



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2018 – 02:18 PM EDT

PDB ID : 4ZCS  
Title : Crystal structure of the C-terminal catalytic domain of Plasmodium falciparum CTP:phosphocholine cytidyltransferase in complex with CDP-choline  
Authors : Guca, E.; Hoh, F.; Guichou, J.-F.; Cerdan, R.  
Deposited on : 2015-04-16  
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

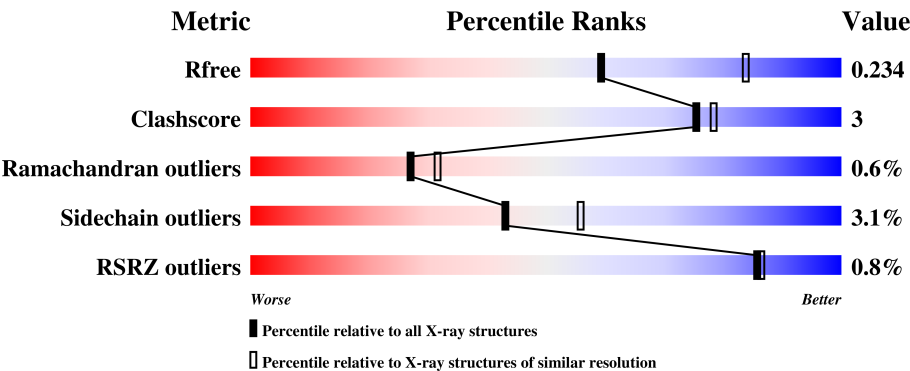
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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 <sub>free</sub>	111664	1259 (2.48-2.44)
Clashscore	122126	1323 (2.48-2.44)
Ramachandran outliers	120053	1314 (2.48-2.44)
Sidechain outliers	120020	1314 (2.48-2.44)
RSRZ outliers	108989	1238 (2.48-2.44)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	180	<div><div>%</div><div><div></div><div>71%</div><div>6%</div><div>.</div><div>22%</div></div></div>
1	B	180	<div><div></div><div>70%</div><div>7%</div><div>..</div><div>22%</div></div>
1	C	180	<div><div>%</div><div><div></div><div>67%</div><div>8%</div><div>.</div><div>24%</div></div></div>
1	D	180	<div><div>2%</div><div><div></div><div>66%</div><div>10%</div><div>..</div><div>23%</div></div></div>
1	E	180	<div><div></div><div>67%</div><div>11%</div><div>.</div><div>22%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	180	<div><div><div>%</div><div><div></div></div><div>73%</div><div><div></div><div></div></div><div>22%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7377 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 Choline-phosphate cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1154	744	193	214	3			
1	C	137	Total	C	N	O	S	0	0	0
			1107	714	184	206	3			
1	E	141	Total	C	N	O	S	0	0	0
			1149	740	192	214	3			
1	B	140	Total	C	N	O	S	0	0	0
			1132	733	187	209	3			
1	D	139	Total	C	N	O	S	0	0	0
			1128	727	187	211	3			
1	F	141	Total	C	N	O	S	0	0	0
			1142	738	186	215	3			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	GLY	-	expression tag	UNP Q8IEE9
A	579	HIS	-	expression tag	UNP Q8IEE9
A	580	MET	-	expression tag	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	GLY	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	PHE	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	PHE	deletion	UNP Q8IEE9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q8IEE9
A	?	-	GLU	deletion	UNP Q8IEE9
A	?	-	GLU	deletion	UNP Q8IEE9
A	?	-	ASN	deletion	UNP Q8IEE9
C	578	GLY	-	expression tag	UNP Q8IEE9
C	579	HIS	-	expression tag	UNP Q8IEE9
C	580	MET	-	expression tag	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	GLY	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	PHE	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	PHE	deletion	UNP Q8IEE9
C	?	-	ASP	deletion	UNP Q8IEE9
C	?	-	GLU	deletion	UNP Q8IEE9
C	?	-	GLU	deletion	UNP Q8IEE9
C	?	-	ASN	deletion	UNP Q8IEE9
E	578	GLY	-	expression tag	UNP Q8IEE9
E	579	HIS	-	expression tag	UNP Q8IEE9
E	580	MET	-	expression tag	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	GLY	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	PHE	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	PHE	deletion	UNP Q8IEE9

