Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2023 – 04:10 PM EST

PDB ID	:	8V4P
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:

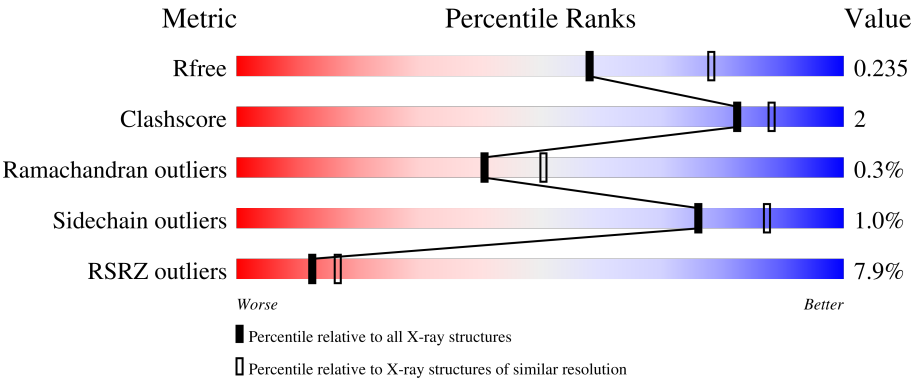
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	2% 90% 6% ·
1	B	686	11% 86% 6% 8%
1	C	686	8% 71% 5% 24%

2 Entry composition (i)

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 Q8NJN3
A	2	HIS	-	expression tag	UNP Q8NJN3
A	3	HIS	-	expression tag	UNP Q8NJN3
A	4	HIS	-	expression tag	UNP Q8NJN3
A	5	HIS	-	expression tag	UNP Q8NJN3
A	6	HIS	-	expression tag	UNP Q8NJN3
A	7	HIS	-	expression tag	UNP Q8NJN3
A	8	HIS	-	expression tag	UNP Q8NJN3
A	9	HIS	-	expression tag	UNP Q8NJN3
A	10	GLU	-	expression tag	UNP Q8NJN3
A	11	ASN	-	expression tag	UNP Q8NJN3
A	12	LEU	-	expression tag	UNP Q8NJN3
A	13	TYR	-	expression tag	UNP Q8NJN3
A	14	PHE	-	expression tag	UNP Q8NJN3
A	15	GLN	-	expression tag	UNP Q8NJN3
A	16	GLY	-	expression tag	UNP Q8NJN3
A	403	ALA	VAL	variant	UNP Q8NJN3
B	1	MET	-	initiating methionine	UNP Q8NJN3
B	2	HIS	-	expression tag	UNP Q8NJN3
B	3	HIS	-	expression tag	UNP Q8NJN3
B	4	HIS	-	expression tag	UNP Q8NJN3
B	5	HIS	-	expression tag	UNP Q8NJN3
B	6	HIS	-	expression tag	UNP Q8NJN3

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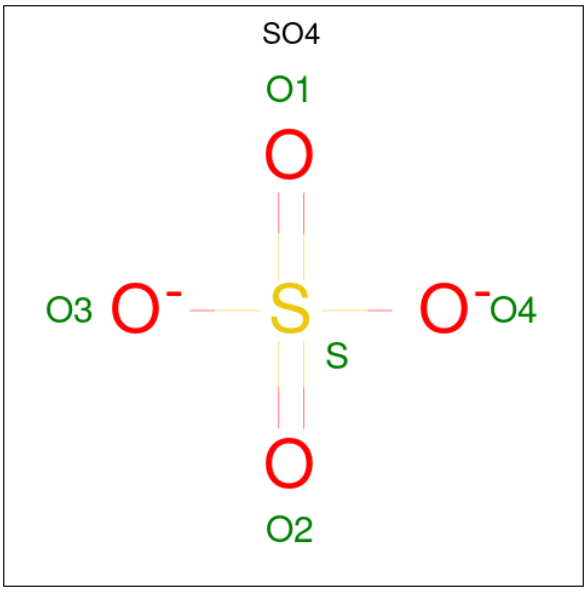
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8NJN3
B	8	HIS	-	expression tag	UNP Q8NJN3
B	9	HIS	-	expression tag	UNP Q8NJN3
B	10	GLU	-	expression tag	UNP Q8NJN3
B	11	ASN	-	expression tag	UNP Q8NJN3
B	12	LEU	-	expression tag	UNP Q8NJN3
B	13	TYR	-	expression tag	UNP Q8NJN3
B	14	PHE	-	expression tag	UNP Q8NJN3
B	15	GLN	-	expression tag	UNP Q8NJN3
B	16	GLY	-	expression tag	UNP Q8NJN3
B	403	ALA	VAL	variant	UNP Q8NJN3
C	1	MET	-	initiating methionine	UNP Q8NJN3
C	2	HIS	-	expression tag	UNP Q8NJN3
C	3	HIS	-	expression tag	UNP Q8NJN3
C	4	HIS	-	expression tag	UNP Q8NJN3
C	5	HIS	-	expression tag	UNP Q8NJN3
C	6	HIS	-	expression tag	UNP Q8NJN3
C	7	HIS	-	expression tag	UNP Q8NJN3
C	8	HIS	-	expression tag	UNP Q8NJN3
C	9	HIS	-	expression tag	UNP Q8NJN3
C	10	GLU	-	expression tag	UNP Q8NJN3
C	11	ASN	-	expression tag	UNP Q8NJN3
C	12	LEU	-	expression tag	UNP Q8NJN3
C	13	TYR	-	expression tag	UNP Q8NJN3
C	14	PHE	-	expression tag	UNP Q8NJN3
C	15	GLN	-	expression tag	UNP Q8NJN3
C	16	GLY	-	expression tag	UNP Q8NJN3
C	403	ALA	VAL	variant	UNP Q8NJN3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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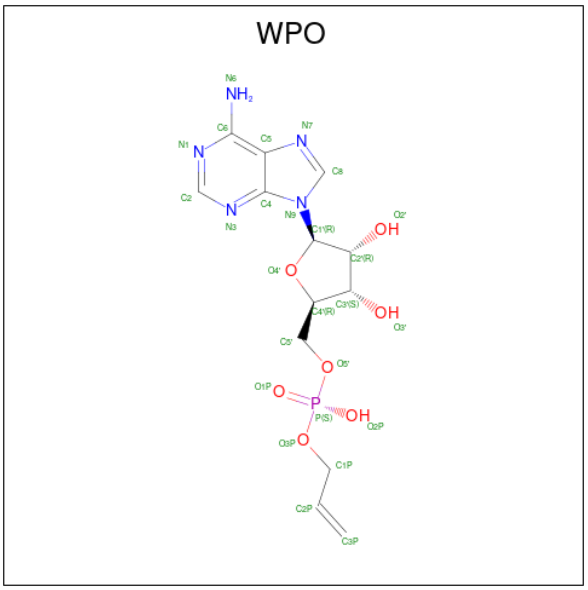
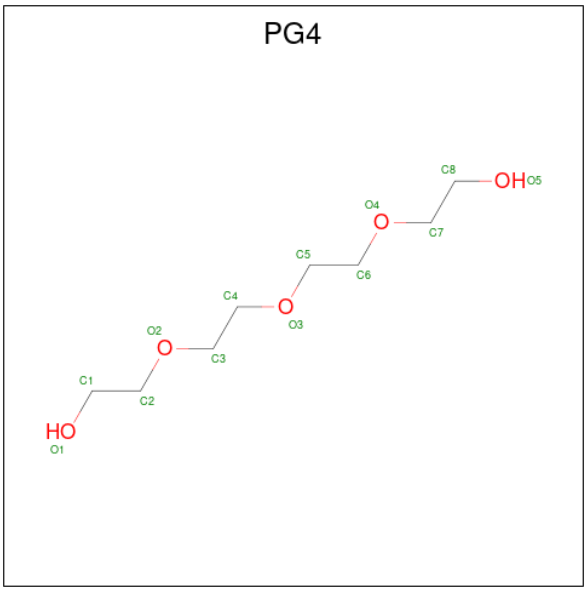
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is 5'-O-{(S)-hydroxy[(prop-2-en-1-yl)oxy]phosphoryl}adenosine (three-letter code: WPO) (formula: $C_{13}H_{18}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 6 is water.

