



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 04:21 PM EST

PDB ID : 7L4G  
Title : Crystal Structure of Acetyl-CoA synthetase in complex with acetyl adenylate from *Cryptococcus neoformans* H99  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2020-12-19  
Resolution : 2.20 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](mailto: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.

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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 : 2.16  
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) : 2.16

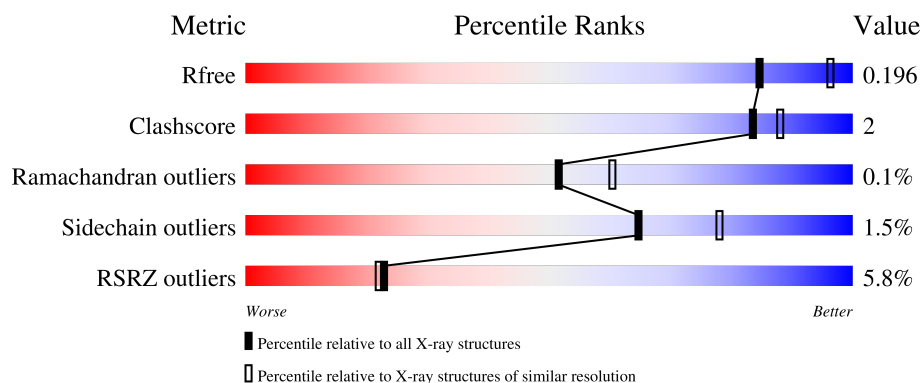
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	<div> <div>4%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	B	694	<div> <div>5%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	C	694	<div> <div>8%</div> <div>84%</div> <div>6%</div> <div>9%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16357 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	656	Total	C	N	O	S	0	5	0
			5116	3261	870	958	27			
1	B	668	Total	C	N	O	S	0	7	0
			5231	3331	891	981	28			
1	C	630	Total	C	N	O	S	0	1	0
			4819	3079	819	896	25			

There are 45 discrepancies between the modelled and reference sequences:

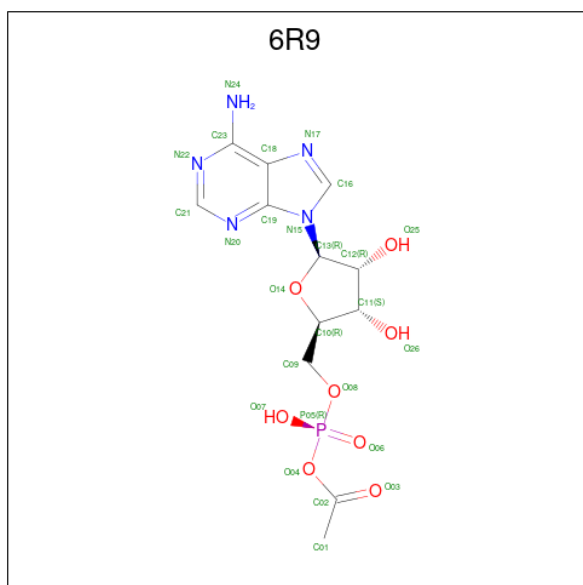
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression 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 [[[2 {R},3 {S},4 {R},5 {R}]-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (three-letter code: 6R9) (formula: C<sub>12</sub>H<sub>16</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	12	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			26	12	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			26	12	5	8	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

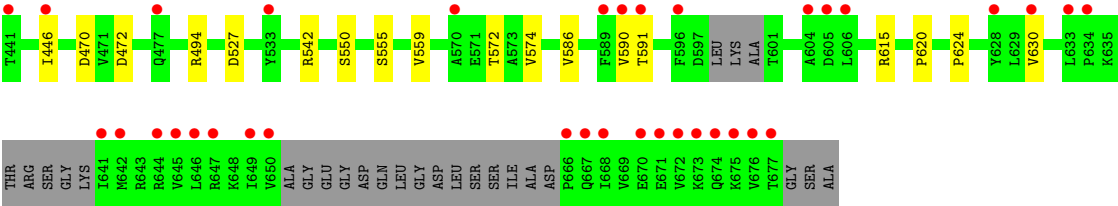
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	389	Total	O	0	2
			391	391		
6	B	398	Total	O	0	4
			401	401		
6	C	239	Total	O	0	1
			240	240		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.39Å 185.75Å 84.88Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	39.06 – 2.20 39.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.06-2.20) 98.1 (39.06-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19RC4-4035	Depositor
R, $R_{free}$	0.155 , 0.196 0.155 , 0.196	Depositor DCC
$R_{free}$ test set	1991 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, K, 6R9, 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	0.40	0/5267	0.59	1/7179 (0.0%)
1	B	0.37	0/5384	0.58	0/7331
1	C	0.36	0/4954	0.57	0/6761
All	All	0.38	0/15605	0.58	1/21271 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	LEU	CA-CB-CG	-5.58	102.47	115.30

