



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 06:09 PM EDT

PDB ID : 9OP3 / pdb\_00009op3  
Title : Structure of Human ADAR2-R2D complexed with dsRNA containing 8-azaN and 2'-Deoxy-2'-fluorouridine  
Authors : Campbell, K.B.; Ouye, R.B.; Wong, B.L.; Jiang, A.; Okada, K.; McKenney, R.J.; Fisher, A.J.; Beal, P.A.  
Deposited on : 2025-05-16  
Resolution : 2.59 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.

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 ⓘ](#)) 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

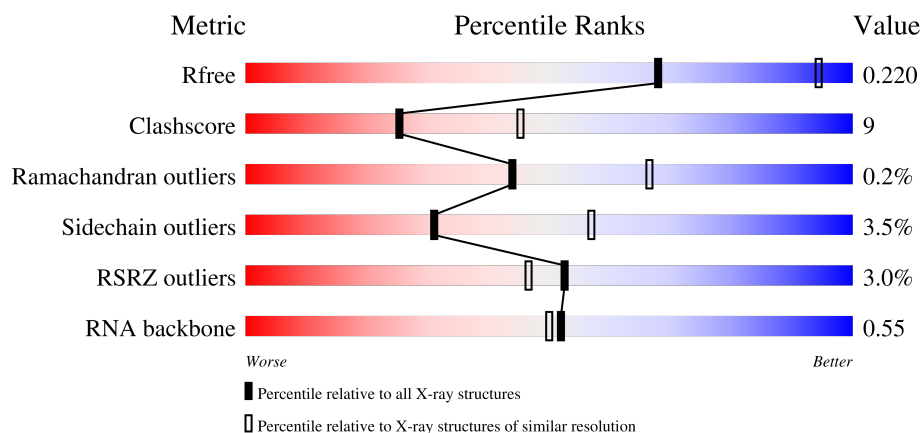
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)
RNA backbone	3690	1025 (2.88-2.32)

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  $\geq 3$ , 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	488	<div> <div>60%</div> <div>18%</div> <div>21%</div> </div>
1	B	488	<div> <div>4%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>
2	C	32	<div> <div>53%</div> <div>44%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	D	32	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: green (75%), yellow (19%), and orange (6%). The percentages are labeled below the bar.

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8083 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 Double-stranded RNA-specific editase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	1	0
			3027	1909	553	554	11			
1	B	455	Total	C	N	O	S	0	0	0
			3553	2245	641	654	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	GLY	-	expression tag	UNP P78563
A	488	GLN	GLU	engineered mutation	UNP P78563
B	214	GLY	-	expression tag	UNP P78563
B	488	GLN	GLU	engineered mutation	UNP P78563

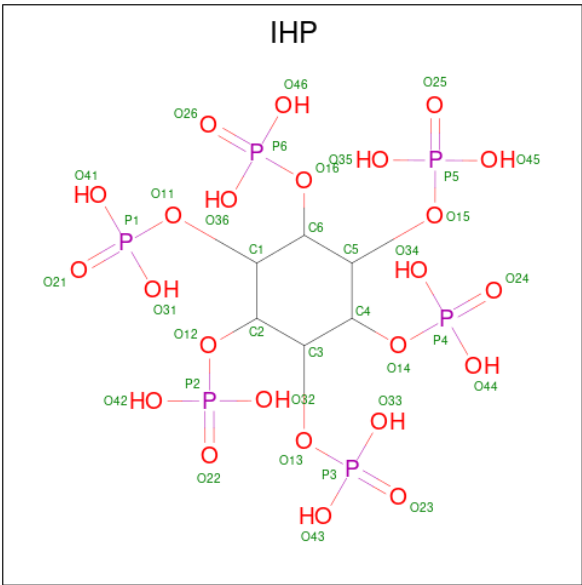
- Molecule 2 is a RNA chain called RNA 32mer Top Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	32	Total	C	N	O	P	0	0	0
			682	304	123	224	31			

- Molecule 3 is a RNA chain called RNA 32mer 2F Bottom Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	32	Total	C	F	N	O	P	0	0
			675	303	1	122	218	31		

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			36	6	24	6		
4	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

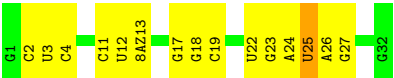
- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

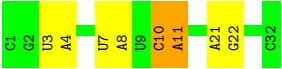
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total	O	0	0
			33	33		
8	B	11	Total	O	0	0
			11	11		
8	C	8	Total	O	0	0
			8	8		
8	D	7	Total	O	0	0
			7	7		





• Molecule 3: RNA 32mer 2F Bottom Strand





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00Å 63.21Å 142.20Å 90.00° 118.13° 90.00°	Depositor
Resolution (Å)	65.70 – 2.59 65.70 – 2.59	Depositor EDS
% Data completeness (in resolution range)	74.9 (65.70-2.59) 74.9 (65.70-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.178 , 0.220 0.178 , 0.220	Depositor DCC
$R_{free}$ test set	1574 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: EDO, ZN, NA, UFT, IHP, 8AZ

