



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:33 PM GMT

PDB ID : 4YFU  
Title : Crystal structure of open Bacillus fragment DNA polymerase bound to DNA and dTTP  
Authors : Wu, E.Y.  
Deposited on : 2015-02-25  
Resolution : 1.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

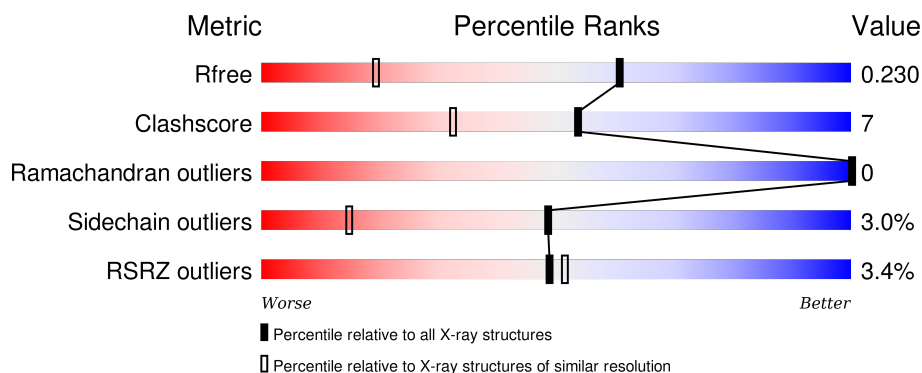
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	580	<div> <div>3%</div> <div>83% 15% •</div> </div>
1	D	580	<div> <div>4%</div> <div>84% 12% ••</div> </div>
2	B	9	<div> <div>44% 33% 11% 11%</div> </div>
2	E	9	<div> <div>44% 11% 33% 11%</div> </div>
3	C	14	<div> <div>57% 21% 21%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SUC	A	902	-	-	-	X
5	SUC	D	901	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11744 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	10	0
			4700	2995	812	873	20			
1	D	580	Total	C	N	O	S	0	13	0
			4719	3011	811	877	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LYS	-	expression tag	UNP E1C9K5
A	456	GLU	ALA	conflict	UNP E1C9K5
A	505	LYS	GLU	conflict	UNP E1C9K5
A	512	GLY	ARG	conflict	UNP E1C9K5
A	550	THR	SER	conflict	UNP E1C9K5
A	598	ALA	ASP	engineered mutation	UNP E1C9K5
A	710	TYR	PHE	engineered mutation	UNP E1C9K5
A	823	HIS	ARG	conflict	UNP E1C9K5
D	297	LYS	-	expression tag	UNP E1C9K5
D	456	GLU	ALA	conflict	UNP E1C9K5
D	505	LYS	GLU	conflict	UNP E1C9K5
D	512	GLY	ARG	conflict	UNP E1C9K5
D	550	THR	SER	conflict	UNP E1C9K5
D	598	ALA	ASP	engineered mutation	UNP E1C9K5
D	710	TYR	PHE	engineered mutation	UNP E1C9K5
D	823	HIS	ARG	conflict	UNP E1C9K5

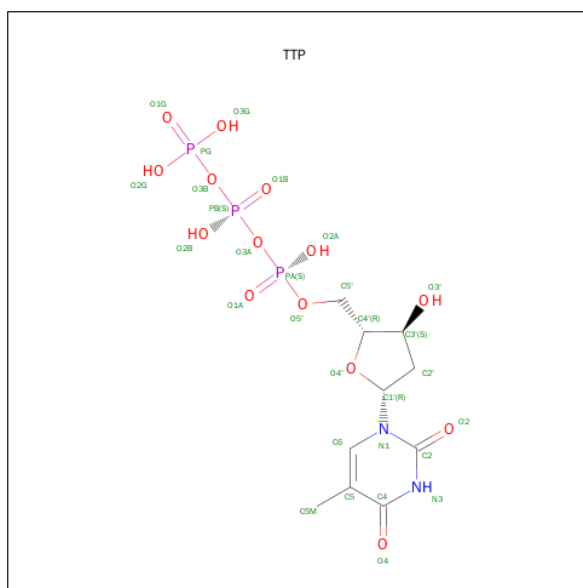
- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
2	E	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 3 is a DNA chain called Template DNA.

