



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:04 AM UTC

PDB ID : 8V4P / pdb_00008v4p
Title : Crystal structure of Acetyl-CoA synthetase 2 in complex with Adenosine-5'-allylphosphate from *Candida albicans*
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-11-29
Resolution : 2.30 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

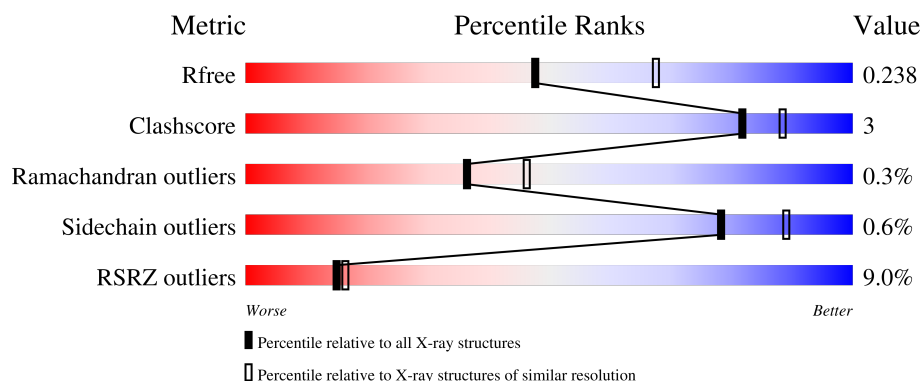
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	686	5% 90% 6% .
1	B	686	9% 87% 6% 8%
1	C	686	11% 71% 5% 24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14592 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	1	0
			5083	3243	863	963	14			
1	B	634	Total	C	N	O	S	0	0	0
			4888	3131	826	918	13			
1	C	523	Total	C	N	O	S	0	0	0
			4044	2598	671	762	13			

There are 51 discrepancies between the modelled and reference sequences:

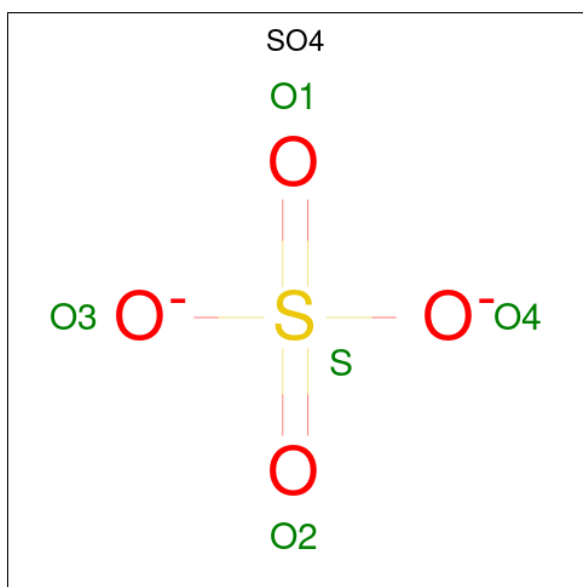
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJJN3
A	2	HIS	-	expression tag	UNP Q8NJJN3
A	3	HIS	-	expression tag	UNP Q8NJJN3
A	4	HIS	-	expression tag	UNP Q8NJJN3
A	5	HIS	-	expression tag	UNP Q8NJJN3
A	6	HIS	-	expression tag	UNP Q8NJJN3
A	7	HIS	-	expression tag	UNP Q8NJJN3
A	8	HIS	-	expression tag	UNP Q8NJJN3
A	9	HIS	-	expression tag	UNP Q8NJJN3
A	10	GLU	-	expression tag	UNP Q8NJJN3
A	11	ASN	-	expression tag	UNP Q8NJJN3
A	12	LEU	-	expression tag	UNP Q8NJJN3
A	13	TYR	-	expression tag	UNP Q8NJJN3
A	14	PHE	-	expression tag	UNP Q8NJJN3
A	15	GLN	-	expression tag	UNP Q8NJJN3
A	16	GLY	-	expression tag	UNP Q8NJJN3
A	403	ALA	VAL	variant	UNP Q8NJJN3
B	1	MET	-	initiating methionine	UNP Q8NJJN3
B	2	HIS	-	expression tag	UNP Q8NJJN3
B	3	HIS	-	expression tag	UNP Q8NJJN3
B	4	HIS	-	expression tag	UNP Q8NJJN3
B	5	HIS	-	expression tag	UNP Q8NJJN3
B	6	HIS	-	expression tag	UNP Q8NJJN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8NJJ3
B	8	HIS	-	expression tag	UNP Q8NJJ3
B	9	HIS	-	expression tag	UNP Q8NJJ3
B	10	GLU	-	expression tag	UNP Q8NJJ3
B	11	ASN	-	expression tag	UNP Q8NJJ3
B	12	LEU	-	expression tag	UNP Q8NJJ3
B	13	TYR	-	expression tag	UNP Q8NJJ3
B	14	PHE	-	expression tag	UNP Q8NJJ3
B	15	GLN	-	expression tag	UNP Q8NJJ3
B	16	GLY	-	expression tag	UNP Q8NJJ3
B	403	ALA	VAL	variant	UNP Q8NJJ3
C	1	MET	-	initiating methionine	UNP Q8NJJ3
C	2	HIS	-	expression tag	UNP Q8NJJ3
C	3	HIS	-	expression tag	UNP Q8NJJ3
C	4	HIS	-	expression tag	UNP Q8NJJ3
C	5	HIS	-	expression tag	UNP Q8NJJ3
C	6	HIS	-	expression tag	UNP Q8NJJ3
C	7	HIS	-	expression tag	UNP Q8NJJ3
C	8	HIS	-	expression tag	UNP Q8NJJ3
C	9	HIS	-	expression tag	UNP Q8NJJ3
C	10	GLU	-	expression tag	UNP Q8NJJ3
C	11	ASN	-	expression tag	UNP Q8NJJ3
C	12	LEU	-	expression tag	UNP Q8NJJ3
C	13	TYR	-	expression tag	UNP Q8NJJ3
C	14	PHE	-	expression tag	UNP Q8NJJ3
C	15	GLN	-	expression tag	UNP Q8NJJ3
C	16	GLY	-	expression tag	UNP Q8NJJ3
C	403	ALA	VAL	variant	UNP Q8NJJ3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

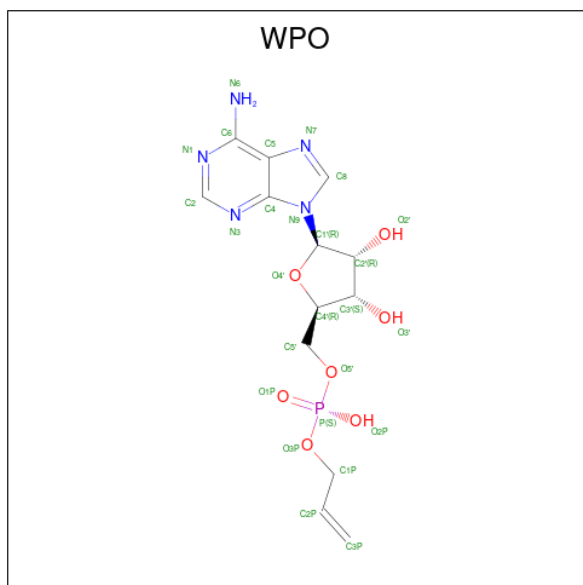
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

