



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:07 pm BST

PDB ID : 4N3N  
Title : Crystal structure of eukaryotic translation initiation factor eIF5B (517-1116) from *Chaetomium thermophilum*, apo form  
Authors : Kuhle, B.; Ficner, R.  
Deposited on : 2013-10-07  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

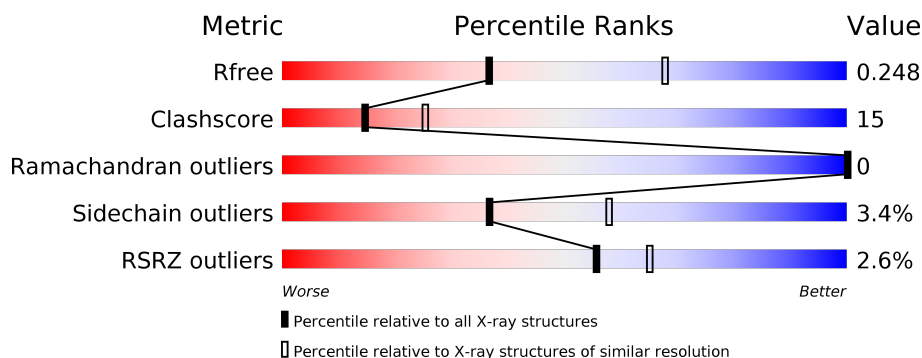
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	603	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4624 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 Eukaryotic translation initiation factor 5B-like protein, eIF5B(517-C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	2	0
			4591	2921	787	861	22			

There are 27 discrepancies between the modelled and reference sequences:

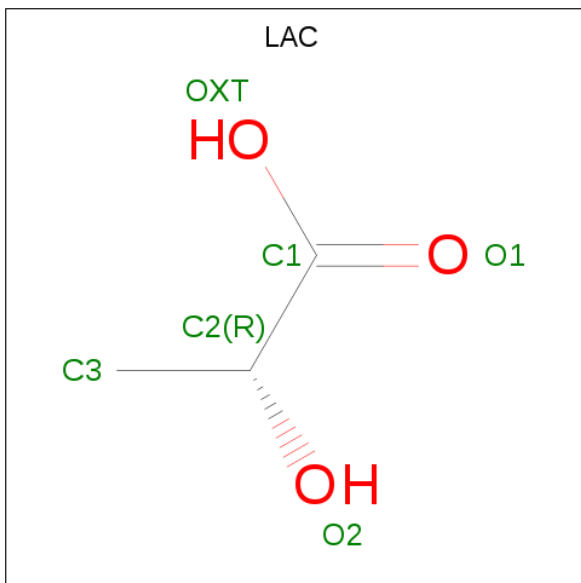
Chain	Residue	Modelled	Actual	Comment	Reference
A	514	SER	-	EXPRESSION TAG	UNP G0S8G9
A	515	HIS	-	EXPRESSION TAG	UNP G0S8G9
A	516	MET	-	EXPRESSION TAG	UNP G0S8G9
A	576	VAL	-	EXPRESSION TAG	UNP G0S8G9
A	577	VAL	-	EXPRESSION TAG	UNP G0S8G9
A	578	ASN	-	EXPRESSION TAG	UNP G0S8G9
A	579	LYS	-	EXPRESSION TAG	UNP G0S8G9
A	580	ASP	-	EXPRESSION TAG	UNP G0S8G9
A	581	GLY	-	EXPRESSION TAG	UNP G0S8G9
A	582	LYS	-	EXPRESSION TAG	UNP G0S8G9
A	583	PHE	-	EXPRESSION TAG	UNP G0S8G9
A	584	GLU	-	EXPRESSION TAG	UNP G0S8G9
A	585	PHE	-	EXPRESSION TAG	UNP G0S8G9
A	586	LYS	-	EXPRESSION TAG	UNP G0S8G9
A	587	VAL	-	EXPRESSION TAG	UNP G0S8G9
A	588	PRO	-	EXPRESSION TAG	UNP G0S8G9
A	589	GLY	-	EXPRESSION TAG	UNP G0S8G9
A	590	LEU	-	EXPRESSION TAG	UNP G0S8G9
A	591	LEU	-	EXPRESSION TAG	UNP G0S8G9
A	592	ILE	-	EXPRESSION TAG	UNP G0S8G9
A	593	ILE	-	EXPRESSION TAG	UNP G0S8G9
A	594	ASP	-	EXPRESSION TAG	UNP G0S8G9
A	595	THR	-	EXPRESSION TAG	UNP G0S8G9
A	596	PRO	-	EXPRESSION TAG	UNP G0S8G9
A	597	GLY	-	EXPRESSION TAG	UNP G0S8G9
A	598	HIS	-	EXPRESSION TAG	UNP G0S8G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	599	GLU	-	EXPRESSION TAG	UNP G0S8G9