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	5116	0	4907	23	0
1	B	5231	0	5046	23	0
1	C	4819	0	4558	26	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	5	0	0	0	0
4	A	24	0	36	2	0
4	B	24	0	36	3	0
4	C	12	0	18	0	0
5	C	1	0	0	0	0
6	A	391	0	0	0	0
6	B	401	0	0	1	0
6	C	240	0	0	2	0
All	All	16357	0	14601	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 2.

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:161:ALA:H	4:B:706:EDO:H22	1.33	0.94
1:A:47:ASN:HA	4:A:706:EDO:H22	1.68	0.76
1:B:548:ASN:HD21	1:B:553:ARG:HG2	1.56	0.71
1:B:297:LYS:NZ	3:B:703:PO4:O4	2.32	0.62
1:A:123:ILE:HD11	1:A:325:ARG:HD3	1.84	0.59
1:B:314:LEU:HD22	1:B:345:PRO:HA	1.84	0.59
1:A:391:ARG:HH11	1:A:594:PRO:HD3	1.69	0.57
1:A:472:ASP:OD2	1:A:494:ARG:HD2	2.05	0.56
1:B:548:ASN:ND2	1:B:553:ARG:HG2	2.19	0.56
1:B:161:ALA:N	4:B:706:EDO:H22	2.12	0.55
1:A:384:THR:HG21	1:A:639:GLY:HA3	1.87	0.55
1:C:472:ASP:OD2	1:C:494:ARG:NE	2.38	0.55
1:A:394:GLU:HG2	1:A:426:PHE:CZ	2.41	0.55
1:C:615:ARG:HG2	1:C:620:PRO:HA	1.88	0.54
1:A:470:ASP:OD2	1:A:494:ARG:HD3	2.08	0.53
1:B:405:LEU:HD13	1:B:408:LEU:HD21	1.91	0.53
1:C:384:THR:OG1	1:C:550:SER:HA	2.09	0.52
1:C:527:ASP:OD1	1:C:542:ARG:HD2	2.10	0.51
1:C:439:TRP:HB3	1:C:446:ILE:HA	1.93	0.51
1:A:617:VAL:HG23	1:A:618:ILE:HG13	1.92	0.51
1:C:224:ALA:HB1	1:C:227:GLN:HG3	1.94	0.50
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.48	0.49
1:C:572:THR:HG22	1:C:590:VAL:HG22	1.96	0.48
1:A:425:ASP:O	1:A:429:LYS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:SER:HB2	1:A:627:ILE:HD12	1.96	0.47
1:A:217:ARG:NH1	1:A:222:THR:OG1	2.47	0.47
1:B:280[B]:SER:OG	1:B:304:ALA:HB3	2.15	0.47
1:C:591:THR:HG22	1:C:630:VAL:HG23	1.97	0.46
1:B:513:GLU:HA	1:B:517:LYS:CG	2.46	0.46
1:C:424:ASN:ND2	6:C:819:HOH:O	2.48	0.46
1:B:321:HIS:HA	4:B:705:EDO:H21	1.97	0.46
1:A:314:LEU:HD22	1:A:345:PRO:HA	1.98	0.45
1:C:365:SER:OG	1:C:369:ASP:OD2	2.34	0.45
1:C:383:PRO:HG3	1:C:410:SER:OG	2.16	0.45
1:A:191:ALA:O	1:A:637:ARG:NH1	2.49	0.45
1:C:291:GLY:O	1:C:555:SER:HB2	2.16	0.45
1:A:603:GLU:HG3	1:A:629:LEU:HD12	1.99	0.45
1:B:368:TRP:HB3	1:B:402:LEU:HD21	1.98	0.45
1:B:635:LYS:O	1:B:663:ILE:HA	2.16	0.45
1:A:577:CYS:HB3	1:A:587:TYR:CE1	2.52	0.45
1:B:597:ASP:HB3	1:B:600:ALA:HB3	1.99	0.45
1:A:70:LYS:HE2	4:A:703:EDO:H21	1.98	0.44
1:C:83:THR:O	1:C:98:PRO:HD2	2.18	0.44
1:C:116[B]:ASN:OD1	6:C:801:HOH:O	2.21	0.44
1:B:271:ALA:HB3	1:C:93:ASP:HB3	1.99	0.44
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.53	0.44
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.53	0.43
1:C:559:VAL:HG12	1:C:574:VAL:HG21	1.99	0.43
1:C:122:ILE:HA	1:C:352:THR:O	2.19	0.43
1:C:470:ASP:OD2	1:C:494:ARG:HD2	2.18	0.43
1:C:586:VAL:HB	1:C:624:PRO:HA	2.00	0.43
1:B:492:VAL:HB	1:B:522:TYR:HB3	2.01	0.43
1:C:381:THR:O	1:C:410:SER:HA	2.19	0.43
1:C:408:LEU:HB3	1:C:423:TYR:CZ	2.54	0.43
1:C:40:PRO:HB2	1:C:321:HIS:CE1	2.54	0.42
1:C:360:VAL:HA	1:C:364:PRO:HA	2.01	0.42
1:B:513:GLU:HA	1:B:517:LYS:HG2	2.01	0.42
1:B:217[B]:ARG:NH2	6:B:812:HOH:O	2.43	0.42
1:B:488:GLU:HG3	1:B:540:LYS:NZ	2.34	0.42
1:B:472:ASP:OD2	1:B:494:ARG:CZ	2.67	0.42
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.54	0.42
1:C:408:LEU:HB3	1:C:423:TYR:CE2	2.54	0.42
1:A:390:ARG:HG3	1:A:422:TRP:CD1	2.55	0.41
1:B:384:THR:OG1	1:B:635:LYS:HD2	2.20	0.41
1:A:146:ARG:O	1:A:150:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:VAL:O	1:A:676:VAL:HG23	2.21	0.41
1:B:63:SER:OG	1:B:85:ARG:NH2	2.53	0.41
1:C:314:LEU:HD22	1:C:345:PRO:HA	2.01	0.41
1:A:554:LEU:HD21	1:A:621:PHE:HE1	1.86	0.41
1:B:42:PRO:HA	1:B:319:ASP:OD2	2.20	0.40
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.90	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	655/694 (94%)	634 (97%)	20 (3%)	1 (0%)	47	55
1	B	673/694 (97%)	656 (98%)	16 (2%)	1 (0%)	51	60
1	C	623/694 (90%)	600 (96%)	23 (4%)	0	100	100
All	All	1951/2082 (94%)	1890 (97%)	59 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	THR
1	A	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	530/576 (92%)	523 (99%)	7 (1%)	69	81
1	B	544/576 (94%)	532 (98%)	12 (2%)	52	65
1	C	484/576 (84%)	477 (99%)	7 (1%)	67	80
All	All	1558/1728 (90%)	1532 (98%)	26 (2%)	65	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	116	ASN
1	A	262	TRP
1	A	277	ARG
1	A	423	TYR
1	A	540	LYS
1	A	580	ASP
1	B	25	ASP
1	B	52	VAL
1	B	76	ASP
1	B	110	ASP
1	B	217[A]	ARG
1	B	217[B]	ARG
1	B	290	SER
1	B	325[A]	ARG
1	B	325[B]	ARG
1	B	416	ASN
1	B	423	TYR
1	B	548	ASN
1	C	51	TYR
1	C	76	ASP
1	C	110	ASP
1	C	116[A]	ASN
1	C	116[B]	ASN
1	C	365	SER
1	C	423	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	430	ASN
1	B	116	ASN

