502	N09	C1-CL	3.06	1.80	1.73
3	B	503	N09	C1-CL	3.05	1.80	1.73
3	B	502	N09	C19-C18	-3.02	1.40	1.45
3	B	502	N09	C1-CL	2.93	1.80	1.73
3	B	503	N09	C19-C18	-2.92	1.40	1.45
3	A	502	N09	C4-N1	-2.88	1.35	1.41
3	B	502	N09	C16-N3	2.86	1.37	1.32
3	D	502	N09	C16-N3	2.84	1.37	1.32
3	B	502	N09	C17-C18	2.84	1.47	1.41
3	B	503	N09	C17-C18	2.80	1.47	1.41
3	A	502	N09	C17-C18	2.78	1.47	1.41
3	A	502	N09	C16-N3	2.70	1.36	1.32
3	D	502	N09	C17-C18	2.68	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	N09	C1-CL	2.66	1.79	1.73
3	B	503	N09	C4-N1	-2.61	1.36	1.41
3	D	502	N09	C4-N1	-2.42	1.36	1.41
3	B	503	N09	C16-N3	2.37	1.36	1.32
3	B	502	N09	O4-C22	2.32	1.26	1.21
3	B	502	N09	C4-N1	-2.17	1.37	1.41
3	B	503	N09	O4-C22	2.13	1.25	1.21
3	D	502	N09	C16-C17	2.10	1.44	1.41

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	N09	C18-C17-C22	-11.27	115.61	122.19
3	A	502	N09	C18-C17-C22	-10.75	115.91	122.19
3	B	503	N09	C18-C17-C22	-10.14	116.26	122.19
3	B	502	N09	C18-C17-C22	-9.56	116.60	122.19
3	B	503	N09	C16-C17-C18	7.98	110.36	104.76
3	A	502	N09	C16-C17-C18	7.41	109.95	104.76
3	B	502	N09	C16-C17-C18	7.40	109.95	104.76
3	D	502	N09	C16-C17-C18	7.13	109.76	104.76
3	B	503	N09	C17-C16-N3	-6.92	103.86	112.45
3	B	503	N09	C16-N3-N2	6.67	111.30	104.95
3	B	502	N09	C17-C16-N3	-6.60	104.25	112.45
3	D	502	N09	C17-C16-N3	-6.45	104.44	112.45
3	A	502	N09	C17-C16-N3	-6.40	104.50	112.45
3	B	502	N09	C16-N3-N2	6.30	110.96	104.95
2	C	501	IMP	C5-C6-N1	6.19	119.69	110.78
3	A	502	N09	O1-C6-C1	6.19	122.44	116.62
2	A	501	IMP	C5-C6-N1	6.06	119.49	110.78
2	B	501	IMP	C5-C6-N1	5.99	119.40	110.78
2	A	501	IMP	C5-C4-N3	-5.94	118.52	127.27
2	D	501	IMP	C5-C6-N1	5.91	119.28	110.78
3	D	502	N09	C16-N3-N2	5.69	110.37	104.95
3	A	502	N09	C16-N3-N2	5.64	110.33	104.95
2	C	501	IMP	C5-C4-N3	-5.64	118.97	127.27
2	C	501	IMP	C2-N3-C4	5.26	120.79	111.53
3	B	503	N09	O1-C6-C1	5.23	121.55	116.62
2	A	501	IMP	C2-N3-C4	5.15	120.59	111.53
2	B	501	IMP	C5-C4-N3	-4.74	120.30	127.27
2	B	501	IMP	C2-N3-C4	4.67	119.75	111.53
2	A	501	IMP	C2-N1-C6	-4.67	118.69	125.09
2	D	501	IMP	C2-N3-C4	4.51	119.46	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	IMP	C2-N1-C6	-4.36	119.12	125.09
2	D	501	IMP	C5-C4-N3	-4.34	120.89	127.27
2	B	501	IMP	C2-N1-C6	-4.28	119.22	125.09
3	B	502	N09	O3-C22-O4	4.12	121.65	116.22
2	D	501	IMP	C2-N1-C6	-3.99	119.62	125.09
2	C	501	IMP	N1-C2-N3	-3.97	120.92	125.50
3	B	503	N09	O3-C22-O4	3.83	121.27	116.22
3	A	502	N09	O3-C22-O4	3.66	121.05	116.22
2	D	501	IMP	N1-C2-N3	-3.65	121.30	125.50
3	B	502	N09	O1-C6-C1	3.57	119.98	116.62
3	B	502	N09	C13-N2-C18	3.55	136.60	129.76
2	B	501	IMP	N1-C2-N3	-3.54	121.42	125.50
2	B	501	IMP	O3P-P-O2P	3.51	120.98	107.80
3	B	503	N09	C13-N2-C18	3.36	136.22	129.76
3	A	502	N09	O1-C6-C5	-3.26	118.46	124.08
3	A	502	N09	C11-C13-N2	-3.24	105.85	111.89
2	A	501	IMP	N1-C2-N3	-3.18	121.84	125.50
3	D	502	N09	C11-C13-N2	-3.14	106.02	111.89
3	B	503	N09	O1-C6-C5	-3.05	118.82	124.08
2	C	501	IMP	C8-N7-C5	3.05	109.69	104.26
3	D	502	N09	C8-O1-C6	2.86	121.71	117.51
2	C	501	IMP	N9-C8-N7	-2.82	108.17	113.40
2	C	501	IMP	N9-C4-N3	2.81	133.29	126.90
3	A	502	N09	C13-N2-C18	2.80	135.16	129.76
3	A	502	N09	C2-C1-C6	-2.73	117.09	120.77
2	A	501	IMP	N9-C4-N3	2.71	133.06	126.90
3	A	502	N09	C6-C1-CL	2.65	122.48	119.44
3	B	503	N09	O2-C11-C13	-2.64	116.40	121.02
2	C	501	IMP	O3P-P-O2P	2.62	117.64	107.80
2	A	501	IMP	C8-N7-C5	2.58	108.86	104.26
3	D	502	N09	C13-N2-C18	2.56	134.68	129.76
2	D	501	IMP	C8-N7-C5	2.53	108.76	104.26
3	D	502	N09	O3-C22-O4	2.52	119.55	116.22
3	D	502	N09	O1-C6-C1	2.51	118.98	116.62
3	A	502	N09	O2-C11-C13	-2.49	116.65	121.02
2	D	501	IMP	O2P-P-O1P	2.48	120.51	110.83
3	B	503	N09	C2-C1-C6	-2.47	117.44	120.77
2	D	501	IMP	N9-C8-N7	-2.45	108.85	113.40
2	B	501	IMP	N9-C8-N7	-2.37	109.00	113.40
2	B	501	IMP	O6-C6-C5	-2.34	120.35	126.53
2	C	501	IMP	C4-C5-N7	-2.30	107.03	110.67
2	B	501	IMP	C8-N7-C5	2.29	108.33	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	N09	C2-C3-C4	2.23	122.87	120.30
2	C	501	IMP	O6-C6-C5	-2.22	120.68	126.53
2	A	501	IMP	O6-C6-C5	-2.21	120.69	126.53
3	B	503	N09	C11-C13-N2	-2.16	107.86	111.89
2	A	501	IMP	C4-C5-N7	-2.12	107.31	110.67
3	A	502	N09	C4-N1-C11	-2.09	123.82	127.52
3	A	502	N09	C4-C5-C6	2.07	121.92	119.27
3	B	502	N09	O1-C6-C5	-2.05	120.54	124.08
3	B	502	N09	O3-C20-C26	2.03	118.95	116.25
2	B	501	IMP	N9-C4-N3	2.01	131.49	126.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	IMP	C5'-O5'-P-O2P
2	A	501	IMP	C5'-O5'-P-O3P
2	B	501	IMP	C5'-O5'-P-O2P
2	D	501	IMP	C5'-O5'-P-O2P
2	D	501	IMP	C5'-O5'-P-O3P
3	A	502	N09	C1-C6-O1-C8
3	B	502	N09	C1-C6-O1-C8
3	B	503	N09	C1-C6-O1-C8
3	D	502	N09	C1-C6-O1-C8
3	B	502	N09	C5-C6-O1-C8
3	B	503	N09	C5-C6-O1-C8
3	D	502	N09	C5-C6-O1-C8
3	A	502	N09	C5-C6-O1-C8
5	D	505	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

