



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2018 – 11:09 PM EST

PDB ID : 6B5E  
Title : Mycobacterium tuberculosis RmlA in complex with dTDP-glucose  
Authors : Brown, H.A.; Holden, H.M.  
Deposited on : 2017-09-29  
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

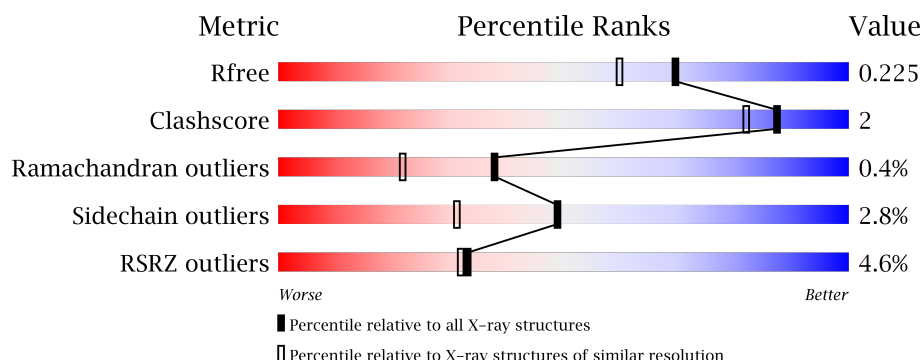
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	296	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	B	296	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	296	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>..</div> </div>
1	D	296	<div> <div>3%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	E	296	<div> <div>5%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	296	<div><div></div><div>6%</div><div>89%</div><div>6%</div><div></div></div>
1	G	296	<div><div></div><div>4%</div><div>89%</div><div>6%</div><div></div></div>
1	H	296	<div><div></div><div>11%</div><div>85%</div><div>8%</div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19586 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 Glucose-1-phosphate thymidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	3	0
			2191	1407	368	410	6			
1	B	286	Total	C	N	O	S	0	2	0
			2219	1423	378	411	7			
1	C	286	Total	C	N	O	S	0	4	0
			2224	1426	378	412	8			
1	D	286	Total	C	N	O	S	0	1	0
			2187	1403	368	409	7			
1	E	286	Total	C	N	O	S	0	5	0
			2214	1423	373	412	6			
1	F	284	Total	C	N	O	S	0	4	0
			2202	1415	370	409	8			
1	G	284	Total	C	N	O	S	0	3	0
			2204	1415	375	407	7			
1	H	279	Total	C	N	O	S	0	0	0
			2142	1376	361	399	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	LEU	-	expression tag	UNP P9WH13
A	290	GLU	-	expression tag	UNP P9WH13
A	291	HIS	-	expression tag	UNP P9WH13
A	292	HIS	-	expression tag	UNP P9WH13
A	293	HIS	-	expression tag	UNP P9WH13
A	294	HIS	-	expression tag	UNP P9WH13
A	295	HIS	-	expression tag	UNP P9WH13
A	296	HIS	-	expression tag	UNP P9WH13
B	289	LEU	-	expression tag	UNP P9WH13
B	290	GLU	-	expression tag	UNP P9WH13
B	291	HIS	-	expression tag	UNP P9WH13
B	292	HIS	-	expression tag	UNP P9WH13
B	293	HIS	-	expression tag	UNP P9WH13

