



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2016 – 05:22 PM EST

PDB ID : 4TSZ
Title : Crystal structure of DNA polymerase sliding clamp from *Pseudomonas aeruginosa* with ligand
Authors : Olieric, V.; Burnouf, D.; Ennifar, E.; Wolff, P.
Deposited on : 2014-06-19
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

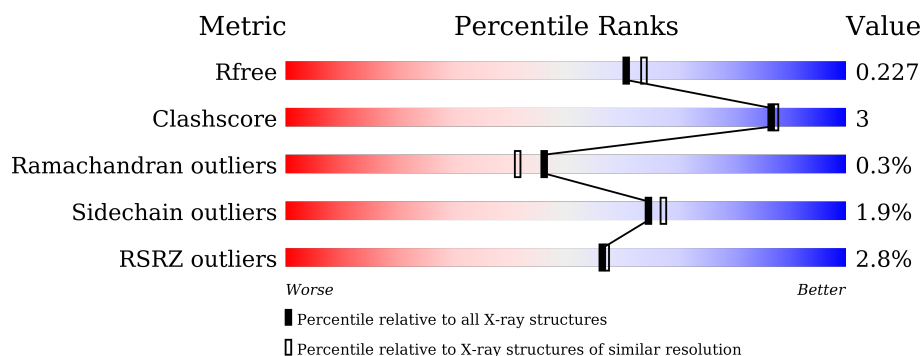
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 ≥ 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	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 9% . </div> </div>
1	B	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 90%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 90% 8% . </div> </div>
1	C	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 90%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 90% 8% .. </div> </div>
1	D	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 89% 9% .. </div> </div>
1	E	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 90%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 90% 8% .. </div> </div>
1	F	368	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 91%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 91% 8% .. </div> </div>


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Mol	Chain	Length	Quality of chain
1	G	368	
1	H	368	
1	I	368	
1	J	368	
1	K	368	
1	L	368	
1	M	368	
1	N	368	
1	O	368	
1	P	368	
2	0	6	
2	1	6	
2	2	6	
2	3	6	
2	4	6	
2	5	6	
2	6	6	
2	Q	6	
2	R	6	
2	S	6	
2	T	6	
2	U	6	
2	V	6	
2	X	6	
2	Y	6	

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Mol	Chain	Length	Quality of chain
2	Z	6	 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47278 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 III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	3	0
			2770	1740	487	534	9			
1	B	363	Total	C	N	O	S	0	2	0
			2743	1726	484	524	9			
1	C	363	Total	C	N	O	S	0	1	0
			2737	1722	482	524	9			
1	D	363	Total	C	N	O	S	0	2	0
			2734	1721	484	520	9			
1	E	363	Total	C	N	O	S	0	2	0
			2741	1724	481	527	9			
1	F	366	Total	C	N	O	S	0	2	0
			2752	1732	485	526	9			
1	G	366	Total	C	N	O	S	0	2	0
			2766	1740	486	531	9			
1	H	366	Total	C	N	O	S	0	2	0
			2758	1736	487	526	9			
1	I	366	Total	C	N	O	S	0	2	0
			2770	1742	486	533	9			
1	J	366	Total	C	N	O	S	0	2	0
			2748	1730	485	524	9			
1	K	363	Total	C	N	O	S	0	1	0
			2742	1725	482	526	9			
1	L	363	Total	C	N	O	S	0	3	0
			2759	1735	488	527	9			
1	M	363	Total	C	N	O	S	0	1	0
			2732	1719	480	524	9			
1	N	366	Total	C	N	O	S	0	2	0
			2748	1730	485	524	9			
1	O	363	Total	C	N	O	S	0	2	0
			2741	1724	481	527	9			
1	P	363	Total	C	N	O	S	0	2	0
			2729	1718	482	520	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP V4MZL6
B	0	HIS	-	expression tag	UNP V4MZL6
C	0	HIS	-	expression tag	UNP V4MZL6
D	0	HIS	-	expression tag	UNP V4MZL6
E	0	HIS	-	expression tag	UNP V4MZL6
F	0	HIS	-	expression tag	UNP V4MZL6
G	0	HIS	-	expression tag	UNP V4MZL6
H	0	HIS	-	expression tag	UNP V4MZL6
I	0	HIS	-	expression tag	UNP V4MZL6
J	0	HIS	-	expression tag	UNP V4MZL6
K	0	HIS	-	expression tag	UNP V4MZL6
L	0	HIS	-	expression tag	UNP V4MZL6
M	0	HIS	-	expression tag	UNP V4MZL6
N	0	HIS	-	expression tag	UNP V4MZL6
O	0	HIS	-	expression tag	UNP V4MZL6
P	0	HIS	-	expression tag	UNP V4MZL6

- Molecule 2 is a protein called ACE-GLN-ALC-ASP-LEU-ZCL peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	R	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	S	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	T	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	U	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	V	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	X	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	Y	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	Z	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	0	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	1	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	3	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	4	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	5	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			
2	6	6	Total	C	Cl	N	O	0	0	0
			53	35	2	6	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	1
			199	199		
3	Q	5	Total	O	0	0
			5	5		
3	B	205	Total	O	0	0
			205	205		
3	R	7	Total	O	0	0
			7	7		
3	C	111	Total	O	0	0
			111	111		
3	S	4	Total	O	0	0
			4	4		
3	D	77	Total	O	0	0
			77	77		
3	T	2	Total	O	0	0
			2	2		
3	E	121	Total	O	0	0
			121	121		
3	U	4	Total	O	0	0
			4	4		
3	F	62	Total	O	0	0
			62	62		
3	V	1	Total	O	0	0
			1	1		
3	G	240	Total	O	0	0
			240	240		
3	X	10	Total	O	0	0
			10	10		

