



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 01:02 PM EDT

PDB ID : 6VFF
Title : Dimer of Human Adenosine Deaminase Acting on dsRNA (ADAR2) mutant E488Q bound to dsRNA sequence derived from human GLI1 gene
Authors : Thuy-boun, A.S.; Fisher, A.J.; Beal, P.A.
Deposited on : 2020-01-03
Resolution : 2.80 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	:	2.14.6
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)	:	2.14.6

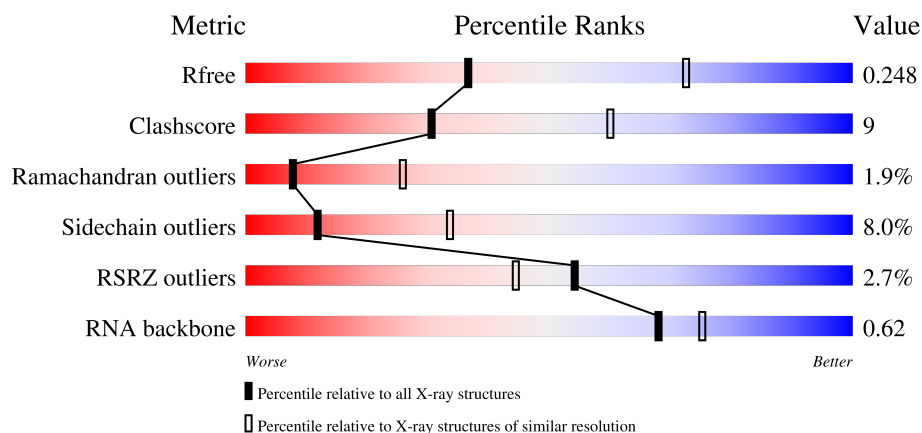
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	488	<div> <div>3%</div> <div>59% 18% 22%</div> </div>
1	B	488	<div> <div>3%</div> <div>58% 27% 11%</div> </div>
2	C	32	<div> <div>13%</div> <div>63% 34%</div> </div>
3	D	32	<div> <div>72% 25%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7870 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	382	Total	C	N	O	S	0	0	0
			2999	1891	545	552	11			
1	B	436	Total	C	N	O	S	0	0	0
			3404	2151	614	626	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

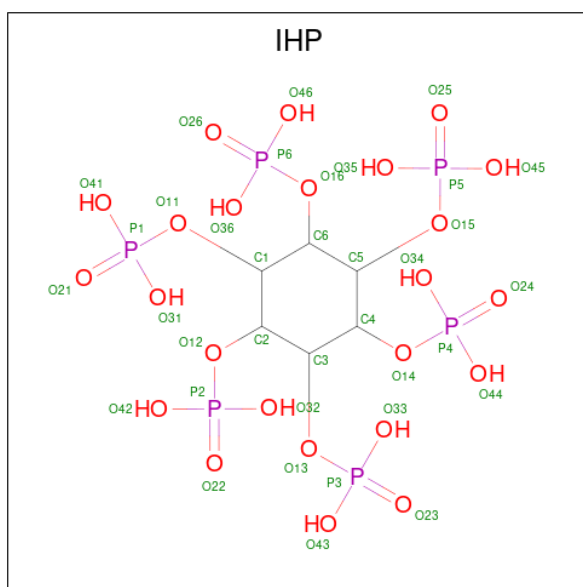
- Molecule 2 is a RNA chain called RNA (5-R(*GP*CP*UP*CP*GP*CP*GP*AP*UP*GP*CP*UP*(8AZ)P*GP*AP*GP*GP*GP*CP*UP*CP*UP*GP*AP*UP*AP*GP*CP*UP*AP*CP*G)-3).

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(5-R(*CP*GP*UP*AP*GP*CP*UP*AP*UP*CP*AP*GP*AP*GP*CP*CP*CP*CP*CP*AP*GP*CP*AP*UP*CP*GP*CP*GP*AP*GP*C)-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	32	Total	C	N	O	P	0	0	0
			675	303	122	219	31			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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 (three-letter code: ZN) (formula: Zn).

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

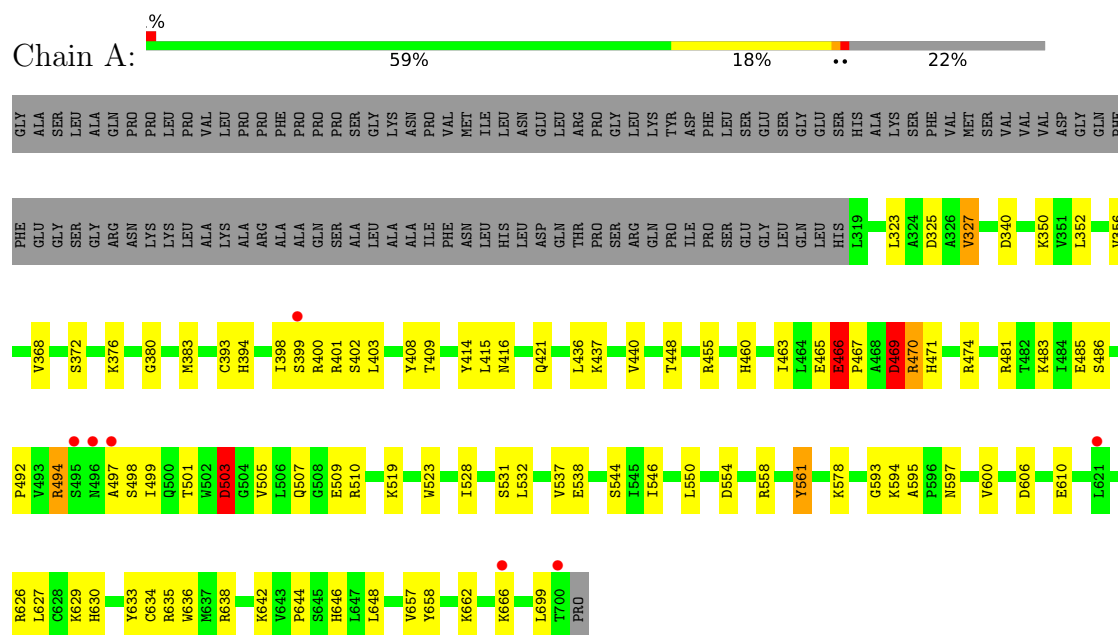
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		

