



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:00 PM UTC

PDB ID : 1RO9 / pdb_00001ro9
Title : CRYSTAL STRUCTURES OF THE CATALYTIC DOMAIN OF PHOSPHO-DIESTERASE 4B2B COMPLEXED WITH 8-Br-AMP
Authors : Xu, R.X.; Rocque, W.J.; Lambert, M.H.; Vanderwall, D.E.; Nolte, R.T.
Deposited on : 2003-12-01
Resolution : 2.13 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

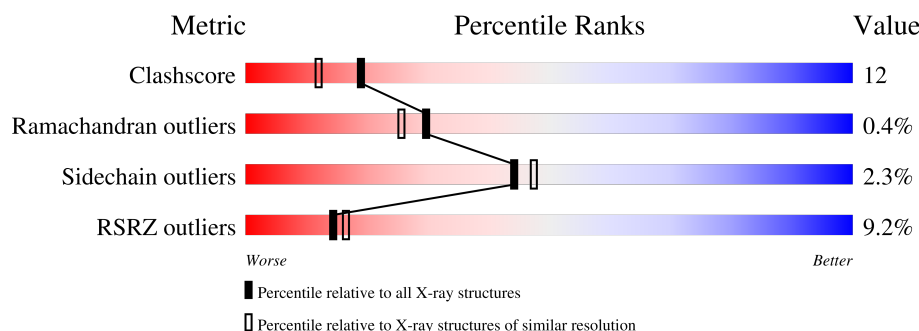
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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))
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	378	6% 69% 19% • 11%
1	B	378	10% 60% 26% •• 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5758 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2724	1718	462	525	19			
1	B	337	Total	C	N	O	S	0	0	0
			2719	1715	461	524	19			

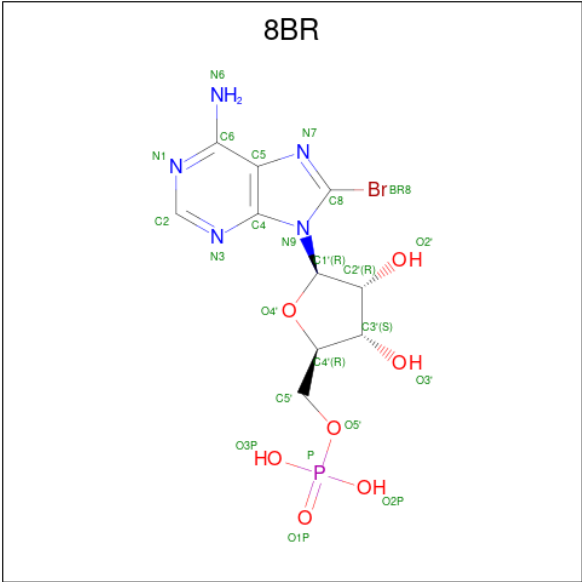
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	initiating methionine	UNP Q07343
A	487	ALA	SER	engineered mutation	UNP Q07343
A	489	ALA	SER	engineered mutation	UNP Q07343
B	151	MET	-	initiating methionine	UNP Q07343
B	487	ALA	SER	engineered mutation	UNP Q07343
B	489	ALA	SER	engineered mutation	UNP Q07343

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 8-BROMO-ADENOSINE-5'-MONOPHOSPHATE (CCD ID: 8BR) (formula: C₁₀H₁₃BrN₅O₇P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	P	0	0
			24	1	10	5	7	1		
3	B	1	Total	Br	C	N	O	P	0	0
			24	1	10	5	7	1		

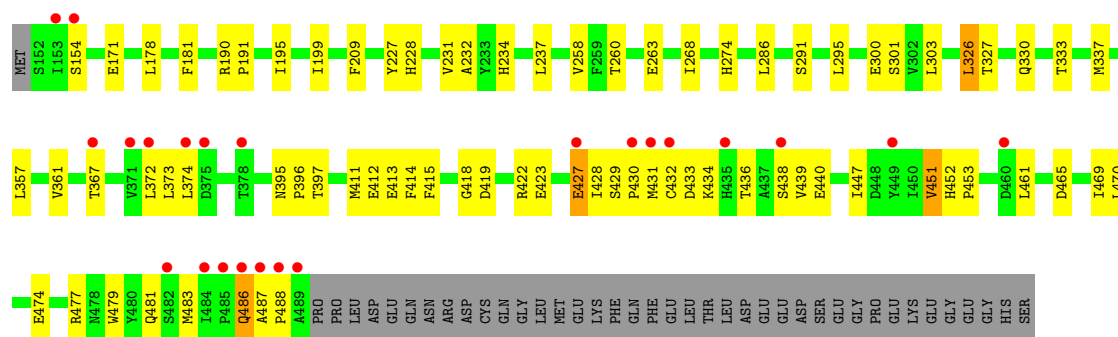
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total	O	0	0
			170	170		
4	B	93	Total	O	0	0
			93	93		

