



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 04:10 AM EDT

PDB ID : 7KNO
Title : Crystal structure of Acetyl-CoA synthetase in complex with adenosine-5'-ethylphosphate from *Cryptococcus neoformans* var. *grubii* serotype A (H99)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-11-05
Resolution : 1.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.35.1
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) : 2.35.1

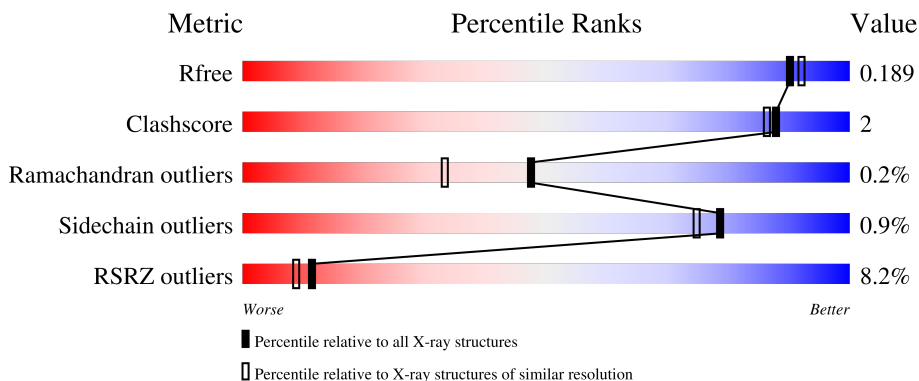
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	694	 4% 91% 2% 3%
1	B	694	 2% 91% 2% 3%
1	C	694	 17% 79% 6% 14%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 16880 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5209	3325	884	972	28	0	12	0
1	B	664	5268	3361	897	981	29	0	18	0
1	C	595	4510	2872	768	846	24	0	4	0

There are 45 discrepancies between the modelled and reference sequences:

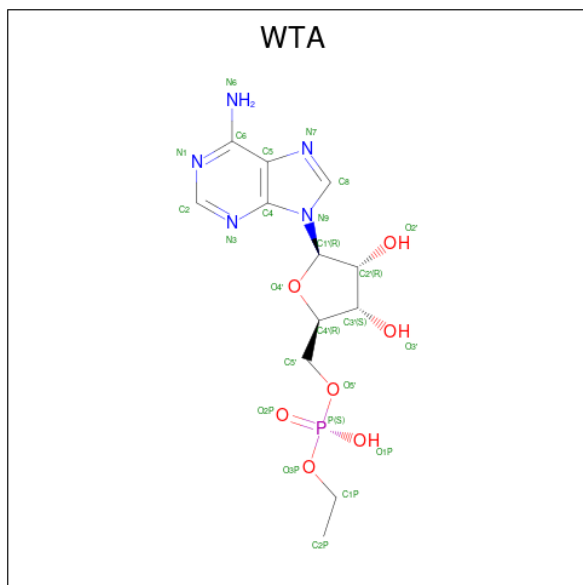
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	initiating methionine	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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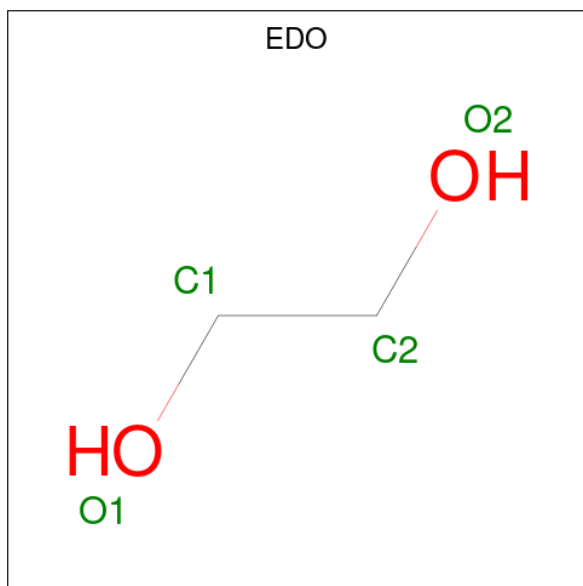
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	initiating methionine	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

- Molecule 2 is 5'-O-[(S)-ethoxy(hydroxy)phosphoryl]adenosine (three-letter code: WTA) (formula: C₁₂H₁₈N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	12	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			25	12	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			25	12	5	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

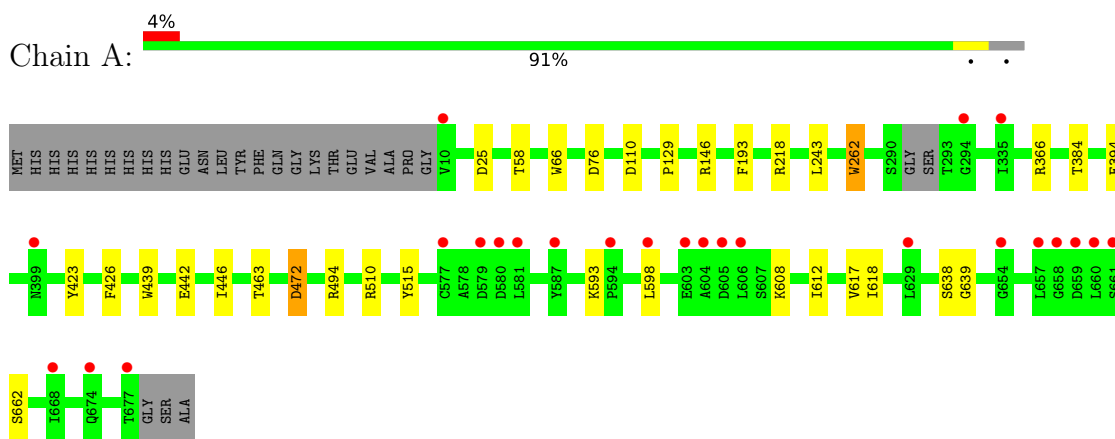
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	684	Total O 696 696	0	14
5	B	714	Total O 723 723	0	9
5	C	337	Total O 342 342	0	5