*Continued on next page...*

*Continued from previous page...*

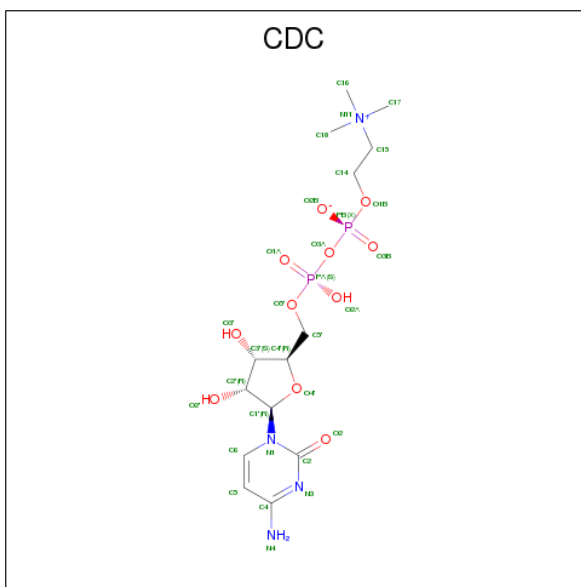
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASP	deletion	UNP Q8IEE9
E	?	-	GLU	deletion	UNP Q8IEE9
E	?	-	GLU	deletion	UNP Q8IEE9
E	?	-	ASN	deletion	UNP Q8IEE9
B	578	GLY	-	expression tag	UNP Q8IEE9
B	579	HIS	-	expression tag	UNP Q8IEE9
B	580	MET	-	expression tag	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	GLY	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	PHE	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	PHE	deletion	UNP Q8IEE9
B	?	-	ASP	deletion	UNP Q8IEE9
B	?	-	GLU	deletion	UNP Q8IEE9
B	?	-	GLU	deletion	UNP Q8IEE9
B	?	-	ASN	deletion	UNP Q8IEE9
D	578	GLY	-	expression tag	UNP Q8IEE9
D	579	HIS	-	expression tag	UNP Q8IEE9
D	580	MET	-	expression tag	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	GLY	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	PHE	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	PHE	deletion	UNP Q8IEE9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP Q8IEE9
D	?	-	GLU	deletion	UNP Q8IEE9
D	?	-	GLU	deletion	UNP Q8IEE9
D	?	-	ASN	deletion	UNP Q8IEE9
F	578	GLY	-	expression tag	UNP Q8IEE9
F	579	HIS	-	expression tag	UNP Q8IEE9
F	580	MET	-	expression tag	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	GLY	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	PHE	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	PHE	deletion	UNP Q8IEE9
F	?	-	ASP	deletion	UNP Q8IEE9
F	?	-	GLU	deletion	UNP Q8IEE9
F	?	-	GLU	deletion	UNP Q8IEE9
F	?	-	ASN	deletion	UNP Q8IEE9

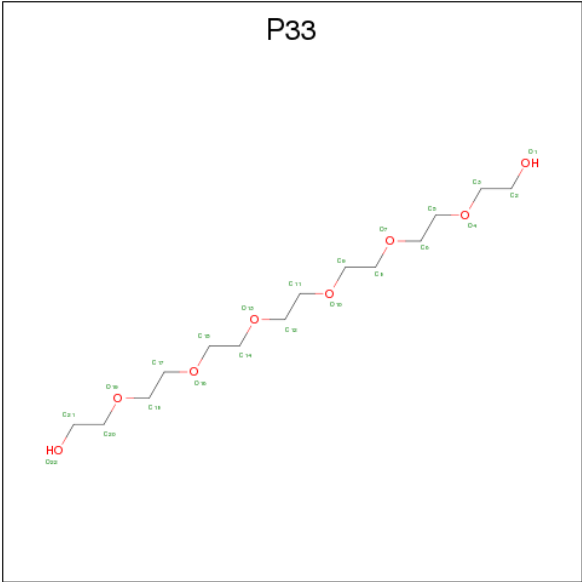
- Molecule 2 is [2-CYTIDYLATE-O'-PHOSPHONYLOXYL]-ETHYL-TRIMETHYL-AMMONIUM (three-letter code: CDC) (formula: C<sub>14</sub>H<sub>26</sub>N<sub>4</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 14	N 4	O 11	P 2	0	0
2	C	1	Total 31	C 14	N 4	O 11	P 2	0	0
2	E	1	Total 31	C 14	N 4	O 11	P 2	0	0
2	B	1	Total 31	C 14	N 4	O 11	P 2	0	0
2	D	1	Total 31	C 14	N 4	O 11	P 2	0	0
2	F	1	Total 31	C 14	N 4	O 11	P 2	0	0

