



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:11 AM EDT

PDB ID : 7KNP
Title : Crystal structure of Acetyl-CoA synthetase in complex with adenosine-5'-butylphosphate from *Cryptococcus neoformans* var. *grubii* serotype A (H99)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-11-05
Resolution : 2.25 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

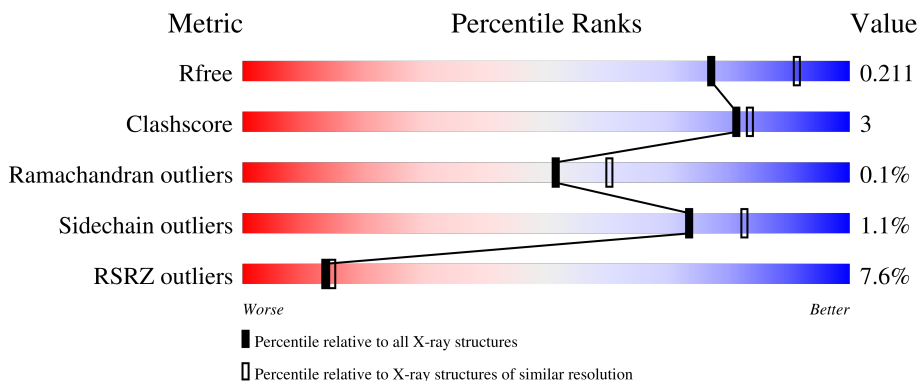
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	 7% 86% 8% 6%
1	B	694	 2% 88% 6% 5%
1	C	694	 12% 68% 5% 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14949 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	653	5003	3190	855	933	25	0	2	0
1	B	658	5111	3259	874	952	26	0	4	0
1	C	511	3874	2468	660	724	22	0	2	0

There are 45 discrepancies between the modelled and reference sequences:

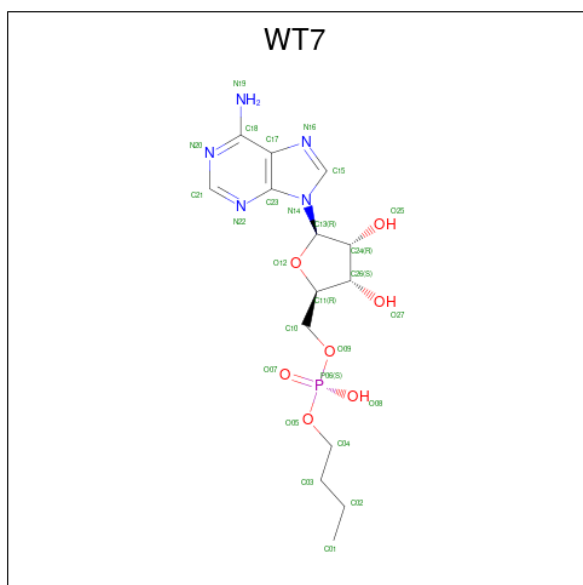
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression 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

Continued on next page...

Continued from previous page...

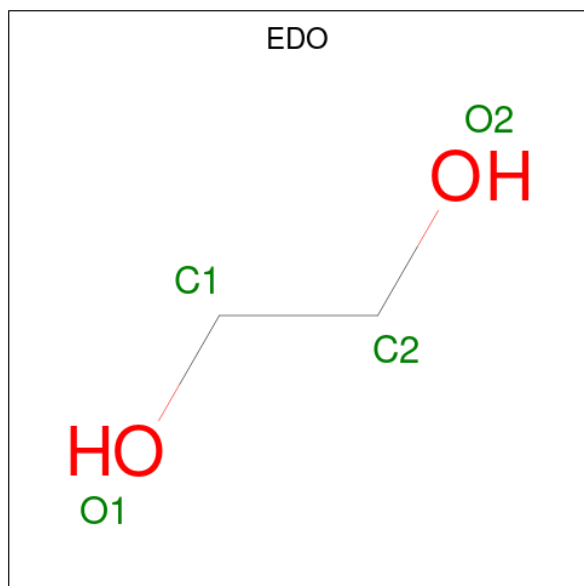
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
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)-butoxy(hydroxy)phosphoryl]adenosine (three-letter code: WT7) (formula: C₁₄H₂₂N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	14	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			27	14	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			27	14	5	7	1		

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



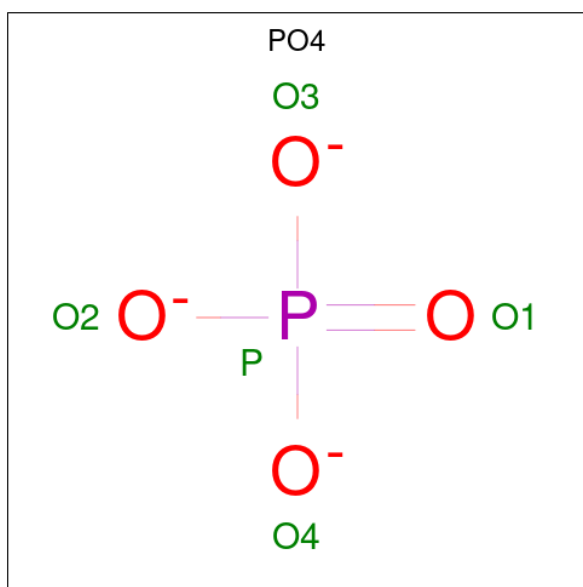
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- 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	B	1	Total O P 5 4 1	0	0