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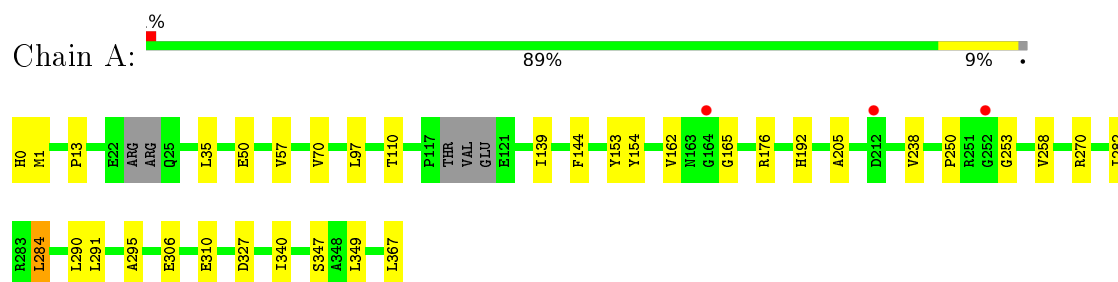
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	201	Total 201	O 201	0	0
3	Y	4	Total 4	O 4	0	0
3	I	211	Total 211	O 211	0	0
3	Z	12	Total 12	O 12	0	0
3	J	202	Total 202	O 202	0	0
3	0	6	Total 6	O 6	0	0
3	K	188	Total 188	O 188	0	0
3	1	4	Total 4	O 4	0	0
3	L	193	Total 194	O 194	0	1
3	2	5	Total 5	O 5	0	0
3	M	124	Total 124	O 124	0	0
3	3	2	Total 2	O 2	0	0
3	N	68	Total 68	O 68	0	0
3	4	3	Total 3	O 3	0	0
3	O	108	Total 108	O 108	0	0
3	5	4	Total 4	O 4	0	0
3	P	73	Total 73	O 73	0	0
3	6	3	Total 3	O 3	0	0

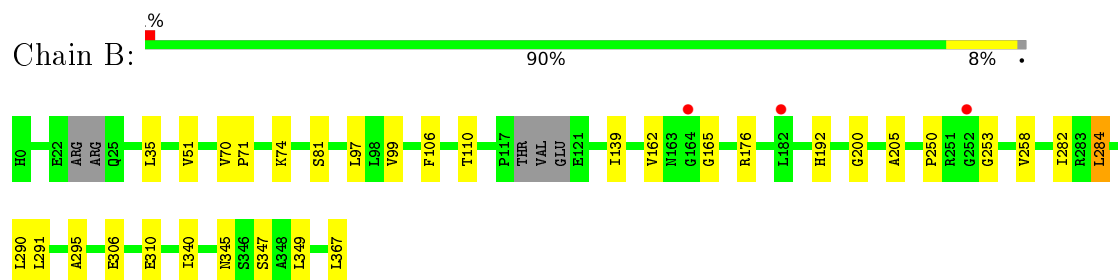
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

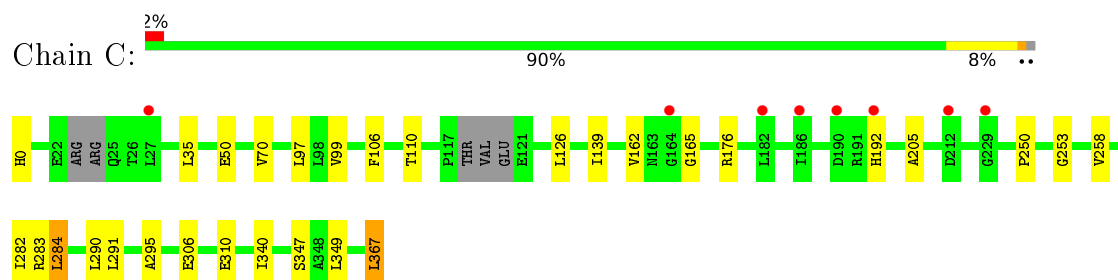
- Molecule 1: DNA polymerase III subunit beta



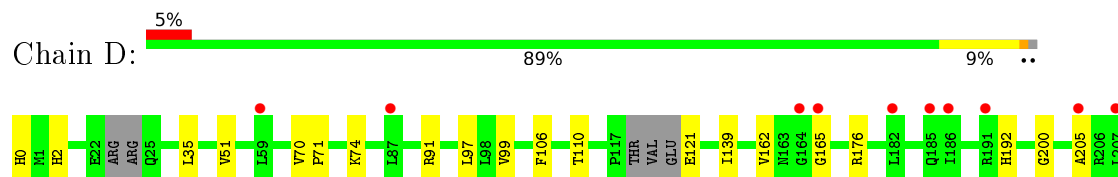
- Molecule 1: DNA polymerase III subunit beta