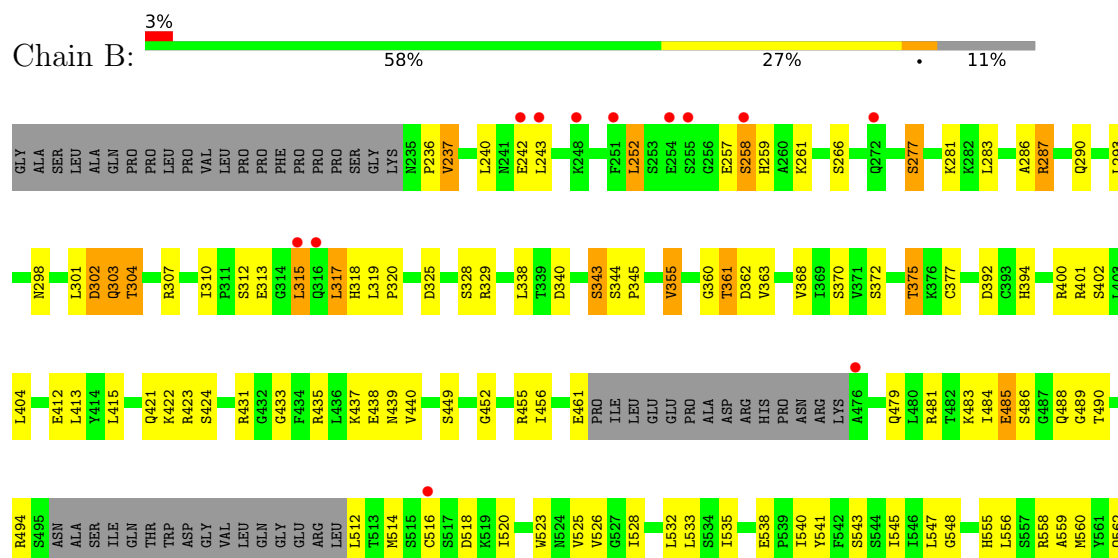
3 Residue-property plots

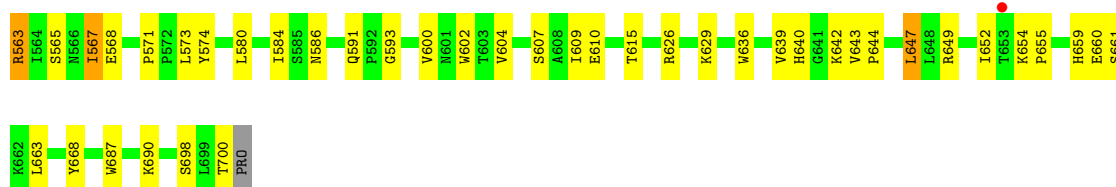
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Double-stranded RNA-specific editase 1



• Molecule 1: Double-stranded RNA-specific editase 1





- Molecule 2: RNA (5-R(*GP*CP*UP*CP*GP*CP*GP*AP*UP*GP*CP*UP*(8AZ)P*GP*AP*GP*GP*GP*CP* UP*CP*UP*GP*AP*UP*AP*GP*CP*UP*AP*CP*G)-3)



- Molecule 3: RNA(5-R(*CP*GP*UP*AP*GP*CP*UP*AP*UP*CP*AP*GP*AP*GP*CP*CP*CP*CP*CP*AP*GP*CP*AP*UP*CP*GP*CP*GP*AP*GP*C)-3)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.00Å 63.21Å 142.20Å 90.00° 118.13° 90.00°	Depositor
Resolution (Å)	37.48 – 2.80 38.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.48-2.80) 97.5 (38.28-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.197 , 0.248 0.199 , 0.248	Depositor DCC
R_{free} test set	1613 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7870	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: ZN, 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	0.46	0/3060	0.65	1/4136 (0.0%)
1	B	0.38	0/3471	0.59	0/4684
2	C	0.64	0/736	1.09	0/1144
3	D	0.61	0/753	1.14	1/1171 (0.1%)
All	All	0.47	0/8020	0.75	2/11135 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	23	C	N1-C2-O2	-6.41	115.05	118.90
1	A	558	ARG	NE-CZ-NH2	-6.22	117.19	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	GLU	Peptide
1	B	485	GLU	Peptide

