



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 9D5K / pdb_00009d5k
Title : Human Adenosine Deaminase Acting on dsRNA (ADAR2-RD) bound to dsRNA containing an expanded cytidine analog at the -1 position of the guide strand
Authors : Fisher, A.J.; Cheng, J.; Manjunath, A.; Campbell, K.
Deposited on : 2024-08-13
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

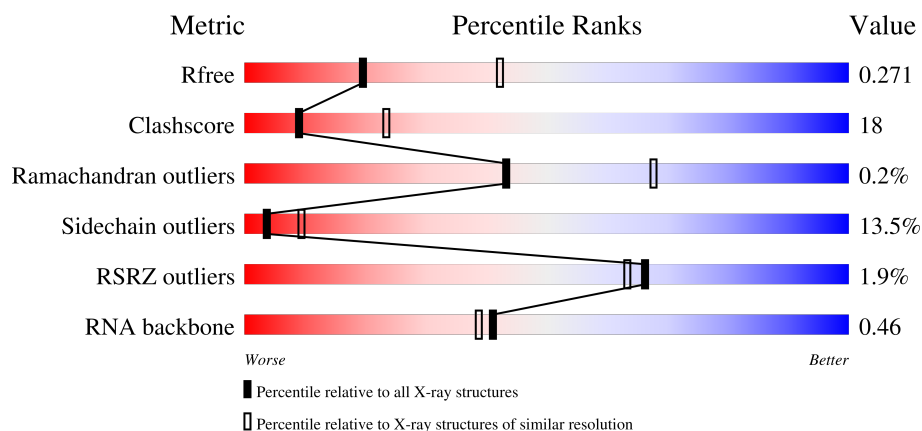
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	487	46% 29% 21%
1	B	487	49% 37% 6% 9%
2	C	32	25% 66% 6%

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Mol	Chain	Length	Quality of chain
3	D	32	 A horizontal bar chart showing the quality of chain D. The bar is divided into two segments: a green segment on the left representing 53% and a yellow segment on the right representing 47%. The percentages are written below their respective segments.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7953 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 Isoform 4 of 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	442	Total	C	N	O	S	0	0	0
			3455	2183	624	635	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	GLN	GLU	engineered mutation	UNP P78563
B	488	GLN	GLU	engineered mutation	UNP P78563

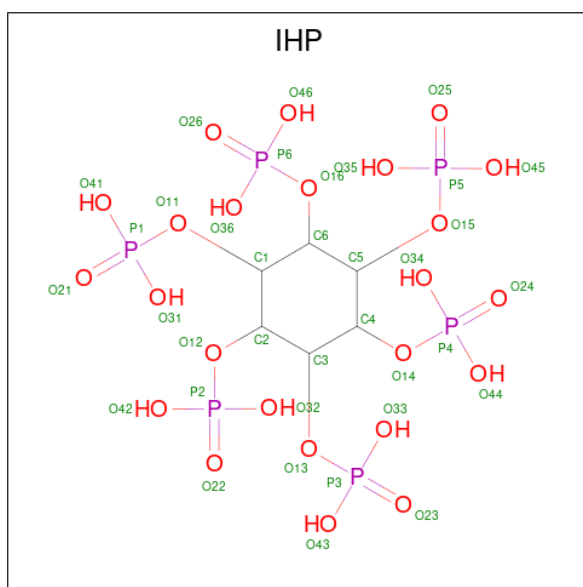
- Molecule 2 is a RNA chain called RNA Top Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	32	Total	C	N	O	P	0	0	0
			685	305	126	223	31			

- Molecule 3 is DNA/RNA hybrid called RNA Bottom Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	32	Total	C	N	O	P	0	0	0
			677	307	120	219	31			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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) (labeled as "Ligand of Interest" by depositor).

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

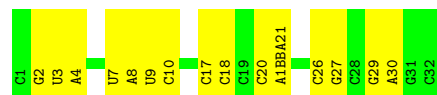
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total 4	O 4	0	0
7	C	6	Total 6	O 6	0	0
7	D	2	Total 2	O 2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.78Å 63.11Å 141.06Å 90.00° 118.54° 90.00°	Depositor
Resolution (Å)	49.46 – 2.70 49.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.46-2.70) 98.2 (49.46-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.221 , 0.268 0.229 , 0.271	Depositor DCC
R_{free} test set	1829 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: 8AZ, ZN, MG, IHP, A1BBA

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	0.78	0/3092	0.98	3/4178 (0.1%)
1	B	0.47	0/3523	0.74	0/4755
2	C	0.55	0/740	0.79	0/1151
3	D	0.60	0/727	0.79	0/1128
All	All	0.62	0/8082	0.85	3/11212 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689	GLU	CA-CB-CG	-5.99	102.13	114.10
1	A	614	ALA	CA-C-N	-5.38	111.72	121.14
1	A	614	ALA	C-N-CA	-5.38	111.72	121.14

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	3027	0	3064	108	0
1	B	3455	0	3497	152	0
2	C	685	0	337	27	0
3	D	677	0	339	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	6	2	0
4	B	36	0	6	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	22	0	0	2	0
7	B	4	0	0	1	0
7	C	6	0	0	0	0
7	D	2	0	0	0	0
All	All	7953	0	7249	279	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 18.

