



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:27 pm BST

PDB ID : 2P4S
Title : Structure of Purine Nucleoside Phosphorylase from *Anopheles gambiae* in complex with DADMe-ImmH
Authors : Rinaldo-Matthis, A.; Almo, S.C.; Schramm, V.L.
Deposited on : 2007-03-13
Resolution : 2.20 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

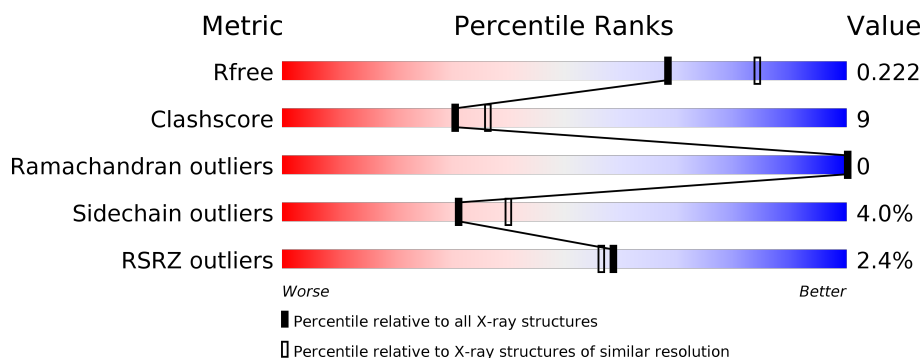
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	373	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 66%, yellow 9%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 66% 9% 24% </div> </div>
1	B	373	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 61%, yellow 12%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 61% 12% 24% </div> </div>
1	C	373	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 62%, yellow 11%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 62% 11% 24% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6986 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			
1	B	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			
1	C	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A4Q998
A	2	GLY	-	EXPRESSION TAG	UNP A4Q998
A	3	SER	-	EXPRESSION TAG	UNP A4Q998
A	4	SER	-	EXPRESSION TAG	UNP A4Q998
A	5	HIS	-	EXPRESSION TAG	UNP A4Q998
A	6	HIS	-	EXPRESSION TAG	UNP A4Q998
A	7	HIS	-	EXPRESSION TAG	UNP A4Q998
A	8	HIS	-	EXPRESSION TAG	UNP A4Q998
A	9	HIS	-	EXPRESSION TAG	UNP A4Q998
A	10	HIS	-	EXPRESSION TAG	UNP A4Q998
A	11	SER	-	EXPRESSION TAG	UNP A4Q998
A	12	SER	-	EXPRESSION TAG	UNP A4Q998
A	13	GLY	-	EXPRESSION TAG	UNP A4Q998
A	14	LEU	-	EXPRESSION TAG	UNP A4Q998
A	15	VAL	-	EXPRESSION TAG	UNP A4Q998
A	16	PRO	-	EXPRESSION TAG	UNP A4Q998
A	17	ARG	-	EXPRESSION TAG	UNP A4Q998
A	18	GLY	-	EXPRESSION TAG	UNP A4Q998
A	19	SER	-	EXPRESSION TAG	UNP A4Q998
A	20	HIS	-	EXPRESSION TAG	UNP A4Q998
B	1	MET	-	EXPRESSION TAG	UNP A4Q998
B	2	GLY	-	EXPRESSION TAG	UNP A4Q998
B	3	SER	-	EXPRESSION TAG	UNP A4Q998

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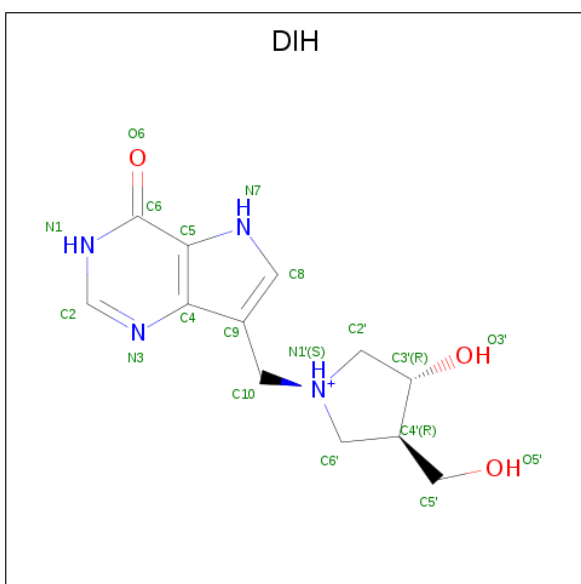
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	EXPRESSION TAG	UNP A4Q998
B	5	HIS	-	EXPRESSION TAG	UNP A4Q998
B	6	HIS	-	EXPRESSION TAG	UNP A4Q998
B	7	HIS	-	EXPRESSION TAG	UNP A4Q998
B	8	HIS	-	EXPRESSION TAG	UNP A4Q998
B	9	HIS	-	EXPRESSION TAG	UNP A4Q998
B	10	HIS	-	EXPRESSION TAG	UNP A4Q998
B	11	SER	-	EXPRESSION TAG	UNP A4Q998
B	12	SER	-	EXPRESSION TAG	UNP A4Q998
B	13	GLY	-	EXPRESSION TAG	UNP A4Q998
B	14	LEU	-	EXPRESSION TAG	UNP A4Q998
B	15	VAL	-	EXPRESSION TAG	UNP A4Q998
B	16	PRO	-	EXPRESSION TAG	UNP A4Q998
B	17	ARG	-	EXPRESSION TAG	UNP A4Q998
B	18	GLY	-	EXPRESSION TAG	UNP A4Q998
B	19	SER	-	EXPRESSION TAG	UNP A4Q998
B	20	HIS	-	EXPRESSION TAG	UNP A4Q998
C	1	MET	-	EXPRESSION TAG	UNP A4Q998
C	2	GLY	-	EXPRESSION TAG	UNP A4Q998
C	3	SER	-	EXPRESSION TAG	UNP A4Q998
C	4	SER	-	EXPRESSION TAG	UNP A4Q998
C	5	HIS	-	EXPRESSION TAG	UNP A4Q998
C	6	HIS	-	EXPRESSION TAG	UNP A4Q998
C	7	HIS	-	EXPRESSION TAG	UNP A4Q998
C	8	HIS	-	EXPRESSION TAG	UNP A4Q998
C	9	HIS	-	EXPRESSION TAG	UNP A4Q998
C	10	HIS	-	EXPRESSION TAG	UNP A4Q998
C	11	SER	-	EXPRESSION TAG	UNP A4Q998
C	12	SER	-	EXPRESSION TAG	UNP A4Q998
C	13	GLY	-	EXPRESSION TAG	UNP A4Q998
C	14	LEU	-	EXPRESSION TAG	UNP A4Q998
C	15	VAL	-	EXPRESSION TAG	UNP A4Q998
C	16	PRO	-	EXPRESSION TAG	UNP A4Q998
C	17	ARG	-	EXPRESSION TAG	UNP A4Q998
C	18	GLY	-	EXPRESSION TAG	UNP A4Q998
C	19	SER	-	EXPRESSION TAG	UNP A4Q998
C	20	HIS	-	EXPRESSION TAG	UNP A4Q998