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Mol	Chain	Res	Type
1	B	548	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	B	706	-	3,3,3	0.61	0	2,2,2	0.18	0
3	PO4	C	702	-	4,4,4	0.82	0	6,6,6	0.55	0
4	EDO	B	708	-	3,3,3	0.56	0	2,2,2	0.38	0
2	6R9	B	701	-	24,28,28	4.10	5 (20%)	26,42,42	1.52	5 (19%)
4	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.31	0
3	PO4	B	702	-	4,4,4	0.80	0	6,6,6	0.46	0
4	EDO	C	703	-	3,3,3	0.51	0	2,2,2	0.28	0
2	6R9	C	701	5	24,28,28	4.29	6 (25%)	26,42,42	1.30	3 (11%)
4	EDO	B	709	-	3,3,3	0.45	0	2,2,2	0.46	0
4	EDO	A	708	-	3,3,3	0.47	0	2,2,2	0.38	0
3	PO4	B	703	-	4,4,4	0.80	0	6,6,6	0.46	0
4	EDO	A	707	-	3,3,3	0.45	0	2,2,2	0.88	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	705	-	3,3,3	0.49	0	2,2,2	0.48	0
4	EDO	A	703	-	3,3,3	0.57	0	2,2,2	0.32	0
4	EDO	B	707	-	3,3,3	0.45	0	2,2,2	0.63	0
4	EDO	C	705	-	3,3,3	0.33	0	2,2,2	0.80	0
3	PO4	A	702	-	4,4,4	0.80	0	6,6,6	0.37	0
4	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.50	0
4	EDO	A	704	-	3,3,3	0.42	0	2,2,2	0.50	0
4	EDO	B	704	-	3,3,3	0.53	0	2,2,2	0.29	0
4	EDO	C	704	-	3,3,3	0.50	0	2,2,2	0.17	0
2	6R9	A	701	-	24,28,28	4.21	5 (20%)	26,42,42	1.50	4 (15%)

