



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2020 – 05:06 PM EST

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 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	:	2.15.1
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)	:	2.15.1

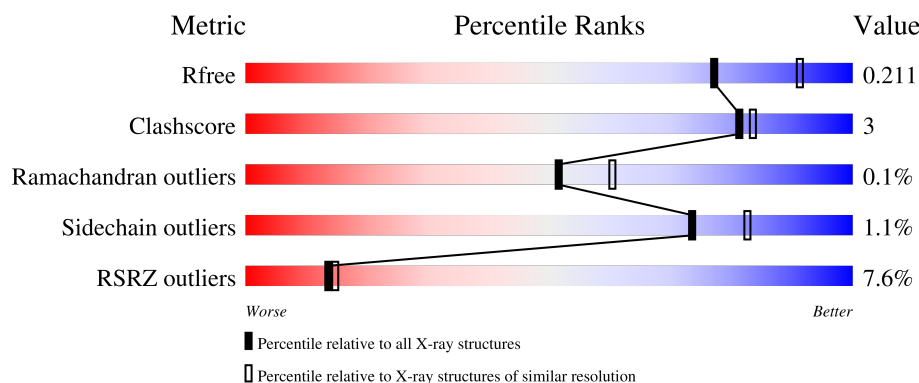
1 Overall quality at a glance

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	
1	B	694	
1	C	694	

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
1	A	653	Total	C	N	O	S	0	2	0
			5003	3190	855	933	25			
1	B	658	Total	C	N	O	S	0	4	0
			5111	3259	874	952	26			
1	C	511	Total	C	N	O	S	0	2	0
			3874	2468	660	724	22			

There are 45 discrepancies between the modelled and reference sequences:

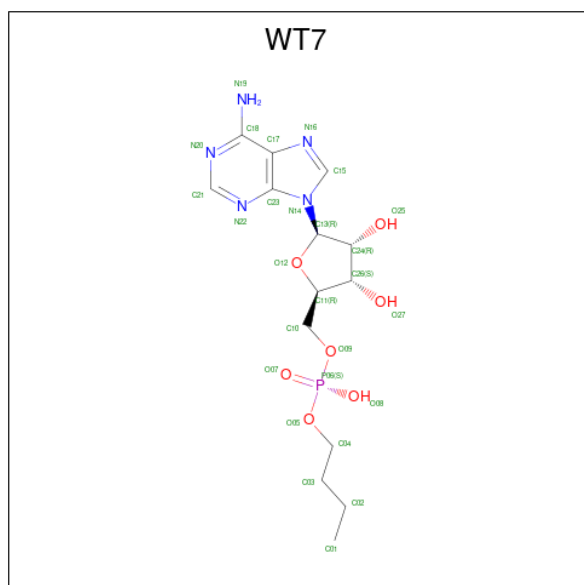
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression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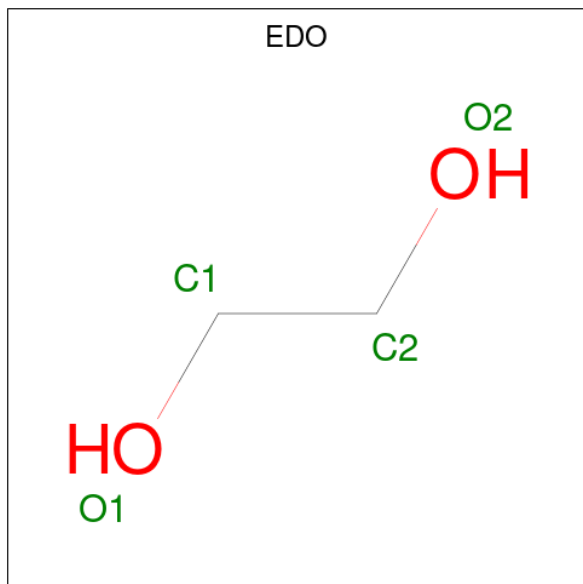
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1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