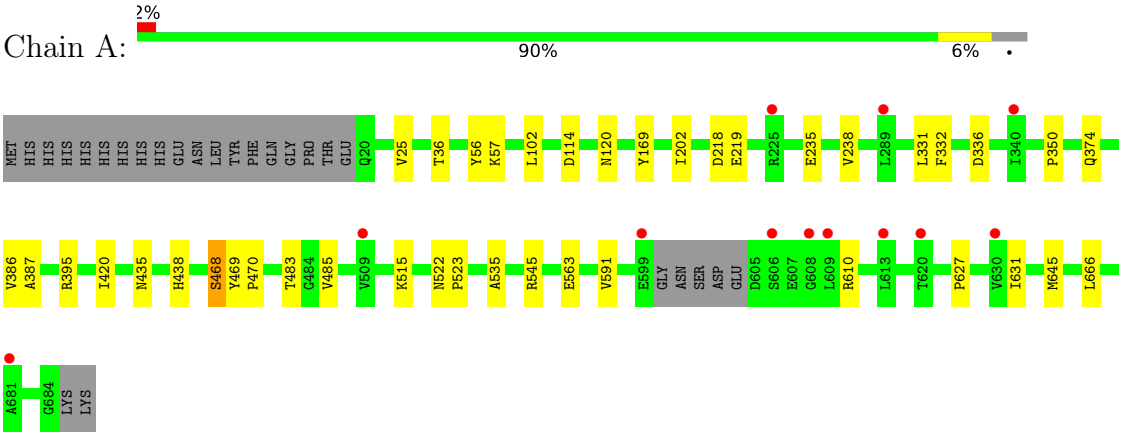
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	183	Total O 183 183	0	0
6	B	156	Total O 156 156	0	0
6	C	27	Total O 27 27	0	0

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.

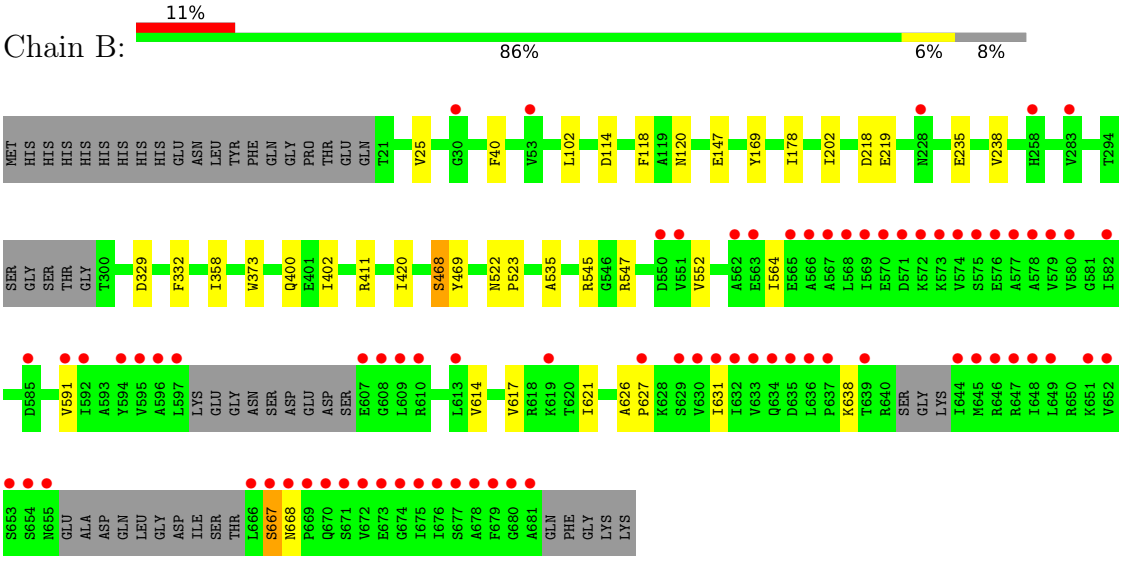
• Molecule 1: Acetyl-coenzyme A synthetase 2

Chain A:



