



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 04:20 PM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

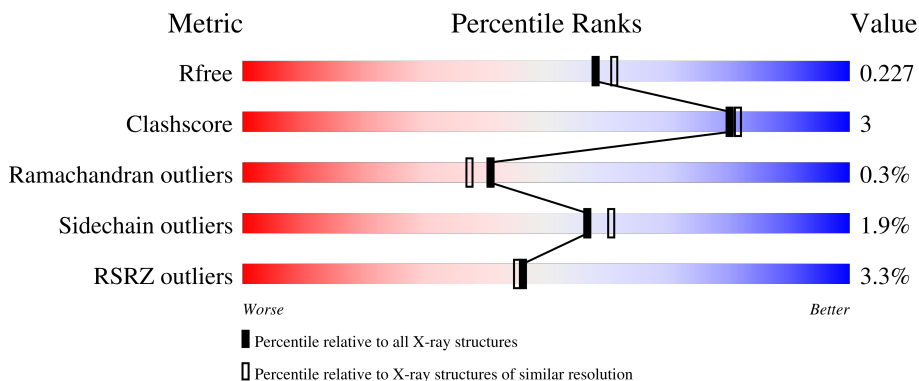
1 Overall quality at a glance

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.



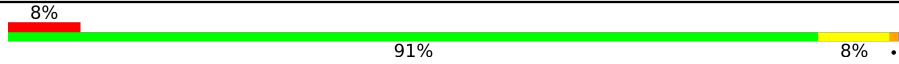
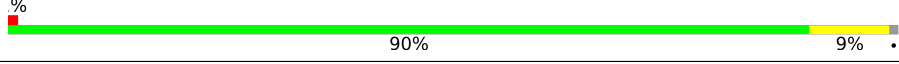
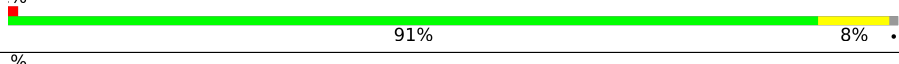
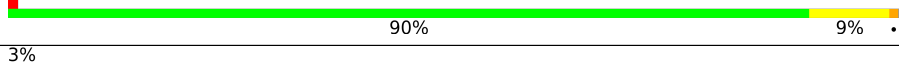
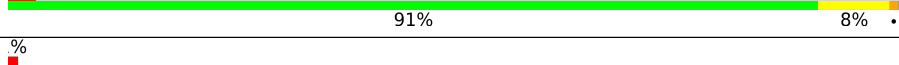
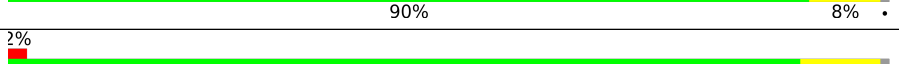
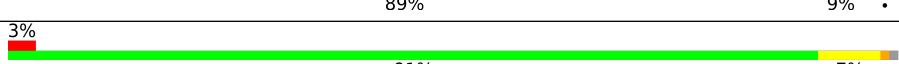
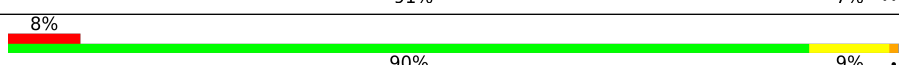
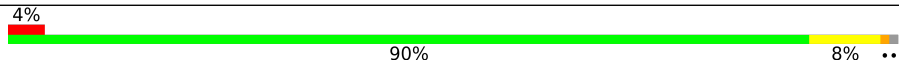
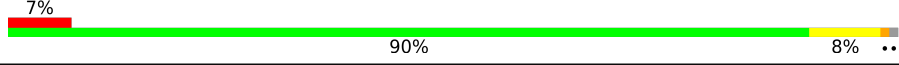

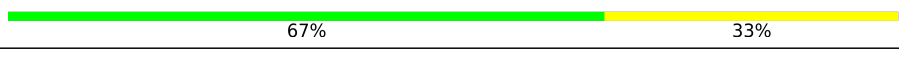
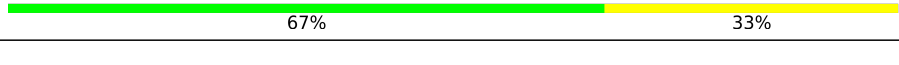


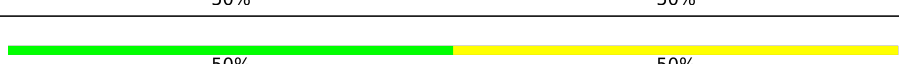



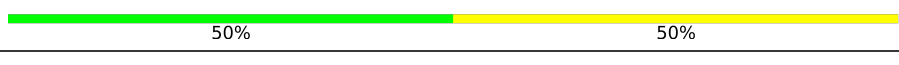





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 89% 9% .
1	B	368	 90% 8% .
1	C	368	 4% 90% 8% ..
1	D	368	 6% 89% 9% ..
1	E	368	 2% 90% 8% ..



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Mol	Chain	Length	Quality of chain
1	F	368	 8% 91% 8% ..
1	G	368	 % 90% 9% .
1	H	368	 % 91% 8% .
1	I	368	 % 90% 9% ..
1	J	368	 3% 91% 8% ..
1	K	368	 % 90% 8% .
1	L	368	 2% 89% 9% .
1	M	368	 3% 91% 7% ..
1	N	368	 8% 90% 9% ..
1	O	368	 4% 90% 8% ..
1	P	368	 7% 90% 8% ..
2	0	6	 67% 33%
2	1	6	 67% 33%
2	2	6	 67% 33%
2	3	6	 50% 50%
2	4	6	 50% 50%
2	5	6	 50% 50%
2	6	6	 50% 50%
2	Q	6	 67% 33%
2	R	6	 67% 33%
2	S	6	 50% 50%
2	T	6	 50% 50%
2	U	6	 33% 67%
2	V	6	 50% 50%
2	X	6	 67% 33%

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Mol	Chain	Length	Quality of chain	
2	Y	6	 67%	33%
2	Z	6	 67%	33%

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

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
			Total	C	Cl	N	O			
2	Q	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	R	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	S	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	T	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	U	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	V	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	X	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	Y	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	Z	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	0	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0
2	1	6	Total 53	C 35	Cl 2	N 6	O 10	0	0	0

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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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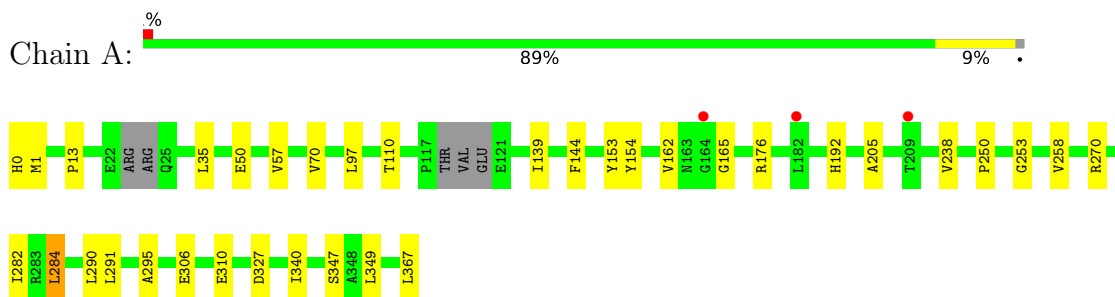
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	201	Total 201	O 201	0	0
3	Y	4	Total 4	O 4	0	0
3	I	211	Total 211	O 211	0	0
3	Z	12	Total 12	O 12	0	0
3	J	202	Total 202	O 202	0	0
3	0	6	Total 6	O 6	0	0
3	K	188	Total 188	O 188	0	0
3	1	4	Total 4	O 4	0	0
3	L	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

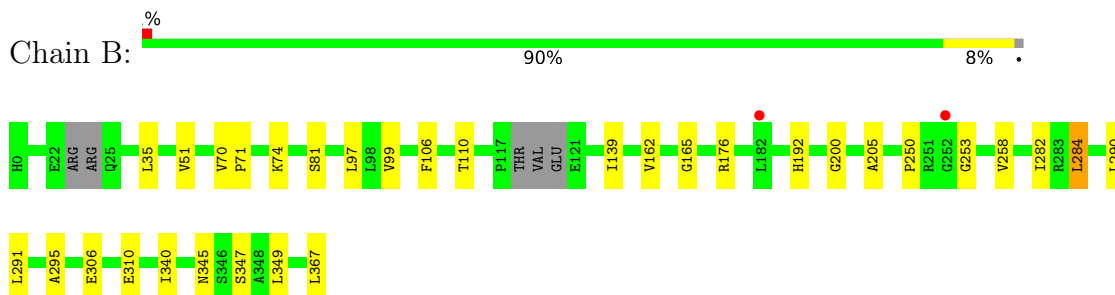
3 Residue-property plots [i](#)