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is 7-[[[(3R,4R)-3-(hydroxymethyl)-4-oxidanyl-pyrrolidin-1-ium-1-yl]methyl]-3,5-dihydropyrrolo[3,2-d]pyrimidin-4-one (three-letter code: DIH) (formula: C₁₂H₁₇N₄O₃).

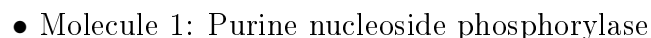
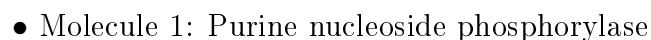


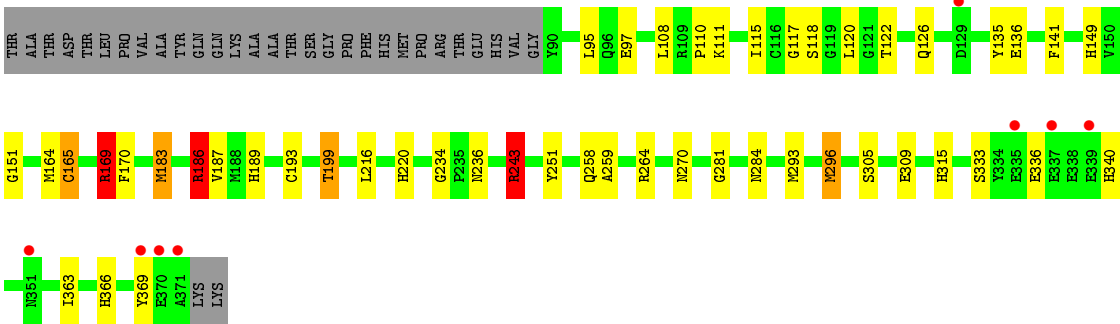
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	12	4	3		
3	B	1	Total	C	N	O	0	0
			19	12	4	3		
3	C	1	Total	C	N	O	0	0
			19	12	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	95	Total	O	0	0
			95	95		
4	C	132	Total	O	0	0
			132	132		

- Molecule 1: Purine nucleoside phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 106.72Å 240.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.9 (8.00-2.20) 93.9 (8.00-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.217 0.182 , 0.222	Depositor DCC
R_{free} test set	3301 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: PO4, DIH

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	0.94	3/2230 (0.1%)	0.79	4/3017 (0.1%)
1	B	0.98	3/2230 (0.1%)	0.88	4/3017 (0.1%)
1	C	1.00	3/2230 (0.1%)	0.97	10/3017 (0.3%)
All	All	0.97	9/6690 (0.1%)	0.88	18/9051 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	CYS	CB-SG	-10.65	1.64	1.82
1	B	316	CYS	CB-SG	-8.98	1.67	1.82
1	B	165	CYS	CB-SG	-8.97	1.67	1.82
1	C	165	CYS	CB-SG	-6.84	1.70	1.82
1	B	238	GLU	CB-CG	-6.13	1.40	1.52
1	A	165	CYS	CB-SG	-5.72	1.72	1.81
1	C	97	GLU	CB-CG	5.37	1.62	1.52
1	A	136	GLU	CG-CD	5.04	1.59	1.51
1	C	369	TYR	CD2-CE2	-5.01	1.31	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ARG	NE-CZ-NH2	-19.52	110.54	120.30
1	B	169	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	C	186	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	C	169	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	B	169	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	186	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	C	243	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	243	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	C	169	ARG	CG-CD-NE	-8.01	94.99	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	169	ARG	CG-CD-NE	-6.57	98.00	111.80
1	A	316	CYS	CB-CA-C	-5.75	98.89	110.40
1	B	243	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	243	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	318	MET	CG-SD-CE	5.52	109.04	100.20
1	C	186	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	264	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	C	186	ARG	CG-CD-NE	5.29	122.91	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2182	0	2145	28	0
1	B	2182	0	2145	46	0
1	C	2182	0	2145	51	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	19	0	17	0	0
3	B	19	0	17	0	0
3	C	19	0	17	0	0
4	A	136	0	0	6	0
4	B	95	0	0	13	0
4	C	132	0	0	10	0
All	All	6986	0	6486	120	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 9.