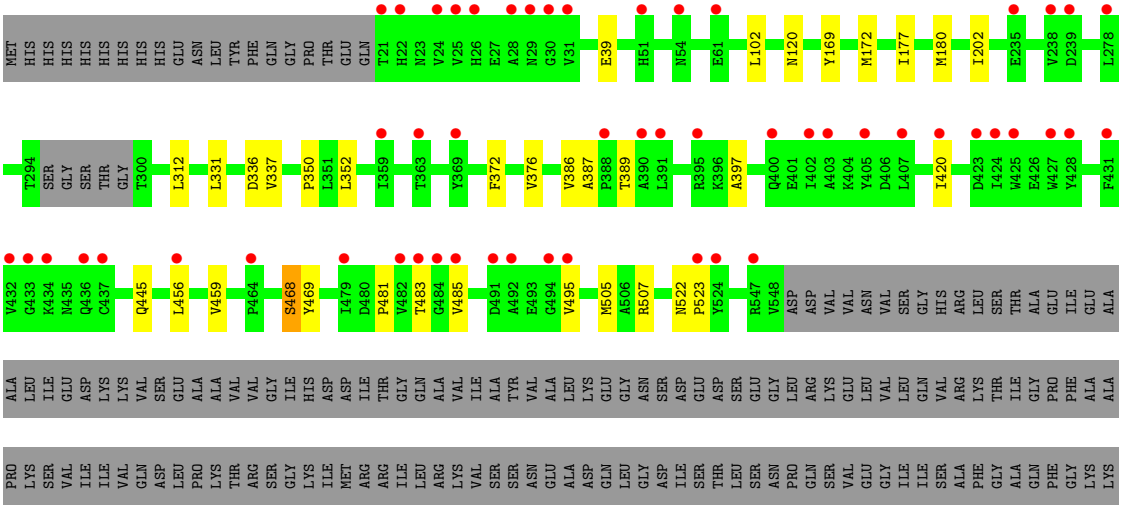
• Molecule 1: Acetyl-coenzyme A synthetase 2

Chain B:



• Molecule 1: Acetyl-coenzyme A synthetase 2

Chain C:


MET HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY PRO THR GLU GLN T21 H22 N23 V24 V25 H26 E27 A28 N29 G30 V31 E39 H51 N54 E61 L102 N120 Y169 M172 I177 M180 I202 E235 V238 D239 L278
T294 SER GLY SER THR GLY T300 L312 L331 D336 V337 P350 L351 L352 I359 T363 Y369 F372 V376 V386 A387 P388 T389 A390 L391 R396 K396 A397 Q400 E401 I402 A403 K404 Y405 D406 L407 I420 D423 I424 W425 E426 W427 Y428 F431
V432 G433 K434 N435 Q436 C437 Q445 L456 V459 P464 S468 Y469 I479 D480 P481 V482 T483 G484 V485 D491 A492 E493 G494 V495 M505 A506 R507 N522 P523 Y524 R547 V548 ASP ASP VAL VAL ASN VAL SER GLY HIS ARG LEU SER THR ALA GLU ILE GLU ALA
ALA LEU ILE GLU ASP LYS LYS VAL SER GLU ALA ALA VAL VAL GLY ILE HIS ASP ASP ILE THR GLY GLN ALA VAL ILE ALA TYR VAL ALA LEU LYS GLU GLY ASN SER ASP GLU ASP SER GLU GLY LEU ARG LYS GLU LEU VAL LEU GLN VAL ARG LYS THR ILE GLY PRO PHE ALA ALA
PRO LYS SER VAL ILE ILE VAL GLN ASP LEU PRO LYS THR ARG SER GLY LYS ILE MET ARG ARG ILE LEU ARG LYS VAL SER SER ASN GLU ALA ASP GLN LEU GLY ASP ILE SER THR LEU SER ASN PRO GLN SER VAL GLU GLY ILE ILE SER ALA PHE GLY ALA GLN PHE GLY LYS LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.211 , 0.238 0.210 , 0.235	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 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PG4, WPO, CL, SO4

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	0.25	0/5215	0.48	0/7103
1	B	0.25	0/5013	0.48	0/6830
1	C	0.24	0/4163	0.44	0/5686
All	All	0.25	0/14391	0.47	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

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	22	0
1	B	4888	0	4741	25	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	68	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 2.

All (68) 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: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: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:A:645:MET:HE3	1:A:666:LEU:HG	1.91	0.52
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:180:MET:HE1	1:C:337:VAL:HG11	1.94	0.49
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: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: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: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
1:C:177:ILE:HA	1:C:180:MET:HE3	2.04	0.40
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%)	47	58
1	B	624/686 (91%)	602 (96%)	20 (3%)	2 (0%)	41	50
1	C	519/686 (76%)	491 (95%)	25 (5%)	3 (1%)	25	31
All	All	1800/2058 (88%)	1733 (96%)	61 (3%)	6 (0%)	41	50

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%)	524 (99%)	7 (1%)	69	82
1	B	510/568 (90%)	506 (99%)	4 (1%)	81	91
1	C	416/568 (73%)	413 (99%)	3 (1%)	84	92
All	All	1457/1704 (86%)	1443 (99%)	14 (1%)	76	87

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

Mol	Chain	Res	Type
1	A	114	ASP
1	A	120	ASN
1	A	332	PHE
1	A	435	ASN
1	A	515	LYS
1	A	545	ARG
1	A	610	ARG
1	B	114	ASP
1	B	120	ASN
1	B	400	GLN
1	B	545	ARG
1	C	120	ASN
1	C	389	THR
1	C	445	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN

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 monosaccharides 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	$\#\|Z\| > 2$
2	SO4	B	702	-	4,4,4	0.61	0	6,6,6	0.05	0
4	WPO	A	709	-	25,28,28	0.65	0	25,41,41	0.71	1 (4%)
4	WPO	C	702	-	25,28,28	0.65	0	25,41,41	0.79	1 (4%)
5	PG4	A	711	-	12,12,12	0.29	0	11,11,11	0.15	0
2	SO4	A	704	-	4,4,4	0.59	0	6,6,6	0.05	0
2	SO4	A	702	-	4,4,4	0.61	0	6,6,6	0.04	0
2	SO4	B	704	-	4,4,4	0.64	0	6,6,6	0.17	0
4	WPO	A	710	-	25,28,28	0.63	0	25,41,41	0.73	1 (4%)
4	WPO	B	707	-	25,28,28	0.66	0	25,41,41	0.77	1 (4%)
2	SO4	B	705	-	4,4,4	0.62	0	6,6,6	0.06	0
2	SO4	A	705	-	4,4,4	0.61	0	6,6,6	0.08	0
5	PG4	B	708	-	9,9,12	0.27	0	8,8,11	0.21	0
2	SO4	B	703	-	4,4,4	0.62	0	6,6,6	0.04	0
2	SO4	A	701	-	4,4,4	0.61	0	6,6,6	0.04	0
2	SO4	B	701	-	4,4,4	0.59	0	6,6,6	0.05	0
4	WPO	C	701	-	25,28,28	0.65	0	25,41,41	0.79	1 (4%)
2	SO4	A	706	-	4,4,4	0.63	0	6,6,6	0.10	0
2	SO4	A	703	-	4,4,4	0.61	0	6,6,6	0.10	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	C	702	-	-	8/11/31/31	0/3/3/3
4	WPO	A	709	-	-	1/11/31/31	0/3/3/3
4	WPO	A	710	-	-	6/11/31/31	0/3/3/3
4	WPO	B	707	-	-	0/11/31/31	0/3/3/3
4	WPO	C	701	-	-	0/11/31/31	0/3/3/3
5	PG4	A	711	-	-	5/10/10/10	-
5	PG4	B	708	-	-	1/7/7/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	701	WPO	C5-C6-N6	2.31	123.86	120.35
4	B	707	WPO	C5-C6-N6	2.28	123.81	120.35
4	A	709	WPO	C5-C6-N6	2.27	123.81	120.35
4	C	702	WPO	C5-C6-N6	2.23	123.75	120.35
4	A	710	WPO	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