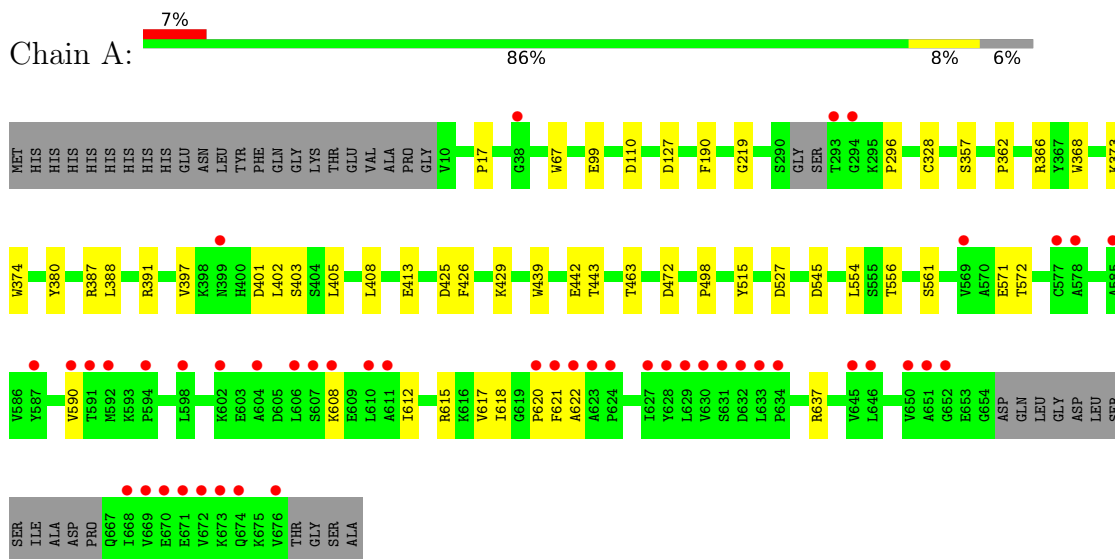
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	341	Total O 341 341	0	0
5	B	333	Total O 336 336	0	3
5	C	145	Total O 145 145	0	0

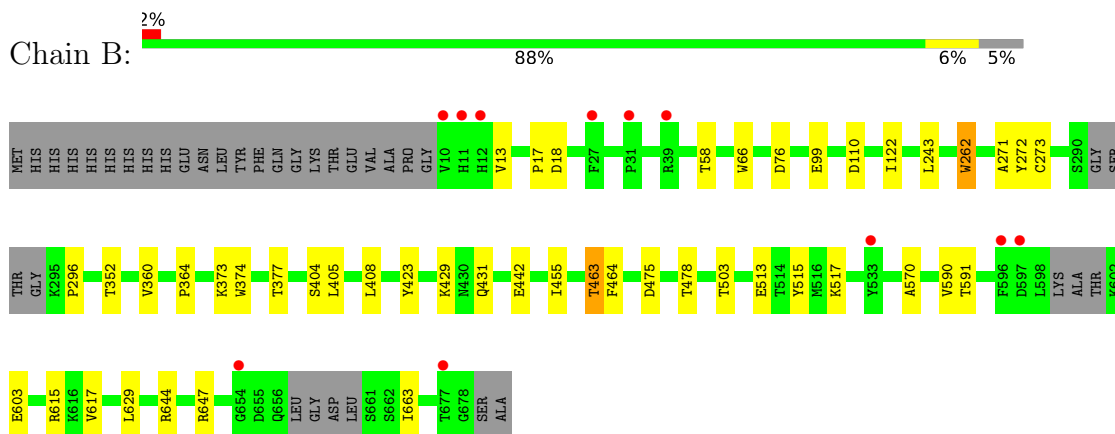
3 Residue-property plots [i](#)