All (279) 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:476:ALA:O	1:B:477:ARG:NH1	2.04	0.90
1:A:424:SER:O	1:A:437:LYS:NZ	2.08	0.87
1:B:327:VAL:HG21	1:B:546:ILE:HG13	1.57	0.86
1:B:235:ASN:ND2	3:D:8:A:O2'	2.13	0.82
1:B:412:GLU:O	1:B:416:ASN:HB2	1.79	0.81
1:B:516:CYS:O	1:B:520:ILE:HG12	1.81	0.81
1:B:259:HIS:O	1:B:591:GLN:NE2	2.16	0.77
1:B:277:SER:O	1:B:287:ARG:NH2	2.15	0.77
1:B:380:GLY:H	1:B:510:ARG:HH22	1.35	0.74
1:B:525:VAL:O	1:B:541:TYR:OH	2.06	0.74
1:A:419:ASP:HA	1:A:422:LYS:HE3	1.68	0.74
1:A:449:SER:HB3	1:A:455:ARG:HG3	1.70	0.73
1:B:594:LYS:HE3	1:B:595:ALA:H	1.52	0.73
1:A:693:GLU:OE1	1:A:693:GLU:N	2.16	0.72
1:B:404:LEU:HD21	1:B:529:GLN:HA	1.71	0.72
1:B:379:ASN:ND2	1:B:381:GLU:OE1	2.24	0.70
1:B:431:ARG:HH11	1:B:431:ARG:HB2	1.56	0.69
1:A:531:SER:O	1:A:534:SER:OG	2.08	0.69
1:A:509:GLU:HG3	1:B:488:GLN:HE21	1.58	0.68
1:A:510:ARG:HD2	1:B:593:GLY:HA2	1.76	0.68
1:B:319:LEU:HB3	1:B:322:VAL:HG13	1.75	0.68
1:B:339:THR:HG23	1:B:342:PHE:H	1.58	0.68
1:A:531:SER:HB3	1:A:668:TYR:CD2	2.28	0.68
1:B:258:SER:OG	1:B:259:HIS:N	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASN:N	1:B:586:ASN:HD22	1.92	0.66
1:B:380:GLY:H	1:B:510:ARG:NH2	1.93	0.66
1:B:552:HIS:CE1	1:B:554:ASP:HB2	2.31	0.66
1:B:656:ASN:O	1:B:698:SER:OG	2.06	0.66
1:A:429:SER:HB3	1:A:432:GLY:O	1.96	0.65
1:A:319:LEU:O	1:A:322:VAL:HG13	1.96	0.65
1:B:662:LYS:NZ	4:B:801:IHP:O24	2.21	0.65
1:A:319:LEU:HD23	1:A:321:GLN:H	1.62	0.64
3:D:3:U:H2'	3:D:4:A:C8	2.33	0.64
1:B:693:GLU:O	1:B:696:GLN:HG2	1.98	0.63
1:B:531:SER:O	1:B:534:SER:OG	2.17	0.63
1:B:319:LEU:O	1:B:322:VAL:HG22	1.98	0.63
1:B:308:GLN:H	1:B:308:GLN:CD	2.06	0.63
1:B:665:ALA:O	1:B:669:GLN:HG2	1.99	0.62
1:B:435:ARG:NH2	1:B:438:GLU:OE2	2.33	0.61
1:B:657:VAL:HG12	1:B:660:GLU:H	1.64	0.61
1:B:272:GLN:HG3	1:B:296:ILE:HD11	1.82	0.61
1:A:447:SER:HA	1:A:548:GLY:HA3	1.83	0.61
1:B:311:PRO:HG3	1:B:580:LEU:HB2	1.83	0.60
1:B:629:LYS:NZ	4:B:801:IHP:O42	2.34	0.60
1:A:462:PRO:HB3	1:A:552:HIS:CE1	2.37	0.60
1:A:446:ILE:HD12	1:A:450:PRO:HG3	1.84	0.59
1:A:325:ASP:OD2	1:A:585:SER:OG	2.20	0.59
1:A:408:TYR:CE1	1:A:533:LEU:HD21	2.37	0.59
2:C:24:A:H2'	2:C:25:U:C6	2.37	0.59
1:B:556:LEU:HD23	1:B:581:LEU:HB3	1.85	0.58
1:B:693:GLU:CD	1:B:693:GLU:H	2.12	0.58
1:A:494:ARG:HB2	1:A:494:ARG:NH1	2.18	0.58
1:B:317:LEU:HD22	1:B:317:LEU:H	1.68	0.58
1:A:475:LYS:NZ	2:C:4:C:OP1	2.26	0.58
1:B:281:LYS:NZ	2:C:19:C:OP1	2.24	0.58
1:B:556:LEU:HG	1:B:581:LEU:HD13	1.86	0.57
1:B:372:SER:HA	1:B:600:VAL:O	2.04	0.57
1:B:555:HIS:HD2	1:B:558:ARG:NH2	2.02	0.57
1:B:690:LYS:HG3	1:B:694:GLN:HE22	1.70	0.57
1:A:560:MET:HE2	1:A:560:MET:HA	1.87	0.57
1:A:325:ASP:O	1:A:329[B]:ARG:HG3	2.05	0.56
2:C:24:A:H2'	2:C:25:U:H6	1.70	0.56
1:B:375:THR:HG23	1:B:595:ALA:HB1	1.87	0.56
1:B:511:LEU:HD22	1:B:691:PRO:HD3	1.87	0.56
1:B:619:ASP:OD1	1:B:622:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:PRO:HG2	7:A:909:HOH:O	2.05	0.56
2:C:22:U:H2'	2:C:23:G:C8	2.39	0.56
1:B:511:LEU:CD2	1:B:691:PRO:HD3	2.36	0.56
1:A:494:ARG:HB2	1:A:494:ARG:HH11	1.70	0.56
1:A:669:GLN:OE1	1:A:672:LYS:HE3	2.06	0.56
1:B:692:THR:OG1	1:B:693:GLU:OE2	2.23	0.56
1:B:698:SER:HB2	1:B:700:THR:HG22	1.88	0.56
1:B:425:ILE:HD12	1:B:436:LEU:HD11	1.87	0.55
1:B:479:GLN:OE1	1:B:479:GLN:N	2.30	0.55
1:B:258:SER:HB3	3:D:18:C:O2'	2.06	0.55
1:B:657:VAL:HG12	1:B:660:GLU:HG2	1.88	0.55
2:C:4:C:H2'	2:C:5:G:C8	2.42	0.55
1:A:403:LEU:HD21	1:A:528:ILE:HD13	1.88	0.54
1:B:308:GLN:HB2	1:B:581:LEU:O	2.07	0.54
1:A:430:GLU:CD	1:A:430:GLU:H	2.16	0.54
1:A:483:LYS:NZ	1:A:516:CYS:SG	2.81	0.54
1:B:310:ILE:HG21	1:B:315:LEU:HD12	1.90	0.54
1:A:531:SER:HB3	1:A:668:TYR:CE2	2.43	0.54
1:B:335:PHE:O	1:B:339:THR:HG22	2.08	0.54
1:B:308:GLN:HA	1:B:551:TYR:OH	2.08	0.53
1:B:640:HIS:O	1:B:643:VAL:HG12	2.08	0.53
1:B:690:LYS:HG3	1:B:691:PRO:HD2	1.89	0.53
1:B:481:ARG:HA	1:B:492:PRO:HA	1.89	0.53
2:C:4:C:H2'	2:C:5:G:H8	1.73	0.53
2:C:26:A:H2'	2:C:27:G:C8	2.44	0.53
1:A:352:LEU:HD12	1:A:372:SER:O	2.09	0.53
1:B:418:LYS:HD3	1:B:421:GLN:OE1	2.08	0.53
1:B:400:ARG:HD3	1:B:523:TRP:CE2	2.42	0.53
1:A:659:HIS:HB2	1:A:695:ASP:HB3	1.90	0.53
1:A:481:ARG:HA	1:A:491:ILE:O	2.09	0.52
1:B:340:ASP:OD1	1:B:343:SER:OG	2.17	0.52
1:A:494:ARG:HH11	1:A:494:ARG:H	1.56	0.52
1:A:529:GLN:H	1:A:529:GLN:CD	2.16	0.52
1:A:569:ASP:OD1	1:A:569:ASP:N	2.43	0.52
1:A:572:PRO:O	1:A:573:LEU:HB2	2.09	0.52
1:B:257:GLU:HA	1:B:261:LYS:HD2	1.91	0.52
1:B:392:ASP:OD2	1:B:397:ILE:HG13	2.10	0.52
1:B:269:VAL:HG11	1:B:292:ALA:HB1	1.90	0.52
1:B:438:GLU:CD	1:B:438:GLU:H	2.17	0.52
1:B:541:TYR:HB3	1:B:577:ASN:ND2	2.24	0.52
2:C:30:A:H2'	2:C:31:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:U:H2'	2:C:4:C:C6	2.45	0.52
1:A:373:THR:O	1:A:599:SER:OG	2.21	0.52
1:B:408:TYR:CE2	1:B:533:LEU:HD21	2.46	0.51
1:B:449:SER:HB3	1:B:455:ARG:HG3	1.92	0.51
2:C:31:C:H2'	2:C:32:G:C8	2.45	0.51
3:D:17:C:H2'	3:D:18:C:O4'	2.10	0.51
1:A:340:ASP:O	1:A:343:SER:OG	2.29	0.51
1:B:255:SER:O	1:B:261:LYS:HG3	2.10	0.51
1:B:405:ARG:CZ	1:B:626:ARG:HD2	2.40	0.51
1:B:345:PRO:O	1:B:348:ARG:HG2	2.10	0.51
1:A:497:ALA:HB2	1:A:686:ALA:HB3	1.93	0.51
1:B:405:ARG:NH2	1:B:606:ASP:OD1	2.44	0.51
2:C:22:U:H2'	2:C:23:G:H8	1.76	0.51
1:A:376:LYS:NZ	2:C:15:A:OP2	2.41	0.51
1:A:484:ILE:HD11	1:A:510:ARG:CZ	2.41	0.51
1:A:462:PRO:HB3	1:A:552:HIS:HE1	1.76	0.50
1:B:338:LEU:HD11	1:B:602:TRP:CD1	2.46	0.50
2:C:3:U:H2'	2:C:4:C:H6	1.77	0.50
1:B:400:ARG:NH2	4:B:801:IHP:O41	2.40	0.50
1:B:532:LEU:HB3	1:B:636:TRP:CD1	2.46	0.50
1:A:372:SER:HA	1:A:600:VAL:O	2.10	0.50
1:A:509:GLU:HG3	1:B:488:GLN:NE2	2.26	0.50
1:B:252:LEU:HD13	1:B:265:MET:HA	1.94	0.50
2:C:2:C:H2'	2:C:3:U:H6	1.76	0.50
2:C:2:C:O2'	2:C:3:U:H5'	2.11	0.50
1:A:320:PRO:HB3	1:A:580:LEU:HD21	1.93	0.50
1:A:325:ASP:O	1:A:329[A]:ARG:HG3	2.12	0.50
1:B:435:ARG:NH1	1:B:436:LEU:O	2.45	0.50
1:B:511:LEU:HG	1:B:512:LEU:N	2.27	0.50
1:A:414:TYR:HD1	1:A:415:LEU:HD23	1.77	0.49
1:B:316:GLN:HG3	1:B:317:LEU:HD22	1.94	0.49
1:B:281:LYS:O	1:B:285:LYS:HG2	2.12	0.49
1:B:338:LEU:HD21	1:B:602:TRP:CD2	2.47	0.49
1:B:378:ILE:HB	1:B:390:LEU:O	2.12	0.49
1:A:644:PRO:HG2	1:A:647:LEU:HD12	1.94	0.49
1:B:377:CYS:SG	1:B:483:LYS:HD3	2.52	0.49
1:A:345:PRO:O	1:A:348:ARG:HB3	2.12	0.49
