



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 04:25 PM EDT

PDB ID : 5TKV  
Title : X-RAY CRYSTAL STRUCTURE OF THE "CLOSED" CONFORMATION OF CTP-INHIBITED E. COLI CYTIDINE TRIPHOSPHATE (CTP) SYNTHETASE  
Authors : Baldwin, E.P.; Endrizzi, J.A.  
Deposited on : 2016-10-07  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (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

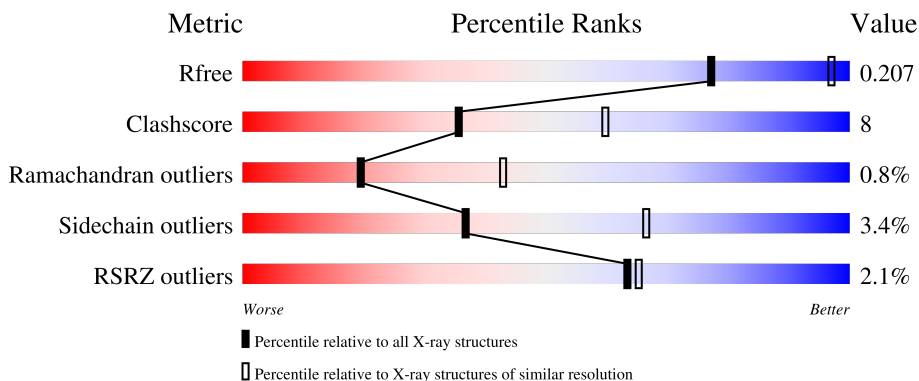
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

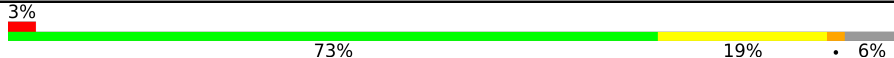
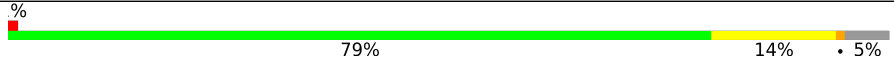
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	565	 3% 73% 19% • 6%
1	B	565	 % 79% 14% • 5%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 8827 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 CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4143	2618	724	781	20	0	0	0
1	B	535	4162	2630	727	785	20	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

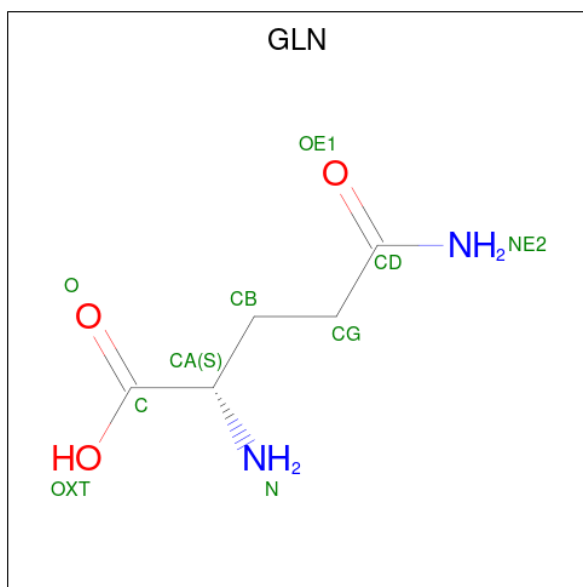
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0A7E5
A	-18	GLY	-	expression tag	UNP P0A7E5
A	-17	SER	-	expression tag	UNP P0A7E5
A	-16	SER	-	expression tag	UNP P0A7E5
A	-15	HIS	-	expression tag	UNP P0A7E5
A	-14	HIS	-	expression tag	UNP P0A7E5
A	-13	HIS	-	expression tag	UNP P0A7E5
A	-12	HIS	-	expression tag	UNP P0A7E5
A	-11	HIS	-	expression tag	UNP P0A7E5
A	-10	HIS	-	expression tag	UNP P0A7E5
A	-9	SER	-	expression tag	UNP P0A7E5
A	-8	SER	-	expression tag	UNP P0A7E5
A	-7	GLY	-	expression tag	UNP P0A7E5
A	-6	LEU	-	expression tag	UNP P0A7E5
A	-5	VAL	-	expression tag	UNP P0A7E5
A	-4	PRO	-	expression tag	UNP P0A7E5
A	-3	ARG	-	expression tag	UNP P0A7E5
A	-2	GLY	-	expression tag	UNP P0A7E5
A	-1	SER	-	expression tag	UNP P0A7E5
A	0	HIS	-	expression tag	UNP P0A7E5
A	268	ALA	CYS	conflict	UNP P0A7E5
B	-19	MET	-	initiating methionine	UNP P0A7E5
B	-18	GLY	-	expression tag	UNP P0A7E5
B	-17	SER	-	expression tag	UNP P0A7E5
B	-16	SER	-	expression tag	UNP P0A7E5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P0A7E5
B	-14	HIS	-	expression tag	UNP P0A7E5
B	-13	HIS	-	expression tag	UNP P0A7E5
B	-12	HIS	-	expression tag	UNP P0A7E5
B	-11	HIS	-	expression tag	UNP P0A7E5
B	-10	HIS	-	expression tag	UNP P0A7E5
B	-9	SER	-	expression tag	UNP P0A7E5
B	-8	SER	-	expression tag	UNP P0A7E5
B	-7	GLY	-	expression tag	UNP P0A7E5
B	-6	LEU	-	expression tag	UNP P0A7E5
B	-5	VAL	-	expression tag	UNP P0A7E5
B	-4	PRO	-	expression tag	UNP P0A7E5
B	-3	ARG	-	expression tag	UNP P0A7E5
B	-2	GLY	-	expression tag	UNP P0A7E5
B	-1	SER	-	expression tag	UNP P0A7E5
B	0	HIS	-	expression tag	UNP P0A7E5
B	268	ALA	CYS	conflict	UNP P0A7E5