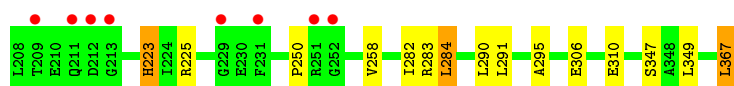


- Molecule 1: DNA polymerase III subunit beta

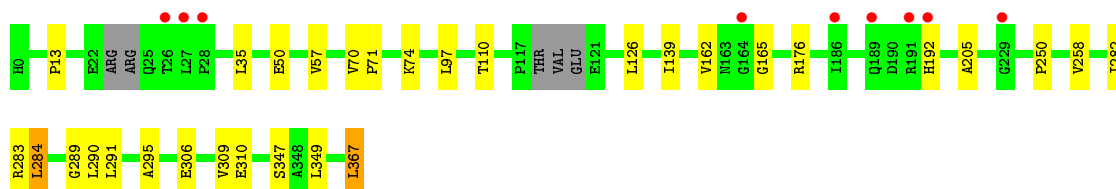
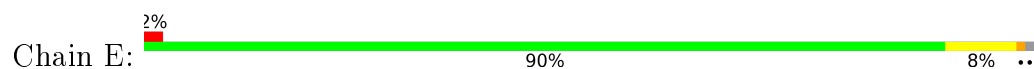


- Molecule 1: DNA polymerase III subunit beta

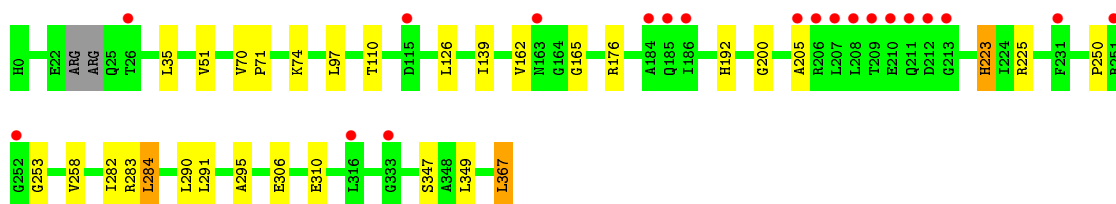
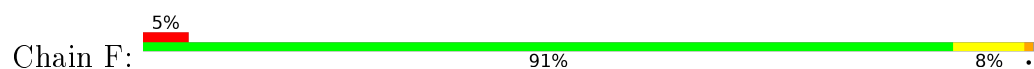




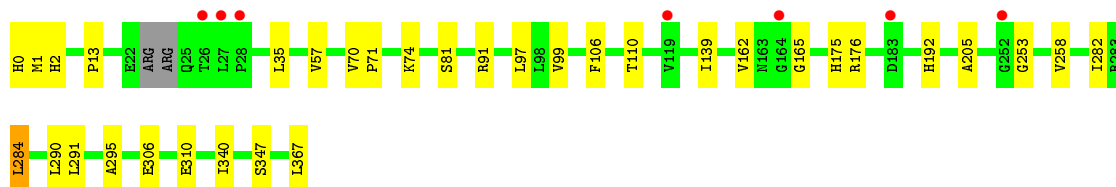
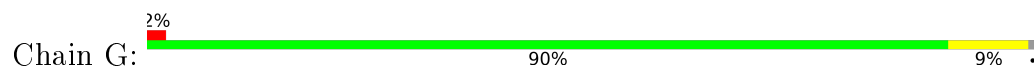
- Molecule 1: DNA polymerase III subunit beta



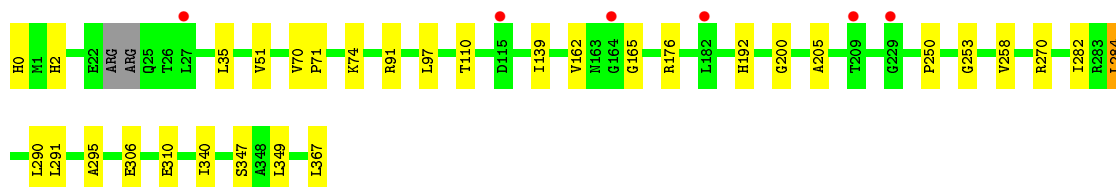
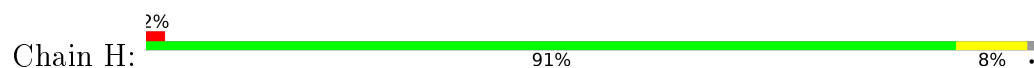
- Molecule 1: DNA polymerase III subunit beta



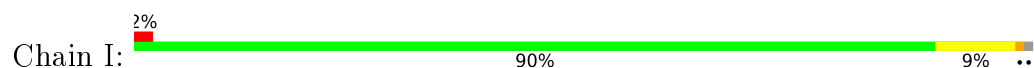
- Molecule 1: DNA polymerase III subunit beta