1:B:690:LYS:HD3	4:B:801:IHP:O45	2.12	0.49
1:A:348:ARG:HG2	1:A:596:PRO:HG3	1.94	0.48
1:A:657:VAL:HG22	1:A:660:GLU:CG	2.43	0.48
1:A:625:SER:C	1:A:627:LEU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLN:CD	1:B:529:GLN:H	2.21	0.48
1:B:637:MET:HE2	1:B:699:LEU:HD12	1.95	0.48
1:A:334:LYS:O	1:A:338:LEU:HG	2.13	0.48
1:B:482:THR:HB	1:B:512:LEU:HB3	1.94	0.48
1:A:441:GLN:HB2	1:A:543:SER:OG	2.13	0.48
1:B:528:ILE:HD11	1:B:540:ILE:HB	1.95	0.48
1:A:662:LYS:NZ	4:A:801:IHP:O42	2.46	0.48
1:B:569:ASP:O	1:B:571:PRO:HD3	2.14	0.48
1:A:532:LEU:HB3	1:A:636:TRP:CD1	2.49	0.48
1:A:350:LYS:HD3	1:A:591:GLN:HB2	1.95	0.47
1:A:488:GLN:HB2	3:D:20:C:O2	2.14	0.47
1:A:514:MET:HG2	1:A:687:TRP:CE2	2.49	0.47
2:C:26:A:H2'	2:C:27:G:H8	1.79	0.47
1:A:418:LYS:HA	1:A:421:GLN:HG2	1.96	0.47
1:B:287:ARG:HG2	1:B:586:ASN:CG	2.40	0.47
1:A:400:ARG:HD3	1:A:523:TRP:CE2	2.49	0.47
1:A:528:ILE:HD11	1:A:540:ILE:CG2	2.43	0.47
1:B:621:LEU:HD23	1:B:623:ARG:NE	2.29	0.47
1:B:268:VAL:HG13	1:B:272:GLN:H	1.80	0.47
1:B:477:ARG:HD2	1:B:479:GLN:HE22	1.79	0.47
2:C:2:C:H2'	2:C:3:U:C6	2.49	0.47
1:B:436:LEU:HD21	1:B:442:PHE:HE1	1.79	0.46
1:B:627:LEU:HD12	1:B:627:LEU:HA	1.77	0.46
2:C:17:G:H2'	2:C:18:G:C8	2.50	0.46
1:B:561:TYR:CD1	1:B:578:LYS:HG2	2.51	0.46
1:A:394:HIS:CE1	1:A:483:LYS:HE3	2.50	0.46
1:B:405:ARG:NH2	1:B:626:ARG:HD2	2.29	0.46
1:A:602:TRP:CD1	1:A:606:ASP:HB2	2.50	0.46
1:B:327:VAL:CG2	1:B:546:ILE:HG13	2.38	0.46
1:A:378:ILE:HG12	1:A:379:ASN:O	2.16	0.46
1:A:405:ARG:HD2	1:A:626:ARG:O	2.15	0.46
1:A:487:GLY:O	2:C:14:G:H1'	2.15	0.46
1:A:417:ASN:C	1:A:418:LYS:HE2	2.41	0.46
1:A:544:SER:HB3	1:A:580:LEU:HB3	1.97	0.46
1:B:301:LEU:HA	1:B:307:ARG:NH2	2.30	0.46
1:B:480:LEU:HB3	1:B:514:MET:HE1	1.97	0.46
1:B:330:LEU:HB3	1:B:368:VAL:CG2	2.46	0.45
1:B:561:TYR:CG	1:B:578:LYS:HG2	2.51	0.45
1:A:327:VAL:HG21	1:A:546:ILE:HG13	1.97	0.45
1:A:396:GLU:OE2	2:C:13:8AZ:O6	2.34	0.45
1:A:486:SER:HB3	2:C:15:A:C1'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HB3	1:B:305:PRO:HD2	1.98	0.45
2:C:8:A:H2'	2:C:9:U:C6	2.51	0.45
1:A:376:LYS:HD2	1:A:597:ASN:HA	1.99	0.45
1:B:491:ILE:HD12	1:B:491:ILE:HA	1.56	0.45
1:B:287:ARG:O	1:B:290:GLN:HG3	2.16	0.45
1:B:572:PRO:O	1:B:573:LEU:HB2	2.17	0.45
1:B:265:MET:HE2	1:B:285:LYS:HD2	1.99	0.45
1:A:571:PRO:HB2	1:A:574:TYR:CD2	2.52	0.44
1:B:268:VAL:HG22	1:B:272:GLN:O	2.16	0.44
1:B:462:PRO:O	1:B:463:ILE:HB	2.17	0.44
1:A:558:ARG:HA	1:A:562:GLN:HB2	2.00	0.44
1:B:481:ARG:HG2	1:B:492:PRO:CA	2.47	0.44
2:C:25:U:H2'	2:C:26:A:O4'	2.17	0.44
1:B:690:LYS:HG2	4:B:801:IHP:O36	2.17	0.44
1:B:446:ILE:HB	1:B:448:THR:O	2.17	0.44
1:A:522:ARG:HD3	1:A:687:TRP:CZ2	2.52	0.44
1:A:693:GLU:H	1:A:693:GLU:CD	2.15	0.44
1:B:629:LYS:HG2	4:B:801:IHP:O42	2.17	0.44
1:A:568:GLU:HB3	1:A:569:ASP:OD1	2.18	0.44
1:B:405:ARG:HH22	1:B:626:ARG:HH11	1.65	0.44
1:A:413:LEU:HD22	1:A:420:ASP:HB3	1.99	0.44
1:A:571:PRO:HB2	1:A:574:TYR:HD2	1.83	0.43
1:B:258:SER:C	1:B:260:ALA:H	2.25	0.43
1:A:540:ILE:HA	7:A:905:HOH:O	2.16	0.43
1:A:486:SER:HB3	2:C:15:A:H1'	1.99	0.43
1:B:396:GLU:OE2	7:B:901:HOH:O	2.21	0.43
1:B:405:ARG:HH22	1:B:626:ARG:NH1	2.16	0.43
1:A:413:LEU:HD12	1:A:424:SER:HA	2.00	0.43
1:A:503:ASP:O	1:B:455:ARG:NH1	2.49	0.43
1:A:514:MET:HG2	1:A:687:TRP:CZ2	2.53	0.43
1:B:571:PRO:HB2	1:B:574:TYR:CD2	2.53	0.43
1:A:486:SER:HB3	2:C:15:A:O2'	2.18	0.43
1:A:498:SER:O	1:A:498:SER:OG	2.33	0.43
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.89	0.43
1:B:554:ASP:O	1:B:557:SER:OG	2.31	0.43
1:B:690:LYS:HD2	1:B:690:LYS:HA	1.79	0.43
3:D:29:G:H2'	3:D:30:A:O4'	2.19	0.43
1:A:481:ARG:HB3	1:A:490:THR:HB	2.00	0.43
1:B:257:GLU:HA	1:B:261:LYS:HB2	2.00	0.43
1:B:514:MET:HG3	1:B:687:TRP:CE2	2.54	0.43
1:B:696:GLN:O	1:B:696:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HA	1:A:596:PRO:HG2	2.00	0.43
1:B:274:PHE:CZ	1:B:295:ALA:HB3	2.54	0.43
2:C:27:G:H2'	2:C:28:C:O4'	2.19	0.42
1:A:426:PHE:O	1:A:437:LYS:HE3	2.19	0.42
1:A:682:ALA:HB3	1:A:684:LEU:HG	2.00	0.42
1:B:334:LYS:HD3	1:B:334:LYS:HA	1.76	0.42
1:B:413:LEU:HD21	1:B:423:ARG:O	2.20	0.42
1:B:521:ALA:O	1:B:524:ASN:N	2.53	0.42
3:D:8:A:H2'	3:D:9:U:O4'	2.20	0.42
1:A:414:TYR:HA	1:A:421:GLN:HA	2.01	0.42
1:A:429:SER:HB2	1:A:435:ARG:HB3	2.01	0.42
1:A:370:SER:HB2	1:A:402:SER:HB3	2.01	0.42
1:A:418:LYS:HE2	1:A:418:LYS:N	2.34	0.42
1:B:244:ARG:HB3	1:B:245:PRO:HD2	2.02	0.42
1:B:392:ASP:OD2	1:B:483:LYS:NZ	2.53	0.42
1:B:488:GLN:OE1	1:B:595:ALA:HB2	2.20	0.42
1:B:555:HIS:CD2	1:B:558:ARG:NH2	2.86	0.42
1:B:648:LEU:HD13	1:B:652:ILE:HG23	2.01	0.42
1:A:338:LEU:HD13	1:A:609:ILE:HG22	2.01	0.42
1:A:621:LEU:HD12	1:A:623:ARG:NE	2.35	0.41
1:A:672:LYS:HE2	4:A:801:IHP:O34	2.19	0.41
1:B:422:LYS:H	1:B:422:LYS:HD3	1.84	0.41
1:A:370:SER:HB2	1:A:602:TRP:O	2.20	0.41
1:A:386:ARG:O	1:A:388:LEU:HG	2.20	0.41
1:A:658:TYR:HB3	1:A:695:ASP:O	2.20	0.41
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.69	0.41
1:A:481:ARG:O	1:A:515:SER:HB3	2.21	0.41
1:A:509:GLU:OE2	1:B:488:GLN:HG3	2.20	0.41
1:B:463:ILE:HD12	1:B:463:ILE:HA	1.87	0.41
3:D:26:C:O2'	3:D:27:G:H5'	2.20	0.41
1:B:350:LYS:HE3	1:B:594:LYS:O	2.20	0.41
1:B:400:ARG:HD3	1:B:523:TRP:CD2	2.55	0.41
1:B:481:ARG:HG2	1:B:492:PRO:HA	2.01	0.41
1:B:495:SER:OG	1:B:496:ASN:N	2.51	0.41
1:A:385:ASP:OD1	1:A:386:ARG:HG3	2.20	0.41
1:B:533:LEU:HA	1:B:533:LEU:HD13	1.79	0.41
1:A:659:HIS:ND1	1:A:659:HIS:C	2.79	0.41
1:B:653:THR:O	1:B:654:LYS:C	2.64	0.41
1:B:350:LYS:HG2	1:B:596:PRO:HD3	2.03	0.41
1:B:431:ARG:HB2	1:B:431:ARG:NH1	2.31	0.41
1:B:452:GLY:O	1:B:456:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:HIS:CE1	1:B:483:LYS:HE2	2.56	0.40
1:A:359:THR:HA	1:A:439:ASN:O	2.21	0.40
1:A:603:THR:HG22	1:A:604:VAL:N	2.36	0.40
1:B:274:PHE:CZ	1:B:292:ALA:HA	2.56	0.40
1:B:302:ASP:O	1:B:307:ARG:NH1	2.53	0.40
1:A:413:LEU:HD22	1:A:413:LEU:O	2.21	0.40
1:B:482:THR:OG1	1:B:512:LEU:HD13	2.21	0.40
1:A:370:SER:CB	1:A:402:SER:HB3	2.52	0.40
1:B:267:VAL:HG12	1:B:268:VAL:H	1.85	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	383/487 (79%)	364 (95%)	18 (5%)	1 (0%)	36	60
1	B	436/487 (90%)	404 (93%)	31 (7%)	1 (0%)	43	68
All	All	819/974 (84%)	768 (94%)	49 (6%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	SER
1	A	467	PRO