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

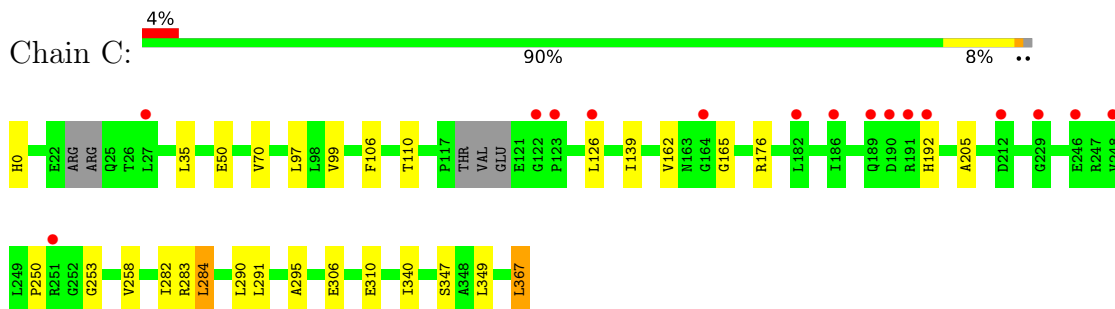
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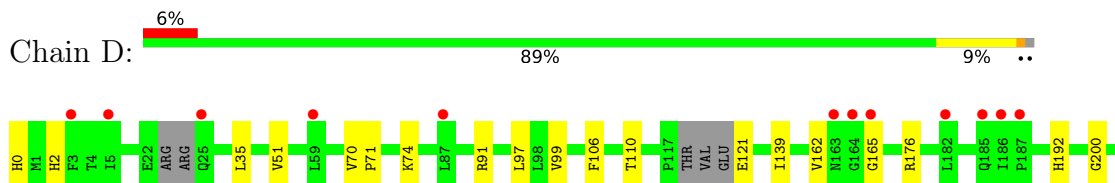
- Molecule 1: DNA polymerase III subunit beta



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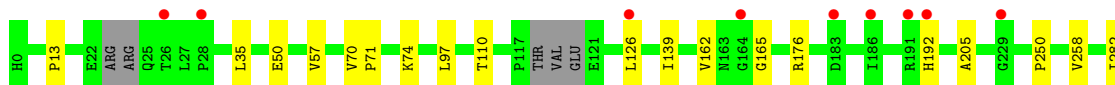
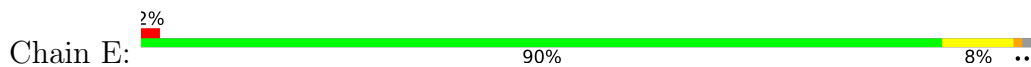


- Molecule 1: DNA polymerase III subunit beta

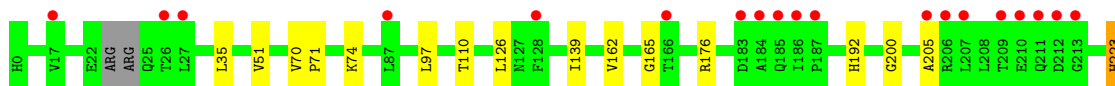
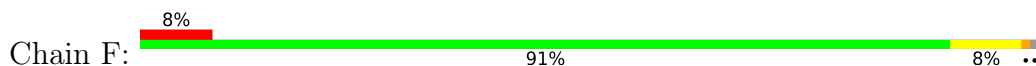




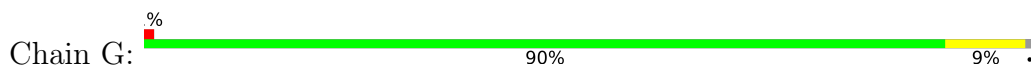
- Molecule 1: DNA polymerase III subunit beta



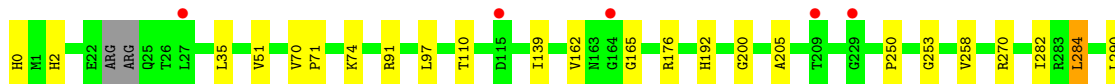
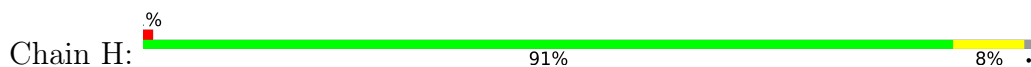
- Molecule 1: DNA polymerase III subunit beta



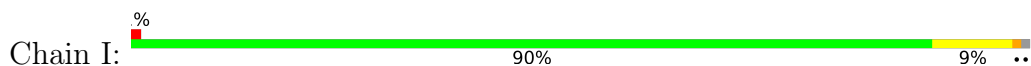
- Molecule 1: DNA polymerase III subunit beta

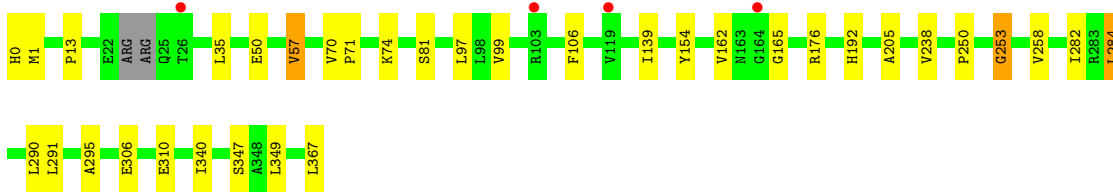


- Molecule 1: DNA polymerase III subunit beta



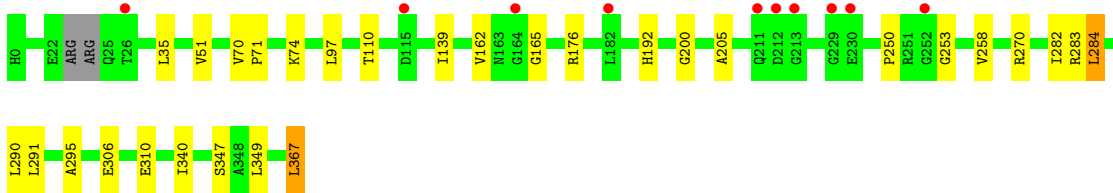
- Molecule 1: DNA polymerase III subunit beta





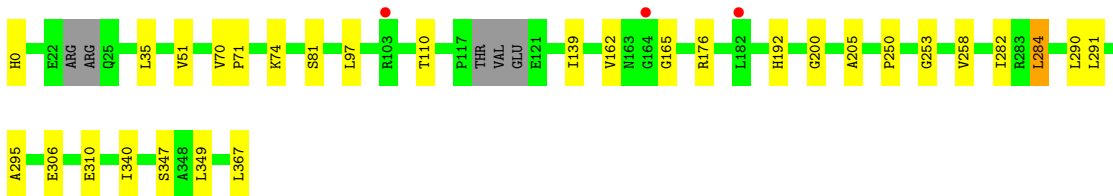
- Molecule 1: DNA polymerase III subunit beta

Chain J: 3% 91% 8% ..



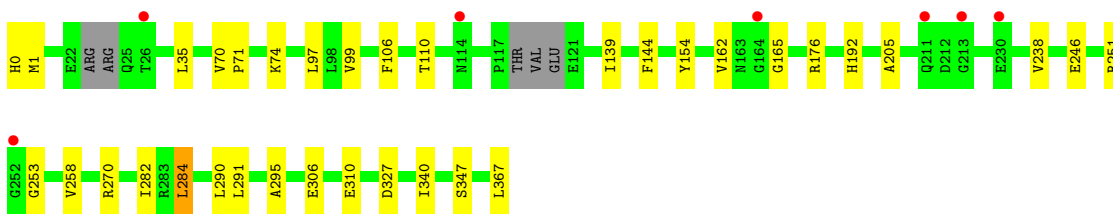
- Molecule 1: DNA polymerase III subunit beta

Chain K: 90% 8% .



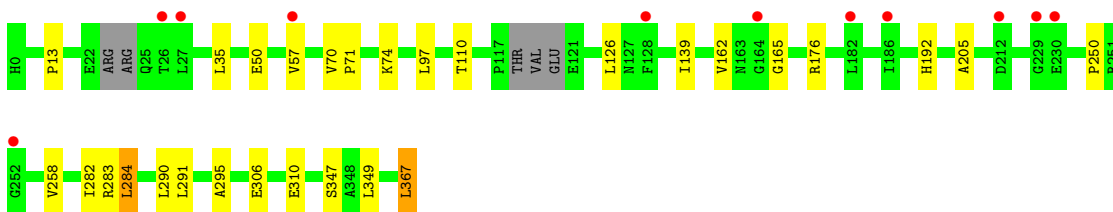
- Molecule 1: DNA polymerase III subunit beta

Chain L: 89% 9% .