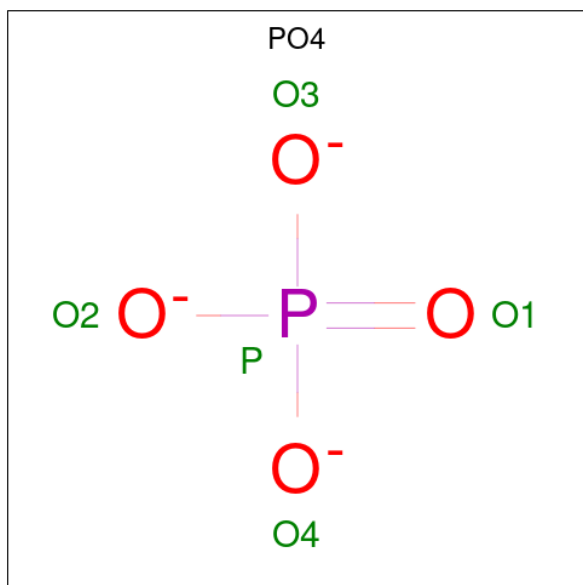
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

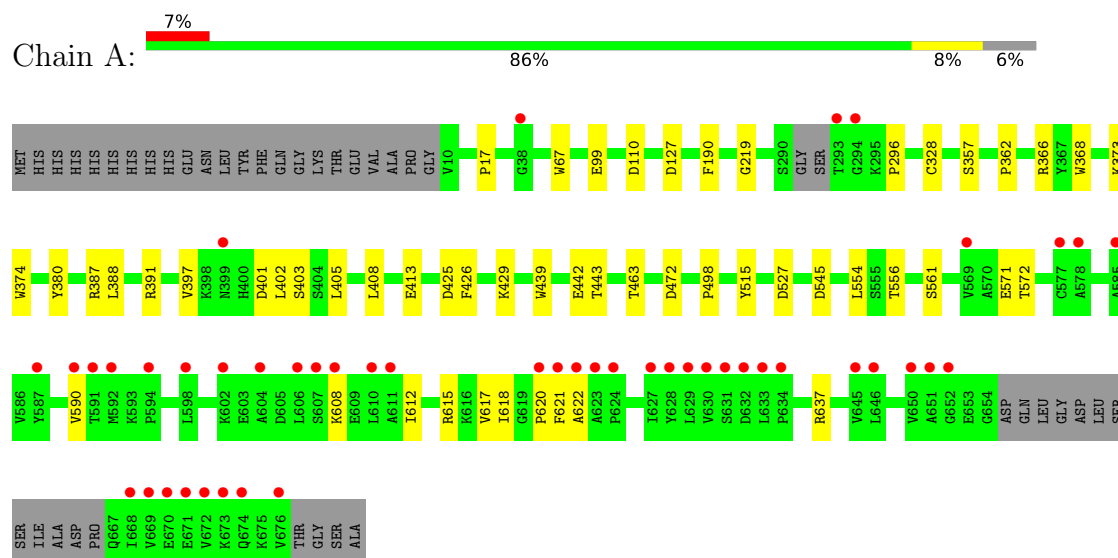
- Molecule 5 is water.

