



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 AM UTC

PDB ID : 1JI2 / pdb\_00001ji2  
Title : Improved X-ray Structure of Thermoactinomyces vulgaris R-47 alpha-Amylase  
2  
Authors : Kamitori, S.; Abe, A.; Ohtaki, A.; Kaji, A.; Tonozuka, T.; Sakano, Y.  
Deposited on : 2001-06-28  
Resolution : 2.30 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.

The types of validation reports are described at

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

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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

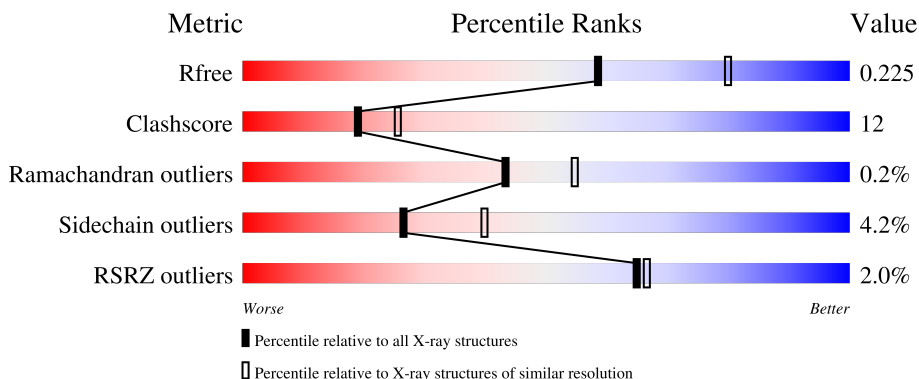
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	585	 3% 75% 23% .
1	B	585	 3% 78% 19% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10450 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
			Total	C	N	O	S			
1	A	585	4776	3056	831	874	15	0	0	0
1	B	585	4776	3056	831	874	15	0	0	0

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

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

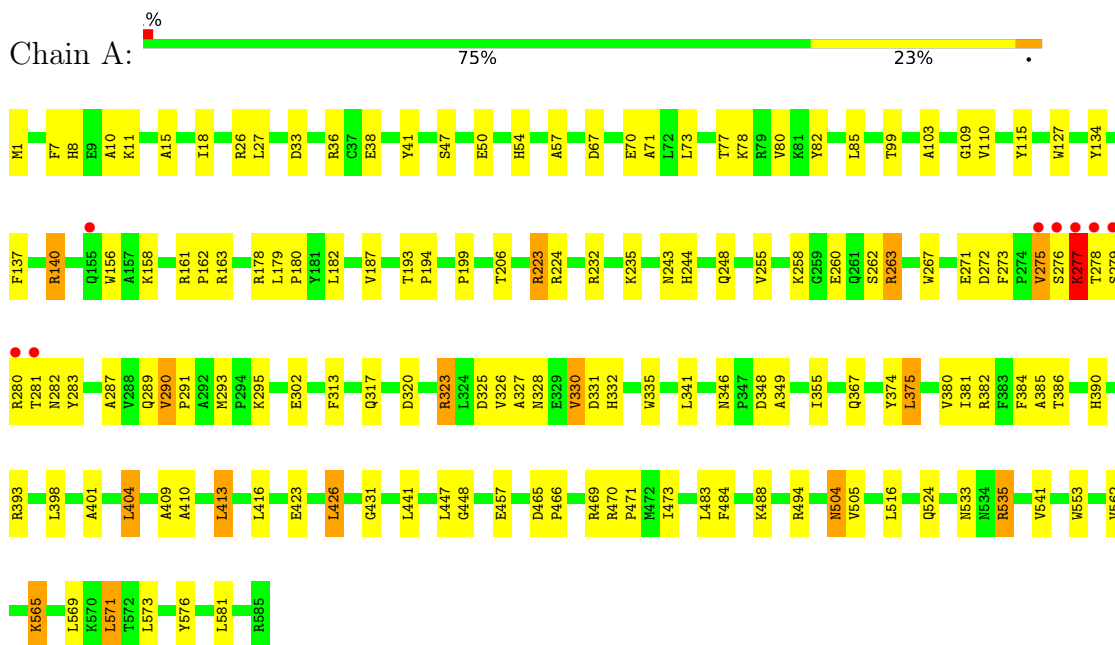
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total 454	O 454	0	0
3	B	442	Total 442	O 442	0	0

