



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:58 PM GMT

PDB ID : 1W19  
Title : LUMAZINE SYNTHASE FROM MYCOBACTERIUM TUBERCULOSIS  
BOUND TO 3-(1,3,7-TRIHYDRO-9-D-RIBITYL-2,6,8-PURINETRION  
E-7-YL) PROPANE 1-PHOSPHATE  
Authors : Morgunova, E.; Meining, W.; Illarionov, B.; Haase, I.; Fischer, M.; Cushman,  
M.; Bacher, A.; Ladenstein, R.  
Deposited on : 2004-06-18  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

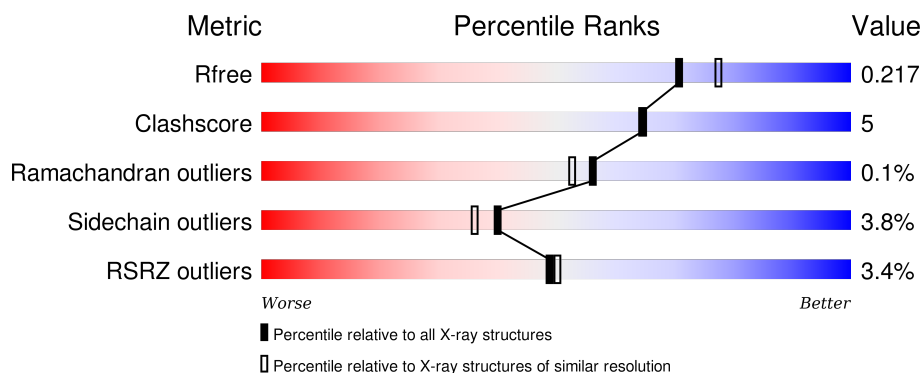
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	160	<div> <div>2%</div> <div>87%</div> <div>8%</div> </div>
1	B	160	<div> <div>3%</div> <div>80%</div> <div>9%</div> <div>8%</div> </div>
1	C	160	<div> <div>3%</div> <div>80%</div> <div>9%</div> <div>9%</div> </div>
1	D	160	<div> <div>5%</div> <div>81%</div> <div>9%</div> <div>8%</div> </div>
1	E	160	<div> <div>3%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>

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
10	D1D	E	1166	-	-	-	X
2	ACY	C	632	-	-	-	X
2	ACY	D	1161	-	-	-	X
2	ACY	E	1161	-	-	-	X
3	DTU	A	1162	-	X	-	X
3	DTU	B	1162	-	X	X	X
7	DTV	C	1161	-	-	-	X
7	DTV	D	1162	-	X	-	X
7	DTV	E	1162	-	-	-	X

## 2 Entry composition [i](#)

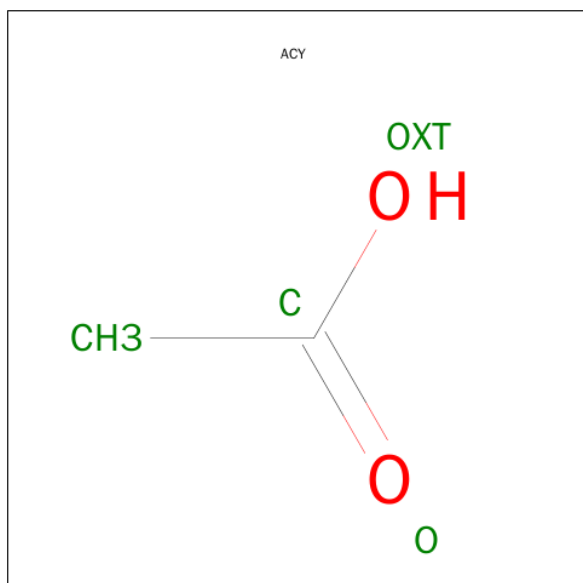
There are 11 unique types of molecules in this entry. The entry contains 6151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	B	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	C	146	Total	C	N	O	S	0	0	0
			1054	651	193	207	3			
1	D	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	E	146	Total	C	N	O	S	0	0	0
			1054	651	193	207	3			

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



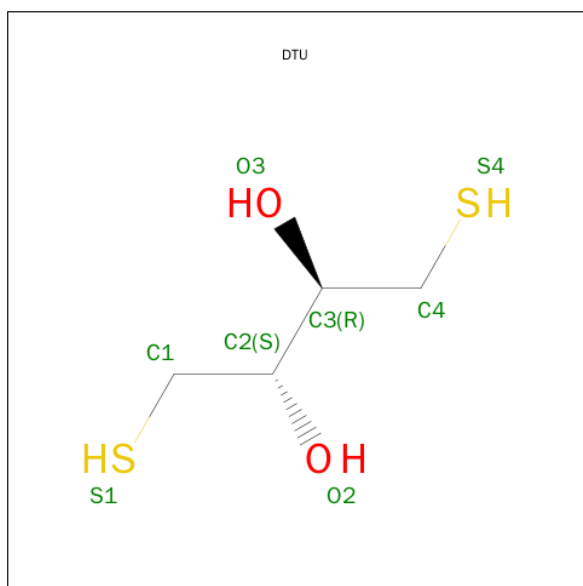
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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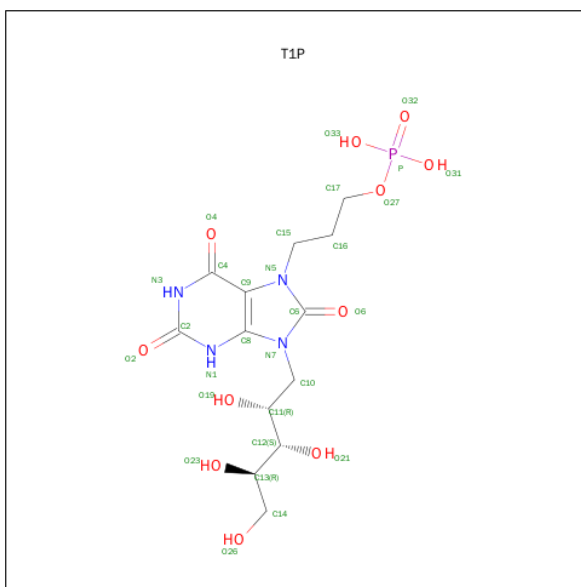
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