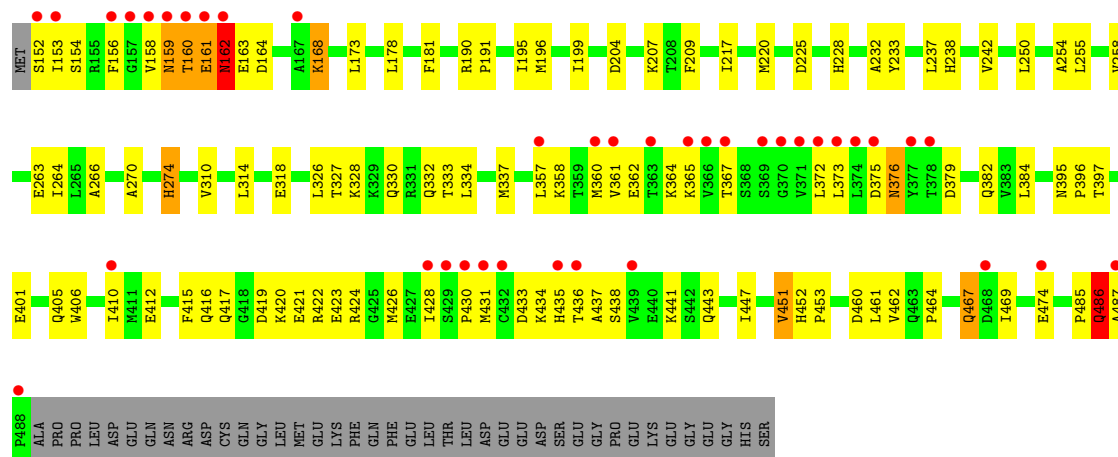
3 Residue-property plots [i](#)

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: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.33Å 159.21Å 108.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.13 20.00 – 2.13	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.13) 93.1 (20.00-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.234 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5758	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: 8BR, ZN

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	0.45	0/2781	0.93	8/3773 (0.2%)
1	B	0.43	0/2776	0.93	7/3766 (0.2%)
All	All	0.44	0/5557	0.93	15/7539 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ALA	N-CA-C	8.16	120.18	111.28
1	A	232	ALA	N-CA-C	7.87	119.85	111.28
1	A	274	HIS	N-CA-C	7.00	121.44	112.34
1	A	227	TYR	N-CA-C	-6.78	99.54	110.32
1	B	159	ASN	N-CA-C	6.45	119.13	111.71
1	A	451	VAL	N-CA-C	6.32	116.49	110.42
1	B	451	VAL	N-CA-C	6.06	116.23	110.42
1	B	161	GLU	N-CA-C	-5.95	106.02	113.28
1	B	375	ASP	N-CA-C	5.74	118.75	111.69
1	A	171	GLU	N-CA-C	-5.69	105.59	112.54
1	A	465	ASP	N-CA-C	5.61	118.12	111.33
1	B	162	ASN	N-CA-C	-5.48	105.96	113.30
1	B	274	HIS	N-CA-C	5.10	118.61	112.38
1	A	326	LEU	N-CA-C	-5.05	103.00	110.48
1	A	231	VAL	N-CA-C	-5.01	100.56	108.23

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	2724	0	2649	41	0
1	B	2719	0	2644	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	11	2	0
3	B	24	0	11	0	0
4	A	170	0	0	3	0
4	B	93	0	0	6	0
All	All	5758	0	5315	128	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 12.

