



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:17 PM GMT

PDB ID : 1WZL  
Title : Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) mutatnt R469L  
Authors : Mizuno, M.; Ichikawa, K.; Tonozuka, T.; Ohtaki, A.; Shimura, Y.; Kamitori, S.; Nishikawa, A.; Sakano, Y.  
Deposited on : 2005-03-06  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

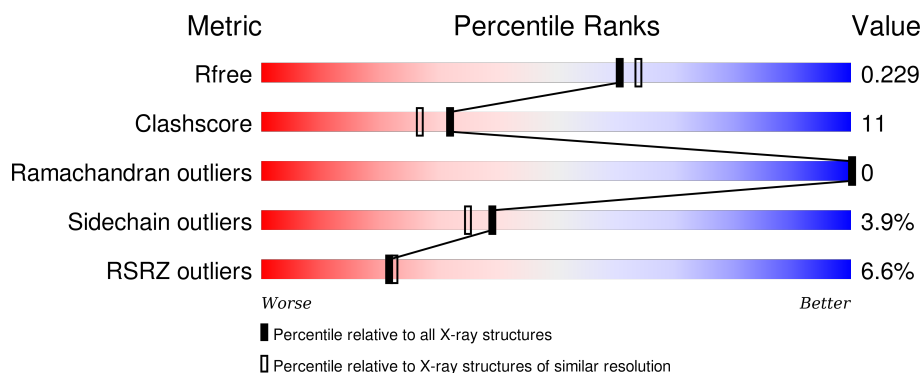
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	585	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10494 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 Alpha-amylase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4772	3056	828	873	15			
1	B	585	Total	C	N	O	S	0	0	0
			4772	3056	828	873	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	LEU	ARG	ENGINEERED	UNP Q08751
B	469	LEU	ARG	ENGINEERED	UNP Q08751

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

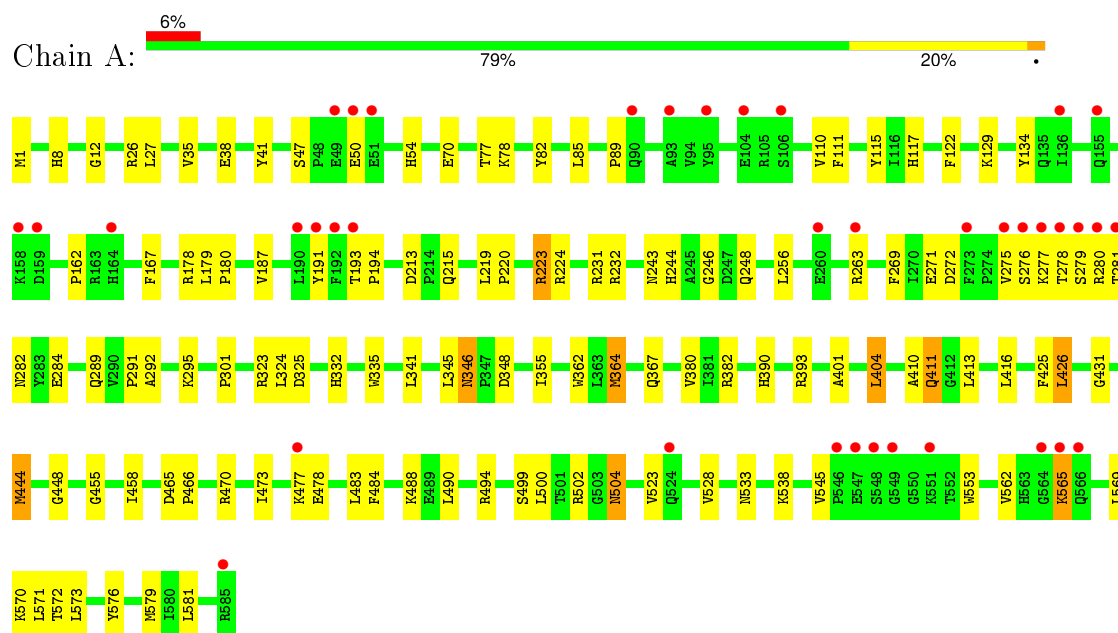
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	494	Total	O	0	0
			494	494		
3	B	454	Total	O	0	0
			454	454		

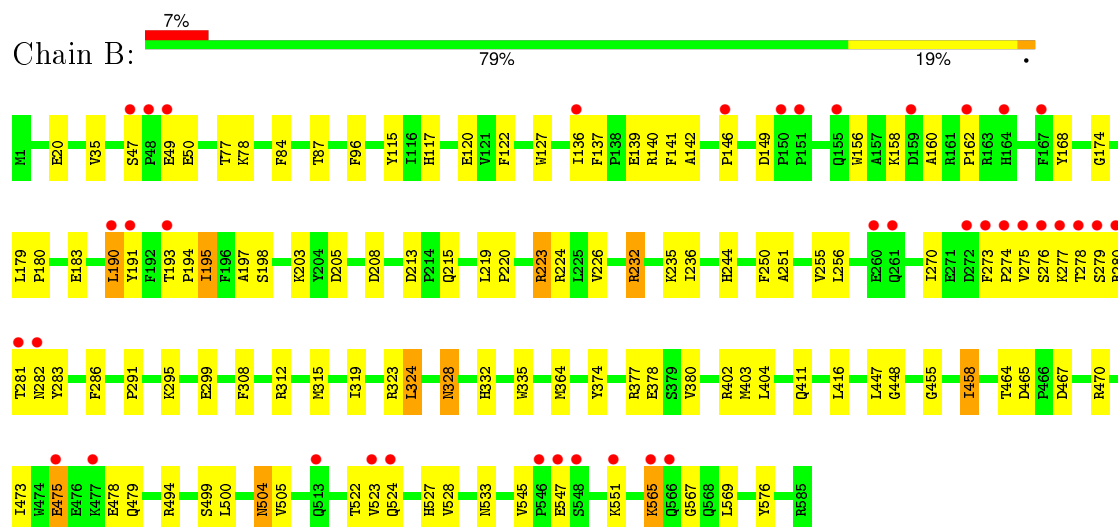
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Alpha-amylase II



#### • Molecule 1: Alpha-amylase II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.87Å 117.91Å 113.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.23 – 2.00 34.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.23-2.00) 99.8 (34.23-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.66 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.229 0.195 , 0.229	Depositor DCC
$R_{free}$ test set	10261 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.1	EDS
Estimated twinning fraction	0.013 for -h,l,k 0.011 for -k,-h,l 0.011 for l,-k,h 0.001 for l,h,k 0.001 for k,l,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102203 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/4902	0.57	0/6638
1	B	0.34	0/4902	0.57	0/6638
All	All	0.34	0/9804	0.57	0/13276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4772	0	4605	99	0