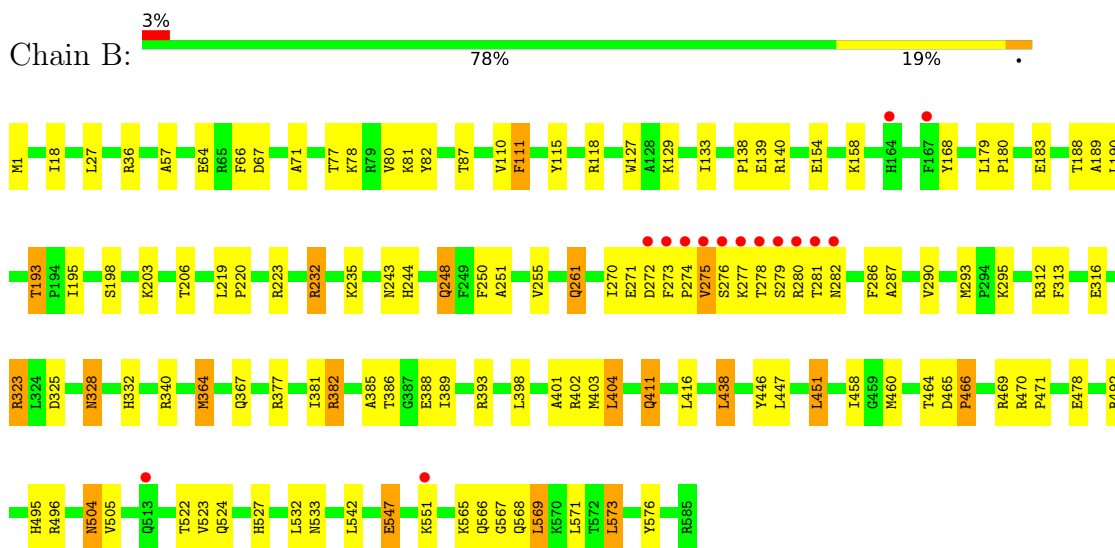
### 3 Residue-property plots i

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.

#### • 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, $\alpha$ , $\beta$ , $\gamma$	112.46Å 117.68Å 112.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.05 – 2.30 37.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.05-2.30) 99.8 (37.05-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.179 , 0.224 0.180 , 0.225	Depositor DCC
$R_{free}$ test set	6776 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k 0.012 for -k,-h,-l 0.013 for l,-k,h 0.003 for l,h,k 0.003 for k,l,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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:  
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	0/4906	0.90	21/6641 (0.3%)
1	B	0.36	0/4906	0.87	12/6641 (0.2%)
All	All	0.37	0/9812	0.89	33/13282 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CA-C-N	7.73	127.79	119.90
1	A	161	ARG	C-N-CA	7.73	127.79	119.90
1	B	18	ILE	N-CA-C	-7.32	105.45	113.43
1	A	290	VAL	CA-C-N	6.88	127.17	119.32
1	A	290	VAL	C-N-CA	6.88	127.17	119.32
1	A	323	ARG	N-CA-C	-6.57	97.81	108.52
1	B	80	VAL	N-CA-C	6.17	116.50	108.35
1	A	524	GLN	CB-CA-C	-6.15	109.50	116.63
1	A	18	ILE	N-CA-C	-6.12	106.75	113.43
1	A	67	ASP	N-CA-C	-5.96	99.99	109.59
1	B	323	ARG	N-CA-C	-5.84	99.00	108.52
1	B	193	THR	N-CA-C	-5.78	101.63	110.07
1	A	275	VAL	N-CA-C	5.74	121.28	109.34
1	B	67	ASP	N-CA-C	-5.73	100.95	110.17
1	B	66	PHE	N-CA-C	5.61	118.21	109.52
1	A	103	ALA	N-CA-C	-5.59	105.96	112.89
1	A	287	ALA	CB-CA-C	-5.57	110.13	116.54
1	A	423	GLU	N-CA-C	-5.53	103.23	110.53
1	B	385	ALA	N-CA-C	5.53	120.02	111.56
1	B	287	ALA	CB-CA-C	-5.50	110.25	116.63
1	A	206	THR	N-CA-C	5.50	118.29	110.10
1	A	80	VAL	N-CA-C	5.43	115.52	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	TRP	N-CA-C	-5.42	106.44	113.16
1	A	7	PHE	N-CA-C	5.38	118.20	109.06
1	B	206	THR	N-CA-C	5.36	117.94	109.96
1	B	275	VAL	N-CA-C	5.35	118.55	111.17
1	A	137	PHE	CA-C-N	5.28	126.44	119.84
1	A	137	PHE	C-N-CA	5.28	126.44	119.84
1	B	111	PHE	N-CA-C	-5.26	103.45	110.55
1	A	137	PHE	N-CA-C	-5.24	98.24	109.81
1	A	331	ASP	N-CA-C	5.21	117.25	110.43
1	B	524	GLN	CB-CA-C	-5.21	110.59	116.63
1	A	140	ARG	N-CA-C	5.03	120.03	112.94