- Molecule 2 is LACTIC ACID (three-letter code: LAC) (formula:  $C_3H_6O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

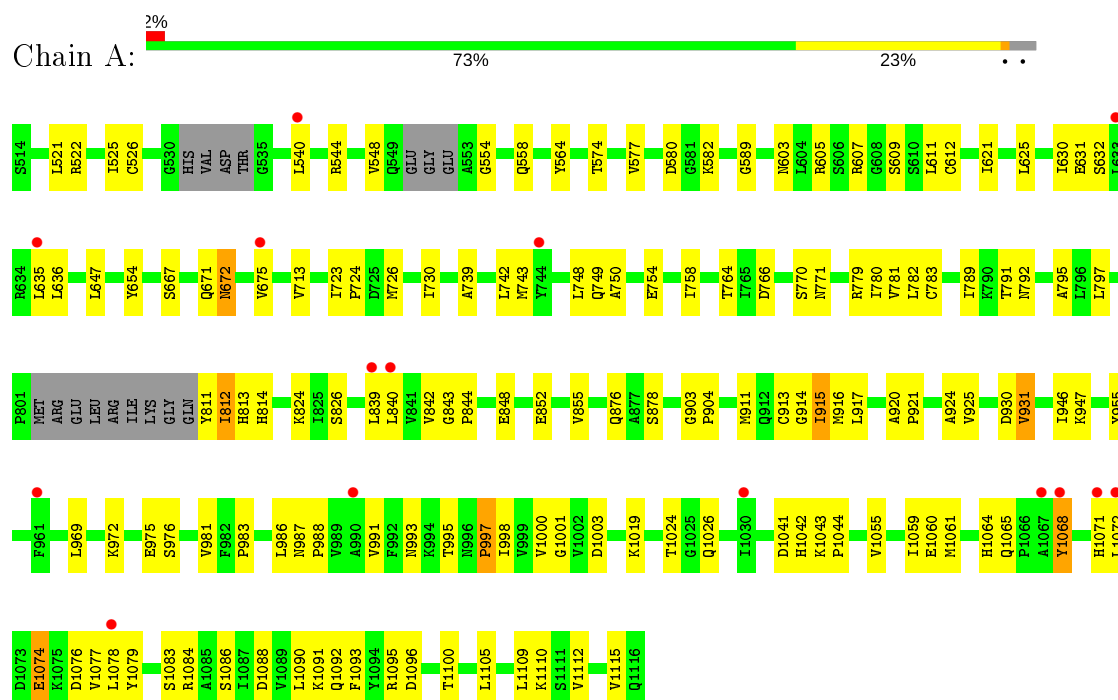
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Eukaryotic translation initiation factor 5B-like protein, eIF5B(517-C)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.47Å 111.47Å 115.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.68 – 2.75 48.27 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.68-2.75) 99.9 (48.27-2.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.193 , 0.238 0.214 , 0.248	Depositor DCC
$R_{free}$ test set	1097 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LAC

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	0.32	3/4663 (0.1%)	0.49	3/6292 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1044	PRO	N-CD	5.27	1.55	1.47
1	A	921	PRO	N-CD	5.08	1.54	1.47
1	A	844	PRO	N-CD	5.07	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	843	GLY	C-N-CD	5.80	140.57	128.40
1	A	920	ALA	C-N-CD	5.74	140.45	128.40
1	A	1043	LYS	C-N-CD	5.60	140.16	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	4591	0	4694	142	0
2	A	6	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	1	0
All	All	4624	0	4699	142	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 15.