1	B	4772	0	4605	102	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	494	0	0	10	0
3	B	454	0	0	10	0
All	All	10494	0	9210	198	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 11.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.30	0.97
1:B:551:LYS:HZ1	1:B:567:GLY:H	1.03	0.93
1:B:139:GLU:HB3	1:B:140:ARG:HH11	1.35	0.88
1:B:455:GLY:HA2	1:B:458:ILE:HD11	1.56	0.87
1:A:277:LYS:HD3	1:A:278:THR:H	1.42	0.84
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.59	0.83
1:A:256:LEU:HD23	1:A:275:VAL:HG23	1.58	0.83
1:B:139:GLU:HB3	1:B:140:ARG:NH1	1.95	0.80
1:B:277:LYS:HG3	1:B:280:ARG:HB3	1.68	0.76
1:A:504:ASN:C	1:A:504:ASN:HD22	1.91	0.74
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.36	0.74
1:B:328:ASN:N	1:B:328:ASN:HD22	1.89	0.71
1:B:255:VAL:HG12	1:B:275:VAL:HG11	1.73	0.70
1:B:158:LYS:HD2	1:B:478:GLU:HB3	1.73	0.70
1:B:499:SER:HB3	1:B:523:VAL:HG12	1.72	0.69
1:A:573:LEU:HD11	1:A:579:MET:HG3	1.74	0.69
1:A:275:VAL:HA	1:A:282:ASN:HD21	1.58	0.68
1:B:551:LYS:NZ	1:B:567:GLY:H	1.88	0.67
1:B:275:VAL:HA	1:B:282:ASN:HD21	1.59	0.67
1:B:193:THR:HB	1:B:194:PRO:HD2	1.75	0.66
1:B:504:ASN:HD22	1:B:504:ASN:C	1.99	0.66
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.76	0.65
1:A:277:LYS:HB3	1:A:280:ARG:HB3	1.77	0.65
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.79	0.64
1:A:277:LYS:HD3	1:A:278:THR:N	2.13	0.63
1:B:551:LYS:HZ1	1:B:567:GLY:N	1.87	0.63
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.29	0.63
1:B:328:ASN:H	1:B:328:ASN:HD22	1.47	0.62
1:B:565:LYS:O	1:B:565:LYS:HD2	2.00	0.62
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.81	0.62
1:B:458:ILE:HD13	1:B:458:ILE:N	2.14	0.62
1:B:458:ILE:H	1:B:458:ILE:HD13	1.64	0.61
1:B:226:VAL:HG22	1:B:236:ILE:HD12	1.82	0.61
1:A:346:ASN:ND2	1:A:348:ASP:H	1.98	0.61
1:A:477:LYS:HD2	1:A:477:LYS:H	1.65	0.61
1:A:364:MET:HE2	1:A:364:MET:HA	1.81	0.61
1:A:499:SER:HB3	1:A:523:VAL:HG12	1.82	0.60
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.83	0.60
1:B:195:ILE:HD13	1:B:195:ILE:H	1.66	0.60