- Molecule 3 is 3,6,9,12,15,18-HEXA OXAICOSANE-1,20-DIOL (three-letter code: P33) (formula:  $C_{14}H_{30}O_8$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			22	14	8		
3	D	1	Total	C	O	0	0
			16	10	6		

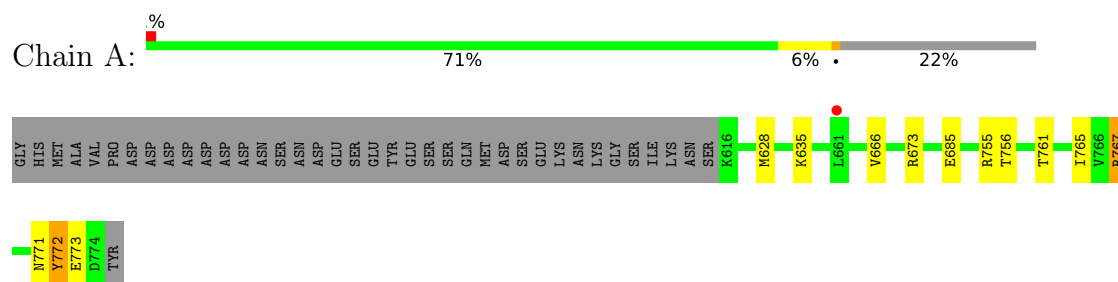
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	C	51	Total	O	0	0
			51	51		
4	E	80	Total	O	0	0
			80	80		
4	B	53	Total	O	0	0
			53	53		
4	D	59	Total	O	0	0
			59	59		
4	F	44	Total	O	0	0
			44	44		

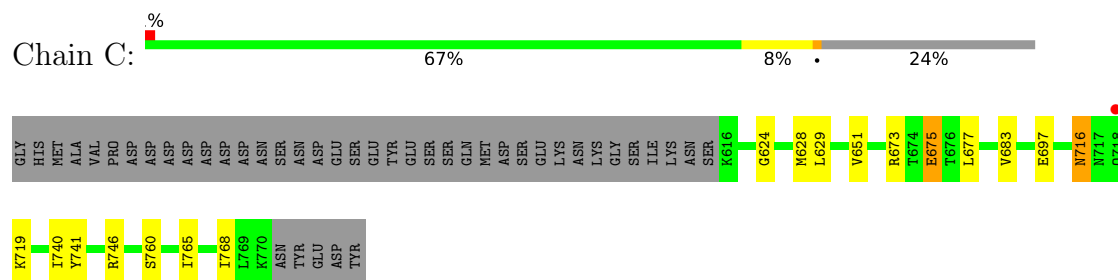
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

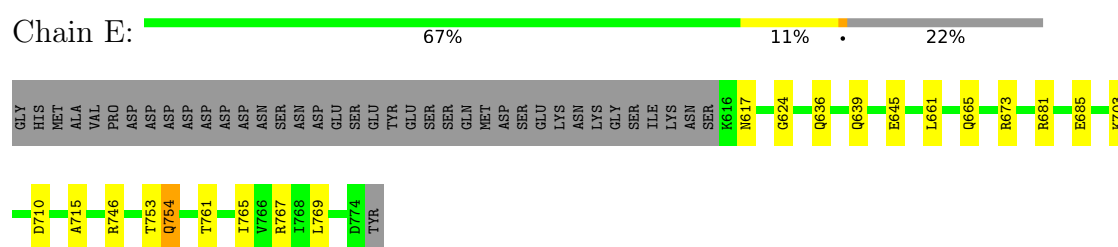
- Molecule 1: Choline-phosphate cytidylyltransferase