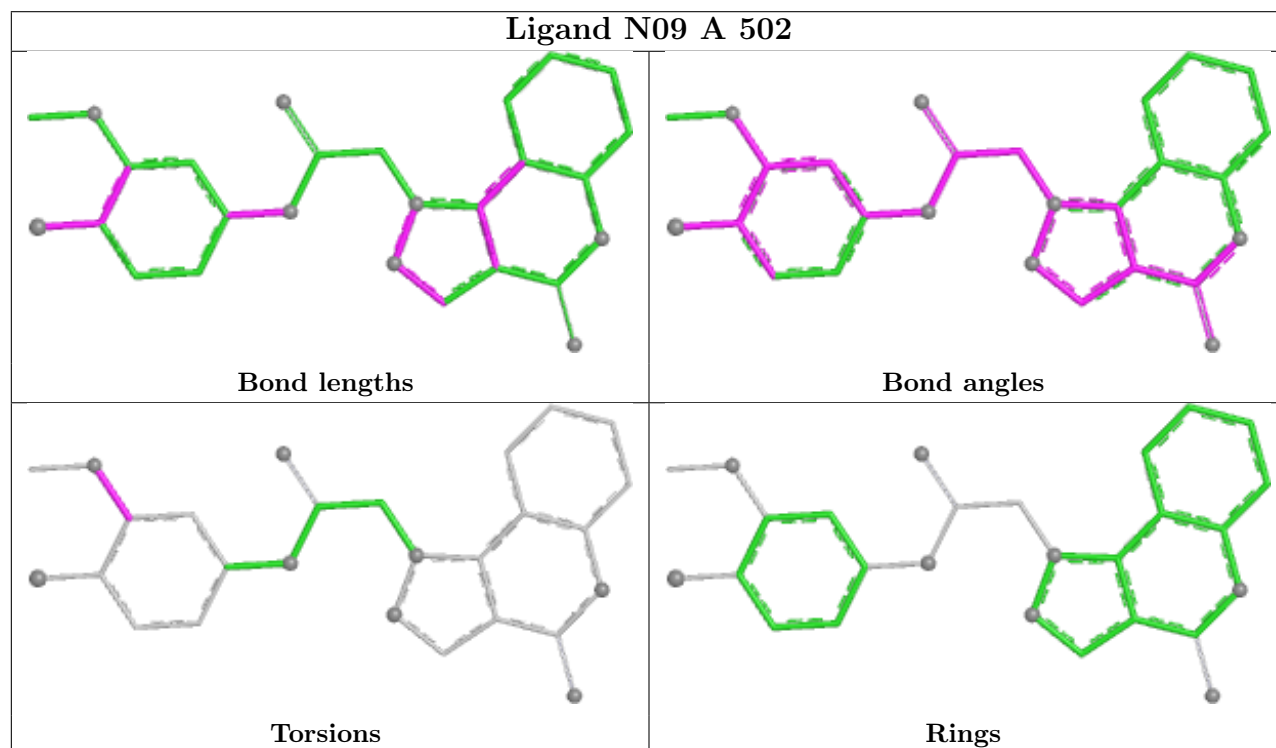
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	IMP	1	0
2	B	501	IMP	2	0
5	D	503	EDO	2	0
2	A	501	IMP	1	0
2	C	501	IMP	1	0
3	D	502	N09	2	0
3	B	503	N09	1	0