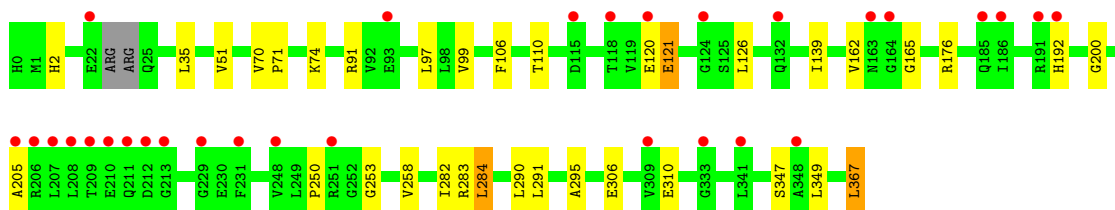
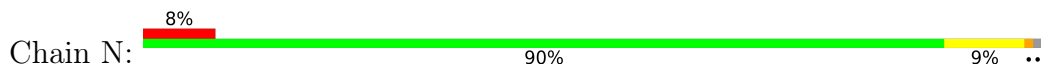


- Molecule 1: DNA polymerase III subunit beta

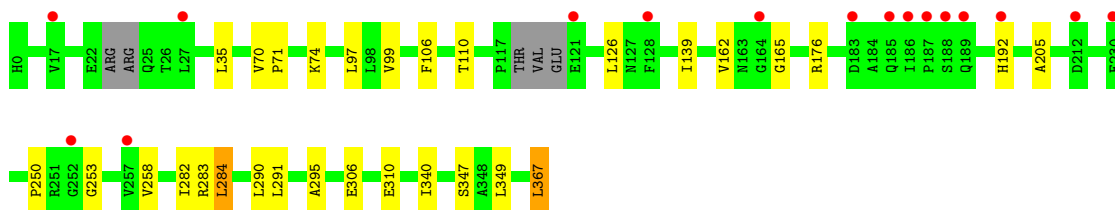
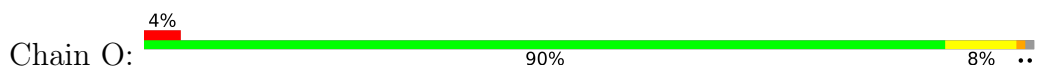
Chain M: 3% 91% 7% ..



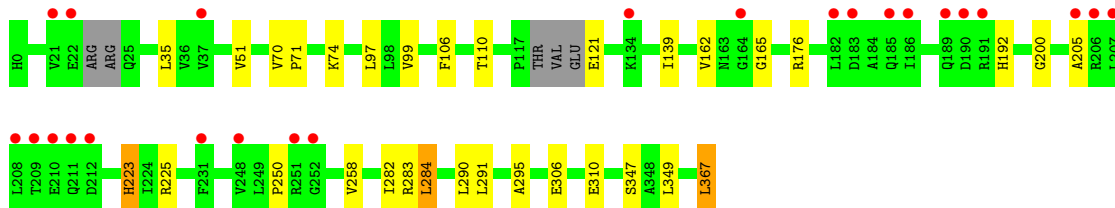
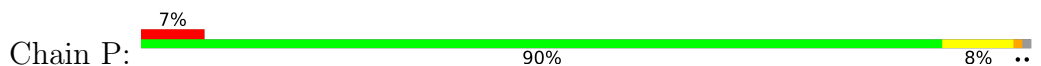
- Molecule 1: DNA polymerase III subunit beta



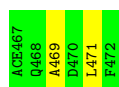
- Molecule 1: DNA polymerase III subunit beta



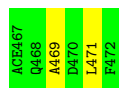
- Molecule 1: DNA polymerase III subunit beta



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

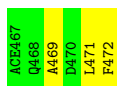


- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

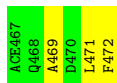


- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide





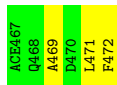
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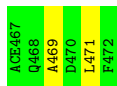
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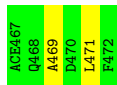
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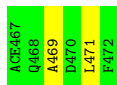
- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



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

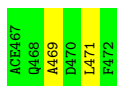


- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

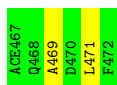


- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide

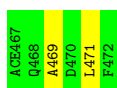




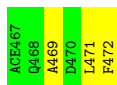
- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



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



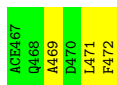
- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



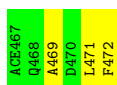
- Molecule 2: ACE-GLN-ALC-ASP-LEU-ZCL peptide



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



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



4 Data and refinement statistics i

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) 95.9 (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)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.202 , 0.222 0.216 , 0.227	Depositor DCC
R_{free} test set	21182 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtrriage
Anisotropy	0.273	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for h,-h-k,-l 0.467 for -h,-k,l 0.016 for -h,h+k,-l	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACE, ALC, ZCL