- Molecule 2 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	5	2	3	0	0
2	B	1	10	5	2	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

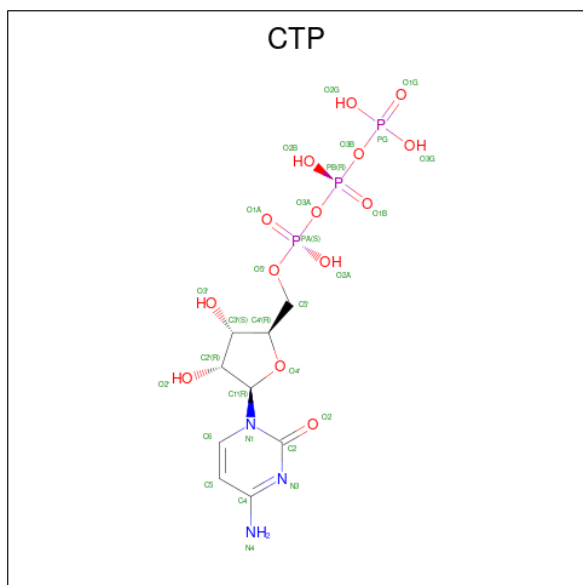


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

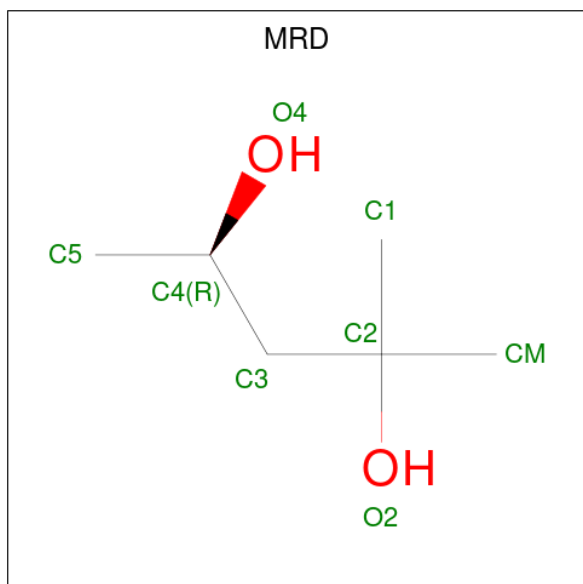
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	29	9	3	14	3	0	0
6	B	1	29	9	3	14	3	0	0

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	8	6	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

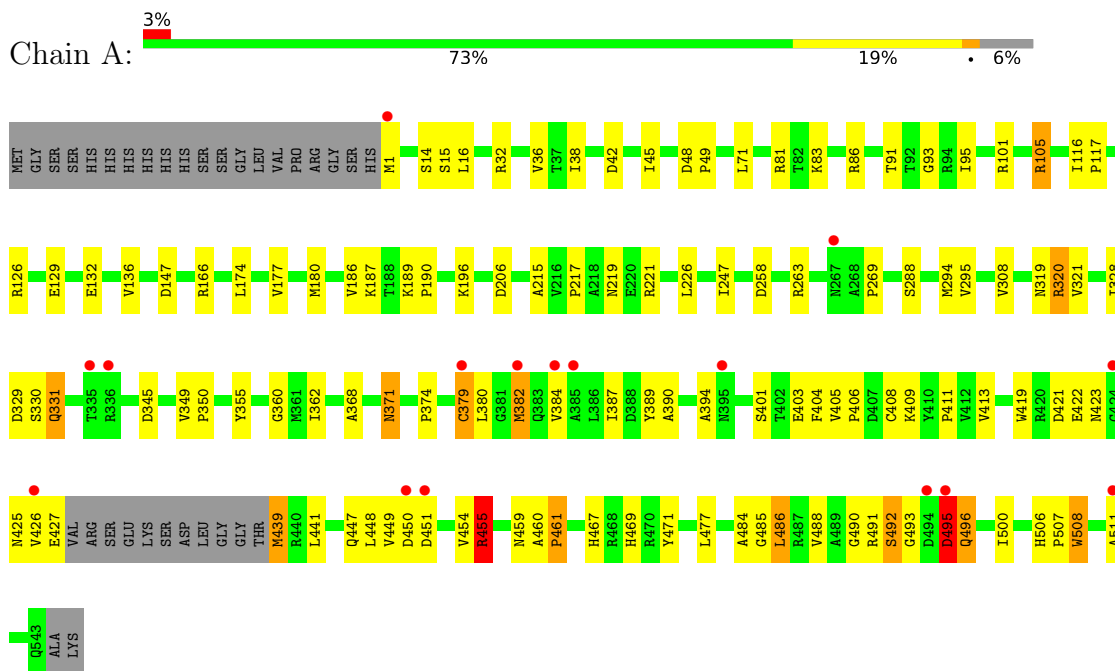
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	165	Total	O	0	0
			165	165		
8	B	205	Total	O	0	0
			205	205		