All (120) 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:136:GLU:HG2	4:C:611:HOH:O	1.59	1.01
1:C:126:GLN:HG2	4:C:633:HOH:O	1.67	0.93
1:C:183:MET:CE	1:C:187:VAL:CG2	2.51	0.88
1:B:186:ARG:HH12	1:B:315:HIS:HD2	1.22	0.88
1:C:281:GLY:HA3	4:C:608:HOH:O	1.73	0.86
1:C:120:LEU:HD13	1:C:199:THR:HG23	1.59	0.84
1:A:149:HIS:HD2	1:A:169:ARG:H	1.22	0.84
1:C:183:MET:CE	1:C:187:VAL:HG21	2.07	0.84
1:C:183:MET:HE2	1:C:187:VAL:HG23	1.60	0.83
1:B:250:THR:CG2	1:B:310:ILE:HD11	2.12	0.78
1:C:186:ARG:HH12	1:C:315:HIS:HD2	1.30	0.78
1:B:106:THR:HG23	1:B:131:ASP:OD2	1.84	0.78
1:C:164:MET:HE3	1:C:193:CYS:SG	2.24	0.77
1:B:250:THR:HG21	1:B:310:ILE:HD11	1.69	0.74
1:C:164:MET:CE	1:C:193:CYS:SG	2.77	0.73
1:C:183:MET:CE	1:C:187:VAL:HG23	2.15	0.73
1:B:142:PRO:HD3	1:B:183:MET:CE	2.20	0.71
1:B:250:THR:CG2	1:B:310:ILE:CD1	2.69	0.70
1:A:164:MET:HE3	1:A:193:CYS:SG	2.33	0.69
1:B:106:THR:HG22	1:B:108:LEU:H	1.56	0.69
1:C:149:HIS:HD2	1:C:169:ARG:H	1.40	0.69
1:C:117:GLY:H	1:C:199:THR:HG22	1.57	0.68
1:C:183:MET:HE1	1:C:187:VAL:HG21	1.75	0.68
1:B:189:HIS:HD2	4:B:550:HOH:O	1.77	0.67
1:B:234:GLY:O	1:B:243:ARG:NH2	2.26	0.67
1:A:230:ASN:HB2	4:A:638:HOH:O	1.97	0.65
1:C:236:ASN:HD21	1:C:315:HIS:CE1	2.15	0.65
1:B:236:ASN:HD21	1:B:315:HIS:CE1	2.15	0.65
1:C:110:PRO:HG2	1:C:164:MET:HE2	1.79	0.63
1:B:220:HIS:HD2	1:B:251:TYR:OH	1.81	0.63
1:B:233:GLN:HB2	4:B:589:HOH:O	2.01	0.60
1:B:233:GLN:CB	4:B:589:HOH:O	2.50	0.60
1:B:220:HIS:HE1	4:C:508:HOH:O	1.85	0.60
1:A:236:ASN:HD21	1:A:315:HIS:HE2	1.50	0.59
1:B:142:PRO:HD3	1:B:183:MET:HE1	1.83	0.59
1:B:194:THR:OG1	1:B:195:HIS:HD2	1.84	0.59
1:C:183:MET:HE1	1:C:187:VAL:CG2	2.29	0.59
1:B:195:HIS:HE1	4:B:541:HOH:O	1.85	0.58
1:B:108:LEU:HD23	1:B:162:PRO:HB3	1.85	0.58
1:B:98:ILE:HD11	1:B:140:HIS:HB2	1.86	0.58
1:A:142:PRO:HD3	1:A:183:MET:HE1	1.85	0.58
1:A:164:MET:CE	1:A:193:CYS:SG	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PRO:HD3	1:B:183:MET:HE3	1.85	0.58
1:C:189:HIS:HD2	4:C:530:HOH:O	1.87	0.58
1:B:186:ARG:HH12	1:B:315:HIS:CD2	2.13	0.57
1:B:340:HIS:HD2	4:B:574:HOH:O	1.88	0.57
1:C:122:THR:HG23	4:C:592:HOH:O	2.05	0.57
1:C:115:ILE:O	1:C:199:THR:HB	2.05	0.57
1:B:233:GLN:HG3	4:B:589:HOH:O	2.04	0.56
1:A:234:GLY:O	1:A:243:ARG:NH2	2.36	0.56
1:A:149:HIS:CD2	1:A:169:ARG:H	2.13	0.56
1:B:189:HIS:CD2	4:B:550:HOH:O	2.56	0.55
1:A:91:THR:HG23	1:A:94:THR:H	1.72	0.55
1:C:164:MET:HE1	1:C:193:CYS:SG	2.45	0.55
1:C:220:HIS:HD2	1:C:251:TYR:OH	1.89	0.55
1:A:118:SER:OG	1:A:149:HIS:HE1	1.89	0.54
1:C:186:ARG:HH12	1:C:315:HIS:CD2	2.20	0.54
1:B:176:TYR:CD1	1:B:180:LYS:HD3	2.44	0.52
1:C:234:GLY:O	1:C:243:ARG:NH2	2.39	0.52
1:A:258:GLN:HG2	1:A:366:HIS:CG	2.45	0.51
1:C:270:ASN:HB3	4:C:512:HOH:O	2.09	0.51
1:C:149:HIS:CD2	1:C:169:ARG:H	2.26	0.51
1:C:169:ARG:HD2	1:C:305:SER:HB2	1.93	0.50
1:C:169:ARG:HD3	1:C:309:GLU:OE2	2.11	0.50
1:A:171:HIS:HE1	2:A:503:PO4:O2	1.94	0.50
1:A:332:MET:HA	4:A:515:HOH:O	2.11	0.49