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

- Molecule 4 is 3-{2,6,8-TRIOXO-9-[(2R,3S,4R)-2,3,4,5-TETRAHYDROXYPENTYL]-1,2,3,6,8,9-HEXAHYDRO-7H-PURIN-7-YL}PROPYL DIHYDROGEN PHOSPHATE (three-letter code: T1P) (formula: C<sub>13</sub>H<sub>21</sub>N<sub>4</sub>O<sub>11</sub>P).

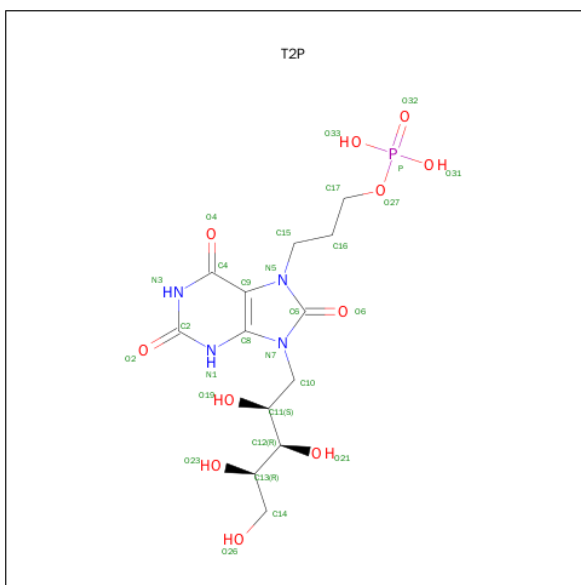


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	13	4	11	1		

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

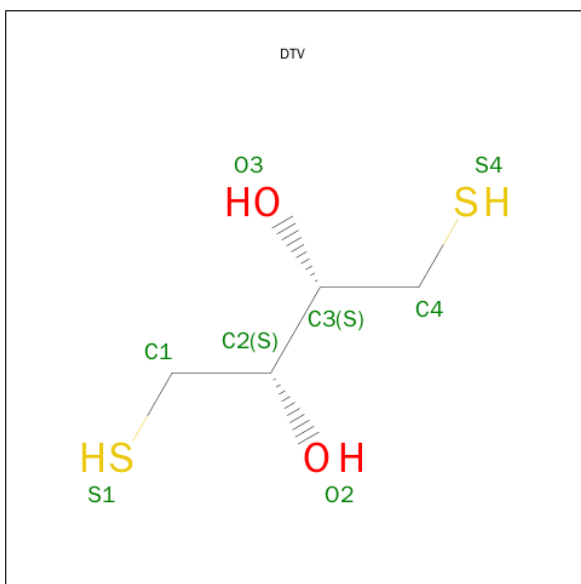
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	K	0	0
			3	3		
5	A	3	Total	K	0	0
			3	3		
5	D	2	Total	K	0	0
			2	2		
5	C	3	Total	K	0	0
			3	3		
5	E	2	Total	K	0	0
			2	2		

- Molecule 6 is 3-{2,6,8-TRIOXO-9-[(2S,3R,4R)-2,3,4,5-TETRAHYDROXYPENTYL]-1,2,3,6,8,9-HEXAHYDRO-7H-PURIN-7-YL}PROPYL DIHYDROGEN PHOSPHATE (three-letter code: T2P) (formula: C<sub>13</sub>H<sub>21</sub>N<sub>4</sub>O<sub>11</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			29	13	4	11	1		

- Molecule 7 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula:  $C_4H_{10}O_2S_2$ ).



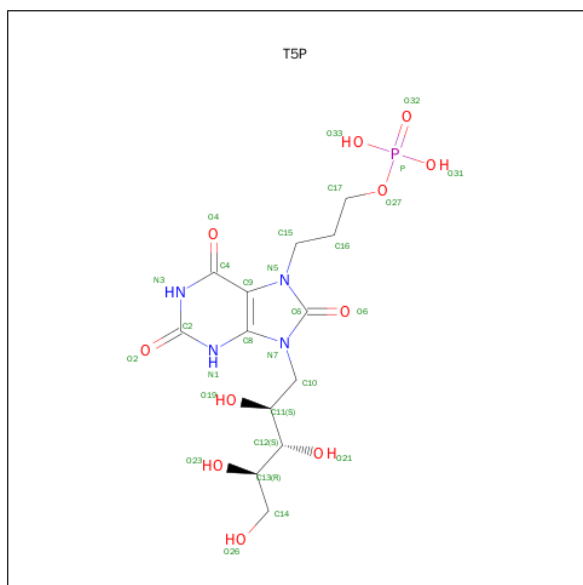
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total 8	C 4	O 2	S 2	0	0
7	D	1	Total 8	C 4	O 2	S 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	O	S	0	0
			8	4	2	2		