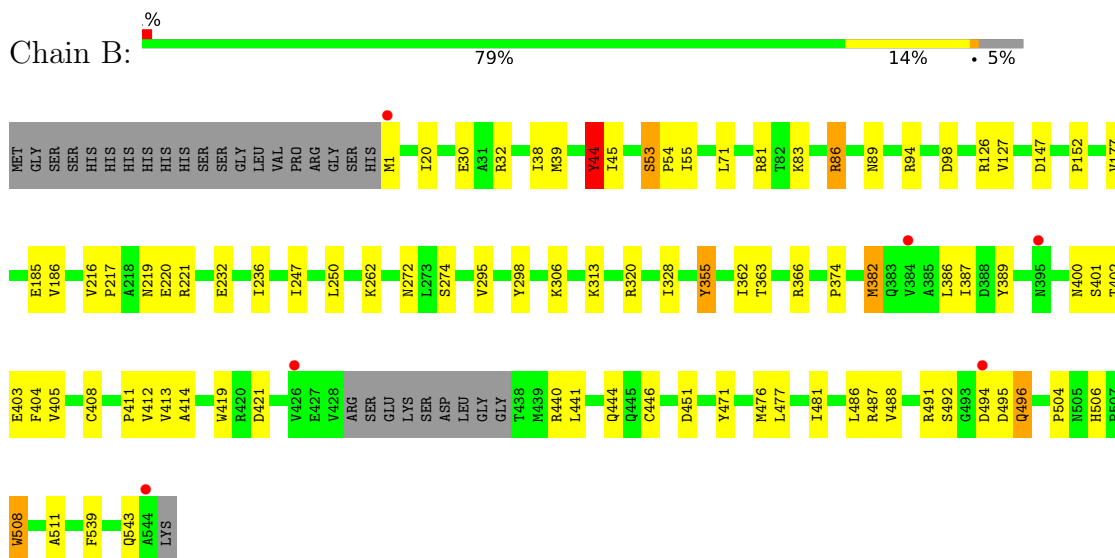
### 3 Residue-property plots i

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: CTP synthase



- Molecule 1: CTP synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.16Å 110.67Å 129.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 2.70 29.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.02-2.70) 98.3 (29.77-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.157 , 0.208 0.159 , 0.207	Depositor DCC
$R_{free}$ test set	3159 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.43% 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: MG, MRD, MPD, SO4, CTP

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	0.81	1/4219 (0.0%)	0.96	11/5716 (0.2%)
1	B	0.81	3/4238 (0.1%)	0.92	3/5743 (0.1%)
All	All	0.81	4/8457 (0.0%)	0.94	14/11459 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	TYR	CB-CG	-6.10	1.42	1.51
1	A	508	TRP	CD2-CE2	5.74	1.48	1.41
1	B	30	GLU	CD-OE1	5.49	1.31	1.25
1	B	508	TRP	CD2-CE2	5.18	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH1	-9.45	115.57	120.30
1	B	32	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	320	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	258	ASP	CB-CG-OD1	7.27	124.85	118.30
1	A	320	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	32	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	263	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	226	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	A	81	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	206	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	A	439	MET	CB-CG-SD	5.24	128.11	112.40
1	B	236	ILE	CG1-CB-CG2	-5.24	99.88	111.40
1	A	455	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	421	ASP	CB-CG-OD1	5.04	122.83	118.30

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	4143	0	4152	77	0
1	B	4162	0	4173	55	0
2	A	10	0	7	1	0
2	B	10	0	7	0	0
3	A	20	0	0	2	0
3	B	20	0	0	1	0
4	A	8	0	14	2	0
4	B	8	0	14	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	58	0	24	2	0
7	B	16	0	28	0	0
8	A	165	0	0	3	0
8	B	205	0	0	10	0
All	All	8827	0	8419	136	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 8.