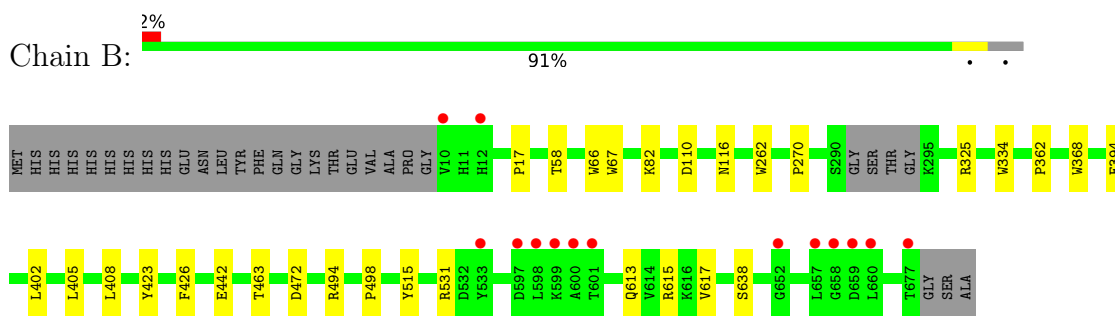
3 Residue-property plots [i](#)

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.

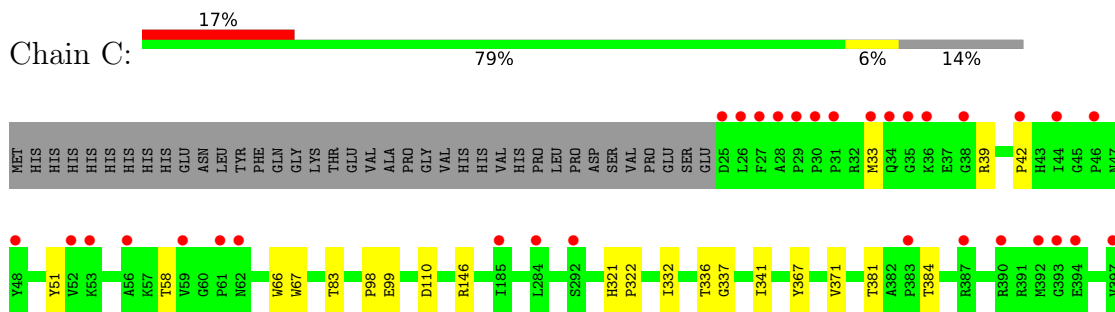
- Molecule 1: Acetyl-coenzyme A synthetase

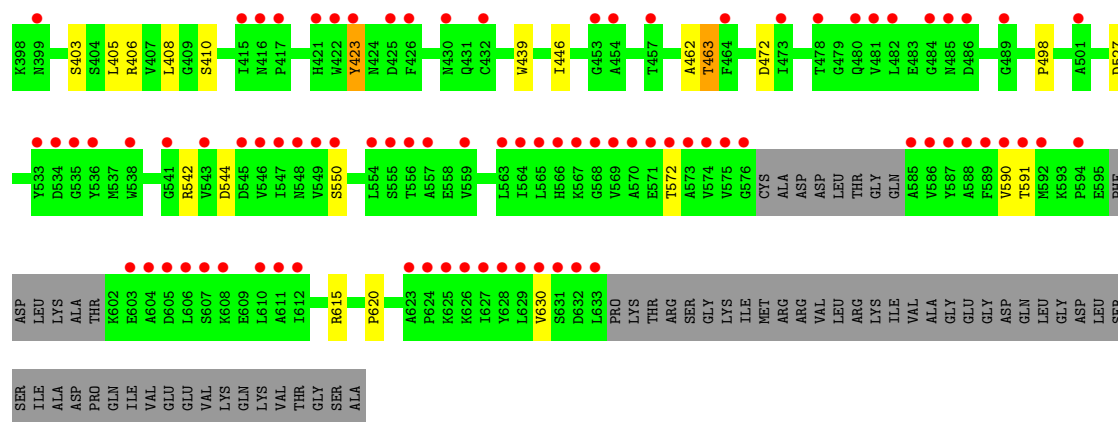


- Molecule 1: Acetyl-coenzyme A synthetase



- Molecule 1: Acetyl-coenzyme A synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.69Å 184.70Å 84.84Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	46.94 – 1.80 46.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.94-1.80) 99.8 (46.94-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.19rc4 4035	Depositor
R, R_{free}	0.164 , 0.190 0.163 , 0.189	Depositor DCC
R_{free} test set	2070 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16880	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PO4, EDO, WTA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/5388	0.64	0/7341
1	B	0.44	0/5460	0.64	0/7432
1	C	0.38	0/4647	0.58	0/6354
All	All	0.43	0/15495	0.62	0/21127