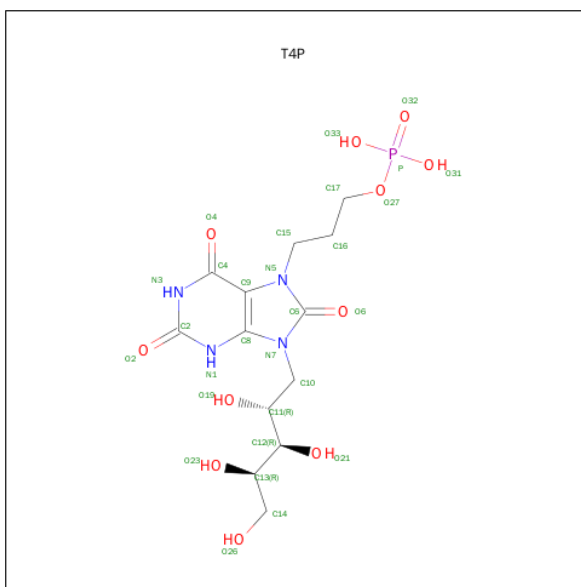
- Molecule 8 is 3-{2,6,8-TRIOXO-9-[(2S,3S,4R)-2,3,4,5-TETRAHYDROXYPENTYL]-1,2,3,6,8,9-HEXAHYDRO-7H-PURIN-7-YL}PROPYL DIHYDROGEN PHOSPHATE (three-letter code: T5P) (formula: C<sub>13</sub>H<sub>21</sub>N<sub>4</sub>O<sub>11</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			29	13	4	11	1		

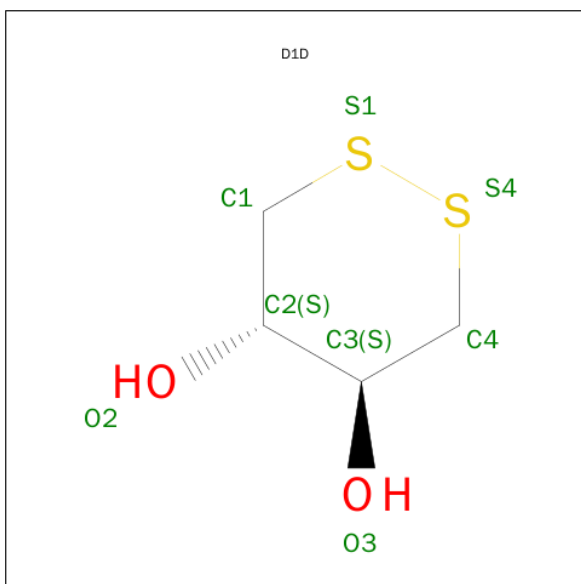
- Molecule 9 is 3-{2,6,8-TRIOXO-9-[(2R,3R,4R)-2,3,4,5-TETRAHYDROXYPENTYL]-1,2,3,6,8,9-HEXAHYDRO-7H-PURIN-7-YL}PROPYL DIHYDROGEN PHOSPHATE (three-letter code: T4P) (formula: C<sub>13</sub>H<sub>21</sub>N<sub>4</sub>O<sub>11</sub>P).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			29	13	4	11	1		
9	E	1	Total	C	N	O	P	0	0
			29	13	4	11	1		

- Molecule 10 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	1	Total	C	O	S	0	0
			8	4	2	2		

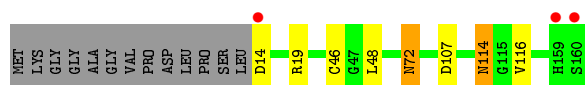
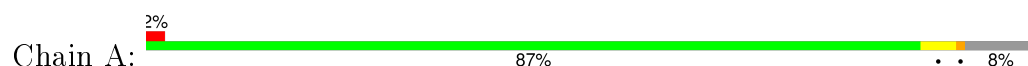
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	136	Total 136	O 136	0	0
11	B	132	Total 132	O 132	0	0
11	C	108	Total 108	O 108	0	0
11	D	122	Total 122	O 122	0	0
11	E	133	Total 133	O 133	0	0

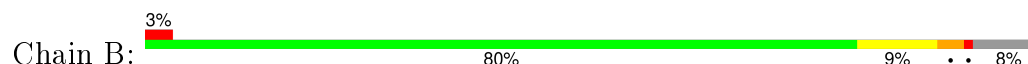
### 3 Residue-property plots [i](#)

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

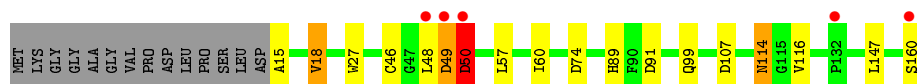
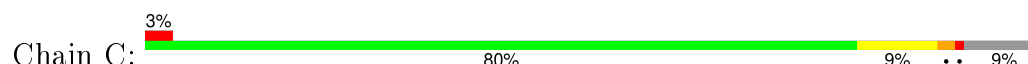
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



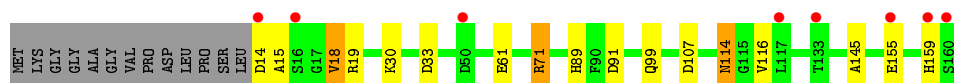
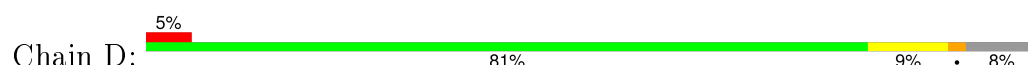
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