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	0.52	0/3092	0.69	0/4178
1	B	0.39	0/3624	0.60	0/4894
2	C	0.42	0/736	0.54	0/1144
3	D	0.46	1/731 (0.1%)	0.58	0/1137
All	All	0.45	1/8183 (0.0%)	0.63	0/11353

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7	UFT	O3'-P	5.89	1.62	1.56

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	3027	0	3064	56	0
1	B	3553	0	3595	75	0
2	C	682	0	336	17	0
3	D	675	0	349	3	0
4	A	36	0	6	2	0
4	B	36	0	6	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	12	0	18	0	0
7	A	1	0	0	0	0
8	A	33	0	0	0	0
8	B	11	0	0	1	0
8	C	8	0	0	0	0
8	D	7	0	0	0	0
All	All	8083	0	7374	146	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 (146) 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:A:362:ASP:HB3	1:A:364:LYS:HG2	1.53	0.89
1:A:349:ARG:NH2	1:A:588:GLU:OE2	2.12	0.81
1:B:305:PRO:HG3	1:B:462:PRO:HB2	1.67	0.77
1:A:327:VAL:HG21	1:A:546:ILE:HD13	1.66	0.76
1:B:303:GLN:OE1	1:B:303:GLN:N	2.24	0.71
1:B:556:LEU:HD23	1:B:581:LEU:HB3	1.72	0.71
1:A:644:PRO:HG2	1:A:647:LEU:HB2	1.74	0.70
1:B:499:ILE:HD11	1:B:689:GLU:H	1.56	0.69
1:B:386:ARG:HG3	1:B:388:LEU:HD13	1.75	0.69
1:A:414:TYR:O	1:A:421:GLN:HG2	1.93	0.68
1:A:316:GLN:HB2	1:A:364:LYS:NZ	2.08	0.68
1:B:667:GLU:H	1:B:667:GLU:CD	2.03	0.66
1:A:331:VAL:HG13	1:A:371:VAL:HG12	1.78	0.63
1:B:555:HIS:CD2	1:B:558:ARG:HH12	2.16	0.63
1:A:537:VAL:HG12	1:A:538:GLU:O	2.00	0.61
1:B:274:PHE:CE1	1:B:292:ALA:HA	2.36	0.61
1:B:690:LYS:HD3	4:B:801:IHP:O36	2.00	0.61
1:B:501:THR:O	1:B:505:VAL:HG22	2.01	0.61
1:B:243:LEU:C	1:B:244:ARG:HD3	2.26	0.60
1:A:453:ASP:OD2	1:A:558:ARG:NE	2.34	0.59
1:B:350:LYS:NZ	1:B:488:GLN:HE22	2.00	0.59
1:B:281:LYS:HE2	2:C:18:G:H5'	1.85	0.59
1:B:319:LEU:HB2	1:B:322:VAL:HG22	1.84	0.58
1:B:279:ARG:NH1	2:C:17:G:OP1	2.37	0.58
1:A:316:GLN:HB2	1:A:364:LYS:HZ1	1.68	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:G:H2'	2:C:19:C:H6	1.69	0.57
1:B:375:THR:HG22	1:B:375:THR:O	2.04	0.57
1:B:386:ARG:NH1	8:B:901:HOH:O	2.38	0.57
1:A:510:ARG:HD2	1:B:593:GLY:HA2	1.88	0.56
1:A:334:LYS:O	1:A:338:LEU:HG	2.06	0.56
1:B:516:CYS:O	1:B:520:ILE:HG13	2.07	0.55
1:B:241:ASN:HA	1:B:247:LEU:HD21	1.87	0.55
1:A:554:ASP:N	1:A:554:ASP:OD1	2.37	0.55
1:A:319:LEU:HD23	1:A:322:VAL:HG12	1.89	0.55
1:B:317:LEU:HD13	1:B:318:HIS:HB2	1.88	0.55
1:B:514:MET:HG3	1:B:687:TRP:CE2	2.42	0.55
2:C:18:G:H2'	2:C:19:C:C6	2.41	0.54
1:A:382:TYR:CE1	1:B:460:HIS:CD2	2.96	0.54