All (142) 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:A:625:LEU:CD2	1:A:630:ILE:HD11	1.77	1.15
1:A:625:LEU:HD21	1:A:630:ILE:CG1	1.76	1.14
1:A:1074:GLU:OE1	1:A:1074:GLU:N	1.88	1.06
1:A:625:LEU:HD21	1:A:630:ILE:CD1	1.89	1.02
1:A:1088:ASP:O	1:A:1092:GLN:HG3	1.63	0.98
1:A:1083:SER:H	1:A:1086:SER:HB3	1.36	0.90
1:A:625:LEU:HD21	1:A:630:ILE:HD11	1.44	0.90
1:A:540:LEU:HD21	1:A:544:ARG:HH11	1.39	0.88
1:A:1068:TYR:CD1	1:A:1072:LEU:HB3	2.12	0.84
1:A:1091:LYS:O	1:A:1095:ARG:HG3	1.81	0.81
1:A:1068:TYR:HA	1:A:1072:LEU:HB2	1.63	0.80
1:A:540:LEU:HD21	1:A:544:ARG:NH1	2.00	0.76
1:A:625:LEU:CD2	1:A:630:ILE:CD1	2.54	0.75
1:A:625:LEU:HD22	1:A:630:ILE:HD11	1.66	0.75
1:A:607:ARG:HH11	1:A:607:ARG:HG2	1.49	0.75
1:A:625:LEU:HD21	1:A:630:ILE:HG13	1.68	0.75
1:A:983:PRO:HB2	1:A:1105:LEU:HD23	1.70	0.73
1:A:1071:HIS:C	1:A:1072:LEU:HD12	2.10	0.72
1:A:840:LEU:HD12	1:A:855:VAL:HB	1.72	0.71
1:A:625:LEU:HD21	1:A:630:ILE:HG12	1.68	0.71
1:A:925:VAL:HG12	1:A:947:LYS:HB2	1.73	0.70
1:A:812:ILE:HD11	1:A:814:HIS:NE2	2.07	0.69
1:A:1061:MET:SD	1:A:1065:GLN:HG3	2.33	0.69
1:A:779:ARG:HB3	1:A:842:VAL:CG1	2.22	0.69
1:A:671:GLN:HB3	1:A:675:VAL:CG2	2.23	0.68
1:A:782:LEU:HA	1:A:855:VAL:HG21	1.74	0.68
1:A:812:ILE:O	1:A:812:ILE:HG13	1.93	0.68
1:A:779:ARG:HB3	1:A:842:VAL:HG12	1.75	0.68
1:A:1083:SER:N	1:A:1086:SER:HB3	2.08	0.68
1:A:654:TYR:O	1:A:675:VAL:HG12	1.94	0.66
1:A:1061:MET:HE2	1:A:1064:HIS:O	1.93	0.66
1:A:621:ILE:HG13	1:A:647:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LEU:HD12	1:A:955:TYR:OH	1.96	0.66
1:A:1084:ARG:HD3	1:A:1084:ARG:O	1.96	0.66
1:A:635:LEU:CD1	1:A:955:TYR:CE2	2.79	0.65
1:A:1061:MET:CE	1:A:1064:HIS:O	2.46	0.64
1:A:1110:LYS:HG2	1:A:1115:VAL:HB	1.80	0.64
1:A:1083:SER:OG	1:A:1086:SER:N	2.31	0.63
1:A:1109:LEU:HA	1:A:1112:VAL:HG13	1.79	0.63
1:A:603:ASN:OD1	1:A:611:LEU:HD12	1.98	0.63
1:A:635:LEU:CD1	1:A:955:TYR:HE2	2.11	0.63
1:A:1041:ASP:O	1:A:1042:HIS:HB2	1.98	0.63
1:A:1019:LYS:HE2	1:A:1076:ASP:OD2	1.99	0.63
1:A:1068:TYR:HD1	1:A:1072:LEU:HB3	1.61	0.62
1:A:972:LYS:HA	1:A:975:GLU:HG2	1.81	0.62
1:A:911:MET:O	1:A:915:ILE:HD13	2.00	0.61
1:A:548:VAL:HG11	1:A:554:GLY:HA3	1.81	0.61
1:A:981:VAL:O	1:A:1090:LEU:HD11	2.00	0.61
1:A:739:ALA:O	1:A:743:MET:HG2	2.01	0.61
1:A:522:ARG:HG2	1:A:742:LEU:O	2.00	0.60
1:A:631:GLU:O	1:A:635:LEU:HD13	2.02	0.60
1:A:1000:VAL:HG11	1:A:1068:TYR:CE2	2.37	0.59
1:A:1068:TYR:O	1:A:1072:LEU:HB2	2.04	0.58
1:A:1071:HIS:O	1:A:1072:LEU:HD12	2.04	0.58
1:A:779:ARG:CG	1:A:842:VAL:CG1	2.82	0.58
1:A:635:LEU:HD11	1:A:955:TYR:CE2	2.38	0.57
1:A:1059:ILE:O	1:A:1065:GLN:NE2	2.34	0.57
1:A:1068:TYR:CD1	1:A:1072:LEU:CB	2.86	0.57
1:A:726:MET:O	1:A:730:ILE:HG12	2.05	0.57
1:A:779:ARG:HG2	1:A:842:VAL:HG11	1.85	0.56
1:A:671:GLN:HB3	1:A:675:VAL:HG21	1.86	0.56
1:A:1064:HIS:CD2	1:A:1065:GLN:N	2.73	0.56
1:A:580:ASP:HB2	1:A:582:LYS:HD3	1.86	0.56
1:A:878:SER:HB3	1:A:930:ASP:O	2.06	0.56
1:A:766:ASP:OD2	1:A:824:LYS:NZ	2.36	0.56
1:A:1096:ASP:N	1:A:1096:ASP:OD1	2.39	0.55
1:A:1000:VAL:HG11	1:A:1068:TYR:HE2	1.70	0.54
1:A:993:ASN:ND2	1:A:995:THR:O	2.40	0.54
1:A:540:LEU:CD2	1:A:544:ARG:NH1	2.70	0.54
1:A:580:ASP:N	1:A:580:ASP:OD1	2.29	0.54
1:A:749:GLN:HB3	1:A:770:SER:HB2	1.89	0.54
1:A:780:ILE:HB	1:A:839:LEU:HD11	1.90	0.53