All (21) 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	C1P-O3P-P-O1P
4	C	702	WPO	C1P-O3P-P-O2P
4	C	702	WPO	C3'-C4'-C5'-O5'
5	B	708	PG4	O3-C5-C6-O4
4	A	709	WPO	O3P-C1P-C2P-C3P
5	A	711	PG4	O4-C7-C8-O5
4	C	702	WPO	C1P-O3P-P-O5'
4	A	710	WPO	O3P-C1P-C2P-C3P
4	A	710	WPO	C2P-C1P-O3P-P
4	C	702	WPO	C2P-C1P-O3P-P
4	C	702	WPO	C5'-O5'-P-O3P
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	C1P-O3P-P-O2P
5	A	711	PG4	O1-C1-C2-O2
4	A	710	WPO	C5'-O5'-P-O1P
4	C	702	WPO	C5'-O5'-P-O1P

There are no ring outliers.

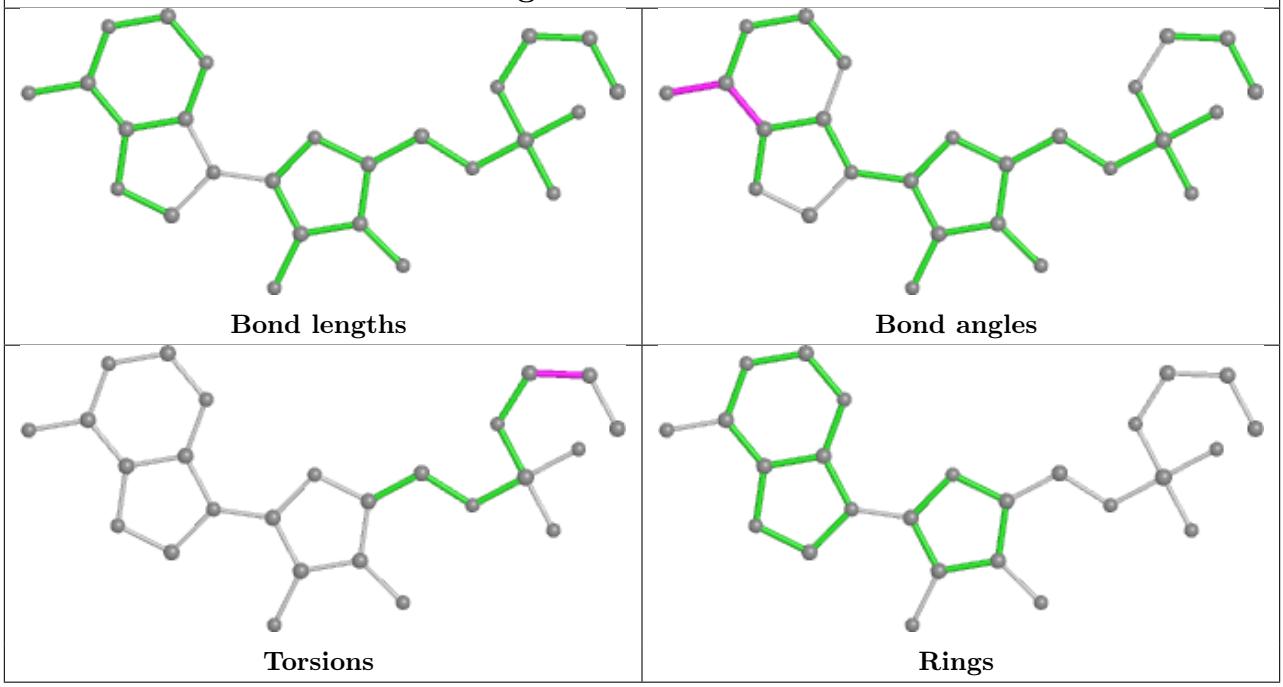
4 monomers are involved in 5 short contacts:

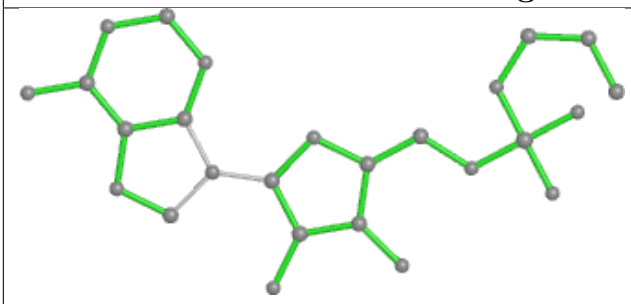
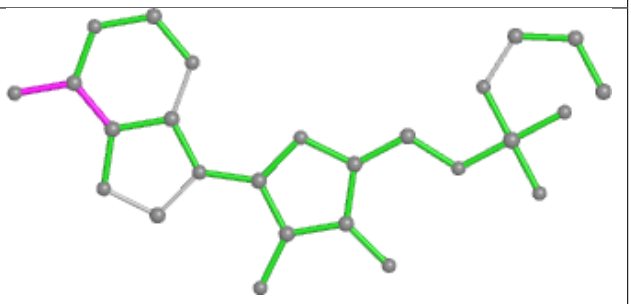
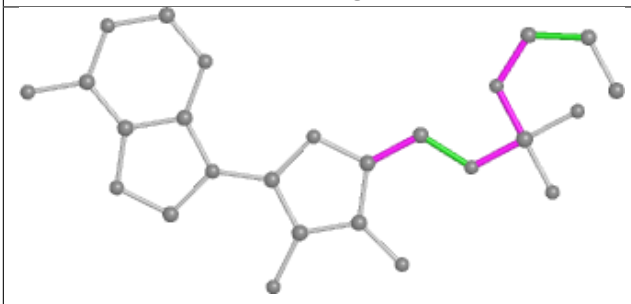
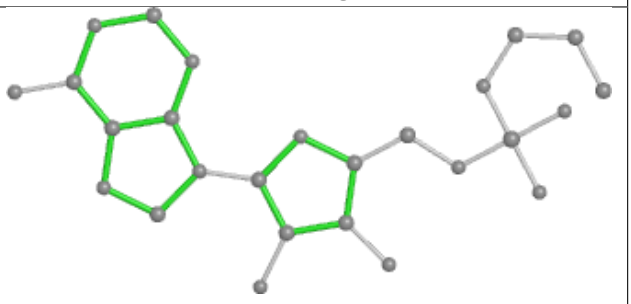
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	WPO	1	0
2	A	704	SO4	1	0
4	A	710	WPO	1	0
5	B	708	PG4	2	0