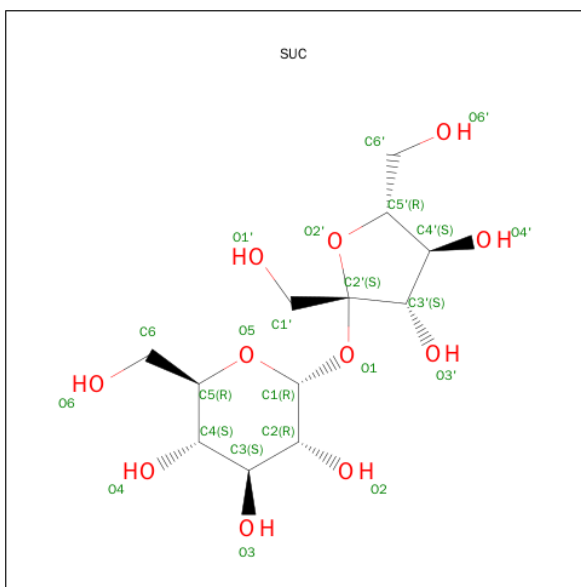
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			
3	F	14	Total	C	N	O	P	0	0	0
			288	137	58	80	13			

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 5 is SUCROSE (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	12	11		
5	D	1	Total	C	O	0	0
			23	12	11		

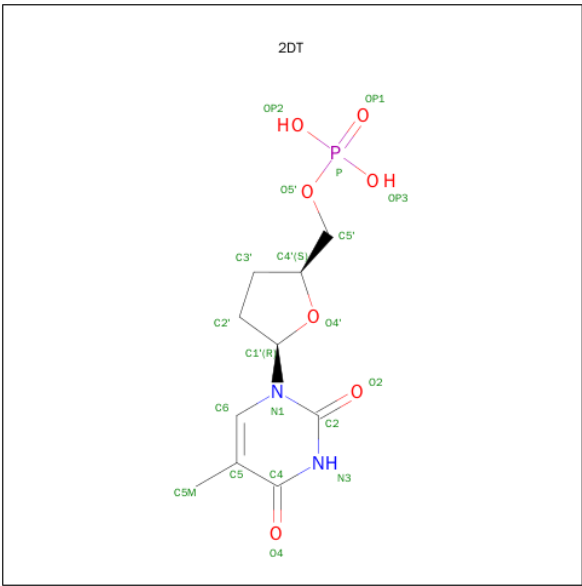
- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 3'-DEOXYTHYMIDINE-5'-MONOPHOSPHATE (three-letter code: 2DT)

(formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			19	10	2	6	1		
7	E	1	Total	C	N	O	P	0	0
			19	10	2	6	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	556	Total	O	0	0
			556	556		
8	D	622	Total	O	0	0
			622	622		
8	B	37	Total	O	0	0
			37	37		
8	C	50	Total	O	0	0
			50	50		
8	E	35	Total	O	0	0
			35	35		
8	F	71	Total	O	0	0
			71	71		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Chain A:

3% 83% 15%

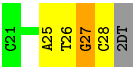
Chain D:

84% 4% 12%

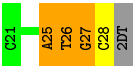
Sample IDs (from left to right): K863, K876, V697, T698, R703, Q704, Y710, Y719, Q723, F735, Y749, M750, R769, R770, I776, R779, T780, F781, W782, R783, R784, S785, F786, A787, E788, R789, M792, D802, I803, R814, L815, R816, E831, A836, E839, E840, N841, E842, R843, R846, L847, E853, R859, Q510, L511, G512, T513, V514, Y519, E525, P531, R578, Q579, L583, Q584, I588, L591, V595, R596, K600, K601, V602, F606, P621, R629, R634, K635, I636, D646, F650, Y654, R660, A663, D669, N670, L671, F690, Q691, V692, S693, E694, D695, F699, G504, K505, E506, L507, A508, E509, K297, K298, L303, A304, D305, R306, F345, D363, D372, F392, D402, D408, D409, K415, M416, K417, Q418, Y419, G430, K431, G432, A433, K434, R435, E440, E456, L457, E458, R459, R466, D471, R472, V475, V495, R499, L500, M503, G504, K505, E506, L507, A508, E509.

Chain B:  44% 33% 11% 11%

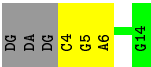




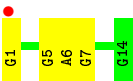
● Molecule 2: Primer DNA



● Molecule 3: Template DNA



● Molecule 3: Template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.23Å 108.10Å 151.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.68 – 1.50 44.68 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.68-1.50) 99.0 (44.68-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.195 , 0.230 0.195 , 0.230	Depositor DCC
$R_{free}$ test set	11140 reflections (4.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 241158 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2DT, CME, TTP, SUC, SO4