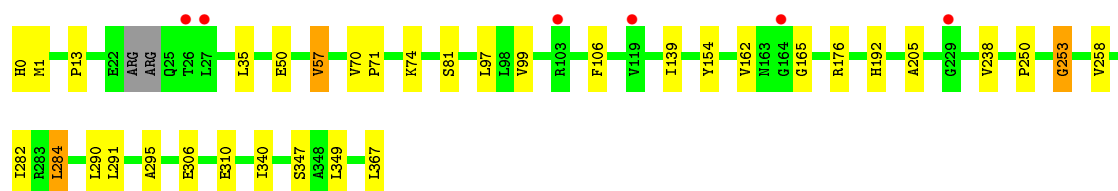


- Molecule 1: DNA polymerase III subunit beta

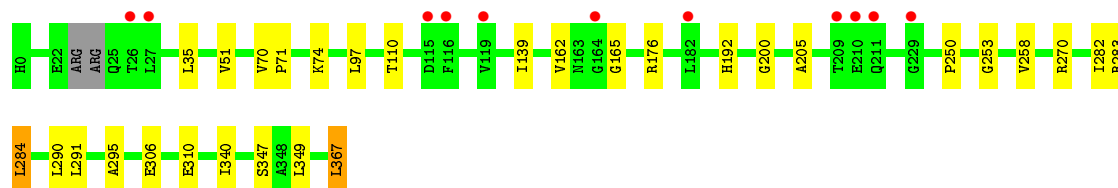


- Molecule 1: DNA polymerase III subunit beta

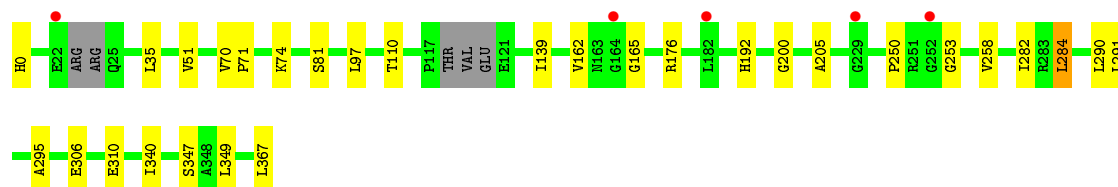




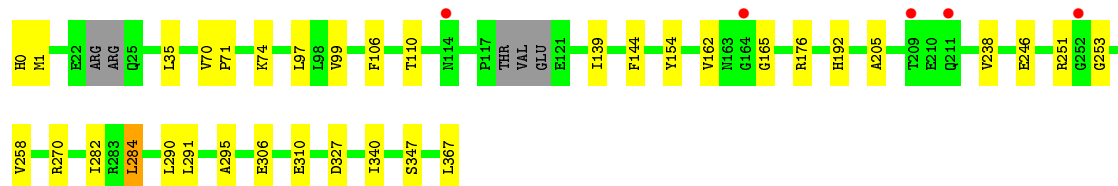
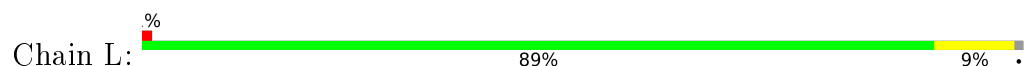
- Molecule 1: DNA polymerase III subunit beta



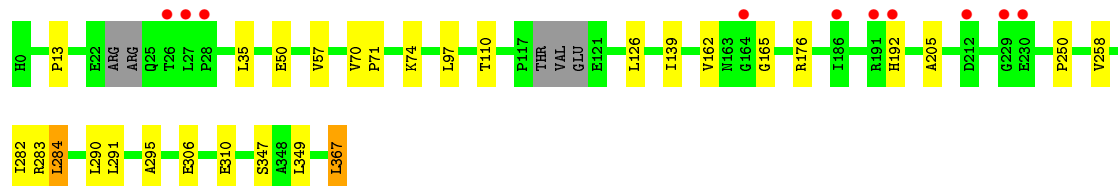
- Molecule 1: DNA polymerase III subunit beta



- Molecule 1: DNA polymerase III subunit beta

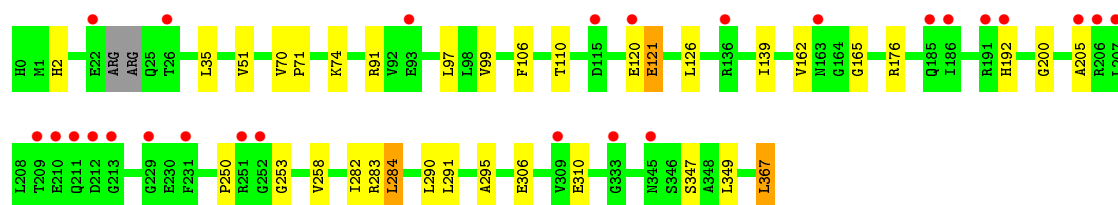


- Molecule 1: DNA polymerase III subunit beta

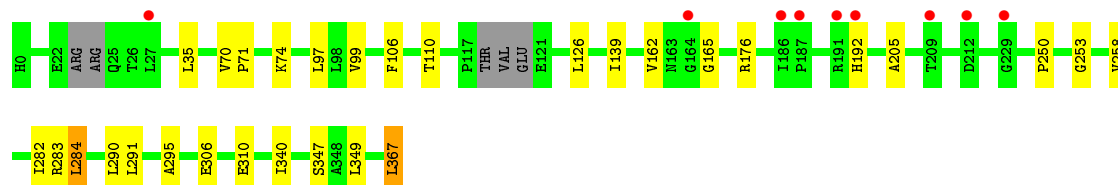
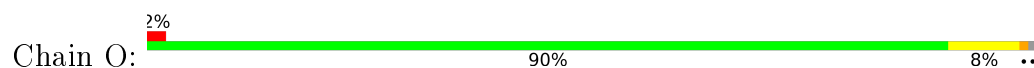


- Molecule 1: DNA polymerase III subunit beta

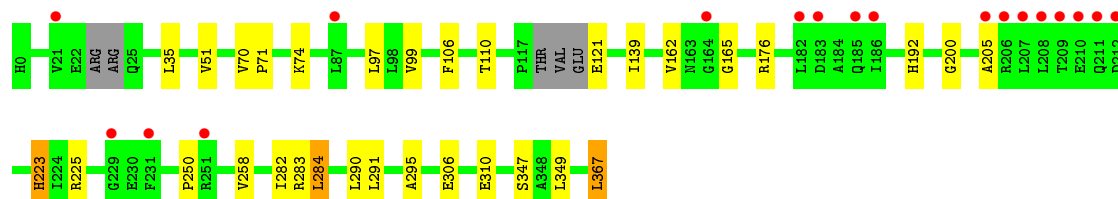
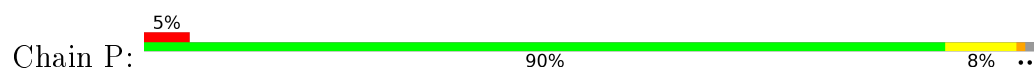