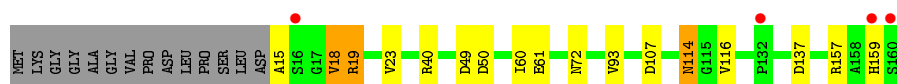
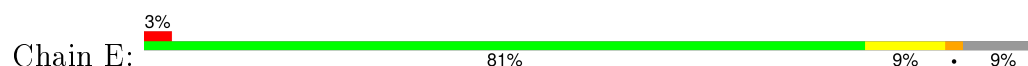
- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



- Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.27Å 80.69Å 86.19Å 90.00° 120.29° 90.00°	Depositor
Resolution (Å)	19.54 – 2.00 19.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.54-2.00) 99.4 (19.93-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.149 , 0.194 0.177 , 0.217	Depositor DCC
$R_{free}$ test set	2661 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 52167 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.69% 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: T5P, K, T4P, D1D, T1P, T2P, ACY, DTV, DTU

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	0.56	0/1074	0.87	3/1467 (0.2%)
1	B	0.56	0/1074	0.93	5/1467 (0.3%)
1	C	0.50	0/1066	0.78	5/1456 (0.3%)
1	D	0.54	0/1074	0.89	8/1467 (0.5%)
1	E	0.55	0/1066	0.88	6/1456 (0.4%)
All	All	0.55	0/5354	0.87	27/7313 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	B	103	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	19	ARG	NE-CZ-NH1	10.17	125.38	120.30
1	E	19	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	D	19	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	107	ASP	CB-CG-OD2	7.46	125.02	118.30
1	E	107	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	19	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	D	71	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	D	107	ASP	CB-CG-OD2	7.00	124.60	118.30
1	D	71	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	C	49	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	50	ASP	CB-CG-OD2	6.03	123.72	118.30
1	E	19	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	19	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	49	ASP	CB-CG-OD2	5.63	123.36	118.30
1	D	33	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	50	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	91	ASP	CB-CG-OD2	5.55	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	107	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	14	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	107	ASP	CB-CG-OD2	5.21	122.98	118.30
1	E	137	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	91	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	74	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	50	ASP	CB-CG-OD2	5.02	122.82	118.30

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	1062	0	1072	6	0
1	B	1062	0	1072	13	0
1	C	1054	0	1069	14	0
1	D	1062	0	1072	10	0
1	E	1054	0	1068	9	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
3	A	8	0	8	0	0
3	B	8	0	7	4	0
4	A	29	0	19	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	B	29	0	19	1	0
7	C	8	0	9	3	0
7	D	8	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	8	0	7	0	0
8	C	29	0	19	1	0
9	D	29	0	18	1	0
9	E	29	0	19	2	0
10	E	8	0	8	0	0
11	A	136	0	0	2	0
11	B	132	0	0	6	0
11	C	108	0	0	2	1
11	D	122	0	0	4	0
11	E	133	0	0	3	0
All	All	6151	0	5508	56	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 5.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:CYS:SG	3:B:1162:DTU:S1	2.31	1.28
7:C:1161:DTV:S4	7:C:1161:DTV:O2	2.16	0.95
3:B:1162:DTU:S4	3:B:1162:DTU:O2	2.26	0.92
1:B:72:ASN:ND2	11:B:2060:HOH:O	2.13	0.82
1:C:46:CYS:SG	7:C:1161:DTV:S1	2.55	0.79
1:B:103:ARG:HD3	1:B:107:ASP:OD1	1.89	0.73
1:D:114:ASN:HD22	1:D:116:VAL:H	1.45	0.65
1:E:60:ILE:HD11	1:E:93:VAL:HA	1.78	0.64
1:D:89:HIS:ND1	11:D:2063:HOH:O	2.31	0.63
1:A:114:ASN:C	1:A:114:ASN:HD22	2.04	0.61
9:E:1163:T4P:O32	11:E:2130:HOH:O	2.17	0.58
1:D:114:ASN:ND2	1:D:116:VAL:H	2.02	0.57
1:C:114:ASN:C	1:C:114:ASN:HD22	2.07	0.56
1:B:28:HIS:CE1	1:B:83:ILE:HD12	2.41	0.55
1:D:114:ASN:C	1:D:114:ASN:HD22	2.11	0.55
1:E:61:GLU:OE1	9:E:1163:T4P:O21	2.26	0.53
1:E:157:ARG:O	1:E:159:HIS:ND1	2.42	0.53
1:B:123:GLU:HG2	1:B:124:GLN:N	2.23	0.52
1:B:154:ARG:NE	11:B:2123:HOH:O	2.42	0.52
1:A:114:ASN:ND2	1:A:116:VAL:H	2.06	0.52
1:C:15:ALA:O	1:C:18:VAL:HG13	2.10	0.52
1:B:99:GLN:NE2	11:B:2075:HOH:O	2.36	0.51
1:E:114:ASN:HD22	1:E:116:VAL:H	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:HA	11:A:2001:HOH:O	2.11	0.51
1:D:114:ASN:ND2	11:D:2090:HOH:O	2.43	0.51
1:C:48:LEU:HD11	1:C:147:LEU:HD21	1.93	0.50
2:B:1161:ACY:H3	11:B:2129:HOH:O	2.11	0.50
1:C:114:ASN:ND2	1:C:116:VAL:H	2.10	0.49
1:C:57:LEU:HD23	1:D:145:ALA:HB2	1.93	0.49
1:E:15:ALA:O	1:E:18:VAL:HG13	2.13	0.48
1:A:72:ASN:HB2	11:A:2058:HOH:O	2.14	0.48
11:B:2074:HOH:O	1:C:99:GLN:HG3	2.13	0.48
1:D:61:GLU:OE1	9:D:1163:T4P:O21	2.32	0.47
1:D:15:ALA:HB1	1:D:18:VAL:HG13	1.97	0.46
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.78	0.46
1:E:114:ASN:HD22	1:E:114:ASN:C	2.19	0.46
7:C:1161:DTV:H4	7:C:1161:DTV:HA	1.35	0.45
1:B:46:CYS:SG	3:B:1162:DTU:H2	2.56	0.45
1:E:72:ASN:HB2	11:E:2061:HOH:O	2.17	0.45
1:E:114:ASN:ND2	1:E:116:VAL:H	2.14	0.45
1:C:60:ILE:HB	8:C:1162:T5P:H12	2.00	0.44
1:B:75:ALA:HB1	1:B:146:ALA:HB1	1.99	0.44
1:C:89:HIS:HE1	11:D:2090:HOH:O	2.01	0.43
1:B:61:GLU:OE2	6:B:1163:T2P:H142	2.18	0.43
1:B:21:ALA:HB2	1:B:73:HIS:CD2	2.53	0.43
1:B:46:CYS:CB	3:B:1162:DTU:S1	3.05	0.43
1:D:155:GLU:O	1:D:159:HIS:HE1	2.02	0.42
1:A:14:ASP:O	1:A:46:CYS:O	2.38	0.41
11:C:2054:HOH:O	1:D:99:GLN:HG3	2.19	0.41
1:C:114:ASN:HD22	1:C:116:VAL:H	1.68	0.41
1:C:49:ASP:O	1:C:50:ASP:C	2.58	0.41
1:B:72:ASN:CG	11:B:2060:HOH:O	2.53	0.41
1:C:89:HIS:CE1	11:D:2090:HOH:O	2.73	0.41
1:A:114:ASN:HD22	1:A:116:VAL:H	1.68	0.41
1:C:27:TRP:HZ3	11:C:2017:HOH:O	2.04	0.40
1:E:19:ARG:HD2	11:E:2003:HOH:O	2.20	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)
11:C:2016:HOH:O	11:C:2016:HOH:O[2_556]	2.16	0.04