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

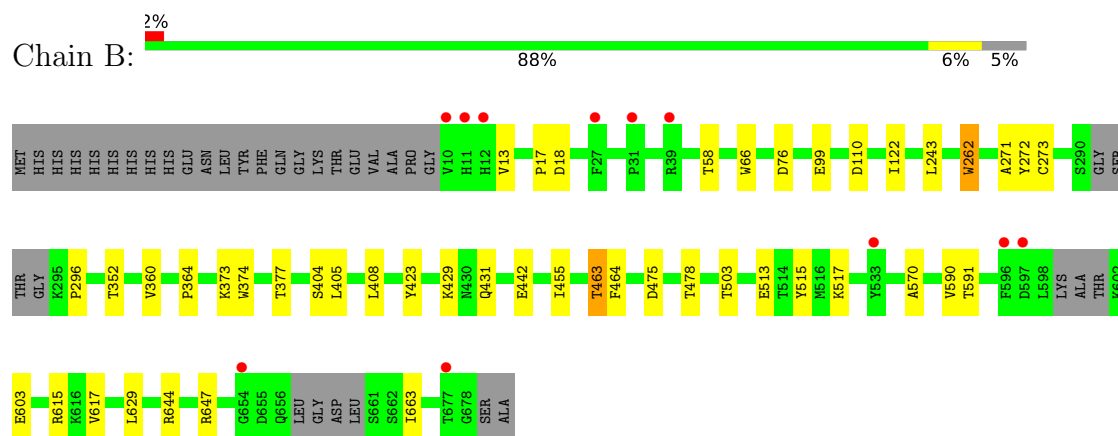
3 Residue-property plots [i](#)

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



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• Molecule 1: Acetyl-coenzyme A synthetase



PHE	ALA	SER	D472	T381	A56	MET
ALA	ALA	ALA	I473	A382	A57	HIS
PRO	ILE	LEU	I474	P383	T58	HIS
LYS	LYS	LEU	D475	T384	V59	HIS
ILE	LYS	LEU	P476	A385	G60	HIS
TYR	ILE	LYS	Q477	I386	W66	HIS
LEU	GLY	GLY	T478	R387	K70	HIS
VAL	VAL	VAL	G479	L388	D93	HIS
VAL	ALA	ALA	Q480	R389	K70	GLU
SER	GLU	GLU	V481	R390	D93	ASN
ASP	THR	THR	L482	R391	T101	LEU
LEU	ALA	ALA	E483	M392	T101	TYR
PRO	VAL	VAL	G484	G393	D10	PHE
LYS	VAL	VAL	V487	L408	D10	GLN
THR	GLY	GLY	E488	G409	K158	GLY
THR	GLY	CYS	G489	S410	R199	LYS
ARG	SER	ALA	V490	V411	T213	THR
GLY	GLY	ASP	L491	G412	G219	GLU
LYS	ASP	ASP	Y519	I415	T222	VAL
ILE	LEU	LEU	Y522	M416	I223	ALA
ILE	THR	THR	F523	E418	A224	PRO
MET	ARG	GLN	F524	A419	Q235	GLY
ARG	VAL	ALA	D527	W420	W276	VAL
VAL	VAL	VAL	G528	W421	S290	HIS
LEU	LEU	VAL	A529	Y423	GLY	VAL
ARG	ARG	THR	A530	N424	THR	HIS
GLY	ALA	MET	R531	D425	GLY	VAL
GLY	GLY	LYS	D532	F426	R295	HIS
GLY	GLY	PRO	Y533	A427	P296	VAL
ASP	ASP	GLU	G535	N430	K297	PRO
GLN	PHE	LEU	Y536	Q431	L314	GLU
LEU	ASP	LEU	M537	C432	R325	SER
GLY	LEU	LEU	H538	A433	I332	GLY
ASP	ASP	LYS	I539	I434	G337	GLY
LEU	ALA	ALA	K540	Y438	T341	ASP
SER	THR	THR	GLY	W439	V360	L26
LYS	LYS	LYS	ARG	L314	K41	F27
ILE	GLU	VAL	VAL	I446	P29	A28
ALA	ALA	ASP	ASP	S447	P30	P29
ASP	PRO	LEU	VAL	I448	R32	F31
PRO	GLN	SER	ILE	P452	M33	R32
ILE	ILE	LYS	ASN	G453	K36	F36
VAL	VAL	GLU	VAL	A454	E37	E37
GLU	GLU	LEU	SER	P459	P40	P40
GLU	ALA	ALA	GLY	G460	K41	K41
VAL	ILE	ILE	HIS	S461	P42	P42
LYS	LYS	GLN	ARG	LEU	H43	H43
GLN	VAL	VAL	VAL	SER	T44	T44
LYS	ARG	LYS	LYS	A462	G45	G45
VAL	VAL	VAL	THR	T463	P46	P46
THR	VAL	VAL	ALA	F464	Y51	Y51
GLY	ILE	GLY	VAL	D470	L379	L379
SER	GLY	VAL	VAL	Y380	Y380	Y380
PRO	ALA	PRO	GLU			