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

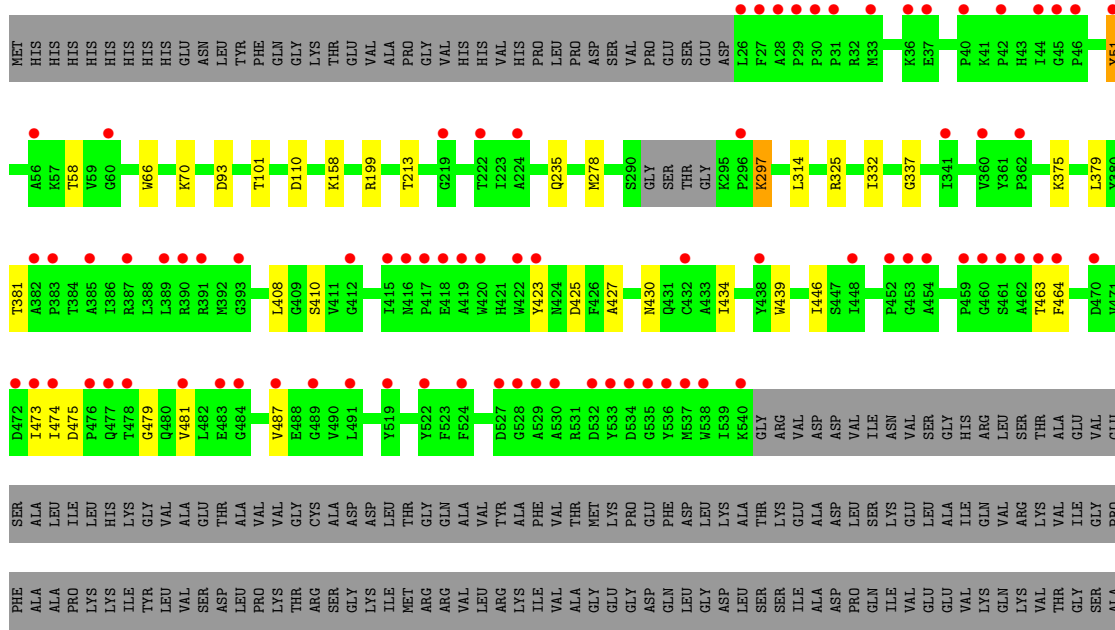


- Molecule 1: Acetyl-coenzyme A synthetase



- 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	72.25Å 184.66Å 85.13Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	40.26 – 2.25 48.42 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.26-2.25) 98.4 (48.42-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.19rc4	Depositor
R, R_{free}	0.176 , 0.213 0.175 , 0.211	Depositor DCC
R_{free} test set	2160 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, WT7, EDO

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	0.41	0/5147	0.59	0/7028
1	B	0.38	0/5264	0.59	0/7174
1	C	0.36	0/3996	0.56	0/5467
All	All	0.38	0/14407	0.58	0/19669

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	5003	0	4722	27	0
1	B	5111	0	4911	25	0
1	C	3874	0	3556	20	0
2	A	27	0	0	1	0
2	B	27	0	0	0	0
2	C	27	0	0	0	0
3	A	16	0	24	1	0
3	B	20	0	30	1	0
3	C	12	0	18	1	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	341	0	0	1	0
5	B	336	0	0	4	0
5	C	145	0	0	1	0
All	All	14949	0	13261	71	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 (71) 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:603:GLU:HG3	1:B:629:LEU:HD12	1.59	0.84
1:B:475:ASP:HB3	1:B:478:THR:HB	1.77	0.67
1:A:387:ARG:NH2	1:A:413:GLU:OE2	2.28	0.64
1:C:158:LYS:NZ	5:C:804:HOH:O	2.35	0.57
1:A:127:ASP:OD1	1:A:219:GLY:N	2.38	0.55
1:C:332:ILE:HA	1:C:337:GLY:HA3	1.88	0.55
1:A:388:LEU:O	1:A:391:ARG:HG2	2.07	0.55
1:A:617:VAL:HG23	1:A:618:ILE:HG13	1.89	0.54
1:B:570:ALA:HB3	1:B:591:THR:HG22	1.89	0.54
1:B:243:LEU:HD11	1:B:262:TRP:HA	1.88	0.54
1:B:590:VAL:HB	1:B:629:LEU:HD23	1.90	0.53
1:A:401:ASP:OD1	1:A:403:SER:OG	2.15	0.52
1:B:373:LYS:HE3	1:B:374:TRP:NE1	2.24	0.52
1:B:17:PRO:HB3	1:B:617:VAL:HG11	1.91	0.52
1:A:373:LYS:HE3	1:A:374:TRP:NE1	2.26	0.51
1:B:513:GLU:HA	1:B:517:LYS:HG3	1.92	0.51
1:C:439:TRP:HB3	1:C:446:ILE:HA	1.92	0.51
1:C:474:ILE:HA	1:C:481:VAL:HA	1.92	0.51
1:B:360:VAL:HA	1:B:364:PRO:HA	1.92	0.51
1:A:362:PRO:HD2	1:A:366:ARG:HD3	1.92	0.51
1:C:199:ARG:NH1	1:C:235:GLN:OE1	2.44	0.51
1:A:615:ARG:HG2	1:A:620:PRO:HA	1.94	0.50
1:A:17:PRO:HD2	1:A:561:SER:HB2	1.94	0.49
1:C:425:ASP:OD1	1:C:430:ASN:ND2	2.39	0.49
1:A:439:TRP:HB2	1:A:443:THR:OG1	2.13	0.49
1:B:603:GLU:OE2	5:B:801:HOH:O	2.19	0.49
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.48	0.49
1:C:381:THR:O	1:C:410:SER:HA	2.12	0.48
1:C:297:LYS:HB3	1:C:297:LYS:HE3	1.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASP:OD1	2:A:701:WT7:O25	2.32	0.47
1:A:99:GLU:HG2	3:C:702:EDO:H21	1.96	0.47
1:A:608:LYS:O	1:A:612:ILE:HD13	2.16	0.46
1:B:271:ALA:HB3	1:C:93:ASP:HB3	1.97	0.46
1:A:328:CYS:HA	1:A:380:TYR:HB3	1.98	0.46
1:C:325:ARG:NH2	1:C:375:LYS:O	2.46	0.45
3:A:702:EDO:H21	1:B:99:GLU:HG2	1.98	0.45
1:B:13:VAL:O	5:B:803:HOH:O	2.21	0.45
1:A:554:LEU:HD21	1:A:621:PHE:HE2	1.82	0.44
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.52	0.44
1:B:455:ILE:HG13	5:B:869:HOH:O	2.17	0.44
1:B:272:TYR:CG	1:B:273:CYS:N	2.86	0.43
1:C:473:ILE:HD12	1:C:487:VAL:HG23	2.00	0.43
1:B:122:ILE:HA	1:B:352:THR:O	2.18	0.43
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.53	0.43
1:A:397:VAL:HG11	1:A:426:PHE:HB3	2.00	0.43
1:C:70:LYS:HD3	1:C:70:LYS:HA	1.85	0.43
1:A:405:LEU:HD13	1:A:408:LEU:HD21	2.01	0.42
1:B:644:ARG:HG3	1:B:647:ARG:HH21	1.83	0.42
1:C:51:TYR:OH	1:C:464:PHE:HB3	2.20	0.42
1:C:423:TYR:O	1:C:427:ALA:HB3	2.20	0.42
1:C:475:ASP:O	1:C:479:GLY:N	2.52	0.42
1:A:296:PRO:HG2	5:A:982:HOH:O	2.20	0.42
1:C:408:LEU:HB2	1:C:434:ILE:HD13	2.01	0.42
1:A:387:ARG:NH2	1:A:571:GLU:OE2	2.42	0.42
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.55	0.42
1:C:101:THR:HA	1:C:278:MET:O	2.20	0.42
1:C:379:LEU:HB3	1:C:408:LEU:HD23	2.01	0.42
1:B:463:THR:OG1	1:B:464:PHE:N	2.52	0.41
1:B:18:ASP:O	5:B:802:HOH:O	2.20	0.41
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.55	0.41
1:A:554:LEU:HD11	1:A:622:ALA:HA	2.03	0.41
1:B:377:THR:HA	1:B:404:SER:O	2.21	0.41
1:A:368:TRP:HB3	1:A:402:LEU:HD21	2.02	0.41
1:B:503:THR:HG21	3:B:704:EDO:H22	2.03	0.41
1:C:463:THR:OG1	1:C:464:PHE:N	2.52	0.41
1:A:425:ASP:O	1:A:429:LYS:HA	2.21	0.41
1:A:545:ASP:HB3	1:A:556:THR:HG21	2.02	0.41
1:B:429:LYS:O	1:B:431:GLN:HG3	2.21	0.41
1:A:190:PHE:CE2	1:A:637:ARG:HB3	2.57	0.40
1:A:572:THR:HG22	1:A:590:VAL:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HD13	1:B:408:LEU:HD21	2.04	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	649/694 (94%)	623 (96%)	25 (4%)	1 (0%)	47	55
1	B	654/694 (94%)	632 (97%)	21 (3%)	1 (0%)	47	55
1	C	509/694 (73%)	488 (96%)	21 (4%)	0	100	100
All	All	1812/2082 (87%)	1743 (96%)	67 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	THR
1	B	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	503/576 (87%)	500 (99%)	3 (1%)	86	91
1	B	529/576 (92%)	521 (98%)	8 (2%)	65	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	377/576 (66%)	372 (99%)	5 (1%)	69 79
All	All	1409/1728 (82%)	1393 (99%)	16 (1%)	73 82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	357	SER
1	A	472	ASP
1	B	76	ASP
1	B	110	ASP
1	B	262	TRP
1	B	296	PRO
1	B	423	TYR
1	B	615[A]	ARG
1	B	615[B]	ARG
1	B	663	ILE
1	C	51	TYR
1	C	110	ASP
1	C	213	THR
1	C	297	LYS
1	C	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	HIS
1	B	116	ASN
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](#)