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.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	471	LEU	Mainchain
2	1	471	LEU	Mainchain
2	2	471	LEU	Mainchain
2	3	471	LEU	Mainchain
2	4	471	LEU	Mainchain
2	5	471	LEU	Mainchain
2	6	471	LEU	Mainchain
2	Q	471	LEU	Mainchain
2	R	471	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	S	471	LEU	Mainchain
2	T	471	LEU	Mainchain
2	U	471	LEU	Mainchain
2	V	471	LEU	Mainchain
2	X	471	LEU	Mainchain
2	Y	471	LEU	Mainchain
2	Z	471	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:L:0:HIS:HD2	1:L:1:MET:H	1.34	0.73
1:I:0:HIS:HD2	1:I:1:MET:H	1.41	0.69
1:G:81:SER:OG	1:H:270:ARG:HG2	2.01	0.60
1:I:81:SER:OG	1:J:270:ARG:HG2	2.02	0.59
1:C:50:GLU:HG3	3:C:479:HOH:O	2.03	0.57
1:I:70:VAL:HG11	1:I:97:LEU:HD22	1.87	0.57
1:P:284:LEU:HG	1:P:291:LEU:HD11	1.87	0.56
1:A:284:LEU:HG	1:A:291:LEU:HD11	1.88	0.56
1:F:284:LEU:HG	1:F:291:LEU:HD11	1.87	0.56
1:D:284:LEU:HG	1:D:291:LEU:HD11	1.87	0.55
1:N:284:LEU:HG	1:N:291:LEU:HD11	1.88	0.55
1:L:284:LEU:HG	1:L:291:LEU:HD11	1.88	0.55
1:K:284:LEU:HG	1:K:291:LEU:HD11	1.89	0.55
1:D:282:ILE:HG22	1:D:295:ALA:HB2	1.89	0.54
1:E:282:ILE:HG22	1:E:295:ALA:HB2	1.89	0.54
1:G:81:SER:O	1:H:270:ARG:NH1	2.38	0.54
1:J:284:LEU:HG	1:J:291:LEU:HD11	1.88	0.54
1:M:70:VAL:HG11	1:M:97:LEU:HD22	1.90	0.54
1:N:282:ILE:HG22	1:N:295:ALA:HB2	1.89	0.54
1:O:282:ILE:HG22	1:O:295:ALA:HB2	1.89	0.54
1:P:282:ILE:HG22	1:P:295:ALA:HB2	1.90	0.54
1:A:282:ILE:HG22	1:A:295:ALA:HB2	1.89	0.54
1:C:282:ILE:HG22	1:C:295:ALA:HB2	1.90	0.54
1:G:70:VAL:HG11	1:G:97:LEU:HD22	1.89	0.54
1:O:284:LEU:HG	1:O:291:LEU:HD11	1.90	0.54
1:E:70:VAL:HG11	1:E:97:LEU:HD22	1.90	0.54
1:H:70:VAL:HG11	1:H:97:LEU:HD22	1.90	0.54
1:E:284:LEU:HG	1:E:291:LEU:HD11	1.88	0.54
1:F:282:ILE:HG22	1:F:295:ALA:HB2	1.90	0.54
1:J:282:ILE:HG22	1:J:295:ALA:HB2	1.89	0.54
1:M:284:LEU:HG	1:M:291:LEU:HD11	1.90	0.54
1:A:270:ARG:HG2	1:B:81:SER:OG	2.07	0.53
1:B:282:ILE:HG22	1:B:295:ALA:HB2	1.90	0.53
1:B:284:LEU:HG	1:B:291:LEU:HD11	1.90	0.53
1:M:282:ILE:HG22	1:M:295:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:LEU:HG	1:H:291:LEU:HD11	1.91	0.53
1:F:70:VAL:HG11	1:F:97:LEU:HD22	1.90	0.53
1:H:282:ILE:HG22	1:H:295:ALA:HB2	1.90	0.53
1:K:70:VAL:HG11	1:K:97:LEU:HD22	1.91	0.53
1:I:282:ILE:HG22	1:I:295:ALA:HB2	1.91	0.53
1:C:284:LEU:HG	1:C:291:LEU:HD11	1.90	0.52
1:G:282:ILE:HG22	1:G:295:ALA:HB2	1.91	0.52
1:G:284:LEU:HG	1:G:291:LEU:HD11	1.90	0.52
1:L:282:ILE:HG22	1:L:295:ALA:HB2	1.91	0.52
1:I:284:LEU:HG	1:I:291:LEU:HD11	1.92	0.52
1:N:70:VAL:HG11	1:N:97:LEU:HD22	1.90	0.52
1:D:70:VAL:HG11	1:D:97:LEU:HD22	1.92	0.52
1:K:81:SER:OG	1:L:270:ARG:HG2	2.10	0.52
1:B:70:VAL:HG11	1:B:97:LEU:HD22	1.91	0.51
1:J:70:VAL:HG11	1:J:97:LEU:HD22	1.91	0.51
1:K:282:ILE:HG22	1:K:295:ALA:HB2	1.92	0.51
1:P:70:VAL:HG11	1:P:97:LEU:HD22	1.91	0.51
1:A:50[A]:GLU:HG3	3:A:586:HOH:O	2.10	0.51
1:A:70:VAL:HG11	1:A:97:LEU:HD22	1.93	0.50
1:I:81:SER:O	1:J:270:ARG:NH1	2.43	0.50
1:L:70:VAL:HG11	1:L:97:LEU:HD22	1.93	0.50
1:B:162:VAL:HG22	1:B:192:HIS:HB3	1.94	0.50
1:K:162:VAL:HG22	1:K:192:HIS:HB3	1.93	0.50
1:P:139:ILE:HG21	1:P:205:ALA:HB2	1.94	0.50
1:O:70:VAL:HG11	1:O:97:LEU:HD22	1.95	0.49
1:D:139:ILE:HG21	1:D:205:ALA:HB2	1.95	0.49
1:A:139:ILE:HG21	1:A:205:ALA:HB2	1.94	0.49
1:A:153:TYR:CE1	2:U:470:ASP:CG	2.86	0.49
1:C:70:VAL:HG11	1:C:97:LEU:HD22	1.94	0.49
1:G:162:VAL:HG22	1:G:192:HIS:HB3	1.95	0.49
1:L:162:VAL:HG22	1:L:192:HIS:HB3	1.95	0.49
1:I:162:VAL:HG22	1:I:192:HIS:HB3	1.95	0.48
1:A:162:VAL:HG22	1:A:192:HIS:HB3	1.95	0.48
1:E:162:VAL:HG22	1:E:192:HIS:HB3	1.96	0.48
1:I:258:VAL:HB	1:I:310:GLU:HB2	1.96	0.48
1:P:250:PRO:HG2	1:P:349:LEU:HB2	1.96	0.47
1:B:258:VAL:HB	1:B:310:GLU:HB2	1.96	0.47
1:H:162:VAL:HG22	1:H:192:HIS:HB3	1.96	0.47
1:N:250:PRO:HG2	1:N:349:LEU:HB2	1.96	0.47
1:F:139:ILE:HG21	1:F:205:ALA:HB2	1.96	0.47
1:K:258:VAL:HB	1:K:310:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PRO:HG2	1:C:349:LEU:HB2	1.96	0.47
1:E:50[A]:GLU:HG3	3:E:495:HOH:O	2.14	0.47
1:J:162:VAL:HG22	1:J:192:HIS:HB3	1.96	0.47
1:M:162:VAL:HG22	1:M:192:HIS:HB3	1.96	0.47
1:C:162:VAL:HG22	1:C:192:HIS:HB3	1.97	0.47
1:N:139:ILE:HG21	1:N:205:ALA:HB2	1.97	0.47
1:N:258:VAL:HB	1:N:310:GLU:HB2	1.97	0.47
1:F:258:VAL:HB	1:F:310:GLU:HB2	1.97	0.47
1:G:258:VAL:HB	1:G:310:GLU:HB2	1.97	0.47
1:J:139:ILE:HG21	1:J:205:ALA:HB2	1.97	0.47
1:L:139:ILE:HG21	1:L:205:ALA:HB2	1.97	0.47
1:A:258:VAL:HB	1:A:310:GLU:HB2	1.97	0.46
1:B:290:LEU:HD11	1:B:306:GLU:HB3	1.98	0.46
1:H:258:VAL:HB	1:H:310:GLU:HB2	1.97	0.46
1:D:250:PRO:HG2	1:D:349:LEU:HB2	1.97	0.46
1:P:162:VAL:HG22	1:P:192:HIS:HB3	1.98	0.46
1:P:223:HIS:HE1	1:P:225:ARG:HB2	1.80	0.46
1:H:139:ILE:HG21	1:H:205:ALA:HB2	1.98	0.46
1:N:51:VAL:HG11	1:N:200:GLY:HA2	1.98	0.46
1:O:250:PRO:HG2	1:O:349:LEU:HB2	1.96	0.46
1:J:51:VAL:HG11	1:J:200:GLY:HA2	1.98	0.46
1:J:258:VAL:HB	1:J:310:GLU:HB2	1.98	0.46
1:N:162:VAL:HG22	1:N:192:HIS:HB3	1.98	0.46
1:F:223:HIS:HE1	1:F:225:ARG:HB2	1.80	0.46
1:D:162:VAL:HG22	1:D:192:HIS:HB3	1.98	0.46
1:D:223:HIS:HE1	1:D:225:ARG:HB2	1.81	0.46
1:E:258:VAL:HB	1:E:310:GLU:HB2	1.98	0.46
1:F:250:PRO:HG2	1:F:349:LEU:HB2	1.97	0.46
1:L:258:VAL:HB	1:L:310:GLU:HB2	1.98	0.46
1:N:120:GLU:O	1:N:121:GLU:HB2	2.16	0.46
1:P:258:VAL:HB	1:P:310:GLU:HB2	1.98	0.46
1:D:258:VAL:HB	1:D:310:GLU:HB2	1.99	0.46
1:M:258:VAL:HB	1:M:310:GLU:HB2	1.98	0.46
1:A:153:TYR:HE1	2:U:470:ASP:CG	2.20	0.45
1:M:250:PRO:HG2	1:M:349:LEU:HB2	1.97	0.45
1:O:162:VAL:HG22	1:O:192:HIS:HB3	1.97	0.45
1:D:51:VAL:HG11	1:D:200:GLY:HA2	1.99	0.45
1:K:290:LEU:HD11	1:K:306:GLU:HB3	1.98	0.45
1:P:51:VAL:HG11	1:P:200:GLY:HA2	1.98	0.45
1:F:162:VAL:HG22	1:F:192:HIS:HB3	1.98	0.45
1:D:290:LEU:HD11	1:D:306:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:VAL:HB	1:O:310:GLU:HB2	1.99	0.45
1:C:258:VAL:HB	1:C:310:GLU:HB2	1.99	0.45
1:E:290:LEU:HD11	1:E:306:GLU:HB3	1.99	0.45
1:E:250:PRO:HG2	1:E:349:LEU:HB2	1.98	0.45
1:L:290:LEU:HD11	1:L:306:GLU:HB3	1.99	0.45
1:F:290:LEU:HD11	1:F:306:GLU:HB3	1.99	0.44
1:K:139:ILE:HG21	1:K:205:ALA:HB2	1.99	0.44
1:B:51:VAL:HG11	1:B:200:GLY:HA2	2.00	0.44
1:H:51:VAL:HG11	1:H:200:GLY:HA2	1.99	0.44
1:C:290:LEU:HD11	1:C:306:GLU:HB3	2.00	0.44
1:G:290:LEU:HD11	1:G:306:GLU:HB3	2.00	0.44
1:J:253:GLY:HA3	1:J:340:ILE:HG22	1.99	0.44
1:N:290:LEU:HD11	1:N:306:GLU:HB3	1.99	0.44
1:F:51:VAL:HG11	1:F:200:GLY:HA2	1.99	0.44
1:P:290:LEU:HD11	1:P:306:GLU:HB3	1.99	0.44
1:C:139:ILE:HG21	1:C:205:ALA:HB2	2.00	0.44
1:H:250:PRO:HG2	1:H:349:LEU:HB2	2.00	0.44
1:M:290:LEU:HD11	1:M:306:GLU:HB3	1.99	0.44
1:G:175:HIS:HE1	3:X:503:HOH:O	2.00	0.43
1:K:250:PRO:HG2	1:K:349:LEU:HB2	2.00	0.43
1:I:290:LEU:HD11	1:I:306:GLU:HB3	2.00	0.43
1:N:71:PRO:HB2	1:N:74:LYS:HB2	2.01	0.43
1:B:70:VAL:HG12	1:B:110:THR:HG22	2.01	0.43
1:E:139:ILE:HG21	1:E:205:ALA:HB2	2.01	0.43
1:I:139:ILE:HG21	1:I:205:ALA:HB2	2.01	0.43
1:J:290:LEU:HD11	1:J:306:GLU:HB3	2.01	0.43
1:K:51:VAL:HG11	1:K:200:GLY:HA2	2.00	0.43
1:P:71:PRO:HB2	1:P:74:LYS:HB2	2.00	0.43
1:N:283:ARG:HG3	1:N:367:LEU:HD21	2.01	0.43
1:O:290:LEU:HD11	1:O:306:GLU:HB3	2.01	0.43
1:P:223:HIS:CE1	1:P:225:ARG:HB2	2.53	0.43
1:A:290:LEU:HD11	1:A:306:GLU:HB3	2.00	0.43
1:C:70:VAL:HG12	1:C:110:THR:HG22	2.01	0.43
1:L:70:VAL:HG12	1:L:110:THR:HG22	2.01	0.43
1:C:283:ARG:HG3	1:C:367:LEU:HD21	2.01	0.42
1:D:223:HIS:CE1	1:D:225:ARG:HB2	2.54	0.42
1:H:290:LEU:HD11	1:H:306:GLU:HB3	2.01	0.42
1:J:70:VAL:HG12	1:J:110:THR:HG22	2.01	0.42
1:A:253:GLY:HA3	1:A:340:ILE:HG22	2.01	0.42
1:C:126:LEU:HD22	1:C:162:VAL:HG21	2.01	0.42
1:M:71:PRO:HB2	1:M:74:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:PRO:HB2	1:E:74:LYS:HB2	2.00	0.42
1:F:283:ARG:HG3	1:F:367:LEU:HD21	2.01	0.42
1:G:139:ILE:HG21	1:G:205:ALA:HB2	2.02	0.42
1:L:253:GLY:HA3	1:L:340:ILE:HG22	2.01	0.42
1:O:126:LEU:HD22	1:O:162:VAL:HG21	2.00	0.42
1:O:139:ILE:HG21	1:O:205:ALA:HB2	2.01	0.42
1:M:139:ILE:HG21	1:M:205:ALA:HB2	2.01	0.42
1:B:71:PRO:HB2	1:B:74:LYS:HB2	2.00	0.42
1:F:223:HIS:CE1	1:F:225:ARG:HB2	2.54	0.42
1:G:71:PRO:HB2	1:G:74:LYS:HB2	2.00	0.42
1:O:70:VAL:HG12	1:O:110:THR:HG22	2.01	0.42
1:B:253:GLY:HA3	1:B:340:ILE:HG22	2.01	0.42
1:E:126:LEU:HD22	1:E:162:VAL:HG21	2.02	0.42
1:H:71:PRO:HB2	1:H:74:LYS:HB2	2.00	0.42
1:K:70:VAL:HG12	1:K:110:THR:HG22	2.01	0.42
1:E:283:ARG:HG3	1:E:367:LEU:HD21	2.02	0.42
1:P:121:GLU:HG3	1:P:223:HIS:CE1	2.55	0.42
1:J:71:PRO:HB2	1:J:74:LYS:HB2	2.01	0.42
1:K:71:PRO:HB2	1:K:74:LYS:HB2	2.01	0.42
1:L:99:VAL:HB	1:L:106:PHE:HB2	2.02	0.42
1:O:283:ARG:HG3	1:O:367:LEU:HD21	2.01	0.42
1:D:71:PRO:HB2	1:D:74:LYS:HB2	2.01	0.41
1:I:13:PRO:HG3	1:I:57:VAL:HG22	2.02	0.41
1:B:345:ASN:ND2	3:B:604:HOH:O	2.52	0.41
1:C:99:VAL:HB	1:C:106:PHE:HB2	2.01	0.41
1:E:13:PRO:HG3	1:E:57:VAL:HG22	2.03	0.41
1:G:13:PRO:HG3	1:G:57:VAL:HG22	2.03	0.41
1:G:253:GLY:HA3	1:G:340:ILE:HG22	2.01	0.41
1:H:253:GLY:HA3	1:H:340:ILE:HG22	2.02	0.41
1:N:126:LEU:HD22	1:N:162:VAL:HG21	2.02	0.41
1:E:70:VAL:HG12	1:E:110:THR:HG22	2.03	0.41
1:F:126:LEU:HD22	1:F:162:VAL:HG21	2.02	0.41
1:J:250:PRO:HG2	1:J:349:LEU:HB2	2.01	0.41
1:P:99:VAL:HB	1:P:106:PHE:HB2	2.02	0.41
1:P:283:ARG:HG3	1:P:367:LEU:HD21	2.03	0.41
1:I:71:PRO:HB2	1:I:74:LYS:HB2	2.02	0.41
1:A:13:PRO:HG3	1:A:57:VAL:HG22	2.03	0.41
1:B:99:VAL:HB	1:B:106:PHE:HB2	2.02	0.41
1:D:283:ARG:HG3	1:D:367:LEU:HD21	2.02	0.41
1:I:253:GLY:HA3	1:I:340:ILE:HG22	2.03	0.41
1:A:250:PRO:HG2	1:A:349:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PRO:HG2	1:B:349:LEU:HB2	2.01	0.41
1:F:71:PRO:HB2	1:F:74:LYS:HB2	2.01	0.41
1:K:253:GLY:HA3	1:K:340:ILE:HG22	2.03	0.41
1:M:13:PRO:HG3	1:M:57:VAL:HG22	2.03	0.41
1:O:71:PRO:HB2	1:O:74:LYS:HB2	2.01	0.41
1:O:253:GLY:HA3	1:O:340:ILE:HG22	2.03	0.41
1:B:139:ILE:HG21	1:B:205:ALA:HB2	2.02	0.41
1:C:253:GLY:HA3	1:C:340:ILE:HG22	2.02	0.41
1:D:70:VAL:HG12	1:D:110:THR:HG22	2.03	0.41
1:D:121:GLU:HG3	1:D:223:HIS:CE1	2.55	0.41
1:G:70:VAL:HG12	1:G:110:THR:HG22	2.03	0.41
1:N:99:VAL:HB	1:N:106:PHE:HB2	2.02	0.41
1:A:70:VAL:HG12	1:A:110:THR:HG22	2.03	0.41
1:I:154:TYR:HA	1:I:238:VAL:HG11	2.03	0.41
1:J:283:ARG:HG3	1:J:367:LEU:HD21	2.03	0.41
1:M:126:LEU:HD22	1:M:162:VAL:HG21	2.02	0.41
1:D:2:HIS:HD2	1:D:91:ARG:HB3	1.86	0.41
1:F:70:VAL:HG12	1:F:110:THR:HG22	2.03	0.41
1:M:70:VAL:HG12	1:M:110:THR:HG22	2.02	0.41
1:A:144:PHE:CD1	1:A:327:ASP:HB3	2.56	0.40
1:D:99:VAL:HB	1:D:106:PHE:HB2	2.02	0.40
1:I:250:PRO:HG2	1:I:349:LEU:HB2	2.03	0.40
1:N:2:HIS:HD2	1:N:91:ARG:HB3	1.86	0.40
1:N:70:VAL:HG12	1:N:110:THR:HG22	2.03	0.40
1:I:99:VAL:HB	1:I:106:PHE:HB2	2.02	0.40
1:O:99:VAL:HB	1:O:106:PHE:HB2	2.02	0.40
1:A:154:TYR:HA	1:A:238:VAL:HG11	2.04	0.40
1:G:2:HIS:HD2	1:G:91:ARG:HB3	1.87	0.40
1:H:2:HIS:HD2	1:H:91:ARG:HB3	1.87	0.40
1:M:283:ARG:HG3	1:M:367:LEU:HD21	2.02	0.40
1:E:289:GLY:HA2	1:E:309:VAL:O	2.21	0.40
1:H:70:VAL:HG12	1:H:110:THR:HG22	2.04	0.40
1:L:71:PRO:HB2	1:L:74:LYS:HB2	2.03	0.40
1:L:246:GLU:O	1:L:251:ARG:NH1	2.55	0.40
1:P:70:VAL:HG12	1:P:110:THR:HG22	2.04	0.40
1:G:99:VAL:HB	1:G:106:PHE:HB2	2.03	0.40
1:L:144:PHE:CD1	1:L:327:ASP:HB3	2.56	0.40
1:L:154:TYR:HA	1:L:238:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/368 (98%)	350 (97%)	9 (2%)	1 (0%)	41	37
1	B	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	41	37
1	C	358/368 (97%)	348 (97%)	9 (2%)	1 (0%)	41	37
1	D	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	41	37
1	E	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	41	37
1	F	364/368 (99%)	355 (98%)	7 (2%)	2 (0%)	29	23
1	G	364/368 (99%)	355 (98%)	8 (2%)	1 (0%)	41	37
1	H	364/368 (99%)	352 (97%)	11 (3%)	1 (0%)	41	37
1	I	364/368 (99%)	353 (97%)	9 (2%)	2 (0%)	29	23
1	J	364/368 (99%)	353 (97%)	10 (3%)	1 (0%)	41	37
1	K	358/368 (97%)	348 (97%)	9 (2%)	1 (0%)	41	37
1	L	360/368 (98%)	349 (97%)	10 (3%)	1 (0%)	41	37
1	M	358/368 (97%)	349 (98%)	8 (2%)	1 (0%)	41	37
1	N	364/368 (99%)	353 (97%)	8 (2%)	3 (1%)	19	13
1	O	359/368 (98%)	349 (97%)	9 (2%)	1 (0%)	41	37
1	P	359/368 (98%)	350 (98%)	8 (2%)	1 (0%)	41	37
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	41	37