1:B:152:ARG:HD2	4:B:566:HOH:O	2.11	0.49
1:C:366:HIS:HD2	4:C:634:HOH:O	1.95	0.49
1:C:110:PRO:CG	1:C:164:MET:HE2	2.41	0.49
1:B:236:ASN:HD21	1:B:315:HIS:HE1	1.58	0.49
1:C:186:ARG:NH1	1:C:315:HIS:HD2	2.06	0.49
1:B:355:THR:HG23	4:B:573:HOH:O	2.12	0.48
1:B:242:PRO:O	1:B:315:HIS:HE1	1.96	0.48
1:C:135:TYR:CE2	1:C:151:GLY:HA2	2.48	0.48
1:C:169:ARG:NH2	1:C:199:THR:O	2.27	0.48
1:C:186:ARG:HH22	1:C:315:HIS:CD2	2.32	0.48
1:C:183:MET:HE3	1:C:187:VAL:HG21	1.93	0.47
1:A:94:THR:O	1:A:97:GLU:HB2	2.15	0.47
1:C:236:ASN:HD21	1:C:315:HIS:HE1	1.58	0.47
1:C:111:LYS:HE2	4:C:555:HOH:O	2.16	0.46
4:A:552:HOH:O	1:C:296:MET:CE	2.63	0.46
1:C:95:LEU:CD2	1:C:183:MET:HG2	2.46	0.46
1:A:297:LEU:HD22	1:B:293:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:HIS:HE1	4:B:522:HOH:O	1.98	0.46
1:A:250:THR:HG23	1:A:314:ARG:HG3	1.97	0.46
1:A:243:ARG:HA	1:A:243:ARG:HD3	1.60	0.45
1:A:314:ARG:HA	1:A:314:ARG:HD2	1.76	0.45
1:A:142:PRO:CD	1:A:183:MET:HE1	2.47	0.45
1:C:118:SER:OG	1:C:149:HIS:HE1	2.00	0.45
1:C:258:GLN:HG2	1:C:366:HIS:CG	2.51	0.45
1:A:171:HIS:HD2	1:A:174:GLU:OE2	1.99	0.44
1:A:110:PRO:HG2	1:A:164:MET:HE2	1.99	0.44
1:A:230:ASN:ND2	4:A:601:HOH:O	2.34	0.44
1:B:142:PRO:CD	1:B:183:MET:HE3	2.47	0.44
1:C:340:HIS:HE1	4:C:529:HOH:O	2.00	0.44
1:B:242:PRO:O	1:B:315:HIS:CE1	2.71	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.84	0.43
1:B:354:LYS:HE3	1:B:354:LYS:HB2	1.53	0.43
1:B:191:ILE:O	4:B:585:HOH:O	2.21	0.43
4:A:511:HOH:O	1:C:220:HIS:HE1	2.00	0.43
1:A:250:THR:HG23	1:A:314:ARG:CG	2.49	0.43
1:B:332:MET:HA	4:B:531:HOH:O	2.18	0.43
1:C:333:SER:OG	1:C:336:GLU:HG3	2.19	0.42
1:B:169:ARG:HD3	1:B:309:GLU:OE2	2.19	0.42
1:B:122:THR:HG23	4:B:535:HOH:O	2.18	0.42
1:C:149:HIS:HD2	1:C:169:ARG:N	2.14	0.42
1:B:230:ASN:HD21	1:C:284:ASN:HD21	1.66	0.42
1:C:111:LYS:HA	1:C:111:LYS:HD3	1.82	0.42
1:C:259:ALA:HB2	1:C:363:ILE:HD11	2.02	0.41
1:B:250:THR:HG23	1:B:314:ARG:HG3	2.03	0.41
1:A:230:ASN:HD21	1:B:284:ASN:ND2	2.19	0.41
1:B:333:SER:OG	1:B:336:GLU:HG3	2.20	0.41
1:B:127:LEU:HD12	1:B:154:VAL:HG12	2.04	0.40
1:A:135:TYR:CE2	1:A:151:GLY:HA2	2.56	0.40
1:C:169:ARG:HG3	1:C:170:PHE:N	2.37	0.40
1:A:110:PRO:HG2	1:A:164:MET:CE	2.51	0.40
1:A:371:ALA:C	4:A:633:HOH:O	2.59	0.40
1:B:264:ARG:HA	1:B:269:GLU:HG3	2.03	0.40
1:B:230:ASN:HD21	1:C:284:ASN:ND2	2.19	0.40
1:B:297:LEU:HD22	1:C:293:MET:HG3	2.04	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	280/373 (75%)	276 (99%)	4 (1%)	0	100	100
1	B	280/373 (75%)	273 (98%)	7 (2%)	0	100	100
1	C	280/373 (75%)	277 (99%)	3 (1%)	0	100	100
All	All	840/1119 (75%)	826 (98%)	14 (2%)	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	234/306 (76%)	229 (98%)	5 (2%)	53	67
1	B	234/306 (76%)	221 (94%)	13 (6%)	21	25
1	C	234/306 (76%)	224 (96%)	10 (4%)	29	36
All	All	702/918 (76%)	674 (96%)	28 (4%)	31	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	129	ASP
1	A	141	PHE
1	A	243	ARG
1	A	333	SER