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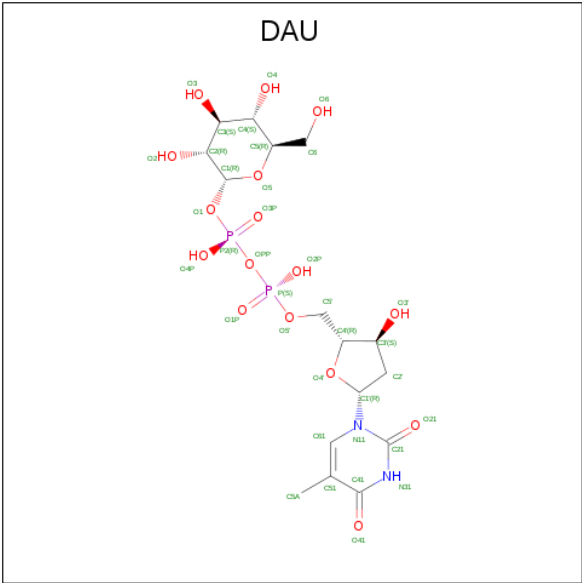
Chain	Residue	Modelled	Actual	Comment	Reference
B	294	HIS	-	expression tag	UNP P9WH13
B	295	HIS	-	expression tag	UNP P9WH13
B	296	HIS	-	expression tag	UNP P9WH13
C	289	LEU	-	expression tag	UNP P9WH13
C	290	GLU	-	expression tag	UNP P9WH13
C	291	HIS	-	expression tag	UNP P9WH13
C	292	HIS	-	expression tag	UNP P9WH13
C	293	HIS	-	expression tag	UNP P9WH13
C	294	HIS	-	expression tag	UNP P9WH13
C	295	HIS	-	expression tag	UNP P9WH13
C	296	HIS	-	expression tag	UNP P9WH13
D	289	LEU	-	expression tag	UNP P9WH13
D	290	GLU	-	expression tag	UNP P9WH13
D	291	HIS	-	expression tag	UNP P9WH13
D	292	HIS	-	expression tag	UNP P9WH13
D	293	HIS	-	expression tag	UNP P9WH13
D	294	HIS	-	expression tag	UNP P9WH13
D	295	HIS	-	expression tag	UNP P9WH13
D	296	HIS	-	expression tag	UNP P9WH13
E	289	LEU	-	expression tag	UNP P9WH13
E	290	GLU	-	expression tag	UNP P9WH13
E	291	HIS	-	expression tag	UNP P9WH13
E	292	HIS	-	expression tag	UNP P9WH13
E	293	HIS	-	expression tag	UNP P9WH13
E	294	HIS	-	expression tag	UNP P9WH13
E	295	HIS	-	expression tag	UNP P9WH13
E	296	HIS	-	expression tag	UNP P9WH13
F	289	LEU	-	expression tag	UNP P9WH13
F	290	GLU	-	expression tag	UNP P9WH13
F	291	HIS	-	expression tag	UNP P9WH13
F	292	HIS	-	expression tag	UNP P9WH13
F	293	HIS	-	expression tag	UNP P9WH13
F	294	HIS	-	expression tag	UNP P9WH13
F	295	HIS	-	expression tag	UNP P9WH13
F	296	HIS	-	expression tag	UNP P9WH13
G	289	LEU	-	expression tag	UNP P9WH13
G	290	GLU	-	expression tag	UNP P9WH13
G	291	HIS	-	expression tag	UNP P9WH13
G	292	HIS	-	expression tag	UNP P9WH13
G	293	HIS	-	expression tag	UNP P9WH13
G	294	HIS	-	expression tag	UNP P9WH13
G	295	HIS	-	expression tag	UNP P9WH13

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Chain	Residue	Modelled	Actual	Comment	Reference
G	296	HIS	-	expression tag	UNP P9WH13
H	289	LEU	-	expression tag	UNP P9WH13
H	290	GLU	-	expression tag	UNP P9WH13
H	291	HIS	-	expression tag	UNP P9WH13
H	292	HIS	-	expression tag	UNP P9WH13
H	293	HIS	-	expression tag	UNP P9WH13
H	294	HIS	-	expression tag	UNP P9WH13
H	295	HIS	-	expression tag	UNP P9WH13
H	296	HIS	-	expression tag	UNP P9WH13

- Molecule 2 is 2'DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>16</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

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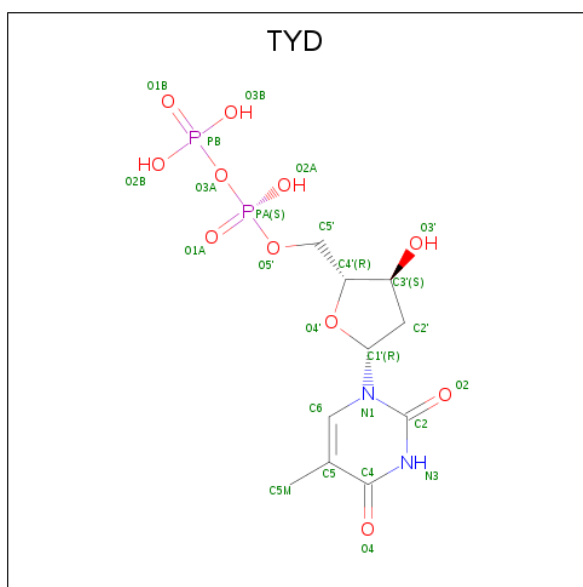
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	G	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	H	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