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	EDO	B	706	-	-	1/1/1/1	-
4	EDO	A	706	-	-	0/1/1/1	-
4	EDO	A	708	-	-	0/1/1/1	-
4	EDO	B	707	-	-	0/1/1/1	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	C	705	-	-	0/1/1/1	-
2	6R9	C	701	5	-	1/9/31/31	0/3/3/3
4	EDO	A	705	-	-	0/1/1/1	-
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	B	704	-	-	1/1/1/1	-
4	EDO	C	704	-	-	0/1/1/1	-
4	EDO	A	707	-	-	1/1/1/1	-
4	EDO	B	705	-	-	0/1/1/1	-
4	EDO	B	708	-	-	0/1/1/1	-
4	EDO	C	703	-	-	0/1/1/1	-
4	EDO	A	703	-	-	0/1/1/1	-
2	6R9	B	701	-	-	1/9/31/31	0/3/3/3
2	6R9	A	701	-	-	1/9/31/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	6R9	O14-C13	15.02	1.62	1.41
2	A	701	6R9	O14-C13	14.28	1.61	1.41
2	B	701	6R9	O14-C13	14.20	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	6R9	C12-C13	-12.33	1.35	1.53
2	C	701	6R9	C12-C13	-12.00	1.35	1.53
2	B	701	6R9	C12-C13	-11.57	1.36	1.53
2	C	701	6R9	O14-C10	-5.88	1.31	1.45
2	B	701	6R9	O14-C10	-5.65	1.32	1.45
2	A	701	6R9	O14-C10	-5.61	1.32	1.45
2	A	701	6R9	P05-O04	3.63	1.68	1.60
2	B	701	6R9	P05-O04	3.51	1.67	1.60
2	C	701	6R9	P05-O04	2.96	1.66	1.60
2	C	701	6R9	C23-N24	2.91	1.44	1.34
2	A	701	6R9	C23-N24	2.89	1.44	1.34
2	B	701	6R9	C23-N24	2.86	1.44	1.34
2	C	701	6R9	C11-C10	2.31	1.58	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	6R9	N20-C21-N22	-4.82	121.15	128.68
2	B	701	6R9	N20-C21-N22	-4.60	121.49	128.68
2	C	701	6R9	N20-C21-N22	-4.16	122.17	128.68
2	A	701	6R9	C13-N15-C19	-2.76	121.79	126.64
2	B	701	6R9	C19-C18-N17	-2.70	106.59	109.40
2	C	701	6R9	C19-C18-N17	-2.59	106.70	109.40
2	B	701	6R9	C13-N15-C19	-2.53	122.20	126.64
2	C	701	6R9	C13-N15-C19	-2.37	122.48	126.64
2	A	701	6R9	O08-C09-C10	-2.26	101.20	108.99
2	B	701	6R9	C11-C12-C13	2.08	104.10	100.98
2	A	701	6R9	C19-C18-N17	-2.05	107.26	109.40
2	B	701	6R9	O08-C09-C10	-2.03	101.99	108.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