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Mol	Chain	Res	Type
1	B	108	LEU
1	B	123	LEU
1	B	141	PHE
1	B	169	ARG
1	B	243	ARG
1	B	256	ASN
1	B	269	GLU
1	B	296	MET
1	B	310	ILE
1	B	343	ASP
1	B	354	LYS
1	B	355	THR
1	B	363	ILE
1	C	108	LEU
1	C	141	PHE
1	C	165	CYS
1	C	169	ARG
1	C	183	MET
1	C	186	ARG
1	C	199	THR
1	C	216	LEU
1	C	243	ARG
1	C	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	171	HIS
1	A	236	ASN
1	A	256	ASN
1	B	189	HIS
1	B	195	HIS
1	B	220	HIS
1	B	236	ASN
1	B	256	ASN
1	B	284	ASN
1	B	315	HIS
1	B	340	HIS
1	B	351	ASN
1	C	149	HIS
1	C	189	HIS

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Mol	Chain	Res	Type
1	C	220	HIS
1	C	236	ASN
1	C	270	ASN
1	C	284	ASN
1	C	315	HIS
1	C	340	HIS
1	C	366	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	DIH	C	402	-	18,21,21	1.52	3 (16%)	15,30,30	2.95	9 (60%)
2	PO4	A	503	-	4,4,4	1.23	0	6,6,6	0.76	0
3	DIH	A	401	-	18,21,21	1.68	3 (16%)	15,30,30	2.79	9 (60%)
2	PO4	C	502	-	4,4,4	1.44	0	6,6,6	0.92	0
3	DIH	B	403	-	18,21,21	1.41	1 (5%)	15,30,30	2.55	8 (53%)
2	PO4	B	501	-	4,4,4	0.90	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	504	-	4,4,4	0.81	0	6,6,6	0.29	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	DIH	A	401	-	-	1/5/18/18	0/3/3/3
3	DIH	C	402	-	-	0/5/18/18	0/3/3/3
3	DIH	B	403	-	-	1/5/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DIH	C6-C5	4.73	1.49	1.41
3	C	402	DIH	C6-C5	4.40	1.48	1.41
3	B	403	DIH	C6-C5	4.39	1.48	1.41
3	A	401	DIH	O6-C6	2.33	1.30	1.24
3	A	401	DIH	C2'-N1'	2.26	1.50	1.47
3	C	402	DIH	C2-N3	2.25	1.35	1.32
3	C	402	DIH	C6'-C4'	2.12	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	DIH	C2-N3-C4	5.77	119.30	114.81
3	A	401	DIH	C2-N1-C6	4.79	123.90	115.88
3	A	401	DIH	C2-N3-C4	4.50	118.31	114.81
3	B	403	DIH	C2-N1-C6	4.30	123.09	115.88
3	C	402	DIH	C6-C5-C4	-4.21	116.78	120.80
3	A	401	DIH	N3-C2-N1	-4.09	122.28	128.68
3	C	402	DIH	N3-C2-N1	-3.97	122.47	128.68
3	B	403	DIH	C6-C5-C4	-3.85	117.12	120.80
3	B	403	DIH	N3-C2-N1	-3.64	122.99	128.68
3	B	403	DIH	C2-N3-C4	3.63	117.63	114.81
3	C	402	DIH	C10-N1'-C6'	3.53	119.26	113.27
3	C	402	DIH	C9-C10-N1'	3.36	118.95	114.14
3	B	403	DIH	C9-C10-N1'	3.26	118.79	114.14
3	A	401	DIH	C10-N1'-C6'	3.24	118.77	113.27
3	A	401	DIH	C6-C5-C4	-3.17	117.77	120.80
3	A	401	DIH	C9-C10-N1'	3.10	118.57	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	DIH	C6'-C4'-C3'	3.02	108.07	103.26
3	C	402	DIH	C2'-N1'-C6'	2.83	108.41	104.19
3	C	402	DIH	C2-N1-C6	2.76	120.51	115.88
3	B	403	DIH	C6'-C4'-C3'	2.49	107.23	103.26
3	A	401	DIH	C6'-C4'-C3'	2.46	107.18	103.26
3	B	403	DIH	C2'-N1'-C6'	2.39	107.74	104.19
3	C	402	DIH	C5-C4-N3	-2.38	122.16	124.92
3	A	401	DIH	C5-C4-N3	-2.32	122.23	124.92
3	B	403	DIH	C5-C4-N3	-2.17	122.39	124.92
3	A	401	DIH	O5'-C5'-C4'	-2.09	106.56	111.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	DIH	C9-C10-N1'-C6'
3	B	403	DIH	C9-C10-N1'-C6'