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	1.16	4/4803 (0.1%)	1.28	38/6487 (0.6%)
1	D	1.29	11/4828 (0.2%)	1.46	54/6524 (0.8%)
2	B	1.06	1/180 (0.6%)	1.98	4/276 (1.4%)
2	E	1.27	3/180 (1.7%)	1.84	5/276 (1.8%)
3	C	1.06	1/253 (0.4%)	1.32	2/388 (0.5%)
3	F	1.16	1/324 (0.3%)	1.21	3/499 (0.6%)
All	All	1.22	21/10568 (0.2%)	1.39	106/14450 (0.7%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	839	GLU	CD-OE1	8.26	1.34	1.25
1	A	382	TRP	CG-CD1	7.13	1.46	1.36
3	C	5	DG	O3'-P	-7.03	1.52	1.61
1	D	853	GLU	CD-OE1	6.72	1.33	1.25
2	B	27	DG	O3'-P	-6.33	1.53	1.61
1	D	749	TYR	CB-CG	6.21	1.60	1.51
1	A	327	TYR	CE1-CZ	6.21	1.46	1.38
1	D	859	ARG	CZ-NH1	5.99	1.40	1.33
2	E	27	DG	P-OP2	-5.84	1.39	1.49
1	D	596	ARG	CZ-NH2	-5.82	1.25	1.33
1	D	419	TYR	CE1-CZ	5.79	1.46	1.38
1	D	578	ARG	CD-NE	-5.74	1.36	1.46
1	D	654	TYR	CE1-CZ	5.43	1.45	1.38
1	D	654	TYR	CB-CG	-5.42	1.43	1.51
2	E	27	DG	O3'-P	-5.36	1.54	1.61
1	D	786	PHE	CG-CD1	5.32	1.46	1.38
1	D	839	GLU	CG-CD	5.28	1.59	1.51
1	A	618	SER	CB-OG	5.24	1.49	1.42
2	E	26	DT	P-OP2	-5.18	1.40	1.49
1	A	578	ARG	CD-NE	-5.17	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	DG	P-OP2	-5.09	1.40	1.49