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%)	290 (88%)	40 (12%)	5	12
1	B	377/415 (91%)	322 (85%)	55 (15%)	3	8
All	All	707/830 (85%)	612 (87%)	95 (13%)	4	9

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	HIS
1	A	322	VAL
1	A	332	LEU
1	A	334	LYS
1	A	356	VAL
1	A	362	ASP
1	A	367	LYS
1	A	409	THR
1	A	413	LEU
1	A	435	ARG
1	A	438	GLU
1	A	446	ILE
1	A	464	LEU
1	A	484	ILE
1	A	486	SER
1	A	488	GLN
1	A	494	ARG
1	A	499	ILE
1	A	500	GLN
1	A	510	ARG
1	A	528	ILE
1	A	535	ILE
1	A	543	SER
1	A	547	LEU
1	A	564	ILE
1	A	569	ASP
1	A	600	VAL
1	A	615	THR
1	A	626	ARG
1	A	635	ARG
1	A	637	MET
1	A	645	SER
1	A	654	LYS

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Mol	Chain	Res	Type
1	A	657	VAL
1	A	659	HIS
1	A	666	LYS
1	A	674	ARG
1	A	680	ILE
1	A	694	GLN
1	A	696	GLN
1	B	237	VAL
1	B	243	LEU
1	B	247	LEU
1	B	249	TYR
1	B	250	ASP
1	B	259	HIS
1	B	267	VAL
1	B	269	VAL
1	B	298	ASN
1	B	310	ILE
1	B	315	LEU
1	B	316	GLN
1	B	317	LEU
1	B	332	LEU
1	B	338	LEU
1	B	348	ARG
1	B	356	VAL
1	B	362	ASP
1	B	365	ASP
1	B	367	LYS
1	B	375	THR
1	B	378	ILE
1	B	386	ARG
1	B	403	LEU
1	B	409	THR
1	B	415	LEU
1	B	419	ASP
1	B	422	LYS
1	B	430	GLU
1	B	431	ARG
1	B	440	VAL
1	B	446	ILE
1	B	449	SER
1	B	455	ARG
1	B	484	ILE

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Mol	Chain	Res	Type
1	B	491	ILE
1	B	494	ARG
1	B	509	GLU
1	B	528	ILE
1	B	533	LEU
1	B	543	SER
1	B	570	LEU
1	B	586	ASN
1	B	594	LYS
1	B	601	ASN
1	B	607	SER
1	B	609	ILE
1	B	615	THR
1	B	627	LEU
1	B	651	LYS
1	B	652	ILE
1	B	657	VAL
1	B	663	LEU
1	B	680	ILE
1	B	690	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	GLN
1	A	473	ASN
1	A	488	GLN
1	A	562	GLN
1	A	591	GLN
1	A	696	GLN
1	B	300	HIS
1	B	410	GLN
1	B	439	ASN
1	B	488	GLN
1	B	577	ASN
1	B	586	ASN
1	B	601	ASN
1	B	659	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	31/32 (96%)	5 (16%)	0
3	D	29/32 (90%)	3 (10%)	0
All	All	60/64 (93%)	8 (13%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	C
2	C	8	A
2	C	13	8AZ
2	C	29	U
2	C	32	G
3	D	2	G
3	D	7	U
3	D	10	C