1:B:303:GLN:O	1:B:305:PRO:HD2	2.08	0.54
1:B:238:MET:O	1:B:242:GLU:HG2	2.09	0.53
1:B:317:LEU:HD12	1:B:323:LEU:HD13	1.91	0.53
1:B:308:GLN:NE2	1:B:321:GLN:HG2	2.24	0.53
1:A:470:ARG:HB2	1:A:471:HIS:HD2	1.74	0.53
1:B:430:GLU:H	1:B:430:GLU:CD	2.16	0.53
1:B:612:ILE:HD11	1:B:625:SER:HB2	1.92	0.52
1:B:400:ARG:O	1:B:403:LEU:HB3	2.10	0.52
1:B:427:GLN:OE1	1:B:435:ARG:NH2	2.34	0.51
1:B:477:ARG:HB2	1:B:479:GLN:OE1	2.11	0.51
1:B:380:GLY:HA2	1:B:383:MET:HG3	1.93	0.51
1:B:317:LEU:HD12	1:B:323:LEU:HB2	1.93	0.50
1:B:274:PHE:CD1	1:B:292:ALA:HA	2.47	0.50
1:A:451:CYS:SG	1:A:483:LYS:HE3	2.51	0.50
2:C:25:U:H2'	2:C:26:A:C8	2.47	0.50
1:B:522:ARG:NH2	4:B:801:IHP:O33	2.45	0.49
1:B:535:ILE:O	1:B:649:ARG:HB2	2.12	0.49
1:A:405:ARG:NH2	1:A:606:ASP:OD2	2.45	0.49
1:B:621:LEU:HD12	1:B:623:ARG:NH1	2.27	0.49
1:A:544:SER:HB3	1:A:580:LEU:HB3	1.95	0.49
1:B:308:GLN:HE22	1:B:321:GLN:HG2	1.76	0.49
1:A:542:PHE:O	1:A:579:PRO:HB3	2.12	0.48
1:A:347:ALA:O	1:A:349:ARG:HG2	2.13	0.48
3:D:3:U:H2'	3:D:4:A:C8	2.48	0.48
1:A:325:ASP:HB3	1:A:329[B]:ARG:HH22	1.78	0.48
1:B:400:ARG:HD2	1:B:523:TRP:CE2	2.49	0.48
1:B:308:GLN:HA	1:B:551:TYR:OH	2.13	0.48
1:A:471:HIS:HB3	1:A:474:ARG:HG3	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ALA:HA	1:B:546:ILE:HD12	1.95	0.47
1:B:555:HIS:HD2	1:B:558:ARG:HH12	1.58	0.47
1:A:373:THR:O	1:A:599:SER:OG	2.27	0.47
1:A:657:VAL:HG22	1:A:660:GLU:HG2	1.95	0.47
2:C:3:U:H2'	2:C:4:C:H6	1.78	0.47
1:A:669:GLN:HE22	1:A:672:LYS:NZ	2.12	0.47
1:B:350:LYS:HZ2	1:B:488:GLN:HE22	1.62	0.46
1:B:237:VAL:HB	3:D:8:A:H5''	1.96	0.46
1:A:430:GLU:H	1:A:430:GLU:CD	2.13	0.46
1:B:392:ASP:OD2	1:B:483:LYS:NZ	2.49	0.46
2:C:23:G:H2'	2:C:24:A:H8	1.81	0.46
1:A:405:ARG:HD3	1:A:626:ARG:O	2.16	0.45
1:A:556:LEU:O	1:A:560:MET:HG2	2.16	0.45
1:B:532:LEU:HB3	1:B:636:TRP:CD1	2.51	0.45
1:A:522:ARG:NH2	1:A:672:LYS:HD2	2.31	0.45
1:A:558:ARG:O	1:A:563:ARG:HG2	2.16	0.45
1:B:659:HIS:CD2	1:B:692:THR:HB	2.51	0.45
2:C:23:G:H2'	2:C:24:A:C8	2.50	0.45
1:A:330:LEU:HB3	1:A:368:VAL:CG2	2.46	0.45
1:B:338:LEU:HB3	1:B:609:ILE:HG23	1.99	0.45
1:B:621:LEU:HD12	1:B:623:ARG:HH12	1.81	0.45
2:C:2:C:O2'	2:C:3:U:H5'	2.16	0.45
2:C:11:C:O2'	2:C:12:U:H5'	2.16	0.45
1:B:500:GLN:OE1	1:B:511:LEU:HA	2.17	0.45
1:A:362:ASP:OD1	1:A:364:LYS:HE2	2.16	0.45
2:C:3:U:H2'	2:C:4:C:C6	2.51	0.45
1:A:357:MET:HE2	1:A:357:MET:HB3	1.82	0.45
3:D:10:C:H5'	3:D:11:A:OP2	2.17	0.45
1:B:490:THR:HG21	1:B:515:SER:HB2	1.99	0.44