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	5209	0	5036	19	0
1	B	5268	0	5124	17	0
1	C	4510	0	4199	24	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
3	A	8	0	12	0	0
3	B	16	0	24	2	0
3	C	8	0	12	0	0
4	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	5	0	0	0	0
5	A	696	0	0	5	0
5	B	723	0	0	5	0
5	C	342	0	0	4	0
All	All	16880	0	14407	59	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 (59) 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:A:638:SER:OG	5:A:801:HOH:O	1.99	0.80
1:A:472:ASP:OD1	5:A:802:HOH:O	2.02	0.76
1:B:531:ARG:NH1	5:B:801:HOH:O	2.16	0.76
1:A:146[B]:ARG:NH2	5:A:803:HOH:O	2.12	0.71
1:C:146[B]:ARG:NH2	5:C:803:HOH:O	2.23	0.71
1:B:325[B]:ARG:NH1	5:B:804:HOH:O	2.24	0.65
1:A:593:LYS:O	5:A:804:HOH:O	2.16	0.63
1:B:82[B]:LYS:HE3	3:B:701:EDO:H22	1.80	0.63
3:B:703:EDO:H21	1:C:99:GLU:HG2	1.81	0.61
1:B:472:ASP:OD2	1:B:494:ARG:NE	2.38	0.56
1:C:384:THR:OG1	1:C:550:SER:HA	2.06	0.55
1:C:408:LEU:HB3	1:C:423:TYR:CZ	2.41	0.55
1:C:336:THR:OG1	5:C:801:HOH:O	2.18	0.54
1:A:384[A]:THR:HG21	1:A:639:GLY:HA3	1.89	0.54
1:C:321:HIS:HB3	1:C:322:PRO:HD2	1.91	0.52
1:B:615[B]:ARG:NE	5:B:818:HOH:O	2.43	0.52
1:C:527:ASP:OD1	1:C:542:ARG:HD2	2.11	0.51
1:B:394:GLU:HG2	1:B:426:PHE:CZ	2.45	0.51
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.48	0.49
1:A:218:ARG:NH2	5:A:815:HOH:O	2.47	0.48
1:C:406:ARG:O	5:C:802:HOH:O	2.20	0.48
1:C:615:ARG:HG2	1:C:620:PRO:HA	1.96	0.47
1:B:613[A]:GLN:OE1	5:B:802:HOH:O	2.19	0.47
1:A:617:VAL:HG23	1:A:618:ILE:HG13	1.96	0.47
1:A:608:LYS:O	1:A:612:ILE:HD13	2.15	0.47
1:C:405:LEU:HD13	1:C:408:LEU:HD21	1.97	0.47
1:A:76:ASP:OD2	1:B:82[B]:LYS:NZ	2.47	0.46
1:C:67:TRP:CZ3	1:C:498:PRO:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:THR:O	1:C:410:SER:HA	2.16	0.46
1:C:591:THR:HG22	1:C:630:VAL:HG23	1.98	0.46
1:A:394:GLU:HG2	1:A:426:PHE:CZ	2.51	0.46
1:C:337:GLY:HA2	1:C:341:ILE:HD12	1.98	0.46
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.51	0.45
1:C:367:TYR:O	1:C:371:VAL:HG23	2.16	0.45
1:C:332:ILE:HA	1:C:337:GLY:HA3	1.99	0.45
1:B:17:PRO:HB3	1:B:617:VAL:HG11	1.98	0.45
1:A:510:ARG:NH2	4:A:703:PO4:O2	2.47	0.44
1:B:368:TRP:HB3	1:B:402:LEU:HD21	1.99	0.44
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.53	0.44
1:A:439:TRP:HB3	1:A:446:ILE:HA	2.00	0.43
1:C:33:MET:HE3	1:C:42:PRO:HB3	2.00	0.43
1:B:334:TRP:CE2	1:B:638:SER:HB2	2.54	0.42
1:A:58:THR:HG22	1:A:66:TRP:CD2	2.53	0.42
1:C:542:ARG:HB3	1:C:544:ASP:OD1	2.17	0.42
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.54	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.87	0.41
1:B:362:PRO:HG2	5:B:1455:HOH:O	2.20	0.41
1:A:472:ASP:OD2	1:A:494[B]:ARG:HD2	2.19	0.41
1:C:462:ALA:O	1:C:463:THR:OG1	2.28	0.41
1:B:405:LEU:HD13	1:B:408:LEU:HD21	2.03	0.41
1:C:83:THR:O	1:C:98:PRO:HD2	2.21	0.41
1:B:67:TRP:CZ3	1:B:498:PRO:HG2	2.55	0.41
1:A:193:PHE:CD1	1:A:662:SER:HB3	2.55	0.40
1:B:270:PRO:HD3	5:C:902:HOH:O	2.21	0.40
1:C:39:ARG:NH2	1:C:403:SER:O	2.48	0.40
1:A:129:PRO:HG3	1:A:366:ARG:CZ	2.51	0.40
1:C:572:THR:HG22	1:C:590:VAL:HG22	2.04	0.40
1:A:243:LEU:HD11	1:A:262:TRP:HA	2.03	0.40
1:C:439:TRP:HB3	1:C:446:ILE:HA	2.02	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	673/694 (97%)	656 (98%)	16 (2%)	1 (0%)	51	36
1	B	678/694 (98%)	661 (98%)	16 (2%)	1 (0%)	51	36
1	C	593/694 (85%)	567 (96%)	25 (4%)	1 (0%)	47	33
All	All	1944/2082 (93%)	1884 (97%)	57 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	THR
1	B	463	THR
1	C	463	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/576 (94%)	538 (99%)	5 (1%)	78	75
1	B	554/576 (96%)	550 (99%)	4 (1%)	84	81
1	C	445/576 (77%)	441 (99%)	4 (1%)	78	75
All	All	1542/1728 (89%)	1529 (99%)	13 (1%)	78	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	110	ASP
1	A	262	TRP
1	A	423	TYR
1	A	472	ASP
1	B	110	ASP
1	B	116	ASN