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	2999	0	3032	52	0
1	B	3404	0	3443	84	0
2	C	682	0	336	7	0
3	D	675	0	350	4	0
4	A	36	0	6	2	0
4	B	36	0	6	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
All	All	7870	0	7173	138	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 (138) 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:258:SER:HA	1:B:261:LYS:HE3	1.52	0.88
1:B:518:ASP:OD1	1:B:563:ARG:NH2	2.14	0.81
1:A:629:LYS:NZ	4:A:801:IHP:O42	2.17	0.78
1:B:281:LYS:NZ	2:C:19:C:OP1	2.21	0.71
1:B:392:ASP:OD2	1:B:483:LYS:NZ	2.23	0.71
1:B:516:CYS:O	1:B:520:ILE:HG13	1.92	0.70
1:B:257:GLU:O	1:B:259:HIS:N	2.24	0.69
1:A:507:GLN:HE21	1:B:455:ARG:HH22	1.43	0.67
1:B:401:ARG:NH2	4:B:801:IHP:O32	2.30	0.64
1:B:318:HIS:HD2	1:B:363:VAL:HG13	1.64	0.63
1:B:558:ARG:HA	1:B:562:GLN:HB2	1.82	0.62
1:A:448:THR:OG1	1:A:455:ARG:NH2	2.34	0.61
1:B:456:ILE:HG13	1:B:481:ARG:NH1	2.18	0.59
1:A:327:VAL:HG21	1:A:546:ILE:HD13	1.84	0.59
1:A:537:VAL:HG12	1:A:538:GLU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:O	1:A:440:VAL:HG12	2.03	0.58
1:B:400:ARG:HD3	1:B:523:TRP:CE2	2.40	0.57
1:B:556:LEU:O	1:B:560:MET:HG2	2.05	0.57
1:B:438:GLU:HG3	1:B:439:ASN:HD22	1.70	0.57
1:B:644:PRO:HG2	1:B:647:LEU:HB2	1.86	0.57
2:C:26:A:H2'	2:C:27:G:C8	2.40	0.57
1:A:436:LEU:HD13	1:A:440:VAL:HG13	1.88	0.56
1:A:356:VAL:HG22	1:A:368:VAL:HA	1.88	0.55
1:B:375:THR:HB	1:B:488:GLN:HE22	1.73	0.54
1:B:377:CYS:SG	1:B:483:LYS:HD3	2.48	0.54
1:A:510:ARG:HD2	1:B:593:GLY:HA2	1.90	0.54
1:B:659:HIS:CE1	1:B:663:LEU:HD11	2.43	0.54
1:B:340:ASP:O	1:B:343:SER:HB3	2.08	0.54
1:A:394:HIS:CE1	1:A:483:LYS:HE2	2.43	0.53
1:B:559:ALA:O	1:B:563:ARG:NH1	2.39	0.53
1:A:485:GLU:HB3	1:A:510:ARG:HB3	1.91	0.53
1:B:573:LEU:HD13	1:B:649:ARG:NH2	2.24	0.52
1:A:380:GLY:O	1:A:383:MET:HG3	2.08	0.52
1:A:400:ARG:HD3	1:A:523:TRP:CE2	2.44	0.52
1:A:594:LYS:HD3	1:A:595:ALA:N	2.25	0.52
1:A:503:ASP:OD2	1:B:490:THR:OG1	2.17	0.52
1:B:277:SER:O	1:B:287:ARG:NH1	2.41	0.52
1:A:507:GLN:HE21	1:B:455:ARG:NH2	2.07	0.52
1:B:437:LYS:O	1:B:440:VAL:HG12	2.09	0.52
1:A:350:LYS:NZ	1:A:593:GLY:O	2.43	0.52
1:A:531:SER:OG	1:A:662:LYS:HG2	2.10	0.51
1:B:394:HIS:CE1	1:B:483:LYS:HE2	2.45	0.51
1:B:312:SER:H	1:B:315:LEU:HD22	1.75	0.51
1:A:352:LEU:HD12	1:A:372:SER:O	2.11	0.50
1:B:413:LEU:HD23	1:B:424:SER:HA	1.91	0.50
1:B:452:GLY:HA2	1:B:481:ARG:HD3	1.92	0.50
1:A:408:TYR:CE1	1:A:636:TRP:HA	2.46	0.50
1:A:501:THR:OG1	1:B:489:GLY:HA3	2.12	0.50
1:B:252:LEU:HD13	1:B:266:SER:HB3	1.93	0.50
1:B:302:ASP:O	1:B:304:THR:N	2.45	0.50
1:B:555:HIS:HA	1:B:558:ARG:NH1	2.26	0.50
1:B:629:LYS:NZ	4:B:801:IHP:O42	2.44	0.49
1:B:526:VAL:HB	1:B:668:TYR:CE2	2.47	0.49
1:B:698:SER:HB2	1:B:700:THR:HG22	1.94	0.49
1:A:507:GLN:HB2	1:B:455:ARG:NH1	2.26	0.49
1:B:548:GLY:HA2	1:B:584:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:O	1:B:580:LEU:HD12	2.12	0.49
1:B:372:SER:HA	1:B:600:VAL:O	2.12	0.49
1:B:610:GLU:OE1	1:B:626:ARG:HG2	2.12	0.49
1:B:355:VAL:CG1	1:B:370:SER:HB3	2.42	0.49
1:B:412:GLU:HG3	1:B:639:VAL:HG12	1.94	0.49
1:A:323:LEU:O	1:A:327:VAL:HG13	2.13	0.48
1:A:376:LYS:HD2	1:A:597:ASN:HA	1.96	0.48
1:A:463:ILE:HG13	1:A:465:GLU:HG2	1.96	0.48
1:A:494:ARG:NE	1:A:497:ALA:HB3	2.28	0.48
1:B:512:LEU:O	1:B:690:LYS:NZ	2.46	0.48
1:B:433:GLY:HA2	1:B:647:LEU:HD23	1.95	0.48
1:B:514:MET:HG3	1:B:687:TRP:CE2	2.48	0.47
1:B:525:VAL:O	1:B:541:TYR:OH	2.14	0.47
1:B:545:ILE:HD13	1:B:560:MET:CE	2.45	0.47