1:B:256:LEU:HD23	1:B:275:VAL:HG23	1.84	0.59
1:A:478:GLU:HG3	3:A:2039:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:NE	3:B:2922:HOH:O	2.36	0.59
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.83	0.58
1:A:426:LEU:HG	3:A:2002:HOH:O	2.03	0.57
1:B:183:GLU:CD	1:B:232:ARG:HG3	2.25	0.57
1:A:565:LYS:HD2	1:A:565:LYS:H	1.70	0.57
1:A:477:LYS:HD2	1:A:477:LYS:N	2.19	0.56
1:B:273:PHE:HA	1:B:274:PRO:C	2.26	0.56
1:A:364:MET:HA	1:A:364:MET:CE	2.36	0.56
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.06	0.56
1:A:504:ASN:ND2	1:A:504:ASN:C	2.57	0.56
1:B:226:VAL:HA	1:B:236:ILE:HD12	1.87	0.55
1:A:364:MET:HE1	3:A:1991:HOH:O	2.06	0.54
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.90	0.54
1:A:289:GLN:O	1:A:291:PRO:HD3	2.08	0.54
1:A:416:LEU:HD23	1:A:416:LEU:H	1.73	0.53
1:B:281:THR:CG2	1:B:291:PRO:HB3	2.39	0.53
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.43	0.53
1:B:195:ILE:HD13	3:B:3013:HOH:O	2.09	0.53
1:A:332:HIS:HE1	3:B:3014:HOH:O	1.90	0.53
1:B:328:ASN:H	1:B:328:ASN:ND2	2.05	0.53
1:B:275:VAL:HG22	3:B:2898:HOH:O	2.07	0.53
1:A:224:ARG:NE	1:A:224:ARG:HA	2.24	0.53
1:B:47:SER:OG	1:B:49:GLU:HG2	2.09	0.52
1:B:140:ARG:CZ	3:B:2922:HOH:O	2.58	0.52
1:A:269:PHE:HB2	1:A:284:GLU:HB3	1.92	0.52
1:B:523:VAL:HG13	1:B:523:VAL:O	2.10	0.52
1:B:504:ASN:ND2	1:B:504:ASN:C	2.63	0.52
1:A:248:GLN:HB2	3:A:1626:HOH:O	2.10	0.52
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.91	0.52
1:B:183:GLU:OE2	1:B:232:ARG:HG3	2.10	0.51
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.75	0.51
1:B:328:ASN:ND2	1:B:328:ASN:N	2.58	0.51
1:A:473:ILE:HD13	3:A:1921:HOH:O	2.10	0.51
1:B:180:PRO:HG3	1:B:232:ARG:NH2	2.12	0.51
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.93	0.51
1:A:35:VAL:HG21	1:A:89:PRO:HA	1.91	0.51
1:B:281:THR:HG22	1:B:291:PRO:HB3	1.91	0.51
1:A:276:SER:O	1:A:277:LYS:HB2	2.11	0.50
1:A:224:ARG:HA	1:A:224:ARG:HE	1.75	0.50
1:B:533:ASN:O	1:B:576:TYR:HA	2.12	0.50
1:B:332:HIS:HE1	3:B:2929:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:VAL:CA	1:B:282:ASN:HD21	2.25	0.49