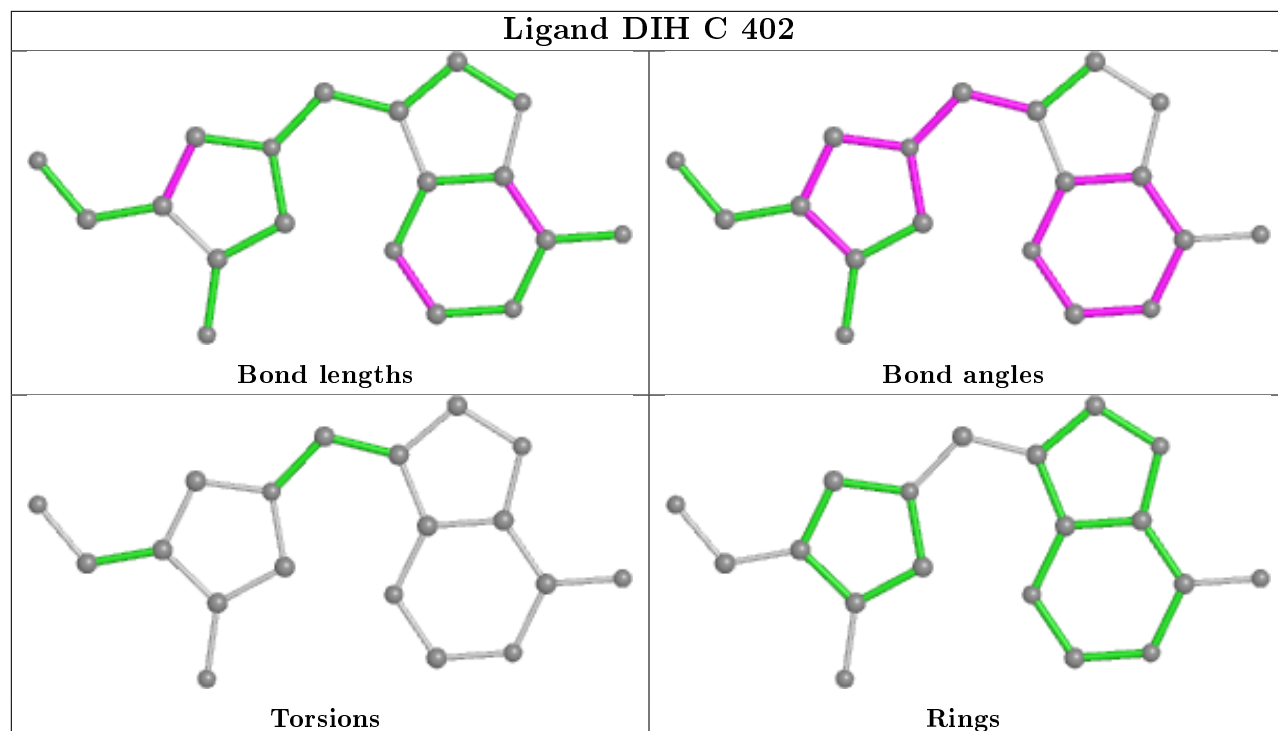
There are no ring outliers.

1 monomer is involved in 1 short contact:

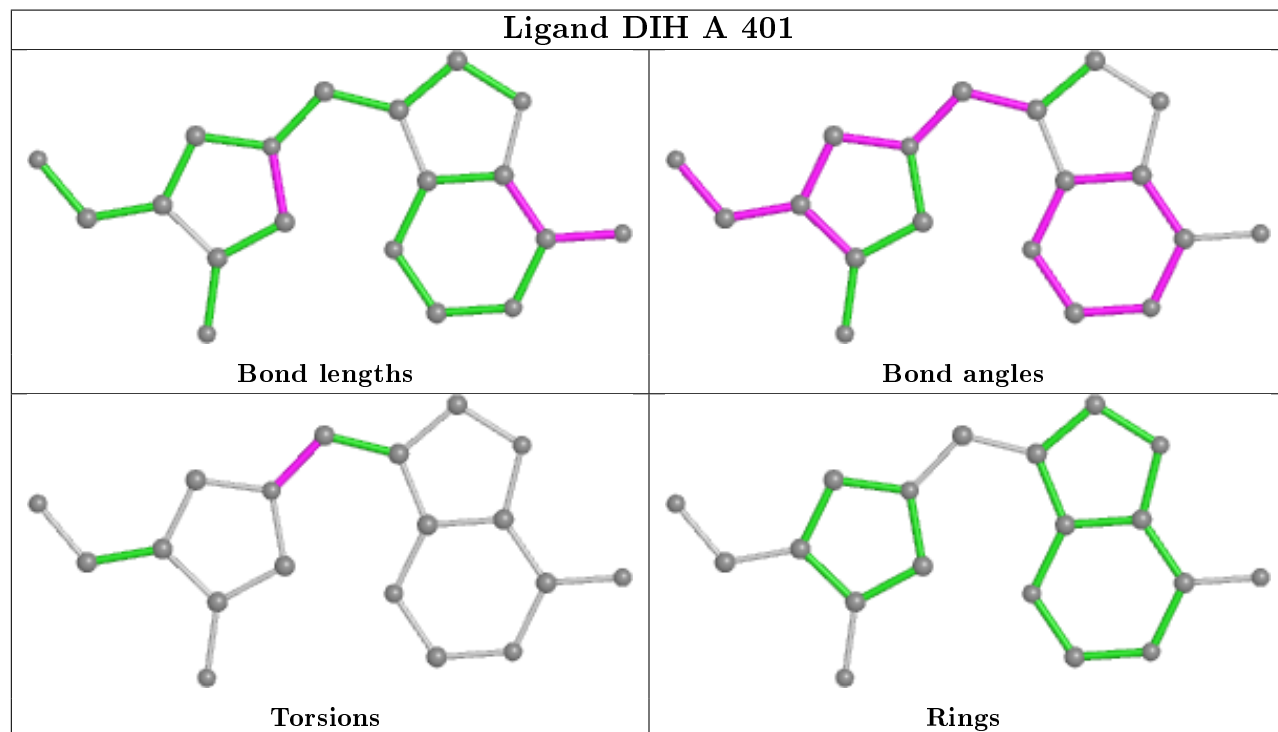
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	PO4	1	0