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	4776	0	4607	114	0
1	B	4776	0	4607	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	454	0	0	8	0
3	B	442	0	0	11	0
All	All	10450	0	9214	221	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 12.

All (221) 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:275:VAL:HA	1:A:282:ASN:HD21	1.29	0.97
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.47	0.94
1:A:224:ARG:HE	1:A:224:ARG:HA	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG11	1:B:293:MET:HE3	1.51	0.92
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.62	0.82
1:B:280:ARG:HE	1:B:281:THR:H	1.26	0.82
1:B:277:LYS:HG3	1:B:280:ARG:HB3	1.60	0.82
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.64	0.80
1:A:290:VAL:HG11	1:A:293:MET:HE3	1.65	0.79
1:B:280:ARG:HE	1:B:281:THR:N	1.80	0.79
1:A:277:LYS:HD2	1:A:280:ARG:HB3	1.65	0.78
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.67	0.76
1:A:140:ARG:HG2	1:A:469:ARG:O	1.86	0.76
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.65	0.75
1:B:328:ASN:N	1:B:328:ASN:HD22	1.83	0.75
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.02	0.74
1:B:551:LYS:NZ	1:B:567:GLY:H	1.86	0.73
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.54	0.72
1:A:504:ASN:C	1:A:504:ASN:HD22	1.95	0.71
1:B:139:GLU:HB3	1:B:140:ARG:HH11	1.55	0.71
1:B:328:ASN:HD22	1:B:328:ASN:H	1.38	0.71
1:A:341:LEU:HD23	1:A:341:LEU:C	2.17	0.69
1:B:504:ASN:C	1:B:504:ASN:HD22	2.01	0.68
1:A:255:VAL:HA	1:A:262:SER:OG	1.93	0.68
1:B:290:VAL:HG11	1:B:293:MET:CE	2.23	0.67
1:B:470:ARG:HG3	3:B:1006:HOH:O	1.94	0.66
1:A:275:VAL:CA	1:A:282:ASN:HD21	2.05	0.66
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.11	0.65
1:B:248:GLN:HG2	3:B:1127:HOH:O	1.97	0.65
1:A:224:ARG:HA	1:A:224:ARG:NE	2.09	0.65
1:B:458:ILE:CD1	1:B:460:MET:HG3	2.27	0.65
1:A:277:LYS:HB2	1:A:277:LYS:NZ	2.13	0.64
1:A:275:VAL:O	1:A:276:SER:HB2	1.98	0.63
1:A:535:ARG:HH21	1:A:535:ARG:HG3	1.62	0.63
1:B:551:LYS:HZ3	1:B:567:GLY:H	1.47	0.63
1:A:263:ARG:HD2	1:A:263:ARG:O	1.98	0.63
1:B:313:PHE:HA	1:B:316:GLU:OE1	1.99	0.63
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.48	0.61
1:B:402:ARG:HG2	1:B:403:MET:HE2	1.82	0.61
1:A:565:LYS:O	1:A:565:LYS:HG2	2.01	0.61
1:A:289:GLN:O	1:A:291:PRO:HD3	2.01	0.61
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.31	0.60
1:A:346:ASN:ND2	1:A:348:ASP:H	1.99	0.60
1:B:495:HIS:HB3	3:B:1152:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:O	1:B:275:VAL:HG21	2.02	0.59
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.02	0.59