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





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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	249	Total	O	0	0
			249	249		
8	B	254	Total	O	0	0
			254	254		
8	C	188	Total	O	0	0
			188	188		
8	D	148	Total	O	0	0
			148	148		
8	E	191	Total	O	0	0
			191	191		
8	F	167	Total	O	0	0
			167	167		

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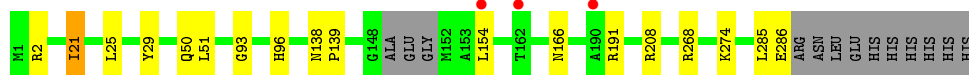
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	181	Total 181	O 181	0	0
8	H	99	Total 99	O 99	0	0

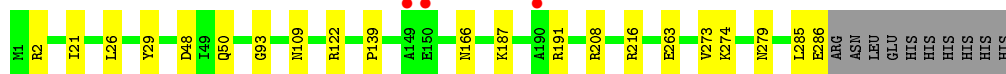
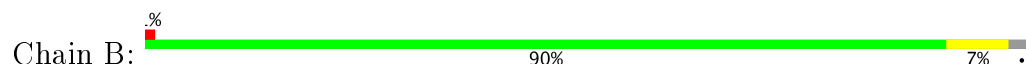
### 3 Residue-property plots [i](#)

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.

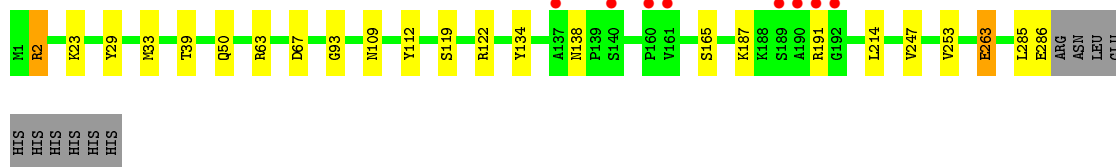
- Molecule 1: Glucose-1-phosphate thymidyltransferase



- Molecule 1: Glucose-1-phosphate thymidyltransferase



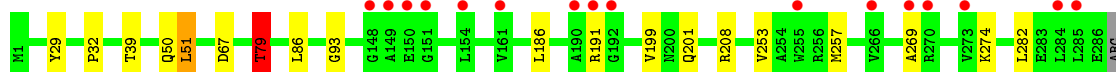
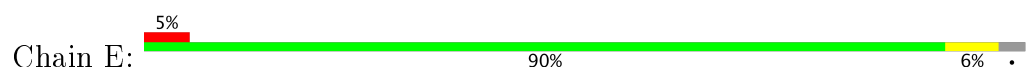
- Molecule 1: Glucose-1-phosphate thymidyltransferase



- Molecule 1: Glucose-1-phosphate thymidyltransferase

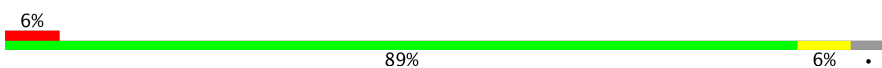


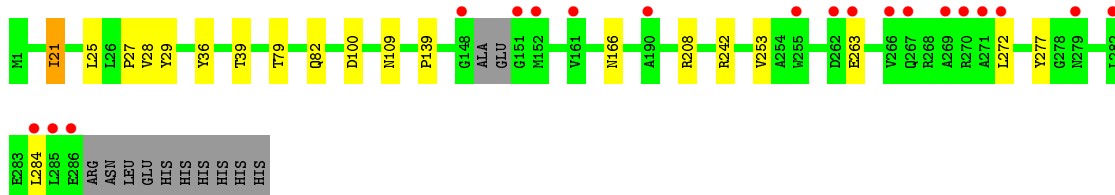
- Molecule 1: Glucose-1-phosphate thymidyltransferase



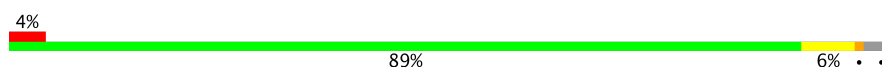
ASN  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: Glucose-1-phosphate thymidyltransferase

Chain F: 