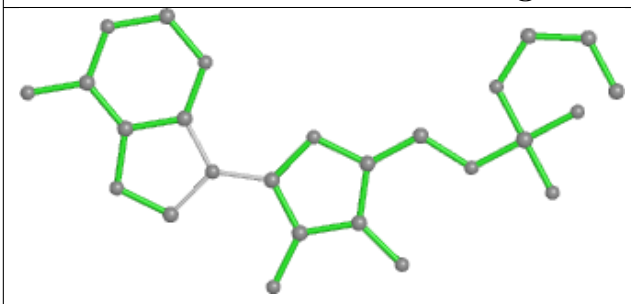
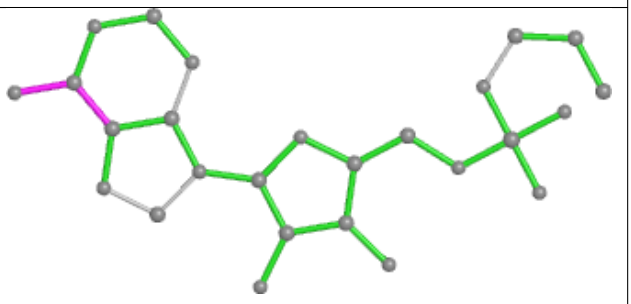
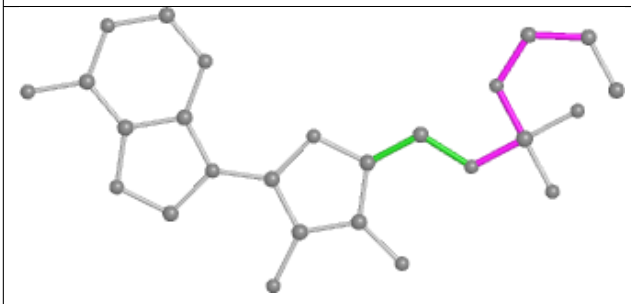
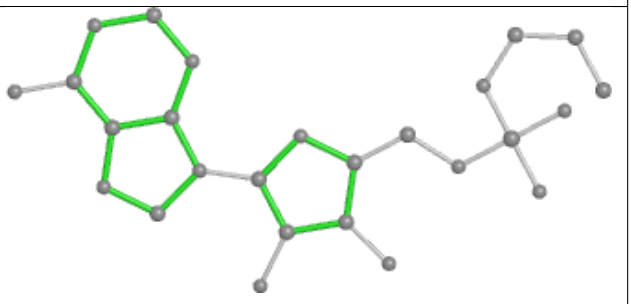
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

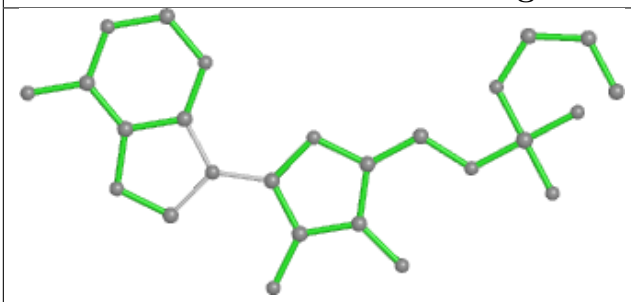
Ligand WPO A 709



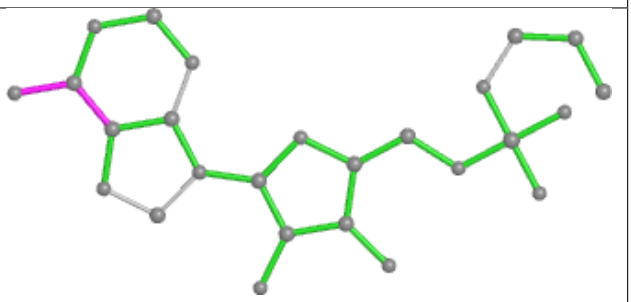
Ligand WPO C 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WPO A 710	
	