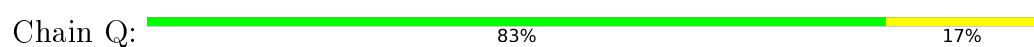
- Molecule 1: DNA polymerase III subunit beta



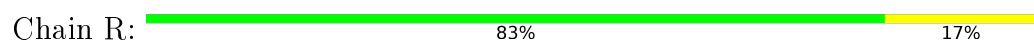
- Molecule 1: DNA polymerase III subunit beta



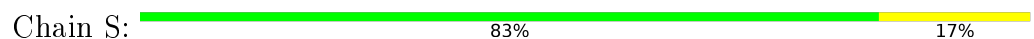
- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain T:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain U:  67% 33%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain V:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain X:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain Y:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain Z:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 0:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 1:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 2:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 3:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 4:  83% 17%




- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 5:  83% 17%



- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

Chain 6:  83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.98Å 85.95Å 272.20Å 90.01° 89.94° 116.56°	Depositor
Resolution (Å)	29.28 – 2.00 49.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.28-2.00) 96.1 (49.33-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.202 , 0.222 0.216 , 0.227	Depositor DCC
R_{free} test set	21178 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l 0.467 for -h,-k,l 0.016 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	47278	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3077e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: ZCL, ALC, ACE

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	0.45	0/2809	0.67	0/3809
1	B	0.46	0/2785	0.66	0/3779
1	C	0.42	0/2776	0.67	0/3766
1	D	0.41	0/2776	0.66	0/3767
1	E	0.42	0/2779	0.66	0/3770
1	F	0.40	0/2794	0.66	0/3794
1	G	0.48	0/2806	0.68	0/3810
1	H	0.46	0/2801	0.66	0/3804
1	I	0.48	0/2810	0.69	0/3815
1	J	0.46	0/2790	0.66	0/3789
1	K	0.46	0/2781	0.67	0/3773
1	L	0.45	0/2801	0.66	0/3799
1	M	0.42	0/2770	0.66	0/3758
1	N	0.40	0/2790	0.66	0/3789
1	O	0.42	0/2779	0.67	0/3770
1	P	0.41	0/2770	0.67	0/3759
2	0	0.37	0/24	0.54	0/30
2	1	0.35	0/24	0.51	0/30
2	2	0.38	0/24	0.55	0/30
2	3	0.41	0/24	0.62	0/30
2	4	0.35	0/24	0.54	0/30
2	5	0.39	0/24	0.56	0/30
2	6	0.26	0/24	0.53	0/30
2	Q	0.38	0/24	0.56	0/30
2	R	0.37	0/24	0.55	0/30
2	S	0.39	0/24	0.56	0/30
2	T	0.30	0/24	0.52	0/30
2	U	0.36	0/24	0.60	0/30
2	V	0.34	0/24	0.54	0/30
2	X	0.46	0/24	0.58	0/30
2	Y	0.34	0/24	0.53	0/30
2	Z	0.45	0/24	0.58	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.44	0/45001	0.66	0/61031

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	0	0	1
2	1	0	1
2	2	0	1
2	3	0	1
2	4	0	1
2	5	0	1
2	6	0	1
2	Q	0	1
2	R	0	1
2	S	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	X	0	1
2	Y	0	1
2	Z	0	1
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Q	471	LEU	Mainchain
2	R	471	LEU	Mainchain
2	S	471	LEU	Mainchain
2	T	471	LEU	Mainchain
2	U	471	LEU	Mainchain

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	2770	0	2747	18	0
1	B	2743	0	2722	15	0
1	C	2737	0	2717	14	0
1	D	2734	0	2713	17	0
1	E	2741	0	2717	15	0
1	F	2752	0	2731	15	0
1	G	2766	0	2742	17	0
1	H	2758	0	2737	15	0
1	I	2770	0	2746	18	0
1	J	2748	0	2727	15	0
1	K	2742	0	2722	13	0
1	L	2759	0	2743	17	0
1	M	2732	0	2712	13	0
1	N	2748	0	2727	16	0
1	O	2741	0	2717	14	0
1	P	2729	0	2708	16	0
2	0	53	0	46	0	0
2	1	53	0	46	0	0
2	2	53	0	46	0	0
2	3	53	0	46	0	0
2	4	53	0	46	0	0
2	5	53	0	46	0	0
2	6	53	0	46	0	0
2	Q	53	0	46	0	0
2	R	53	0	46	0	0
2	S	53	0	46	0	0
2	T	53	0	46	0	0
2	U	53	0	46	2	0
2	V	53	0	46	0	0
2	X	53	0	46	0	0
2	Y	53	0	46	0	0
2	Z	53	0	46	0	0
3	0	6	0	0	0	0
3	1	4	0	0	0	0
3	2	5	0	0	0	0
3	3	2	0	0	0	0
3	4	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5	4	0	0	0	0
3	6	3	0	0	0	0
3	A	199	0	0	1	0
3	B	205	0	0	1	0
3	C	111	0	0	1	0
3	D	77	0	0	0	0
3	E	121	0	0	1	0
3	F	62	0	0	0	0
3	G	240	0	0	0	0
3	H	201	0	0	0	0
3	I	211	0	0	1	0
3	J	202	0	0	0	0
3	K	188	0	0	0	0
3	L	194	0	0	0	0
3	M	124	0	0	0	0
3	N	68	0	0	0	0
3	O	108	0	0	0	0
3	P	73	0	0	0	0
3	Q	5	0	0	0	0
3	R	7	0	0	0	0
3	S	4	0	0	0	0
3	T	2	0	0	0	0
3	U	4	0	0	0	0
3	V	1	0	0	0	0
3	X	10	0	0	1	0
3	Y	4	0	0	0	0
3	Z	12	0	0	0	0
All	All	47278	0	44364	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 242 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:L:0:HIS:CD2	1:L:1:MET:H	1.96	0.83
1:I:0:HIS:CD2	1:I:1:MET:H	1.98	0.82
1:A:0:HIS:CD2	1:A:1:MET:H	2.00	0.79
1:I:50[A]:GLU:HG2	3:I:586:HOH:O	1.85	0.76
1:G:0:HIS:CD2	1:G:1:MET:H	2.04	0.75