All (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
1	C	165	GLY
1	D	165	GLY
1	E	165	GLY
1	F	165	GLY
1	G	165	GLY
1	H	165	GLY
1	I	165	GLY
1	J	165	GLY
1	L	165	GLY
1	M	165	GLY
1	N	165	GLY
1	O	165	GLY
1	P	165	GLY
1	F	253	GLY
1	N	253	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%)	55	58
1	B	290/318 (91%)	284 (98%)	6 (2%)	53	57
1	C	290/318 (91%)	283 (98%)	7 (2%)	49	51
1	D	288/318 (91%)	280 (97%)	8 (3%)	43	44
1	E	290/318 (91%)	284 (98%)	6 (2%)	53	57
1	F	290/318 (91%)	283 (98%)	7 (2%)	49	51
1	G	293/318 (92%)	287 (98%)	6 (2%)	55	58
1	H	291/318 (92%)	284 (98%)	7 (2%)	49	51
1	I	294/318 (92%)	287 (98%)	7 (2%)	49	51
1	J	289/318 (91%)	283 (98%)	6 (2%)	53	57
1	K	291/318 (92%)	284 (98%)	7 (2%)	49	51
1	L	293/318 (92%)	287 (98%)	6 (2%)	55	58
1	M	289/318 (91%)	282 (98%)	7 (2%)	49	51
1	N	289/318 (91%)	283 (98%)	6 (2%)	53	57
1	O	290/318 (91%)	284 (98%)	6 (2%)	53	57
1	P	287/318 (90%)	280 (98%)	7 (2%)	49	51
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	4697/5136 (92%)	4592 (98%)	105 (2%)	57	55