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$
2	8AZ	C	13	2,5	18,24,25	2.67	5 (27%)	19,35,38	1.94	5 (26%)
3	A1BBA	D	21	3	23,26,27	1.90	4 (17%)	33,38,41	1.83	10 (30%)

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	-	5/7/35/36	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1BBA	D	21	3	-	0/7/21/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	13	8AZ	C2-N1	7.59	1.47	1.34
2	C	13	8AZ	N7-N8	6.15	1.42	1.32
3	D	21	A1BBA	C3-C4	5.86	1.49	1.41
3	D	21	A1BBA	C4-C5	4.99	1.47	1.40
2	C	13	8AZ	N9-N8	3.79	1.40	1.35
2	C	13	8AZ	C2-N3	2.82	1.35	1.30
3	D	21	A1BBA	C1-C1'	-2.48	1.47	1.51
2	C	13	8AZ	C4-N9	-2.17	1.33	1.35
3	D	21	A1BBA	C6-C5	-2.12	1.36	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	8AZ	C5-C4-N3	-4.94	119.83	127.24
3	D	21	A1BBA	C6-C1-C2	3.74	123.19	118.09
3	D	21	A1BBA	C4-C3-C23	-3.63	115.92	119.42
2	C	13	8AZ	N1-C2-N3	-3.38	118.43	125.78
3	D	21	A1BBA	C19-C5-C4	3.32	124.99	121.02
3	D	21	A1BBA	C3-C23-N22	3.23	118.34	114.93
3	D	21	A1BBA	C3-C4-N20	-2.62	119.74	122.33
2	C	13	8AZ	O3'-C3'-C4'	-2.54	103.79	111.08
3	D	21	A1BBA	C2-C3-C23	2.51	124.77	120.09
2	C	13	8AZ	O3'-C3'-C2'	-2.25	104.62	111.82
2	C	13	8AZ	C2-N3-C4	2.21	115.42	111.53
3	D	21	A1BBA	C3-C4-C5	-2.12	118.78	120.56
3	D	21	A1BBA	O25-C23-N22	-2.10	118.13	120.62
3	D	21	A1BBA	C6-C1-C1'	-2.06	112.52	120.26
3	D	21	A1BBA	C5-C4-N20	2.03	121.45	117.46

There are no chirality outliers.

All (5) 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'
2	C	13	8AZ	O4'-C1'-N9-N8

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Mol	Chain	Res	Type	Atoms
2	C	13	8AZ	O4'-C1'-N9-C4
2	C	13	8AZ	C2'-C1'-N9-N8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	13	8AZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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	B	801	-	36,36,36	0.81	0	60,60,60	0.86	2 (3%)
4	IHP	A	801	6	36,36,36	0.77	1 (2%)	60,60,60	1.51	11 (18%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IHP	B	801	-	-	2/30/54/54	0/1/1/1
4	IHP	A	801	6	-	1/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	IHP	P2-O22	2.36	1.57	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	IHP	O15-P5-O25	-4.93	91.76	109.33
4	A	801	IHP	O42-P2-O12	-3.13	93.65	105.85
4	A	801	IHP	O11-P1-O21	-3.12	98.20	109.33
4	A	801	IHP	O44-P4-O14	3.00	117.53	105.85
4	A	801	IHP	P1-O11-C1	-2.96	115.54	123.43
4	A	801	IHP	O32-P2-O12	2.46	115.44	105.85
4	A	801	IHP	O35-P5-O15	2.39	115.14	105.85
4	A	801	IHP	O34-P4-O14	-2.22	97.19	105.85
4	A	801	IHP	P2-O12-C2	-2.16	117.66	123.43
4	B	801	IHP	O36-P6-O16	2.08	113.96	105.85
4	B	801	IHP	P6-O16-C6	-2.08	117.88	123.43
4	A	801	IHP	O14-P4-O24	-2.02	102.14	109.33
4	A	801	IHP	O15-C5-C4	-2.00	104.51	108.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	IHP	C2-O12-P2-O32
4	A	801	IHP	C4-O14-P4-O34
4	B	801	IHP	C6-O16-P6-O36

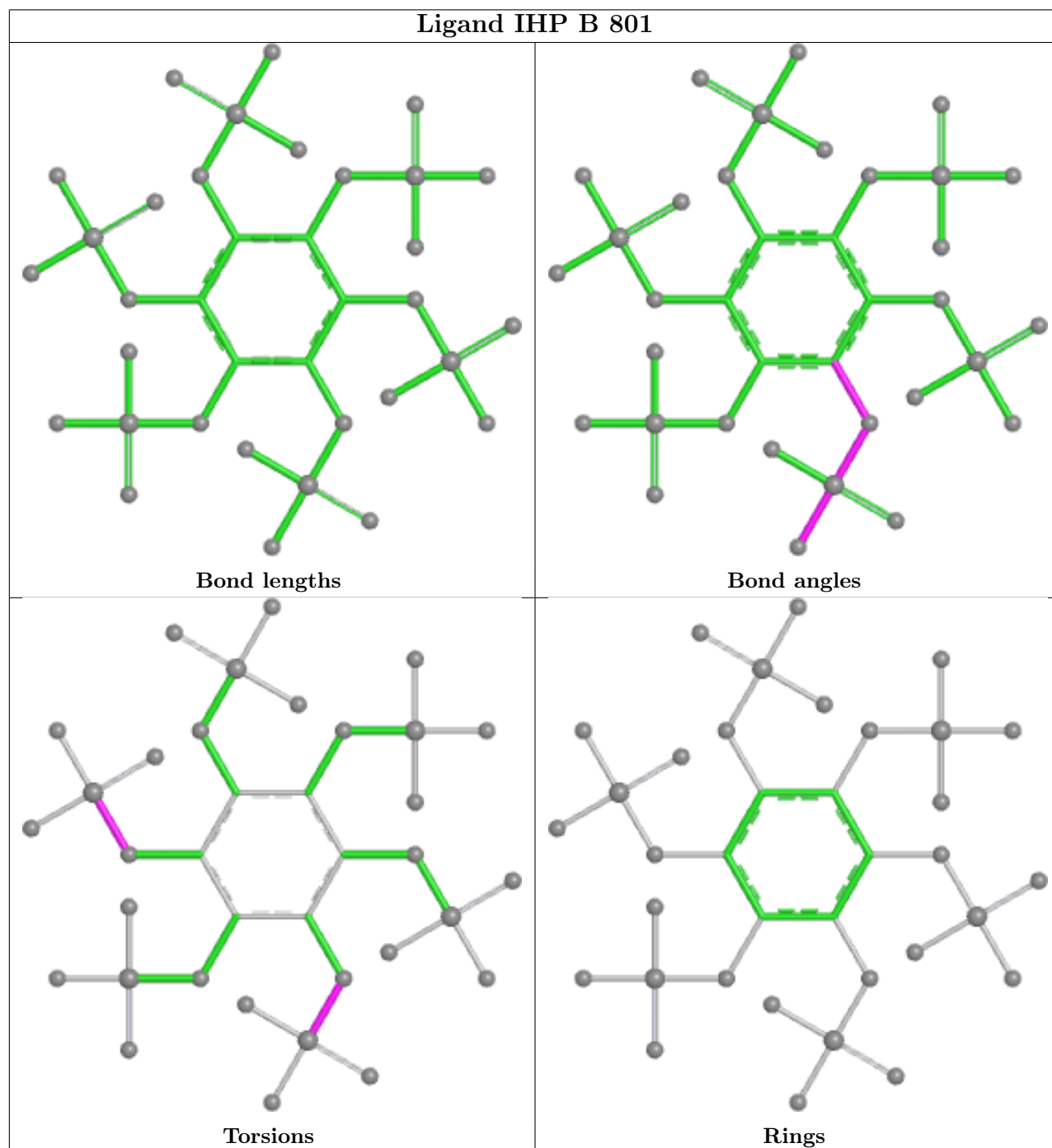
There are no ring outliers.