1:B:569:LEU:HD22	1:B:571:LEU:HG	1.85	0.59
1:B:364:MET:HE3	1:B:364:MET:HA	1.84	0.59
1:B:382:ARG:NH2	1:B:389:ILE:HD13	2.18	0.59
1:B:328:ASN:H	1:B:328:ASN:ND2	2.00	0.58
1:A:416:LEU:H	1:A:416:LEU:HD23	1.67	0.58
1:A:280:ARG:O	1:A:281:THR:HG23	2.04	0.58
1:A:276:SER:O	1:A:277:LYS:HB2	2.03	0.58
1:B:82:TYR:C	1:B:110:VAL:HG23	2.28	0.58
1:A:277:LYS:HD2	1:A:280:ARG:CB	2.32	0.58
1:A:272:ASP:O	1:A:282:ASN:ND2	2.35	0.57
1:A:271:GLU:HG2	1:A:282:ASN:O	2.04	0.57
1:B:139:GLU:HB3	1:B:140:ARG:NH1	2.19	0.57
1:B:547:GLU:CG	1:B:551:LYS:HE2	2.29	0.57
1:A:409:ALA:O	1:A:413:LEU:HD13	2.04	0.57
1:A:504:ASN:C	1:A:504:ASN:ND2	2.59	0.57
1:A:224:ARG:HE	1:A:224:ARG:CA	2.10	0.56
1:A:280:ARG:HA	1:A:289:GLN:OE1	2.06	0.56
1:A:401:ALA:HA	1:A:404:LEU:HD22	1.87	0.56
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.87	0.56
1:B:382:ARG:HH22	1:B:389:ILE:HD13	1.71	0.56
1:B:551:LYS:HZ1	1:B:566:GLN:N	2.04	0.55
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.41	0.55
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.70	0.55
1:B:110:VAL:HG22	1:B:111:PHE:O	2.07	0.55
1:B:158:LYS:HD2	1:B:478:GLU:HB3	1.89	0.55
1:B:386:THR:OG1	1:B:388:GLU:HG3	2.07	0.54
1:A:346:ASN:HD22	1:A:346:ASN:C	2.15	0.54
1:B:273:PHE:HA	1:B:274:PRO:C	2.32	0.54
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.88	0.54
1:A:533:ASN:O	1:A:576:TYR:HA	2.07	0.54
1:A:27:LEU:C	1:A:27:LEU:HD23	2.33	0.54
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.38	0.54
1:A:390:HIS:CD2	1:A:393:ARG:H	2.26	0.53
1:A:8:HIS:HD2	1:A:26:ARG:O	1.92	0.53
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.91	0.53
1:A:535:ARG:HG3	1:A:535:ARG:NH2	2.23	0.53
1:A:278:THR:O	1:A:279:SER:HB2	2.08	0.53
1:A:390:HIS:HD2	1:A:393:ARG:H	1.57	0.53
1:A:223:ARG:HD2	1:A:317:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.92	0.53
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.44	0.53
1:A:277:LYS:HB2	1:A:277:LYS:HZ2	1.73	0.52
1:A:382:ARG:HD3	3:A:1412:HOH:O	2.09	0.52
1:B:255:VAL:HG11	1:B:270:ILE:HD11	1.90	0.52
1:A:11:LYS:N	1:A:15:ALA:HB3	2.25	0.52
1:A:258:LYS:HE3	3:A:1305:HOH:O	2.08	0.52
1:B:82:TYR:N	1:B:110:VAL:CG2	2.73	0.52
1:B:504:ASN:C	1:B:504:ASN:ND2	2.67	0.52
1:B:312:ARG:O	1:B:316:GLU:HG3	2.10	0.52
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.93	0.52
1:B:401:ALA:HA	1:B:404:LEU:HD22	1.91	0.52
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.91	0.52
3:A:1374:HOH:O	1:B:340:ARG:HG3	2.10	0.51
1:B:82:TYR:O	1:B:110:VAL:HG23	2.11	0.51
1:B:278:THR:O	1:B:279:SER:HB2	2.10	0.51
1:A:1:MET:HB2	1:A:33:ASP:OD2	2.10	0.51