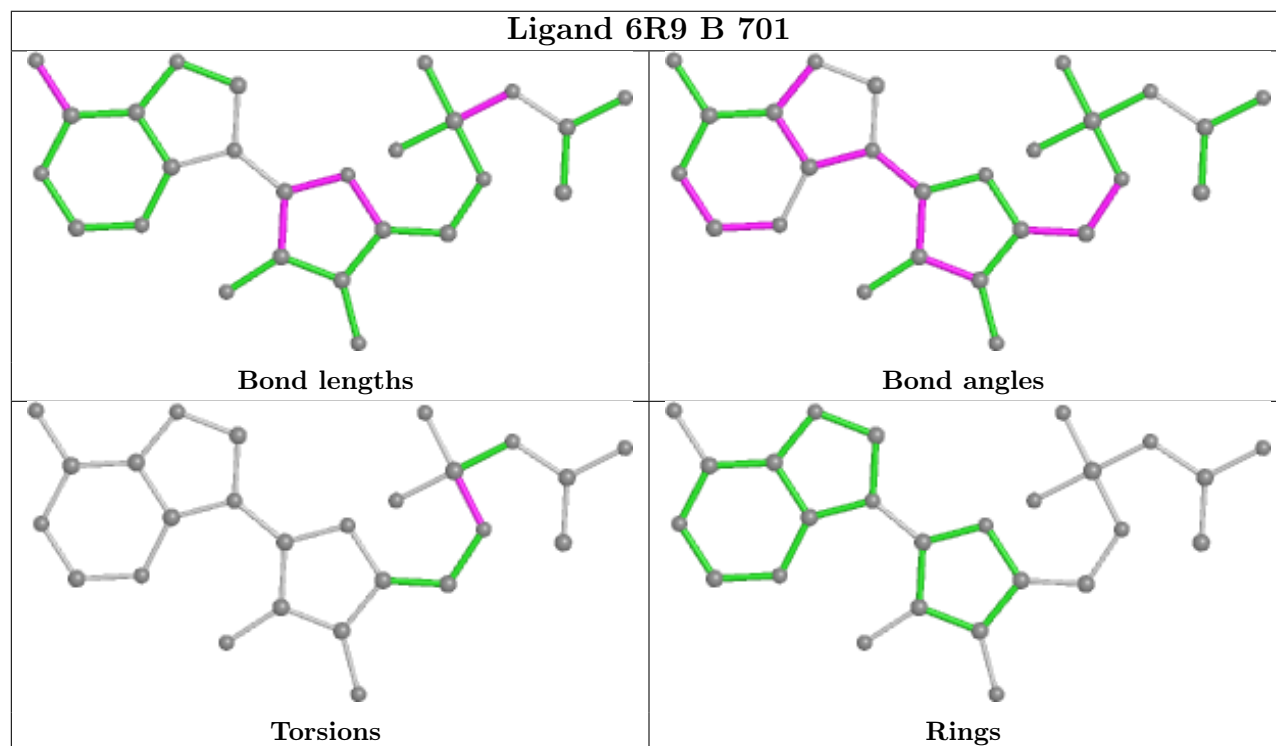
Mol	Chain	Res	Type	Atoms
2	C	701	6R9	C09-O08-P05-O04
4	B	706	EDO	O1-C1-C2-O2
4	B	704	EDO	O1-C1-C2-O2
2	A	701	6R9	C02-O04-P05-O08
4	A	707	EDO	O1-C1-C2-O2
2	B	701	6R9	C09-O08-P05-O06

