



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:17 AM UTC

PDB ID : 1WZL / pdb_00001wzl
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

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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

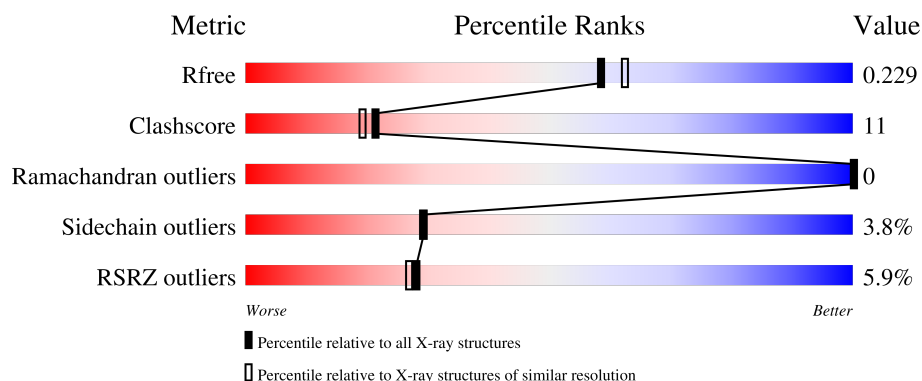
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	585	5% 76% 21% .
1	B	585	7% 77% 21% .

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 mutation	UNP Q08751
B	469	LEU	ARG	engineered mutation	UNP Q08751

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

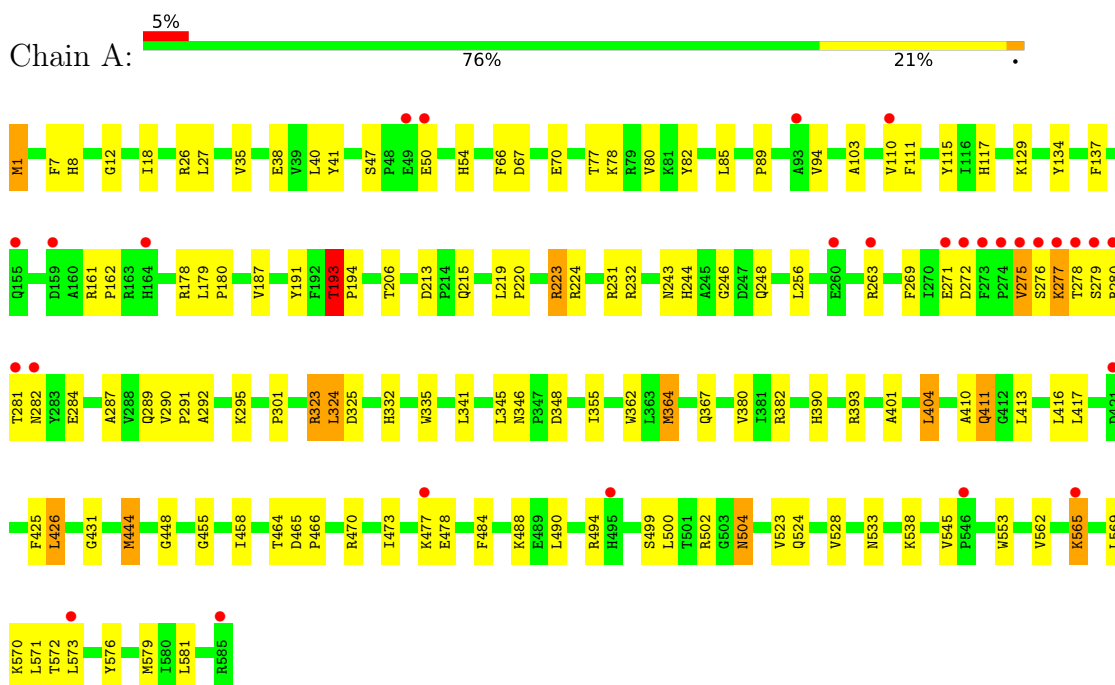
- Molecule 3 is water.