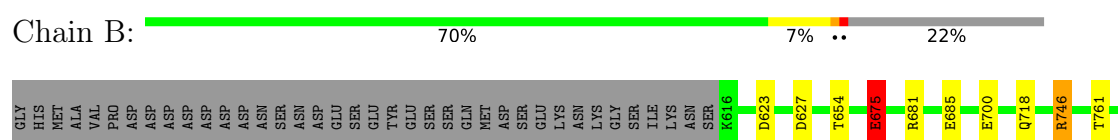
- Molecule 1: Choline-phosphate cytidylyltransferase



- Molecule 1: Choline-phosphate cytidylyltransferase

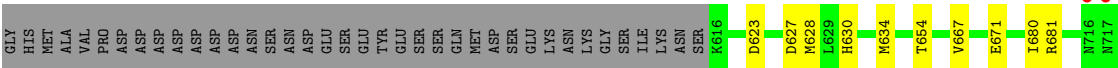


- Molecule 1: Choline-phosphate cytidylyltransferase

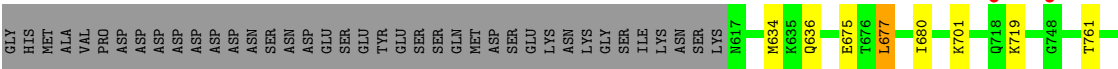




● Molecule 1: Choline-phosphate cytidylyltransferase



● Molecule 1: Choline-phosphate cytidylyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.63Å 149.13Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.67 – 2.45 56.83 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (113.67-2.45) 99.6 (56.83-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.32	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.181 , 0.234 0.188 , 0.234	Depositor DCC
$R_{free}$ test set	2808 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 27.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P33, CDC

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	1.00	1/1181 (0.1%)	1.01	4/1600 (0.2%)
1	B	0.98	1/1156 (0.1%)	0.97	3/1568 (0.2%)
1	C	0.96	1/1130 (0.1%)	0.96	3/1534 (0.2%)
1	D	0.85	0/1152	0.95	4/1564 (0.3%)
1	E	0.97	1/1173 (0.1%)	0.91	2/1590 (0.1%)
1	F	0.85	0/1167	0.83	1/1586 (0.1%)
All	All	0.94	4/6959 (0.1%)	0.94	17/9442 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	675	GLU	CD-OE1	6.86	1.33	1.25
1	E	685	GLU	CD-OE2	6.61	1.32	1.25
1	B	675	GLU	CD-OE2	5.69	1.31	1.25
1	A	685	GLU	CD-OE2	5.05	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH1	6.53	123.57	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	746	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	F	677	LEU	CA-CB-CG	6.30	129.78	115.30
1	A	755	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	746	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	623	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	E	673	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	746	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	673	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	627	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	673	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	746	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	627	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	767	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	E	681	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	772	TYR	CB-CA-C	5.24	120.88	110.40
1	D	760	SER	N-CA-CB	5.17	118.25	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	770	LYS	Peptide
1	E	715	ALA	Peptide