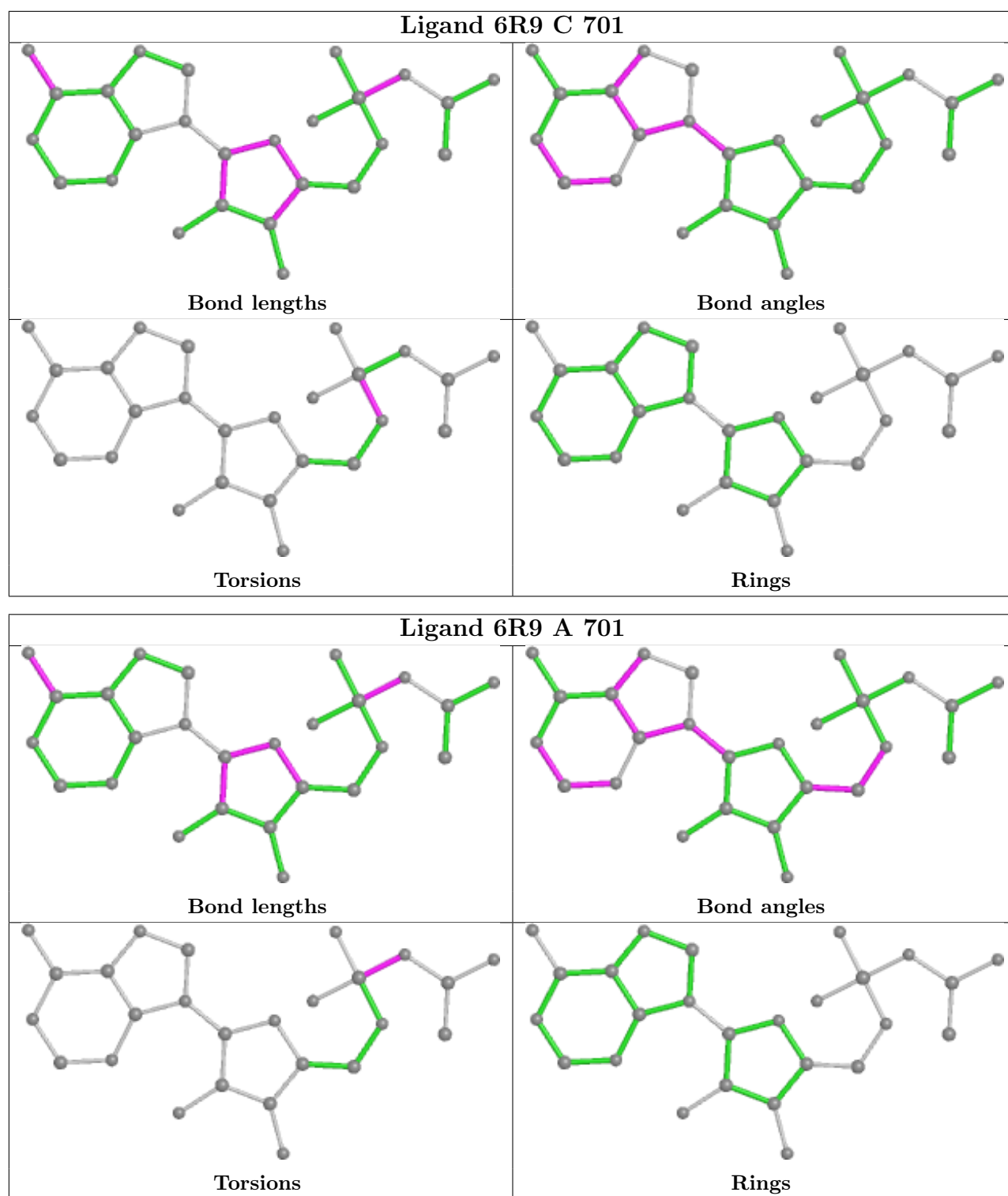
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	EDO	2	0
4	A	706	EDO	1	0
3	B	703	PO4	1	0
4	B	705	EDO	1	0
4	A	703	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	656/694 (94%)	-0.21	25 (3%)	40	38	25, 40, 76, 111	0
1	B	668/694 (96%)	-0.16	34 (5%)	28	26	26, 40, 75, 127	0
1	C	630/694 (90%)	0.10	55 (8%)	10	8	27, 50, 83, 132	0
All	All	1954/2082 (93%)	-0.09	114 (5%)	23	22	25, 42, 80, 132	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	THR	6.2
1	B	601	THR	6.2
1	C	676	VAL	5.8
1	C	677	THR	5.7
1	B	291	GLY	5.7
1	B	600	ALA	5.6
1	C	675	LYS	5.3
1	C	646	LEU	4.8
1	B	292	SER	4.6
1	C	672	VAL	4.5
1	B	294	GLY	4.5
1	C	604	ALA	4.4
1	C	642	MET	4.2
1	C	335	ILE	4.2
1	B	411	VAL	4.1
1	C	596	PHE	4.0
1	C	650	VAL	3.9
1	C	606	LEU	3.8
1	B	639	GLY	3.7
1	C	649	ILE	3.7
1	C	666	PRO	3.6
1	C	589	PHE	3.6
1	B	334	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	628	TYR	3.4
1	C	645	VAL	3.3
1	B	340	TYR	3.2
1	A	677	THR	3.2
1	C	411	VAL	3.2
1	C	633	LEU	3.2
1	B	599	LYS	3.1
1	B	381	THR	3.1
1	A	665	ASP	3.0
1	C	340	TYR	3.0
1	C	533	TYR	3.0
1	B	380	TYR	3.0
1	A	654	GLY	3.0
1	C	590	VAL	3.0
1	B	336	THR	3.0
1	C	634	PRO	2.9
1	C	336	THR	2.9
1	A	335	ILE	2.8
1	C	337	GLY	2.8
1	B	382	ALA	2.8
1	C	570	ALA	2.8
1	C	668	ILE	2.8
1	C	38	GLY	2.8
1	B	595	GLU	2.8
1	C	26	LEU	2.7
1	A	336	THR	2.7
1	C	591	THR	2.7
1	A	652	GLY	2.7
1	B	410	SER	2.7
1	C	644	ARG	2.7
1	A	674	GLN	2.7
1	A	330	ALA	2.7
1	A	341	ILE	2.6
1	C	674	GLN	2.6
1	B	10	VAL	2.6
1	C	412	GLY	2.6
1	B	409	GLY	2.6
1	C	670	GLU	2.6
1	A	533	TYR	2.5
1	B	657	LEU	2.5
1	B	439	TRP	2.5
1	B	597	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	437	THR	2.5
1	C	641	ILE	2.5
1	C	667	GLN	2.5
1	B	335	ILE	2.5
1	C	647	ARG	2.4
1	B	446	ILE	2.4
1	A	580	ASP	2.4
1	C	339	SER	2.4
1	C	630	VAL	2.4
1	A	655	ASP	2.4
1	C	439	TRP	2.3
1	A	411	VAL	2.3
1	B	669	VAL	2.3
1	C	341	ILE	2.3
1	C	673	LYS	2.3
1	A	334	TRP	2.3
1	C	422	TRP	2.3
1	A	332	ILE	2.3
1	C	338	HIS	2.2
1	B	435	VAL	2.2
1	C	61	PRO	2.2
1	C	441	THR	2.2
1	A	594	PRO	2.2
1	B	330	ALA	2.2
1	C	306	TYR	2.2
1	B	342	ILE	2.2
1	C	25	ASP	2.2
1	B	596	PHE	2.1
1	C	314	LEU	2.1
1	A	333	GLY	2.1
1	C	380	TYR	2.1
1	A	579	ASP	2.1
1	A	399	ASN	2.1
1	B	339	SER	2.1
1	B	328	CYS	2.1
1	A	339	SER	2.1
1	A	668	ILE	2.1
1	C	446	ILE	2.1
1	A	577	CYS	2.1
1	C	328	CYS	2.1
1	C	477	GLN	2.1
1	C	426	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	2.1
1	A	338	HIS	2.1
1	C	671	GLU	2.1
1	A	581	LEU	2.1
1	B	314	LEU	2.1
1	B	654	GLY	2.0
1	C	605	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	C	705	4/4	0.87	0.15	40,43,44,51	0
4	EDO	A	703	4/4	0.88	0.27	45,50,53,55	0
4	EDO	A	707	4/4	0.88	0.11	48,53,55,57	0
4	EDO	C	704	4/4	0.88	0.12	49,52,56,58	0
4	EDO	B	706	4/4	0.90	0.15	38,41,46,46	0
4	EDO	A	704	4/4	0.91	0.15	36,39,41,47	0
4	EDO	B	704	4/4	0.91	0.20	55,57,58,59	0
4	EDO	B	708	4/4	0.91	0.15	42,42,44,48	0
4	EDO	B	705	4/4	0.92	0.11	42,46,47,50	0
4	EDO	B	709	4/4	0.92	0.17	44,48,49,50	0
4	EDO	C	703	4/4	0.92	0.16	49,50,54,56	0
3	PO4	A	702	5/5	0.93	0.38	54,70,74,78	0
3	PO4	C	702	5/5	0.93	0.19	68,76,84,84	0
2	6R9	C	701	26/26	0.94	0.16	40,48,51,51	0
4	EDO	B	707	4/4	0.95	0.15	44,44,47,48	0
3	PO4	B	702	5/5	0.96	0.12	60,62,72,74	0