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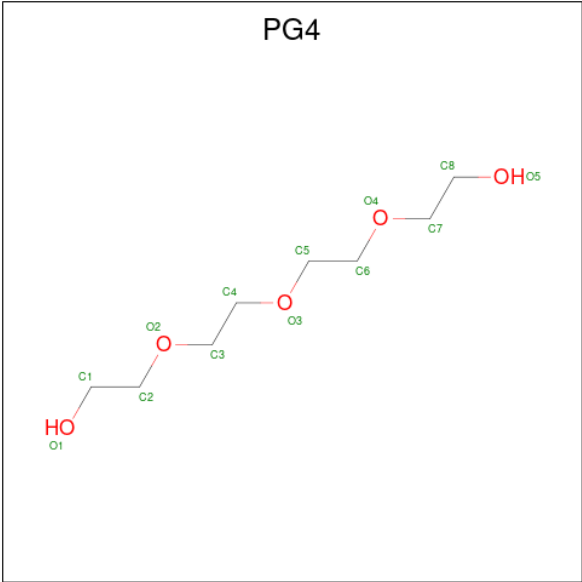
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 5'-O-[(S)-hydroxy[(prop-2-en-1-yl)oxy]phosphoryl]adenosine (CCD ID: WPO) (formula: C₁₃H₁₈N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
4	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			10	6	4		

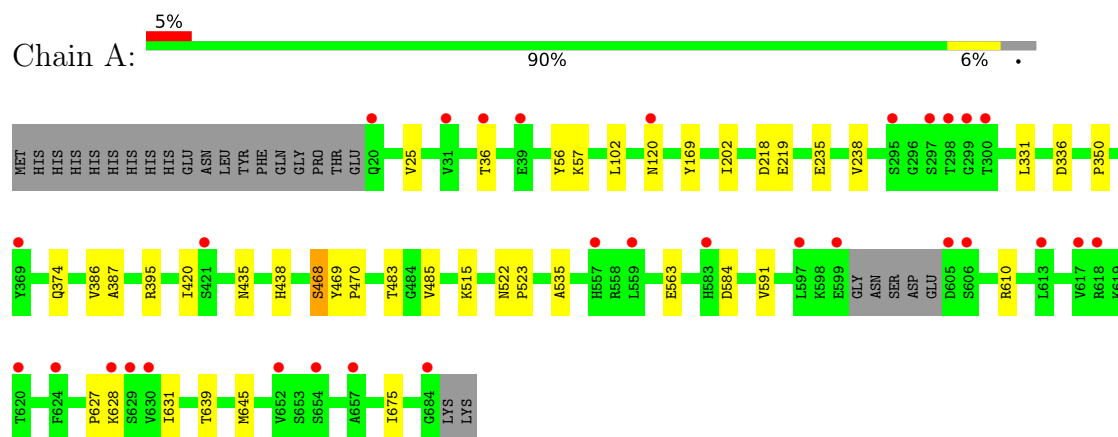
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	156	Total	O	0	0
			156	156		
6	C	27	Total	O	0	0
			27	27		

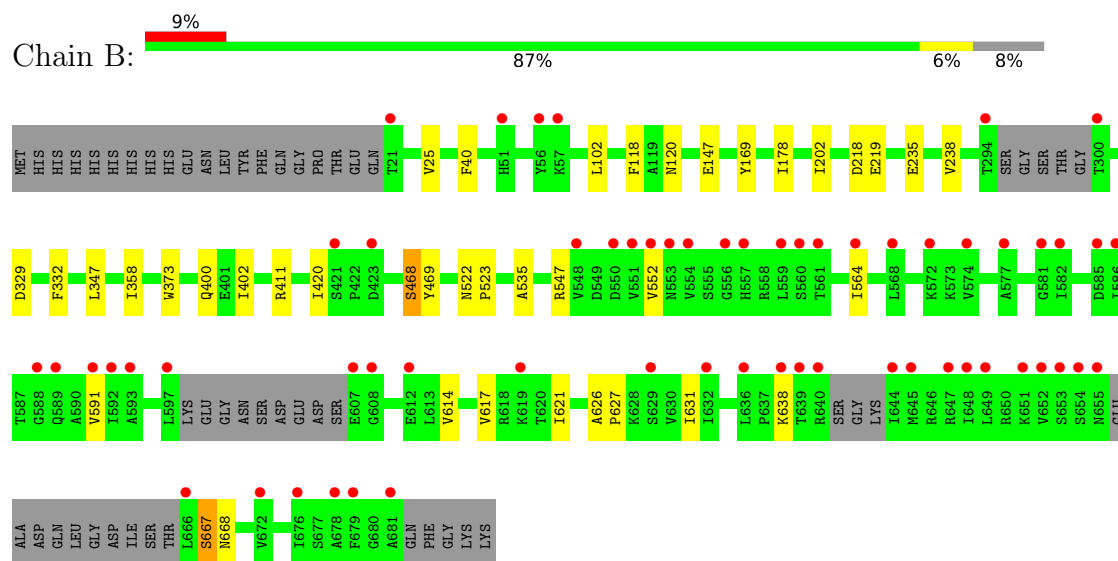
3 Residue-property plots [i](#)

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: Acetyl-coenzyme A synthetase 2

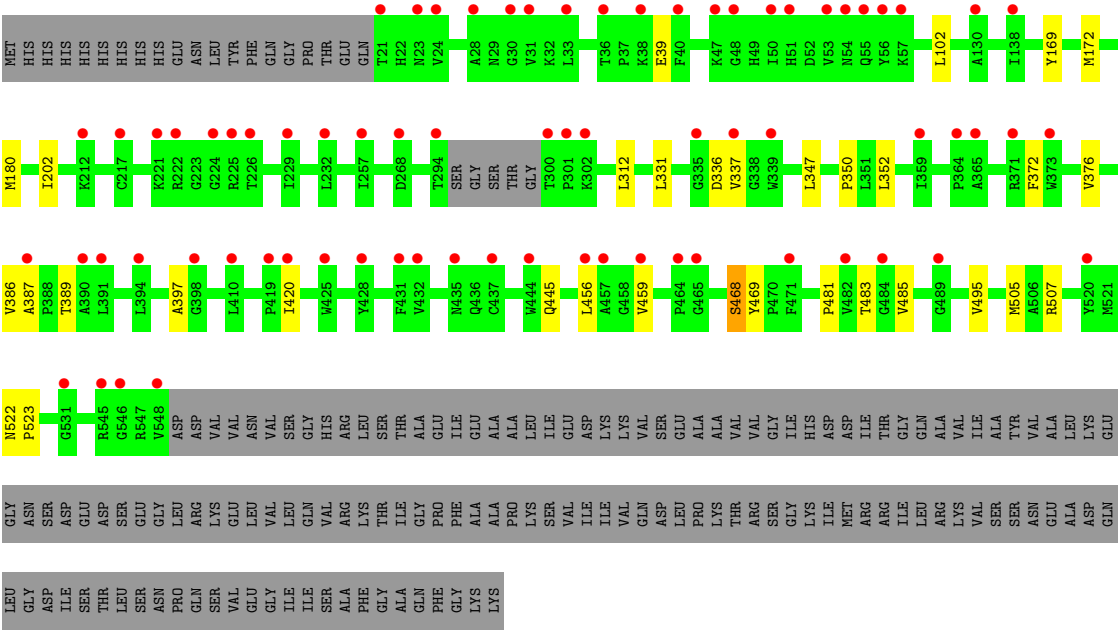


• Molecule 1: Acetyl-coenzyme A synthetase 2



• Molecule 1: Acetyl-coenzyme A synthetase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.54Å 138.54Å 543.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.51 – 2.30 49.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.51-2.30) 100.0 (49.51-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.211 , 0.238 0.213 , 0.238	Depositor DCC
R_{free} test set	6792 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14592	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WPO, SO4, CL, PG4