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Mol	Chain	Res	Type
1	B	262	TRP
1	B	423	TYR
1	C	51	TYR
1	C	110	ASP
1	C	423	TYR
1	C	472	ASP

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	116	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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	702	-	3,3,3	0.53	0	2,2,2	0.58	0
4	PO4	A	703	-	4,4,4	0.93	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.54	0
4	PO4	B	706	-	4,4,4	0.90	0	6,6,6	0.44	0
4	PO4	B	707	-	4,4,4	0.95	0	6,6,6	0.39	0
2	WTA	B	702	-	24,27,27	1.05	2 (8%)	26,40,40	0.98	1 (3%)
3	EDO	B	703	-	3,3,3	0.49	0	2,2,2	0.41	0
4	PO4	C	704	-	4,4,4	0.86	0	6,6,6	0.41	0
2	WTA	A	701	-	24,27,27	1.07	2 (8%)	26,40,40	0.90	1 (3%)
3	EDO	C	703	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	B	705	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	B	701	-	3,3,3	0.55	0	2,2,2	0.30	0
3	EDO	B	704	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	C	702	-	3,3,3	0.48	0	2,2,2	0.41	0
2	WTA	C	701	-	24,27,27	1.07	2 (8%)	26,40,40	1.23	3 (11%)
4	PO4	A	704	-	4,4,4	0.85	0	6,6,6	0.42	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
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
2	WTA	B	702	-	-	0/10/30/30	0/3/3/3
3	EDO	B	703	-	-	0/1/1/1	-
2	WTA	A	701	-	-	0/10/30/30	0/3/3/3
3	EDO	C	703	-	-	1/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	B	701	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
2	WTA	C	701	-	-	1/10/30/30	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	WTA	O4'-C1'	3.10	1.45	1.41
2	C	701	WTA	C8-N7	-2.77	1.29	1.34
2	B	702	WTA	O4'-C1'	2.56	1.44	1.41
2	C	701	WTA	O4'-C1'	2.53	1.44	1.41
2	A	701	WTA	C8-N7	-2.32	1.30	1.34
2	B	702	WTA	C8-N7	-2.27	1.30	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	WTA	O4'-C1'-C2'	-2.85	102.75	106.93
2	C	701	WTA	C3'-C2'-C1'	2.78	105.17	100.98
2	B	702	WTA	N3-C2-N1	-2.40	124.93	128.68
2	C	701	WTA	O3P-P-O2P	2.40	118.44	109.07
2	A	701	WTA	C1'-N9-C4	-2.06	123.02	126.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