1:B:47:SER:O	1:B:50:GLU:HB2	2.12	0.49
1:A:401:ALA:O	1:A:404:LEU:HB2	2.13	0.49
1:B:278:THR:O	1:B:279:SER:HB2	2.13	0.49
1:B:473:ILE:HD13	3:B:3017:HOH:O	2.12	0.49
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.48	0.48
1:A:346:ASN:HD22	1:A:346:ASN:C	2.15	0.48
1:B:77:THR:O	1:B:78:LYS:HB2	2.13	0.48
1:B:308:PHE:O	1:B:312:ARG:HG3	2.14	0.48
1:B:374:TYR:O	1:B:378:GLU:HG3	2.12	0.48
1:B:35:VAL:HG22	1:B:87:THR:O	2.13	0.48
1:A:278:THR:O	1:A:279:SER:HB2	2.13	0.48
1:A:301:PRO:HG3	3:A:1983:HOH:O	2.14	0.47
1:A:477:LYS:CD	1:A:477:LYS:H	2.26	0.47
1:A:12:GLY:HA2	1:A:364:MET:HE1	1.96	0.47
1:B:140:ARG:NE	1:B:168:TYR:HD2	2.12	0.47
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.49	0.47
1:A:444:MET:HG2	1:A:490:LEU:HB3	1.97	0.47
1:A:275:VAL:O	1:A:276:SER:HB2	2.15	0.47
1:A:346:ASN:HD21	1:A:348:ASP:HB2	1.80	0.47
1:A:565:LYS:O	1:A:565:LYS:HG2	2.15	0.47
1:B:276:SER:HB2	1:B:283:TYR:HE2	1.79	0.47
1:A:523:VAL:HG13	1:A:523:VAL:O	2.15	0.47
1:B:416:LEU:H	1:B:416:LEU:HD23	1.80	0.47
1:A:232:ARG:NE	3:A:1676:HOH:O	2.41	0.47
1:B:255:VAL:HG11	1:B:270:ILE:HD11	1.97	0.47
1:B:448:GLY:O	1:B:494:ARG:NH2	2.48	0.47
1:B:141:PHE:HB3	3:B:2642:HOH:O	2.14	0.47
1:A:458:ILE:HD12	1:A:473:ILE:HB	1.96	0.46
1:B:226:VAL:HA	1:B:236:ILE:CD1	2.46	0.46
1:B:139:GLU:O	1:B:140:ARG:HD3	2.15	0.46
1:A:8:HIS:HD2	1:A:26:ARG:O	1.99	0.46
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.99	0.45
1:B:522:THR:OG1	1:B:527:HIS:HD2	2.00	0.45
1:B:140:ARG:HE	1:B:168:TYR:HD2	1.65	0.45
1:B:464:THR:O	1:B:465:ASP:C	2.55	0.45
1:A:411:GLN:NE2	3:A:1775:HOH:O	2.49	0.45
1:A:533:ASN:O	1:A:576:TYR:HA	2.16	0.45
1:A:401:ALA:HA	1:A:404:LEU:HD22	1.99	0.45
1:A:341:LEU:O	1:A:345:LEU:HD13	2.17	0.45
1:A:272:ASP:O	1:A:282:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ARG:HG2	1:B:403:MET:CE	2.47	0.44
1:A:219:LEU:HB2	1:A:220:PRO:HD3	2.00	0.44
1:A:380:VAL:HG12	1:A:425:PHE:CZ	2.53	0.44
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.29	0.44
1:B:255:VAL:CG1	1:B:275:VAL:HG11	2.46	0.44
1:A:382:ARG:HD3	3:A:1955:HOH:O	2.17	0.44