All (136) 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:306:LYS:HD2	8:B:754:HOH:O	1.67	0.94
1:A:493:GLY:O	1:A:496:GLN:NE2	2.00	0.92
1:A:455:ARG:HH11	1:A:455:ARG:HG3	1.35	0.90
1:B:487:ARG:NH2	1:B:504:PRO:HB3	1.90	0.85
3:B:609:SO4:O1	8:B:701:HOH:O	1.93	0.85
1:B:487:ARG:HH21	1:B:504:PRO:HB3	1.41	0.85
1:A:455:ARG:HH11	1:A:455:ARG:CG	1.96	0.78
1:B:81:ARG:HD2	8:B:797:HOH:O	1.87	0.75
1:A:426:VAL:O	1:A:427:GLU:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:CYS:HB2	8:B:860:HOH:O	1.91	0.70
3:A:602:SO4:O4	8:A:701:HOH:O	2.10	0.69
1:A:382:MET:HA	1:A:511:ALA:HB1	1.76	0.66
1:A:455:ARG:HG3	1:A:455:ARG:NH1	2.05	0.64
1:B:98:ASP:OD2	1:B:126:ARG:NH1	2.27	0.63
1:B:295:VAL:HG22	1:B:328:ILE:HB	1.80	0.62
1:B:247:ILE:HD11	4:B:607:MPD:H4	1.81	0.62
1:A:105:ARG:HG3	1:A:105:ARG:O	1.99	0.62
1:A:389:TYR:CE2	1:A:486:LEU:HB2	2.35	0.61
1:A:411:PRO:HD2	1:A:477:LEU:HD11	1.83	0.61
1:B:487:ARG:HH21	1:B:504:PRO:CB	2.14	0.60
1:A:409:LYS:HE2	1:A:422:GLU:HB2	1.85	0.59
1:B:232:GLU:HG2	8:B:855:HOH:O	2.03	0.59
1:B:71:LEU:C	1:B:71:LEU:HD12	2.23	0.58
1:A:295:VAL:HG12	1:A:330:SER:HB3	1.85	0.58
1:A:368:ALA:O	1:A:506:HIS:HE1	1.85	0.58
1:A:405:VAL:HG12	1:A:408:CYS:HB3	1.86	0.58
1:B:419:TRP:C	1:B:476:MET:HE3	2.25	0.57
1:B:177:VAL:HG12	1:B:186:VAL:HB	1.87	0.57
1:B:389:TYR:CE2	1:B:486:LEU:HB2	2.39	0.57
1:B:411:PRO:HD2	1:B:477:LEU:HD11	1.87	0.56
1:B:362:ILE:HD13	1:B:387:ILE:HG21	1.88	0.55
1:A:371:ASN:N	1:A:371:ASN:OD1	2.39	0.55
1:A:247:ILE:HD11	4:A:604:MPD:H4	1.88	0.55
1:A:294:MET:HE2	1:A:308:VAL:HG11	1.90	0.54
1:A:389:TYR:OH	1:A:485:GLY:HA3	2.09	0.53
1:A:495:ASP:O	1:A:496:GLN:C	2.46	0.53
1:A:460:ALA:HB1	1:A:461:PRO:HD2	1.90	0.53
4:A:604:MPD:O4	4:A:604:MPD:O2	2.24	0.52
1:B:86:ARG:NH1	1:B:89:ASN:O	2.43	0.52
1:A:177:VAL:HG12	1:A:186:VAL:HB	1.92	0.51
1:B:355:TYR:CD1	1:B:404:PHE:HB3	2.45	0.51
1:A:355:TYR:CD1	1:A:404:PHE:HB3	2.45	0.51
1:B:374:PRO:HB3	1:B:508:TRP:HB3	1.93	0.51
1:B:44:TYR:HE2	8:B:867:HOH:O	1.94	0.51
1:A:413:VAL:HG12	1:A:471:TYR:HB3	1.92	0.51
1:B:402:THR:HG23	1:B:414:ALA:HB2	1.93	0.51
1:B:362:ILE:CD1	1:B:387:ILE:HG21	2.42	0.50
1:B:363:THR:O	1:B:366:ARG:HB3	2.11	0.50
1:B:216:VAL:O	1:B:221:ARG:NH1	2.45	0.50
1:A:439:MET:O	1:A:439:MET:HG2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG22	1:A:136:VAL:HB	1.94	0.49
1:A:320:ARG:NH2	8:A:706:HOH:O	2.44	0.49
1:A:423:ASN:HB2	1:A:425:ASN:OD1	2.13	0.49
1:B:217:PRO:HD2	1:B:220:GLU:HG3	1.93	0.49
1:A:449:VAL:HG21	1:A:488:VAL:O	2.13	0.48
1:A:450:ASP:HA	1:A:455:ARG:HD3	1.95	0.48
1:A:45:ILE:O	1:A:93:GLY:HA3	2.13	0.48
1:A:180:MET:HG2	1:A:187:LYS:HG3	1.95	0.48
1:B:440:ARG:HH11	1:B:444:GLN:HE22	1.60	0.48
1:B:147:ASP:HB3	6:B:603:CTP:C2	2.48	0.48
1:A:295:VAL:HA	1:A:328:ILE:O	2.14	0.47
1:B:401:SER:HA	1:B:413:VAL:O	2.14	0.47
1:A:401:SER:HA	1:A:413:VAL:O	2.15	0.47
1:B:94:ARG:CD	8:B:849:HOH:O	2.61	0.47
1:A:426:VAL:O	1:A:427:GLU:CB	2.60	0.46
1:B:382:MET:HA	1:B:511:ALA:HB1	1.96	0.46
1:A:379:CYS:O	1:A:380:LEU:C	2.53	0.46
1:A:448:LEU:HD22	1:A:454:VAL:HG12	1.95	0.46
1:A:492:SER:OG	1:A:493:GLY:N	2.46	0.46
1:B:320:ARG:HA	8:B:747:HOH:O	2.15	0.46
1:A:403:GLU:HB2	1:A:471:TYR:CZ	2.51	0.46
1:B:400:ASN:OD1	1:B:401:SER:N	2.39	0.46
1:B:403:GLU:HB2	1:B:471:TYR:CZ	2.50	0.46
1:B:39:MET:HE2	1:B:127:VAL:HG22	1.98	0.46
1:A:374:PRO:HB3	1:A:508:TRP:HB3	1.98	0.46
1:A:441:LEU:HA	1:A:467:HIS:O	2.16	0.45
1:A:95:ILE:CD1	1:A:126:ARG:HD2	2.46	0.45
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.76	0.45
1:A:16:LEU:HD13	1:A:174:LEU:HB3	1.98	0.45
1:A:215:ALA:O	1:A:217:PRO:HD3	2.16	0.45
1:A:294:MET:HE2	1:A:308:VAL:CG1	2.47	0.45
1:A:129:GLU:O	1:A:132:GLU:HG2	2.15	0.45
1:B:412:VAL:HG23	1:B:413:VAL:HG23	1.99	0.45
1:A:189:LYS:HB3	1:A:190:PRO:HD3	1.98	0.44
1:B:94:ARG:HD2	8:B:849:HOH:O	2.16	0.44
1:A:71:LEU:HD12	1:A:71:LEU:C	2.37	0.44
1:A:506:HIS:HD2	1:A:508:TRP:H	1.66	0.44
1:A:401:SER:HB2	1:A:413:VAL:HB	1.99	0.44
1:B:495:ASP:O	1:B:496:GLN:C	2.56	0.44
1:A:14:SER:O	1:A:15:SER:HB2	2.18	0.44
1:A:345:ASP:O	1:A:374:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:HD13	1:A:387:ILE:HG21	1.99	0.44
1:A:447:GLN:O	1:A:490:GLY:HA2	2.17	0.44
1:B:488:VAL:HG11	1:B:491:ARG:CZ	2.48	0.43
1:B:374:PRO:HA	1:B:506:HIS:HE1	1.83	0.43
1:A:380:LEU:O	1:A:384:VAL:HG13	2.18	0.43
1:A:95:ILE:HD11	1:A:126:ARG:HD2	2.00	0.43
1:A:390:ALA:HA	1:A:394:ALA:HB3	2.01	0.43
1:B:152:PRO:HG2	8:B:702:HOH:O	2.17	0.43
1:B:419:TRP:HB3	1:B:476:MET:HE3	2.00	0.43
1:A:147:ASP:HB3	6:B:601:CTP:C2	2.54	0.43
1:A:319:ASN:O	1:A:321:VAL:HG23	2.18	0.43
1:A:349:VAL:HA	1:A:350:PRO:HD3	1.90	0.42
1:B:83:LYS:HD3	1:B:83:LYS:HA	1.83	0.42
1:A:405:VAL:HG12	1:A:405:VAL:O	2.19	0.42
3:A:603:SO4:O4	8:A:702:HOH:O	2.22	0.42
1:A:42:ASP:O	1:A:91:THR:HA	2.19	0.42
1:B:272:ASN:OD1	1:B:274:SER:OG	2.36	0.42
1:A:83:LYS:HD3	1:A:83:LYS:HA	1.83	0.42
1:A:32:ARG:HD3	1:A:269:PRO:O	2.19	0.42
1:B:313:LYS:HB3	1:B:313:LYS:HE2	1.83	0.42
1:A:405:VAL:HA	1:A:406:PRO:HD3	1.85	0.42
1:A:329:ASP:OD1	1:A:331:GLN:HB2	2.19	0.42
1:A:403:GLU:HB2	1:A:471:TYR:CE1	2.55	0.42
1:A:506:HIS:CD2	1:A:507:PRO:HD2	2.55	0.42
1:B:217:PRO:HD2	1:B:220:GLU:CG	2.50	0.41
1:A:187:LYS:HE3	1:A:187:LYS:HB3	1.77	0.41
1:A:166:ARG:HG2	1:A:166:ARG:O	2.20	0.41
1:A:294:MET:HE1	1:A:308:VAL:HG12	2.02	0.41
1:A:330:SER:O	1:A:360:GLY:HA3	2.21	0.41
1:A:459:ASN:O	1:A:459:ASN:OD1	2.38	0.41
1:B:405:VAL:HG23	1:B:408:CYS:HB3	2.02	0.41
1:B:539:PHE:CD1	1:B:539:PHE:C	2.93	0.41
1:A:491:ARG:HD2	1:A:496:GLN:HB3	2.01	0.41
1:B:54:PRO:HG2	1:B:298:TYR:CZ	2.56	0.41
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.85	0.41
1:B:38:ILE:HG21	1:B:38:ILE:HD13	1.81	0.41
1:A:469:HIS:HB2	2:A:601:GLN:OXT	2.21	0.41
1:A:488:VAL:HG11	1:A:491:ARG:HH11	1.86	0.40
1:B:539:PHE:O	1:B:543:GLN:HG2	2.20	0.40
1:A:48:ASP:HB2	1:A:49:PRO:HD2	2.03	0.40
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:TRP:HB3	1:B:476:MET:CE	2.51	0.40
1:A:116:ILE:HA	1:A:117:PRO:HA	1.80	0.40
1:B:45:ILE:O	1:B:45:ILE:HG22	2.20	0.40
1:B:53:SER:OG	1:B:55:ILE:HG12	2.21	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	528/565 (94%)	488 (92%)	34 (6%)	6 (1%)	14	34
1	B	531/565 (94%)	508 (96%)	21 (4%)	2 (0%)	34	60
All	All	1059/1130 (94%)	996 (94%)	55 (5%)	8 (1%)	19	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	SER
1	A	496	GLN
1	B	496	GLN
1	B	492	SER
1	A	484	ALA
1	A	419	TRP
1	A	461	PRO
1	A	495	ASP