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

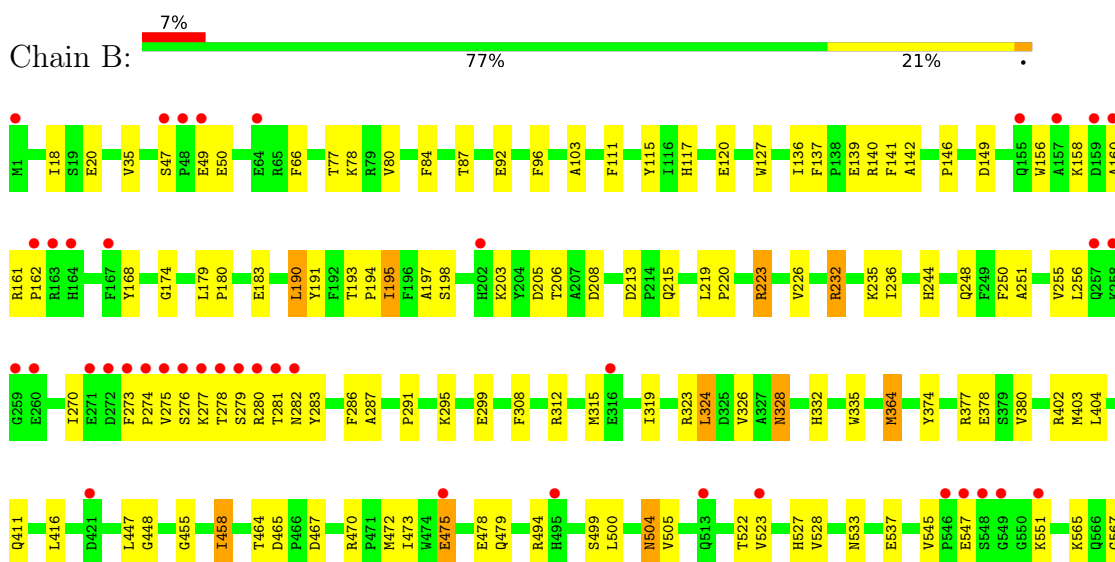
3 Residue-property plots

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.

• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
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
F_o, F_c correlation	0.94	EDS
Total number of atoms	10494	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.37	0/4902	0.88	19/6638 (0.3%)
1	B	0.36	0/4902	0.84	9/6638 (0.1%)
All	All	0.36	0/9804	0.86	28/13276 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CA-C-N	8.43	128.50	119.90
1	A	161	ARG	C-N-CA	8.43	128.50	119.90
1	A	275	VAL	N-CA-C	7.74	118.78	106.32
1	B	111	PHE	N-CA-C	-7.50	100.42	110.55
1	A	18	ILE	N-CA-C	-7.42	105.97	113.47
1	B	18	ILE	N-CA-C	-7.36	105.41	113.43
1	B	80	VAL	N-CA-C	6.22	116.56	108.35
1	A	290	VAL	CA-C-N	6.21	126.40	119.32
1	A	290	VAL	C-N-CA	6.21	126.40	119.32
1	B	103	ALA	N-CA-C	-5.92	106.02	113.18
1	A	323	ARG	N-CA-C	-5.85	98.87	108.41
1	A	524	GLN	CB-CA-C	-5.69	110.03	116.63
1	B	161	ARG	CA-C-N	5.58	125.59	119.90
1	B	161	ARG	C-N-CA	5.58	125.59	119.90
1	A	287	ALA	CB-CA-C	-5.57	110.14	116.54
1	B	287	ALA	CB-CA-C	-5.49	110.26	116.63
1	A	417	LEU	N-CA-C	-5.47	107.15	113.88
1	A	103	ALA	N-CA-C	-5.34	106.27	112.89
1	A	7	PHE	N-CA-C	5.27	117.39	109.23
1	A	324	LEU	N-CA-C	5.27	117.31	108.73
1	A	80	VAL	N-CA-C	5.22	115.89	108.42
1	A	137	PHE	N-CA-C	-5.21	98.29	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	PHE	N-CA-C	5.19	117.57	109.52
1	A	66	PHE	N-CA-C	5.18	118.03	109.85
1	A	193	THR	N-CA-C	-5.16	101.52	109.41
1	A	206	THR	N-CA-C	5.07	117.66	110.10
1	B	206	THR	N-CA-C	5.06	117.49	109.96
1	A	67	ASP	N-CA-C	-5.03	101.49	109.59