Bond lengths	Bond angles
	
Torsions	Rings

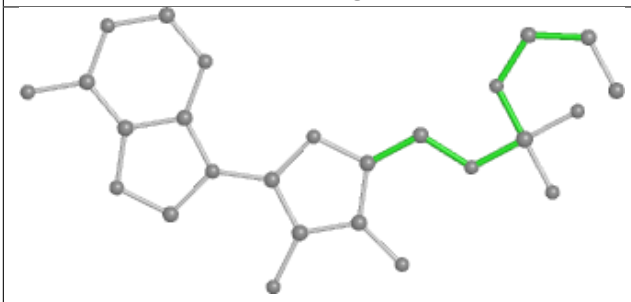
Ligand WPO B 707



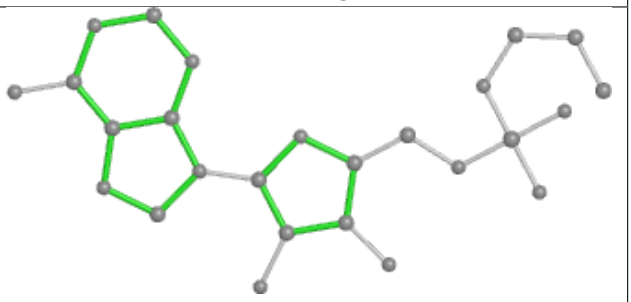
Bond lengths



Bond angles

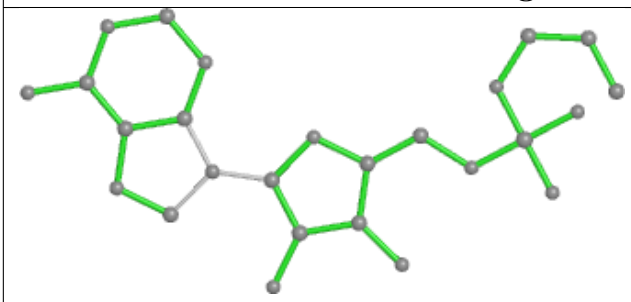


Torsions

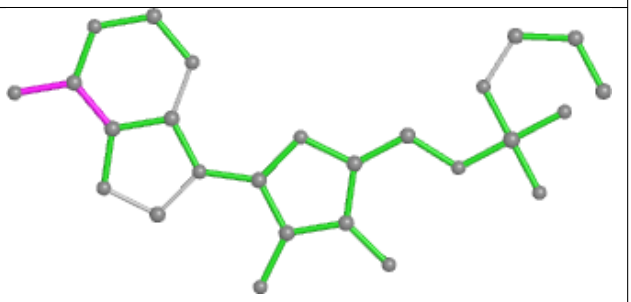


Rings

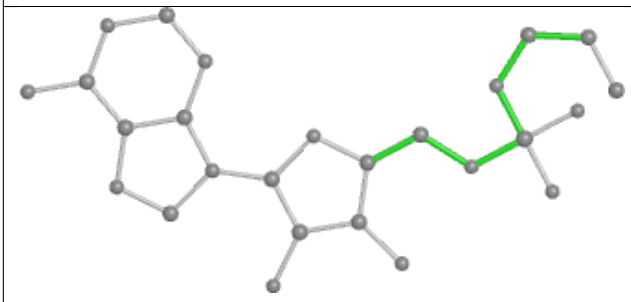
Ligand WPO C 701



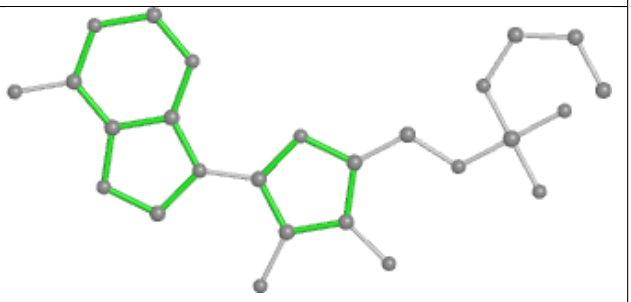
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.23	12 (1%) 68 74	42, 61, 88, 148	0
1	B	634/686 (92%)	0.64	77 (12%) 4 6	43, 62, 145, 191	0
1	C	523/686 (76%)	0.58	54 (10%) 6 9	57, 97, 141, 175	0
All	All	1817/2058 (88%)	0.47	143 (7%) 12 17	42, 67, 135, 191	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	LEU	11.0
1	B	672	VAL	10.1
1	B	679	PHE	8.5
1	B	676	ILE	8.3
1	B	632	ILE	8.3
1	B	644	ILE	8.2
1	B	678	ALA	7.6
1	B	595	VAL	7.5
1	B	675	ILE	7.3
1	B	631	ILE	7.0
1	B	550	ASP	6.9
1	C	28	ALA	6.7
1	B	597	LEU	6.6
1	B	633	VAL	6.3
1	B	671	SER	6.1
1	B	635	ASP	6.1
1	B	637	PRO	6.0
1	C	25	VAL	5.7
1	C	482	VAL	5.7
1	B	574	VAL	5.6
1	B	596	ALA	5.5
1	B	668	ASN	5.4
1	B	567	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	646	ARG	5.1
1	B	674	GLY	5.1
1	B	669	PRO	5.1
1	C	24	VAL	5.0
1	B	673	GLU	5.0
1	C	437	CYS	5.0
1	B	670	GLN	4.9
1	B	639	THR	4.9
1	B	569	ILE	4.8
1	B	613	LEU	4.7
1	B	648	ILE	4.6
1	B	680	GLY	4.6
1	C	431	PHE	4.6
1	B	575	SER	4.6
1	B	645	MET	4.5
1	C	420	ILE	4.5
1	B	667	SER	4.5
1	B	629	SER	4.4
1	B	677	SER	4.3
1	C	432	VAL	4.3
1	B	572	LYS	4.3
1	B	634	GLN	4.2
1	B	610	ARG	4.2
1	C	492	ALA	4.0
1	B	652	VAL	4.0
1	C	405	TYR	3.9
1	B	576	GLU	3.9
1	B	609	LEU	3.9
1	B	573	LYS	3.8
1	B	571	ASP	3.8
1	C	427	TRP	3.8
1	C	30	GLY	3.8
1	B	568	LEU	3.8
1	C	391	LEU	3.7
1	B	591	VAL	3.7
1	C	26	HIS	3.7
1	B	562	ALA	3.7
1	B	653	SER	3.7
1	B	594	TYR	3.7
1	C	403	ALA	3.6
1	C	436	GLN	3.6
1	C	485	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	258	HIS	3.5
1	B	630	VAL	3.5
1	B	570	GLU	3.5
1	C	21	THR	3.5
1	C	494	GLY	3.4
1	B	578	ALA	3.3
1	B	566	ALA	3.3
1	C	479	ILE	3.3
1	C	54	ASN	3.3
1	A	609	LEU	3.2
1	C	464	PRO	3.2
1	B	30	GLY	3.2
1	C	390	ALA	3.2
1	C	22	HIS	3.2
1	C	400	GLN	3.2
1	B	655	ASN	3.1
1	C	407	LEU	3.1
1	C	402	ILE	3.1
1	C	29	ASN	3.1
1	C	31	VAL	3.1
1	C	484	GLY	3.1
1	A	340	ILE	3.1
1	A	613	LEU	3.1
1	B	654	SER	3.0
1	C	428	TYR	3.0
1	B	651	LYS	3.0
1	B	592	ILE	3.0
1	A	681	ALA	2.9
1	B	647	ARG	2.8
1	C	424	ILE	2.8
1	B	681	ALA	2.7
1	C	483	THR	2.7
1	C	51	HIS	2.7
1	C	433	GLY	2.7
1	C	61	GLU	2.7
1	B	579	VAL	2.7
1	C	363	THR	2.7
1	C	425	TRP	2.6
1	B	53	VAL	2.6
1	A	606	SER	2.6
1	B	577	ALA	2.6
1	C	388	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	225	ARG	2.6
1	C	395	ARG	2.6
1	C	278	LEU	2.5
1	B	649	LEU	2.5
1	B	627	PRO	2.5
1	B	585	ASP	2.5
1	C	491	ASP	2.4
1	B	582	ILE	2.4
1	B	283	VAL	2.3
1	C	423	ASP	2.3
1	C	235	GLU	2.3
1	A	289	LEU	2.3
1	C	369	TYR	2.3
1	A	620	THR	2.3
1	A	630	VAL	2.3
1	C	523	PRO	2.3
1	B	607	GLU	2.2
1	A	608	GLY	2.2
1	C	239	ASP	2.2
1	C	495	VAL	2.2
1	B	608	GLY	2.2
1	A	599	GLU	2.2
1	B	666	LEU	2.2
1	B	580	VAL	2.2
1	B	563	GLU	2.2
1	B	619	LYS	2.1
1	C	456	LEU	2.1
1	B	228	ASN	2.1
1	C	547	ARG	2.1
1	B	551	VAL	2.1
1	C	238	VAL	2.1
1	C	359	ILE	2.1
1	C	524	TYR	2.1
1	B	565	GLU	2.0
1	A	509	VAL	2.0
1	C	434	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 monosaccharides in this entry.