1:A:600:VAL:HA	1:A:610:GLU:O	2.13	0.47
1:B:400:ARG:HD3	1:B:523:TRP:CZ2	2.49	0.47
1:A:414:TYR:HA	1:A:421:GLN:HA	1.96	0.47
1:A:634:CYS:O	1:A:638:ARG:HG3	2.15	0.47
1:B:325:ASP:O	1:B:329:ARG:HG3	2.15	0.47
2:C:26:A:H2'	2:C:27:G:H8	1.78	0.47
1:A:629:LYS:HZ2	1:A:658:TYR:HE2	1.63	0.46
1:B:360:GLY:O	1:B:362:ASP:N	2.47	0.46
1:B:639:VAL:O	1:B:643:VAL:HG12	2.14	0.46
3:D:18:C:H2'	3:D:19:C:O4'	2.16	0.46
1:A:486:SER:HB2	2:C:15:A:O2'	2.16	0.46
1:B:449:SER:HA	1:B:547:LEU:HD13	1.97	0.46
1:B:571:PRO:HB2	1:B:574:TYR:CD2	2.52	0.45
1:B:242:GLU:HG3	1:B:243:LEU:HD12	1.98	0.45
1:B:640:HIS:CE1	1:B:655:PRO:HG3	2.51	0.45
1:A:469:ASP:O	1:A:470:ARG:HB2	2.15	0.45
1:B:344:SER:OG	1:B:345:PRO:HD2	2.15	0.45
1:A:523:TRP:HB3	1:A:528:ILE:HG22	1.99	0.45
1:B:237:VAL:HG12	1:B:286:ALA:HA	1.99	0.45
1:B:302:ASP:OD1	1:B:302:ASP:N	2.47	0.45
1:B:545:ILE:HD13	1:B:560:MET:HE2	1.98	0.45
1:B:559:ALA:HA	1:B:563:ARG:HD3	1.99	0.45
3:D:21:A:C2	3:D:22:G:C4	3.04	0.45
1:A:403:LEU:HD23	1:A:528:ILE:HD13	1.99	0.45
1:A:393:CYS:HA	1:A:398:ILE:HD11	1.99	0.44
1:A:409:THR:OG1	1:A:635:ARG:NH2	2.50	0.44
1:A:561:TYR:CD2	1:A:578:LYS:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASP:OD1	1:A:554:ASP:N	2.50	0.44
1:B:317:LEU:HD12	1:B:363:VAL:HG12	1.99	0.44
1:A:630:HIS:CE1	1:A:699:LEU:HD23	2.53	0.44
1:A:519:LYS:NZ	4:A:801:IHP:O31	2.35	0.44
1:B:375:THR:HB	1:B:488:GLN:NE2	2.32	0.44
1:A:414:TYR:HD1	1:A:415:LEU:HD23	1.83	0.43
3:D:15:C:H2'	3:D:16:C:C6	2.53	0.43
1:A:644:PRO:HB2	1:A:646:HIS:ND1	2.32	0.43
1:B:319:LEU:H	1:B:319:LEU:HD12	1.83	0.43
1:A:401:ARG:NH2	1:A:627:LEU:O	2.43	0.43
1:B:654:LYS:O	1:B:654:LYS:HD3	2.19	0.43
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.83	0.43
1:A:494:ARG:HE	1:A:497:ALA:HB3	1.83	0.43
1:B:528:ILE:C	1:B:528:ILE:HD12	2.40	0.42
1:B:240:LEU:HB2	1:B:293:LEU:HD21	2.01	0.42
1:B:318:HIS:NE2	1:B:361:THR:O	2.52	0.42
1:B:404:LEU:HD22	1:B:533:LEU:HD12	2.01	0.42
1:B:479:GLN:HG2	1:B:479:GLN:H	1.56	0.42
1:B:535:ILE:O	1:B:649:ARG:HB2	2.19	0.42
1:A:481:ARG:NH1	1:A:492:PRO:HD3	2.34	0.42
1:A:471:HIS:HB3	1:A:474:ARG:HG3	2.01	0.42
1:B:338:LEU:HD22	1:B:609:ILE:HG23	2.02	0.42
1:B:629:LYS:HZ3	4:B:801:IHP:P2	2.42	0.42
1:B:532:LEU:HB3	1:B:636:TRP:CD1	2.54	0.42
1:B:415:LEU:O	1:B:642:LYS:HE3	2.19	0.42
1:A:507:GLN:NE2	1:B:455:ARG:HH12	2.17	0.42
1:B:567:ILE:HG13	1:B:568:GLU:N	2.35	0.41
1:B:431:ARG:HD2	1:B:538:GLU:OE2	2.20	0.41
1:B:571:PRO:HB2	1:B:574:TYR:HD2	1.85	0.41
2:C:32:G:OP2	2:C:32:G:H8	2.03	0.41
1:A:466:GLU:OE2	1:A:466:GLU:HA	2.20	0.41
1:B:488:GLN:HA	1:B:488:GLN:OE1	2.20	0.41
1:A:606:ASP:HB3	1:A:626:ARG:HH12	1.85	0.41
2:C:11:C:O2'	2:C:12:U:H5'	2.21	0.41
3:D:3:U:H2'	3:D:4:A:C8	2.56	0.41
1:B:528:ILE:HG13	1:B:540:ILE:O	2.21	0.41
1:B:602:TRP:CZ2	1:B:604:VAL:HA	2.55	0.41
2:C:3:U:H2'	2:C:4:C:C6	2.56	0.41
1:B:355:VAL:HG13	1:B:370:SER:HB3	2.01	0.40
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.89	0.40
1:A:460:HIS:C	1:A:550:LEU:HD22	2.42	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	380/488 (78%)	360 (95%)	13 (3%)	7 (2%)	8	28
1	B	430/488 (88%)	394 (92%)	28 (6%)	8 (2%)	8	26
All	All	810/976 (83%)	754 (93%)	41 (5%)	15 (2%)	8	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	PRO
1	A	469	ASP
1	B	258	SER
1	B	361	THR
1	B	486	SER
1	A	340	ASP
1	A	503	ASP
1	B	236	PRO
1	B	303	GLN
1	A	561	TYR
1	A	470	ARG
1	A	499	ILE
1	B	252	LEU
1	B	320	PRO
1	B	304	THR