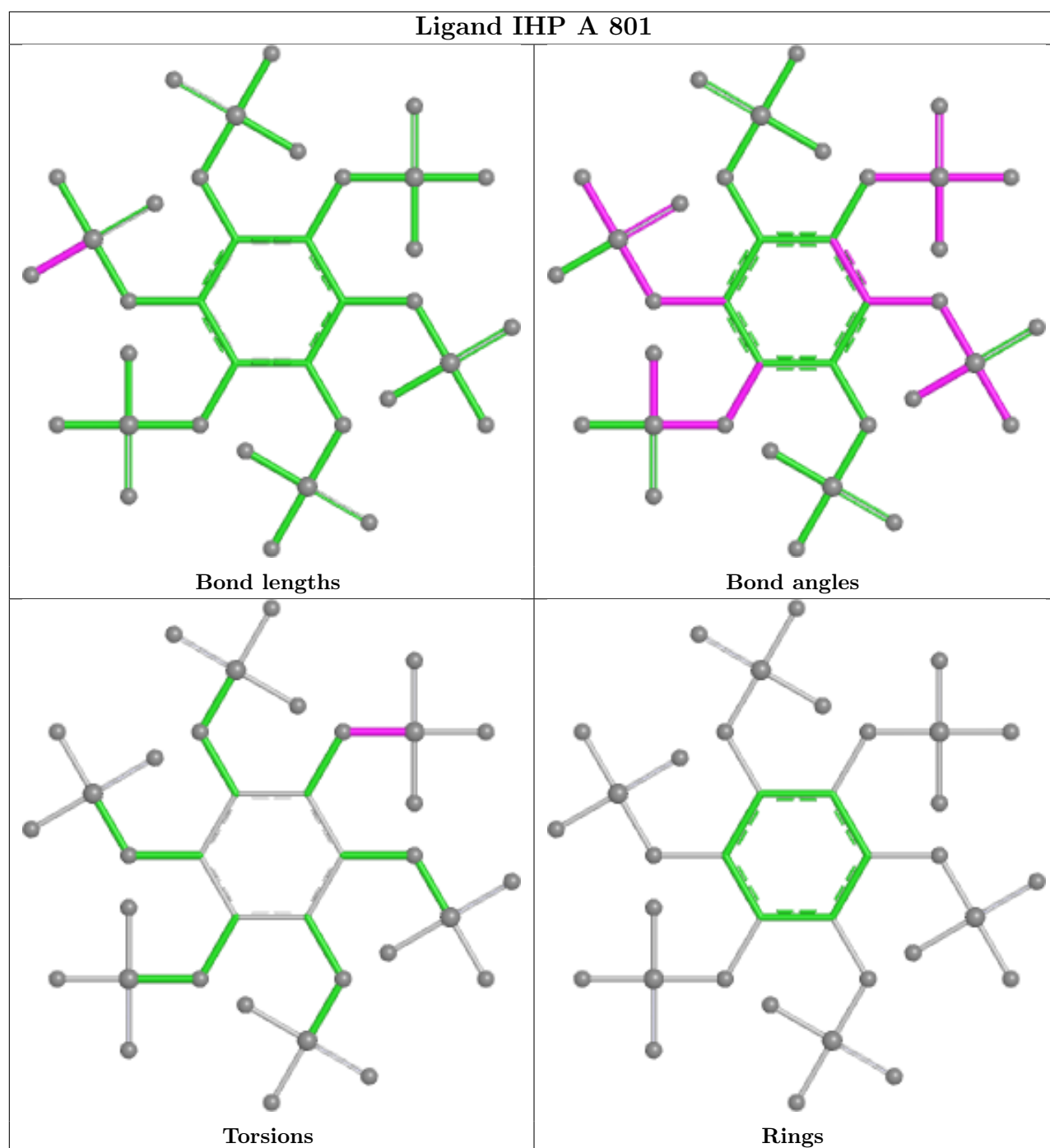
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	IHP	6	0
4	A	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.





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	384/487 (78%)	0.03	7 (1%) 67 65	57, 81, 134, 231	1 (0%)
1	B	442/487 (90%)	0.23	10 (2%) 61 58	83, 136, 191, 236	0
2	C	31/32 (96%)	-0.71	0 100 100	76, 117, 170, 171	0
3	D	31/32 (96%)	-0.75	0 100 100	73, 129, 162, 163	0
All	All	888/1038 (85%)	0.08	17 (1%) 66 63	57, 111, 184, 236	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	663	LEU	3.6
1	A	507	GLN	2.9
1	B	621	LEU	2.9
1	A	497	ALA	2.7
1	A	463	ILE	2.6
1	A	499	ILE	2.6
1	B	415	LEU	2.5
1	B	598	PHE	2.5
1	A	498	SER	2.4
1	B	476	ALA	2.4
1	B	675	LEU	2.3
1	A	652	ILE	2.2
1	B	596	PRO	2.2
1	B	700	THR	2.1
1	B	442	PHE	2.1
1	B	528	ILE	2.1
1	B	540	ILE	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
3	A1BBA	D	21	24/25	0.95	0.09	75,78,92,98	0
2	8AZ	C	13	22/23	0.96	0.07	64,70,72,73	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

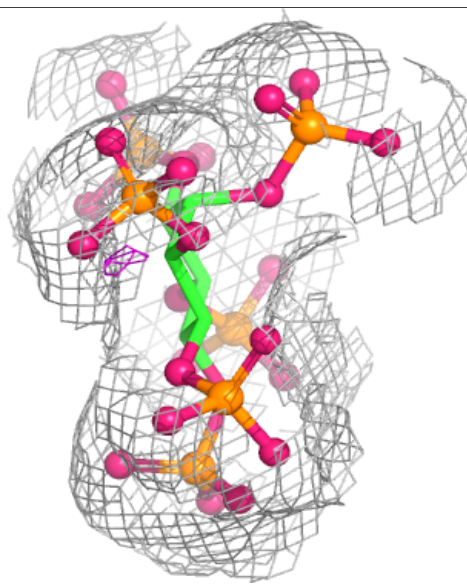
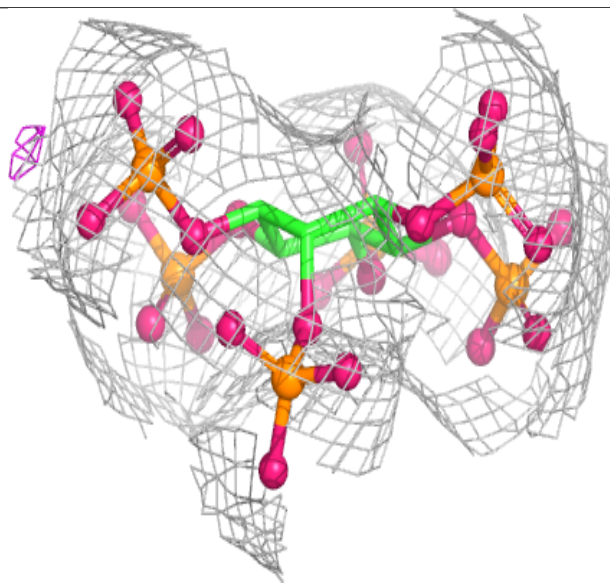
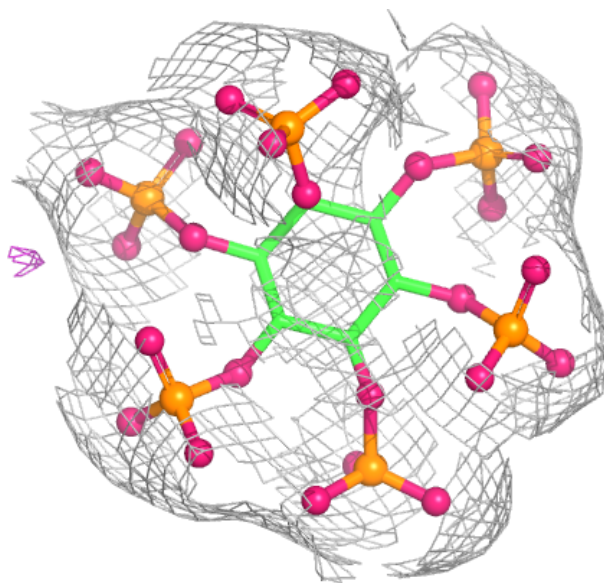
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.94	0.06	105,119,128,131	0
6	MG	A	803	1/1	0.94	0.06	82,82,82,82	0
4	IHP	A	801	36/36	0.96	0.06	54,65,70,87	0
5	ZN	A	802	1/1	0.99	0.03	63,63,63,63	0
5	ZN	B	802	1/1	1.00	0.02	79,79,79,79	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.