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	DA	O5'-P-OP2	-18.39	88.63	110.70
1	D	843	ARG	NE-CZ-NH2	-15.91	112.35	120.30
2	B	25	DA	O5'-P-OP1	14.92	128.60	110.70
1	D	578	ARG	NE-CZ-NH2	-14.80	112.90	120.30
1	D	843	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	D	578	ARG	NE-CZ-NH1	13.79	127.20	120.30
1	D	846	ARG	CG-CD-NE	13.47	140.08	111.80
1	A	578	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	D	770	ARG	NE-CZ-NH2	12.46	126.53	120.30
1	D	859	ARG	NE-CZ-NH1	12.16	126.38	120.30
2	E	25	DA	C5'-C4'-C3'	11.59	134.96	114.10
1	D	596	ARG	NE-CZ-NH2	-11.38	114.61	120.30
2	E	25	DA	P-O5'-C5'	11.36	139.08	120.90
1	A	596	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	D	843	ARG	CD-NE-CZ	11.22	139.31	123.60
1	D	769	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	372	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	A	601	LYS	CD-CE-NZ	-9.02	90.97	111.70
1	D	660	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	748	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	467	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	466	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	601	LYS	CD-CE-NZ	-8.50	92.16	111.70
3	C	6	DA	O5'-P-OP2	-8.28	98.24	105.70
1	D	596	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	769	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	D	629	ARG	NE-CZ-NH1	8.05	124.33	120.30
2	E	25	DA	O4'-C4'-C3'	-7.62	101.43	106.00
1	D	408	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	687	MET	CG-SD-CE	7.52	112.23	100.20
1	D	859	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	831	GLU	CA-CB-CG	7.32	129.50	113.40
1	D	606	PHE	CB-CG-CD2	-7.31	115.68	120.80
1	A	490	PHE	CB-CG-CD2	-7.28	115.70	120.80
2	E	25	DA	O5'-P-OP2	-7.26	99.17	105.70
1	D	372	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	D	846	ARG	NE-CZ-NH2	7.16	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	786	PHE	CB-CG-CD1	7.15	125.80	120.80
1	D	750[A]	MET	CG-SD-CE	6.98	111.37	100.20
1	D	750[B]	MET	CG-SD-CE	6.98	111.37	100.20
1	D	802	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	769	ARG	NE-CZ-NH1	6.89	123.74	120.30
3	F	6	DA	O5'-P-OP2	-6.89	99.50	105.70
2	E	25	DA	C4'-C3'-C2'	-6.75	97.03	103.10
1	A	591	LEU	CA-CB-CG	6.70	130.70	115.30
1	D	472	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	402	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	459	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	F	7	DG	O4'-C4'-C3'	-6.51	101.90	104.50
1	D	457	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	D	306	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	735	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	D	578	ARG	CB-CG-CD	-6.21	95.46	111.60
1	D	792	MET	CG-SD-CE	-6.20	90.28	100.20
1	A	832	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	A	629	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	615	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	408	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	B	27	DG	O5'-P-OP2	-5.85	100.43	105.70
1	A	347	ARG	NE-CZ-NH1	5.83	123.21	120.30
2	B	28	DC	O5'-P-OP2	-5.80	100.48	105.70
1	D	650	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	A	634	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	D	847[A]	LEU	CA-CB-CG	5.73	128.48	115.30
1	D	847[B]	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	354	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	327	TYR	CG-CD1-CE1	5.67	125.83	121.30
1	A	485	LEU	CB-CG-CD2	5.66	120.62	111.00
1	A	343	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	409	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	629	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	660	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	507	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	477	LEU	CB-CG-CD2	5.56	120.46	111.00
3	F	6	DA	OP1-P-OP2	5.55	127.93	119.60
1	D	843	ARG	CG-CD-NE	-5.54	100.17	111.80
1	D	392	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	A	735	PHE	CB-CG-CD2	-5.51	116.95	120.80
1	A	467	ARG	NE-CZ-NH2	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	TYR	CG-CD2-CE2	-5.45	116.94	121.30
1	A	676	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	748	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	363	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	561	LEU	CB-CG-CD1	5.27	119.95	111.00
1	D	802	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	719	TYR	CB-CG-CD1	5.26	124.15	121.00
1	A	544	LEU	CB-CG-CD1	5.25	119.93	111.00
1	A	786	PHE	CB-CG-CD1	5.24	124.47	120.80
1	D	471	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	D	816	LYS	CB-CG-CD	5.23	125.19	111.60
1	D	784	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	762	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	A	676	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	583	LEU	CB-CG-CD1	-5.20	102.17	111.00
1	A	490	PHE	CD1-CE1-CZ	-5.19	113.87	120.10
1	A	771	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	507	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	363	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	669	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	363	ASP	CB-CG-OD1	5.16	122.94	118.30
3	C	5	DG	C2'-C3'-O3'	-5.15	95.62	112.60
1	D	583	LEU	CB-CG-CD2	5.10	119.67	111.00
1	D	475	VAL	CA-CB-CG2	-5.09	103.27	110.90
1	A	507	LEU	CA-CB-CG	5.07	126.96	115.30
1	D	459	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	853	GLU	OE1-CD-OE2	5.01	129.31	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4700	0	4794	54	0
1	D	4719	0	4817	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	161	0	91	2	0
2	E	161	0	91	6	0
3	C	226	0	124	1	0
3	F	288	0	158	1	0
4	A	29	0	13	2	0
5	A	23	0	22	1	0
5	D	23	0	22	2	0
6	D	5	0	0	0	0
7	B	19	0	13	1	0
7	E	19	0	13	0	0
8	A	556	0	0	15	1
8	B	37	0	0	0	0
8	C	50	0	0	1	0
8	D	622	0	0	32	1
8	E	35	0	0	1	0
8	F	71	0	0	1	0
All	All	11744	0	10158	134	1

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 7.