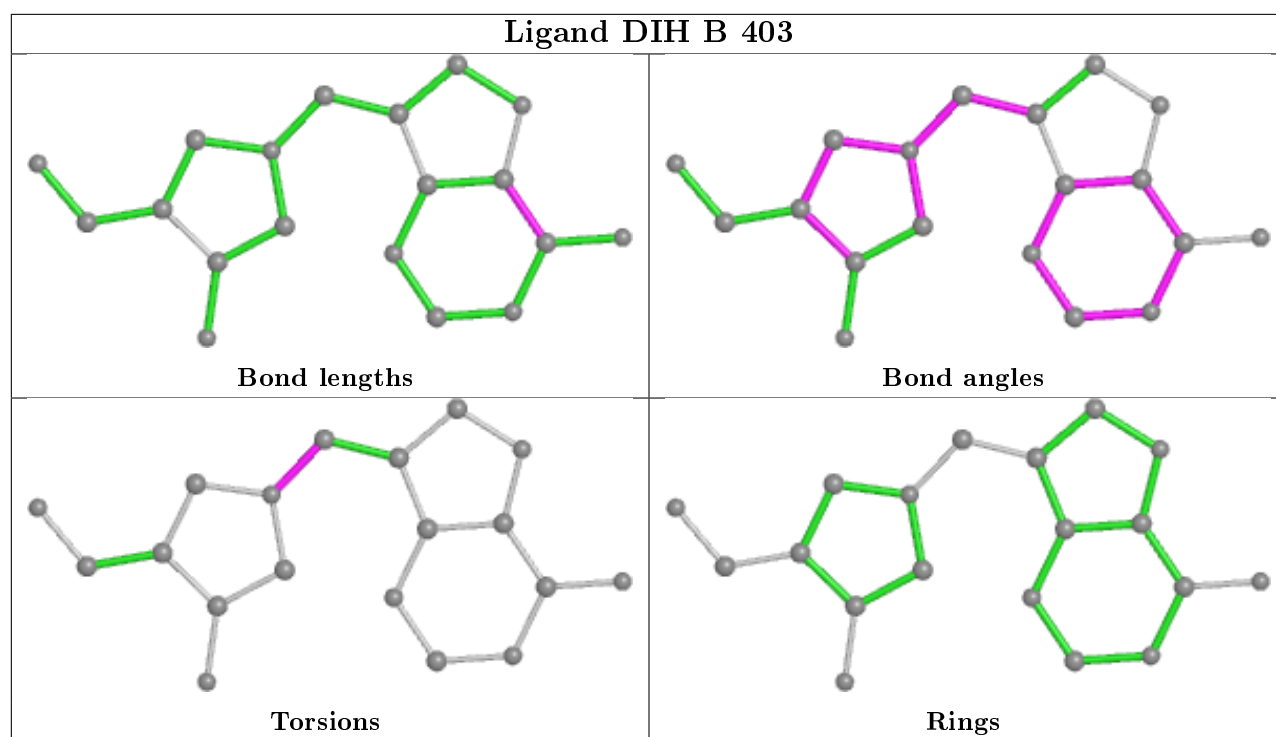
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DIH C 402



Ligand DIH A 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	282/373 (75%)	-0.67	3 (1%) 80 79	12, 23, 38, 50	0
1	B	282/373 (75%)	-0.49	9 (3%) 47 45	14, 25, 42, 49	0
1	C	282/373 (75%)	-0.71	8 (2%) 53 51	13, 20, 35, 55	0
All	All	846/1119 (75%)	-0.63	20 (2%) 59 56	12, 22, 40, 55	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	ALA	5.7
1	C	369	TYR	4.8
1	B	369	TYR	4.0
1	A	369	TYR	3.9
1	C	371	ALA	3.4
1	C	337	GLU	3.2
1	C	339	GLU	3.0
1	B	337	GLU	2.9
1	B	370	GLU	2.9
1	B	107	GLU	2.9
1	C	351	ASN	2.9
1	C	129	ASP	2.9
1	B	354	LYS	2.8
1	B	129	ASP	2.5
1	A	93	ASP	2.5
1	B	93	ASP	2.5
1	B	343	ASP	2.5
1	C	335	GLU	2.4
1	A	339	GLU	2.4
1	C	370	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