## 5.2 Too-close contacts

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	1154	0	1162	6	0
1	B	1132	0	1127	10	0
1	C	1107	0	1103	10	0
1	D	1128	0	1121	13	0
1	E	1149	0	1151	9	0
1	F	1142	0	1122	6	0
2	A	31	0	25	1	0
2	B	31	0	25	3	0
2	C	31	0	25	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	25	1	0
2	E	31	0	25	3	0
2	F	31	0	25	3	0
3	B	22	0	30	1	0
3	D	16	0	20	0	0
4	A	54	0	0	0	0
4	B	53	0	0	1	0
4	C	51	0	0	0	0
4	D	59	0	0	3	0
4	E	80	0	0	1	0
4	F	44	0	0	0	0
All	All	7377	0	6986	48	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 (48) 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:C:624:GLY:HA2	2:C:801:CDC:H142	1.70	0.72
1:A:761:THR:HG23	1:B:761:THR:HG23	1.75	0.69
1:E:761:THR:HG23	1:F:761:THR:HG23	1.75	0.68
1:E:639:GLN:HE22	1:E:754:GLN:H	1.42	0.68
1:D:681:ARG:NH2	4:D:902:HOH:O	2.26	0.67
1:E:617:ASN:ND2	4:E:901:HOH:O	2.30	0.64
1:D:630:HIS:CD2	1:D:760:SER:HA	2.36	0.61
1:B:654:THR:HG21	2:B:801:CDC:H172	1.83	0.60
1:D:760:SER:OG	4:D:901:HOH:O	2.17	0.59
1:C:628:MET:HG2	1:D:764:LEU:HD13	1.87	0.56
1:C:740:ILE:HD11	2:C:801:CDC:H173	1.88	0.55
1:E:624:GLY:HA2	2:E:801:CDC:H141	1.87	0.55
1:E:765:ILE:CG1	1:F:765:ILE:HG13	2.39	0.52
1:E:765:ILE:HG12	1:F:765:ILE:HG13	1.92	0.52
2:F:801:CDC:O1B	2:F:801:CDC:H163	2.11	0.51
1:D:763:ASP:HB2	4:D:901:HOH:O	2.12	0.49
1:E:710:ASP:HA	1:E:753:THR:O	2.14	0.47
1:C:768:ILE:HG12	1:D:667:VAL:HG22	1.96	0.47
1:A:765:ILE:HG13	1:B:765:ILE:HG13	1.96	0.47
1:B:623:ASP:OD2	2:B:801:CDC:H162	2.15	0.46
1:C:716:ASN:HD21	1:C:719:LYS:HB2	1.80	0.46
1:A:765:ILE:HG13	1:B:765:ILE:CG1	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:TYR:OH	2:C:801:CDC:H152	2.16	0.45
1:C:765:ILE:HG13	1:D:765:ILE:CD1	2.46	0.45
2:C:801:CDC:C16	2:C:801:CDC:O1B	2.65	0.45
1:D:634:MET:HG2	1:D:680:ILE:HD12	1.99	0.45
1:C:628:MET:O	1:C:629:LEU:C	2.57	0.43
1:A:771:ASN:O	1:A:773:GLU:N	2.51	0.43
2:A:801:CDC:H183	2:A:801:CDC:O1B	2.17	0.43
2:E:801:CDC:O1B	2:E:801:CDC:H163	2.18	0.43
1:F:773:GLU:H	1:F:773:GLU:CD	2.20	0.43
2:F:801:CDC:O1B	2:F:801:CDC:C16	2.66	0.43
1:B:675:GLU:HG2	4:B:923:HOH:O	2.19	0.43
1:D:654:THR:HG21	2:D:801:CDC:H162	2.00	0.43
1:F:636:GLN:HG3	2:F:801:CDC:H1'	2.01	0.42
1:A:628:MET:HG2	1:B:764:LEU:HD13	2.01	0.42
1:E:746:ARG:HD2	1:B:681:ARG:NH1	2.35	0.42
1:C:765:ILE:HG13	1:D:765:ILE:HG13	2.01	0.42
1:B:772:TYR:O	1:B:773:GLU:CB	2.68	0.41
1:B:685:GLU:OE1	3:B:802:P33:O4	2.38	0.41
1:E:636:GLN:HG3	2:E:801:CDC:H1'	2.03	0.41
1:A:635:LYS:HE2	1:A:756:THR:HG21	2.03	0.41
1:D:759:VAL:O	1:D:760:SER:CB	2.69	0.41
2:B:801:CDC:H173	2:B:801:CDC:H142	1.76	0.40
1:C:651:VAL:HG21	1:C:683:VAL:HG22	2.01	0.40
1:D:771:ASN:O	1:D:772:TYR:HB2	2.20	0.40
1:F:634:MET:HG2	1:F:680:ILE:HD12	2.03	0.40
1:D:628:MET:CE	1:D:667:VAL:HG21	2.51	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	140/180 (78%)	136 (97%)	3 (2%)	1 (1%)	24	28
1	B	138/180 (77%)	134 (97%)	3 (2%)	1 (1%)	24	28
1	C	135/180 (75%)	131 (97%)	4 (3%)	0	100	100
1	D	137/180 (76%)	130 (95%)	5 (4%)	2 (2%)	11	10
1	E	139/180 (77%)	135 (97%)	4 (3%)	0	100	100
1	F	139/180 (77%)	135 (97%)	3 (2%)	1 (1%)	24	28
All	All	828/1080 (77%)	801 (97%)	22 (3%)	5 (1%)	27	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	718	GLN
1	D	760	SER
1	F	701	LYS
1	D	770	LYS
1	A	772	TYR