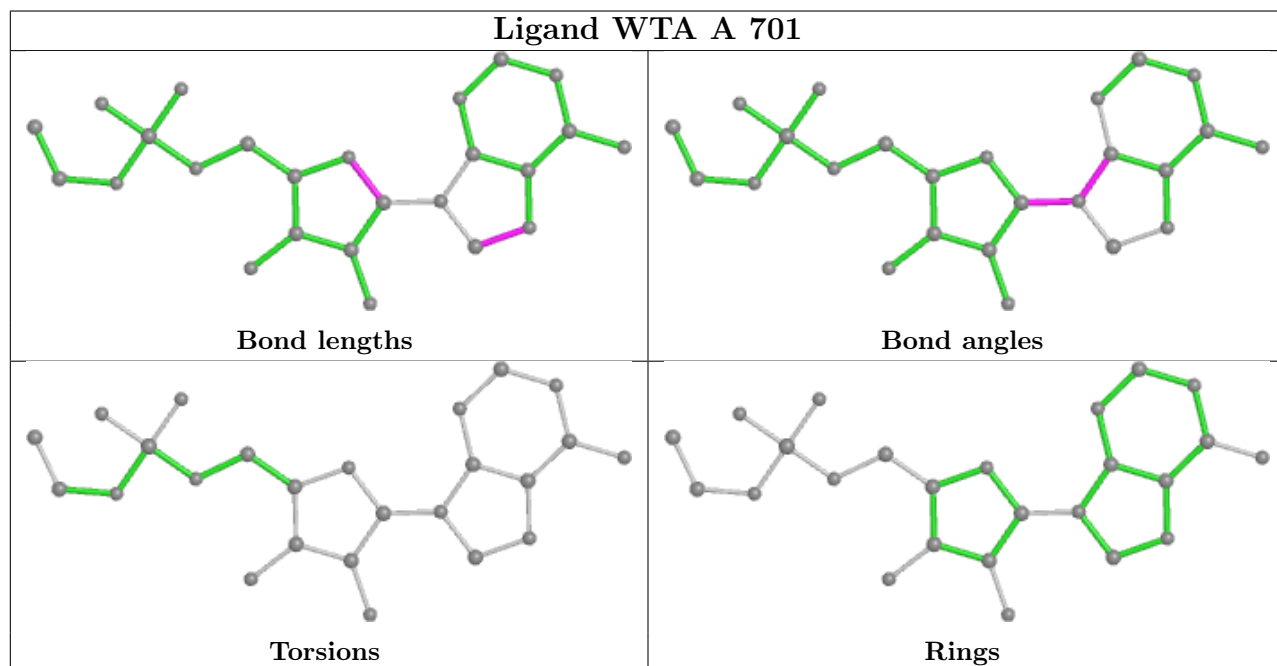
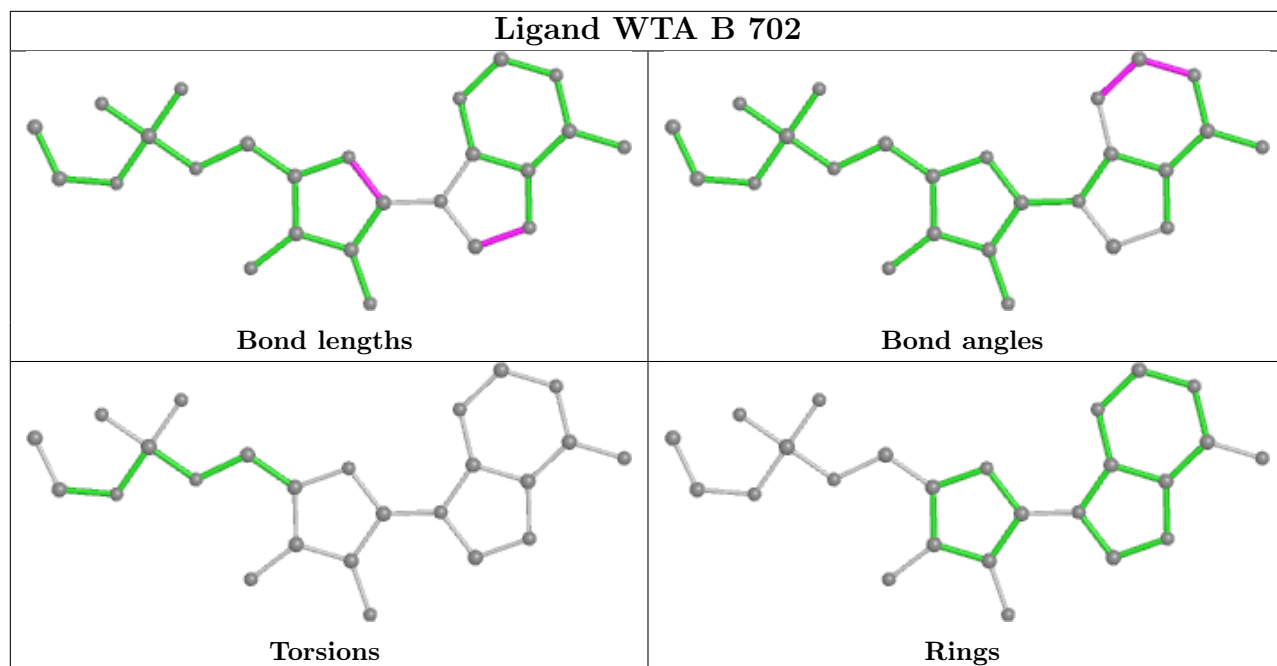
Mol	Chain	Res	Type	Atoms
2	C	701	WTA	C1P-O3P-P-O2P
3	C	703	EDO	O1-C1-C2-O2