17 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	B	703	-	3,3,3	0.50	0	2,2,2	0.25	0
4	PO4	A	706	-	4,4,4	0.85	0	6,6,6	0.54	0
3	EDO	A	703	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	C	702	-	3,3,3	0.38	0	2,2,2	0.56	0
3	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.58	0
3	EDO	B	704	-	3,3,3	0.81	0	2,2,2	0.45	0
3	EDO	C	703	-	3,3,3	0.50	0	2,2,2	0.19	0
2	WT7	B	701	-	26,29,29	0.98	1 (3%)	28,42,42	0.81	1 (3%)
3	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.16	0
3	EDO	B	706	-	3,3,3	0.36	0	2,2,2	0.46	0
4	PO4	B	707	-	4,4,4	0.82	0	6,6,6	0.49	0
2	WT7	A	701	-	26,29,29	1.01	3 (11%)	28,42,42	0.85	1 (3%)
3	EDO	C	704	-	3,3,3	0.41	0	2,2,2	0.34	0
2	WT7	C	701	-	26,29,29	1.02	2 (7%)	28,42,42	0.84	0
3	EDO	B	705	-	3,3,3	0.47	0	2,2,2	0.22	0
3	EDO	A	702	-	3,3,3	0.37	0	2,2,2	0.64	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	B	703	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
2	WT7	B	701	-	-	1/12/32/32	0/3/3/3
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
2	WT7	A	701	-	-	3/12/32/32	0/3/3/3
3	EDO	C	704	-	-	1/1/1/1	-
2	WT7	C	701	-	-	7/12/32/32	0/3/3/3
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	WT7	C15-N16	-2.43	1.30	1.34
2	B	701	WT7	C15-N16	-2.41	1.30	1.34
2	A	701	WT7	C15-N16	-2.41	1.30	1.34
2	C	701	WT7	C24-C13	2.20	1.57	1.53
2	A	701	WT7	C24-C13	2.19	1.57	1.53
2	A	701	WT7	P06-O05	2.01	1.67	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	WT7	O08-P06-O07	2.06	122.41	112.24
2	B	701	WT7	O08-P06-O07	2.03	122.27	112.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	WT7	C10-O09-P06-O08
2	C	701	WT7	C04-O05-P06-O07
2	B	701	WT7	C01-C02-C03-C04
2	C	701	WT7	C02-C03-C04-O05
3	C	704	EDO	O1-C1-C2-O2
2	C	701	WT7	O09-C10-C11-C26
2	C	701	WT7	C01-C02-C03-C04

Continued on next page...