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	176	ARG
1	A	284	LEU
1	A	347[A]	SER
1	A	347[B]	SER
1	A	367	LEU
1	B	35	LEU
1	B	176	ARG
1	B	284	LEU
1	B	347[A]	SER
1	B	347[B]	SER
1	B	367	LEU
1	C	0	HIS
1	C	35	LEU
1	C	176	ARG
1	C	284	LEU
1	C	347[A]	SER
1	C	347[B]	SER
1	C	367	LEU
1	D	0	HIS
1	D	35	LEU
1	D	176	ARG
1	D	223	HIS
1	D	284	LEU
1	D	347[A]	SER
1	D	347[B]	SER
1	D	367	LEU
1	E	35	LEU
1	E	176	ARG
1	E	284	LEU
1	E	347[A]	SER
1	E	347[B]	SER
1	E	367	LEU
1	F	35	LEU
1	F	176	ARG
1	F	223	HIS

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Mol	Chain	Res	Type
1	F	284	LEU
1	F	347[A]	SER
1	F	347[B]	SER
1	F	367	LEU
1	G	35	LEU
1	G	176	ARG
1	G	284	LEU
1	G	347[A]	SER
1	G	347[B]	SER
1	G	367	LEU
1	H	0	HIS
1	H	35	LEU
1	H	176	ARG
1	H	284	LEU
1	H	347[A]	SER
1	H	347[B]	SER
1	H	367	LEU
1	I	35	LEU
1	I	57	VAL
1	I	176	ARG
1	I	284	LEU
1	I	347[A]	SER
1	I	347[B]	SER
1	I	367	LEU
1	J	35	LEU
1	J	176	ARG
1	J	284	LEU
1	J	347[A]	SER
1	J	347[B]	SER
1	J	367	LEU
1	K	0	HIS
1	K	35	LEU
1	K	176	ARG
1	K	284	LEU
1	K	347[A]	SER
1	K	347[B]	SER
1	K	367	LEU
1	L	35	LEU
1	L	176	ARG
1	L	284	LEU
1	L	347[A]	SER
1	L	347[B]	SER

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Mol	Chain	Res	Type
1	L	367	LEU
1	M	35	LEU
1	M	50	GLU
1	M	176	ARG
1	M	284	LEU
1	M	347[A]	SER
1	M	347[B]	SER
1	M	367	LEU
1	N	35	LEU
1	N	176	ARG
1	N	284	LEU
1	N	347[A]	SER
1	N	347[B]	SER
1	N	367	LEU
1	O	35	LEU
1	O	176	ARG
1	O	284	LEU
1	O	347[A]	SER
1	O	347[B]	SER
1	O	367	LEU
1	P	35	LEU
1	P	176	ARG
1	P	223	HIS
1	P	284	LEU
1	P	347[A]	SER
1	P	347[B]	SER
1	P	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	40	GLN
1	A	114	ASN
1	A	175	HIS
1	A	285	GLN
1	A	345	ASN
1	B	40	GLN
1	B	175	HIS
1	B	262	GLN
1	B	285	GLN
1	B	345	ASN

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Mol	Chain	Res	Type
1	C	40	GLN
1	C	175	HIS
1	C	285	GLN
1	C	345	ASN
1	D	40	GLN
1	D	175	HIS
1	D	223	HIS
1	D	285	GLN
1	D	345	ASN
2	T	468	GLN
1	E	40	GLN
1	E	175	HIS
1	E	262	GLN
1	E	285	GLN
1	E	345	ASN
2	U	468	GLN
1	F	40	GLN
1	F	175	HIS
1	F	223	HIS
1	F	285	GLN
1	F	345	ASN
2	V	468	GLN
1	G	0	HIS
1	G	40	GLN
1	G	175	HIS
1	G	262	GLN
1	G	285	GLN
1	G	345	ASN
1	H	40	GLN
1	H	127	ASN
1	H	175	HIS
1	H	285	GLN
1	H	345	ASN
1	I	0	HIS
1	I	40	GLN
1	I	114	ASN
1	I	175	HIS
1	I	262	GLN
1	I	285	GLN
1	I	345	ASN
1	J	40	GLN
1	J	114	ASN