## 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	145/160 (91%)	144 (99%)	1 (1%)	0	100	100
1	B	145/160 (91%)	142 (98%)	3 (2%)	0	100	100
1	C	144/160 (90%)	141 (98%)	2 (1%)	1 (1%)	26	19
1	D	145/160 (91%)	142 (98%)	3 (2%)	0	100	100
1	E	144/160 (90%)	141 (98%)	3 (2%)	0	100	100
All	All	723/800 (90%)	710 (98%)	12 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	ASP

### 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	111/120 (92%)	108 (97%)	3 (3%)	52	52
1	B	111/120 (92%)	105 (95%)	6 (5%)	27	21
1	C	110/120 (92%)	106 (96%)	4 (4%)	42	39
1	D	111/120 (92%)	107 (96%)	4 (4%)	42	39
1	E	110/120 (92%)	106 (96%)	4 (4%)	42	39
All	All	553/600 (92%)	532 (96%)	21 (4%)	40	36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	72	ASN
1	A	114	ASN
1	B	14	ASP
1	B	18	VAL
1	B	72	ASN
1	B	103	ARG
1	B	123	GLU
1	B	131	LEU
1	C	18	VAL
1	C	50	ASP
1	C	114	ASN
1	C	160	SER
1	D	18	VAL
1	D	30	LYS
1	D	71	ARG
1	D	114	ASN
1	E	18	VAL
1	E	23	VAL
1	E	40	ARG
1	E	114	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	114	ASN
1	B	72	ASN
1	B	99	GLN
1	C	99	GLN
1	C	114	ASN
1	D	72	ASN
1	D	89	HIS
1	D	99	GLN
1	D	114	ASN
1	E	99	GLN
1	E	114	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 13 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ACY	A	1161	-	1,3,3	1.15	0	0,3,3	0.00	-
3	DTU	A	1162	-	7,7,7	6.31	7 (100%)	4,8,8	8.81	3 (75%)
4	T1P	A	1163	-	27,30,30	3.31	4 (14%)	29,44,44	2.94	13 (44%)
2	ACY	B	1161	-	1,3,3	1.55	0	0,3,3	0.00	-
3	DTU	B	1162	-	7,7,7	6.01	7 (100%)	4,8,8	7.35	3 (75%)
6	T2P	B	1163	-	27,30,30	3.05	3 (11%)	29,44,44	2.85	14 (48%)
7	DTV	C	1161	-	7,7,7	6.05	6 (85%)	4,8,8	8.66	3 (75%)
8	T5P	C	1162	-	27,30,30	2.93	3 (11%)	29,44,44	2.48	11 (37%)
2	ACY	C	632	-	1,3,3	1.08	0	0,3,3	0.00	-
2	ACY	D	1161	-	1,3,3	1.31	0	0,3,3	0.00	-
7	DTV	D	1162	-	7,7,7	6.21	6 (85%)	4,8,8	8.29	4 (100%)
9	T4P	D	1163	-	27,30,30	3.19	5 (18%)	29,44,44	3.36	12 (41%)
2	ACY	E	1161	-	1,3,3	0.31	0	0,3,3	0.00	-
7	DTV	E	1162	-	7,7,7	6.14	5 (71%)	4,8,8	6.94	4 (100%)
9	T4P	E	1163	-	27,30,30	3.32	5 (18%)	29,44,44	3.17	15 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	D1D	E	1166	-	6,8,8	0.92	1 (16%)	6,10,10	5.14	6 (100%)