1:B:693:GLU:H	1:B:693:GLU:CD	2.26	0.44
2:C:22:U:H2'	2:C:23:G:C8	2.52	0.44
1:A:430:GLU:OE2	1:A:430:GLU:N	2.30	0.44
1:A:493:VAL:HG11	1:A:686:ALA:O	2.18	0.44
1:B:308:GLN:OE1	1:B:308:GLN:N	2.51	0.44
1:A:438:GLU:N	1:A:438:GLU:OE2	2.50	0.44
1:B:388:LEU:O	1:B:618:LYS:HE2	2.17	0.44
1:A:410:GLN:OE1	1:A:425:ILE:HG23	2.18	0.43
2:C:2:C:H2'	2:C:3:U:H6	1.83	0.43
2:C:22:U:H2'	2:C:23:G:H8	1.82	0.43
2:C:24:A:H2'	2:C:25:U:C6	2.53	0.43
1:B:390:LEU:HD21	1:B:627:LEU:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:HA3	1:A:649:ARG:HG3	1.99	0.43
1:B:620:GLU:C	1:B:621:LEU:HD23	2.44	0.43
1:A:470:ARG:HB2	1:A:471:HIS:CD2	2.53	0.43
1:A:352:LEU:HD12	1:A:372:SER:O	2.19	0.43
1:A:625:SER:C	1:A:627:LEU:H	2.27	0.42
1:B:478:GLY:O	1:B:684:LEU:HD13	2.19	0.42
1:A:658:TYR:OH	4:A:801:IHP:O42	2.32	0.42
1:B:550:LEU:HD23	1:B:550:LEU:HA	1.87	0.42
1:B:266:SER:OG	1:B:274:PHE:O	2.25	0.42
1:B:481:ARG:HA	1:B:492:PRO:HA	2.01	0.42
1:A:529:GLN:H	1:A:529:GLN:CD	2.28	0.42
1:B:235:ASN:O	1:B:239:ILE:HG12	2.20	0.42
1:B:480:LEU:HD11	1:B:679:PHE:CG	2.54	0.42
1:B:677:THR:O	1:B:681:LYS:HG2	2.18	0.42
1:A:377:CYS:SG	1:A:483:LYS:HD3	2.60	0.41
1:A:449:SER:O	1:A:455:ARG:NH1	2.52	0.41
1:A:523:TRP:HB3	1:A:528:ILE:HG22	2.02	0.41
1:B:243:LEU:O	1:B:244:ARG:HD3	2.20	0.41
1:B:400:ARG:NH2	1:B:404:LEU:HD11	2.35	0.41
1:A:350:LYS:HG3	1:A:595:ALA:HA	2.01	0.41
1:A:462:PRO:HB3	1:A:552:HIS:CE1	2.55	0.41
1:B:349:ARG:HD2	1:B:349:ARG:C	2.46	0.41
1:A:394:HIS:CE1	1:A:483:LYS:HE2	2.55	0.41
1:B:403:LEU:O	1:B:406:PHE:HB3	2.21	0.41
1:B:244:ARG:O	1:B:246:GLY:N	2.54	0.41
2:C:25:U:H2'	2:C:26:A:H8	1.83	0.41
1:A:514:MET:HG3	1:A:687:TRP:CE2	2.56	0.41
1:B:514:MET:HG3	1:B:687:TRP:CZ2	2.56	0.41
2:C:2:C:H2'	2:C:3:U:C6	2.56	0.41
1:B:676:PHE:HE2	1:B:689:GLU:OE1	2.04	0.41
1:A:460:HIS:C	1:A:550:LEU:HD22	2.46	0.40
1:B:635:ARG:O	1:B:639:VAL:HG23	2.21	0.40
4:A:801:IHP:O26	4:A:801:IHP:O21	2.40	0.40
1:B:449:SER:HB3	1:B:455:ARG:HG3	2.03	0.40
1:A:621:LEU:HD13	1:A:623:ARG:HH21	1.87	0.40
1:B:532:LEU:HD21	1:B:662:LYS:HG2	2.04	0.40
1:A:660:GLU:O	1:A:661:SER:C	2.64	0.40
1:A:693:GLU:OE1	1:B:481:ARG:NH2	2.51	0.40
1:A:400:ARG:HD2	1:A:528:ILE:O	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	383/488 (78%)	368 (96%)	15 (4%)	0	100	100
1	B	451/488 (92%)	435 (96%)	14 (3%)	2 (0%)	30	52
All	All	834/976 (86%)	803 (96%)	29 (4%)	2 (0%)	44	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	LEU
1	B	304	THR