1:B:64:GLU:HG3	1:B:393:ARG:NH2	2.25	0.51
1:A:277:LYS:HB3	1:A:280:ARG:O	2.11	0.51
1:A:199:PRO:HG3	1:A:248:GLN:HG3	1.91	0.51
1:B:438:LEU:HD22	1:B:532:LEU:HD22	1.93	0.51
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.92	0.51
1:B:188:THR:HG21	3:B:1286:HOH:O	2.10	0.51
1:A:401:ALA:O	1:A:404:LEU:HB2	2.11	0.51
1:B:504:ASN:HD21	1:B:522:THR:HB	1.76	0.50
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.12	0.50
1:B:138:PRO:HG2	3:B:1103:HOH:O	2.10	0.50
1:B:573:LEU:N	1:B:573:LEU:HD22	2.26	0.50
1:A:38:GLU:OE1	1:A:54:HIS:HD2	1.95	0.50
1:A:416:LEU:H	1:A:416:LEU:CD2	2.24	0.49
1:B:276:SER:OG	1:B:277:LYS:N	2.44	0.49
1:A:341:LEU:C	1:A:341:LEU:CD2	2.85	0.49
1:B:154:GLU:HG3	3:B:1236:HOH:O	2.12	0.48
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.46	0.48
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.43	0.48
1:A:99:THR:OG1	1:A:109:GLY:HA3	2.14	0.48
1:B:118:ARG:NH1	3:B:1075:HOH:O	2.46	0.48
1:A:193:THR:HB	1:A:194:PRO:CD	2.44	0.47
1:A:163:ARG:HB2	1:A:163:ARG:NH1	2.29	0.47
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.78	0.47
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HD12	1:B:189:ALA:HB3	1.97	0.47
1:B:551:LYS:HZ1	1:B:567:GLY:H	1.60	0.47
1:B:565:LYS:HD2	1:B:565:LYS:O	2.15	0.47
1:B:183:GLU:CD	1:B:232:ARG:HG3	2.40	0.47
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.96	0.47
1:B:382:ARG:HH21	1:B:382:ARG:HB2	1.80	0.47
1:B:458:ILE:HD11	1:B:460:MET:HG3	1.96	0.47
1:A:277:LYS:CD	1:A:280:ARG:HB3	2.42	0.46
1:B:133:ILE:HB	1:B:451:LEU:HD23	1.98	0.46
1:A:82:TYR:N	1:A:110:VAL:HG22	2.30	0.46
1:A:330:VAL:HG11	1:A:335:TRP:CZ2	2.50	0.46
1:B:183:GLU:OE2	1:B:232:ARG:HG3	2.15	0.46
1:A:273:PHE:CD1	1:A:275:VAL:HG23	2.51	0.46
1:B:243:ASN:HD21	1:B:295:LYS:NZ	2.13	0.46
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.15	0.46
1:B:492:ARG:HG2	1:B:496:ARG:CZ	2.46	0.46
1:A:127:TRP:CG	1:A:235:LYS:HE2	2.50	0.46
1:A:565:LYS:HE3	3:A:1413:HOH:O	2.15	0.46
1:B:275:VAL:O	1:B:276:SER:HB2	2.15	0.45
3:A:1326:HOH:O	1:B:332:HIS:HE1	1.99	0.45
1:B:271:GLU:HB2	1:B:282:ASN:O	2.15	0.45
1:B:464:THR:O	1:B:465:ASP:C	2.59	0.45
1:B:542:LEU:HD21	1:B:568:GLN:HE22	1.81	0.45
1:B:81:LYS:HB2	1:B:110:VAL:HG21	1.98	0.45
1:B:193:THR:O	1:B:195:ILE:HG23	2.17	0.45
1:A:11:LYS:HE3	3:B:1422:HOH:O	2.17	0.45
1:A:179:LEU:N	1:A:180:PRO:CD	2.79	0.45
1:A:516:LEU:C	1:A:516:LEU:HD23	2.41	0.45
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.99	0.45
1:A:232:ARG:NE	3:A:1082:HOH:O	2.36	0.45
1:B:77:THR:O	1:B:78:LYS:HB2	2.17	0.45
1:B:118:ARG:HG2	1:B:118:ARG:NH1	2.32	0.45