- Molecule 1: Glucose-1-phosphate thymidyltransferase

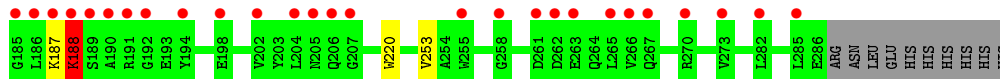
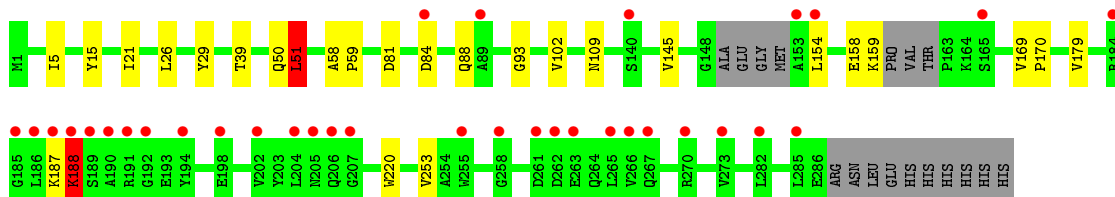
Chain G: 



ARG  
ASN  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: Glucose-1-phosphate thymidyltransferase

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.32Å 111.26Å 290.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 37.82 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-1.85) 97.8 (37.82-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15.80 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.171 , 0.218 0.182 , 0.225	Depositor DCC
$R_{free}$ test set	9779 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: MG, CL, TYD, NA, EDO, DAU

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	0.73	0/2247	0.82	0/3054
1	B	0.72	0/2273	0.84	1/3086 (0.0%)
1	C	0.63	0/2284	0.76	2/3099 (0.1%)
1	D	0.56	0/2238	0.74	1/3043 (0.0%)
1	E	0.66	1/2277 (0.0%)	0.79	4/3096 (0.1%)
1	F	0.61	0/2261	0.75	2/3070 (0.1%)
1	G	0.58	0/2260	0.77	2/3069 (0.1%)
1	H	0.59	0/2187	0.74	3/2969 (0.1%)
All	All	0.64	1/18027 (0.0%)	0.78	15/24486 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	THR	CB-CG2	-5.35	1.34	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	270	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	G	270	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	F	100	ASP	CB-CG-OD1	7.62	125.15	118.30
1	H	188	LYS	N-CA-C	6.79	129.32	111.00
1	E	208	ARG	NE-CZ-NH2	6.09	123.35	120.30

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	2191	0	2178	10	0
1	B	2219	0	2225	9	0
1	C	2224	0	2225	12	0
1	D	2187	0	2162	6	0
1	E	2214	0	2217	8	0
1	F	2202	0	2208	11	0
1	G	2204	0	2210	15	0
1	H	2142	0	2126	19	0
2	A	36	0	24	1	0
2	B	36	0	24	0	0
2	C	36	0	24	1	0
2	D	36	0	24	0	0
2	E	72	0	48	0	0
2	F	72	0	48	0	0
2	G	36	0	24	0	0
2	H	36	0	24	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	25	0	13	0	0
4	B	25	0	13	0	0
4	C	25	0	13	0	0
4	D	25	0	13	0	0
4	G	25	0	13	0	0
4	H	25	0	13	0	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	249	0	0	3	0
8	B	254	0	0	1	0
8	C	188	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	148	0	0	0	0
8	E	191	0	0	2	0
8	F	167	0	0	1	0
8	G	181	0	0	2	0
8	H	99	0	0	0	0
All	All	19586	0	17875	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 87 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:G:268[B]:ARG:HG3	1:G:268[B]:ARG:HH21	1.01	1.13
1:A:21:ILE:HD12	1:B:21:ILE:HD12	1.36	1.08
1:A:268[B]:ARG:NH1	8:A:401:HOH:O	1.91	0.95
1:F:21:ILE:HD12	1:H:21:ILE:HD12	1.50	0.92
1:G:268[B]:ARG:NH2	1:G:268[B]:ARG:HG3	1.81	0.88

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	282/296 (95%)	279 (99%)	2 (1%)	1 (0%)	38	22
1	B	286/296 (97%)	282 (99%)	3 (1%)	1 (0%)	44	29
1	C	288/296 (97%)	282 (98%)	5 (2%)	1 (0%)	44	29
1	D	285/296 (96%)	279 (98%)	5 (2%)	1 (0%)	38	22
1	E	289/296 (98%)	285 (99%)	3 (1%)	1 (0%)	44	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	284/296 (96%)	279 (98%)	4 (1%)	1 (0%)	38	22
1	G	283/296 (96%)	280 (99%)	2 (1%)	1 (0%)	38	22
1	H	273/296 (92%)	264 (97%)	7 (3%)	2 (1%)	25	10
All	All	2270/2368 (96%)	2230 (98%)	31 (1%)	9 (0%)	38	22