### 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	330/415 (80%)	317 (96%)	13 (4%)	27	53
1	B	387/415 (93%)	374 (97%)	13 (3%)	32	58
All	All	717/830 (86%)	691 (96%)	26 (4%)	31	56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	A	329[A]	ARG
1	A	329[B]	ARG
1	A	364	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	409	THR
1	A	470	ARG
1	A	477	ARG
1	A	494	ARG
1	A	562	GLN
1	A	600	VAL
1	A	645	SER
1	A	647	LEU
1	A	657	VAL
1	B	247	LEU
1	B	266	SER
1	B	302	ASP
1	B	318	HIS
1	B	358	THR
1	B	399	SER
1	B	423	ARG
1	B	455	ARG
1	B	458	SER
1	B	499	ILE
1	B	601	ASN
1	B	612	ILE
1	B	625	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	HIS
1	A	479	GLN
1	A	566	ASN
1	A	669	GLN
1	B	488	GLN
1	B	500	GLN
1	B	552	HIS
1	B	555	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	31/32 (96%)	2 (6%)	0
3	D	29/32 (90%)	4 (13%)	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	60/64 (93%)	6 (10%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	25	U
2	C	27	G
3	D	10	C
3	D	11	A
3	D	21	A
3	D	22	G

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UFT	D	7	3,2	18,21,22	0.25	0	25,30,33	0.41	0
2	8AZ	C	13	5,2	16,24,25	2.67	4 (25%)	12,35,38	1.07	1 (8%)

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	UFT	D	7	3,2	-	2/7/25/26	0/2/2/2
2	8AZ	C	13	5,2	-	2/3/35/36	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	13	8AZ	C2-N1	8.53	1.48	1.34
2	C	13	8AZ	N7-N8	4.11	1.41	1.34
2	C	13	8AZ	C2-N3	3.40	1.35	1.29
2	C	13	8AZ	N8-N9	2.88	1.39	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	8AZ	O3'-C3'-C2'	-2.18	104.83	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	7	UFT	O4'-C4'-C5'-O5'
3	D	7	UFT	C3'-C4'-C5'-O5'
2	C	13	8AZ	O4'-C4'-C5'-O5'
2	C	13	8AZ	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z  > 2$
6	EDO	A	805	-	3,3,3	0.39	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	IHP	A	801	7	36,36,36	1.34	7 (19%)	60,60,60	0.90	0
4	IHP	B	801	-	36,36,36	0.84	2 (5%)	60,60,60	0.90	3 (5%)
6	EDO	A	804	-	3,3,3	0.30	0	2,2,2	0.32	0
6	EDO	A	803	-	3,3,3	0.33	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
6	EDO	A	805	-	-	1/1/1/1	-
4	IHP	A	801	7	-	1/30/54/54	0/1/1/1
4	IHP	B	801	-	-	2/30/54/54	0/1/1/1
6	EDO	A	804	-	-	0/1/1/1	-
6	EDO	A	803	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	IHP	P1-O11	3.52	1.65	1.59
4	A	801	IHP	P4-O14	3.40	1.65	1.59
4	A	801	IHP	P2-O22	2.47	1.58	1.50
4	B	801	IHP	P1-O11	2.18	1.63	1.59
4	B	801	IHP	P4-O14	2.09	1.63	1.59
4	A	801	IHP	P3-O13	2.09	1.63	1.59
4	A	801	IHP	P5-O15	2.06	1.63	1.59
4	A	801	IHP	P2-O12	2.05	1.63	1.59
4	A	801	IHP	P4-O24	2.00	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	IHP	O12-P2-O22	-2.76	99.51	109.33
4	B	801	IHP	P6-O16-C6	-2.59	116.51	123.43
4	B	801	IHP	P3-O13-C3	-2.42	116.96	123.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	IHP	C1-O11-P1-O21
6	A	805	EDO	O1-C1-C2-O2
4	B	801	IHP	C5-O15-P5-O45
6	A	803	EDO	O1-C1-C2-O2
4	A	801	IHP	C1-O11-P1-O21

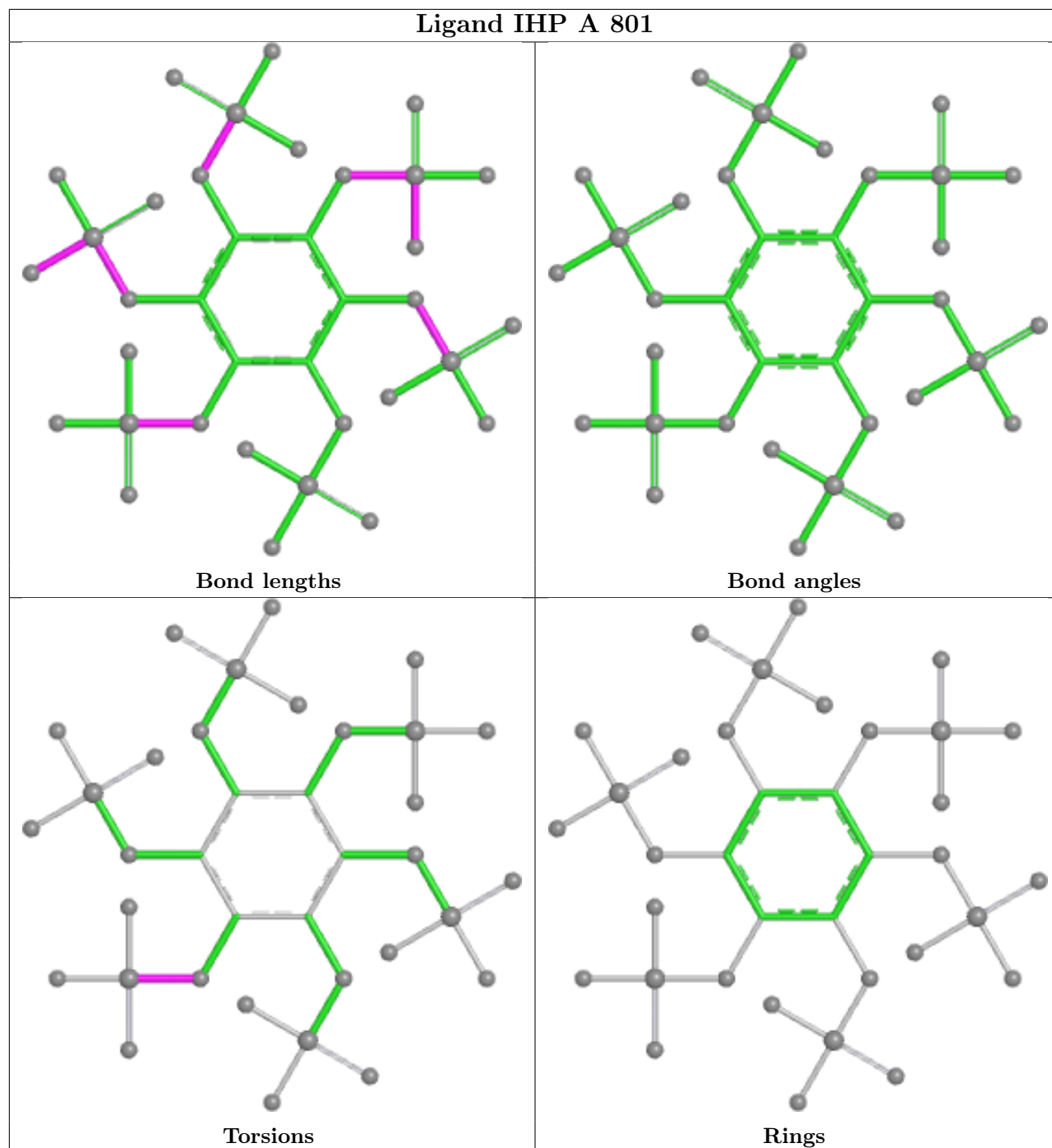
There are no ring outliers.