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)	Xtriage
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	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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, EDO, WT7

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

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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:HE3	1:C:297:LYS:HB3	1.67	0.47

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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

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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

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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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
3	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.16	0
4	PO4	A	706	-	4,4,4	0.85	0	6,6,6	0.54	0
2	WT7	B	701	-	26,29,29	0.98	1 (3%)	28,42,42	0.81	1 (3%)
4	PO4	B	707	-	4,4,4	0.82	0	6,6,6	0.49	0
3	EDO	C	704	-	3,3,3	0.41	0	2,2,2	0.34	0
3	EDO	B	704	-	3,3,3	0.81	0	2,2,2	0.45	0
3	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	C	703	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	B	705	-	3,3,3	0.47	0	2,2,2	0.22	0
3	EDO	A	703	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	A	702	-	3,3,3	0.37	0	2,2,2	0.64	0
3	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.58	0
2	WT7	A	701	-	26,29,29	1.01	3 (11%)	28,42,42	0.85	1 (3%)
3	EDO	C	702	-	3,3,3	0.38	0	2,2,2	0.56	0
3	EDO	B	706	-	3,3,3	0.36	0	2,2,2	0.46	0
2	WT7	C	701	-	26,29,29	1.02	2 (7%)	28,42,42	0.84	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	705	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WT7	B	701	-	-	1/12/32/32	0/3/3/3
3	EDO	C	704	-	-	1/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
2	WT7	A	701	-	-	3/12/32/32	0/3/3/3
3	EDO	A	702	-	-	0/1/1/1	-
2	WT7	C	701	-	-	7/12/32/32	0/3/3/3
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	B	706	-	-	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	C	701	WT7	C04-O05-P06-O07
2	A	701	WT7	C10-O09-P06-O08
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