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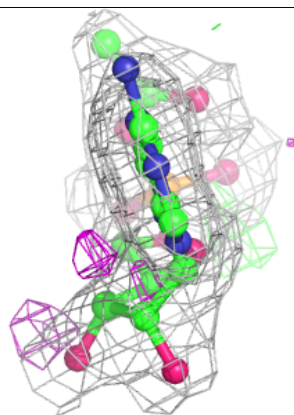
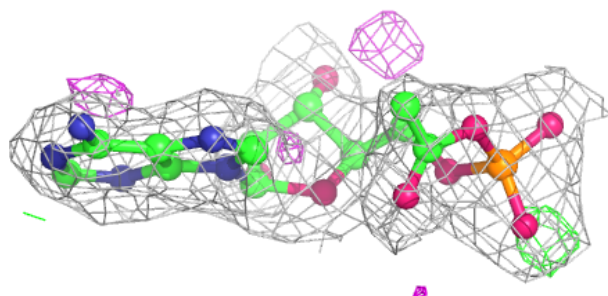
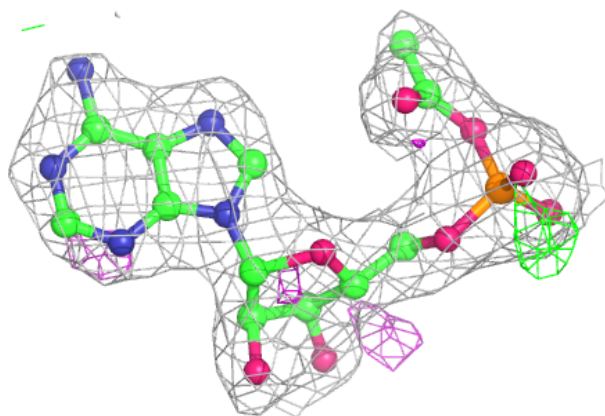
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	706	4/4	0.96	0.30	40,44,45,49	0
4	EDO	A	705	4/4	0.96	0.07	34,40,41,45	0
4	EDO	A	708	4/4	0.97	0.08	39,40,42,42	0
3	PO4	B	703	5/5	0.97	0.29	65,76,84,87	0
2	6R9	A	701	26/26	0.97	0.18	26,31,36,40	0
2	6R9	B	701	26/26	0.98	0.20	29,32,35,37	0
5	K	C	706	1/1	0.99	0.09	48,48,48,48	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.