Continued from previous page...

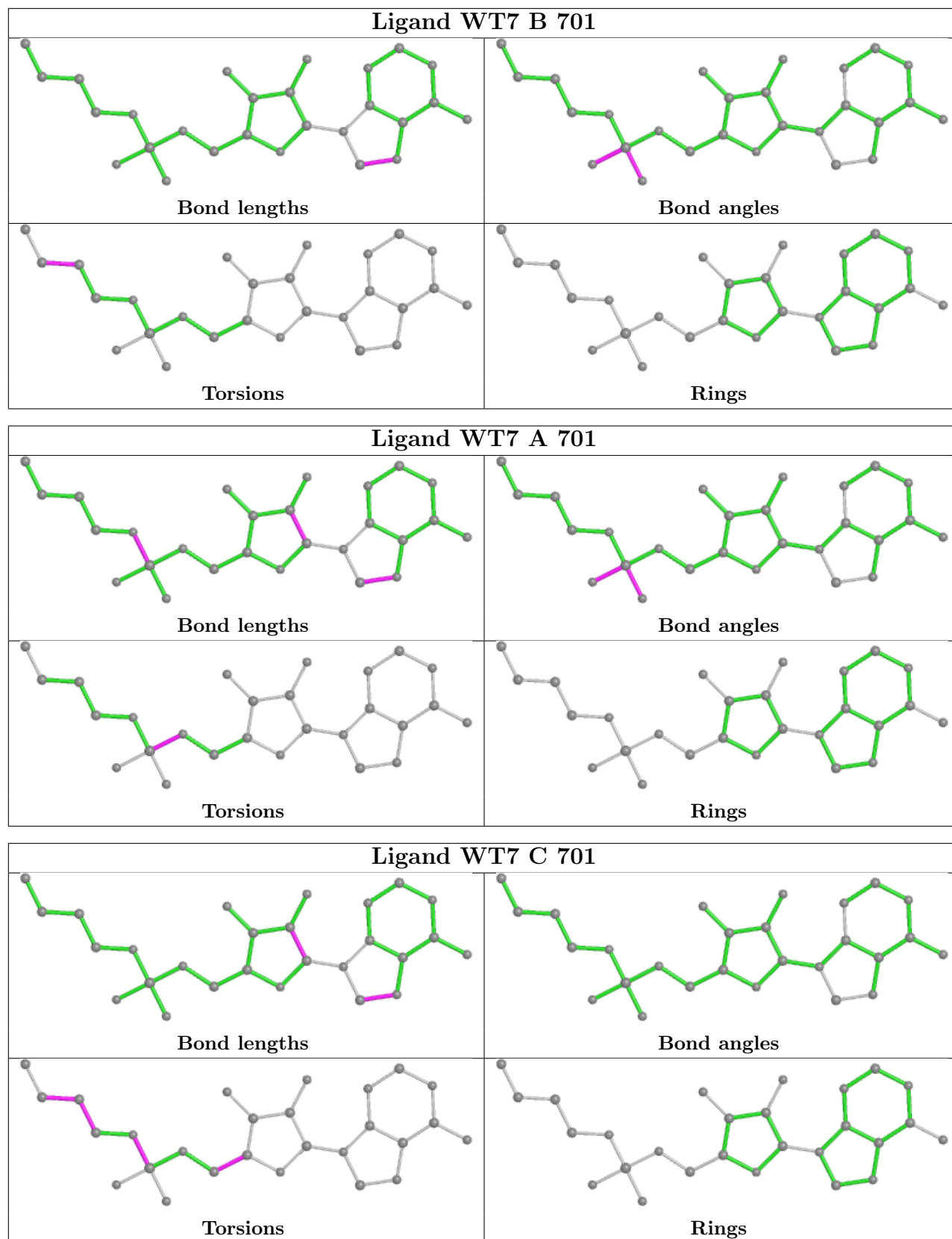
Mol	Chain	Res	Type	Atoms
2	C	701	WT7	O09-C10-C11-O12
3	B	704	EDO	O1-C1-C2-O2
2	C	701	WT7	C04-O05-P06-O09
2	A	701	WT7	C10-O09-P06-O05
3	A	704	EDO	O1-C1-C2-O2
2	A	701	WT7	C10-O09-P06-O07
2	C	701	WT7	C04-O05-P06-O08