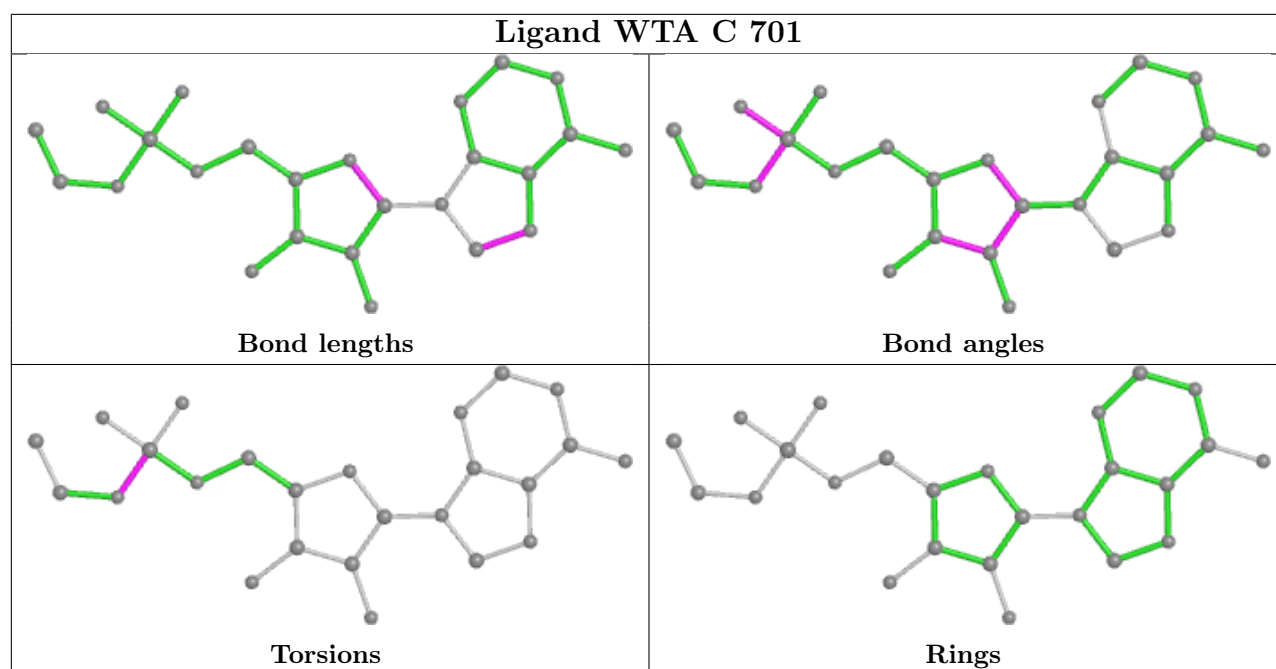
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	PO4	1	0
3	B	703	EDO	1	0
3	B	701	EDO	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 [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	666/694 (95%)	-0.01	25 (3%) 40 35	15, 30, 62, 90	0
1	B	664/694 (95%)	-0.21	14 (2%) 63 59	16, 29, 50, 83	0
1	C	595/694 (85%)	0.92	118 (19%) 1 0	19, 51, 86, 108	0
All	All	1925/2082 (92%)	0.21	157 (8%) 11 9	15, 34, 76, 108	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	633	LEU	7.8
1	C	604	ALA	7.2
1	C	628	TYR	6.8
1	C	585	ALA	6.4
1	C	589	PHE	6.3
1	C	586	VAL	6.2
1	C	627	ILE	5.7
1	C	590	VAL	5.7
1	C	630	VAL	5.7
1	C	575	VAL	5.6
1	C	606	LEU	5.5
1	C	629	LEU	5.4
1	C	576	GLY	5.4
1	C	422	TRP	5.2
1	C	534	ASP	5.2
1	C	568	GLY	5.1
1	C	607	SER	5.1
1	C	572	THR	5.0
1	C	541	GLY	5.0
1	C	549	VAL	5.0
1	C	570	ALA	4.8
1	C	631	SER	4.7
1	B	10	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	601	THR	4.6
1	C	454	ALA	4.6
1	C	591	THR	4.6
1	C	573	ALA	4.6
1	C	417	PRO	4.5
1	C	545	ASP	4.4
1	C	26	LEU	4.4
1	C	611	ALA	4.3
1	C	610	LEU	4.3
1	C	574	VAL	4.2
1	C	588	ALA	4.2
1	B	599	LYS	4.2
1	B	600	ALA	4.2
1	C	27	PHE	4.0
1	C	543	VAL	3.9
1	C	31	PRO	3.9
1	C	564	ILE	3.9
1	A	577	CYS	3.9
1	A	629	LEU	3.8
1	A	657	LEU	3.8
1	C	484	GLY	3.8
1	C	554	LEU	3.8
1	A	677	THR	3.8
1	A	658	GLY	3.7
1	C	28	ALA	3.7
1	C	603	GLU	3.7
1	C	535	GLY	3.6
1	A	654	GLY	3.6
1	C	36	LYS	3.5
1	C	612	ILE	3.5
1	C	587	TYR	3.5
1	C	52	VAL	3.5
1	A	659	ASP	3.5
1	C	565	LEU	3.5
1	C	567	LYS	3.4
1	C	48	TYR	3.4
1	C	46	PRO	3.4
1	C	632	ASP	3.4
1	A	399	ASN	3.4
1	A	660	LEU	3.3
1	C	624	PRO	3.3
1	A	580	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	3.2
1	A	10	VAL	3.2
1	C	626	LYS	3.2
1	C	605	ASP	3.2
1	C	569	VAL	3.2
1	C	566	HIS	3.2
1	C	42	PRO	3.1
1	C	25	ASP	3.1
1	C	594	PRO	3.1
1	C	486	ASP	3.1
1	C	38	GLY	3.0
1	B	658	GLY	3.0
1	C	592	MET	3.0
1	C	61	PRO	3.0
1	C	30	PRO	3.0
1	C	432	CYS	3.0
1	C	550	SER	3.0
1	C	557	ALA	3.0
1	B	677	THR	3.0
1	C	556	THR	2.9
1	C	399	ASN	2.9
1	A	581	LEU	2.9
1	C	56	ALA	2.9
1	C	546	VAL	2.9
1	B	598	LEU	2.9
1	C	571	GLU	2.8
1	C	547	ILE	2.8
1	C	473	ILE	2.8
1	C	34	GLN	2.8
1	C	423	TYR	2.8
1	A	606	LEU	2.8
1	C	284	LEU	2.8
1	C	625	LYS	2.7
1	B	12	HIS	2.7
1	A	661	SER	2.7
1	C	608	LYS	2.7
1	C	416	ASN	2.7
1	A	594	PRO	2.7
1	A	604	ALA	2.6
1	A	335	ILE	2.6
1	C	464	PHE	2.6
1	C	453	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	559	VAL	2.6
1	C	421	HIS	2.5
1	C	501	ALA	2.5
1	C	53	LYS	2.5
1	C	425	ASP	2.5
1	B	533	TYR	2.5
1	C	548	ASN	2.4
1	C	426	PHE	2.4
1	B	657	LEU	2.4
1	A	294	GLY	2.4
1	C	390	ARG	2.4
1	A	603	GLU	2.4
1	B	597	ASP	2.4
1	A	598	LEU	2.4
1	C	387	ARG	2.4
1	C	485	ASN	2.4
1	A	587	TYR	2.4
1	C	185	ILE	2.4
1	C	481	VAL	2.4
1	C	482	LEU	2.3
1	C	536	TYR	2.3
1	C	392	MET	2.3
1	C	29	PRO	2.3
1	C	383	PRO	2.3
1	C	533	TYR	2.3
1	C	33	MET	2.3
1	A	674	GLN	2.3
1	C	457	THR	2.3
1	C	62	ASN	2.2
1	B	659	ASP	2.2
1	C	430	ASN	2.2
1	C	563	LEU	2.2
1	C	292	SER	2.2
1	C	397	VAL	2.2
1	C	35	GLY	2.1
1	C	555	SER	2.1
1	B	652	GLY	2.1
1	C	480	GLN	2.1
1	C	538	TRP	2.1
1	C	489	GLY	2.1
1	C	59	VAL	2.1
1	B	660	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	605	ASP	2.0
1	C	623	ALA	2.0
1	C	393	GLY	2.0
1	A	668	ILE	2.0
1	C	415	ILE	2.0
1	A	579	ASP	2.0
1	C	394	GLU	2.0
1	C	478	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