### 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	449/477 (94%)	433 (96%)	16 (4%)	35	64
1	B	451/477 (94%)	436 (97%)	15 (3%)	38	67
All	All	900/954 (94%)	869 (97%)	31 (3%)	37	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	86	ARG
1	A	101	ARG
1	A	105	ARG
1	A	196	LYS
1	A	219	ASN
1	A	288	SER
1	A	331	GLN
1	A	371	ASN
1	A	379	CYS
1	A	382	MET
1	A	451	ASP
1	A	455	ARG
1	A	486	LEU
1	A	495	ASP
1	A	500	ILE
1	B	1	MET
1	B	20	ILE
1	B	44	TYR
1	B	53	SER
1	B	86	ARG
1	B	185	GLU
1	B	219	ASN
1	B	250	LEU
1	B	262	LYS
1	B	355	TYR
1	B	382	MET
1	B	421	ASP
1	B	451	ASP
1	B	481	ILE
1	B	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	459	ASN
1	A	506	HIS
1	B	324	ASN
1	B	444	GLN
1	B	447	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLN	A	601	-	8,9,9	1.02	1 (12%)	10,11,11	1.10	1 (10%)
4	MPD	A	604	-	7,7,7	0.56	0	9,10,10	1.27	1 (11%)
2	GLN	B	604	-	8,9,9	0.99	0	10,11,11	1.41	2 (20%)
3	SO4	A	605	-	4,4,4	0.32	0	6,6,6	0.22	0
3	SO4	B	605	-	4,4,4	0.62	0	6,6,6	0.99	0
3	SO4	A	603	-	4,4,4	0.55	0	6,6,6	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CTP	B	603	5	26,30,30	0.86	0	39,47,47	1.07	4 (10%)
7	MRD	B	610	-	7,7,7	0.76	0	9,10,10	1.78	2 (22%)
3	SO4	A	606	-	4,4,4	0.46	0	6,6,6	0.70	0
4	MPD	B	607	-	7,7,7	1.50	2 (28%)	9,10,10	1.13	1 (11%)
6	CTP	B	601	5	26,30,30	0.90	0	39,47,47	1.33	4 (10%)
3	SO4	B	608	-	4,4,4	0.54	0	6,6,6	0.51	0
3	SO4	B	609	-	4,4,4	0.12	0	6,6,6	0.32	0
7	MRD	B	611	-	7,7,7	1.28	1 (14%)	9,10,10	0.93	0
3	SO4	A	602	-	4,4,4	0.80	0	6,6,6	1.27	1 (16%)
3	SO4	B	606	-	4,4,4	0.53	0	6,6,6	0.83	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
2	GLN	A	601	-	-	0/9/9/9	-
4	MPD	A	604	-	-	3/5/5/5	-
2	GLN	B	604	-	-	0/9/9/9	-
7	MRD	B	610	-	-	1/5/5/5	-
4	MPD	B	607	-	-	2/5/5/5	-
6	CTP	B	601	5	-	4/22/38/38	0/2/2/2
7	MRD	B	611	-	-	0/5/5/5	-
6	CTP	B	603	5	-	3/22/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	607	MPD	O2-C2	2.99	1.52	1.44
4	B	607	MPD	CM-C2	-2.53	1.44	1.52
7	B	611	MRD	O4-C4	2.45	1.53	1.43
2	A	601	GLN	OXT-C	-2.16	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	610	MRD	O4-C4-C3	3.72	126.38	111.36
2	B	604	GLN	OXT-C-O	-3.30	116.59	124.09
6	B	601	CTP	O3G-PG-O2G	2.84	118.50	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	MPD	O2-C2-CM	2.77	116.98	108.08
7	B	610	MRD	O4-C4-C5	-2.53	98.41	109.38
6	B	601	CTP	O2-C2-N3	-2.51	118.24	122.33
2	B	604	GLN	OXT-C-CA	2.47	121.79	113.38
2	A	601	GLN	OXT-C-O	-2.43	118.56	124.09
6	B	603	CTP	O2G-PG-O1G	2.35	119.87	110.68
6	B	601	CTP	PB-O3A-PA	-2.22	125.22	132.83
6	B	603	CTP	C2'-C1'-N1	2.16	119.34	113.22
3	A	602	SO4	O4-S-O1	-2.09	98.38	109.31
4	B	607	MPD	O2-C2-C1	-2.08	101.41	108.08
6	B	601	CTP	O2B-PB-O1B	2.04	122.33	112.24
6	B	603	CTP	PB-O3A-PA	-2.02	125.88	132.83
6	B	603	CTP	O3B-PG-O1G	-2.02	99.98	111.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	603	CTP	PB-O3B-PG-O3G
6	B	601	CTP	PB-O3B-PG-O1G
6	B	601	CTP	PB-O3B-PG-O3G
6	B	603	CTP	PB-O3A-PA-O1A
4	A	604	MPD	C2-C3-C4-C5
4	A	604	MPD	C2-C3-C4-O4
4	A	604	MPD	CM-C2-C3-C4
6	B	601	CTP	PB-O3A-PA-O2A
6	B	601	CTP	PB-O3A-PA-O1A
6	B	603	CTP	PB-O3A-PA-O2A
4	B	607	MPD	C2-C3-C4-C5
7	B	610	MRD	C2-C3-C4-C5
4	B	607	MPD	C2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 9 short contacts:

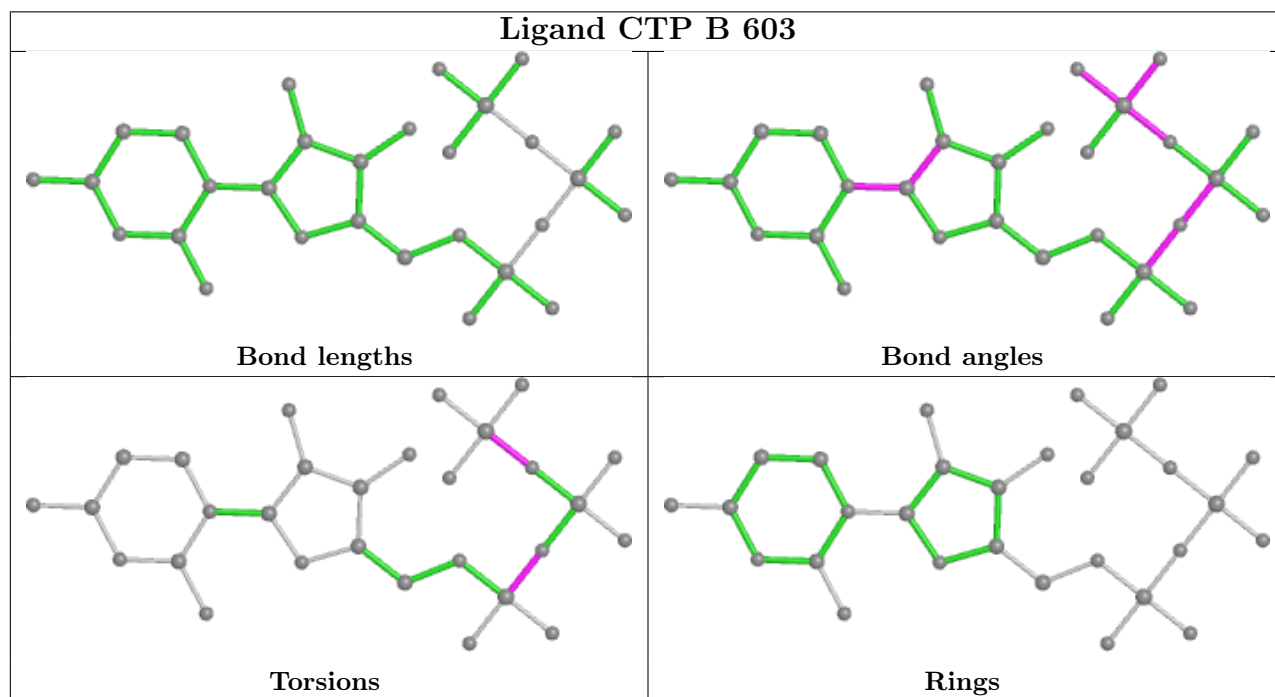
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLN	1	0
4	A	604	MPD	2	0
3	A	603	SO4	1	0
6	B	603	CTP	1	0
4	B	607	MPD	1	0