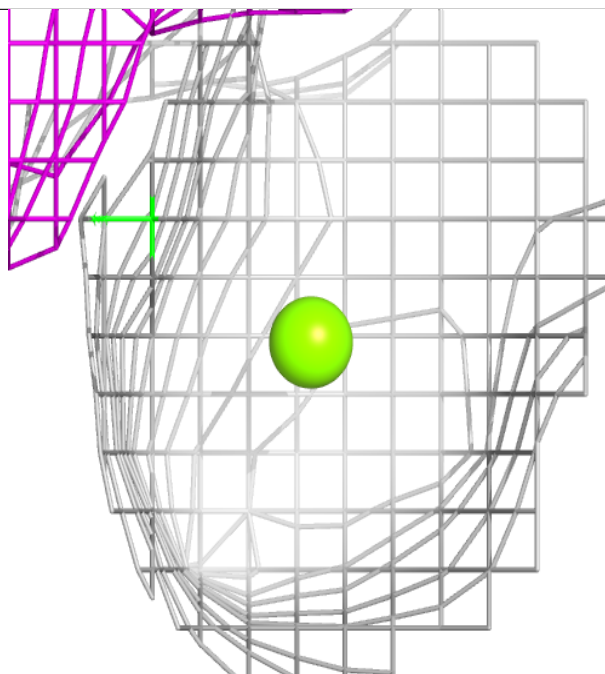
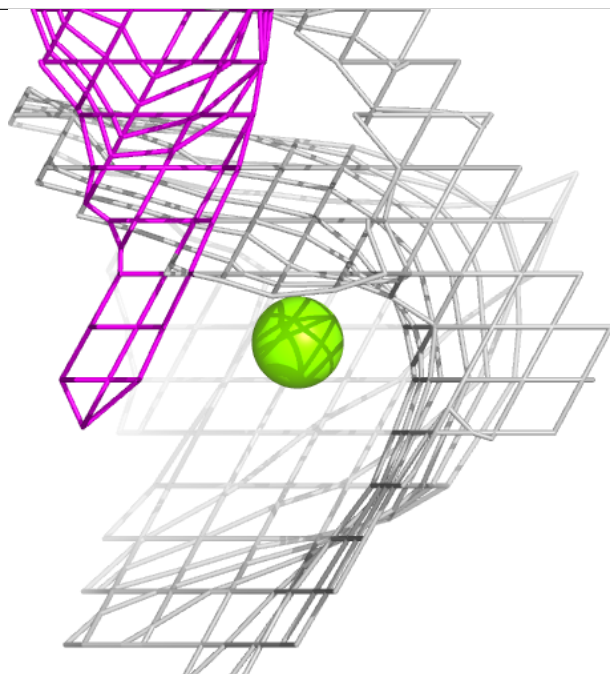
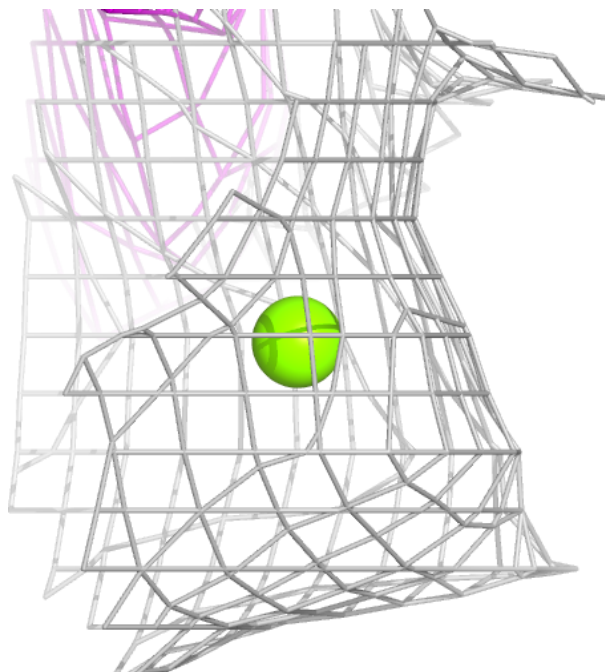
Electron density around IHP B 801:

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



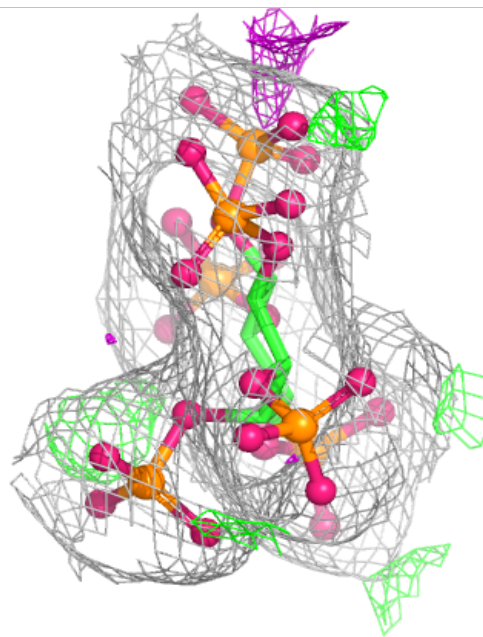
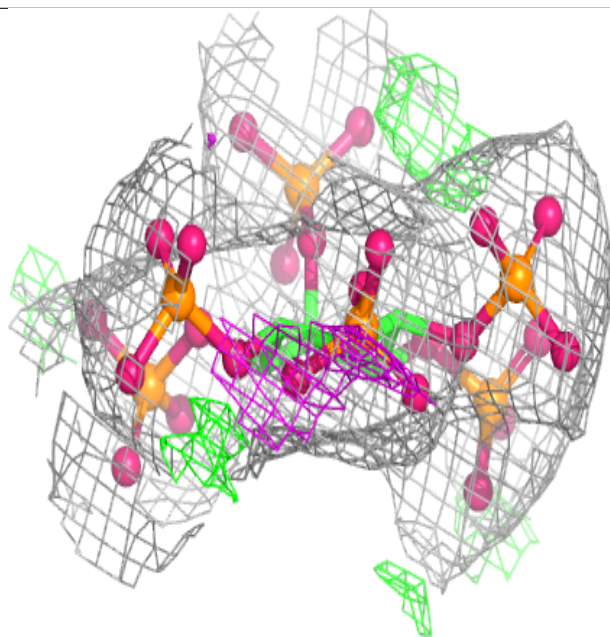
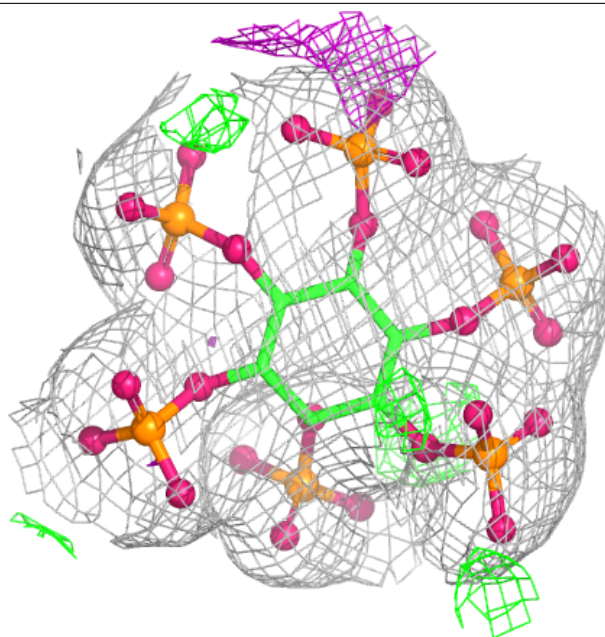
Electron density around MG A 803:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