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	327/415 (79%)	310 (95%)	17 (5%)	23	55
1	B	371/415 (89%)	332 (90%)	39 (10%)	7	20
All	All	698/830 (84%)	642 (92%)	56 (8%)	12	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ASP
1	A	327	VAL
1	A	399	SER
1	A	402	SER
1	A	416	ASN
1	A	466	GLU
1	A	469	ASP
1	A	494	ARG
1	A	498	SER
1	A	503	ASP
1	A	505	VAL
1	A	509	GLU
1	A	544	SER
1	A	633	TYR
1	A	642	LYS
1	A	657	VAL
1	A	666	LYS
1	B	237	VAL
1	B	277	SER
1	B	283	LEU
1	B	287	ARG
1	B	290	GLN
1	B	298	ASN
1	B	301	LEU
1	B	302	ASP
1	B	303	GLN
1	B	307	ARG
1	B	313	GLU
1	B	315	LEU
1	B	317	LEU
1	B	328	SER
1	B	343	SER
1	B	355	VAL
1	B	368	VAL

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Mol	Chain	Res	Type
1	B	375	THR
1	B	402	SER
1	B	421	GLN
1	B	422	LYS
1	B	423	ARG
1	B	435	ARG
1	B	461	GLU
1	B	484	ILE
1	B	485	GLU
1	B	494	ARG
1	B	543	SER
1	B	563	ARG
1	B	565	SER
1	B	567	ILE
1	B	586	ASN
1	B	591	GLN
1	B	607	SER
1	B	615	THR
1	B	647	LEU
1	B	652	ILE
1	B	660	GLU
1	B	661	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	A	659	HIS
1	B	318	HIS
1	B	659	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	30/32 (93%)	4 (13%)	0
3	D	31/32 (96%)	1 (3%)	0
All	All	61/64 (95%)	5 (8%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	8	A
2	C	24	A
2	C	29	U
2	C	32	G
3	D	22	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	8AZ	C	13	2,5	17,24,25	0.72	0	14,35,38	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8AZ	C	13	2,5	-	2/3/35/36	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	IHP	A	801	-	36,36,36	1.15	2 (5%)	54,60,60	2.26	19 (35%)
4	IHP	B	801	-	36,36,36	1.18	3 (8%)	54,60,60	2.20	14 (25%)

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
4	IHP	A	801	-	-	5/30/54/54	0/1/1/1
4	IHP	B	801	-	-	5/30/54/54	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	IHP	P1-O11	3.70	1.66	1.59
4	A	801	IHP	P1-O11	2.86	1.64	1.59
4	B	801	IHP	P3-O13	2.82	1.64	1.59
4	A	801	IHP	P3-O13	2.74	1.64	1.59
4	B	801	IHP	C6-C5	2.17	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	IHP	C3-C2-C1	6.27	124.14	110.41
4	A	801	IHP	C3-C2-C1	5.58	122.64	110.41
4	B	801	IHP	C6-C5-C4	5.29	122.00	110.41
4	B	801	IHP	O11-C1-C2	4.97	120.40	108.69
4	B	801	IHP	O13-C3-C4	4.93	120.31	108.69
4	A	801	IHP	O11-C1-C2	4.77	119.93	108.69
4	A	801	IHP	C5-C4-C3	4.67	120.63	110.41
4	B	801	IHP	C5-C6-C1	4.56	120.40	110.41
4	A	801	IHP	C5-C6-C1	4.43	120.10	110.41
4	A	801	IHP	O13-C3-C4	4.28	118.78	108.69
4	A	801	IHP	C6-C5-C4	4.26	119.74	110.41
4	A	801	IHP	O13-C3-C2	3.98	118.06	108.69
4	A	801	IHP	O15-P5-O25	-3.95	94.16	109.39
4	B	801	IHP	O13-C3-C2	3.93	117.95	108.69
4	B	801	IHP	C5-C4-C3	3.47	118.00	110.41
4	B	801	IHP	O46-P6-O36	3.29	120.20	107.64
4	B	801	IHP	O12-C2-C1	3.07	115.93	108.69
4	A	801	IHP	O14-C4-C5	3.07	115.92	108.69
4	A	801	IHP	O44-P4-O34	3.04	119.26	107.64
4	B	801	IHP	O14-C4-C3	2.97	115.68	108.69
4	B	801	IHP	O32-P2-O22	2.94	122.18	110.68
4	A	801	IHP	O12-P2-O22	-2.84	98.42	109.39
4	A	801	IHP	O11-C1-C6	2.81	115.31	108.69
4	A	801	IHP	O15-C5-C4	2.79	115.26	108.69
4	B	801	IHP	O45-P5-O15	-2.55	94.57	105.99
4	B	801	IHP	O16-C6-C5	2.50	114.59	108.69
4	A	801	IHP	O11-P1-O21	-2.46	99.90	109.39
4	A	801	IHP	O32-P2-O22	2.37	119.94	110.68
4	A	801	IHP	O35-P5-O15	2.33	116.43	105.99
4	A	801	IHP	O12-C2-C1	2.22	113.93	108.69
4	A	801	IHP	O16-C6-C5	2.14	113.74	108.69
4	A	801	IHP	O43-P3-O33	2.05	115.47	107.64
4	B	801	IHP	O11-C1-C6	2.05	113.52	108.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	IHP	C2-O12-P2-O22
4	A	801	IHP	C3-O13-P3-O23
4	A	801	IHP	C5-O15-P5-O25

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Mol	Chain	Res	Type	Atoms
4	A	801	IHP	C2-O12-P2-O32
4	B	801	IHP	C3-O13-P3-O43
4	B	801	IHP	C6-O16-P6-O46
4	A	801	IHP	C1-O11-P1-O21
4	B	801	IHP	C1-O11-P1-O21
4	B	801	IHP	C4-O14-P4-O34
4	B	801	IHP	C5-O15-P5-O45