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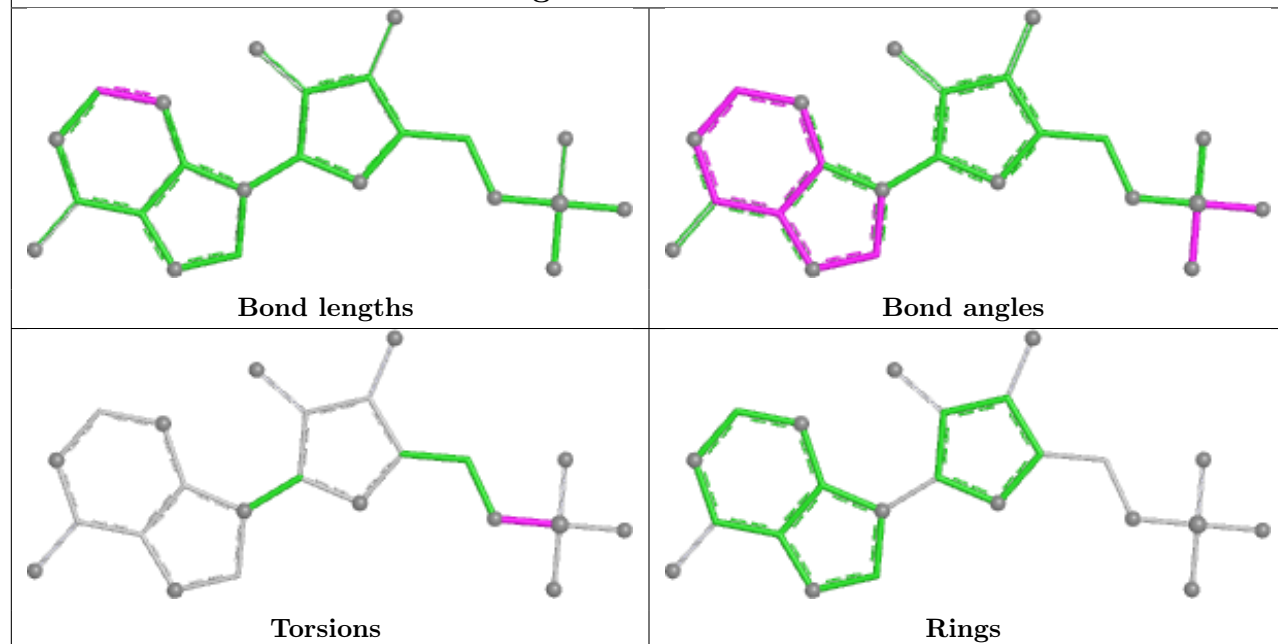
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	EDO	2	0

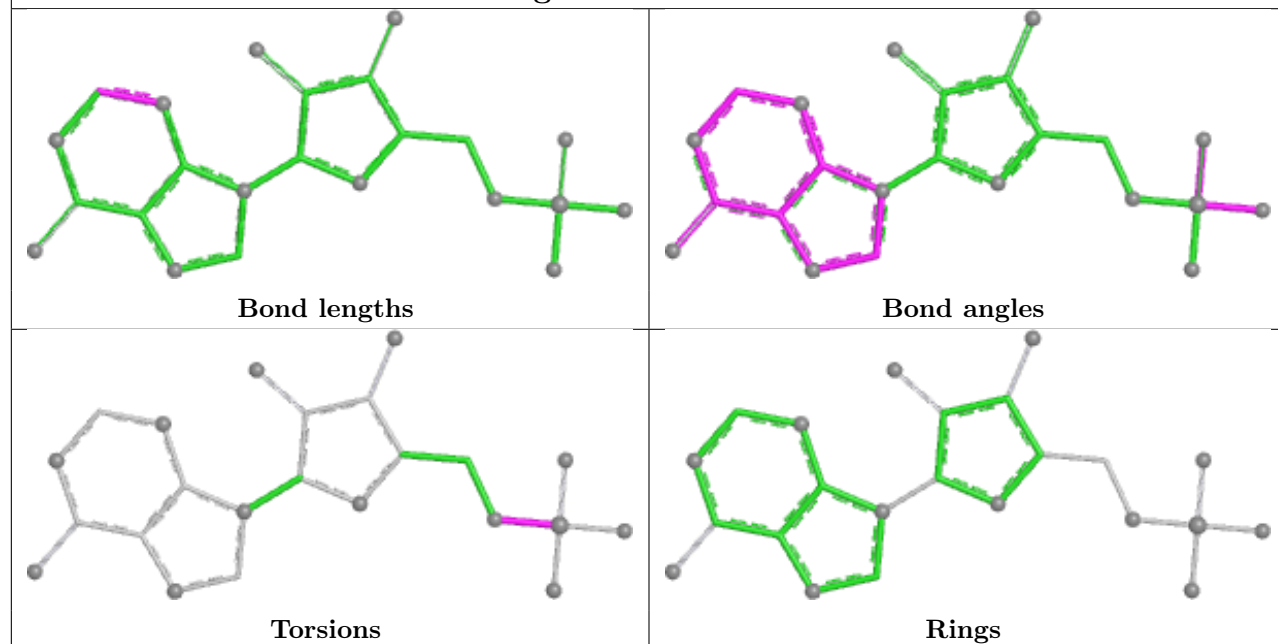
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