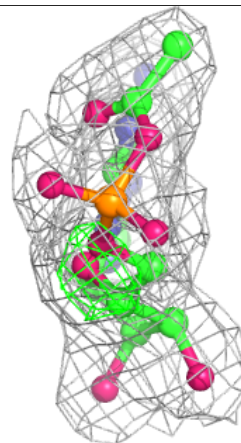
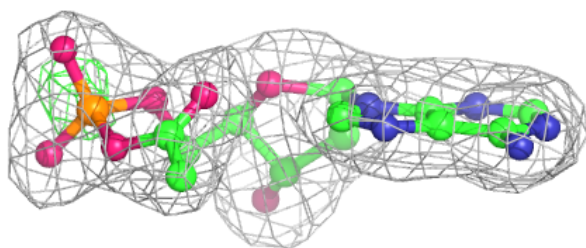
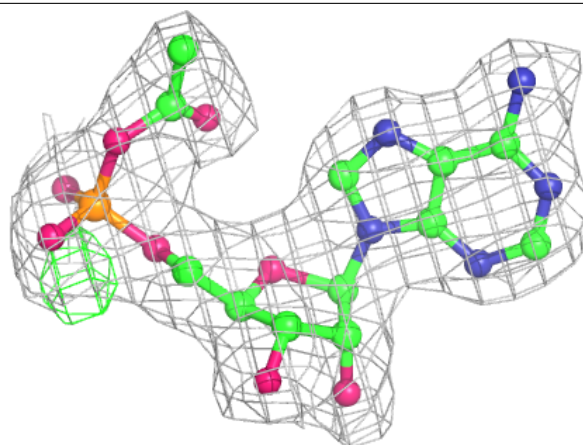
**Electron density around 6R9 C 701:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



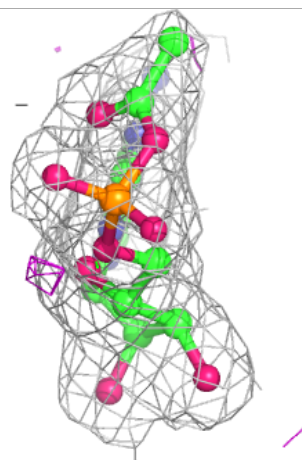
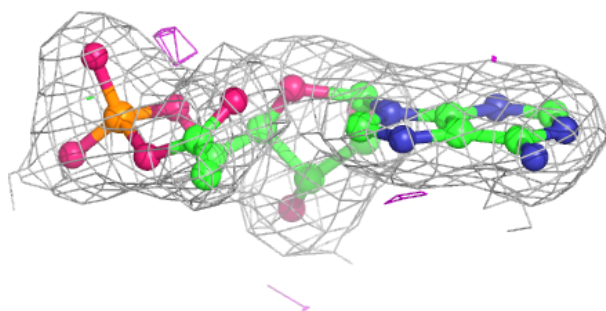
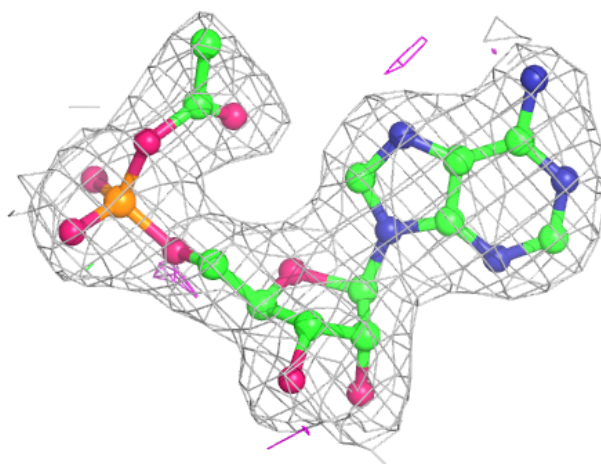
**Electron density around 6R9 A 701:**

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



**Electron density around 6R9 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.