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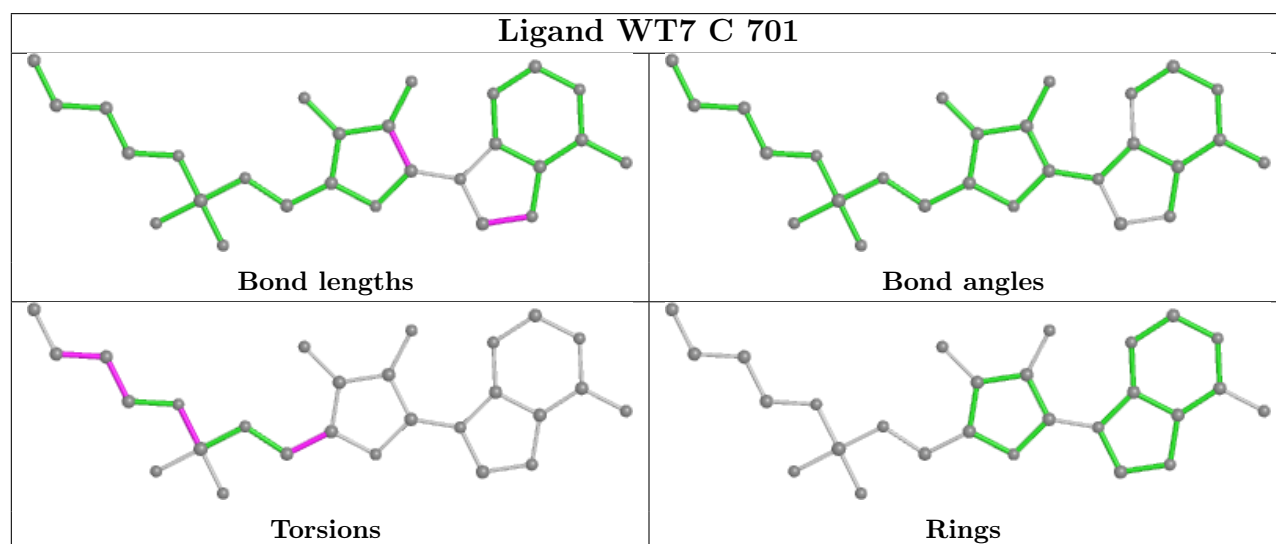
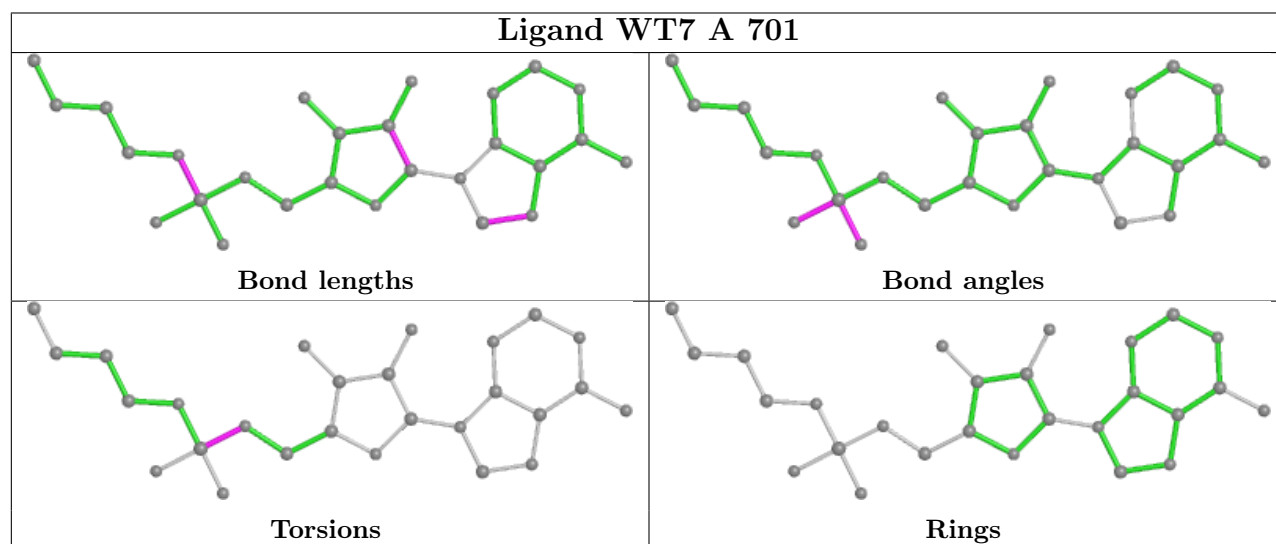
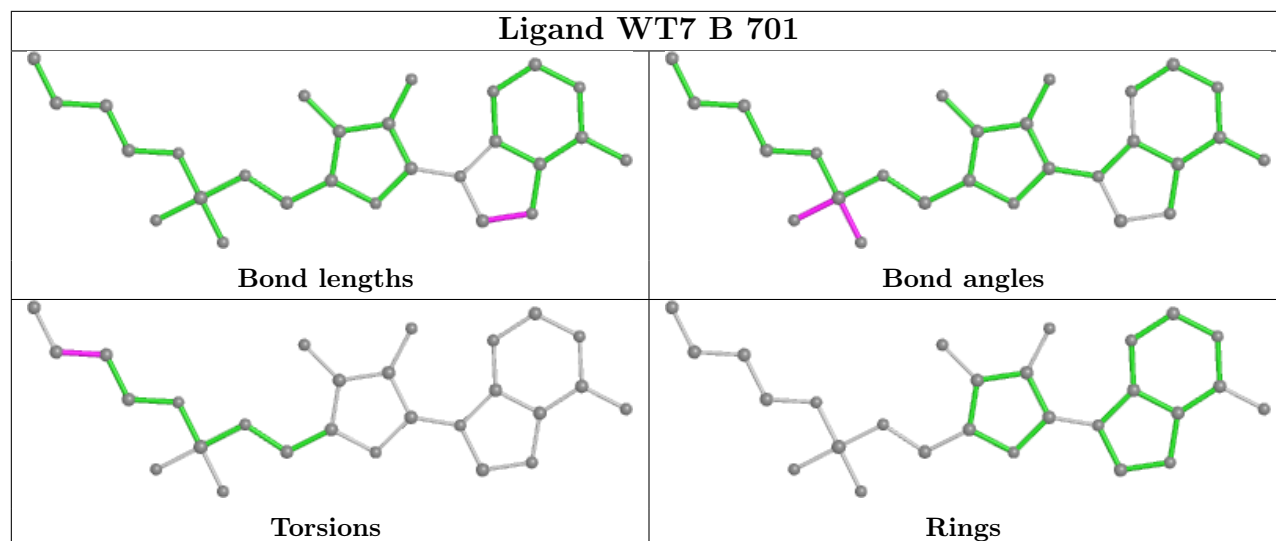
Mol	Chain	Res	Type	Atoms
2	C	701	WT7	O09-C10-C11-O12
3	B	704	EDO	O1-C1-C2-O2
2	C	701	WT7	C04-O05-P06-O09
2	A	701	WT7	C10-O09-P06-O05
3	A	704	EDO	O1-C1-C2-O2
2	C	701	WT7	C04-O05-P06-O08
2	A	701	WT7	C10-O09-P06-O07