All (128) 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:406:TRP:O	1:B:410:ILE:HD12	1.66	0.93
1:B:376:ASN:HD22	1:B:376:ASN:H	1.20	0.89
1:B:160:THR:HA	1:B:163:GLU:HG2	1.56	0.88
1:B:160:THR:HA	1:B:163:GLU:CG	2.05	0.87
1:B:152:SER:HB3	1:B:217:ILE:HD12	1.58	0.85
1:B:365:LYS:HB2	4:B:549:HOH:O	1.82	0.79
1:A:487:ALA:HB1	1:A:488:PRO:HA	1.70	0.74
1:B:373:LEU:HB3	4:B:549:HOH:O	1.88	0.74
1:B:158:VAL:HG12	1:B:162:ASN:OD1	1.88	0.72
1:B:434:LYS:HD3	1:B:434:LYS:O	1.90	0.72
1:B:406:TRP:C	1:B:410:ILE:HD12	2.15	0.72
1:A:412:GLU:HG2	4:A:627:HOH:O	1.91	0.71
1:B:419:ASP:O	1:B:423:GLU:HG3	1.90	0.71
1:B:376:ASN:HD22	1:B:376:ASN:N	1.89	0.70
1:A:397:THR:HB	1:A:469:ILE:HG23	1.72	0.70
1:B:412:GLU:O	1:B:416:GLN:HG3	1.90	0.69
1:A:291:SER:O	1:A:295:LEU:HD13	1.95	0.67
1:A:300:GLU:HB2	4:A:691:HOH:O	1.95	0.66
1:A:333:THR:HG22	1:A:337:MET:HE2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:HB	1:B:469:ILE:HG23	1.76	0.66
1:B:486:GLN:NE2	1:B:487:ALA:H	1.94	0.65
1:B:263:GLU:HA	1:B:337:MET:HE1	1.80	0.62
1:B:467:GLN:HG2	4:B:597:HOH:O	1.98	0.62
1:B:395:ASN:HB2	1:B:396:PRO:HD3	1.81	0.62
1:A:411:MET:HE2	1:A:439:VAL:HG22	1.82	0.61
1:A:470:LEU:O	1:A:474:GLU:HG3	2.01	0.61
1:B:233:TYR:CD1	1:B:410:ILE:HG13	2.36	0.60
1:A:258:VAL:HG11	1:A:374:LEU:HD12	1.83	0.60
1:B:334:LEU:C	1:B:334:LEU:HD23	2.27	0.60
1:B:376:ASN:H	1:B:376:ASN:ND2	1.96	0.59
1:B:196:MET:HG3	1:B:220:MET:HE2	1.83	0.58
1:A:477:ARG:NH1	1:A:481:GLN:OE1	2.36	0.58
1:B:367:THR:HG22	1:B:373:LEU:HD13	1.86	0.58
1:B:164:ASP:HB2	4:B:596:HOH:O	2.04	0.57
1:B:422:ARG:HB2	1:B:428:ILE:HD11	1.85	0.57
1:B:401:GLU:O	1:B:405:GLN:HG3	2.05	0.57
1:A:427:GLU:H	1:A:427:GLU:CD	2.13	0.56
1:B:204:ASP:OD1	1:B:207:LYS:HD2	2.06	0.56
1:A:429:SER:HB3	1:A:430:PRO:HD2	1.88	0.56
1:B:333:THR:O	1:B:337:MET:HG3	2.05	0.55
1:B:376:ASN:HD21	1:B:379:ASP:CG	2.13	0.55
1:B:420:LYS:O	1:B:424:ARG:HG3	2.06	0.55
1:A:419:ASP:O	1:A:423:GLU:HG3	2.07	0.55
1:B:376:ASN:ND2	1:B:379:ASP:HB2	2.23	0.54
1:B:159:ASN:O	1:B:160:THR:CB	2.55	0.54
1:B:486:GLN:NE2	1:B:487:ALA:N	2.55	0.54
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.91	0.53
1:B:160:THR:O	1:B:163:GLU:HB2	2.09	0.53
1:A:395:ASN:HB2	1:A:396:PRO:HD3	1.91	0.52
1:B:254:ALA:O	1:B:372:LEU:HB2	2.09	0.52
1:B:318:GLU:HB3	4:B:542:HOH:O	2.10	0.52
1:B:486:GLN:CD	1:B:487:ALA:H	2.18	0.52
1:B:173:LEU:HA	1:B:178:LEU:HD12	1.92	0.52
1:A:479:TRP:O	1:A:483:MET:HG2	2.09	0.52
1:B:195:ILE:O	1:B:199:ILE:HG13	2.10	0.51
1:B:373:LEU:HD23	4:B:549:HOH:O	2.08	0.51
1:A:430:PRO:O	1:A:431:MET:HB2	2.11	0.51
1:B:196:MET:HG3	1:B:220:MET:CE	2.40	0.51
1:B:485:PRO:O	1:B:487:ALA:N	2.44	0.50
1:B:376:ASN:HD21	1:B:379:ASP:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:O	1:B:153:ILE:HG13	2.12	0.50
1:B:433:ASP:HB3	1:B:436:THR:HB	1.94	0.49
1:B:173:LEU:HA	1:B:178:LEU:CD1	2.43	0.49
1:B:360:MET:HE2	1:B:382:GLN:CD	2.37	0.49
1:B:357:LEU:O	1:B:360:MET:HB3	2.13	0.49
1:B:238:HIS:O	1:B:242:VAL:HG23	2.12	0.48
1:A:327:THR:OG1	1:A:330:GLN:HG3	2.14	0.48
1:A:181:PHE:CD1	1:A:237:LEU:HD21	2.48	0.48
1:B:417:GLN:O	1:B:421:GLU:HG3	2.14	0.47
1:A:367:THR:HG22	1:A:373:LEU:HD21	1.97	0.47