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	ACY	A	1161	-	-	0/0/0/0	0/0/0/0
3	DTU	A	1162	-	-	0/8/8/8	0/0/0/0
4	T1P	A	1163	-	-	0/22/54/54	0/2/2/2
2	ACY	B	1161	-	-	0/0/0/0	0/0/0/0
3	DTU	B	1162	-	-	0/8/8/8	0/0/0/0
6	T2P	B	1163	-	-	0/22/54/54	0/2/2/2
7	DTV	C	1161	-	-	0/8/8/8	0/0/0/0
8	T5P	C	1162	-	-	0/22/54/54	0/2/2/2
2	ACY	C	632	-	-	0/0/0/0	0/0/0/0
2	ACY	D	1161	-	-	0/0/0/0	0/0/0/0
7	DTV	D	1162	-	-	0/8/8/8	0/0/0/0
9	T4P	D	1163	-	-	0/22/54/54	0/2/2/2
2	ACY	E	1161	-	-	0/0/0/0	0/0/0/0
7	DTV	E	1162	-	-	0/8/8/8	0/0/0/0
9	T4P	E	1163	-	-	0/22/54/54	0/2/2/2
10	D1D	E	1166	-	-	0/0/11/11	0/0/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1162	DTU	O3-C3	-14.84	1.10	1.43
7	D	1162	DTV	O3-C3	-14.66	1.10	1.43
7	E	1162	DTV	O3-C3	-14.50	1.10	1.43
3	B	1162	DTU	O3-C3	-14.39	1.11	1.43
7	C	1161	DTV	O3-C3	-14.34	1.11	1.43
4	A	1163	T1P	C9-N5	-11.72	1.31	1.46
9	E	1163	T4P	C9-N5	-11.70	1.31	1.46
4	A	1163	T1P	C8-N7	-11.16	1.32	1.45
6	B	1163	T2P	C8-N7	-11.12	1.32	1.45
9	E	1163	T4P	C8-N7	-11.04	1.32	1.45
9	D	1163	T4P	C8-N7	-10.87	1.32	1.45
9	D	1163	T4P	C9-N5	-10.80	1.32	1.46
8	C	1162	T5P	C8-N7	-10.31	1.33	1.45
6	B	1163	T2P	C9-N5	-10.02	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1162	T5P	C9-N5	-9.77	1.34	1.46
3	A	1162	DTU	C1-S1	-4.19	1.72	1.81
7	C	1161	DTV	C1-S1	-4.03	1.72	1.81
7	E	1162	DTV	C1-S1	-4.02	1.72	1.81
7	D	1162	DTV	C1-S1	-3.83	1.72	1.81
7	E	1162	DTV	C3-C2	-3.43	1.43	1.52
7	C	1161	DTV	C1-C2	-3.43	1.41	1.51
7	E	1162	DTV	C1-C2	-3.33	1.42	1.51
3	A	1162	DTU	C1-C2	-3.31	1.42	1.51
7	D	1162	DTV	C1-C2	-3.30	1.42	1.51
7	D	1162	DTV	C3-C2	-3.28	1.44	1.52
7	D	1162	DTV	O2-C2	-3.26	1.36	1.43
3	B	1162	DTU	C1-S1	-3.19	1.74	1.81
7	E	1162	DTV	O2-C2	-3.06	1.36	1.43
3	A	1162	DTU	C3-C2	-3.03	1.44	1.52
3	B	1162	DTU	C1-C2	-2.96	1.43	1.51
3	B	1162	DTU	O2-C2	-2.93	1.36	1.43
7	C	1161	DTV	C3-C2	-2.89	1.45	1.52
3	A	1162	DTU	O2-C2	-2.89	1.36	1.43
3	B	1162	DTU	C3-C2	-2.87	1.45	1.52
4	A	1163	T1P	C4-N3	-2.64	1.32	1.37
7	C	1161	DTV	O2-C2	-2.58	1.37	1.43
3	A	1162	DTU	C4-S4	-2.46	1.76	1.81
3	A	1162	DTU	C4-C3	-2.42	1.44	1.51
9	D	1163	T4P	C6-N7	-2.35	1.32	1.37
3	B	1162	DTU	C4-S4	-2.30	1.76	1.81
9	D	1163	T4P	C10-C11	-2.20	1.49	1.52
9	E	1163	T4P	C4-N3	-2.17	1.33	1.37
7	D	1162	DTV	C4-C3	-2.15	1.45	1.51
3	B	1162	DTU	C4-C3	-2.12	1.45	1.51
7	C	1161	DTV	C4-S4	-2.10	1.76	1.81
9	E	1163	T4P	C6-N7	-2.07	1.33	1.37
10	E	1166	D1D	C3-C2	2.18	1.55	1.52
9	E	1163	T4P	O6-C6	2.83	1.28	1.22
9	D	1163	T4P	O6-C6	2.88	1.28	1.22
4	A	1163	T1P	O6-C6	2.95	1.28	1.22
6	B	1163	T2P	O6-C6	3.41	1.29	1.22
8	C	1162	T5P	O6-C6	3.76	1.29	1.22