### 5.3.2 Protein sidechains ⓘ

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	126/164 (77%)	124 (98%)	2 (2%)	65	76
1	B	120/164 (73%)	117 (98%)	3 (2%)	50	63
1	C	119/164 (73%)	114 (96%)	5 (4%)	32	43
1	D	122/164 (74%)	120 (98%)	2 (2%)	65	76
1	E	125/164 (76%)	118 (94%)	7 (6%)	23	30
1	F	122/164 (74%)	118 (97%)	4 (3%)	41	53
All	All	734/984 (75%)	711 (97%)	23 (3%)	43	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	666	VAL
1	A	767	ARG
1	C	675	GLU
1	C	677	LEU
1	C	697	GLU
1	C	716	ASN
1	C	760	SER
1	E	645	GLU
1	E	661	LEU
1	E	665	GLN
1	E	703	LYS
1	E	754	GLN
1	E	767	ARG
1	E	769	LEU
1	B	675	GLU
1	B	700	GLU
1	B	746	ARG
1	D	671	GLU
1	D	762	THR
1	F	675	GLU
1	F	677	LEU
1	F	719	LYS
1	F	773	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	665	GLN
1	C	716	ASN
1	E	639	GLN
1	E	665	GLN
1	B	617	ASN
1	D	617	ASN
1	F	665	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
2	CDC	A	801	-	26,32,32	1.33	3 (11%)	32,49,49	1.31	3 (9%)
2	CDC	B	801	-	26,32,32	1.12	1 (3%)	32,49,49	1.51	5 (15%)
3	P33	B	802	-	21,21,21	0.89	0	20,20,20	0.73	0
2	CDC	C	801	-	26,32,32	1.42	5 (19%)	32,49,49	1.16	3 (9%)
2	CDC	D	801	-	26,32,32	1.27	4 (15%)	32,49,49	1.51	4 (12%)
3	P33	D	802	-	15,15,21	1.13	0	14,14,20	1.03	1 (7%)
2	CDC	E	801	-	26,32,32	1.84	3 (11%)	32,49,49	1.42	4 (12%)
2	CDC	F	801	-	26,32,32	1.65	3 (11%)	32,49,49	1.37	2 (6%)