1:B:20:GLU:HB2	3:B:2897:HOH:O	2.17	0.43
1:B:276:SER:HA	1:B:282:ASN:OD1	2.18	0.43
1:A:426:LEU:HD22	1:A:431:GLY:HA2	2.00	0.43
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.54	0.43
1:A:553:TRP:HB2	1:A:562:VAL:CG2	2.47	0.43
1:B:213:ASP:OD1	1:B:215:GLN:HG2	2.18	0.43
1:A:82:TYR:O	1:A:110:VAL:HG23	2.18	0.43
1:A:565:LYS:HD2	1:A:565:LYS:N	2.32	0.43
1:A:77:THR:O	1:A:78:LYS:HB2	2.18	0.43
1:B:117:HIS:HB2	1:B:120:GLU:HG3	2.01	0.43
1:B:377:ARG:O	1:B:380:VAL:HG22	2.18	0.43
1:B:179:LEU:N	1:B:180:PRO:CD	2.81	0.43
1:B:504:ASN:HD21	1:B:522:THR:HB	1.82	0.43
1:A:455:GLY:O	1:A:458:ILE:HG13	2.19	0.43
1:B:136:ILE:HD12	1:B:190:LEU:HG	2.01	0.43
1:A:117:HIS:HB3	1:B:299:GLU:OE2	2.18	0.43
1:A:573:LEU:CD1	1:A:579:MET:HG3	2.47	0.43
1:B:160:ALA:O	1:B:162:PRO:HD3	2.18	0.43
1:A:41:TYR:HB3	1:A:82:TYR:HB3	2.00	0.43
1:A:246:GLY:HA2	1:A:292:ALA:O	2.19	0.43
1:A:271:GLU:HG2	1:A:282:ASN:O	2.18	0.43
1:A:573:LEU:HD11	1:A:579:MET:CG	2.46	0.43
1:A:179:LEU:N	1:A:180:PRO:CD	2.82	0.43
1:A:553:TRP:HB3	1:A:581:LEU:HB3	2.01	0.43
1:A:213:ASP:OD1	1:A:215:GLN:HG2	2.19	0.43
1:A:82:TYR:C	1:A:110:VAL:HG23	2.39	0.42
1:A:193:THR:HB	1:A:194:PRO:CD	2.49	0.42
1:A:223:ARG:NH1	1:A:223:ARG:HB3	2.34	0.42
1:B:315:MET:HA	1:B:319:ILE:HG12	2.01	0.42
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.54	0.42
1:A:465:ASP:HA	1:A:466:PRO:HA	1.85	0.42
1:B:475:GLU:O	1:B:479:GLN:HG3	2.19	0.42
1:B:275:VAL:O	1:B:276:SER:HB2	2.19	0.42
1:A:416:LEU:H	1:A:416:LEU:CD2	2.33	0.42
1:B:223:ARG:NH2	1:B:223:ARG:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HA	1:A:413:LEU:HG	2.01	0.42
1:B:197:ALA:HB3	1:B:208:ASP:HB3	2.01	0.42
1:B:402:ARG:HG2	1:B:403:MET:HE3	2.02	0.42
1:A:27:LEU:C	1:A:27:LEU:HD23	2.39	0.41
1:B:142:ALA:O	1:B:174:GLY:HA3	2.19	0.41
1:B:256:LEU:HA	1:B:275:VAL:HG21	2.02	0.41
1:A:346:ASN:HD22	1:A:348:ASP:H	1.68	0.41
1:B:467:ASP:OD1	1:B:470:ARG:HD3	2.20	0.41
1:A:545:VAL:O	1:A:545:VAL:HG23	2.20	0.41
1:B:545:VAL:HG23	1:B:545:VAL:O	2.20	0.41
1:A:277:LYS:HD2	1:A:280:ARG:HB3	2.01	0.41
1:A:448:GLY:O	1:A:494:ARG:NH2	2.54	0.41