All (88) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1162	DTU	C3-C4-S4	-13.14	92.12	113.91
7	C	1161	DTV	C2-C1-S1	-12.71	92.84	113.91
7	D	1162	DTV	C2-C1-S1	-11.21	95.32	113.91
3	A	1162	DTU	C2-C1-S1	-11.20	95.34	113.91
7	D	1162	DTV	C3-C4-S4	-11.16	95.40	113.91
7	C	1161	DTV	C3-C4-S4	-10.88	95.87	113.91
7	E	1162	DTV	C2-C1-S1	-10.81	95.99	113.91
3	B	1162	DTU	C3-C4-S4	-10.78	96.04	113.91
3	B	1162	DTU	C2-C1-S1	-9.18	98.70	113.91
7	E	1162	DTV	C3-C4-S4	-7.75	101.06	113.91
9	D	1163	T4P	O6-C6-N7	-6.02	117.22	125.80
6	B	1163	T2P	C10-C11-C12	-5.10	95.24	109.82
10	E	1166	D1D	O2-C2-C1	-4.41	102.40	110.05
9	E	1163	T4P	C9-N5-C6	-4.38	103.30	111.88
9	D	1163	T4P	C9-N5-C6	-4.33	103.39	111.88
9	E	1163	T4P	O6-C6-N7	-4.20	119.82	125.80
4	A	1163	T1P	O6-C6-N7	-4.17	119.87	125.80
6	B	1163	T2P	C9-N5-C6	-4.16	103.74	111.88
4	A	1163	T1P	C9-N5-C6	-4.09	103.86	111.88
8	C	1162	T5P	O6-C6-N7	-3.98	120.13	125.80
10	E	1166	D1D	O3-C3-C4	-3.85	103.36	110.05
8	C	1162	T5P	C9-N5-C6	-3.63	104.77	111.88
4	A	1163	T1P	O21-C12-C11	-3.44	100.08	108.75
6	B	1163	T2P	O6-C6-N7	-3.25	121.17	125.80
9	D	1163	T4P	O27-P-O32	-2.91	99.73	107.14
6	B	1163	T2P	O6-C6-N5	-2.83	121.76	125.80
10	E	1166	D1D	O2-C2-C3	-2.77	104.06	110.27
8	C	1162	T5P	O2-C2-N1	-2.66	116.69	122.86
4	A	1163	T1P	O27-P-O32	-2.64	100.42	107.14
4	A	1163	T1P	O2-C2-N1	-2.61	116.78	122.86
7	D	1162	DTV	O2-C2-C3	-2.56	104.57	109.79
9	E	1163	T4P	O6-C6-N5	-2.55	122.17	125.80
9	E	1163	T4P	C15-C16-C17	-2.53	102.94	113.32
4	A	1163	T1P	O6-C6-N5	-2.48	122.26	125.80
9	D	1163	T4P	C15-C16-C17	-2.47	103.21	113.32
10	E	1166	D1D	O3-C3-C2	-2.39	104.91	110.27
9	E	1163	T4P	O31-P-O27	-2.38	99.70	106.56
4	A	1163	T1P	C15-C16-C17	-2.35	103.67	113.32
7	E	1162	DTV	O2-C2-C3	-2.35	104.99	109.79
9	D	1163	T4P	O2-C2-N1	-2.20	117.74	122.86
8	C	1162	T5P	O6-C6-N5	-2.13	122.77	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1163	T4P	C10-C11-C12	-2.10	103.82	109.82
6	B	1163	T2P	O2-C2-N1	-2.02	118.16	122.86
6	B	1163	T2P	C15-C16-C17	-2.00	105.10	113.32
9	E	1163	T4P	C16-C15-N5	2.08	116.50	113.52
4	A	1163	T1P	O31-P-O33	2.13	115.50	107.38
8	C	1162	T5P	O31-P-O33	2.14	115.51	107.38
4	A	1163	T1P	C9-C4-N3	2.14	118.89	116.31
9	E	1163	T4P	C9-C4-N3	2.22	118.99	116.31
6	B	1163	T2P	C16-C15-N5	2.27	116.78	113.52
6	B	1163	T2P	O19-C11-C10	2.28	115.84	110.45
8	C	1162	T5P	C9-C4-N3	2.30	119.09	116.31
9	D	1163	T4P	O31-P-O33	2.45	116.72	107.38
9	E	1163	T4P	O21-C12-C13	2.46	114.95	108.75
4	A	1163	T1P	O19-C11-C10	2.46	116.26	110.45
6	B	1163	T2P	C9-C4-N3	2.57	119.41	116.31
9	E	1163	T4P	O31-P-O33	2.71	117.69	107.38
8	C	1162	T5P	C16-C15-N5	2.86	117.61	113.52
6	B	1163	T2P	O21-C12-C13	2.96	116.21	108.75
6	B	1163	T2P	O19-C11-C12	3.08	116.77	109.02
7	E	1162	DTV	O3-C3-C2	3.17	116.27	109.79
8	C	1162	T5P	C10-N7-C6	3.22	129.01	122.19
9	D	1163	T4P	O21-C12-C13	3.31	117.08	108.75
3	B	1162	DTU	O3-C3-C2	3.51	116.95	109.79
3	A	1162	DTU	O3-C3-C2	3.52	116.98	109.79
8	C	1162	T5P	C10-N7-C8	3.54	129.58	124.10
9	E	1163	T4P	O23-C13-C12	4.07	119.25	109.02
7	C	1161	DTV	O3-C3-C2	4.22	118.42	109.79
9	D	1163	T4P	O23-C13-C12	4.27	119.75	109.02
7	D	1162	DTV	O3-C3-C2	4.28	118.53	109.79
9	D	1163	T4P	O19-C11-C12	4.77	121.01	109.02
8	C	1162	T5P	N3-C2-N1	5.22	121.85	116.14
9	E	1163	T4P	O19-C11-C12	5.23	122.16	109.02
6	B	1163	T2P	C10-N7-C8	5.28	132.27	124.10
9	E	1163	T4P	N3-C2-N1	5.60	122.27	116.14
9	D	1163	T4P	N3-C2-N1	5.75	122.44	116.14
4	A	1163	T1P	N3-C2-N1	5.77	122.46	116.14
6	B	1163	T2P	N3-C2-N1	5.89	122.59	116.14
10	E	1166	D1D	C1-C2-C3	6.97	126.93	112.51
4	A	1163	T1P	C10-N7-C8	7.05	135.01	124.10
6	B	1163	T2P	N7-C6-N5	7.16	117.00	108.36
8	C	1162	T5P	N7-C6-N5	7.21	117.07	108.36
9	E	1163	T4P	C10-N7-C8	7.56	135.79	124.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1163	T1P	N7-C6-N5	7.86	117.85	108.36
10	E	1166	D1D	C4-C3-C2	7.91	128.86	112.51
9	D	1163	T4P	N7-C6-N5	7.93	117.93	108.36
9	E	1163	T4P	N7-C6-N5	7.99	118.00	108.36
9	D	1163	T4P	C10-N7-C8	8.57	137.36	124.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1161	ACY	1	0
3	B	1162	DTU	4	0
6	B	1163	T2P	1	0
7	C	1161	DTV	3	0
8	C	1162	T5P	1	0
9	D	1163	T4P	1	0
9	E	1163	T4P	2	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	147/160 (91%)	-0.27	3 (2%) 68 69	6, 12, 21, 37	0
1	B	147/160 (91%)	-0.21	5 (3%) 49 50	9, 12, 21, 31	0
1	C	146/160 (91%)	-0.01	5 (3%) 49 50	8, 13, 20, 26	0
1	D	147/160 (91%)	-0.12	8 (5%) 29 31	7, 12, 20, 33	0
1	E	146/160 (91%)	-0.24	4 (2%) 58 58	8, 12, 21, 29	0
All	All	733/800 (91%)	-0.17	25 (3%) 49 50	6, 12, 21, 37	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	SER	7.3
1	A	14	ASP	6.8
1	D	160	SER	4.8
1	D	14	ASP	3.9
1	A	160	SER	3.9
1	C	49	ASP	3.4
1	E	159	HIS	3.4
1	A	159	HIS	3.3
1	E	160	SER	3.1
1	E	16	SER	3.0
1	D	159	HIS	3.0
1	C	132	PRO	3.0
1	B	160	SER	2.9
1	C	48	LEU	2.8
1	B	16	SER	2.6
1	D	16	SER	2.5
1	D	133	THR	2.3
1	E	132	PRO	2.3
1	B	14	ASP	2.2
1	B	159	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	117	LEU	2.1
1	D	117	LEU	2.1
1	D	155	GLU	2.1
1	D	50	ASP	2.1
1	C	50	ASP	2.1