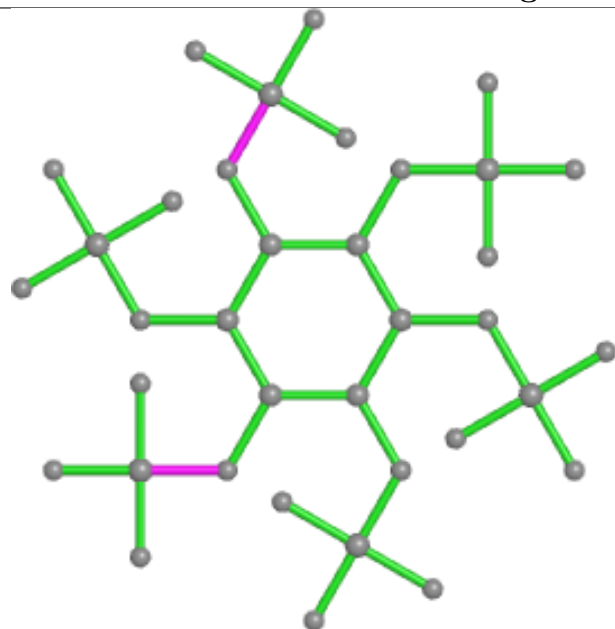
There are no ring outliers.

2 monomers are involved in 5 short contacts:

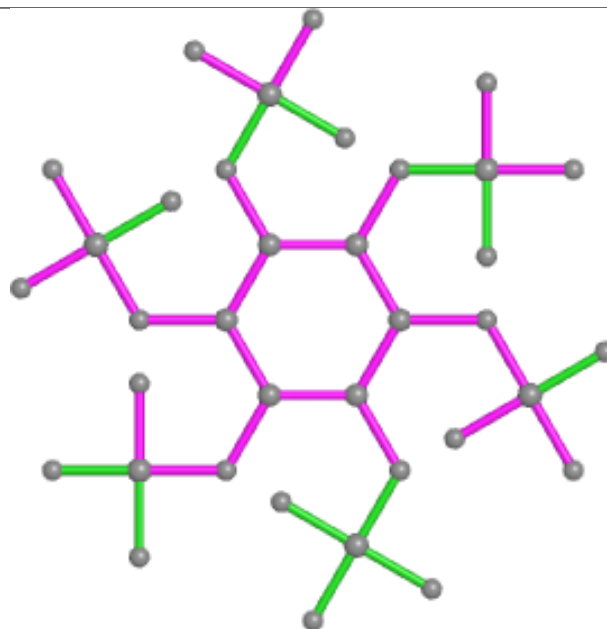
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	IHP	2	0
4	B	801	IHP	3	0

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.