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	188	LYS
1	G	29	TYR
1	A	29	TYR
1	B	29	TYR
1	C	29	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	226/237 (95%)	220 (97%)	6 (3%)	50	33
1	B	229/237 (97%)	222 (97%)	7 (3%)	45	27
1	C	229/237 (97%)	223 (97%)	6 (3%)	51	34
1	D	223/237 (94%)	216 (97%)	7 (3%)	45	27
1	E	229/237 (97%)	221 (96%)	8 (4%)	41	21
1	F	229/237 (97%)	222 (97%)	7 (3%)	45	27
1	G	228/237 (96%)	222 (97%)	6 (3%)	51	34
1	H	219/237 (92%)	214 (98%)	5 (2%)	56	39
All	All	1812/1896 (96%)	1760 (97%)	52 (3%)	49	30

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	181	GLU

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Mol	Chain	Res	Type
1	E	67	ASP
1	H	81	ASP
1	D	191	ARG
1	E	32	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	201	GLN
1	E	205	ASN
1	H	50	GLN
1	E	50	GLN
1	E	200	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	DAU	A	301	3	30,38,38	1.13	2 (6%)	42,58,58	2.14	6 (14%)
4	TYD	A	303	-	24,26,26	2.24	5 (20%)	28,40,40	1.66	6 (21%)
6	EDO	A	305	-	3,3,3	0.57	0	2,2,2	0.39	0
2	DAU	B	301	3	30,38,38	0.89	1 (3%)	42,58,58	1.75	6 (14%)
4	TYD	B	304	-	24,26,26	2.31	4 (16%)	28,40,40	1.67	6 (21%)
2	DAU	C	301	3	30,38,38	0.82	1 (3%)	42,58,58	2.18	9 (21%)
4	TYD	C	303	-	24,26,26	2.31	3 (12%)	28,40,40	1.69	5 (17%)
2	DAU	D	301	3	30,38,38	0.75	1 (3%)	42,58,58	1.89	5 (11%)
4	TYD	D	303	-	24,26,26	2.30	3 (12%)	28,40,40	1.78	7 (25%)
2	DAU	E	301	3	30,38,38	1.06	3 (10%)	42,58,58	1.99	7 (16%)
2	DAU	E	302	-	30,38,38	0.67	0	42,58,58	1.83	5 (11%)
2	DAU	F	301	3	30,38,38	0.60	0	42,58,58	2.17	5 (11%)
2	DAU	F	302	-	30,38,38	0.70	0	42,58,58	1.77	3 (7%)
2	DAU	G	301	3	30,38,38	0.75	1 (3%)	42,58,58	1.95	4 (9%)
4	TYD	G	303	-	24,26,26	2.38	5 (20%)	28,40,40	1.55	5 (17%)
2	DAU	H	301	3	30,38,38	0.74	1 (3%)	42,58,58	2.03	6 (14%)
4	TYD	H	303	-	24,26,26	2.30	3 (12%)	28,40,40	1.84	9 (32%)

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	DAU	A	301	3	-	0/19/55/55	0/3/3/3
4	TYD	A	303	-	-	0/16/28/28	0/2/2/2
6	EDO	A	305	-	-	0/1/1/1	0/0/0/0
2	DAU	B	301	3	-	0/19/55/55	0/3/3/3
4	TYD	B	304	-	-	0/16/28/28	0/2/2/2
2	DAU	C	301	3	-	0/19/55/55	0/3/3/3
4	TYD	C	303	-	-	0/16/28/28	0/2/2/2
2	DAU	D	301	3	-	0/19/55/55	0/3/3/3
4	TYD	D	303	-	-	0/16/28/28	0/2/2/2
2	DAU	E	301	3	-	0/19/55/55	0/3/3/3
2	DAU	E	302	-	-	0/19/55/55	0/3/3/3
2	DAU	F	301	3	-	0/19/55/55	0/3/3/3
2	DAU	F	302	-	-	0/19/55/55	0/3/3/3
2	DAU	G	301	3	-	0/19/55/55	0/3/3/3
4	TYD	G	303	-	-	0/16/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAU	H	301	3	-	0/19/55/55	0/3/3/3
4	TYD	H	303	-	-	0/16/28/28	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	TYD	C6-N1	-8.81	1.35	1.46
4	C	303	TYD	C6-N1	-8.79	1.35	1.46
4	H	303	TYD	C6-N1	-8.78	1.35	1.46
4	G	303	TYD	C6-N1	-8.38	1.35	1.46
4	B	304	TYD	C6-N1	-8.38	1.35	1.46