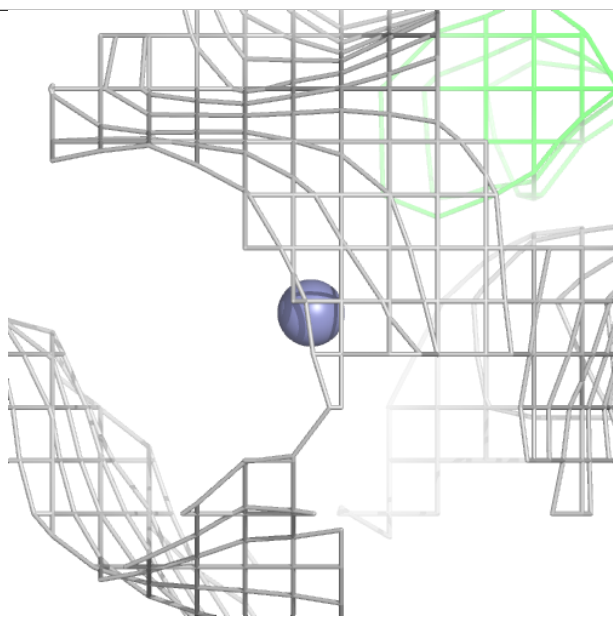
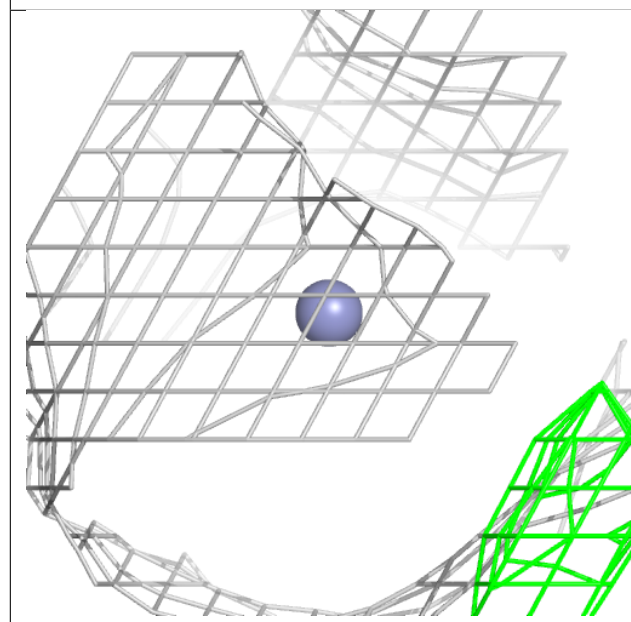
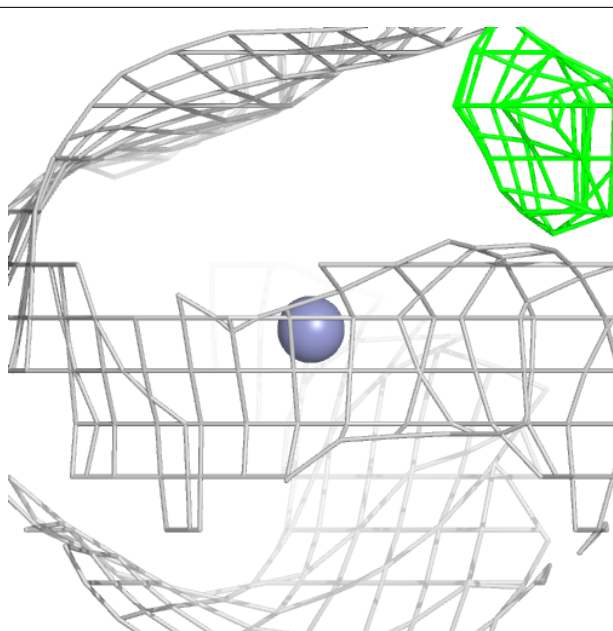
Electron density around IHP A 801:

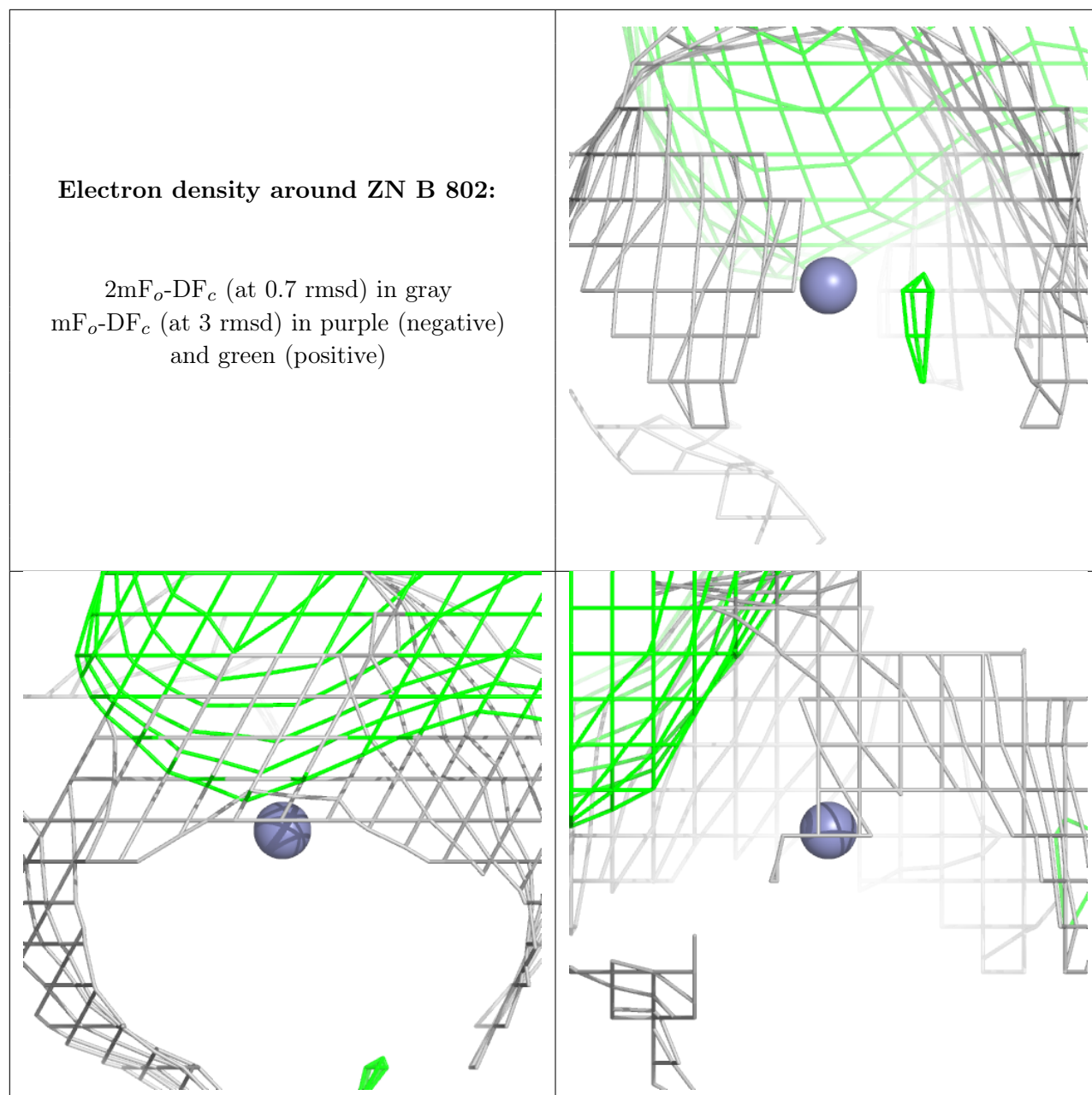
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 802:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.