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	0.11	0/5215	0.30	0/7103
1	B	0.10	0/5013	0.29	0/6830
1	C	0.09	0/4163	0.24	0/5686
All	All	0.10	0/14391	0.28	0/19619

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5083	0	4924	23	0
1	B	4888	0	4741	26	0
1	C	4044	0	3831	22	0
2	A	30	0	0	1	0
2	B	25	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	52	0	0	1	0
4	B	26	0	0	0	0
4	C	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	13	0	18	0	0
5	B	10	0	13	2	0
6	A	183	0	0	3	0
6	B	156	0	0	0	0
6	C	27	0	0	0	0
All	All	14592	0	13527	70	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 3.

All (70) 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:547:ARG:HH22	5:B:708:PG4:H72	1.50	0.75
1:A:331:LEU:HD23	1:A:350:PRO:HG3	1.72	0.71
1:C:180:MET:HE1	1:C:337:VAL:HG11	1.73	0.70
1:C:331:LEU:HD23	1:C:350:PRO:HG3	1.74	0.68
1:C:180:MET:CE	1:C:337:VAL:HG11	2.27	0.65
1:A:591:VAL:HG23	1:A:627:PRO:HA	1.82	0.62
1:C:481:PRO:HG3	1:C:495:VAL:HG23	1.81	0.61
1:B:617:VAL:HG13	1:B:621:ILE:HD12	1.83	0.60
1:C:180:MET:SD	1:C:337:VAL:HG11	2.40	0.60
1:C:39:GLU:N	1:C:39:GLU:OE1	2.35	0.57
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.40	0.56
1:C:169:TYR:CE1	1:C:202:ILE:HD11	2.40	0.56
1:C:468:SER:OG	1:C:469:TYR:N	2.39	0.55
1:A:483:THR:OG1	1:A:485:VAL:HG22	2.07	0.55
1:B:591:VAL:HG23	1:B:627:PRO:HA	1.88	0.54
1:A:639:THR:HG22	1:A:645:MET:HE2	1.90	0.54
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.43	0.54
1:B:147:GLU:HG2	1:B:178:ILE:HD13	1.89	0.54
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.43	0.53
1:C:337:VAL:O	1:C:337:VAL:HG12	2.08	0.53
1:B:40:PHE:CD2	1:B:411:ARG:HG2	2.43	0.53
1:B:638:LYS:O	1:B:667:SER:OG	2.26	0.52
1:C:172:MET:SD	1:C:337:VAL:HG23	2.50	0.51
1:C:336:ASP:OD2	4:C:702:WPO:O2'	2.30	0.49
1:B:468:SER:OG	1:B:469:TYR:N	2.45	0.48
1:C:505:MET:O	1:C:507:ARG:NH1	2.45	0.48
1:B:329:ASP:OD1	1:B:411:ARG:NH2	2.46	0.48
1:C:522:ASN:N	1:C:523:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:HG22	1:A:438:HIS:ND1	2.30	0.47
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.50	0.47
1:A:57:LYS:NZ	6:A:808:HOH:O	2.48	0.47
1:A:522:ASN:N	1:A:523:PRO:CD	2.79	0.46
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.98	0.46
1:C:372:PHE:O	1:C:376:VAL:HG23	2.16	0.46
1:A:631:ILE:HD12	1:A:631:ILE:N	2.31	0.46
1:B:522:ASN:N	1:B:523:PRO:CD	2.79	0.45
1:A:395:ARG:NH2	2:A:704:SO4:O2	2.38	0.45
1:A:25:VAL:HG22	1:A:535:ALA:HB1	1.99	0.45
1:A:56:TYR:OH	1:A:470:PRO:O	2.35	0.45
1:A:468:SER:OG	1:A:469:TYR:N	2.50	0.45
1:A:235:GLU:O	1:A:238:VAL:HG12	2.17	0.44
1:C:347:LEU:C	1:C:347:LEU:HD23	2.42	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.17	0.44
1:B:631:ILE:HD12	1:B:631:ILE:N	2.33	0.44
1:A:584:ASP:OD1	1:A:628:LYS:NZ	2.47	0.44
1:A:420:ILE:O	1:A:420:ILE:HG23	2.18	0.44
1:C:483:THR:OG1	1:C:485:VAL:HG22	2.18	0.44
1:B:552:VAL:HG11	1:B:591:VAL:HG13	1.99	0.43
1:C:386:VAL:HG22	1:C:387:ALA:N	2.33	0.43
1:A:386:VAL:HG22	1:A:387:ALA:N	2.33	0.43
1:C:456:LEU:HD12	1:C:456:LEU:N	2.33	0.43
1:B:373:TRP:NE1	1:B:402:ILE:HG12	2.33	0.43
1:C:102:LEU:H	1:C:102:LEU:HD12	1.83	0.43
1:A:336:ASP:OD2	4:A:710:WPO:O2'	2.36	0.43
1:B:102:LEU:HD12	1:B:102:LEU:N	2.34	0.42
1:B:564:ILE:HA	1:B:621:ILE:HD11	2.02	0.42
1:C:420:ILE:O	1:C:420:ILE:HG23	2.19	0.42
1:B:332:PHE:HB2	1:B:358:ILE:HD12	2.02	0.42
1:A:563:GLU:OE1	6:A:801:HOH:O	2.22	0.42
1:B:614:VAL:HG13	1:B:626:ALA:HB1	2.02	0.42
1:B:102:LEU:HD12	1:B:102:LEU:H	1.85	0.41
1:C:312:LEU:HD22	1:C:352:LEU:HD11	2.02	0.41
1:B:667:SER:OG	1:B:668:ASN:N	2.53	0.41
1:A:102:LEU:HD12	1:A:102:LEU:H	1.86	0.41
1:A:374:GLN:NE2	6:A:810:HOH:O	2.50	0.41
1:B:347:LEU:HD23	1:B:347:LEU:C	2.46	0.41
1:A:218:ASP:OD1	1:A:219:GLU:N	2.49	0.40
1:B:235:GLU:O	1:B:238:VAL:HG12	2.21	0.40
1:B:547:ARG:NH2	5:B:708:PG4:H72	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASP:OD1	1:B:219:GLU:N	2.50	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	657/686 (96%)	640 (97%)	16 (2%)	1 (0%)	43	55
1	B	624/686 (91%)	602 (96%)	20 (3%)	2 (0%)	36	46
1	C	519/686 (76%)	491 (95%)	25 (5%)	3 (1%)	21	27
All	All	1800/2058 (88%)	1733 (96%)	61 (3%)	6 (0%)	36	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	B	667	SER
1	C	468	SER
1	B	468	SER
1	C	397	ALA
1	C	459	VAL