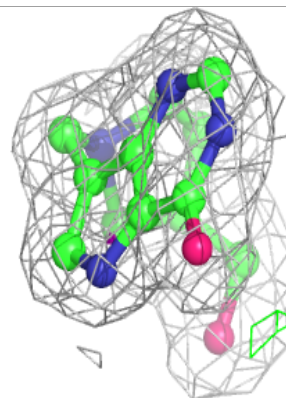
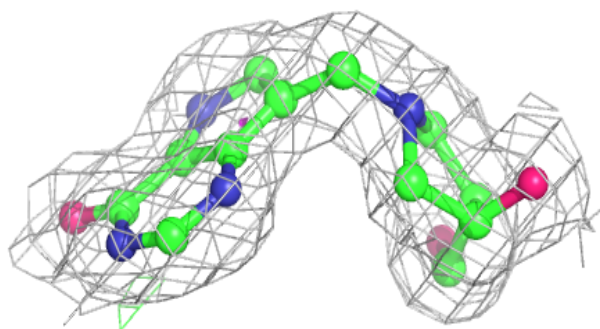
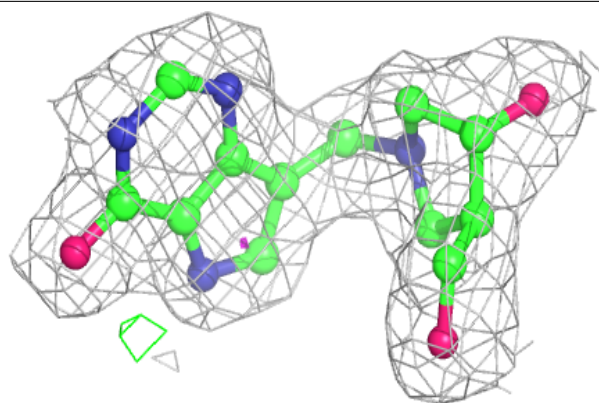
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	A	504	5/5	0.93	0.12	81,81,83,83	0
3	DIH	A	401	19/19	0.98	0.07	12,14,18,18	0
3	DIH	B	403	19/19	0.98	0.06	14,17,19,22	0
3	DIH	C	402	19/19	0.98	0.06	15,17,20,21	0
2	PO4	A	503	5/5	0.99	0.05	16,16,17,17	0
2	PO4	B	501	5/5	0.99	0.05	18,19,20,21	0
2	PO4	C	502	5/5	0.99	0.05	14,14,18,20	0

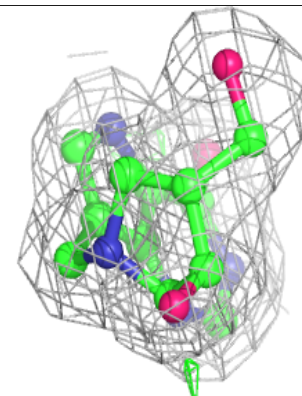
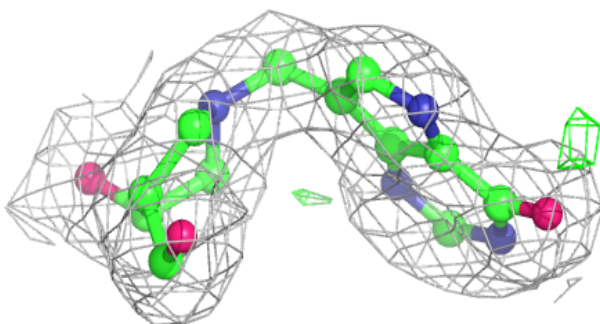
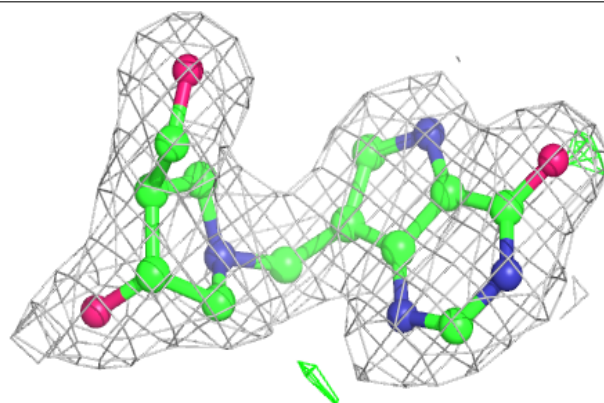
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DIH A 401:

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

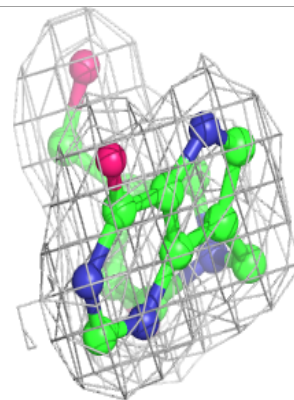
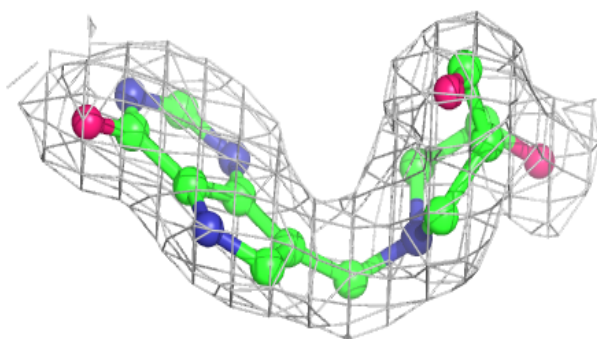
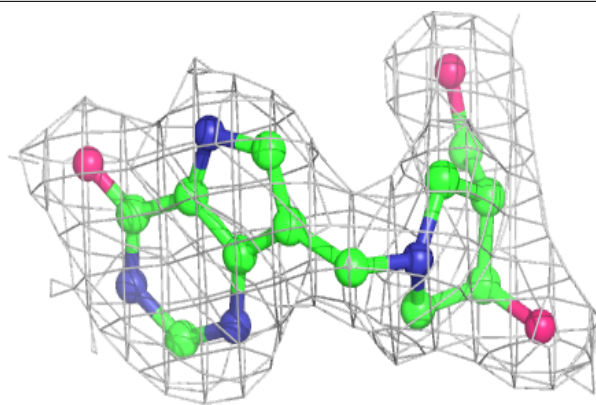
**Electron density around DIH B 403:**

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



Electron density around DIH C 402:

$2mF_o-DF_c$ (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.