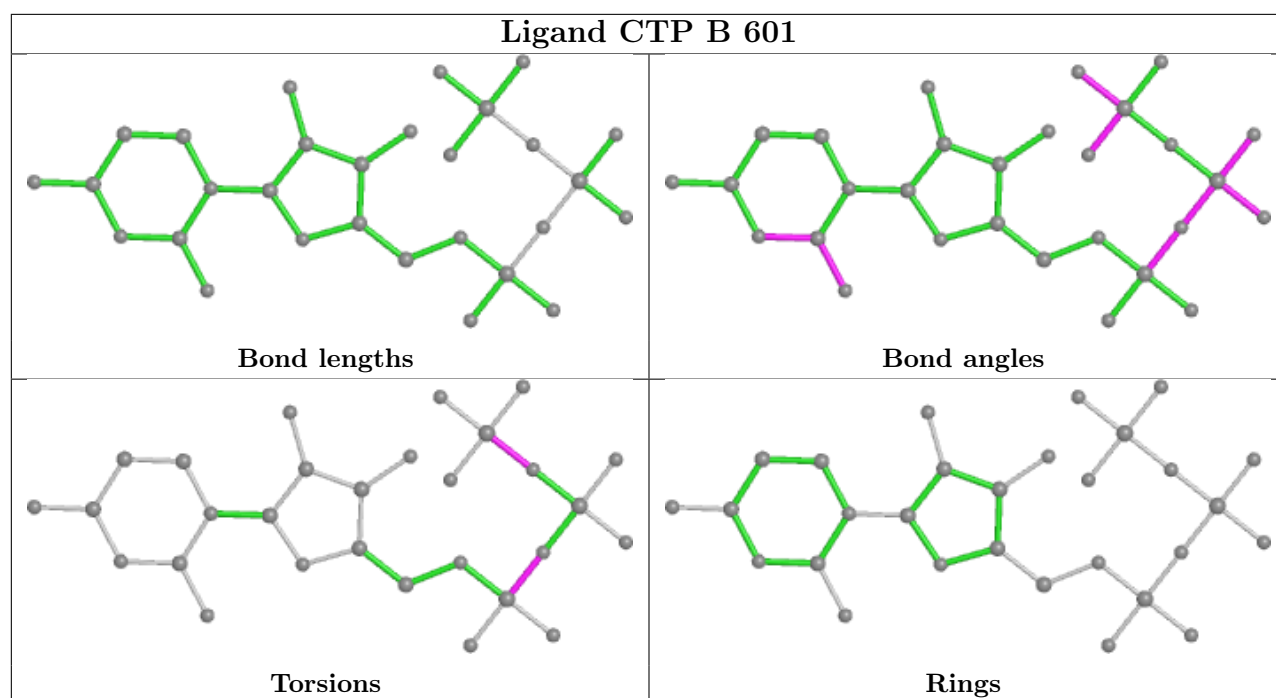
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	CTP	1	0
3	B	609	SO4	1	0
3	A	602	SO4	1	0

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, 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	532/565 (94%)	-0.42	16 (3%) 50 51	20, 43, 86, 123	0
1	B	535/565 (94%)	-0.58	6 (1%) 80 82	18, 40, 79, 126	0
All	All	1067/1130 (94%)	-0.50	22 (2%) 63 65	18, 42, 84, 126	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ASP	3.4
1	A	384	VAL	3.3
1	A	395	ASN	3.0
1	B	544	ALA	3.0
1	A	495	ASP	2.9
1	A	511	ALA	2.8
1	B	494	ASP	2.8
1	B	426	VAL	2.7
1	A	382	MET	2.7
1	B	395	ASN	2.6
1	A	1	MET	2.5
1	A	385	ALA	2.4
1	A	267	ASN	2.4
1	A	424	GLY	2.4
1	A	426	VAL	2.4
1	B	1	MET	2.3
1	A	335	THR	2.2
1	A	451	ASP	2.2
1	A	450	ASP	2.2
1	B	384	VAL	2.1
1	A	336	ARG	2.1
1	A	379	CYS	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.