1:A:1083:SER:H	1:A:1086:SER:CB	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:ARG:CB	1:A:842:VAL:HG12	2.39	0.53
1:A:983:PRO:HB2	1:A:1105:LEU:CD2	2.37	0.52
1:A:621:ILE:HD12	1:A:647:LEU:HD21	1.91	0.52
1:A:812:ILE:CD1	1:A:814:HIS:NE2	2.73	0.52
1:A:671:GLN:HB3	1:A:675:VAL:HG23	1.91	0.52
1:A:915:ILE:N	1:A:915:ILE:CD1	2.73	0.52
1:A:813:HIS:N	1:A:813:HIS:CD2	2.78	0.51
1:A:913:CYS:O	1:A:916:MET:HB2	2.11	0.51
1:A:916:MET:HB3	1:A:924:ALA:HB2	1.93	0.51
1:A:1068:TYR:CA	1:A:1072:LEU:HB2	2.36	0.50
1:A:754:GLU:HB2	1:A:766:ASP:HB2	1.92	0.50
1:A:1064:HIS:HD2	1:A:1065:GLN:N	2.09	0.50
1:A:797:LEU:HB2	1:A:824:LYS:HB3	1.93	0.50
1:A:1019:LYS:CE	1:A:1076:ASP:OD2	2.60	0.50
1:A:607:ARG:NH1	1:A:607:ARG:HG2	2.21	0.50
1:A:779:ARG:CG	1:A:842:VAL:HG11	2.42	0.50
1:A:842:VAL:HG13	1:A:842:VAL:O	2.12	0.49
1:A:607:ARG:CG	1:A:607:ARG:HH11	2.22	0.49
1:A:621:ILE:CD1	1:A:647:LEU:HD21	2.42	0.49
1:A:1019:LYS:NZ	1:A:1076:ASP:OD2	2.45	0.48
1:A:876:GLN:NE2	1:A:903:GLY:O	2.46	0.48
1:A:779:ARG:CB	1:A:842:VAL:CG1	2.91	0.48
1:A:997:PRO:HB3	1:A:1060:GLU:HB3	1.95	0.48
1:A:917:LEU:HD11	1:A:946:ILE:HD11	1.96	0.47
1:A:812:ILE:HD11	1:A:814:HIS:CE1	2.49	0.47
1:A:758:ILE:HG13	1:A:824:LYS:HE2	1.97	0.47
1:A:1077:VAL:HG12	1:A:1078:LEU:N	2.29	0.47
1:A:781:VAL:HA	1:A:789:ILE:O	2.15	0.47
1:A:667:SER:O	1:A:671:GLN:HG2	2.16	0.46
1:A:609:SER:HA	1:A:612:CYS:O	2.15	0.46
1:A:750:ALA:HB3	1:A:839:LEU:HB3	1.98	0.46
1:A:811:TYR:N	3:A:1324:HOH:O	2.48	0.45
1:A:904:PRO:HA	1:A:931:VAL:HG13	1.97	0.45
1:A:1074:GLU:H	1:A:1074:GLU:CD	2.15	0.44
1:A:713:VAL:HG11	1:A:726:MET:HB2	1.99	0.44
1:A:1000:VAL:CG1	1:A:1068:TYR:HE2	2.31	0.44
1:A:621:ILE:CG1	1:A:647:LEU:HD11	2.45	0.44
1:A:672:ASN:O	1:A:675:VAL:HG22	2.17	0.44
1:A:1092:GLN:HB2	1:A:1093:PHE:CE2	2.52	0.44
1:A:779:ARG:HG2	1:A:842:VAL:CG1	2.46	0.44
1:A:1068:TYR:CE1	1:A:1072:LEU:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:ILE:N	1:A:915:ILE:HD12	2.32	0.43
1:A:1000:VAL:CG1	1:A:1068:TYR:CE2	3.01	0.43
1:A:635:LEU:HD12	1:A:955:TYR:CE2	2.53	0.43
1:A:987:ASN:HA	1:A:988:PRO:HD3	1.89	0.43
1:A:764:THR:OG1	1:A:824:LYS:HE3	2.19	0.43
1:A:911:MET:O	1:A:914:GLY:N	2.52	0.43
1:A:564:TYR:OH	1:A:589:GLY:HA3	2.19	0.43
1:A:1092:GLN:HB2	1:A:1093:PHE:CD2	2.54	0.42
1:A:1001:GLY:HA2	1:A:1055:VAL:O	2.19	0.42
1:A:1084:ARG:HD3	1:A:1084:ARG:C	2.39	0.42
1:A:574:THR:O	1:A:577:VAL:HG23	2.18	0.42
1:A:748:LEU:HD12	1:A:771:ASN:O	2.20	0.42
1:A:991:VAL:HG22	1:A:1000:VAL:HG12	2.02	0.42
1:A:795:ALA:HB3	1:A:826:SER:HB3	2.01	0.42
1:A:1024:THR:OG1	1:A:1026:GLN:HG2	2.19	0.41
1:A:986:LEU:HB2	1:A:1078:LEU:HB2	2.01	0.41
1:A:632:SER:O	1:A:636:LEU:HG	2.20	0.41
1:A:848:GLU:O	1:A:852:GLU:HG3	2.20	0.41
1:A:779:ARG:CG	1:A:842:VAL:HG12	2.50	0.41
1:A:972:LYS:HB2	1:A:972:LYS:HE3	1.79	0.41
1:A:975:GLU:HG3	1:A:976:SER:N	2.35	0.41
1:A:1068:TYR:CE1	1:A:1072:LEU:HD23	2.56	0.41
1:A:1064:HIS:CD2	1:A:1064:HIS:C	2.93	0.40
1:A:791:THR:OG1	1:A:792:ASN:N	2.54	0.40
1:A:723:ILE:N	1:A:724:PRO:HD2	2.36	0.40
1:A:995:THR:HA	1:A:998:ILE:HG12	2.02	0.40
1:A:522:ARG:NH2	1:A:743:MET:O	2.54	0.40
1:A:839:LEU:HD12	1:A:840:LEU:N	2.36	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	581/603 (96%)	574 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	507/522 (97%)	490 (97%)	17 (3%)	37	58