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Mol	Chain	Res	Type
1	J	127	ASN
1	J	175	HIS
1	J	285	GLN
1	J	345	ASN
1	K	40	GLN
1	K	127	ASN
1	K	175	HIS
1	K	262	GLN
1	K	285	GLN
1	K	345	ASN
1	L	0	HIS
1	L	40	GLN
1	L	114	ASN
1	L	175	HIS
1	L	285	GLN
1	L	345	ASN
1	M	40	GLN
1	M	175	HIS
1	M	285	GLN
1	M	345	ASN
1	N	40	GLN
1	N	175	HIS
1	N	285	GLN
1	N	345	ASN
2	4	468	GLN
1	O	40	GLN
1	O	175	HIS
1	O	285	GLN
1	O	345	ASN
1	P	40	GLN
1	P	175	HIS
1	P	285	GLN
1	P	345	ASN
2	6	468	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	ZCL	Z	472	2	13,14,14	0.38	0	18,19,19	0.25	0
2	ZCL	4	472	2	13,14,14	0.91	1 (7%)	18,19,19	0.77	2 (11%)
2	ALC	3	469	2	9,11,12	0.44	0	10,13,15	0.88	1 (10%)
2	ZCL	5	472	2	13,14,14	0.91	1 (7%)	18,19,19	0.78	2 (11%)
2	ALC	Z	469	2	9,11,12	0.47	0	10,13,15	0.88	1 (10%)
2	ZCL	Y	472	2	13,14,14	0.44	0	18,19,19	0.28	0
2	ZCL	6	472	2	13,14,14	0.92	1 (7%)	18,19,19	0.79	2 (11%)
2	ZCL	R	472	2	13,14,14	0.42	0	18,19,19	0.32	0
2	ZCL	U	472	2	13,14,14	0.89	1 (7%)	18,19,19	0.81	2 (11%)
2	ZCL	X	472	2	13,14,14	0.46	0	18,19,19	0.27	0
2	ZCL	0	472	2	13,14,14	0.43	0	18,19,19	0.30	0
2	ZCL	V	472	2	13,14,14	0.92	1 (7%)	18,19,19	0.76	2 (11%)
2	ZCL	Q	472	2	13,14,14	0.37	0	18,19,19	0.32	0
2	ALC	5	469	2	9,11,12	0.42	0	10,13,15	0.79	1 (10%)
2	ALC	Y	469	2	9,11,12	0.47	0	10,13,15	0.97	1 (10%)
2	ALC	X	469	2	9,11,12	0.44	0	10,13,15	0.94	1 (10%)
2	ALC	R	469	2	9,11,12	0.42	0	10,13,15	0.98	1 (10%)
2	ALC	1	469	2	9,11,12	0.42	0	10,13,15	0.90	1 (10%)
2	ALC	Q	469	2	9,11,12	0.44	0	10,13,15	0.92	1 (10%)
2	ALC	U	469	2	9,11,12	0.40	0	10,13,15	0.93	1 (10%)
2	ALC	T	469	2	9,11,12	0.41	0	10,13,15	0.78	1 (10%)
2	ALC	S	469	2	9,11,12	0.41	0	10,13,15	0.82	1 (10%)
2	ZCL	1	472	2	13,14,14	0.41	0	18,19,19	0.32	0
2	ZCL	S	472	2	13,14,14	0.91	1 (7%)	18,19,19	0.77	2 (11%)
2	ALC	2	469	2	9,11,12	0.42	0	10,13,15	0.96	1 (10%)
2	ALC	4	469	2	9,11,12	0.44	0	10,13,15	0.87	1 (10%)
2	ZCL	T	472	2	13,14,14	0.93	1 (7%)	18,19,19	0.78	2 (11%)
2	ALC	V	469	2	9,11,12	0.42	0	10,13,15	0.86	1 (10%)
2	ALC	6	469	2	9,11,12	0.42	0	10,13,15	0.79	1 (10%)
2	ALC	0	469	2	9,11,12	0.48	0	10,13,15	0.87	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZCL	3	472	2	13,14,14	0.94	1 (7%)	18,19,19	0.79	2 (11%)
2	ZCL	2	472	2	13,14,14	0.34	0	18,19,19	0.32	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	ZCL	Z	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	4	472	2	-	0/8/8/8	0/1/1/1
2	ALC	3	469	2	-	0/5/14/16	0/1/1/1
2	ZCL	5	472	2	-	0/8/8/8	0/1/1/1
2	ALC	Z	469	2	-	0/5/14/16	0/1/1/1
2	ZCL	Y	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	6	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	R	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	U	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	X	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	0	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	V	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	Q	472	2	-	0/8/8/8	0/1/1/1
2	ALC	5	469	2	-	0/5/14/16	0/1/1/1
2	ALC	Y	469	2	-	0/5/14/16	0/1/1/1
2	ALC	X	469	2	-	0/5/14/16	0/1/1/1
2	ALC	R	469	2	-	0/5/14/16	0/1/1/1
2	ALC	1	469	2	-	0/5/14/16	0/1/1/1
2	ALC	Q	469	2	-	0/5/14/16	0/1/1/1
2	ALC	U	469	2	-	0/5/14/16	0/1/1/1
2	ALC	T	469	2	-	0/5/14/16	0/1/1/1
2	ALC	S	469	2	-	0/5/14/16	0/1/1/1
2	ZCL	1	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	S	472	2	-	0/8/8/8	0/1/1/1
2	ALC	2	469	2	-	0/5/14/16	0/1/1/1
2	ALC	4	469	2	-	0/5/14/16	0/1/1/1
2	ZCL	T	472	2	-	0/8/8/8	0/1/1/1
2	ALC	V	469	2	-	0/5/14/16	0/1/1/1
2	ALC	6	469	2	-	0/5/14/16	0/1/1/1
2	ALC	0	469	2	-	0/5/14/16	0/1/1/1
2	ZCL	3	472	2	-	0/8/8/8	0/1/1/1
2	ZCL	2	472	2	-	0/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	472	ZCL	O-C	2.97	1.31	1.22
2	3	472	ZCL	O-C	2.97	1.31	1.22
2	6	472	ZCL	O-C	2.91	1.31	1.22
2	V	472	ZCL	O-C	2.85	1.30	1.22
2	S	472	ZCL	O-C	2.85	1.30	1.22
2	5	472	ZCL	O-C	2.84	1.30	1.22
2	U	472	ZCL	O-C	2.82	1.30	1.22
2	4	472	ZCL	O-C	2.77	1.30	1.22

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	469	ALC	CB-CA-N	2.87	116.71	110.32
2	X	469	ALC	CB-CA-N	2.85	116.68	110.32
2	Y	469	ALC	CB-CA-N	2.83	116.63	110.32
2	2	469	ALC	CB-CA-N	2.83	116.61	110.32
2	Q	469	ALC	CB-CA-N	2.81	116.57	110.32
2	U	469	ALC	CB-CA-N	2.80	116.55	110.32
2	1	469	ALC	CB-CA-N	2.70	116.34	110.32
2	Z	469	ALC	CB-CA-N	2.68	116.29	110.32
2	4	469	ALC	CB-CA-N	2.68	116.29	110.32
2	V	469	ALC	CB-CA-N	2.66	116.26	110.32
2	3	469	ALC	CB-CA-N	2.64	116.19	110.32
2	0	469	ALC	CB-CA-N	2.61	116.13	110.32
2	S	469	ALC	CB-CA-N	2.44	115.76	110.32
2	6	469	ALC	CB-CA-N	2.42	115.71	110.32
2	5	469	ALC	CB-CA-N	2.39	115.65	110.32
2	T	469	ALC	CB-CA-N	2.39	115.65	110.32
2	U	472	ZCL	O-C-CA	-2.35	113.86	122.14
2	3	472	ZCL	O-C-CA	-2.33	113.92	122.14
2	6	472	ZCL	O-C-CA	-2.30	114.02	122.14
2	T	472	ZCL	O-C-CA	-2.29	114.06	122.14
2	5	472	ZCL	O-C-CA	-2.25	114.21	122.14
2	U	472	ZCL	OXT-C-CA	2.22	120.95	113.38
2	S	472	ZCL	O-C-CA	-2.22	114.31	122.14
2	3	472	ZCL	OXT-C-CA	2.21	120.91	113.38
2	4	472	ZCL	O-C-CA	-2.21	114.34	122.14
2	V	472	ZCL	O-C-CA	-2.20	114.39	122.14
2	6	472	ZCL	OXT-C-CA	2.17	120.76	113.38
2	5	472	ZCL	OXT-C-CA	2.16	120.75	113.38
2	T	472	ZCL	OXT-C-CA	2.16	120.73	113.38
2	S	472	ZCL	OXT-C-CA	2.14	120.68	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	472	ZCL	OXT-C-CA	2.13	120.63	113.38
2	V	472	ZCL	OXT-C-CA	2.10	120.55	113.38