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	103	0
1	B	4772	0	4605	104	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	204	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 (204) 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:551:LYS:HZ1	1:B:567:GLY:H	1.00	1.00
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.30	0.97
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASN:HD22	1:A:504:ASN:C	1.91	0.79
1:B:277:LYS:HG3	1:B:280:ARG:HB3	1.68	0.76
1:A:364:MET:HE2	1:A:364:MET:HA	1.68	0.74
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.36	0.74
1:B:328:ASN:HD22	1:B:328:ASN:N	1.89	0.71
1:B:504:ASN:C	1:B:504:ASN:HD22	1.99	0.70
1:B:551:LYS:HZ1	1:B:567:GLY:N	1.84	0.70
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: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: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:447:LEU:HB2	1:B:505:VAL:CG2	2.29	0.63
1:B:328:ASN:HD22	1:B:328:ASN:H	1.47	0.62
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.81	0.62
1:B:565:LYS:O	1:B:565:LYS:HD2	2.00	0.62
1:B:458:ILE:N	1:B:458:ILE:HD13	2.14	0.62
1:B:183:GLU:CD	1:B:232:ARG:HG3	2.25	0.62
1:B:458:ILE:HD13	1:B:458:ILE:H	1.64	0.61
1:A:504:ASN:C	1:A:504:ASN:ND2	2.57	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:H	1:A:477:LYS:HD2	1.65	0.61
1:B:273:PHE:HA	1:B:274:PRO:C	2.26	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:H	1:B:195:ILE:HD13	1.66	0.60
1:B:364:MET:HA	1:B:364:MET:HE3	1.83	0.59
1:A:478:GLU:HG3	3:A:2039:HOH:O	2.01	0.59
1:B:256:LEU:HD23	1:B:275:VAL:HG23	1.84	0.59
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:A:565:LYS:H	1:A:565:LYS:HD2	1.70	0.57
1:B:504:ASN:C	1:B:504:ASN:ND2	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HD2	1:A:477:LYS:N	2.19	0.56
1:A:1:MET:HE3	1:A:94:VAL:HG12	1.87	0.56
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.06	0.56
1:B:226:VAL:HA	1:B:236:ILE:HD12	1.87	0.55
1:A:346:ASN:HD22	1:A:346:ASN:C	2.15	0.55
1:A:289:GLN:O	1:A:291:PRO:HD3	2.08	0.54
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.90	0.54
1:B:551:LYS:NZ	1:B:567:GLY:H	1.88	0.54
1:A:364:MET:HA	1:A:364:MET:CE	2.36	0.53
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:A:269:PHE:HB2	1:A:284:GLU:HB3	1.92	0.52
1:B:140:ARG:CZ	3:B:2922:HOH:O	2.58	0.52
1:B:523:VAL:HG13	1:B:523:VAL:O	2.10	0.52
1:A:248:GLN:HB2	3:A:1626:HOH:O	2.10	0.52
1:A:12:GLY:HA2	1:A:364:MET:HE1	1.90	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: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:35:VAL:HG21	1:A:89:PRO:HA	1.91	0.51
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.93	0.51
1:B:281:THR:HG22	1:B:291:PRO:HB3	1.91	0.51
1:A:224:ARG:HA	1:A:224:ARG:HE	1.75	0.50
1:A:276:SER:O	1:A:277:LYS:HB2	2.11	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
1:B:464:THR:O	1:B:465:ASP:C	2.55	0.49
1:A:401:ALA:O	1:A:404:LEU:HB2	2.13	0.49
1:B:47:SER:O	1:B:50:GLU:HB2	2.12	0.49
1:B:275:VAL:CA	1:B:282:ASN:HD21	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.48	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:H	1:A:477:LYS:CD	2.26	0.47
1:B:140:ARG:NE	1:B:168:TYR:HD2	2.12	0.47
1:A:82:TYR:C	1:A:110:VAL:HG23	2.39	0.47
1:A:444:MET:HG2	1:A:490:LEU:HB3	1.97	0.47
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.49	0.47
1:B:458:ILE:HD11	1:B:472:MET:HE1	1.95	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:A:232:ARG:NE	3:A:1676:HOH:O	2.41	0.47