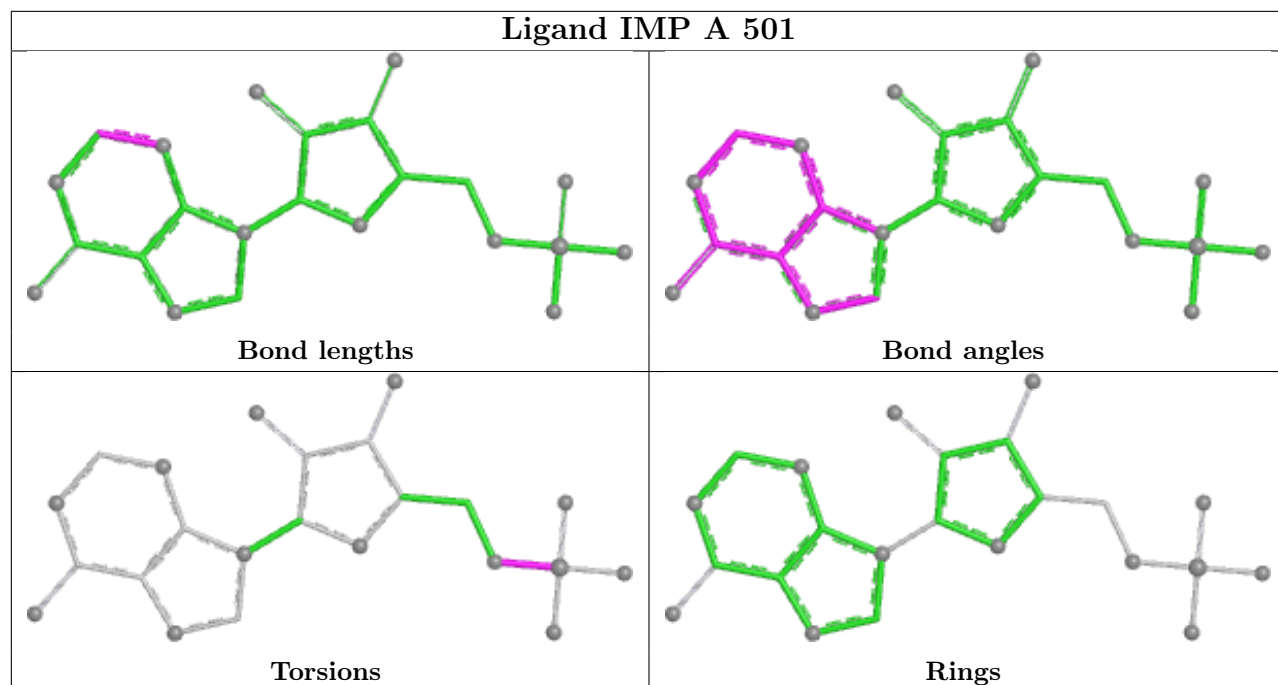
Ligand IMP D 501



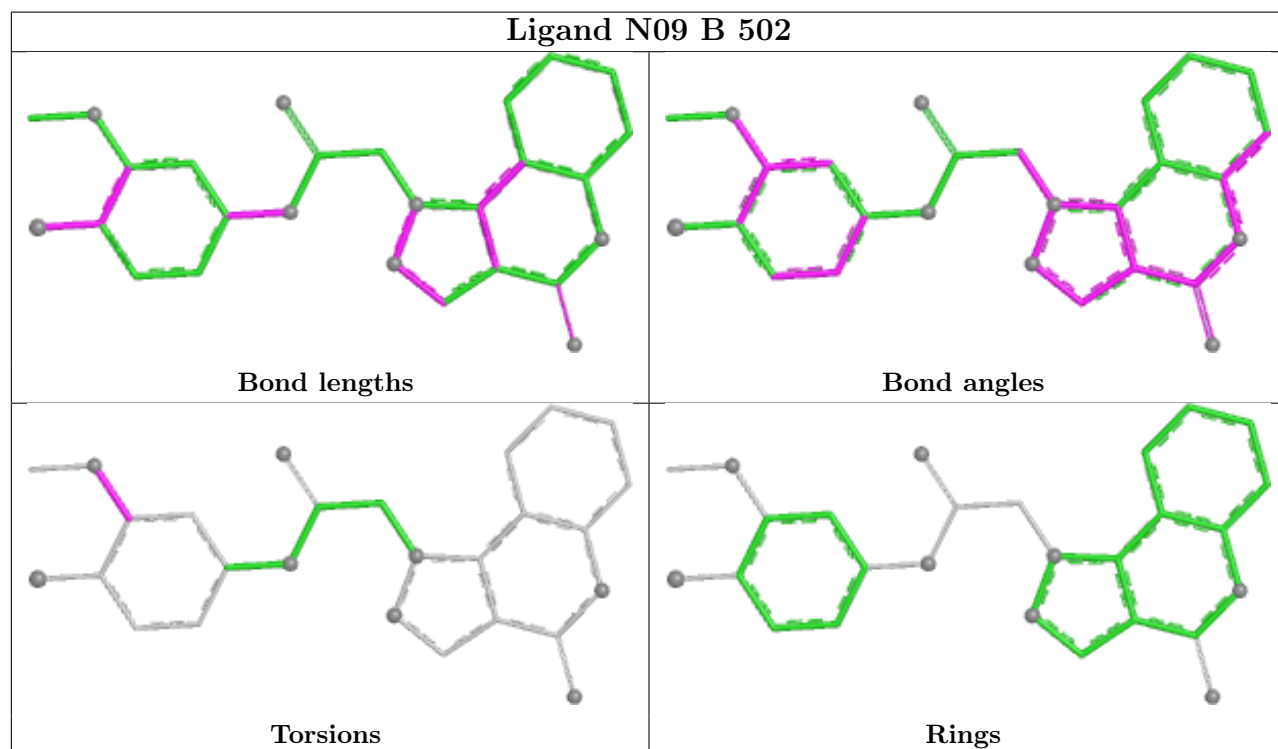
Ligand IMP B 501



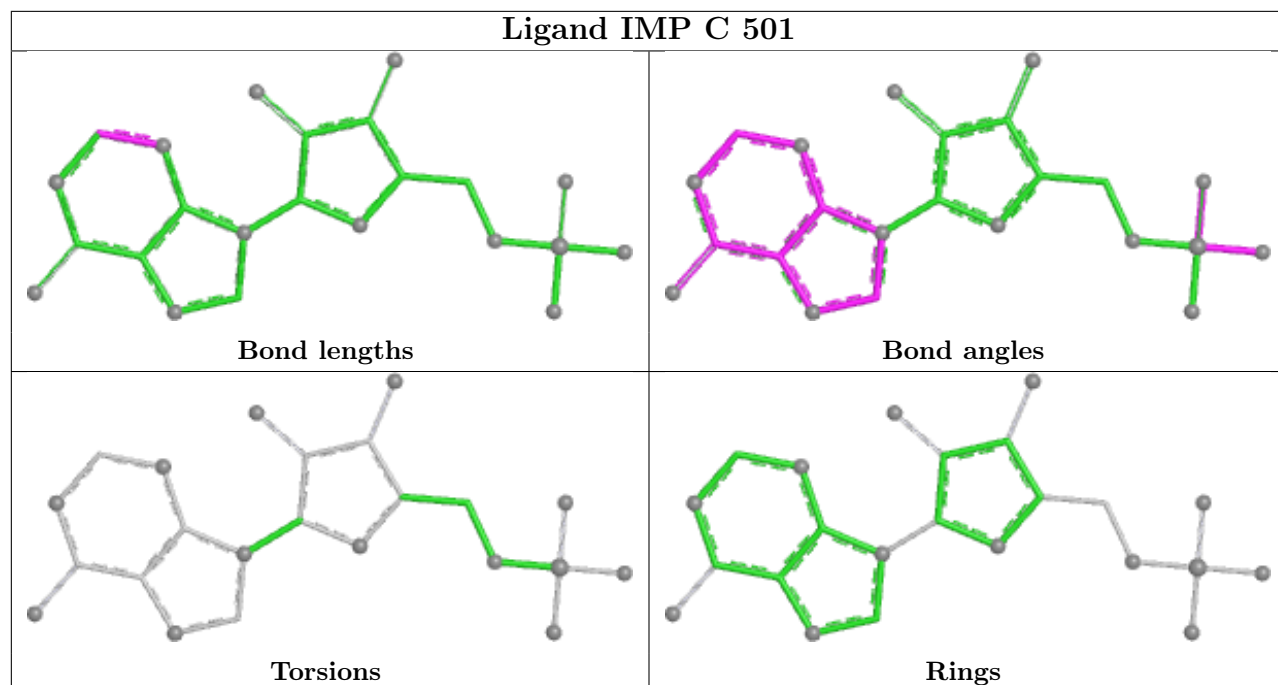
Ligand IMP A 501



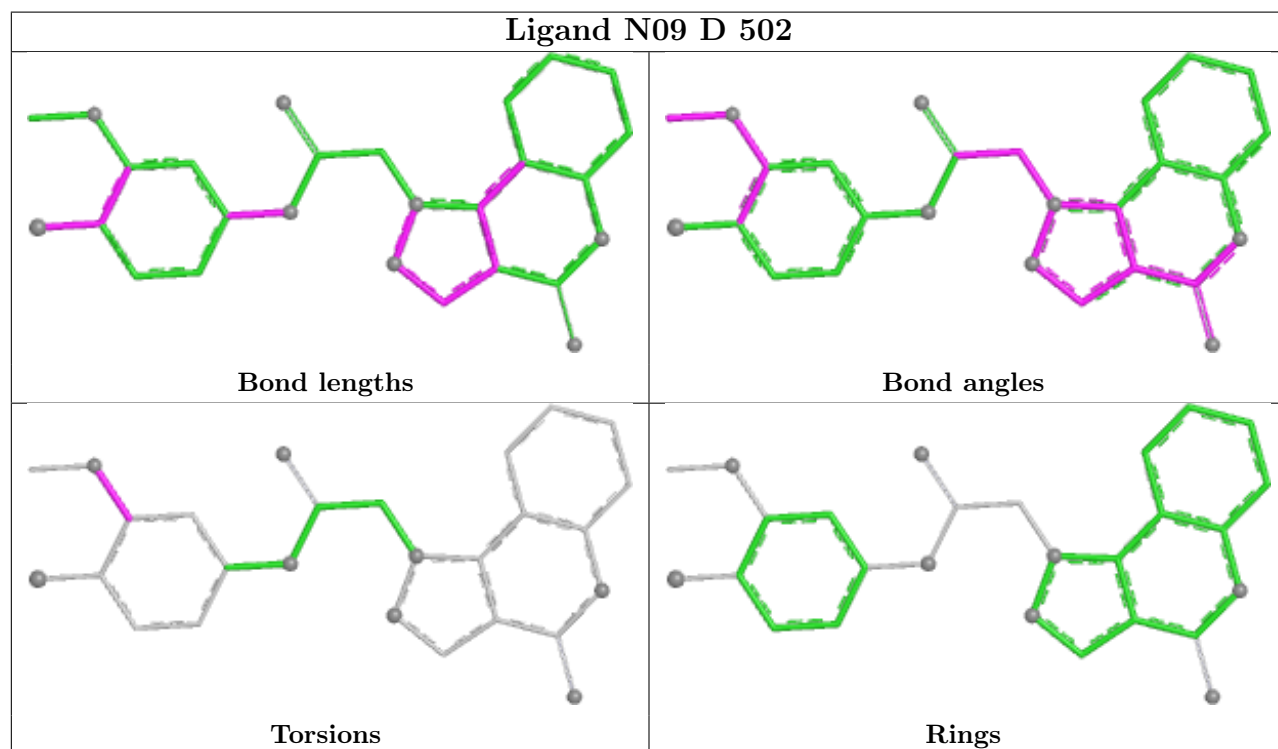
Ligand N09 B 502

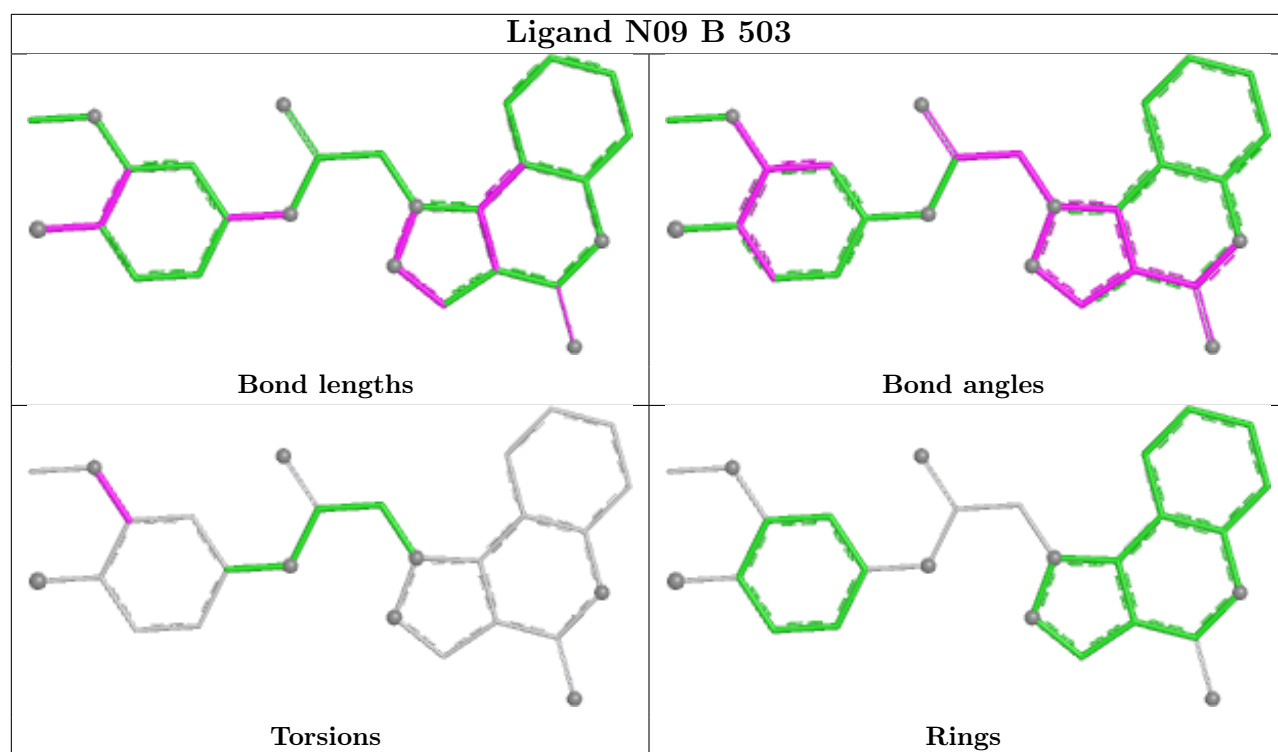


Ligand IMP C 501



Ligand N09 D 502





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	342/361 (94%)	0.40	19 (5%)	30 26	12, 51, 87, 128	2 (0%)
1	B	345/361 (95%)	0.31	11 (3%)	50 47	16, 50, 82, 142	2 (0%)
1	C	345/361 (95%)	0.33	15 (4%)	40 35	24, 49, 88, 115	1 (0%)
1	D	346/361 (95%)	0.31	16 (4%)	37 33	24, 49, 85, 123	1 (0%)
All	All	1378/1444 (95%)	0.34	61 (4%)	39 34	12, 49, 88, 142	6 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	ALA	5.0
1	B	163	ASP	4.9
1	A	287	GLU	4.6
1	C	0	ALA	4.4
1	D	163	ASP	4.3
1	A	64	ARG	4.2
1	D	287	GLU	4.1