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	360/368 (98%)	350 (97%)	9 (2%)	1 (0%)	46	41
1	B	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	46	41
1	C	358/368 (97%)	348 (97%)	9 (2%)	1 (0%)	46	41
1	D	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	46	41
1	E	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	46	41
1	F	364/368 (99%)	355 (98%)	7 (2%)	2 (0%)	34	26
1	G	364/368 (99%)	355 (98%)	8 (2%)	1 (0%)	46	41
1	H	364/368 (99%)	352 (97%)	11 (3%)	1 (0%)	46	41
1	I	364/368 (99%)	353 (97%)	9 (2%)	2 (0%)	34	26
1	J	364/368 (99%)	353 (97%)	10 (3%)	1 (0%)	46	41
1	K	358/368 (97%)	348 (97%)	9 (2%)	1 (0%)	46	41
1	L	360/368 (98%)	349 (97%)	10 (3%)	1 (0%)	46	41
1	M	358/368 (97%)	349 (98%)	8 (2%)	1 (0%)	46	41
1	N	364/368 (99%)	353 (97%)	8 (2%)	3 (1%)	24	15
1	O	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	46	41
1	P	359/368 (98%)	350 (98%)	8 (2%)	1 (0%)	46	41
2	0	3/6 (50%)	3 (100%)	0	0	100	100
2	1	3/6 (50%)	3 (100%)	0	0	100	100
2	2	3/6 (50%)	3 (100%)	0	0	100	100
2	3	3/6 (50%)	3 (100%)	0	0	100	100
2	4	3/6 (50%)	3 (100%)	0	0	100	100
2	5	3/6 (50%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	3/6 (50%)	3 (100%)	0	0	100	100
2	Q	3/6 (50%)	3 (100%)	0	0	100	100
2	R	3/6 (50%)	3 (100%)	0	0	100	100
2	S	3/6 (50%)	3 (100%)	0	0	100	100
2	T	3/6 (50%)	3 (100%)	0	0	100	100
2	U	3/6 (50%)	3 (100%)	0	0	100	100
2	V	3/6 (50%)	3 (100%)	0	0	100	100
2	X	3/6 (50%)	3 (100%)	0	0	100	100
2	Y	3/6 (50%)	3 (100%)	0	0	100	100
2	Z	3/6 (50%)	3 (100%)	0	0	100	100
All	All	5821/5984 (97%)	5659 (97%)	142 (2%)	20 (0%)	46	41

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	121	GLU
1	I	253	GLY
1	K	165	GLY
1	A	165	GLY
1	B	165	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/318 (93%)	289 (98%)	6 (2%)	63	65
1	B	290/318 (91%)	284 (98%)	6 (2%)	61	63
1	C	290/318 (91%)	283 (98%)	7 (2%)	57	58
1	D	288/318 (91%)	280 (97%)	8 (3%)	51	50
1	E	290/318 (91%)	284 (98%)	6 (2%)	61	63
1	F	290/318 (91%)	283 (98%)	7 (2%)	57	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	293/318 (92%)	287 (98%)	6 (2%)	63	65
1	H	291/318 (92%)	284 (98%)	7 (2%)	57	58
1	I	294/318 (92%)	287 (98%)	7 (2%)	57	58
1	J	289/318 (91%)	283 (98%)	6 (2%)	61	63
1	K	291/318 (92%)	284 (98%)	7 (2%)	57	58
1	L	293/318 (92%)	287 (98%)	6 (2%)	63	65
1	M	289/318 (91%)	282 (98%)	7 (2%)	57	58
1	N	289/318 (91%)	283 (98%)	6 (2%)	61	63
1	O	290/318 (91%)	284 (98%)	6 (2%)	61	63
1	P	287/318 (90%)	280 (98%)	7 (2%)	57	58
2	0	3/3 (100%)	3 (100%)	0	100	100
2	1	3/3 (100%)	3 (100%)	0	100	100
2	2	3/3 (100%)	3 (100%)	0	100	100
2	3	3/3 (100%)	3 (100%)	0	100	100
2	4	3/3 (100%)	3 (100%)	0	100	100
2	5	3/3 (100%)	3 (100%)	0	100	100
2	6	3/3 (100%)	3 (100%)	0	100	100
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
2	S	3/3 (100%)	3 (100%)	0	100	100
2	T	3/3 (100%)	3 (100%)	0	100	100
2	U	3/3 (100%)	3 (100%)	0	100	100
2	V	3/3 (100%)	3 (100%)	0	100	100
2	X	3/3 (100%)	3 (100%)	0	100	100
2	Y	3/3 (100%)	3 (100%)	0	100	100
2	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	4697/5136 (92%)	4592 (98%)	105 (2%)	65	62