1:A:523:VAL:O	1:A:523:VAL:HG13	2.15	0.47
1:B:276:SER:HB2	1:B:283:TYR:HE2	1.79	0.47
1:B:416:LEU:H	1:B:416:LEU:HD23	1.80	0.47
1:B:141:PHE:HB3	3:B:2642:HOH:O	2.14	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:A:458:ILE:HD12	1:A:473:ILE:HB	1.96	0.46
1:A:27:LEU:C	1:A:27:LEU:HD23	2.39	0.46
1:A:275:VAL:O	1:A:276:SER:HB2	2.15	0.46
1:B:226:VAL:HA	1:B:236:ILE:CD1	2.46	0.46
1:A:8:HIS:HD2	1:A:26:ARG:O	1.99	0.46
1:B:139:GLU:O	1:B:140:ARG:HD3	2.15	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:A:346:ASN:ND2	1:A:346:ASN:C	2.75	0.45
1:B:140:ARG:HE	1:B:168:TYR:HD2	1.65	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:341:LEU:O	1:A:345:LEU:HD13	2.17	0.45
1:A:401:ALA:HA	1:A:404:LEU:HD22	1.99	0.45
1:A:272:ASP:O	1:A:282:ASN:ND2	2.50	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:ARG:HG2	1:B:403:MET:HE2	2.00	0.44
1:B:20:GLU:HB2	3:B:2897:HOH:O	2.17	0.43
1:B:328:ASN:N	1:B:328:ASN:ND2	2.58	0.43
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.54	0.43
1:A:426:LEU:HD22	1:A:431:GLY:HA2	2.00	0.43
1:A:553:TRP:HB2	1:A:562:VAL:CG2	2.47	0.43
1:B:276:SER:HA	1:B:282:ASN:OD1	2.18	0.43
1:A:82:TYR:O	1:A:110:VAL:HG23	2.18	0.43
1:B:213:ASP:OD1	1:B:215:GLN:HG2	2.18	0.43
1:A:77:THR:O	1:A:78:LYS:HB2	2.18	0.43
1:A:565:LYS:HD2	1:A:565:LYS:N	2.32	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:A:117:HIS:HB3	1:B:299:GLU:OE2	2.18	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: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: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: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:179:LEU:N	1:A:180:PRO:CD	2.82	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: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:193:THR:HB	1:A:194:PRO:CD	2.49	0.42
1:A:278:THR:C	1:A:280:ARG:H	2.27	0.42
1:A:223:ARG:HB3	1:A:223:ARG:NH1	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:A:410:ALA:HA	1:A:413:LEU:HG	2.01	0.42
1:A:416:LEU:H	1:A:416:LEU:CD2	2.33	0.42
1:B:197:ALA:HB3	1:B:208:ASP:HB3	2.01	0.42
1:B:223:ARG:HB3	1:B:223:ARG:NH2	2.35	0.42
1:B:275:VAL:O	1:B:276:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:MET:HE1	3:A:1991:HOH:O	2.19	0.41
1:B:142:ALA:O	1:B:174:GLY:HA3	2.19	0.41
1:A:346:ASN:HD22	1:A:348:ASP:H	1.68	0.41
1:B:256:LEU:HA	1:B:275:VAL:HG21	2.02	0.41
1:A:545:VAL:HG23	1:A:545:VAL:O	2.20	0.41
1:B:467:ASP:OD1	1:B:470:ARG:HD3	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:A:464:THR:O	1:A:465:ASP:C	2.63	0.41
1:B:205:ASP:OD1	1:B:205:ASP:N	2.51	0.41
1:A:355:ILE:HD13	1:A:362:TRP:CE3	2.55	0.41
1:B:156:TRP:HB2	3:B:2980:HOH:O	2.21	0.41
1:B:250:PHE:CG	1:B:251:ALA:N	2.88	0.41
1:B:324:LEU:HD13	1:B:335:TRP:CH2	2.56	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:A:390:HIS:CD2	1:A:393:ARG:H	2.39	0.41
1:B:195:ILE:HD13	1:B:195:ILE:N	2.35	0.41
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.55	0.41
1:A:38:GLU:OE1	1:A:54:HIS:HD2	2.04	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:178:ARG:HH21	1:A:178:ARG:HG2	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:278:THR:C	1:A:280:ARG:N	2.80	0.40
1:A:500:LEU:HD21	1:A:528:VAL:HG11	2.03	0.40
1:A:570:LYS:O	1:A:571:LEU:HD12	2.21	0.40
1:A:134:TYR:HB2	1:A:187:VAL:HG11	2.04	0.40
1:B:276:SER:OG	1:B:277:LYS:N	2.54	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%)	475 (96%)	18 (4%)	30	30
1	B	493/493 (100%)	474 (96%)	19 (4%)	28	28
All	All	986/986 (100%)	949 (96%)	37 (4%)	29	29