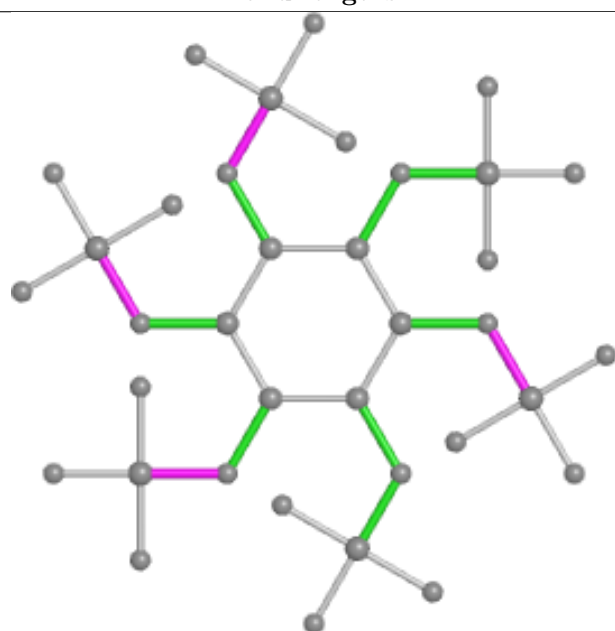
Ligand IHP A 801



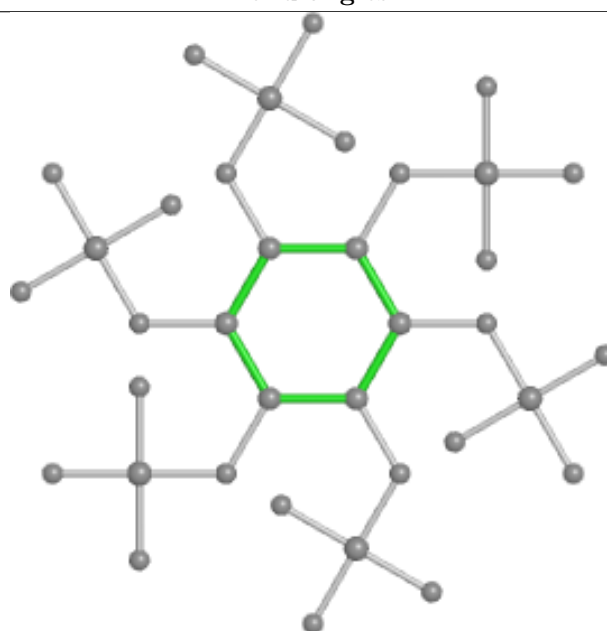
Bond lengths



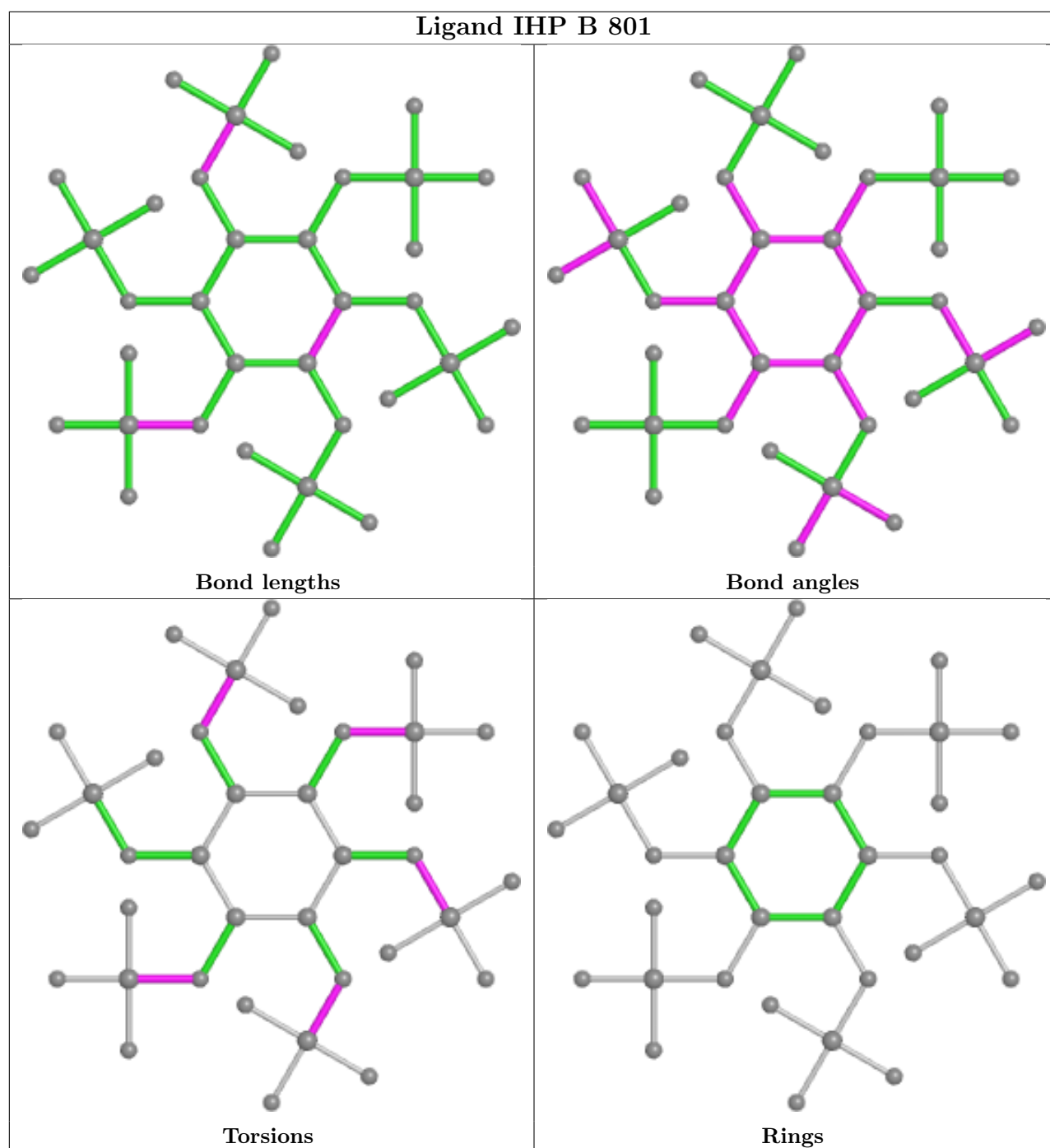
Bond angles



Torsions



Rings



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	382/488 (78%)	-0.09	7 (1%) 68 61	45, 63, 98, 118	0
1	B	436/488 (89%)	0.05	13 (2%) 50 40	58, 82, 126, 137	0
2	C	31/32 (96%)	0.50	4 (12%) 3 2	58, 78, 148, 151	0
3	D	32/32 (100%)	0.30	0 100 100	53, 88, 144, 150	0
All	All	881/1040 (84%)	0.02	24 (2%) 54 44	45, 74, 125, 151	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	ALA	6.6
1	A	496	ASN	5.0
1	A	700	THR	4.8
1	B	258	SER	4.3
1	B	255	SER	4.1
1	B	315	LEU	3.6
1	B	248	LYS	3.4
2	C	27	G	3.1
1	B	254	GLU	2.9
1	A	495	SER	2.7
1	B	476	ALA	2.7
1	B	251	PHE	2.7
1	B	316	GLN	2.7
2	C	26	A	2.6
1	B	242	GLU	2.5
1	B	653	THR	2.4
1	A	666	LYS	2.4
1	A	399	SER	2.3
1	B	243	LEU	2.3
1	B	272	GLN	2.2
2	C	30	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	621	LEU	2.1
2	C	28	C	2.0
1	B	516	CYS	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, 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(Å ²)	Q<0.9
2	8AZ	C	13	22/23	0.97	0.13	49,60,70,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