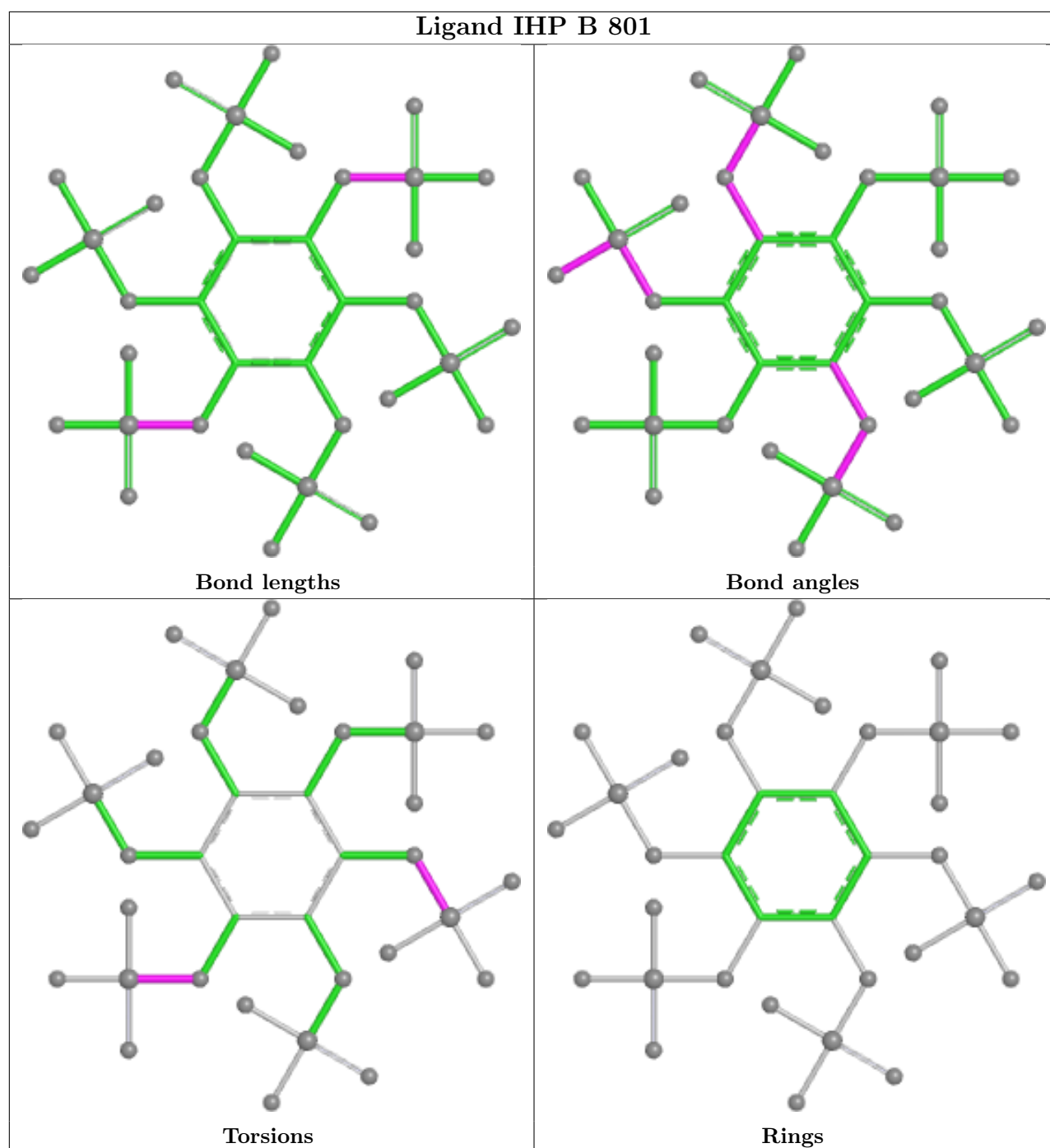
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	IHP	2	0
4	B	801	IHP	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 IHP A 801