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	EDO	1	0
3	B	704	EDO	1	0
2	A	701	WT7	1	0
3	A	702	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	653/694 (94%)	0.18	47 (7%) 15 16	22, 46, 99, 123	0
1	B	658/694 (94%)	-0.02	11 (1%) 70 73	25, 45, 75, 101	0
1	C	511/694 (73%)	0.75	81 (15%) 1 1	26, 64, 112, 140	0
All	All	1822/2082 (87%)	0.27	139 (7%) 13 15	22, 50, 103, 140	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	GLY	7.1
1	C	417	PRO	6.8
1	A	591	THR	6.5
1	C	415	ILE	6.3
1	A	669	VAL	6.0
1	A	672	VAL	5.9
1	C	481	VAL	5.5
1	C	484	GLY	5.4
1	C	459	PRO	5.2
1	C	36	LYS	5.2
1	C	460	GLY	5.1
1	C	383	PRO	5.0
1	C	389	LEU	5.0
1	A	630	VAL	5.0
1	C	29	PRO	4.9
1	A	577	CYS	4.9
1	C	487	VAL	4.7
1	C	534	ASP	4.7
1	A	633	LEU	4.7
1	C	461	SER	4.6
1	C	529	ALA	4.5
1	A	611	ALA	4.4
1	C	537	MET	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	606	LEU	4.4
1	C	390	ARG	4.3
1	A	631	SER	4.2
1	C	438	TYR	4.2
1	A	628	TYR	4.1
1	C	536	TYR	4.1
1	C	528	GLY	4.1
1	C	391	ARG	4.0
1	B	10	VAL	4.0
1	A	604	ALA	3.9
1	C	538	TRP	3.9
1	C	33	MET	3.9
1	C	44	ILE	3.8
1	A	668	ILE	3.8
1	C	477	GLN	3.7
1	A	652	GLY	3.7
1	C	452	PRO	3.7
1	A	602	LYS	3.6
1	A	38	GLY	3.6
1	C	530	ALA	3.6
1	C	483	GLU	3.6
1	C	463	THR	3.6
1	A	598	LEU	3.5
1	B	533	TYR	3.5
1	A	569	VAL	3.5
1	B	597	ASP	3.5
1	A	293	THR	3.4
1	C	535	GLY	3.4
1	A	629	LEU	3.4
1	C	454	ALA	3.4
1	A	646	LEU	3.3
1	C	491	LEU	3.3
1	A	650	VAL	3.3
1	C	478	THR	3.3
1	A	578	ALA	3.2
1	A	294	GLY	3.2
1	A	627	ILE	3.2
1	A	621	PHE	3.2
1	C	422	TRP	3.1
1	C	46	PRO	3.1
1	C	418	GLU	3.1
1	C	533	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	30	PRO	3.1
1	C	519	TYR	3.1
1	C	473	ILE	3.1
1	C	56	ALA	3.1
1	C	224	ALA	3.0
1	C	524	PHE	3.0
1	A	590	VAL	3.0
1	B	11	HIS	3.0
1	C	532	ASP	3.0
1	A	674	GLN	3.0
1	A	622	ALA	2.9
1	C	382	ALA	2.9
1	A	587	TYR	2.9
1	A	610	LEU	2.9
1	C	420	TRP	2.9
1	B	31	PRO	2.9
1	C	474	ILE	2.8
1	A	399	ASN	2.8
1	A	670	GLU	2.8
1	A	585	ALA	2.8
1	C	419	ALA	2.8
1	C	45	GLY	2.8
1	C	527	ASP	2.8
1	B	596	PHE	2.8
1	C	27	PHE	2.8
1	C	31	PRO	2.8
1	C	385	ALA	2.8
1	C	462	ALA	2.8
1	A	607	SER	2.7
1	C	60	GLY	2.7
1	A	632	ASP	2.7
1	C	540	LYS	2.7
1	C	432	CYS	2.7
1	C	464	PHE	2.7
1	C	40	PRO	2.6
1	C	42	PRO	2.6
1	A	673	LYS	2.6
1	A	592	MET	2.6
1	C	28	ALA	2.6
1	A	676	VAL	2.5
1	C	448	ILE	2.5
1	B	12	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	387[A]	ARG	2.5
1	C	360	VAL	2.4
1	A	671	GLU	2.4
1	C	393	GLY	2.4
1	C	522	TYR	2.4
1	A	624	PRO	2.4
1	C	412	GLY	2.4
1	C	472	ASP	2.4
1	C	51	TYR	2.4
1	C	37	GLU	2.4
1	C	219	GLY	2.3
1	A	645	VAL	2.3
1	B	39	ARG	2.3
1	C	423	TYR	2.3
1	A	623	ALA	2.3
1	B	677	THR	2.3
1	A	651	ALA	2.3
1	C	416	ASN	2.2
1	B	654	GLY	2.2
1	A	594	PRO	2.2
1	C	362	PRO	2.2
1	B	27	PHE	2.2
1	C	26	LEU	2.2
1	A	620	PRO	2.2
1	C	296	PRO	2.2
1	C	222	THR	2.1
1	C	453	GLY	2.1
1	A	634	PRO	2.1
1	A	608	LYS	2.0
1	C	341	ILE	2.0
1	C	476	PRO	2.0
1	C	470	ASP	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](#)