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	531/568 (94%)	526 (99%)	5 (1%)	70	84
1	B	510/568 (90%)	508 (100%)	2 (0%)	84	92
1	C	416/568 (73%)	414 (100%)	2 (0%)	81	90
All	All	1457/1704 (86%)	1448 (99%)	9 (1%)	78	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	435	ASN
1	A	515	LYS
1	A	610	ARG
1	A	675	ILE
1	B	120	ASN
1	B	400	GLN
1	C	389	THR
1	C	445	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	46	ASN
1	B	26	HIS
1	B	46	ASN
1	B	445	GLN
1	B	557	HIS
1	C	51	HIS
1	C	120	ASN
1	C	374	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	WPO	B	707	-	28,28,28	0.36	0	38,41,41	0.46	0
2	SO4	A	701	-	4,4,4	0.68	0	6,6,6	0.07	0
2	SO4	B	705	-	4,4,4	0.69	0	6,6,6	0.08	0
4	WPO	A	709	-	28,28,28	0.36	0	38,41,41	0.39	0
2	SO4	B	703	-	4,4,4	0.69	0	6,6,6	0.07	0
2	SO4	A	703	-	4,4,4	0.68	0	6,6,6	0.06	0
2	SO4	B	704	-	4,4,4	0.71	0	6,6,6	0.11	0
4	WPO	C	702	-	28,28,28	0.37	0	38,41,41	0.48	0
2	SO4	A	702	-	4,4,4	0.68	0	6,6,6	0.07	0
2	SO4	B	702	-	4,4,4	0.68	0	6,6,6	0.06	0
2	SO4	A	706	-	4,4,4	0.70	0	6,6,6	0.11	0
5	PG4	B	708	-	9,9,12	0.28	0	8,8,11	0.21	0
2	SO4	A	705	-	4,4,4	0.69	0	6,6,6	0.11	0
4	WPO	A	710	-	28,28,28	0.35	0	38,41,41	0.46	0
2	SO4	B	701	-	4,4,4	0.67	0	6,6,6	0.08	0
4	WPO	C	701	-	28,28,28	0.37	0	38,41,41	0.45	0
2	SO4	A	704	-	4,4,4	0.67	0	6,6,6	0.07	0
5	PG4	A	711	-	12,12,12	0.30	0	11,11,11	0.15	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
4	WPO	B	707	-	-	0/15/31/31	0/3/3/3
4	WPO	A	709	-	-	1/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	708	-	-	1/7/7/10	-
4	WPO	A	710	-	-	9/15/31/31	0/3/3/3
4	WPO	C	701	-	-	0/15/31/31	0/3/3/3
4	WPO	C	702	-	-	10/15/31/31	0/3/3/3
5	PG4	A	711	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

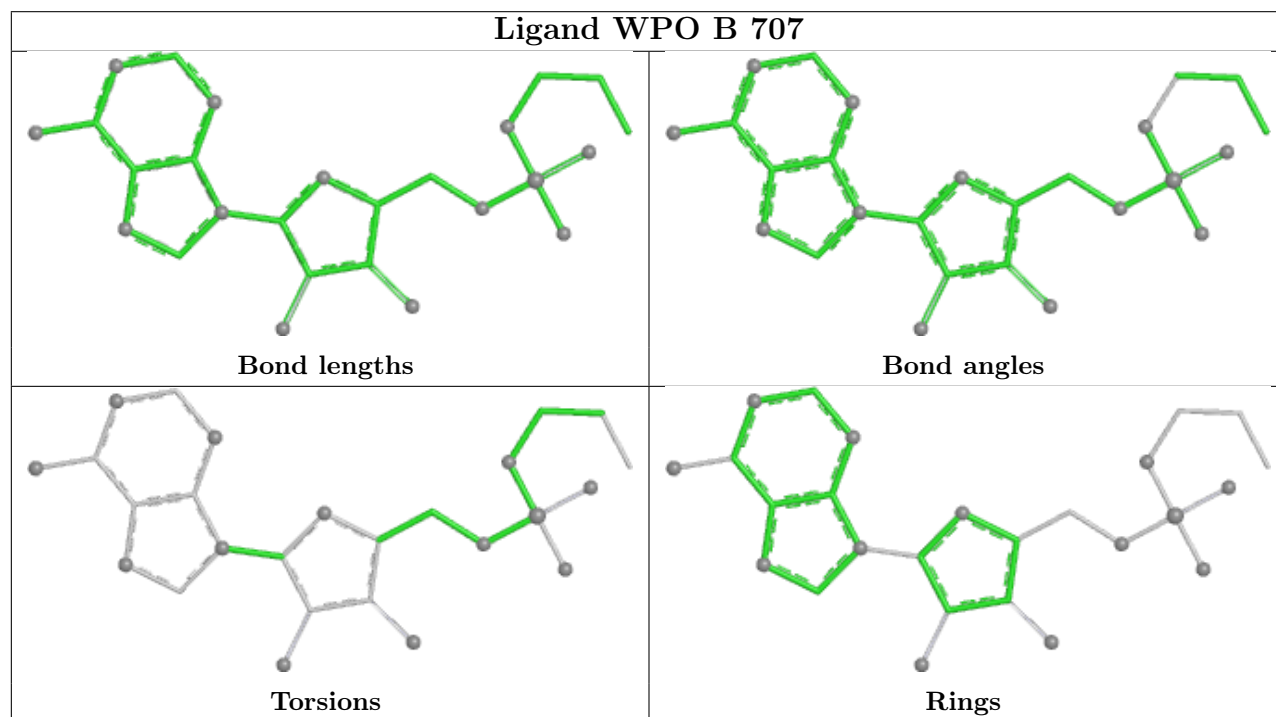
Mol	Chain	Res	Type	Atoms
4	A	710	WPO	C1P-O3P-P-O5'
4	A	710	WPO	C1P-O3P-P-O1P
4	C	702	WPO	O4'-C4'-C5'-O5'
4	C	702	WPO	C5'-O5'-P-O3P
4	C	702	WPO	C1P-O3P-P-O5'
4	C	702	WPO	C1P-O3P-P-O1P
4	C	702	WPO	C1P-O3P-P-O2P
5	B	708	PG4	O3-C5-C6-O4
5	A	711	PG4	O4-C7-C8-O5
4	A	709	WPO	O3P-C1P-C2P-C3P
4	C	702	WPO	C3'-C4'-C5'-O5'
4	A	710	WPO	C2P-C1P-O3P-P
4	C	702	WPO	C2P-C1P-O3P-P
4	A	710	WPO	O3P-C1P-C2P-C3P
5	A	711	PG4	O3-C5-C6-O4
5	A	711	PG4	C3-C4-O3-C5
5	A	711	PG4	C4-C3-O2-C2
4	A	710	WPO	C2'-C1'-N9-C8
4	C	702	WPO	C2'-C1'-N9-C8
4	A	710	WPO	C5'-O5'-P-O1P
4	A	710	WPO	C1P-O3P-P-O2P
5	A	711	PG4	O1-C1-C2-O2
4	A	710	WPO	C2'-C1'-N9-C4
4	A	710	WPO	O4'-C1'-N9-C8
4	C	702	WPO	O4'-C1'-N9-C8
4	C	702	WPO	C2'-C1'-N9-C4