All (134) 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:D:749:TYR:CE2	1:D:750[A]:MET:CE	2.41	1.04
1:D:418:GLN:HG2	8:D:1093:HOH:O	1.64	0.96
1:D:843:ARG:HD2	8:D:1496:HOH:O	1.66	0.95
1:D:792:MET:HB3	8:D:1354:HOH:O	1.69	0.92
1:A:690:PHE:HZ	1:A:704:GLN:NE2	1.72	0.87
1:D:781:PHE:HD2	8:D:1605:HOH:O	1.57	0.87
1:D:749:TYR:HE2	1:D:750[A]:MET:CE	1.85	0.86
1:D:749:TYR:CE2	1:D:750[A]:MET:HE2	2.11	0.84
1:A:315:LYS:HE2	8:A:1147:HOH:O	1.77	0.84
1:D:846:ARG:HD2	8:D:1015:HOH:O	1.79	0.81
1:A:690:PHE:HZ	1:A:704:GLN:HE21	1.30	0.79
1:D:507:LEU:O	8:D:1546:HOH:O	1.99	0.79
1:D:749:TYR:CD2	1:D:750[A]:MET:HE3	2.19	0.77
1:D:749:TYR:CD2	1:D:750[A]:MET:CE	2.69	0.76
1:D:843:ARG:CD	8:D:1496:HOH:O	2.30	0.74
1:D:578:ARG:NH2	2:E:25:DA:H5"	2.03	0.74
1:D:749:TYR:CE2	1:D:750[A]:MET:HE3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:PHE:CZ	1:A:704:GLN:NE2	2.56	0.72
1:D:646:ASP:N	1:D:646:ASP:OD1	2.25	0.70
1:D:591:LEU:O	1:D:595[A]:VAL:HG23	1.91	0.70
1:D:816:LYS:HG2	8:D:1472:HOH:O	1.94	0.67
1:D:792:MET:CB	8:D:1354:HOH:O	2.33	0.67
1:A:525:GLU:HB3	8:A:1135:HOH:O	1.93	0.67
1:D:596:ARG:CZ	8:D:1593:HOH:O	2.46	0.62
1:A:697:VAL:HA	1:A:701:MET:HE1	1.81	0.62
1:D:456:GLU:HG2	8:D:1341:HOH:O	1.99	0.62
1:A:594:VAL:HG13	8:A:1409:HOH:O	2.02	0.60
1:A:408:ASP:HB2	5:A:902:SUC:H1'1	1.84	0.59
1:D:584:GLN:CD	8:D:1390:HOH:O	2.41	0.58
1:D:814:ARG:NH1	8:D:1585:HOH:O	2.34	0.58
1:A:517:ARG:HD3	8:A:1323:HOH:O	2.03	0.57
1:D:749:TYR:HD2	1:D:750[A]:MET:HE3	1.69	0.57
1:D:749:TYR:HE2	1:D:750[A]:MET:HE1	1.69	0.57
1:A:784[B]:ARG:NH2	8:A:1163:HOH:O	2.26	0.57
1:A:456:GLU:HG2	8:A:1290:HOH:O	2.04	0.56
1:D:710:TYR:HD1	8:D:1409:HOH:O	1.89	0.56
1:A:750[A]:MET:SD	1:A:792[A]:MET:HB3	2.46	0.56
1:A:692:VAL:HG21	1:A:701:MET:CE	2.36	0.56
1:A:766[A]:LEU:HG	8:A:1350:HOH:O	2.06	0.56
1:D:692:VAL:HB	1:D:696:GLU:HG3	1.87	0.56
1:D:690:PHE:HZ	1:D:704:GLN:NE2	2.04	0.55
1:D:511:LEU:N	8:D:1546:HOH:O	2.38	0.55
1:A:766[A]:LEU:HD12	1:A:799:SER:HB3	1.88	0.55
1:D:789:ARG:NH1	8:D:1424:HOH:O	2.36	0.55
1:A:779:ARG:NH1	8:A:1002:HOH:O	2.39	0.55
1:D:788:GLU:O	1:D:792:MET:HG3	2.06	0.55
3:F:1:DG:N2	8:F:102:HOH:O	2.41	0.54
4:A:901:TTP:H2'2	8:A:1261:HOH:O	2.06	0.54
4:A:901:TTP:C2'	8:A:1261:HOH:O	2.56	0.54
1:A:692:VAL:HB	1:A:696:GLU:HB2	1.91	0.53
1:D:507:LEU:HB3	8:D:1390:HOH:O	2.09	0.53
1:A:779:ARG:O	1:A:784[A]:ARG:NH2	2.42	0.52
1:A:415:LYS:HD3	8:A:1497:HOH:O	2.10	0.52
1:A:551:LYS:HG3	1:A:552:THR:HG23	1.92	0.52
1:A:561:LEU:HG	1:A:571:VAL:HG13	1.92	0.51
1:D:749:TYR:CD2	1:D:750[A]:MET:HE2	2.37	0.51
1:A:730:LYS:NZ	8:A:1004:HOH:O	2.43	0.51
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:LEU:HB3	8:D:1484:HOH:O	2.11	0.51
1:A:741:GLU:HG2	8:A:1095:HOH:O	2.11	0.51
1:A:629:ARG:NH2	7:B:101:2DT:OP1	2.44	0.50
2:E:26:DT:H2'	2:E:27:DG:C8	2.47	0.49
1:D:503[A]:MET:CE	8:D:1275:HOH:O	2.59	0.49
1:A:853:GLU:HG3	1:A:864:VAL:HG23	1.95	0.49
1:A:776:ILE:O	1:A:784[B]:ARG:HG3	2.14	0.48
1:D:303:LEU:HD13	1:D:345:PHE:HD2	1.78	0.48
1:A:580:LEU:HD21	1:A:632:GLU:OE1	2.13	0.48
1:D:690:PHE:CZ	1:D:704:GLN:NE2	2.81	0.48