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	DAU	O4'-C1'-N11	-6.94	96.08	107.78
2	C	301	DAU	O4'-C1'-N11	-6.57	96.72	107.78
2	F	301	DAU	C51-C41-N31	-6.24	118.36	125.24
2	E	302	DAU	C51-C41-N31	-6.17	118.43	125.24
2	F	302	DAU	C51-C41-N31	-6.08	118.53	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	DAU	1	0
2	C	301	DAU	1	0
2	H	301	DAU	1	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 ⓘ

### 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	283/296 (95%)	-0.19	3 (1%) 80 81	10, 18, 41, 70	0
1	B	286/296 (96%)	-0.23	3 (1%) 82 82	9, 17, 37, 69	0
1	C	286/296 (96%)	-0.02	8 (2%) 53 52	14, 23, 50, 88	0
1	D	286/296 (96%)	0.14	9 (3%) 49 47	14, 28, 50, 84	0
1	E	286/296 (96%)	0.04	16 (5%) 25 24	13, 22, 54, 72	0
1	F	284/296 (95%)	0.20	19 (6%) 19 18	14, 25, 51, 77	0
1	G	284/296 (95%)	-0.06	12 (4%) 37 35	13, 23, 43, 59	0
1	H	279/296 (94%)	0.72	34 (12%) 5 5	15, 35, 63, 102	0
All	All	2274/2368 (96%)	0.07	104 (4%) 33 32	9, 23, 51, 102	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	ARG	6.8
1	E	149	ALA	6.4
1	C	190	ALA	6.0
1	B	190	ALA	5.6
1	H	186	LEU	5.5

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	TYD	H	303	25/25	0.94	0.11	0.41	29,33,38,41	0
6	EDO	A	305	4/4	0.96	0.10	0.32	23,24,26,29	0
4	TYD	A	303	25/25	0.97	0.08	-0.13	18,20,25,29	0
4	TYD	C	303	25/25	0.96	0.09	-0.19	23,26,32,35	0
7	NA	C	304	1/1	0.99	0.08	-0.27	17,17,17,17	0
2	DAU	F	302	36/36	0.97	0.08	-0.30	20,24,40,42	0
2	DAU	E	302	36/36	0.97	0.09	-0.36	20,28,50,57	0
2	DAU	B	301	36/36	0.98	0.08	-0.47	9,12,15,16	0
2	DAU	C	301	36/36	0.96	0.09	-0.50	19,22,27,28	0
4	TYD	B	304	25/25	0.97	0.07	-0.60	16,19,22,27	0
2	DAU	H	301	36/36	0.93	0.12	-0.72	21,30,39,43	0
4	TYD	G	303	25/25	0.97	0.07	-0.97	24,28,33,34	0
2	DAU	A	301	36/36	0.98	0.07	-0.98	12,15,18,20	0
4	TYD	D	303	25/25	0.97	0.08	-1.10	24,27,32,36	0
2	DAU	G	301	36/36	0.98	0.07	-1.15	13,16,19,21	0
2	DAU	D	301	36/36	0.97	0.07	-1.23	19,23,26,30	0
2	DAU	E	301	36/36	0.98	0.06	-1.35	12,16,18,19	0
2	DAU	F	301	36/36	0.98	0.07	-1.35	17,21,26,27	0
5	CL	A	304	1/1	1.00	0.06	-2.43	19,19,19,19	0
3	MG	B	303	1/1	0.95	0.07	-2.96	34,34,34,34	0
7	NA	B	305	1/1	0.96	0.20	-	32,32,32,32	0
3	MG	G	302	1/1	1.00	0.06	-	14,14,14,14	0
3	MG	F	303	1/1	0.99	0.09	-	18,18,18,18	0
3	MG	B	302	1/1	1.00	0.06	-	10,10,10,10	0
3	MG	D	302	1/1	0.99	0.06	-	17,17,17,17	0
3	MG	A	302	1/1	0.99	0.06	-	12,12,12,12	0
3	MG	C	302	1/1	0.99	0.07	-	20,20,20,20	0
3	MG	E	303	1/1	0.99	0.03	-	17,17,17,17	0
3	MG	H	302	1/1	0.95	0.07	-	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.