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	LEU
1	I	347[B]	SER

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Mol	Chain	Res	Type
1	O	367	LEU
1	H	176	ARG
1	I	35	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	GLN
1	I	262	GLN
1	O	285	GLN
1	H	127	ASN
1	I	0	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 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	$\# Z > 2$
2	ALC	0	469	2	9,11,12	0.53	0	11,13,15	0.97	1 (9%)
2	ZCL	0	472	2	11,14,14	0.20	0	14,19,19	0.24	0
2	ALC	1	469	2	9,11,12	0.49	0	11,13,15	1.00	2 (18%)
2	ZCL	1	472	2	11,14,14	0.23	0	14,19,19	0.24	0
2	ALC	2	469	2	9,11,12	0.49	0	11,13,15	1.03	2 (18%)
2	ZCL	2	472	2	11,14,14	0.20	0	14,19,19	0.26	0
2	ALC	3	469	2	9,11,12	0.44	0	11,13,15	1.01	2 (18%)
2	ZCL	3	472	2	11,14,14	0.22	0	14,19,19	0.19	0
2	ALC	4	469	2	9,11,12	0.44	0	11,13,15	1.00	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZCL	4	472	2	11,14,14	0.19	0	14,19,19	0.20	0
2	ALC	5	469	2	9,11,12	0.43	0	11,13,15	0.96	2 (18%)
2	ZCL	5	472	2	11,14,14	0.21	0	14,19,19	0.21	0
2	ALC	6	469	2	9,11,12	0.45	0	11,13,15	0.95	2 (18%)
2	ZCL	6	472	2	11,14,14	0.20	0	14,19,19	0.20	0
2	ALC	Q	469	2	9,11,12	0.46	0	11,13,15	1.03	2 (18%)
2	ZCL	Q	472	2	11,14,14	0.20	0	14,19,19	0.25	0
2	ALC	R	469	2	9,11,12	0.54	0	11,13,15	1.05	2 (18%)
2	ZCL	R	472	2	11,14,14	0.23	0	14,19,19	0.24	0
2	ALC	S	469	2	9,11,12	0.43	0	11,13,15	0.99	2 (18%)
2	ZCL	S	472	2	11,14,14	0.21	0	14,19,19	0.22	0
2	ALC	T	469	2	9,11,12	0.46	0	11,13,15	0.96	2 (18%)
2	ZCL	T	472	2	11,14,14	0.19	0	14,19,19	0.19	0
2	ALC	U	469	2	9,11,12	0.40	0	11,13,15	1.05	2 (18%)
2	ZCL	U	472	2	11,14,14	0.22	0	14,19,19	0.22	0
2	ALC	V	469	2	9,11,12	0.43	0	11,13,15	1.00	2 (18%)
2	ZCL	V	472	2	11,14,14	0.17	0	14,19,19	0.20	0
2	ALC	X	469	2	9,11,12	0.47	0	11,13,15	1.02	1 (9%)
2	ZCL	X	472	2	11,14,14	0.27	0	14,19,19	0.20	0
2	ALC	Y	469	2	9,11,12	0.54	0	11,13,15	1.02	1 (9%)
2	ZCL	Y	472	2	11,14,14	0.20	0	14,19,19	0.20	0
2	ALC	Z	469	2	9,11,12	0.50	0	11,13,15	0.98	1 (9%)
2	ZCL	Z	472	2	11,14,14	0.23	0	14,19,19	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALC	0	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	0	472	2	-	0/4/8/8	0/1/1/1
2	ALC	1	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	1	472	2	-	0/4/8/8	0/1/1/1
2	ALC	2	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	2	472	2	-	0/4/8/8	0/1/1/1
2	ALC	3	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	3	472	2	-	0/4/8/8	0/1/1/1
2	ALC	4	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	4	472	2	-	0/4/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALC	5	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	5	472	2	-	0/4/8/8	0/1/1/1
2	ALC	6	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	6	472	2	-	0/4/8/8	0/1/1/1
2	ALC	Q	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	Q	472	2	-	0/4/8/8	0/1/1/1
2	ALC	R	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	R	472	2	-	0/4/8/8	0/1/1/1
2	ALC	S	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	S	472	2	-	0/4/8/8	0/1/1/1
2	ALC	T	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	T	472	2	-	0/4/8/8	0/1/1/1
2	ALC	U	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	U	472	2	-	0/4/8/8	0/1/1/1
2	ALC	V	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	V	472	2	-	0/4/8/8	0/1/1/1
2	ALC	X	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	X	472	2	-	0/4/8/8	0/1/1/1
2	ALC	Y	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	Y	472	2	-	0/4/8/8	0/1/1/1
2	ALC	Z	469	2	-	0/4/14/16	0/1/1/1
2	ZCL	Z	472	2	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	469	ALC	O-C-CA	-2.20	119.83	125.72
2	5	469	ALC	O-C-CA	-2.14	119.98	125.72
2	U	469	ALC	O-C-CA	-2.14	119.99	125.72
2	T	469	ALC	O-C-CA	-2.13	120.00	125.72
2	V	469	ALC	O-C-CA	-2.10	120.09	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	363/368 (98%)	-0.23	3 (0%) 87 88	25, 39, 66, 96	0
1	B	363/368 (98%)	-0.19	3 (0%) 87 88	22, 41, 64, 96	0
1	C	363/368 (98%)	-0.04	8 (2%) 65 66	33, 53, 81, 116	0
1	D	363/368 (98%)	0.15	18 (4%) 32 34	35, 58, 85, 105	0
1	E	363/368 (98%)	-0.13	9 (2%) 61 61	30, 49, 74, 101	0
1	F	366/368 (99%)	0.23	20 (5%) 29 30	42, 58, 87, 108	0
1	G	366/368 (99%)	-0.20	7 (1%) 70 70	20, 36, 60, 89	0
1	H	366/368 (99%)	-0.20	6 (1%) 74 75	25, 38, 61, 90	0
1	I	366/368 (99%)	-0.21	6 (1%) 74 75	21, 35, 62, 92	0
1	J	366/368 (99%)	-0.18	11 (3%) 54 55	26, 38, 62, 97	0
1	K	363/368 (98%)	-0.21	5 (1%) 78 78	22, 41, 64, 97	0
1	L	363/368 (98%)	-0.22	5 (1%) 78 78	24, 39, 66, 95	0
1	M	363/368 (98%)	-0.13	10 (2%) 56 57	32, 49, 76, 105	0
1	N	366/368 (99%)	0.27	26 (7%) 19 20	42, 59, 88, 108	0
1	O	363/368 (98%)	-0.02	9 (2%) 61 61	33, 54, 80, 115	0
1	P	363/368 (98%)	0.16	18 (4%) 32 34	36, 59, 85, 103	0
2	0	3/6 (50%)	-0.61	0 100 100	39, 39, 43, 50	0
2	1	3/6 (50%)	-0.32	0 100 100	38, 38, 41, 47	0
2	2	3/6 (50%)	-0.55	0 100 100	34, 34, 39, 48	0
2	3	3/6 (50%)	-0.41	0 100 100	43, 43, 44, 55	0
2	4	3/6 (50%)	-0.08	0 100 100	53, 53, 69, 70	0
2	5	3/6 (50%)	-0.27	0 100 100	46, 46, 59, 62	0
2	6	3/6 (50%)	-0.46	0 100 100	46, 46, 58, 60	0
2	Q	3/6 (50%)	-0.51	0 100 100	34, 34, 38, 47	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	R	3/6 (50%)	-0.32	0	100	100	37, 37, 42, 46	0
2	S	3/6 (50%)	-0.21	0	100	100	44, 44, 57, 59	0
2	T	3/6 (50%)	-0.34	0	100	100	44, 44, 60, 65	0
2	U	3/6 (50%)	-0.13	0	100	100	43, 43, 45, 52	0
2	V	3/6 (50%)	0.29	0	100	100	55, 55, 64, 70	0
2	X	3/6 (50%)	-0.42	0	100	100	30, 30, 30, 43	0
2	Y	3/6 (50%)	-0.56	0	100	100	39, 39, 42, 48	0
2	Z	3/6 (50%)	-0.33	0	100	100	31, 31, 33, 43	0
All	All	5874/5984 (98%)	-0.07	164 (2%)	56	57	20, 47, 78, 116	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	212	ASP	8.2
1	D	212	ASP	8.0
1	O	186	ILE	7.9
1	F	211	GLN	6.9
1	N	120	GLU	6.4