1:D:583:LEU:HD21	8:D:1325:HOH:O	2.14	0.48
1:A:823:HIS:HE1	1:A:835:GLU:OE2	1.96	0.48
1:D:634:ARG:HH21	1:D:876:LYS:HD3	1.78	0.48
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.29	0.47
1:D:588:ILE:HD11	1:D:636:ILE:HD11	1.96	0.47
1:D:846:ARG:HD2	1:D:846:ARG:HH11	1.59	0.47
1:D:588:ILE:HD11	1:D:636:ILE:CD1	2.45	0.47
1:D:431:LYS:HD2	1:D:435:ARG:HD3	1.96	0.47
1:A:511:LEU:O	1:A:515:GLU:HB2	2.14	0.47
1:D:634:ARG:NH2	1:D:876:LYS:HD3	2.29	0.47
1:A:692:VAL:HG21	1:A:701:MET:HE3	1.96	0.47
1:D:691:GLN:CG	8:D:1418:HOH:O	2.63	0.47
1:A:415:LYS:HA	1:A:415:LYS:HD2	1.62	0.46
1:D:495:VAL:HG11	1:D:500:LEU:HD11	1.96	0.46
1:D:629:ARG:NH2	2:E:28:DC:OP2	2.48	0.46
2:E:25:DA:H2''	8:E:232:HOH:O	2.14	0.46
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.97	0.46
1:D:588:ILE:CD1	1:D:636:ILE:CD1	2.94	0.45
1:D:600:LYS:HD3	8:D:1590:HOH:O	2.16	0.45
1:A:668:ASP:O	1:A:672:MET:HG3	2.17	0.45
1:A:648:LEU:HD12	1:A:841:MET:HG3	1.99	0.45
1:D:408:ASP:HB2	5:D:901:SUC:H1'1	1.99	0.45
1:A:405:GLN:HB3	1:A:407:VAL:HG23	1.99	0.45
1:D:595[A]:VAL:HG22	1:D:602[A]:VAL:HG13	1.98	0.45
1:D:596:ARG:NH1	8:D:1593:HOH:O	2.50	0.45
1:A:701:MET:HE2	1:A:701:MET:HB3	1.88	0.45
1:A:770:ARG:HH12	1:D:472:ARG:NH1	2.15	0.44
1:D:719:TYR:O	1:D:723:GLN:HG2	2.17	0.44
1:D:506:GLU:HG3	1:D:507:LEU:N	2.31	0.44
1:A:849:PRO:HG3	1:A:866:TYR:CD1	2.53	0.44
1:D:416:MET:SD	8:D:1609:HOH:O	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LYS:HG2	2:B:26:DT:H2''	2.00	0.43
1:A:596:ARG:HD3	1:A:603:HIS:CD2	2.53	0.43
1:D:816:LYS:CD	8:D:1472:HOH:O	2.66	0.43
1:D:816:LYS:CG	8:D:1472:HOH:O	2.60	0.43
1:D:690:PHE:HZ	1:D:704:GLN:HE21	1.67	0.43
1:A:579:GLN:HG2	2:B:27:DG:OP1	2.18	0.43
1:D:663:ALA:HB2	1:D:671:LEU:HG	2.00	0.43
1:A:823:HIS:CE1	1:A:835:GLU:OE2	2.72	0.42
1:A:712:ILE:HD13	8:A:1465:HOH:O	2.18	0.42
1:A:588:ILE:HD11	1:A:636:ILE:HD13	2.01	0.42
1:D:298:LYS:HD2	8:D:1313:HOH:O	2.19	0.42
1:A:665:ILE:HD12	1:A:796[A]:ILE:HD13	2.00	0.42
1:D:836:ALA:HB3	1:D:841:MET:CE	2.49	0.42
1:D:435:ARG:HD2	1:D:435:ARG:HA	1.42	0.42
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.68	0.42
1:D:440:GLU:HG3	8:D:1163:HOH:O	2.19	0.42
1:A:779:ARG:C	1:A:784[A]:ARG:HH21	2.23	0.42
1:A:326:ASN:HD22	1:A:620:GLU:CD	2.23	0.42
1:D:519:TYR:CD2	1:D:525:GLU:HG2	2.55	0.42
1:D:418:GLN:HA	8:D:1532:HOH:O	2.19	0.42
1:D:433:ALA:HA	1:D:434:LYS:HA	1.81	0.42
3:C:4:DC:H6	8:C:108:HOH:O	2.01	0.41
1:D:584:GLN:NE2	8:D:1390:HOH:O	2.52	0.41
1:D:531:PRO:HG3	2:E:25:DA:H5'	2.02	0.41
1:D:863:LYS:HE2	8:D:1302:HOH:O	2.20	0.41
1:D:602[B]:VAL:HG11	1:D:621:PRO:HG3	2.02	0.41
1:D:298:LYS:HE2	1:D:298:LYS:HB3	1.91	0.41
1:A:315:LYS:CE	8:A:1147:HOH:O	2.50	0.41
1:A:692:VAL:HG21	1:A:701:MET:HE1	2.03	0.41
1:A:762:TYR:CD1	1:A:770:ARG:HG3	2.55	0.41
1:A:495:VAL:CG1	1:A:500:LEU:HD22	2.51	0.41
1:D:691:GLN:HG3	8:D:1418:HOH:O	2.21	0.40
1:D:579:GLN:HG2	2:E:27:DG:OP1	2.21	0.40
5:D:901:SUC:H1	5:D:901:SUC:H1'2	1.92	0.40
1:A:515:GLU:HG2	1:A:519:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1001:HOH:O	8:D:1067:HOH:O[2_745]	1.99	0.21