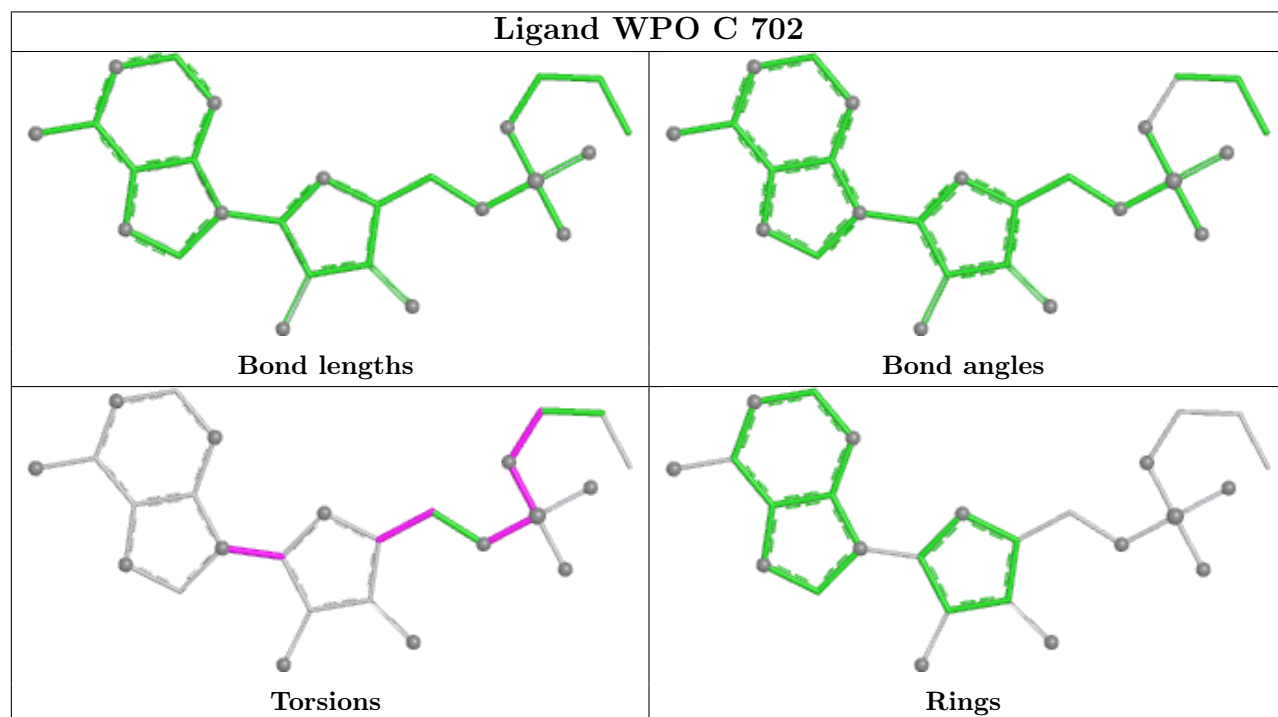
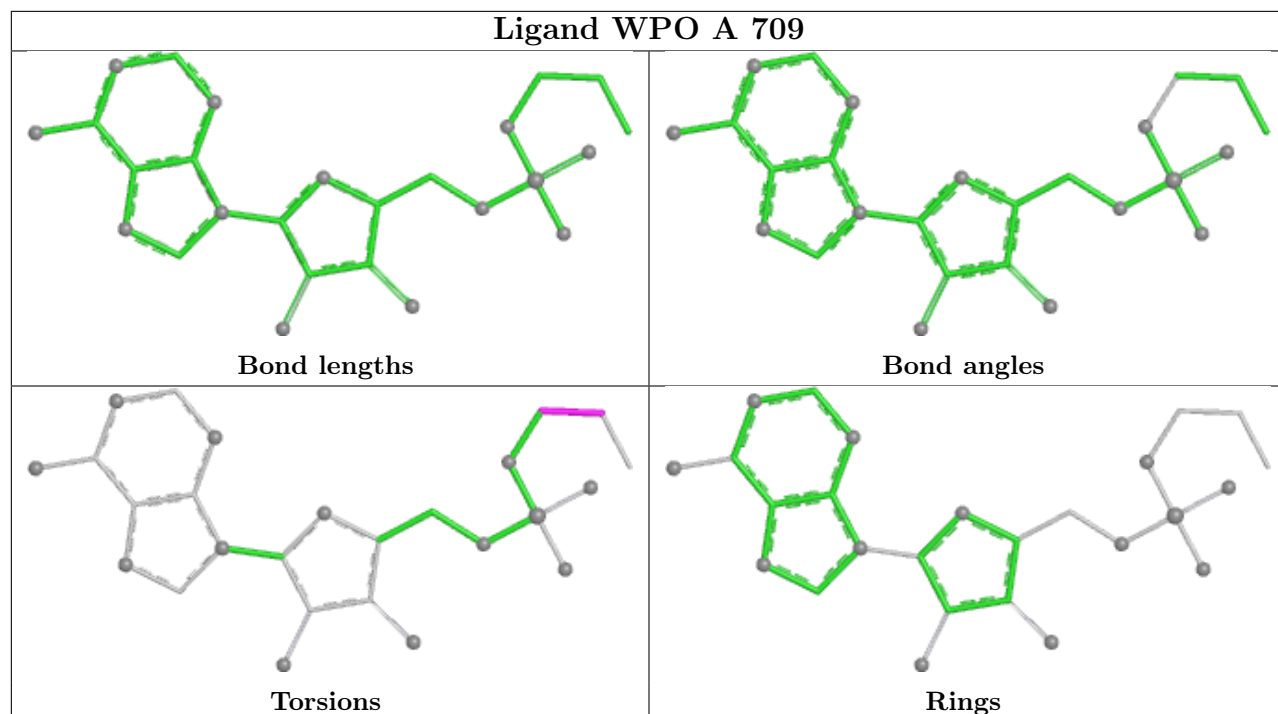
There are no ring outliers.