6.4 Ligands (i)

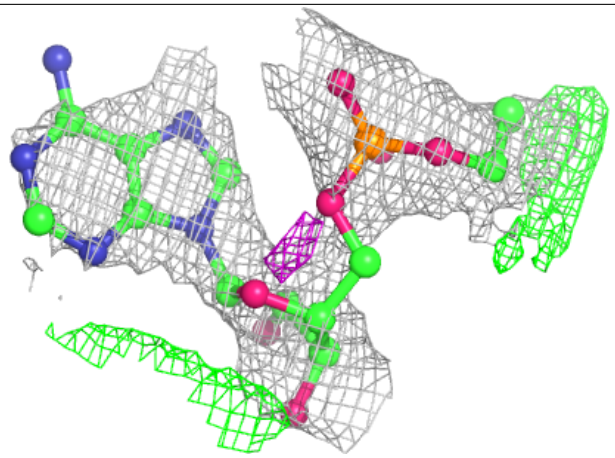
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

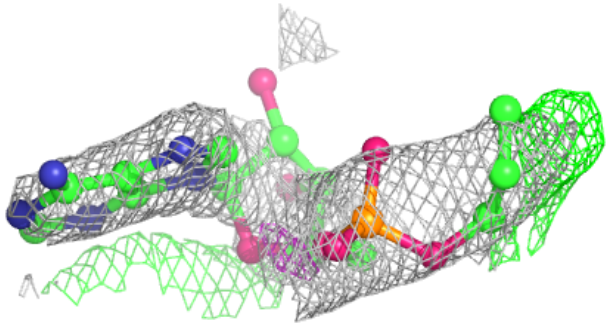
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	708	1/1	0.47	0.36	123,123,123,123	0
4	WPO	C	702	26/26	0.66	0.38	101,112,127,134	26
2	SO4	B	704	5/5	0.71	0.26	64,65,67,99	0
2	SO4	A	706	5/5	0.73	0.27	63,68,75,99	0
5	PG4	A	711	13/13	0.80	0.32	62,70,88,91	0
2	SO4	B	701	5/5	0.82	0.24	117,119,124,125	0
5	PG4	B	708	10/13	0.82	0.19	78,82,86,94	0
4	WPO	C	701	26/26	0.83	0.18	94,106,115,157	0
3	CL	B	706	1/1	0.84	0.11	91,91,91,91	0
4	WPO	A	710	26/26	0.84	0.23	59,71,76,83	26
2	SO4	B	703	5/5	0.84	0.22	89,91,113,118	0
2	SO4	A	702	5/5	0.85	0.17	78,96,103,124	0
2	SO4	B	702	5/5	0.89	0.22	71,83,95,106	0
2	SO4	A	704	5/5	0.89	0.33	82,88,98,109	0
2	SO4	B	705	5/5	0.92	0.17	67,70,85,88	0
2	SO4	A	703	5/5	0.92	0.12	74,87,102,104	0
2	SO4	A	701	5/5	0.95	0.18	87,90,108,114	0
3	CL	A	707	1/1	0.96	0.17	85,85,85,85	0
2	SO4	A	705	5/5	0.96	0.10	65,66,71,75	0
4	WPO	A	709	26/26	0.98	0.18	43,48,52,53	0
4	WPO	B	707	26/26	0.98	0.15	49,54,61,65	0

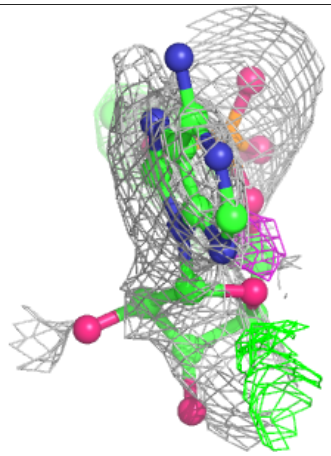
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

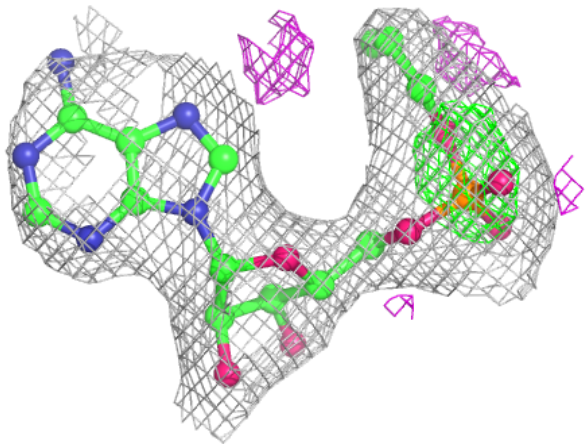


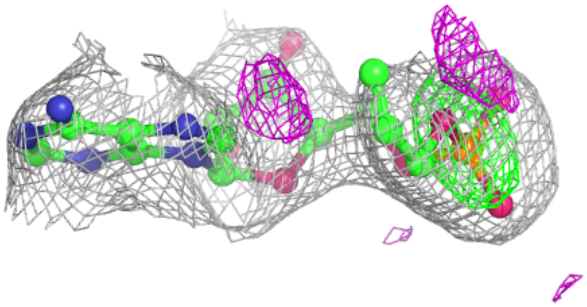


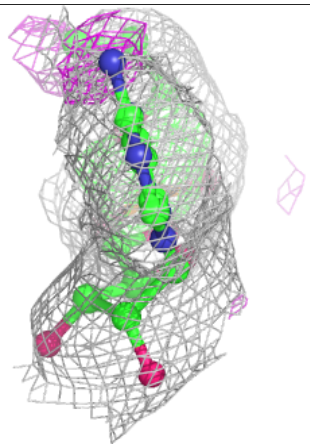


Electron density around WPO C 701:

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

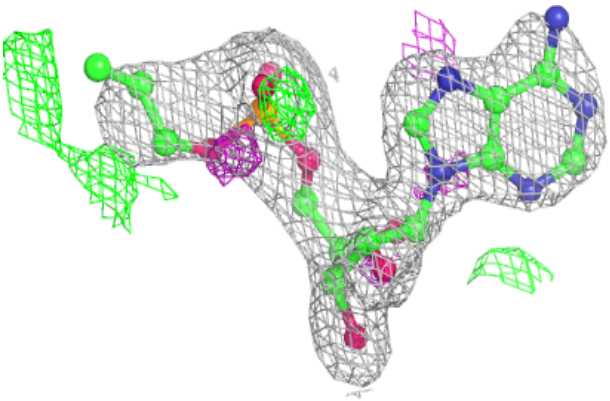


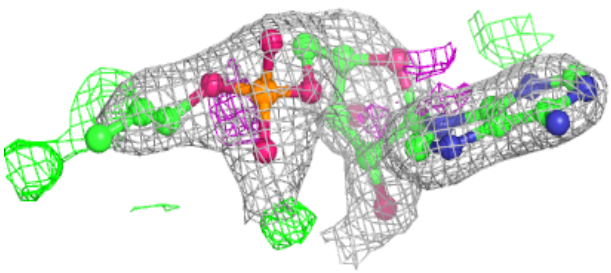


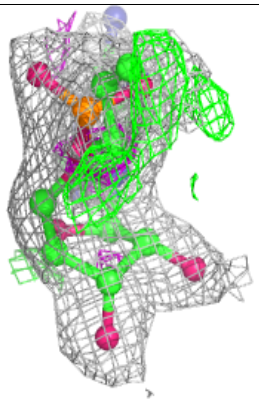


Electron density around WPO A 710:

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

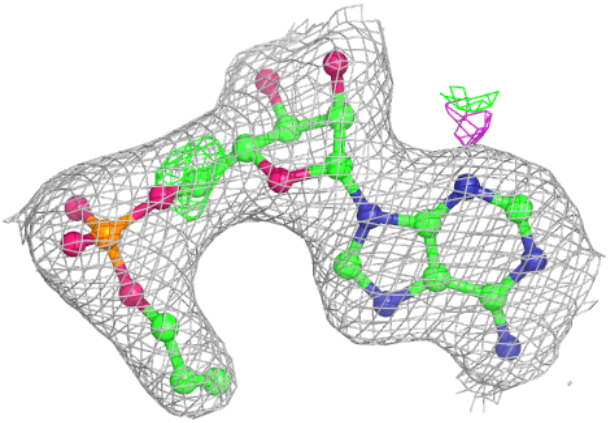


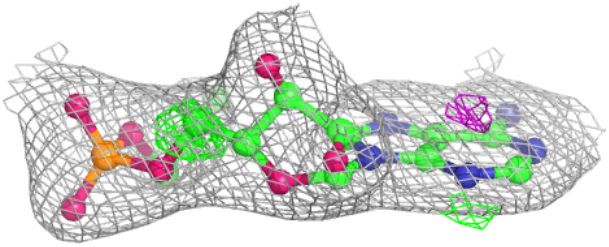


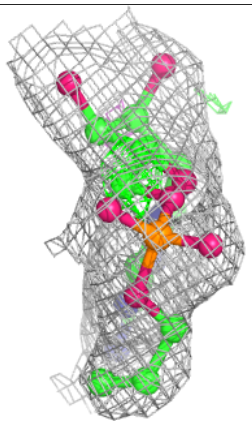


Electron density around WPO A 709:

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

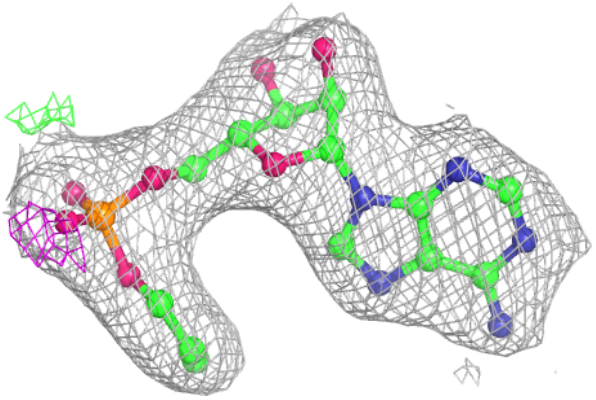


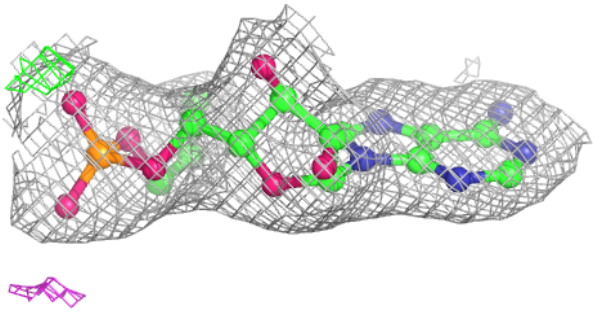


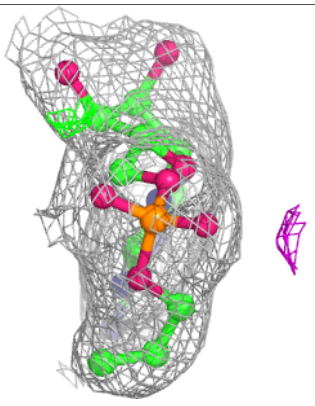


Electron density around WPO B 707:

$2mF_o$-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.