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	586/580 (101%)	574 (98%)	12 (2%)	0	100	100
1	D	590/580 (102%)	574 (97%)	16 (3%)	0	100	100
All	All	1176/1160 (101%)	1148 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	504/495 (102%)	489 (97%)	15 (3%)	48	15
1	D	507/495 (102%)	491 (97%)	16 (3%)	46	13
All	All	1011/990 (102%)	980 (97%)	31 (3%)	48	14

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

Mol	Chain	Res	Type
1	A	303	LEU
1	A	415	LYS
1	A	420	GLU
1	A	500	LEU
1	A	507	LEU
1	A	544	LEU
1	A	561	LEU
1	A	566	PRO

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Mol	Chain	Res	Type
1	A	591	LEU
1	A	677	ARG
1	A	699	PRO
1	A	784[A]	ARG
1	A	784[B]	ARG
1	A	837	PRO
1	A	846	ARG
1	D	298	LYS
1	D	303	LEU
1	D	415	LYS
1	D	431	LYS
1	D	434	LYS
1	D	435	ARG
1	D	499	ARG
1	D	506	GLU
1	D	511	LEU
1	D	513	THR
1	D	629	ARG
1	D	703	ARG
1	D	776	ILE
1	D	816	LYS
1	D	846	ARG
1	D	863	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	691	GLN
1	A	704	GLN
1	A	726	ASN
1	A	755	GLN
1	A	823	HIS
1	D	704	GLN
1	D	768	HIS
1	D	867	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	388	1	7,9,10	0.64	0	6,9,11	1.56	1 (16%)
1	CME	D	388	1	7,9,10	0.54	0	6,9,11	1.66	2 (33%)

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
1	CME	A	388	1	-	0/5/8/10	0/0/0/0
1	CME	D	388	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	388	CME	CB-SG-SD	-2.89	98.33	103.95
1	A	388	CME	O-C-CA	-2.66	118.59	125.72
1	D	388	CME	O-C-CA	-2.31	119.52	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 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$
4	TTP	A	901	-	21,30,30	0.78	0	26,47,47	2.70	7 (26%)
5	SUC	A	902	-	24,24,24	0.88	0	36,36,36	1.20	3 (8%)
7	2DT	B	101	2	11,20,21	1.30	2 (18%)	12,28,31	2.26	4 (33%)
5	SUC	D	901	-	24,24,24	0.89	1 (4%)	36,36,36	1.27	4 (11%)
6	SO4	D	902	-	4,4,4	0.73	0	6,6,6	1.39	1 (16%)
7	2DT	E	101	2	11,20,21	1.72	3 (27%)	12,28,31	2.42	3 (25%)