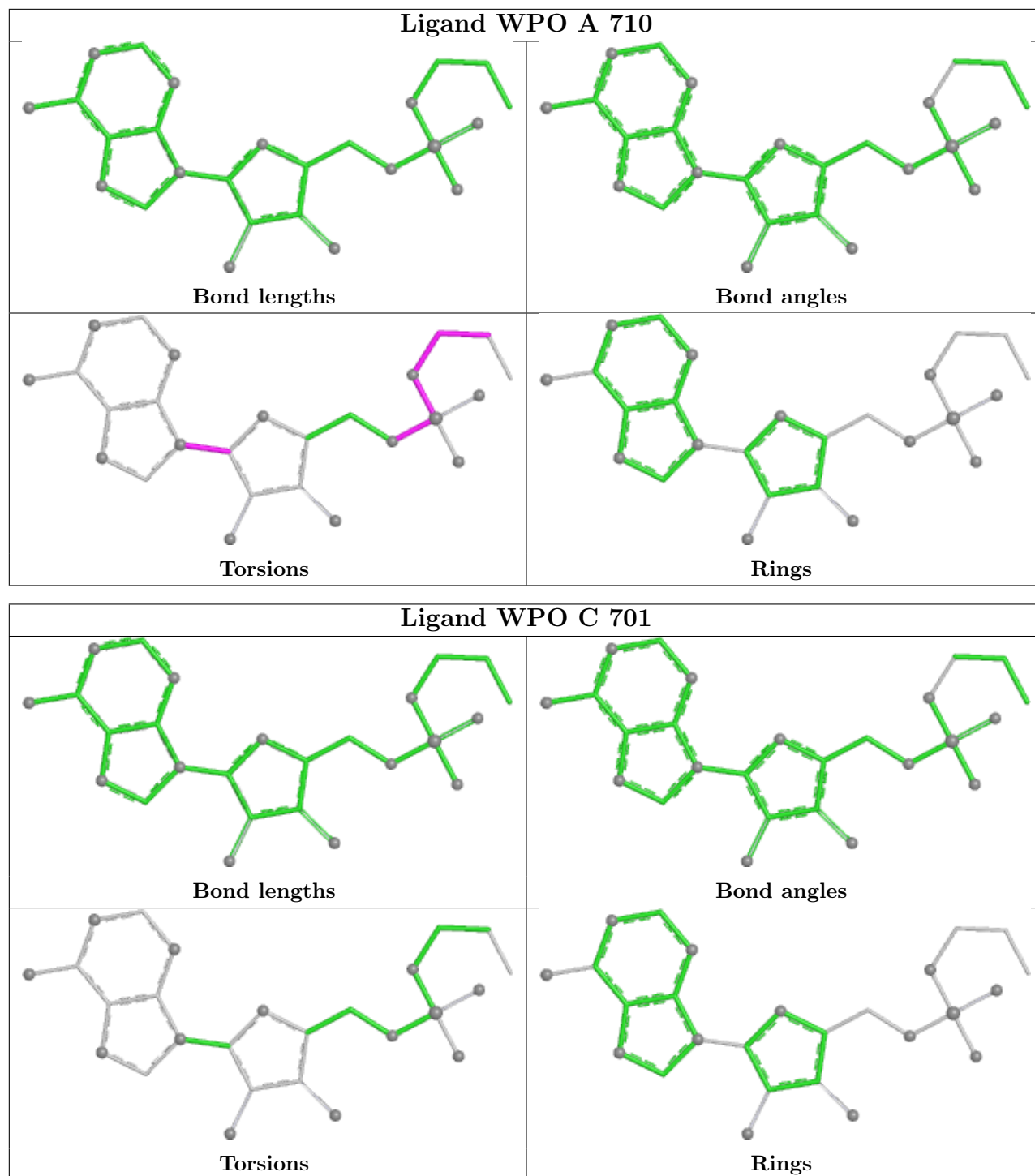
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	WPO	1	0
5	B	708	PG4	2	0
4	A	710	WPO	1	0
2	A	704	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	660/686 (96%)	0.29	31 (4%)	36	38	42, 61, 88, 148	1 (0%)
1	B	634/686 (92%)	0.46	60 (9%)	14	15	43, 62, 145, 191	0
1	C	523/686 (76%)	1.09	73 (13%)	6	7	57, 97, 141, 175	0
All	All	1817/2058 (88%)	0.58	164 (9%)	15	16	42, 67, 135, 191	1 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	666	LEU	6.9
1	A	605	ASP	6.0
1	A	20	GLN	5.0
1	B	681	ALA	4.9
1	C	364	PRO	4.9
1	B	640	ARG	4.9
1	A	684	GLY	4.7
1	C	294	THR	4.6
1	C	21	THR	4.5
1	B	648	ILE	4.4
1	B	672	VAL	4.2
1	C	435	ASN	4.1
1	B	647	ARG	4.1
1	B	300	THR	4.0
1	C	548	VAL	4.0
1	B	561	THR	4.0
1	C	387	ALA	3.9
1	B	636	LEU	3.8
1	C	359	ILE	3.7
1	B	294	THR	3.7
1	B	593	ALA	3.7
1	A	39[A]	GLU	3.7
1	C	23	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	51	HIS	3.6
1	C	257	ILE	3.6
1	C	419	PRO	3.6
1	B	592	ILE	3.6
1	B	560	SER	3.6
1	B	21	THR	3.6
1	C	482	VAL	3.6
1	C	226	THR	3.5
1	B	551	VAL	3.5
1	C	225	ARG	3.4
1	C	30	GLY	3.4
1	B	676	ILE	3.4
1	C	54	ASN	3.4
1	C	53	VAL	3.3
1	B	652	VAL	3.3
1	B	639	THR	3.3
1	B	607	GLU	3.2
1	B	554	VAL	3.2
1	C	546	GLY	3.2
1	C	138	ILE	3.2
1	A	657	ALA	3.1
1	A	620	THR	3.1
1	C	337	VAL	3.1
1	B	644	ILE	3.1
1	C	47	LYS	3.1
1	A	597	LEU	3.1
1	B	582	ILE	3.1
1	B	581	GLY	3.1
1	C	28	ALA	3.1
1	C	36	THR	3.0
1	B	586	ILE	3.0
1	C	489	GLY	3.0
1	B	550	ASP	3.0
1	A	624	PHE	3.0
1	A	421	SER	2.9
1	B	651	LYS	2.9
1	C	425	TRP	2.9
1	B	556	GLY	2.8
1	C	300	THR	2.8
1	C	222	ARG	2.8
1	C	437	CYS	2.8
1	B	553	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	577	ALA	2.8
1	B	564	ILE	2.7
1	C	50	ILE	2.7
1	C	531	GLY	2.7
1	C	24	VAL	2.7
1	A	629	SER	2.7
1	B	645	MET	2.7
1	C	55	GLN	2.7
1	A	298	THR	2.7
1	C	57	LYS	2.7
1	C	224	GLY	2.7
1	A	559	LEU	2.7
1	A	652	VAL	2.6
1	A	297	SER	2.6
1	B	632	ILE	2.6
1	C	410	LEU	2.6
1	C	431	PHE	2.6
1	C	428	TYR	2.6
1	C	432	VAL	2.6
1	C	459	VAL	2.6
1	A	295	SER	2.6
1	B	629	SER	2.6
1	C	302	LYS	2.6
1	C	301	PRO	2.6
1	C	365	ALA	2.5
1	B	608	GLY	2.5
1	B	591	VAL	2.5
1	C	31	VAL	2.5
1	C	56	TYR	2.5
1	A	599	GLU	2.5
1	B	559	LEU	2.5
1	B	638	LYS	2.5
1	C	40	PHE	2.5
1	A	617	VAL	2.5
1	C	420	ILE	2.5
1	A	613	LEU	2.5
1	B	649	LEU	2.5
1	C	38	LYS	2.5
1	C	221	LYS	2.5
1	A	369	TYR	2.5
1	B	654	SER	2.4
1	C	229	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	212	LYS	2.4
1	A	654	SER	2.4
1	B	552	VAL	2.4
1	B	57	LYS	2.4
1	B	568	LEU	2.4
1	C	545	ARG	2.4
1	C	335	GLY	2.4
1	C	217	CYS	2.4
1	C	444	TRP	2.4
1	B	557	HIS	2.4
1	A	36	THR	2.4
1	A	606	SER	2.4
1	B	548	VAL	2.4
1	B	574	VAL	2.4
1	A	120	ASN	2.3
1	C	464	PRO	2.3
1	B	56	TYR	2.3
1	B	612	GLU	2.3
1	B	679	PHE	2.3
1	A	557	HIS	2.3
1	C	232	LEU	2.3
1	B	585	ASP	2.3
1	C	48	GLY	2.3
1	A	299	GLY	2.2
1	B	421	SER	2.2
1	C	130	ALA	2.2
1	C	390	ALA	2.2
1	B	653	SER	2.2
1	C	398	GLY	2.2
1	C	465	GLY	2.2
1	A	300	THR	2.2
1	C	339	TRP	2.1
1	B	423	ASP	2.1
1	C	457	ALA	2.1
1	A	618	ARG	2.1
1	B	619	LYS	2.1
1	A	31	VAL	2.1
1	C	471	PHE	2.1
1	B	588	GLY	2.1
1	B	597	LEU	2.1
1	C	33	LEU	2.1
1	C	391	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	394	LEU	2.1
1	C	268	ASP	2.1
1	C	520	TYR	2.1
1	B	51	HIS	2.1
1	B	589	GLN	2.1
1	C	371	ARG	2.1
1	A	583	HIS	2.1
1	A	630	VAL	2.1
1	C	373	TRP	2.1
1	B	572	LYS	2.0
1	B	678	ALA	2.0
1	C	484	GLY	2.0
1	B	655	ASN	2.0
1	C	456	LEU	2.0
1	A	628	LYS	2.0