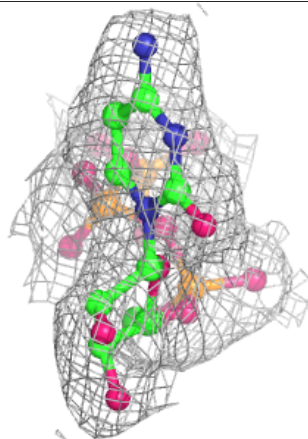
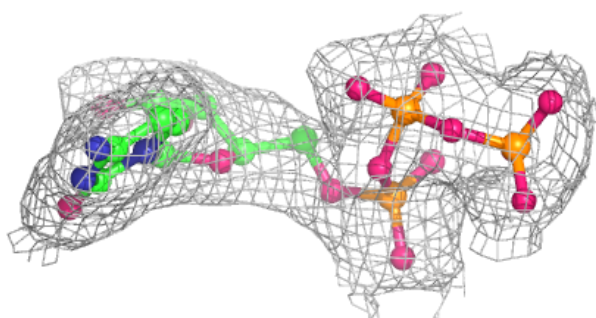
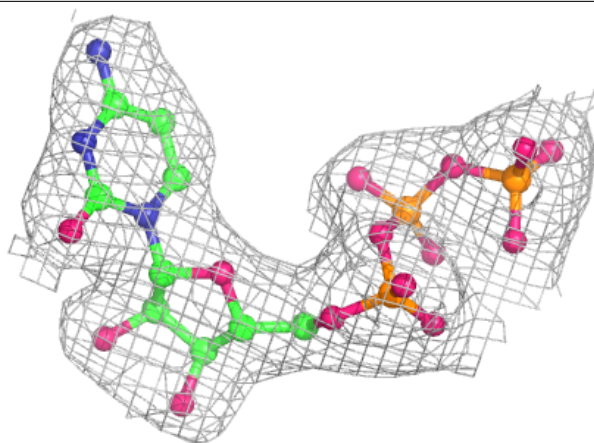
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MRD	B	610	8/8	0.80	0.34	57,72,92,98	0
4	MPD	B	607	8/8	0.90	0.26	51,59,72,76	0
3	SO4	A	605	5/5	0.93	0.16	49,51,65,67	5
3	SO4	B	608	5/5	0.93	0.16	31,34,53,56	5
2	GLN	A	601	10/10	0.93	0.22	52,58,68,70	0
3	SO4	A	603	5/5	0.93	0.34	21,32,38,46	5
2	GLN	B	604	10/10	0.94	0.20	42,45,65,68	0
4	MPD	A	604	8/8	0.94	0.17	42,63,78,79	0
7	MRD	B	611	8/8	0.94	0.29	47,64,69,74	0
3	SO4	B	606	5/5	0.95	0.31	20,29,42,43	5
3	SO4	A	606	5/5	0.95	0.11	35,35,41,48	5
3	SO4	A	602	5/5	0.97	0.16	37,40,65,65	0
3	SO4	B	609	5/5	0.98	0.10	34,34,37,39	5
3	SO4	B	605	5/5	0.99	0.14	34,38,50,61	0
5	MG	A	607	1/1	0.99	0.04	34,34,34,34	0
6	CTP	B	603	29/29	1.00	0.08	16,24,31,35	0
5	MG	B	602	1/1	1.00	0.04	40,40,40,40	0
6	CTP	B	601	29/29	1.00	0.08	17,23,30,32	0

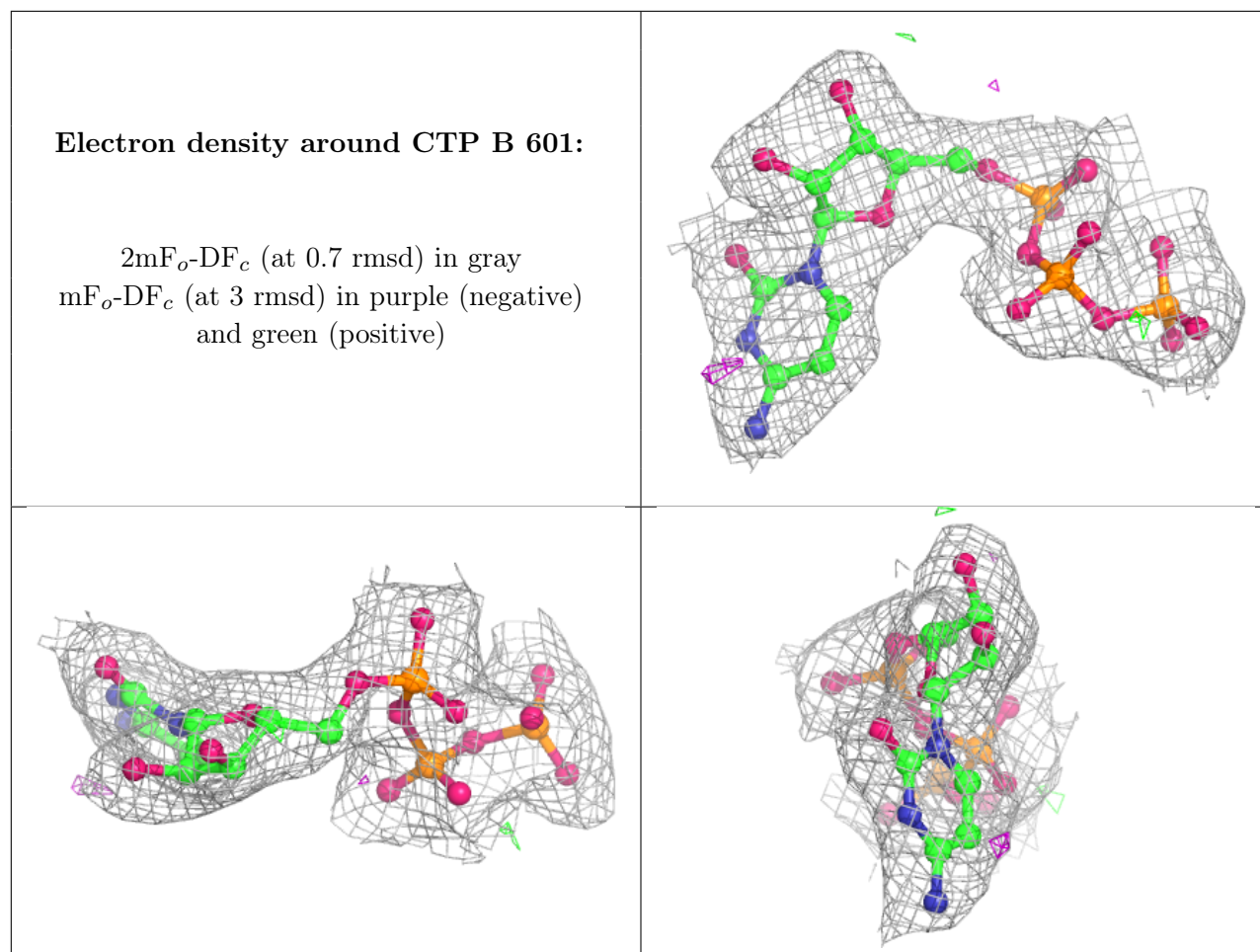
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around CTP B 603:**

$2mF_o-DF_c$  (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.