1:B:159:ASN:O	1:B:160:THR:HB	2.14	0.47
1:A:418:GLY:HA3	1:A:432:CYS:O	2.14	0.47
1:A:422:ARG:HB2	1:A:428:ILE:HD11	1.96	0.47
1:B:443:GLN:O	1:B:447:ILE:HG13	2.15	0.47
1:B:228:HIS:N	1:B:228:HIS:CD2	2.80	0.47
1:A:234:HIS:NE2	3:A:531:8BR:O2P	2.42	0.47
1:B:160:THR:HA	1:B:163:GLU:HG3	1.92	0.47
1:A:357:LEU:O	1:A:361:VAL:HG23	2.15	0.47
1:B:452:HIS:HB3	1:B:453:PRO:HD3	1.96	0.46
1:A:447:ILE:HA	1:A:451:VAL:HB	1.97	0.46
1:B:416:GLN:O	1:B:420:LYS:HG3	2.15	0.46
1:B:361:VAL:O	1:B:364:LYS:HG2	2.15	0.45
1:B:376:ASN:HD21	1:B:379:ASP:CB	2.29	0.45
1:B:485:PRO:C	1:B:486:GLN:HG3	2.40	0.45
1:A:300:GLU:O	1:A:301:SER:C	2.60	0.45
1:B:204:ASP:CG	1:B:207:LYS:HD2	2.41	0.45
1:B:266:ALA:CB	1:B:337:MET:HE3	2.47	0.45
1:A:199:ILE:HG21	1:A:268:ILE:HD13	1.99	0.45
1:B:328:LYS:O	1:B:332:GLN:HG3	2.17	0.45
1:B:431:MET:HA	1:B:437:ALA:HB2	1.99	0.44
1:B:421:GLU:HB3	1:B:426:MET:HB2	2.00	0.44
1:A:440:GLU:H	1:A:440:GLU:CD	2.26	0.44
1:B:190:ARG:N	1:B:191:PRO:CD	2.80	0.44
1:A:414:PHE:HZ	3:A:531:8BR:O2'	2.01	0.43
1:A:433:ASP:HB3	1:A:436:THR:OG1	2.18	0.43
1:B:376:ASN:ND2	1:B:379:ASP:OD2	2.39	0.43
1:B:361:VAL:HG22	1:B:461:LEU:HB2	2.01	0.43
1:B:152:SER:HB3	1:B:217:ILE:CD1	2.40	0.43
1:B:168:LYS:O	1:B:168:LYS:HD3	2.19	0.43
1:B:438:SER:HB3	1:B:441:LYS:HB2	2.00	0.43
1:B:415:PHE:CD2	1:B:434:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:CD1	1:A:326:LEU:HD22	2.54	0.43
1:B:447:ILE:HA	1:B:451:VAL:HB	2.01	0.42
1:B:327:THR:OG1	1:B:330:GLN:HG3	2.18	0.42
1:B:358:LYS:O	1:B:362:GLU:HG3	2.20	0.42
1:A:415:PHE:CE1	1:A:434:LYS:HA	2.54	0.42
1:B:310:VAL:O	1:B:314:LEU:HG	2.19	0.42
1:A:286:LEU:HD11	1:A:303:LEU:HD21	2.01	0.42
1:B:250:LEU:HD13	1:B:264:ILE:HG23	2.01	0.42
1:A:438:SER:HB3	4:A:654:HOH:O	2.18	0.41
1:B:360:MET:HE1	1:B:379:ASP:HA	2.01	0.41
1:A:190:ARG:N	1:A:191:PRO:CD	2.83	0.41
1:B:263:GLU:HB3	1:B:384:LEU:HD11	2.01	0.41
1:A:234:HIS:ND1	1:A:413:GLU:OE2	2.54	0.41
1:A:228:HIS:N	1:A:228:HIS:CD2	2.88	0.41
1:B:209:PHE:CD1	1:B:326:LEU:HD22	2.56	0.41
1:A:260:THR:OG1	1:A:263:GLU:HG3	2.20	0.41
1:A:477:ARG:NH2	1:A:481:GLN:OE1	2.53	0.41
1:A:195:ILE:O	1:A:199:ILE:HG13	2.20	0.41
1:A:372:LEU:HD21	1:A:461:LEU:O	2.21	0.41
1:B:154:SER:C	1:B:156:PHE:H	2.29	0.41
1:B:204:ASP:OD2	1:B:207:LYS:HD2	2.20	0.41
1:B:255:LEU:C	1:B:258:VAL:HG23	2.45	0.41
1:B:270:ALA:O	1:B:274:HIS:HB3	2.21	0.41
1:B:430:PRO:O	1:B:431:MET:HB2	2.21	0.41
1:B:181:PHE:CD1	1:B:237:LEU:HD21	2.57	0.40
1:B:254:ALA:HB3	1:B:462:VAL:HB	2.02	0.40
1:B:361:VAL:HG11	1:B:460:ASP:CG	2.45	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	336/378 (89%)	322 (96%)	13 (4%)	1 (0%)	36	33
1	B	335/378 (89%)	319 (95%)	14 (4%)	2 (1%)	21	15
All	All	671/756 (89%)	641 (96%)	27 (4%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLN
1	B	486	GLN
1	B	160	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	305/341 (89%)	301 (99%)	4 (1%)	61	67
1	B	305/341 (89%)	295 (97%)	10 (3%)	33	33
All	All	610/682 (89%)	596 (98%)	14 (2%)	44	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	SER
1	A	178	LEU
1	A	427	GLU
1	A	486	GLN
1	B	161	GLU
1	B	162	ASN
1	B	168	LYS
1	B	225	ASP
1	B	376	ASN
1	B	435	HIS
1	B	464	PRO
1	B	467	GLN
1	B	474	GLU