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	EDO	1	0
3	A	702	EDO	1	0
2	A	701	WT7	1	0
3	C	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

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	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

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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

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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

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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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

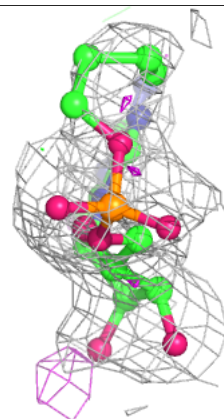
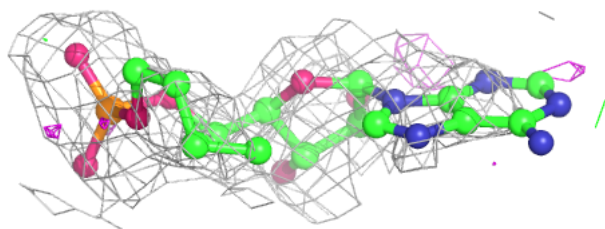
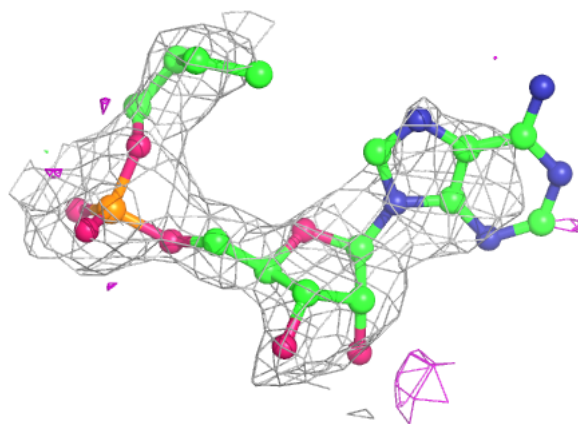
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	705	4/4	0.92	0.38	47,48,50,53	0
3	EDO	B	703	4/4	0.92	0.14	53,54,56,59	0
3	EDO	A	702	4/4	0.95	0.19	33,36,40,40	0
3	EDO	A	703	4/4	0.95	0.13	40,43,45,47	0
3	EDO	A	705	4/4	0.96	0.25	39,39,42,46	0
2	WT7	A	701	27/27	0.96	0.14	29,33,40,40	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.