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	LEU
1	A	85	LEU
1	A	191	TYR
1	A	193	THR
1	A	223	ARG
1	A	263	ARG
1	A	277	LYS
1	A	281	THR
1	A	323	ARG
1	A	325	ASP
1	A	364	MET
1	A	404	LEU
1	A	411	GLN

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Mol	Chain	Res	Type
1	A	426	LEU
1	A	444	MET
1	A	504	ASN
1	A	565	LYS
1	B	92	GLU
1	B	190	LEU
1	B	191	TYR
1	B	195	ILE
1	B	223	ARG
1	B	232	ARG
1	B	248	GLN
1	B	323	ARG
1	B	324	LEU
1	B	326	VAL
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	537	GLU
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	22	GLN
1	A	54	HIS
1	A	135	GLN
1	A	155	GLN
1	A	164	HIS
1	A	244	HIS
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	411	GLN
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS

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Mol	Chain	Res	Type
1	A	544	GLN
1	B	164	HIS
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	495	HIS
1	B	504	ASN
1	B	509	HIS
1	B	527	HIS
1	B	544	GLN
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 oligosaccharides 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

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

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, 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	585/585 (100%)	0.18	28 (4%)	35	34	14, 21, 42, 76	0
1	B	585/585 (100%)	0.23	41 (7%)	22	21	13, 22, 44, 81	0
All	All	1170/1170 (100%)	0.21	69 (5%)	28	27	13, 22, 44, 81	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	VAL	9.7
1	A	278	THR	7.6
1	B	278	THR	7.2
1	A	279	SER	6.2
1	A	275	VAL	5.9
1	B	280	ARG	5.4
1	B	279	SER	5.3
1	B	276	SER	4.6
1	A	276	SER	4.6
1	A	281	THR	4.5
1	B	277	LYS	4.5
1	B	274	PRO	4.2
1	B	260	GLU	4.2
1	B	281	THR	4.1
1	B	282	ASN	4.0
1	A	280	ARG	3.9
1	A	277	LYS	3.9
1	B	523	VAL	3.7
1	B	551	LYS	3.5
1	B	273	PHE	3.4
1	B	272	ASP	3.4
1	A	273	PHE	3.3
1	A	585	ARG	3.1
1	A	155	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	47	SER	3.0
1	B	259	GLY	3.0
1	B	49	GLU	3.0
1	A	274	PRO	3.0
1	B	495	HIS	3.0
1	A	50	GLU	2.9
1	B	162	PRO	2.9
1	B	48	PRO	2.8
1	B	548	SER	2.7
1	A	272	ASP	2.7
1	B	421	ASP	2.7
1	A	495	HIS	2.7
1	B	257	GLN	2.6
1	B	547	GLU	2.6
1	A	159	ASP	2.6
1	A	260	GLU	2.6
1	A	164	HIS	2.6
1	A	546	PRO	2.5
1	A	565	LYS	2.5
1	B	546	PRO	2.5
1	B	159	ASP	2.4
1	B	258	LYS	2.4
1	B	64	GLU	2.4
1	B	1	MET	2.4
1	A	263	ARG	2.4
1	A	49	GLU	2.4
1	A	271	GLU	2.3
1	B	513	GLN	2.3
1	B	163	ARG	2.3
1	B	164	HIS	2.3
1	B	155	GLN	2.3
1	B	316	GLU	2.2
1	B	475	GLU	2.2
1	A	421	ASP	2.2
1	A	573	LEU	2.2
1	B	271	GLU	2.1
1	B	202	HIS	2.1
1	A	93	ALA	2.1
1	A	477	LYS	2.1
1	B	157	ALA	2.1
1	A	282	ASN	2.1
1	A	110	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	2.1
1	B	167	PHE	2.0
1	B	549	GLY	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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
2	CA	A	1601	1/1	0.98	0.03	19,19,19,19	0
2	CA	B	2601	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.