1:B:205:ASP:OD1	1:B:205:ASP:N	2.51	0.41
1:B:324:LEU:HD13	1:B:335:TRP:CH2	2.56	0.41
1:B:156:TRP:HB2	3:B:2980:HOH:O	2.21	0.41
1:A:355:ILE:HD13	1:A:362:TRP:CE3	2.55	0.41
1:B:250:PHE:CG	1:B:251:ALA:N	2.88	0.41
1:B:137:PHE:HE1	1:B:140:ARG:NH1	2.18	0.41
1:B:500:LEU:HD21	1:B:528:VAL:HG11	2.03	0.41
1:B:195:ILE:N	1:B:195:ILE:HD13	2.35	0.41
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.55	0.41
1:A:390:HIS:CD2	1:A:393:ARG:H	2.39	0.41
1:A:231:ARG:NH2	3:A:1869:HOH:O	2.52	0.41
1:B:146:PRO:HA	1:B:149:ASP:OD2	2.20	0.41
1:A:38:GLU:OE1	1:A:54:HIS:HD2	2.04	0.41
1:A:346:ASN:C	1:A:346:ASN:ND2	2.75	0.41
1:A:178:ARG:HG2	1:A:178:ARG:HH21	1.86	0.40
1:B:127:TRP:CD2	1:B:235:LYS:HD2	2.56	0.40
1:A:538:LYS:HE2	1:A:572:THR:HG21	2.03	0.40
1:A:570:LYS:O	1:A:571:LEU:HD12	2.21	0.40
1:A:500:LEU:HD21	1:A:528:VAL:HG11	2.03	0.40
1:B:276:SER:OG	1:B:277:LYS:N	2.54	0.40
1:A:134:TYR:HB2	1:A:187:VAL:HG11	2.04	0.40
1:A:110:VAL:HG22	1:A:111:PHE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	560 (96%)	23 (4%)	0	100	100
1	B	583/585 (100%)	567 (97%)	16 (3%)	0	100	100
All	All	1166/1170 (100%)	1127 (97%)	39 (3%)	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	493/493 (100%)	474 (96%)	19 (4%)	39	35
1	B	493/493 (100%)	474 (96%)	19 (4%)	39	35
All	All	986/986 (100%)	948 (96%)	38 (4%)	39	35

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	85	LEU
1	A	122	PHE
1	A	167	PHE
1	A	191	TYR
1	A	223	ARG
1	A	263	ARG
1	A	281	THR

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Mol	Chain	Res	Type
1	A	323	ARG
1	A	325	ASP
1	A	346	ASN
1	A	364	MET
1	A	404	LEU
1	A	411	GLN
1	A	426	LEU
1	A	444	MET
1	A	483	LEU
1	A	504	ASN
1	A	565	LYS
1	B	122	PHE
1	B	190	LEU
1	B	191	TYR
1	B	195	ILE
1	B	223	ARG
1	B	224	ARG
1	B	232	ARG
1	B	323	ARG
1	B	324	LEU
1	B	328	ASN
1	B	364	MET
1	B	404	LEU
1	B	411	GLN
1	B	458	ILE
1	B	475	GLU
1	B	504	ASN
1	B	524	GLN
1	B	565	LYS
1	B	569	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	54	HIS
1	A	135	GLN
1	A	155	GLN
1	A	201	HIS
1	A	244	HIS
1	A	332	HIS
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	367	GLN