1	A	60	VAL	3.9
1	B	395	VAL	3.8
1	D	324	ASN	3.7
1	C	2	GLY	3.6
1	D	292	GLY	3.6
1	A	291	ILE	3.5
1	C	163	ASP	3.5
1	C	310	SER	3.4
1	B	0	ALA	3.3
1	A	301	GLY	3.3
1	D	298	TYR	3.2
1	D	-1	ASN	3.0
1	D	295	VAL	2.8
1	B	324	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	84	VAL	2.8
1	A	324	ASN	2.7
1	A	397	ASN	2.7
1	B	292	GLY	2.7
1	A	163	ASP	2.6
1	C	1	MET	2.6
1	C	399	SER	2.6
1	A	74	ASN	2.5
1	D	399	SER	2.5
1	C	91	GLY	2.4
1	C	324	ASN	2.4
1	B	325	LYS	2.4
1	A	325	LYS	2.4
1	A	294	THR	2.4
1	B	290	LEU	2.4
1	C	136	ARG	2.3
1	B	310	SER	2.3
1	C	291	ILE	2.3
1	D	296	TYR	2.3
1	D	396	MET	2.3
1	A	63	ALA	2.2
1	B	392	VAL	2.2
1	B	291	ILE	2.2
1	A	392	VAL	2.2
1	D	291	ILE	2.2
1	D	293	ASP	2.2
1	A	307	ALA	2.2
1	C	84	VAL	2.1
1	B	296	TYR	2.1
1	D	294	THR	2.1
1	A	288	LYS	2.1
1	C	325	LYS	2.1
1	A	399	SER	2.1
1	C	397	ASN	2.1
1	C	392	VAL	2.0
1	A	292	GLY	2.0