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

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(Å ²)	Q<0.9
2	SO4	A	706	5/5	0.52	0.20	63,68,75,99	0
2	SO4	B	704	5/5	0.56	0.20	64,65,67,99	0
4	WPO	C	702	26/26	0.59	0.22	101,112,127,134	26
2	SO4	A	704	5/5	0.65	0.15	82,88,98,109	0
2	SO4	B	703	5/5	0.65	0.14	89,91,113,118	0
3	CL	A	708	1/1	0.67	0.27	123,123,123,123	0
2	SO4	A	702	5/5	0.72	0.14	78,96,103,124	0
5	PG4	A	711	13/13	0.73	0.26	62,70,88,91	0

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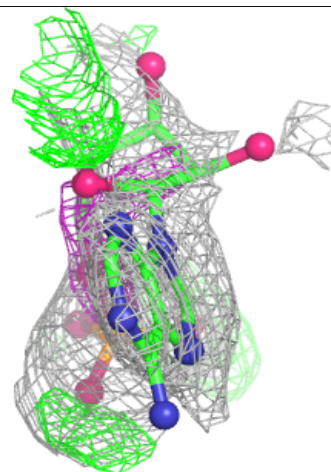
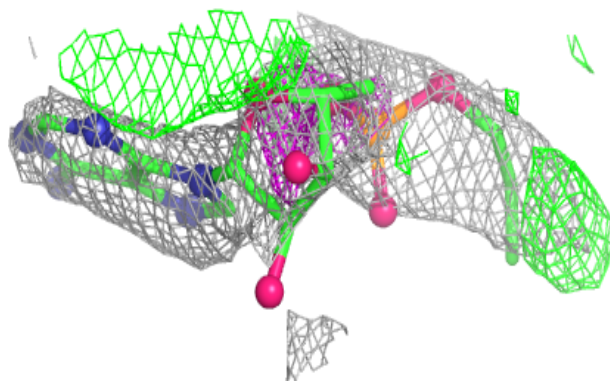
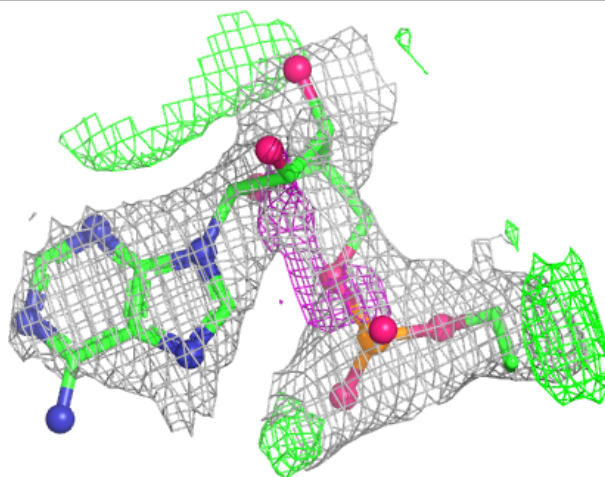
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	703	5/5	0.75	0.14	74,87,102,104	0
2	SO4	B	702	5/5	0.77	0.18	71,83,95,106	0
2	SO4	B	701	5/5	0.77	0.11	117,119,124,125	0
2	SO4	B	705	5/5	0.80	0.11	67,70,85,88	0
4	WPO	A	710	26/26	0.83	0.18	59,71,76,83	26
4	WPO	C	701	26/26	0.84	0.16	94,106,115,157	0
5	PG4	B	708	10/13	0.85	0.17	78,82,86,94	0
2	SO4	A	701	5/5	0.86	0.13	87,90,108,114	0
2	SO4	A	705	5/5	0.88	0.27	65,66,71,75	0
3	CL	B	706	1/1	0.90	0.17	91,91,91,91	0
3	CL	A	707	1/1	0.96	0.22	85,85,85,85	0
4	WPO	A	709	26/26	0.97	0.07	43,48,52,53	0
4	WPO	B	707	26/26	0.97	0.07	49,54,61,65	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.