1	A	390	HIS
1	A	411	GLN
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS
1	A	544	GLN
1	B	135	GLN
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	504	ASN
1	B	509	HIS
1	B	527	HIS
1	B	566	GLN
1	B	568	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	585/585 (100%)	0.28	38 (6%)	22 23	14, 21, 42, 76	0
1	B	585/585 (100%)	0.39	39 (6%)	21 22	13, 22, 44, 81	0
All	All	1170/1170 (100%)	0.34	77 (6%)	22 22	13, 22, 44, 81	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	VAL	14.0
1	B	278	THR	12.9
1	A	279	SER	12.5
1	B	279	SER	12.4
1	A	278	THR	12.3
1	B	280	ARG	9.6
1	B	274	PRO	6.7
1	B	276	SER	6.2
1	A	277	LYS	6.1
1	B	277	LYS	6.0
1	A	280	ARG	5.8
1	B	548	SER	5.4
1	B	273	PHE	4.6
1	A	565	LYS	4.6
1	A	276	SER	4.6
1	B	155	GLN	4.4
1	B	272	ASP	4.4
1	B	281	THR	3.9
1	B	547	GLU	3.8
1	B	159	ASP	3.7
1	A	585	ARG	3.6
1	B	566	GLN	3.6
1	A	275	VAL	3.5
1	B	260	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	523	VAL	3.3
1	B	261	GLN	3.2
1	B	551	LYS	3.2
1	B	546	PRO	3.1
1	A	93	ALA	3.1
1	A	106	SER	3.1
1	A	548	SER	3.1
1	B	164	HIS	3.0
1	A	547	GLU	2.9
1	B	190	LEU	2.9
1	B	282	ASN	2.9
1	A	263	ARG	2.9
1	B	49	GLU	2.8
1	A	546	PRO	2.8
1	A	549	GLY	2.8
1	A	159	ASP	2.7
1	B	513	GLN	2.6
1	A	551	LYS	2.6
1	B	475	GLU	2.6
1	A	95	TYR	2.5
1	A	164	HIS	2.5
1	A	155	GLN	2.5
1	A	566	GLN	2.5
1	A	192	PHE	2.5
1	A	564	GLY	2.4
1	B	146	PRO	2.4
1	A	50	GLU	2.4
1	A	524	GLN	2.4
1	B	167	PHE	2.4
1	A	477	LYS	2.4
1	A	136	ILE	2.4
1	A	90	GLN	2.4
1	B	150	PRO	2.4
1	A	104	GLU	2.4
1	B	48	PRO	2.3
1	A	191	TYR	2.3
1	B	151	PRO	2.3
1	B	191	TYR	2.3
1	A	49	GLU	2.3
1	B	193	THR	2.2
1	B	477	LYS	2.2
1	A	51	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	524	GLN	2.1
1	A	158	LYS	2.1
1	A	260	GLU	2.1
1	B	47	SER	2.1
1	A	190	LEU	2.1
1	A	273	PHE	2.1
1	A	193	THR	2.1
1	B	162	PRO	2.1
1	B	565	LYS	2.0
1	A	281	THR	2.0
1	B	136	ILE	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	1601	1/1	0.99	0.07	-2.26	19,19,19,19	0
2	CA	B	2601	1/1	0.99	0.04	-2.59	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.