1	C	287	GLU	2.0
1	A	75	MET	2.0
1	D	326	MET	2.0
1	D	290	LEU	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](#)

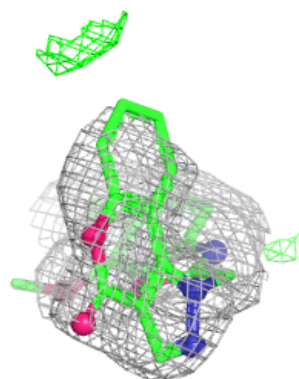
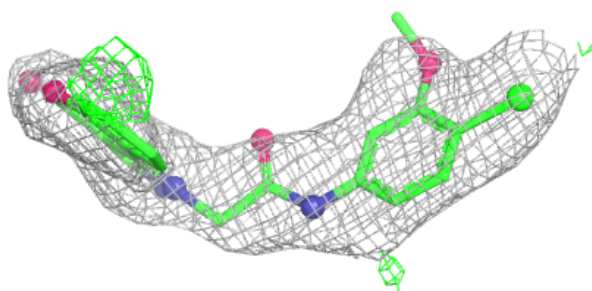
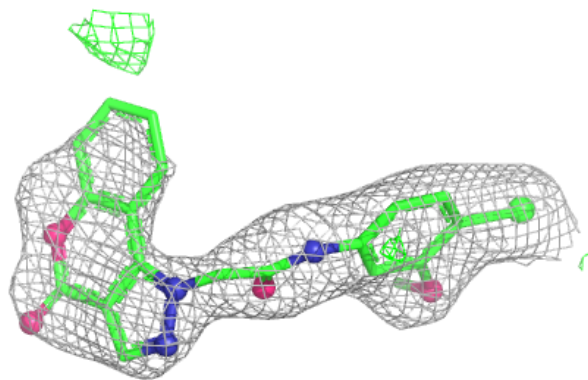
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	503	4/4	0.68	0.20	59,60,61,61	0
4	ACY	B	504	4/4	0.86	0.19	67,68,68,68	0
3	N09	B	503	27/27	0.88	0.14	53,65,70,71	0
3	N09	B	502	27/27	0.89	0.11	51,59,62,82	0
5	EDO	D	505	4/4	0.89	0.11	48,49,50,50	0
3	N09	A	502	27/27	0.90	0.12	58,68,69,70	0
6	FMT	D	504	3/3	0.91	0.11	52,52,53,54	0
5	EDO	C	502	4/4	0.92	0.12	46,47,48,48	0
3	N09	D	502	27/27	0.93	0.10	46,55,58,65	0
2	IMP	C	501	23/23	0.95	0.08	35,37,41,43	0
2	IMP	A	501	23/23	0.95	0.08	33,37,45,47	0
2	IMP	D	501	23/23	0.96	0.07	29,35,39,40	0
2	IMP	B	501	23/23	0.97	0.07	28,33,38,41	0