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	TTP	A	901	-	-	0/18/34/34	0/2/2/2
5	SUC	A	902	-	-	0/12/51/51	0/2/2/2
7	2DT	B	101	2	-	0/3/18/19	0/2/2/2
5	SUC	D	901	-	-	0/12/51/51	0/2/2/2
6	SO4	D	902	-	-	0/0/0/0	0/0/0/0
7	2DT	E	101	2	-	0/3/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	101	2DT	C3'-C2'	-2.94	1.45	1.54
7	B	101	2DT	C5M-C5	2.21	1.55	1.51
7	B	101	2DT	C4-N3	2.27	1.37	1.33
5	D	901	SUC	O3'-C3'	2.40	1.47	1.42
7	E	101	2DT	C5M-C5	2.41	1.55	1.51
7	E	101	2DT	C4-N3	2.59	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	TTP	C5-C4-N3	-7.53	119.03	125.35
7	E	101	2DT	C5-C4-N3	-6.40	119.98	125.35
7	B	101	2DT	C5-C4-N3	-5.60	120.65	125.35
5	A	902	SUC	O6'-C6'-C5'	-4.49	96.30	111.30
5	D	901	SUC	C2'-O1-C1	-3.14	108.93	117.45
5	D	901	SUC	O6'-C6'-C5'	-2.96	101.41	111.30
4	A	901	TTP	C5M-C5-C4	-2.96	116.68	119.97
5	D	901	SUC	O5-C1-C2	-2.79	104.47	110.28
5	A	902	SUC	O3'-C3'-C4'	-2.57	104.28	113.43
4	A	901	TTP	O3'-C3'-C2'	-2.52	102.26	110.74
6	D	902	SO4	O2-S-O1	-2.34	101.77	109.59
5	A	902	SUC	O2-C2-C1	-2.30	104.91	110.01
7	E	101	2DT	O4'-C1'-C2'	-2.26	104.17	106.63
5	D	901	SUC	O6-C6-C5	2.00	117.99	111.30
4	A	901	TTP	C2'-C3'-C4'	2.11	107.06	102.77
4	A	901	TTP	O2B-PB-O3B	2.14	114.45	105.27
7	B	101	2DT	O4'-C4'-C5'	2.17	112.79	109.52
7	B	101	2DT	C2'-C1'-N1	2.72	117.80	112.49
7	B	101	2DT	C4-N3-C2	2.86	117.54	115.16
4	A	901	TTP	C5M-C5-C6	2.92	124.56	118.63
7	E	101	2DT	C3'-C2'-C1'	3.97	107.25	102.75
4	A	901	TTP	C4-N3-C2	8.68	122.40	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	TTP	2	0
5	A	902	SUC	1	0
7	B	101	2DT	1	0
5	D	901	SUC	2	0

## 5.7 Other polymers ⓘ

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	578/580 (99%)	-0.05	16 (2%) 56 59	14, 27, 45, 67	3 (0%)
1	D	579/580 (99%)	0.15	24 (4%) 41 43	11, 24, 49, 89	1 (0%)
2	B	8/9 (88%)	-0.41	0 100 100	22, 26, 30, 37	0
2	E	8/9 (88%)	-0.40	0 100 100	17, 24, 31, 51	0
3	C	11/14 (78%)	-0.44	0 100 100	17, 22, 37, 45	0
3	F	14/14 (100%)	0.09	1 (7%) 19 19	14, 23, 41, 46	0
All	All	1198/1206 (99%)	0.04	41 (3%) 49 51	11, 25, 47, 89	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	GLY	6.3
1	D	602[A]	VAL	5.3
1	D	434	LYS	4.1
1	D	693	SER	4.0
1	A	523	GLY	3.9
1	D	508	ALA	3.6
1	D	509	GLU	3.6
1	A	298	LYS	3.5
1	D	504	GLY	3.5
1	A	647	TRP	3.2
1	D	514	VAL	3.2
3	F	1	DG	3.1
1	D	695	ASP	3.1
1	D	433	ALA	3.1
1	D	430	GLY	3.0
1	D	505	LYS	2.7
1	D	512	GLY	2.7
1	D	692	VAL	2.7
1	A	868	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	854[A]	GLN	2.6
1	D	431	LYS	2.5
1	A	505	LYS	2.4
1	D	305	ASP	2.4
1	A	819	ARG	2.4
1	D	803	ILE	2.4
1	D	306	ARG	2.3
1	A	846	ARG	2.3
1	D	698	THR	2.2
1	D	782	ASN	2.2
1	A	519	TYR	2.2
1	A	431	LYS	2.2
1	A	836	ALA	2.1
1	D	297	LYS	2.1
1	A	509	GLU	2.1
1	A	842	GLU	2.1
1	D	779	ARG	2.1
1	A	689	ILE	2.1
1	A	525	GLU	2.1
1	D	691	GLN	2.0
1	A	551	LYS	2.0
1	D	781	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CME	D	388	10/11	0.96	0.09	-	18,26,45,49	0
1	CME	A	388	10/11	0.95	0.10	-	19,22,55,68	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SUC	A	902	23/23	0.81	0.17	4.09	29,36,41,45	0
5	SUC	D	901	23/23	0.81	0.17	3.54	15,19,21,24	23
4	TTP	A	901	29/29	0.93	0.11	1.86	28,35,43,43	29
7	2DT	B	101	19/20	0.98	0.08	0.18	20,22,28,32	0
6	SO4	D	902	5/5	0.97	0.10	0.01	36,38,50,50	0
7	2DT	E	101	19/20	0.98	0.08	-0.42	16,18,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.