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Mol	Chain	Res	Type
1	B	486	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	284	GLN
1	A	316	GLN
1	A	332	GLN
1	A	386	ASN
1	A	416	GLN
1	A	463	GLN
1	B	165	HIS
1	B	182	ASN
1	B	284	GLN
1	B	376	ASN
1	B	382	GLN
1	B	463	GLN
1	B	467	GLN
1	B	486	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
3	8BR	B	531	-	26,26,26	1.53	6 (23%)	38,40,40	1.65	10 (26%)
3	8BR	A	531	-	26,26,26	1.66	9 (34%)	38,40,40	1.71	10 (26%)

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	8BR	B	531	-	-	6/10/26/26	0/3/3/3
3	8BR	A	531	-	-	5/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	531	8BR	P-O3P	-3.28	1.42	1.54
3	A	531	8BR	C8-N7	3.17	1.35	1.29
3	B	531	8BR	P-O3P	-3.13	1.43	1.54
3	A	531	8BR	C1'-N9	3.09	1.51	1.45
3	B	531	8BR	C1'-N9	3.07	1.50	1.45
3	B	531	8BR	C8-N7	2.81	1.35	1.29
3	B	531	8BR	C5-C4	2.79	1.44	1.39
3	A	531	8BR	C5-C4	2.76	1.44	1.39
3	A	531	8BR	C4-N3	2.43	1.39	1.34
3	A	531	8BR	C2-N1	2.27	1.38	1.33
3	A	531	8BR	BR8-C8	2.25	1.90	1.86
3	B	531	8BR	C2-N1	2.09	1.37	1.33
3	A	531	8BR	P-O2P	-2.06	1.47	1.54
3	A	531	8BR	C4-N9	2.06	1.41	1.38
3	B	531	8BR	C4-N3	2.03	1.38	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	531	8BR	C6-C5-N7	4.17	135.86	131.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	531	8BR	C6-C5-N7	3.84	135.53	131.72
3	B	531	8BR	C5-C4-N3	-3.37	122.08	126.72
3	A	531	8BR	C5-C4-N3	-3.35	122.10	126.72
3	A	531	8BR	N3-C2-N1	-3.22	123.71	128.58
3	A	531	8BR	C5-N7-C8	3.22	106.37	103.22
3	A	531	8BR	C4-C5-N7	-3.20	107.64	110.91
3	A	531	8BR	C5-C4-N9	3.12	107.59	105.63
3	B	531	8BR	N3-C2-N1	-3.05	123.96	128.58
3	B	531	8BR	C4-C5-N7	-3.05	107.79	110.91
3	A	531	8BR	BR8-C8-N9	2.96	124.91	121.97
3	B	531	8BR	C5-C4-N9	2.94	107.48	105.63
3	B	531	8BR	C5-N7-C8	2.93	106.08	103.22
3	B	531	8BR	BR8-C8-N9	2.52	124.48	121.97
3	A	531	8BR	C2-N3-C4	2.31	117.48	111.83
3	B	531	8BR	C2-N3-C4	2.18	117.16	111.83
3	B	531	8BR	N3-C4-N9	2.16	130.44	127.33
3	A	531	8BR	O5'-P-O1P	2.10	112.13	106.44
3	A	531	8BR	N3-C4-N9	2.06	130.30	127.33
3	B	531	8BR	O4'-C1'-N9	2.01	111.08	108.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