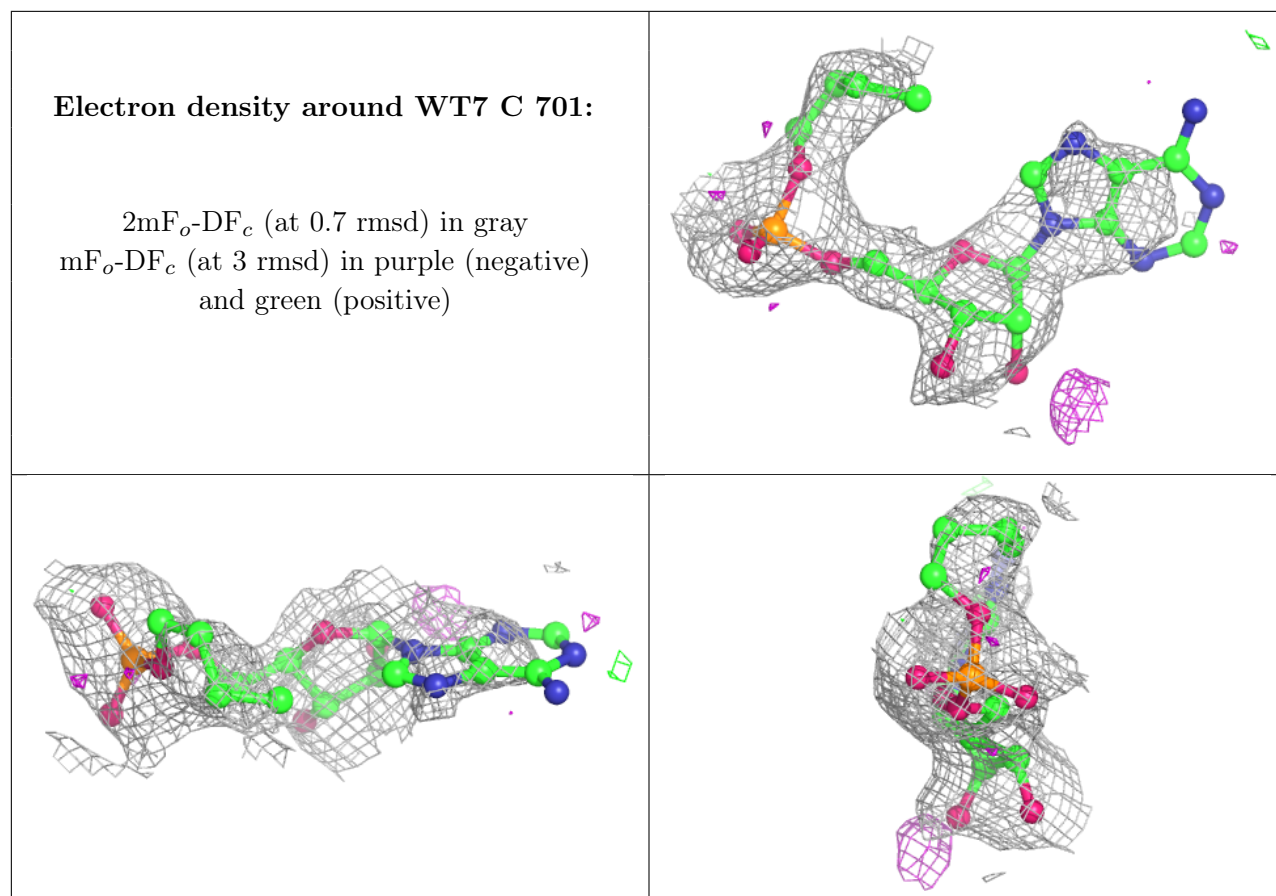
There are no monosaccharides in this entry.

6.4 Ligands

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.

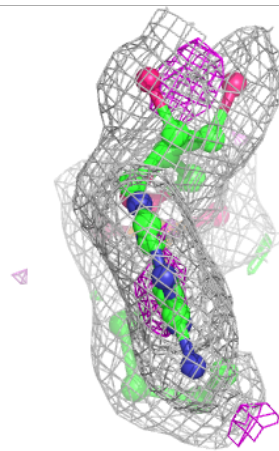
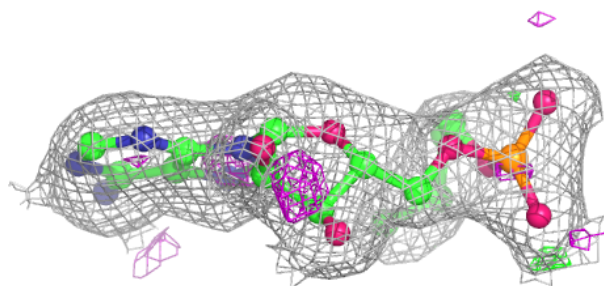
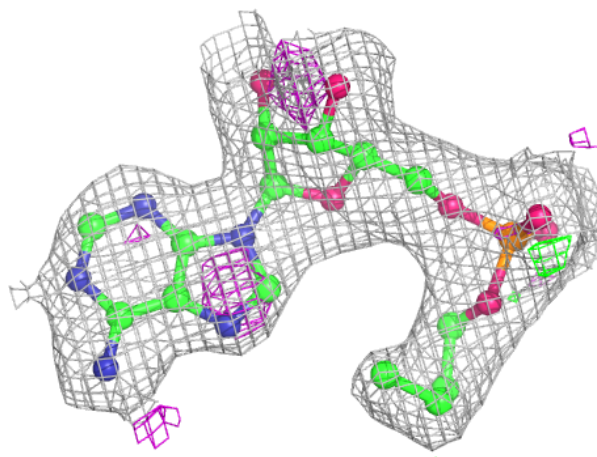
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WT7	C	701	27/27	0.77	0.33	63,85,95,98	27
3	EDO	A	704	4/4	0.82	0.33	50,56,56,56	0
3	EDO	B	704	4/4	0.82	0.21	31,35,40,43	0
3	EDO	C	703	4/4	0.83	0.19	63,66,67,72	0
3	EDO	C	704	4/4	0.83	0.29	54,60,60,63	0
4	PO4	A	706	5/5	0.87	0.20	51,54,61,65	5
3	EDO	B	702	4/4	0.88	0.14	49,51,52,57	0
4	PO4	B	707	5/5	0.89	0.19	64,68,82,84	5
3	EDO	B	703	4/4	0.92	0.14	53,54,56,59	0
3	EDO	B	705	4/4	0.92	0.38	47,48,50,53	0
3	EDO	A	703	4/4	0.95	0.13	40,43,45,47	0
3	EDO	A	702	4/4	0.95	0.19	33,36,40,40	0
2	WT7	A	701	27/27	0.96	0.14	29,33,40,40	0
3	EDO	A	705	4/4	0.96	0.25	39,39,42,46	0
2	WT7	B	701	27/27	0.97	0.15	26,33,37,38	0
3	EDO	C	702	4/4	0.97	0.09	36,40,43,47	0
3	EDO	B	706	4/4	0.98	0.12	47,48,50,51	0