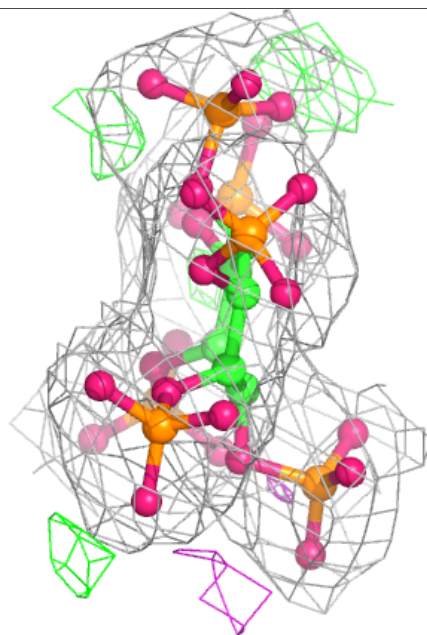
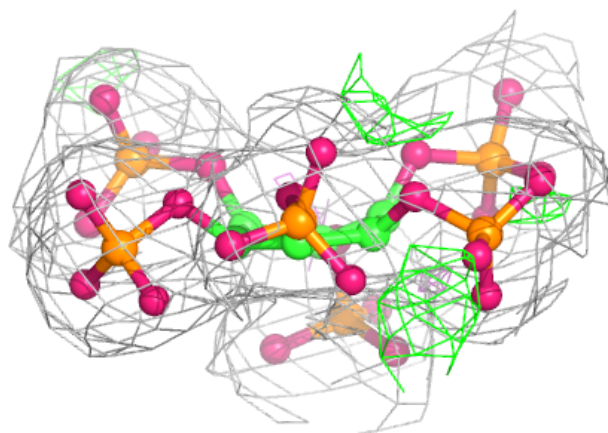
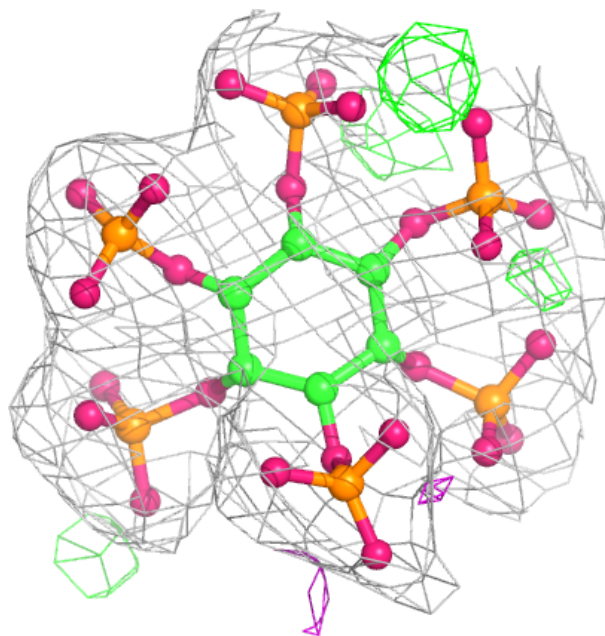
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IHP	B	801	36/36	0.95	0.24	56,71,85,86	0
4	IHP	A	801	36/36	0.97	0.25	40,54,64,65	0
5	ZN	B	802	1/1	0.99	0.20	57,57,57,57	0
5	ZN	A	802	1/1	1.00	0.21	56,56,56,56	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.

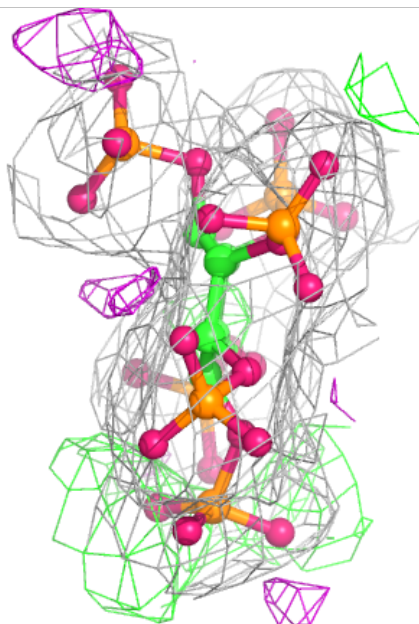
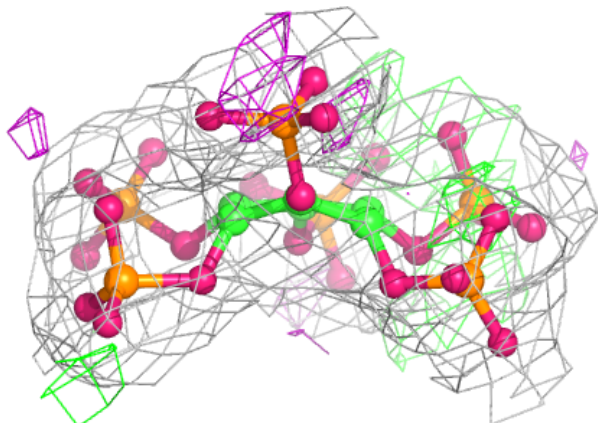
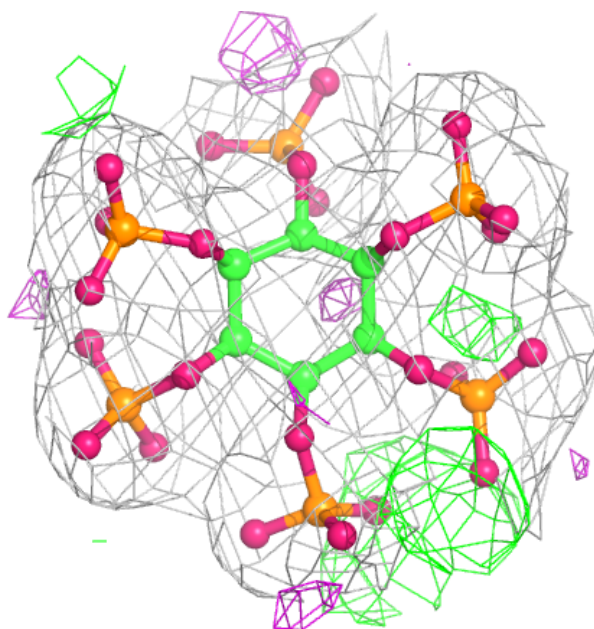
Electron density around IHP B 801:

$2mF_o-DF_c$ (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.