## 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. 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
2	ACY	E	1161	4/4	0.51	0.35	20.77	24,24,24,24	0
10	D1D	E	1166	8/8	0.62	0.23	18.46	27,27,28,29	0
7	DTV	E	1162	8/8	0.83	0.41	15.69	20,23,26,28	0
7	DTV	C	1161	8/8	0.81	0.47	15.40	27,30,31,32	0
2	ACY	D	1161	4/4	0.76	0.30	10.07	25,25,25,25	0
2	ACY	C	632	4/4	0.69	0.21	5.79	27,28,28,28	0
3	DTU	B	1162	8/8	0.65	0.44	5.44	17,22,25,25	0
7	DTV	D	1162	8/8	0.80	0.43	2.89	19,21,23,24	0
3	DTU	A	1162	8/8	0.77	0.43	1.78	19,21,22,22	0
6	T2P	B	1163	29/29	0.92	0.18	1.78	9,14,17,20	0
8	T5P	C	1162	29/29	0.95	0.15	1.15	9,13,15,15	0
9	T4P	D	1163	29/29	0.95	0.15	1.15	9,12,15,18	0
4	T1P	A	1163	29/29	0.95	0.13	0.84	10,14,15,15	0
9	T4P	E	1163	29/29	0.95	0.13	0.67	9,13,15,17	0
5	K	D	1164	1/1	1.00	0.04	-1.70	17,17,17,17	0
5	K	C	1165	1/1	0.98	0.04	-1.81	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K	B	1166	1/1	0.99	0.04	-2.22	29,29,29,29	0
5	K	C	1164	1/1	0.97	0.06	-2.41	39,39,39,39	0
5	K	E	1165	1/1	0.99	0.03	-2.53	27,27,27,27	0
5	K	B	1164	1/1	1.00	0.02	-2.62	19,19,19,19	0
5	K	E	1164	1/1	1.00	0.03	-2.79	14,14,14,14	0
5	K	B	1165	1/1	1.00	0.04	-2.96	23,23,23,23	0
5	K	D	1165	1/1	0.99	0.04	-3.06	29,29,29,29	0
5	K	A	1165	1/1	0.99	0.04	-3.19	21,21,21,21	0
5	K	A	1164	1/1	1.00	0.02	-3.88	16,16,16,16	0
5	K	C	1163	1/1	1.00	0.02	-3.88	19,19,19,19	0
2	ACY	A	1161	4/4	0.77	0.25	-	30,30,30,30	0
5	K	A	1166	1/1	0.99	0.04	-	25,25,25,25	1
2	ACY	B	1161	4/4	0.71	0.33	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.