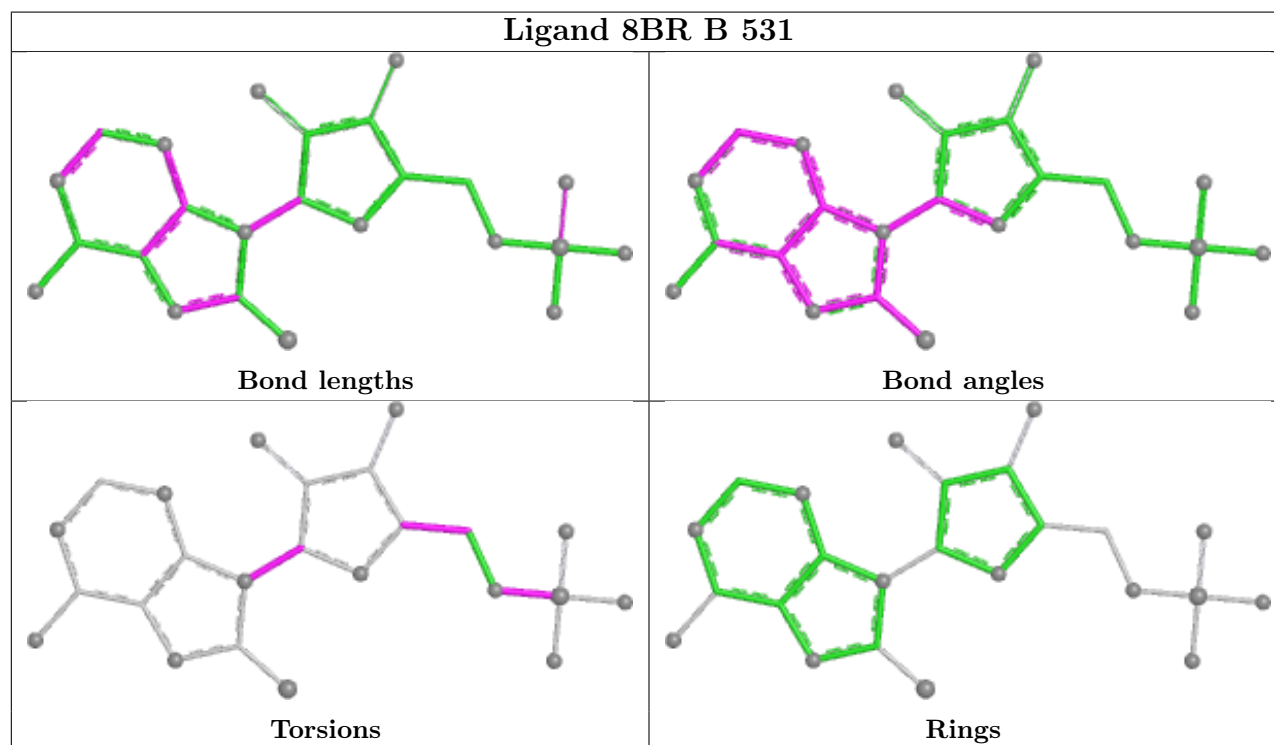
Mol	Chain	Res	Type	Atoms
3	A	531	8BR	C5'-O5'-P-O2P
3	A	531	8BR	C5'-O5'-P-O3P
3	B	531	8BR	O4'-C1'-N9-C4
3	B	531	8BR	C2'-C1'-N9-C4
3	A	531	8BR	O4'-C1'-N9-C4
3	A	531	8BR	C2'-C1'-N9-C4
3	B	531	8BR	C2'-C1'-N9-C8
3	B	531	8BR	C5'-O5'-P-O2P
3	B	531	8BR	C3'-C4'-C5'-O5'
3	B	531	8BR	O4'-C1'-N9-C8
3	A	531	8BR	C2'-C1'-N9-C8