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	CDC	A	801	-	-	0/20/40/40	0/2/2/2
2	CDC	B	801	-	-	0/20/40/40	0/2/2/2
3	P33	B	802	-	-	0/19/19/19	0/0/0/0
2	CDC	C	801	-	-	0/20/40/40	0/2/2/2
2	CDC	D	801	-	-	0/20/40/40	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P33	D	802	-	-	0/13/13/19	0/0/0/0
2	CDC	E	801	-	-	0/20/40/40	0/2/2/2
2	CDC	F	801	-	-	0/20/40/40	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	CDC	O1B-C14	-3.30	1.32	1.45
2	C	801	CDC	PB-O1B	-2.36	1.49	1.59
2	D	801	CDC	O2'-C2'	-2.31	1.37	1.43
2	D	801	CDC	C5-C4	-2.21	1.35	1.41
2	C	801	CDC	PA-O1A	-2.13	1.43	1.50
2	D	801	CDC	C3'-C2'	-2.09	1.47	1.53
2	C	801	CDC	PA-O2A	-2.08	1.45	1.55
2	A	801	CDC	O4'-C4'	2.16	1.49	1.45
2	F	801	CDC	O4'-C1'	2.21	1.44	1.41
2	C	801	CDC	C4-N3	2.38	1.39	1.35
2	D	801	CDC	C6-N1	2.45	1.39	1.35
2	E	801	CDC	O4'-C1'	2.58	1.44	1.41
2	A	801	CDC	C4-N3	3.00	1.40	1.35
2	F	801	CDC	C6-N1	3.35	1.40	1.35
2	E	801	CDC	O4'-C4'	3.44	1.52	1.45
2	A	801	CDC	C6-N1	3.77	1.40	1.35
2	C	801	CDC	C6-N1	3.92	1.41	1.35
2	F	801	CDC	C2-N3	4.01	1.46	1.38
2	E	801	CDC	C6-N1	6.80	1.44	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	CDC	C4'-O4'-C1'	-4.54	105.09	109.83
2	D	801	CDC	C5-C4-N3	-4.04	116.95	121.69
2	E	801	CDC	C4'-O4'-C1'	-3.91	105.75	109.83
2	B	801	CDC	C14-C15-N11	-3.52	103.81	115.81
2	B	801	CDC	O4'-C4'-C5'	-3.35	98.21	109.39
2	E	801	CDC	C5-C4-N3	-2.95	118.23	121.69
2	A	801	CDC	C5-C4-N3	-2.89	118.30	121.69
2	C	801	CDC	PB-O3A-PA	-2.74	123.42	132.63
2	C	801	CDC	O2B-PB-O1B	-2.40	96.58	107.75
2	B	801	CDC	PB-O1B-C14	-2.08	111.33	121.59
2	F	801	CDC	C18-N11-C16	2.01	114.06	108.96
2	C	801	CDC	O4'-C1'-N1	2.08	112.18	108.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	P33	C9-O10-C11	2.08	122.44	113.30
2	E	801	CDC	C5-C4-N4	2.14	124.98	121.17
2	D	801	CDC	N4-C4-N3	2.22	120.19	116.56
2	B	801	CDC	O4'-C1'-N1	2.74	113.49	108.05
2	A	801	CDC	O1B-PB-O3B	2.85	120.20	109.07
2	D	801	CDC	O1B-PB-O3B	3.05	120.97	109.07
2	B	801	CDC	N4-C4-N3	3.09	121.62	116.56
2	A	801	CDC	N4-C4-N3	3.22	121.82	116.56
2	E	801	CDC	O4'-C1'-N1	3.66	115.31	108.05
2	F	801	CDC	N4-C4-N3	3.68	122.58	116.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CDC	1	0
2	B	801	CDC	3	0
3	B	802	P33	1	0
2	C	801	CDC	4	0
2	D	801	CDC	1	0
2	E	801	CDC	3	0
2	F	801	CDC	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	141/180 (78%)	-0.38	1 (0%) 87 88	24, 36, 62, 92	2 (1%)
1	B	140/180 (77%)	-0.51	0 100 100	26, 41, 74, 95	1 (0%)
1	C	137/180 (76%)	-0.35	1 (0%) 87 88	27, 39, 73, 119	1 (0%)
1	D	139/180 (77%)	-0.33	3 (2%) 62 58	30, 44, 85, 119	0
1	E	141/180 (78%)	-0.39	0 100 100	23, 35, 69, 88	1 (0%)
1	F	141/180 (78%)	-0.27	2 (1%) 75 73	27, 49, 77, 108	0
All	All	839/1080 (77%)	-0.37	7 (0%) 86 86	23, 40, 77, 119	5 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	718	GLN	4.5
1	D	716	ASN	4.2
1	F	718	GLN	3.6
1	A	661	LEU	3.0
1	D	717	ASN	2.6
1	D	738	GLU	2.3
1	F	748	GLY	2.2

### 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
3	P33	B	802	22/22	0.82	0.18	61,85,97,101	0
3	P33	D	802	16/22	0.86	0.13	58,66,77,78	0
2	CDC	B	801	31/31	0.98	0.12	28,32,42,44	0
2	CDC	F	801	31/31	0.99	0.12	32,37,43,46	0
2	CDC	A	801	31/31	0.99	0.13	20,27,42,49	0
2	CDC	D	801	31/31	0.99	0.13	29,33,42,43	0
2	CDC	C	801	31/31	0.99	0.13	24,30,45,46	0
2	CDC	E	801	31/31	0.99	0.13	20,32,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.