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 monosaccharides 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%)	-0.30	3 (0%) 86 85	24, 39, 66, 96	0
1	B	363/368 (98%)	-0.23	2 (0%) 89 88	22, 41, 64, 96	0
1	C	363/368 (98%)	0.01	16 (4%) 34 33	33, 53, 81, 116	0
1	D	363/368 (98%)	0.25	23 (6%) 20 19	35, 58, 85, 105	0
1	E	363/368 (98%)	-0.12	9 (2%) 57 56	30, 49, 74, 101	0
1	F	366/368 (99%)	0.32	29 (7%) 12 11	42, 58, 87, 108	0
1	G	366/368 (99%)	-0.29	3 (0%) 86 85	20, 36, 60, 89	0
1	H	366/368 (99%)	-0.32	5 (1%) 75 74	25, 38, 61, 90	0
1	I	366/368 (99%)	-0.33	4 (1%) 80 79	21, 35, 62, 92	0
1	J	366/368 (99%)	-0.21	10 (2%) 54 53	26, 38, 62, 97	0
1	K	363/368 (98%)	-0.32	3 (0%) 86 85	22, 41, 64, 97	0
1	L	363/368 (98%)	-0.25	7 (1%) 66 65	24, 39, 66, 95	0
1	M	363/368 (98%)	-0.10	11 (3%) 50 49	32, 49, 76, 105	0
1	N	366/368 (99%)	0.32	30 (8%) 11 11	42, 58, 88, 108	0
1	O	363/368 (98%)	0.04	16 (4%) 34 33	33, 54, 80, 115	0
1	P	363/368 (98%)	0.28	24 (6%) 18 17	36, 59, 85, 103	0
2	0	3/6 (50%)	-0.75	0 100 100	39, 39, 43, 50	0
2	1	3/6 (50%)	-0.63	0 100 100	38, 38, 41, 47	0
2	2	3/6 (50%)	-0.76	0 100 100	34, 34, 39, 48	0
2	3	3/6 (50%)	-0.28	0 100 100	43, 43, 44, 55	0
2	4	3/6 (50%)	-0.06	0 100 100	53, 53, 69, 70	0
2	5	3/6 (50%)	-0.44	0 100 100	46, 46, 59, 62	0
2	6	3/6 (50%)	-0.32	0 100 100	46, 46, 58, 60	0
2	Q	3/6 (50%)	-0.56	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%)	-0.64	0 100 100	37, 37, 42, 46	0
2	S	3/6 (50%)	-0.04	0 100 100	44, 44, 57, 59	0
2	T	3/6 (50%)	-0.54	0 100 100	44, 44, 60, 65	0
2	U	3/6 (50%)	-0.44	0 100 100	43, 43, 45, 52	0
2	V	3/6 (50%)	0.31	0 100 100	55, 55, 64, 70	0
2	X	3/6 (50%)	-0.63	0 100 100	30, 30, 30, 43	0
2	Y	3/6 (50%)	-0.61	0 100 100	39, 39, 42, 48	0
2	Z	3/6 (50%)	-0.53	0 100 100	31, 31, 33, 43	0
All	All	5874/5984 (98%)	-0.08	195 (3%) 46 45	20, 47, 78, 116	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	212	ASP	13.1
1	O	186	ILE	11.5
1	P	211	GLN	8.7
1	F	186	ILE	6.5
1	N	251	ARG	6.4
1	P	251	ARG	6.3
1	F	211	GLN	6.1
1	N	115	ASP	5.9
1	D	212	ASP	5.6
1	P	210	GLU	5.6
1	D	186	ILE	5.5
1	F	212	ASP	5.4
1	G	26	THR	5.3
1	N	210	GLU	5.3
1	D	231	PHE	5.2
1	H	115	ASP	5.1
1	N	211	GLN	5.1
1	D	205	ALA	5.0
1	F	231	PHE	5.0
1	F	213	GLY	4.9
1	C	186	ILE	4.9
1	N	309	VAL	4.8
1	E	191	ARG	4.6
1	N	231	PHE	4.5
1	P	207	LEU	4.5
1	C	191	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	N	22	GLU	4.5
1	D	252	GLY	4.4
1	E	164	GLY	4.4
1	F	210	GLU	4.4
1	N	212	ASP	4.4
1	M	164	GLY	4.3
1	I	26	THR	4.2
1	F	207	LEU	4.2
1	C	192	HIS	4.1
1	F	205	ALA	4.1
1	L	230	GLU	4.1
1	O	187	PRO	4.0
1	P	186	ILE	4.0
1	P	209	THR	4.0
1	F	26	THR	3.9
1	I	119	VAL	3.9
1	H	209	THR	3.9
1	D	187	PRO	3.9
1	P	231	PHE	3.9
1	M	186	ILE	3.9
1	N	207	LEU	3.8
1	F	209	THR	3.8
1	D	185	GLN	3.7
1	F	185	GLN	3.7
1	N	209	THR	3.7
1	M	26	THR	3.7
1	N	205	ALA	3.6
1	F	257	VAL	3.6
1	C	251	ARG	3.6
1	N	120	GLU	3.5
1	P	208	LEU	3.5
1	C	122	GLY	3.5
1	N	206	ARG	3.5
1	D	207	LEU	3.5
1	L	211	GLN	3.5
1	M	27	LEU	3.5
1	D	87	LEU	3.5
1	N	191	ARG	3.4
1	P	206	ARG	3.4
1	N	186	ILE	3.4
1	O	188	SER	3.4
1	P	164	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	190	ASP	3.4
1	H	229	GLY	3.3
1	M	252	GLY	3.2
1	E	26	THR	3.2
1	O	230	GLU	3.2
1	E	192	HIS	3.2
1	K	182	LEU	3.2
1	M	230	GLU	3.1
1	J	213	GLY	3.0
1	F	187	PRO	3.0
1	D	5	ILE	3.0
1	J	164	GLY	3.0
1	N	229	GLY	3.0
1	D	257	VAL	3.0
1	C	164	GLY	2.9
1	D	182	LEU	2.9
1	O	164	GLY	2.9
1	A	209	THR	2.9
1	P	191	ARG	2.9
1	L	26	THR	2.9
1	P	182	LEU	2.9
1	D	165	GLY	2.9
1	E	183	ASP	2.9
1	J	115	ASP	2.9
1	C	212	ASP	2.8
1	N	185	GLN	2.8
1	O	212	ASP	2.8
1	D	253	GLY	2.8
1	L	252	GLY	2.8
1	M	212	ASP	2.8
1	B	252	GLY	2.8
1	P	22	GLU	2.8
1	N	248	VAL	2.7
1	D	164	GLY	2.7
1	N	213	GLY	2.7
1	D	211	GLN	2.7
1	P	134	LYS	2.7
1	N	163	ASN	2.7
1	P	205	ALA	2.7
1	F	166	THR	2.7
1	O	257	VAL	2.7
1	F	339	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	LEU	2.7
1	E	126	LEU	2.7
1	O	121	GLU	2.6
1	A	164	GLY	2.6
1	F	252	GLY	2.6
1	J	212	ASP	2.6
1	F	316	LEU	2.6
1	I	164	GLY	2.6
1	N	208	LEU	2.6
1	N	93	GLU	2.6
1	C	126	LEU	2.6
1	G	28	PRO	2.5
1	P	37	VAL	2.5
1	J	230	GLU	2.5
1	F	128	PHE	2.5
1	L	213	GLY	2.5
1	F	184	ALA	2.5
1	P	183	ASP	2.5
1	G	164	GLY	2.5
1	F	17	VAL	2.5
1	C	189	GLN	2.5
1	P	185	GLN	2.4
1	I	103	ARG	2.4
1	O	189	GLN	2.4
1	J	26	THR	2.4
1	F	27	LEU	2.4
1	C	190	ASP	2.4
1	N	192	HIS	2.4
1	A	182	LEU	2.3
1	D	259	GLY	2.3
1	N	118	THR	2.3
1	D	25	GLN	2.3
1	O	128	PHE	2.3
1	L	164	GLY	2.3
1	D	59	LEU	2.3
1	D	353	ALA	2.3
1	D	163	ASN	2.3
1	N	341	LEU	2.3
1	P	248	VAL	2.3
1	O	183	ASP	2.3
1	C	229	GLY	2.3
1	J	211	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	27	LEU	2.2
1	D	215	VAL	2.2
1	L	114	ASN	2.2
1	O	185	GLN	2.2
1	F	253	GLY	2.2
1	O	252	GLY	2.2
1	J	182	LEU	2.2
1	O	27	LEU	2.2
1	K	103	ARG	2.2
1	C	123	PRO	2.2
1	J	252	GLY	2.2
1	K	164	GLY	2.2
1	O	192	HIS	2.2
1	P	21	VAL	2.2
1	B	182	LEU	2.2
1	E	186	ILE	2.2
1	C	27	LEU	2.2
1	C	248	VAL	2.2
1	F	183	ASP	2.2
1	C	246	GLU	2.1
1	E	229	GLY	2.1
1	F	87	LEU	2.1
1	M	182	LEU	2.1
1	J	229	GLY	2.1
1	N	164	GLY	2.1
1	F	341	LEU	2.1
1	F	230	GLU	2.1
1	P	252	GLY	2.1
1	D	3	PHE	2.1
1	O	17	VAL	2.1
1	M	128	PHE	2.1
1	H	164	GLY	2.1
1	M	229	GLY	2.1
1	N	124	GLY	2.1
1	N	333	GLY	2.1
1	F	206	ARG	2.0
1	F	308	GLN	2.0
1	M	57	VAL	2.0
1	N	348	ALA	2.0
1	F	251	ARG	2.0
1	N	132	GLN	2.0
1	E	28	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	189	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
2	ZCL	T	472	14/14	0.69	0.18	86,90,106,108	0
2	ZCL	S	472	14/14	0.75	0.17	83,89,109,110	0
2	ZCL	V	472	14/14	0.77	0.17	79,84,103,106	0
2	ZCL	4	472	14/14	0.78	0.23	83,85,108,111	0
2	ZCL	6	472	14/14	0.79	0.15	75,78,91,93	0
2	ZCL	5	472	14/14	0.81	0.19	88,91,112,113	0
2	ZCL	1	472	14/14	0.81	0.13	49,54,65,67	0
2	ZCL	R	472	14/14	0.82	0.11	51,55,70,71	0
2	ZCL	Q	472	14/14	0.86	0.14	43,55,63,66	0
2	ZCL	Y	472	14/14	0.86	0.15	46,53,63,66	0
2	ZCL	3	472	14/14	0.87	0.11	52,55,62,63	0
2	ZCL	Z	472	14/14	0.88	0.10	27,39,42,46	0
2	ZCL	0	472	14/14	0.90	0.10	46,51,62,64	0
2	ZCL	U	472	14/14	0.90	0.12	50,52,69,69	0
2	ALC	0	469	11/12	0.90	0.11	39,44,48,49	0
2	ZCL	2	472	14/14	0.91	0.09	42,55,61,64	0
2	ALC	Y	469	11/12	0.92	0.11	38,42,49,49	0
2	ALC	X	469	11/12	0.92	0.09	31,36,41,42	0
2	ALC	6	469	11/12	0.92	0.13	49,55,62,63	0
2	ALC	5	469	11/12	0.93	0.15	49,55,64,65	0
2	ALC	R	469	11/12	0.93	0.11	34,38,50,51	0
2	ZCL	X	472	14/14	0.93	0.08	29,38,41,45	0
2	ALC	3	469	11/12	0.93	0.13	46,50,54,55	0
2	ALC	T	469	11/12	0.94	0.12	48,54,63,65	0
2	ALC	V	469	11/12	0.94	0.19	56,64,67,68	0
2	ALC	Q	469	11/12	0.94	0.11	33,37,41,41	0
2	ALC	S	469	11/12	0.94	0.12	47,54,66,67	0
2	ALC	Z	469	11/12	0.95	0.09	30,34,44,44	0
2	ALC	1	469	11/12	0.96	0.12	36,40,51,53	0
2	ALC	4	469	11/12	0.96	0.13	56,62,66,66	0
2	ALC	U	469	11/12	0.97	0.10	43,46,53,53	0
2	ALC	2	469	11/12	0.97	0.07	34,38,46,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.