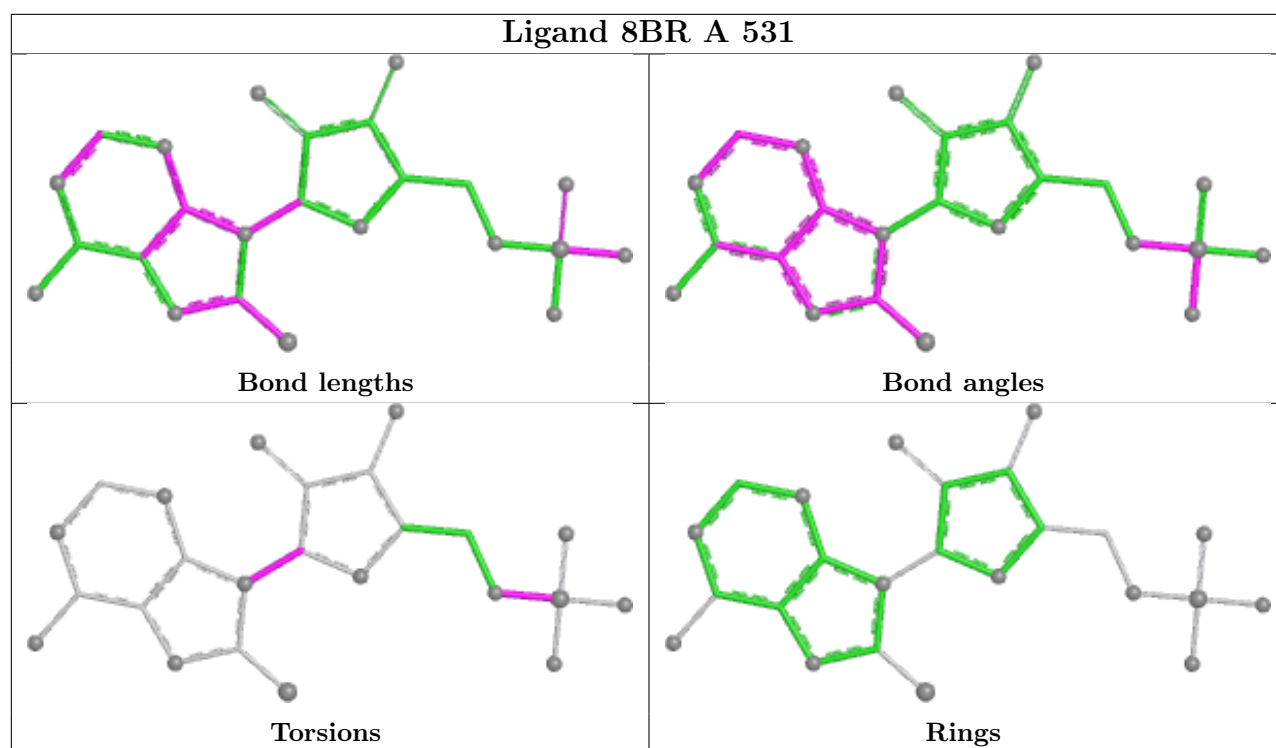
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	531	8BR	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	338/378 (89%)	0.27	23 (6%) 23 27	18, 31, 66, 87	0
1	B	337/378 (89%)	0.79	39 (11%) 9 11	23, 41, 73, 86	0
All	All	675/756 (89%)	0.53	62 (9%) 14 16	18, 37, 69, 87	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	ALA	5.9
1	A	488	PRO	5.4
1	A	487	ALA	5.0
1	B	488	PRO	5.0
1	B	160	THR	4.8
1	B	159	ASN	4.3
1	B	430	PRO	4.3
1	B	435	HIS	4.3
1	B	429	SER	4.2
1	A	431	MET	4.2
1	B	156	PHE	3.7
1	B	152	SER	3.7
1	B	369	SER	3.6
1	B	158	VAL	3.6
1	A	486	GLN	3.6
1	B	153	ILE	3.5
1	B	157	GLY	3.5
1	B	361	VAL	3.4
1	B	374	LEU	3.4
1	B	431	MET	3.3
1	B	370	GLY	3.3
1	B	432	CYS	3.3
1	A	482	SER	3.3
1	A	435	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	ALA	3.1
1	B	360	MET	3.1
1	A	153	ILE	3.0
1	B	439	VAL	3.0
1	B	366	VAL	2.9
1	B	372	LEU	2.9
1	B	371	VAL	2.8
1	B	161	GLU	2.8
1	A	430	PRO	2.8
1	B	365	LYS	2.7
1	A	374	LEU	2.7
1	A	460	ASP	2.6
1	A	484	ILE	2.6
1	A	449	TYR	2.6
1	B	378	THR	2.6
1	B	436	THR	2.5
1	A	154	SER	2.5
1	B	377	TYR	2.5
1	A	375	ASP	2.5
1	B	375	ASP	2.4
1	B	410	ILE	2.4
1	B	363	THR	2.4
1	A	371	VAL	2.4
1	B	428	ILE	2.4
1	A	427	GLU	2.3
1	A	372	LEU	2.3
1	B	167	ALA	2.3
1	B	373	LEU	2.3
1	B	162	ASN	2.2
1	B	468	ASP	2.2
1	B	357	LEU	2.2
1	A	485	PRO	2.1
1	A	432	CYS	2.1
1	A	438	SER	2.1
1	A	367	THR	2.1
1	B	367	THR	2.1
1	B	474	GLU	2.0
1	A	378	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