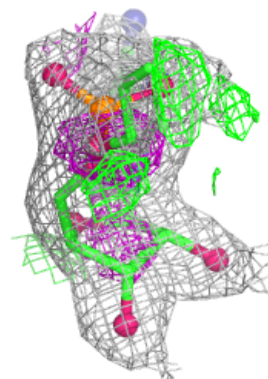
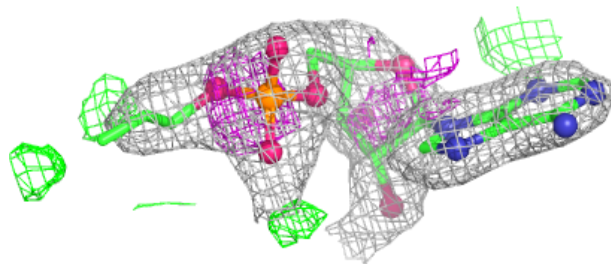
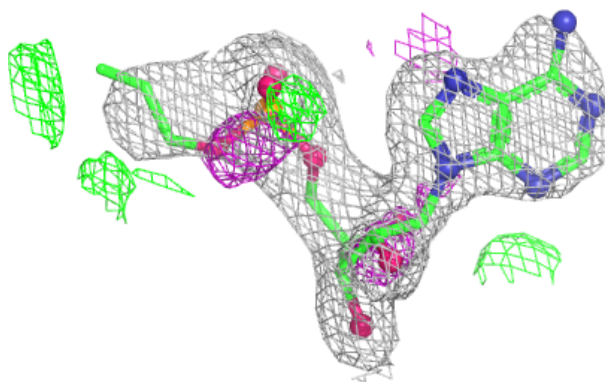
Electron density around WPO C 702:

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



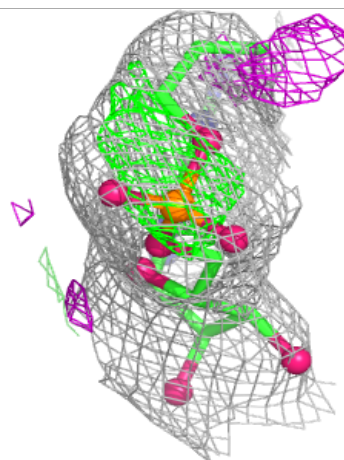
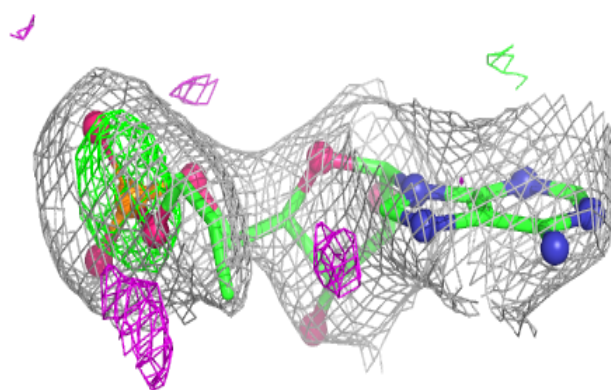
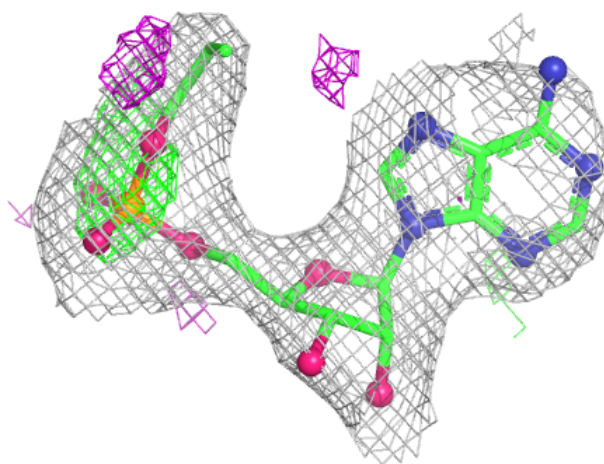
Electron density around WPO A 710:

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



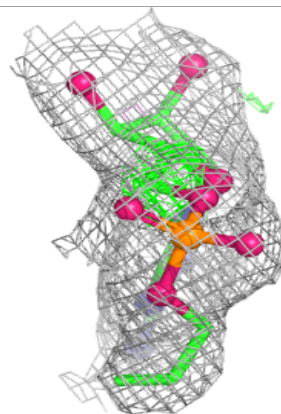
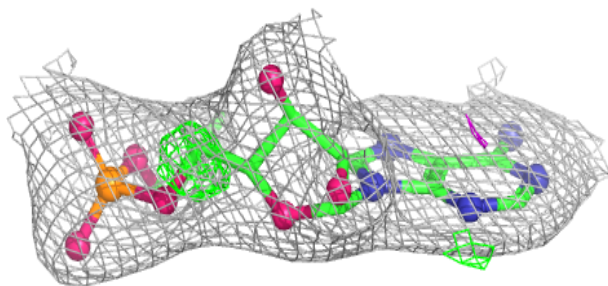
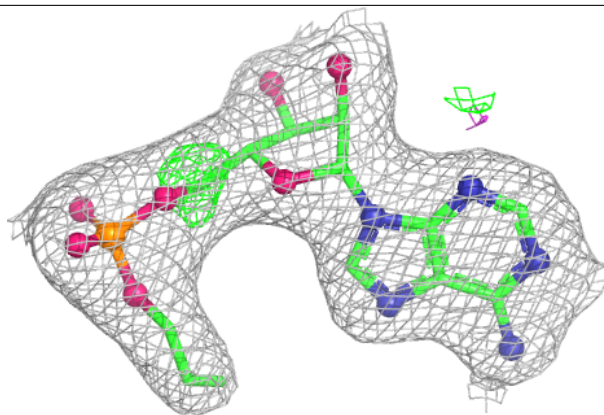
Electron density around WPO C 701:

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

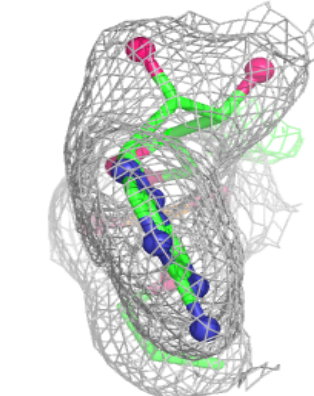
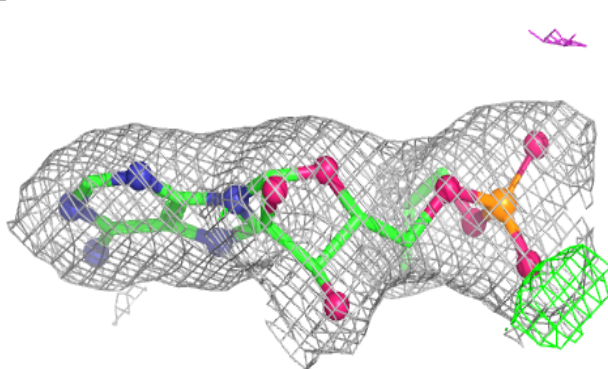
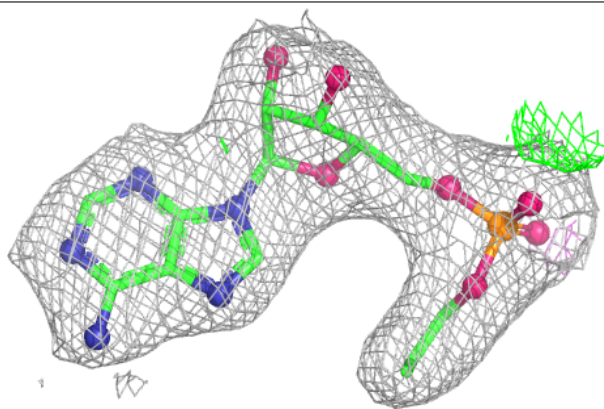


Electron density around WPO A 709:

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

**Electron density around WPO B 707:**

$2mF_o-DF_c$ (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.