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	384/488 (78%)	-0.44	6 (1%) 70 65	32, 47, 93, 137	1 (0%)
1	B	455/488 (93%)	0.14	21 (4%) 38 32	45, 74, 140, 261	0
2	C	31/32 (96%)	-0.80	0 100 100	43, 71, 127, 142	0
3	D	31/32 (96%)	-0.73	0 100 100	39, 72, 118, 121	0
All	All	901/1040 (86%)	-0.17	27 (2%) 52 46	32, 62, 129, 261	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	ILE	4.0
1	A	497	ALA	3.9
1	B	499	ILE	3.7
1	B	497	ALA	3.4
1	A	317	LEU	3.4
1	B	488	GLN	3.4
1	B	476	ALA	3.3
1	B	501	THR	3.3
1	B	505	VAL	3.2
1	A	498	SER	3.0
1	A	496	ASN	3.0
1	B	299	LEU	2.9
1	B	692	THR	2.9
1	B	462	PRO	2.8
1	B	319	LEU	2.8
1	B	700	THR	2.8
1	B	502	TRP	2.8
1	B	511	LEU	2.6
1	B	506	LEU	2.6
1	B	504	GLY	2.5
1	B	301	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	500	GLN	2.2
1	B	315	LEU	2.1
1	A	319	LEU	2.1
1	B	654	LYS	2.1
1	A	466	GLU	2.1
1	B	653	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
3	UFT	D	7	20/21	0.86	0.10	100,107,110,112	0
2	8AZ	C	13	22/23	0.97	0.06	34,39,45,50	0

## 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, 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(Å <sup>2</sup> )	Q<0.9
6	EDO	A	805	4/4	0.82	0.15	66,66,70,76	0
6	EDO	A	804	4/4	0.90	0.12	59,60,62,65	0
4	IHP	B	801	36/36	0.95	0.07	46,65,78,83	0
6	EDO	A	803	4/4	0.96	0.10	48,49,51,62	0
7	NA	A	806	1/1	0.97	0.08	38,38,38,38	0
4	IHP	A	801	36/36	0.98	0.05	24,36,44,48	0
5	ZN	A	802	1/1	0.99	0.01	39,39,39,39	0
5	ZN	B	802	1/1	1.00	0.02	52,52,52,52	0

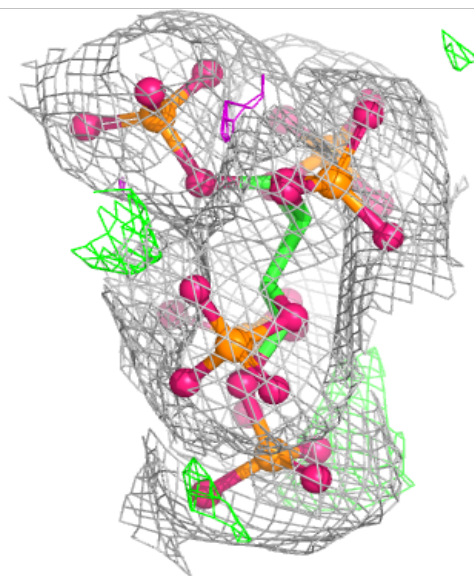
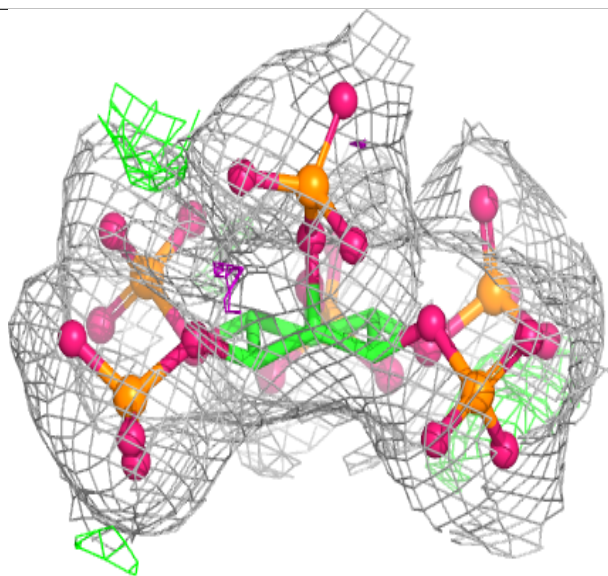
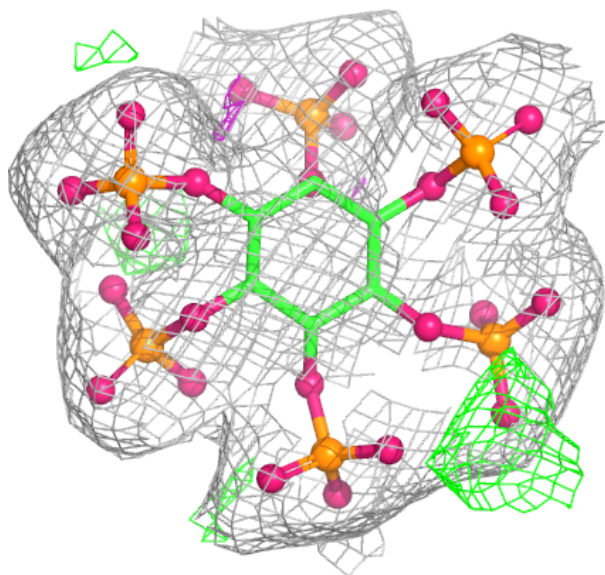
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