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	LEU
1	A	525	ILE
1	A	526	CYS
1	A	558	GLN
1	A	605	ARG
1	A	672	ASN
1	A	783	CYS
1	A	812	ILE
1	A	915	ILE
1	A	931	VAL
1	A	969	LEU
1	A	997	PRO
1	A	1003	ASP
1	A	1068	TYR
1	A	1074	GLU
1	A	1079	TYR
1	A	1100	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	813	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1064	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	LAC	A	1201	-	2,5,5	0.18	0	3,6,6	0.35	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	LAC	A	1201	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	587/603 (97%)	0.20	15 (2%) 56 65	33, 61, 94, 134	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1072	LEU	3.8
1	A	1078	LEU	3.7
1	A	961	PHE	3.5
1	A	744	TYR	2.8
1	A	1071	HIS	2.7
1	A	840	LEU	2.5
1	A	1068	TYR	2.5
1	A	839	LEU	2.3
1	A	675	VAL	2.3
1	A	635	LEU	2.2
1	A	1067	ALA	2.1
1	A	633	LEU	2.1
1	A	1030	ILE	2.1
1	A	990	ALA	2.0
1	A	540	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LAC	A	1201	6/6	0.96	0.18	39,45,48,54	0

## 6.5 Other polymers

There are no such residues in this entry.