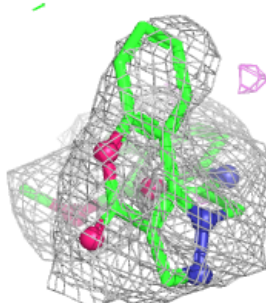
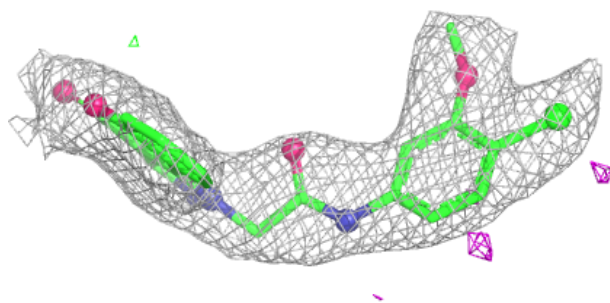
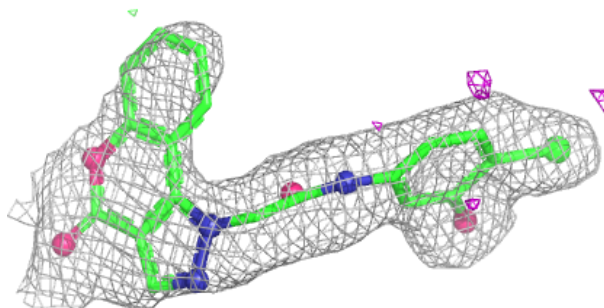
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N09 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)

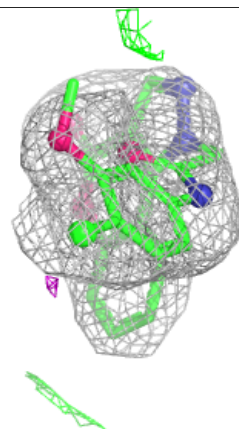
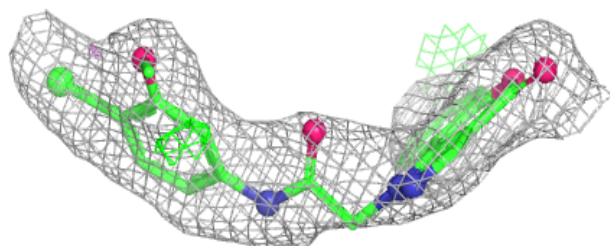
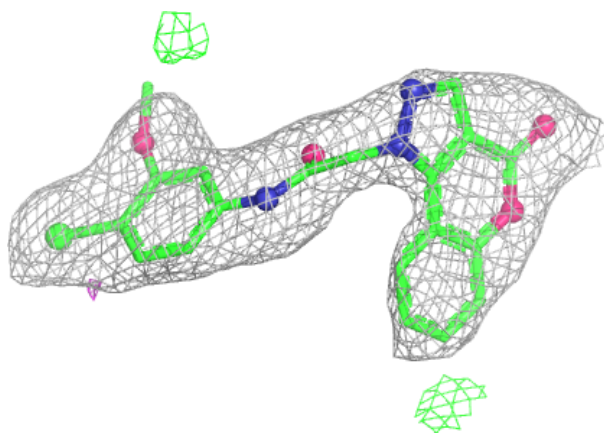
**Electron density around N09 B 502:**

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

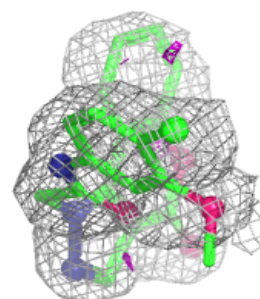
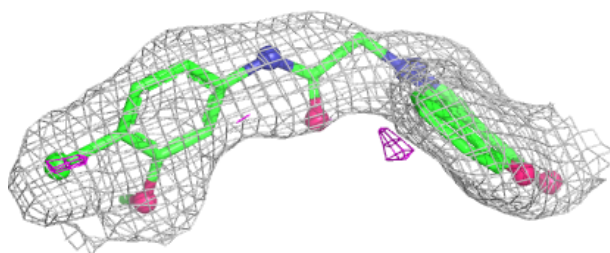
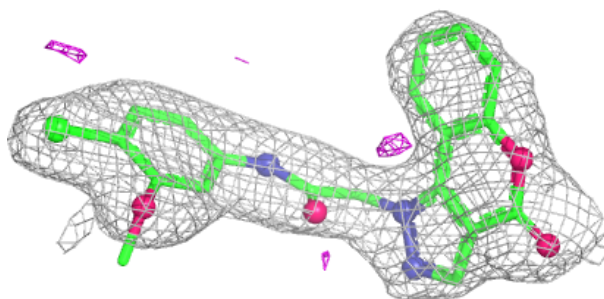


Electron density around N09 A 502:

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

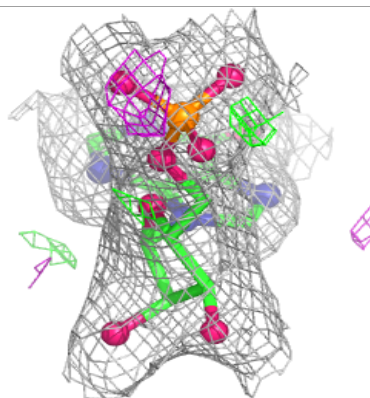
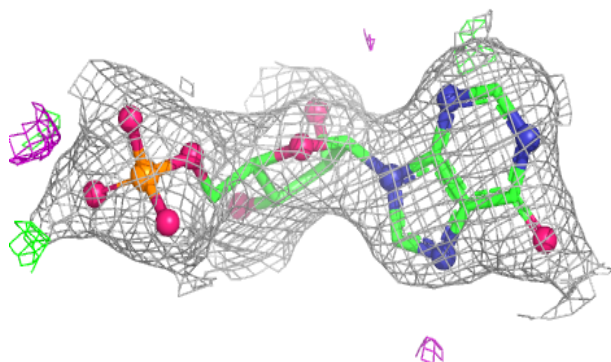
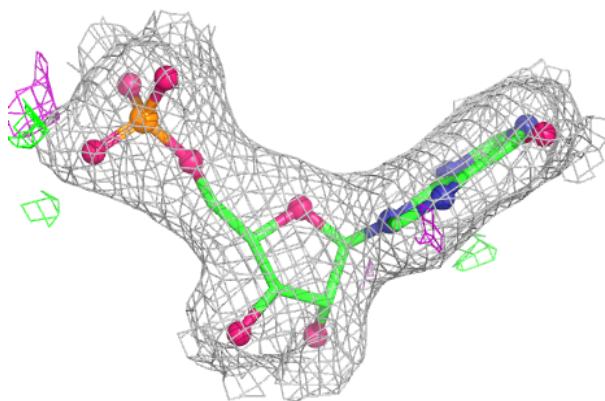
**Electron density around N09 D 502:**