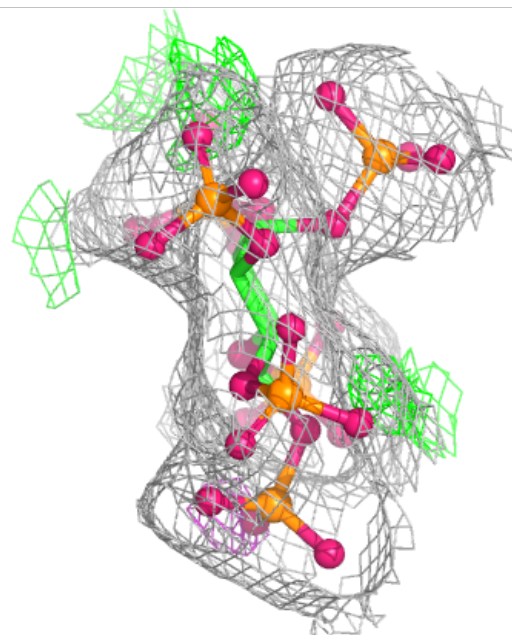
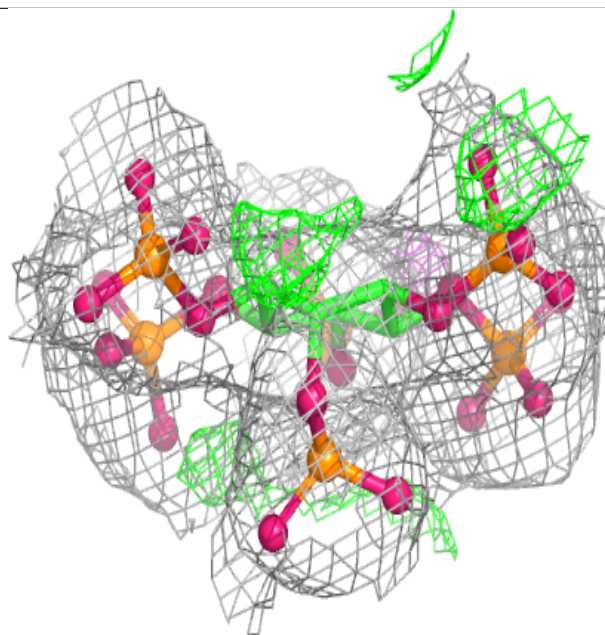
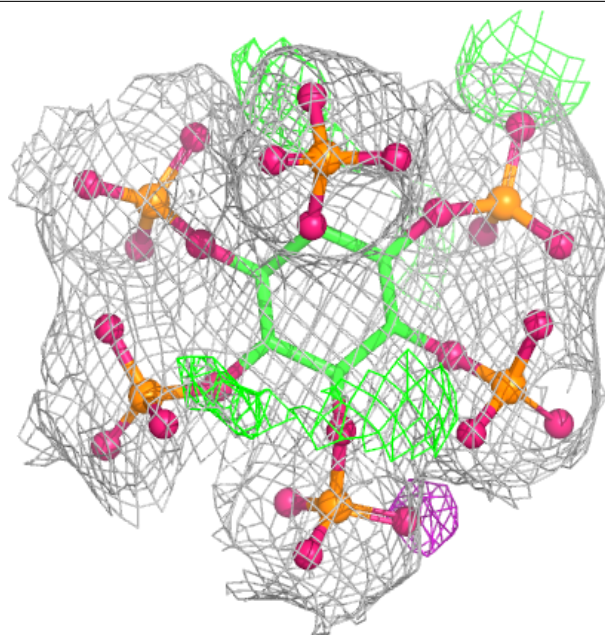
**Electron density around IHP B 801:**

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



**Electron density around IHP A 801:**

$2mF_o-DF_c$  (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.