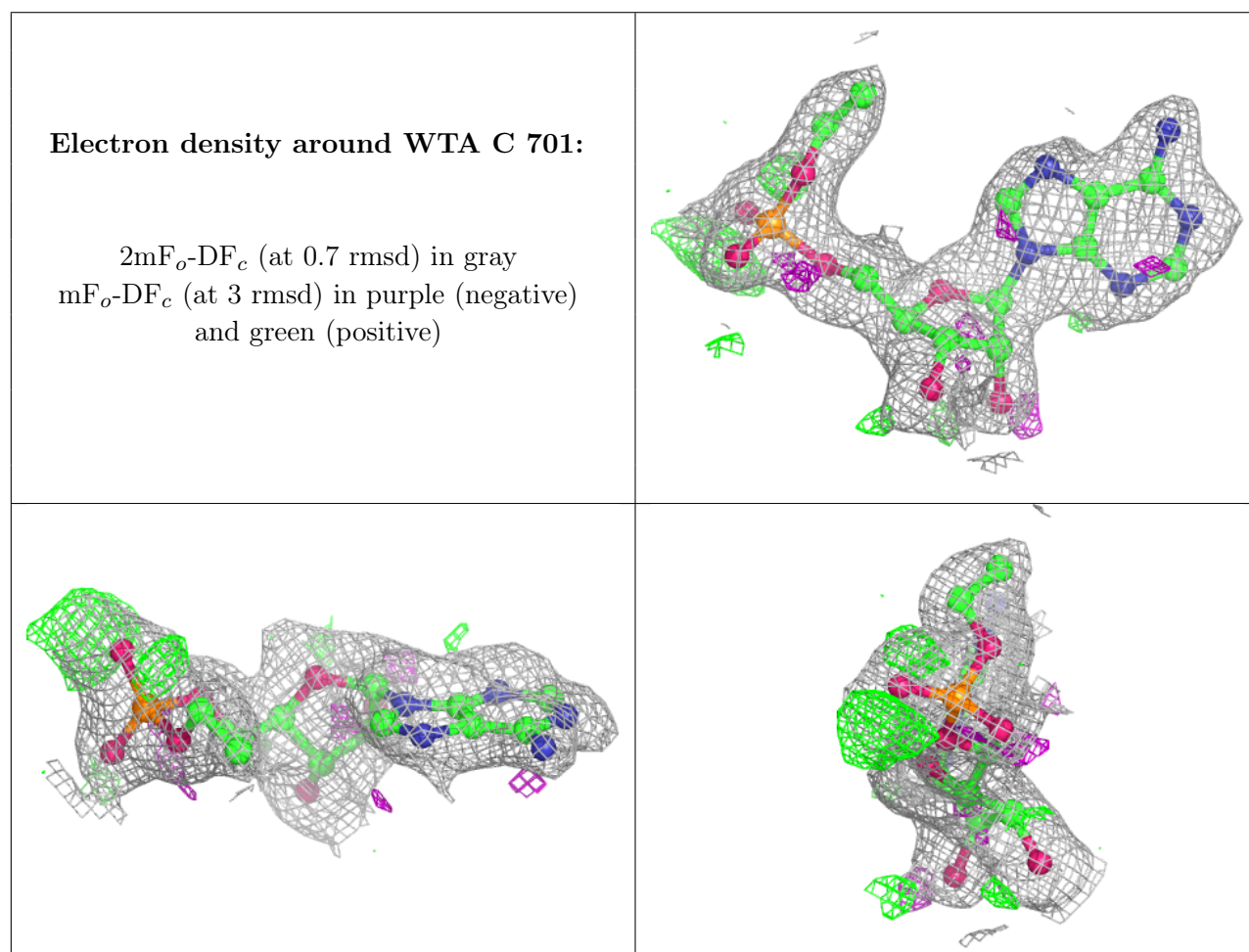
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	707	5/5	0.86	0.14	43,45,51,59	5
4	PO4	A	704	5/5	0.87	0.18	43,45,54,56	5
2	WTA	C	701	25/25	0.90	0.13	33,48,55,57	0
3	EDO	C	702	4/4	0.90	0.11	53,54,55,57	0
4	PO4	C	704	5/5	0.91	0.20	66,69,75,78	5
3	EDO	C	703	4/4	0.92	0.12	60,63,64,64	0
3	EDO	B	705	4/4	0.92	0.18	46,51,55,59	0
4	PO4	B	706	5/5	0.94	0.12	32,33,40,40	5
4	PO4	A	703	5/5	0.94	0.16	29,42,43,44	5
3	EDO	B	701	4/4	0.94	0.10	26,27,28,43	0
3	EDO	A	705	4/4	0.95	0.09	32,33,36,36	0
3	EDO	B	704	4/4	0.95	0.08	39,41,41,46	0
3	EDO	B	703	4/4	0.96	0.10	34,37,37,50	0
3	EDO	A	702	4/4	0.96	0.11	33,33,36,40	0
2	WTA	A	701	25/25	0.98	0.14	15,19,22,22	0