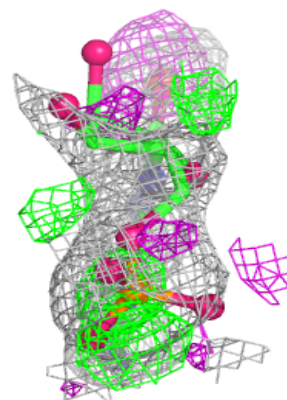
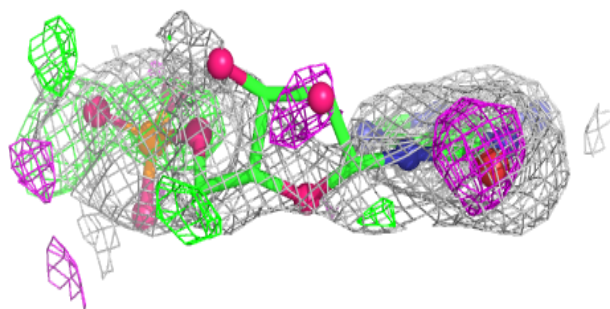
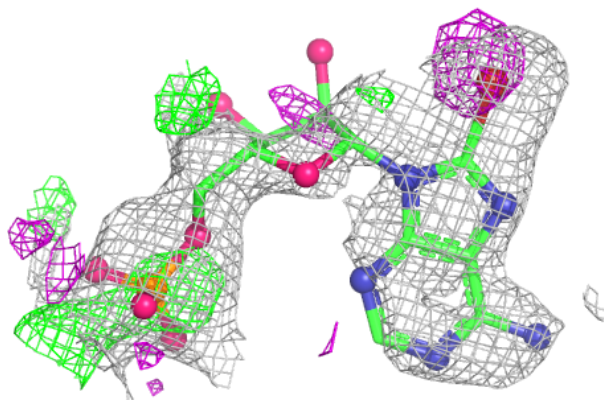
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	8BR	B	531	24/24	0.76	0.21	84,91,94,98	0
3	8BR	A	531	24/24	0.83	0.17	65,79,82,86	0
2	ZN	B	529	1/1	0.97	0.03	39,39,39,39	0
2	ZN	B	530	1/1	0.97	0.10	61,61,61,61	0
2	ZN	A	529	1/1	0.98	0.04	35,35,35,35	0
2	ZN	A	530	1/1	0.98	0.14	58,58,58,58	0

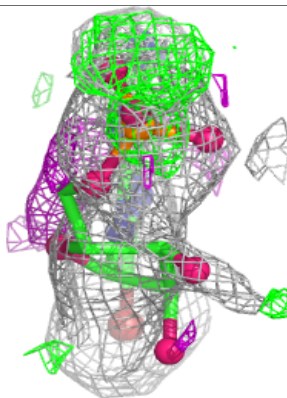
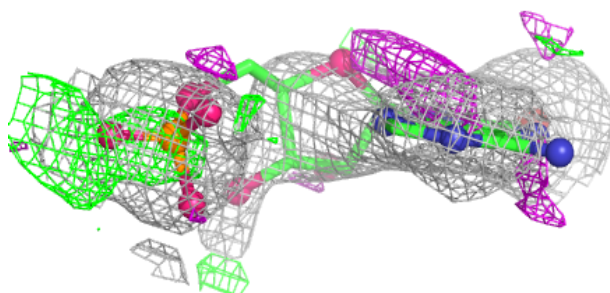
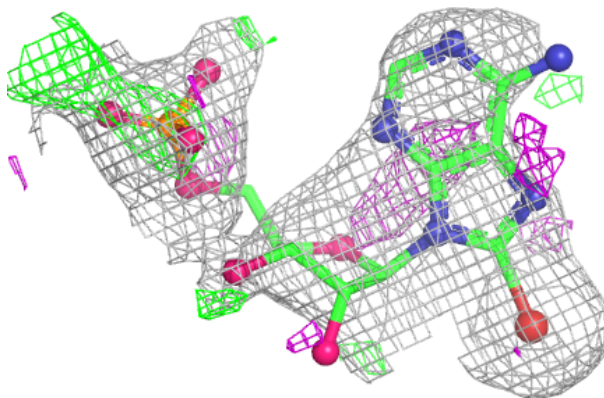
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8BR B 531:

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

**Electron density around 8BR A 531:**

$2mF_o-DF_c$ (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.