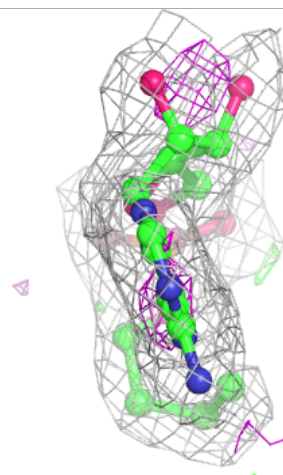
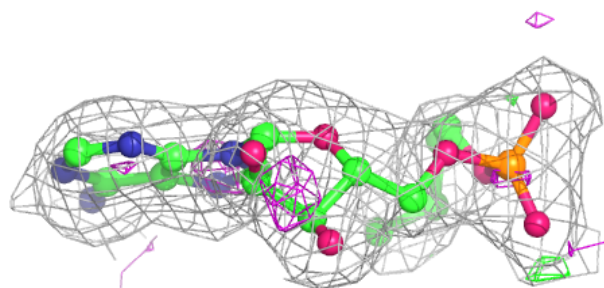
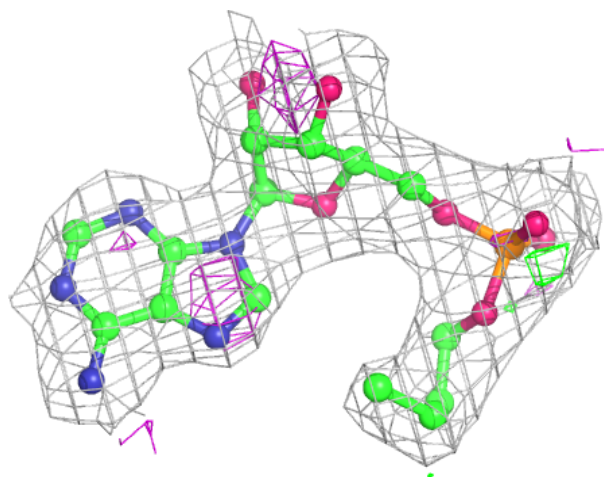
Electron density around WT7 C 701:

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



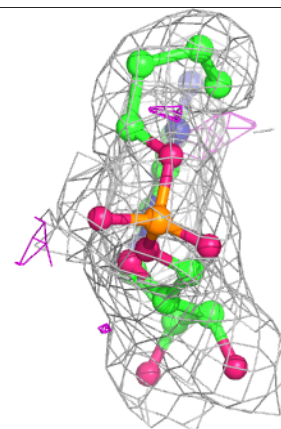
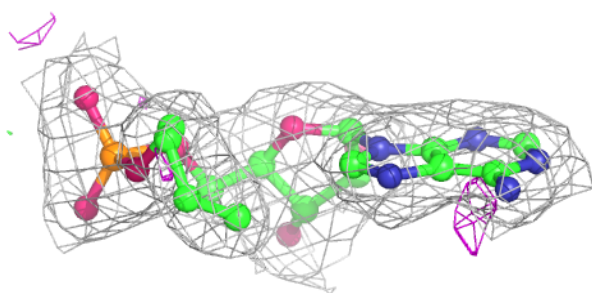
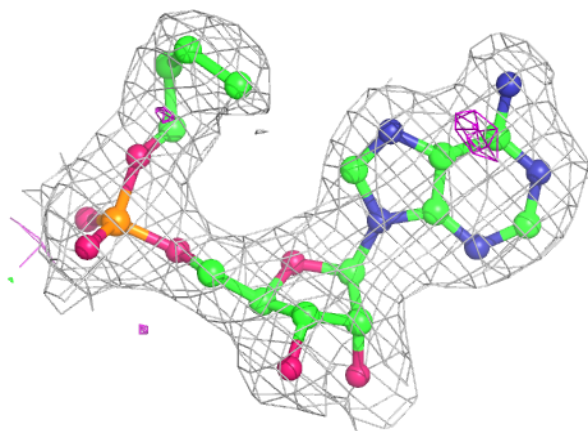
Electron density around WT7 A 701:

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



Electron density around WT7 B 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.