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

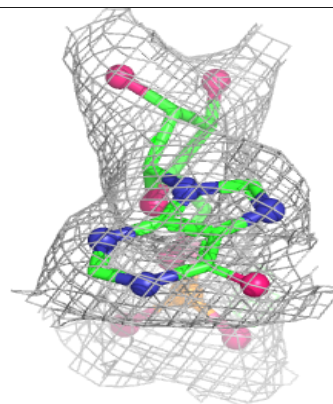
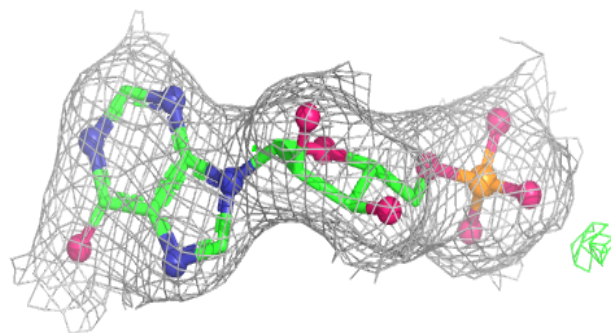
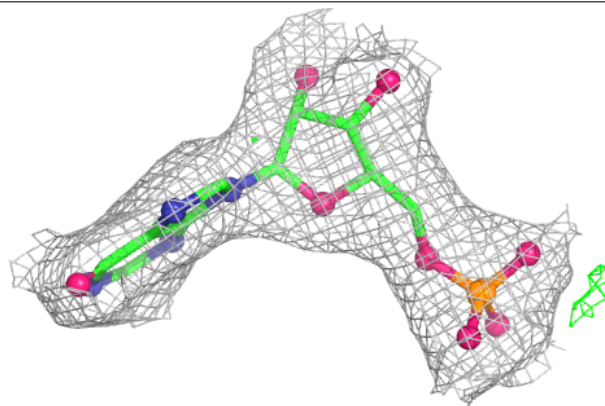


Electron density around IMP C 501:

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

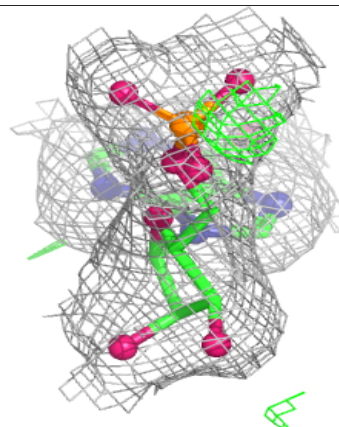
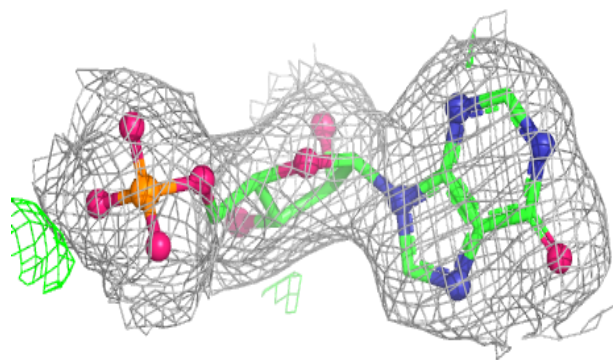
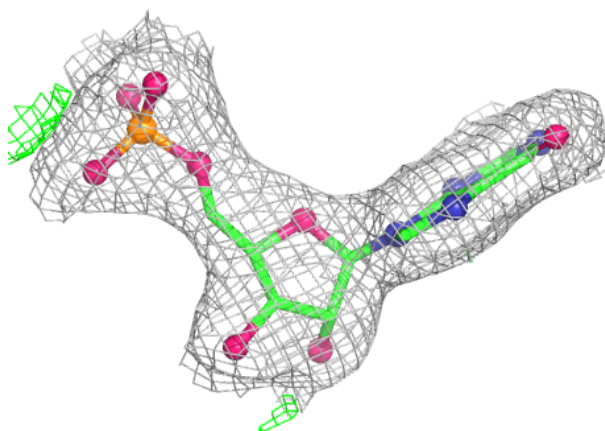
**Electron density around IMP A 501:**

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



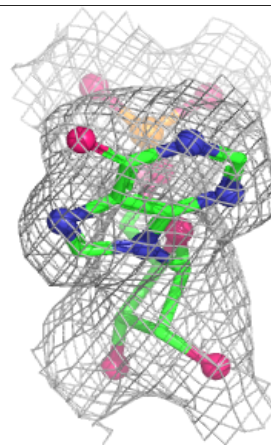
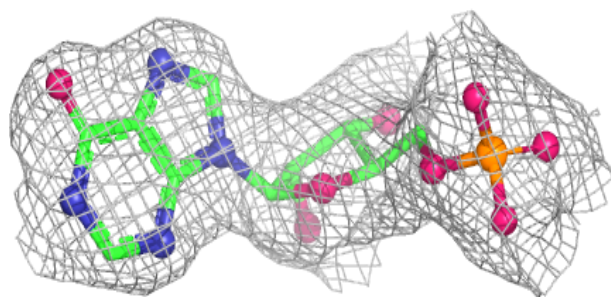
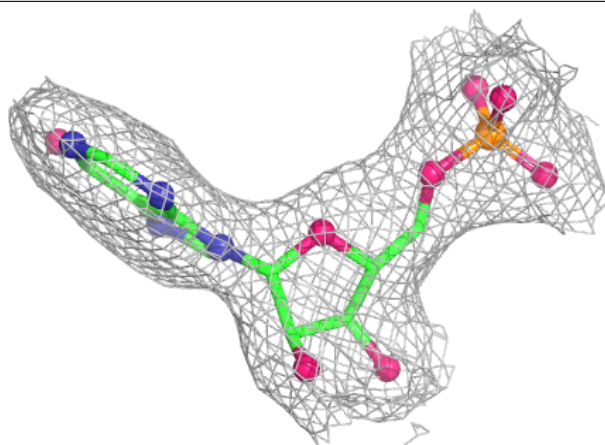
Electron density around IMP D 501:

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



Electron density around IMP B 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 [i](#)

There are no such residues in this entry.