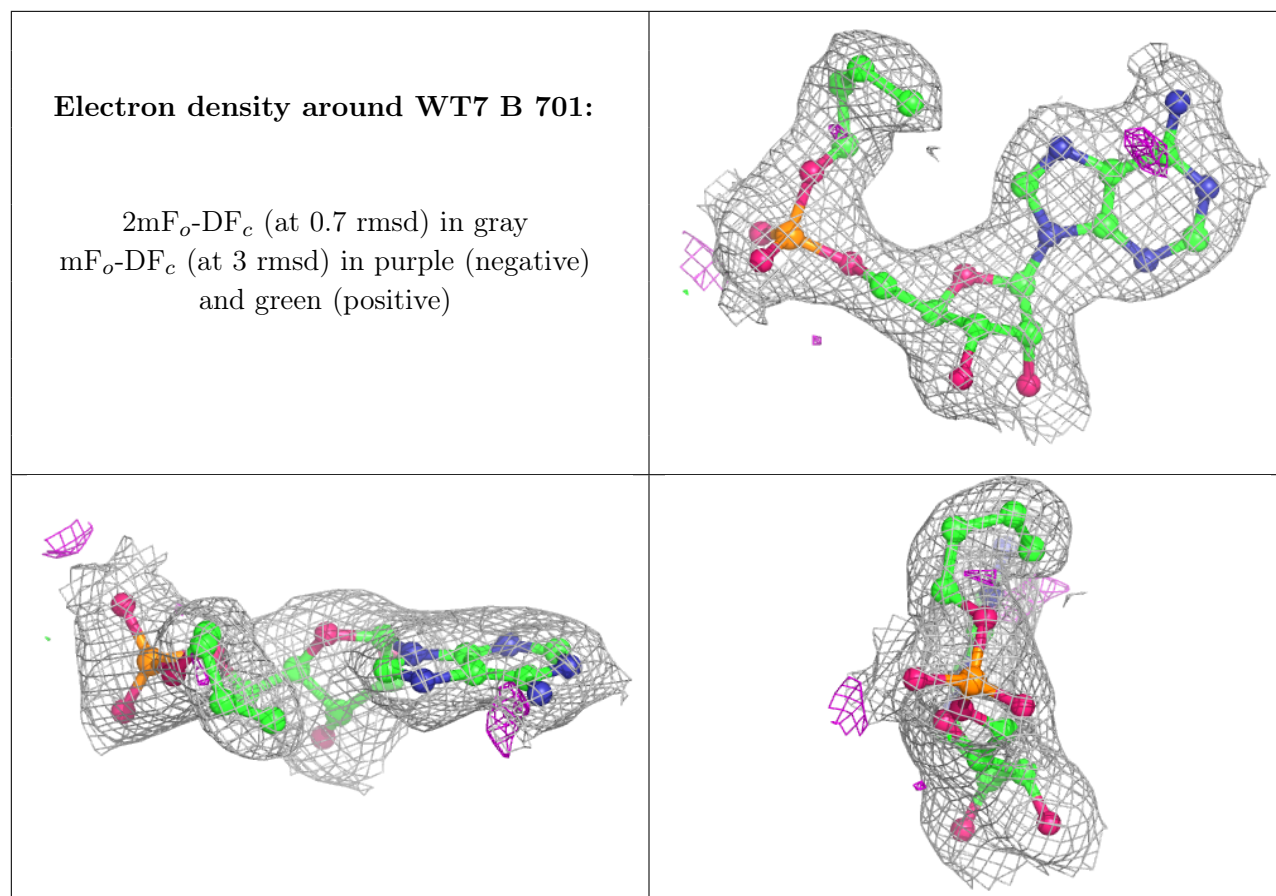
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around WT7 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.