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, 95th 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 ²)	Q<0.9
2	ALC	Q	469	11/12	0.96	0.12	-	33,37,41,41	0
2	ALC	5	469	11/12	0.95	0.14	-	49,55,64,65	0
2	ZCL	T	472	14/14	0.75	0.17	-	86,90,106,108	0
2	ZCL	S	472	14/14	0.79	0.18	-	83,89,109,110	0
2	ALC	Y	469	11/12	0.93	0.13	-	38,42,49,49	0
2	ZCL	1	472	14/14	0.82	0.14	-	49,54,65,67	0
2	ZCL	U	472	14/14	0.91	0.11	-	50,52,69,69	0
2	ALC	3	469	11/12	0.97	0.11	-	46,50,54,55	0
2	ALC	X	469	11/12	0.95	0.10	-	31,36,41,42	0
2	ALC	U	469	11/12	0.97	0.09	-	43,46,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZCL	4	472	14/14	0.78	0.21	-	83,85,108,111	0
2	ALC	4	469	11/12	0.95	0.17	-	56,62,66,66	0
2	ZCL	3	472	14/14	0.91	0.11	-	52,55,62,63	0
2	ZCL	V	472	14/14	0.78	0.20	-	79,84,103,106	0
2	ZCL	5	472	14/14	0.80	0.16	-	88,91,112,113	0
2	ALC	S	469	11/12	0.95	0.14	-	47,54,66,67	0
2	ALC	0	469	11/12	0.95	0.12	-	39,44,48,49	0
2	ALC	T	469	11/12	0.95	0.12	-	48,54,63,65	0
2	ALC	2	469	11/12	0.96	0.11	-	34,38,46,47	0
2	ZCL	X	472	14/14	0.91	0.10	-	29,38,41,45	0
2	ALC	6	469	11/12	0.94	0.11	-	49,55,62,63	0
2	ZCL	R	472	14/14	0.83	0.12	-	51,55,70,71	0
2	ZCL	6	472	14/14	0.77	0.17	-	75,78,91,93	0
2	ALC	1	469	11/12	0.97	0.14	-	36,40,51,53	0
2	ZCL	Y	472	14/14	0.89	0.12	-	46,53,63,66	0
2	ALC	Z	469	11/12	0.96	0.09	-	30,34,44,44	0
2	ZCL	Z	472	14/14	0.89	0.11	-	27,39,42,46	0
2	ALC	R	469	11/12	0.96	0.14	-	34,38,50,51	0
2	ALC	V	469	11/12	0.95	0.20	-	56,64,67,68	0
2	ZCL	2	472	14/14	0.91	0.12	-	42,55,61,64	0
2	ZCL	Q	472	14/14	0.87	0.11	-	43,55,63,66	0
2	ZCL	0	472	14/14	0.91	0.11	-	46,51,62,64	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.