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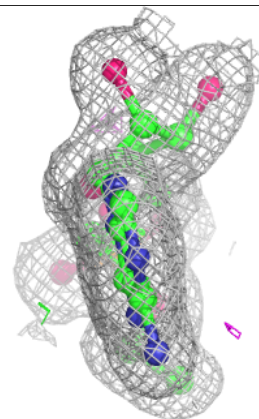
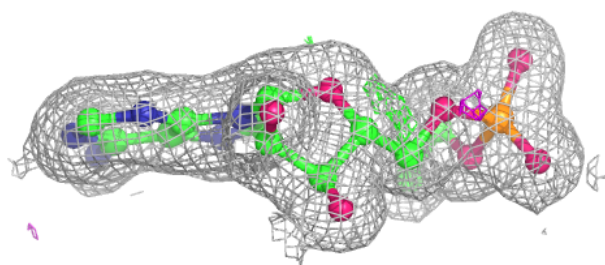
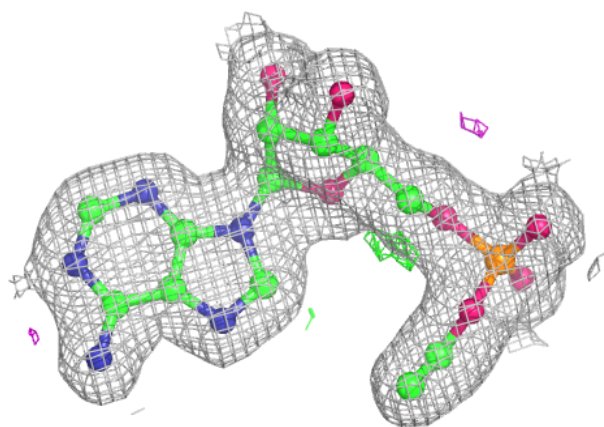
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	WTA	B	702	25/25	0.98	0.13	16,20,22,22	0

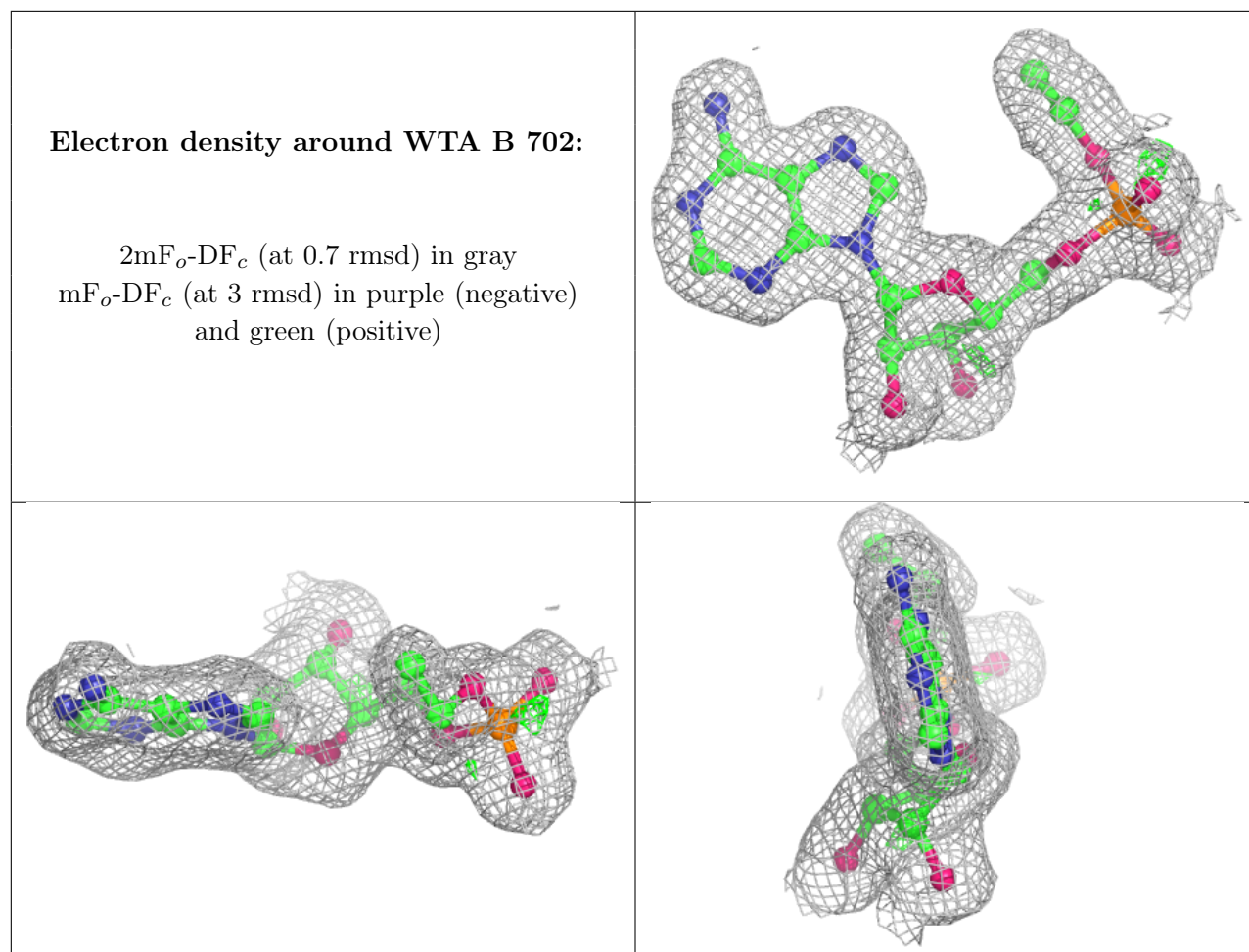
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around WTA A 701:

$2mF_o-DF_c$ (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.