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.52	0.45
1:B:523:VAL:O	1:B:523:VAL:HG13	2.16	0.45
1:A:320:ASP:O	1:A:349:ALA:HA	2.17	0.45
1:A:441:LEU:C	1:A:441:LEU:HD23	2.42	0.45
1:B:140:ARG:HG3	1:B:469:ARG:O	2.17	0.44
1:B:382:ARG:HH21	1:B:382:ARG:CB	2.30	0.44
1:A:77:THR:O	1:A:78:LYS:HB2	2.17	0.44
1:B:118:ARG:NH1	3:B:1086:HOH:O	2.50	0.44
1:B:458:ILE:HD12	1:B:460:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:HG3	1:A:272:ASP:N	2.31	0.44
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.48	0.44
1:A:326:VAL:HG22	3:A:1269:HOH:O	2.18	0.44
1:B:127:TRP:CG	1:B:235:LYS:HE3	2.52	0.44
1:A:275:VAL:O	1:A:275:VAL:HG12	2.17	0.44
1:A:277:LYS:HD2	1:A:280:ARG:CG	2.47	0.44
1:B:1:MET:N	3:B:1140:HOH:O	2.49	0.44
1:B:179:LEU:N	1:B:180:PRO:CD	2.81	0.44
1:B:328:ASN:N	1:B:328:ASN:ND2	2.54	0.44
1:B:533:ASN:O	1:B:576:TYR:HA	2.18	0.44
1:B:127:TRP:CE3	1:B:235:LYS:HD2	2.53	0.44
1:A:346:ASN:ND2	1:A:346:ASN:C	2.75	0.43
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.52	0.43
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.52	0.43
1:B:27:LEU:HD23	1:B:27:LEU:C	2.43	0.43
1:B:129:LYS:HA	1:B:411:GLN:OE1	2.19	0.43
1:A:313:PHE:O	1:A:317:GLN:HG2	2.17	0.43
1:A:381:ILE:O	1:A:385:ALA:HB3	2.18	0.43
1:A:127:TRP:CD1	1:A:235:LYS:HE2	2.54	0.43
1:A:426:LEU:HD22	1:A:431:GLY:HA2	2.00	0.43
1:A:134:TYR:HB2	1:A:187:VAL:HG11	1.99	0.43
1:B:36:ARG:HB3	1:B:87:THR:HB	2.01	0.43
1:B:168:TYR:CD1	1:B:471:PRO:HG3	2.53	0.43
1:A:565:LYS:H	1:A:565:LYS:HD2	1.84	0.43
1:A:10:ALA:C	1:A:15:ALA:HB3	2.43	0.43
1:A:380:VAL:HG13	1:A:384:PHE:CD1	2.54	0.43
1:A:41:TYR:HB3	1:A:82:TYR:HB3	2.00	0.42
1:A:275:VAL:HG13	1:A:283:TYR:HD2	1.84	0.42
1:B:140:ARG:NH2	3:B:1241:HOH:O	2.52	0.42
1:A:330:VAL:HG11	1:A:335:TRP:HZ2	1.83	0.42
1:B:280:ARG:NE	1:B:281:THR:H	2.06	0.42
1:A:327:ALA:O	1:A:330:VAL:HG13	2.19	0.42
1:B:250:PHE:CG	1:B:251:ALA:N	2.88	0.42
1:A:275:VAL:O	1:A:276:SER:CB	2.66	0.42
1:A:158:LYS:HE3	1:A:473:ILE:HD13	2.02	0.41
1:A:457:GLU:OE1	1:A:457:GLU:N	2.46	0.41
1:A:275:VAL:CG1	1:A:283:TYR:CD2	3.03	0.41
1:A:178:ARG:HA	1:A:178:ARG:HD3	1.90	0.41
1:B:416:LEU:CD2	1:B:416:LEU:H	2.34	0.41
1:A:276:SER:OG	1:A:277:LYS:N	2.53	0.41
1:A:26:ARG:NE	3:A:1449:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TRP:HB2	1:A:562:VAL:CG2	2.50	0.41
1:A:82:TYR:H	1:A:110:VAL:HG22	1.85	0.41
1:A:448:GLY:O	1:A:494:ARG:NH2	2.54	0.41
1:B:261:GLN:H	1:B:261:GLN:NE2	2.18	0.41
1:B:272:ASP:O	1:B:282:ASN:ND2	2.52	0.41
1:B:57:ALA:HB2	1:B:71:ALA:HB2	2.02	0.40
1:B:416:LEU:H	1:B:416:LEU:HD23	1.86	0.40
1:B:465:ASP:HA	1:B:466:PRO:HA	1.94	0.40
1:A:263:ARG:HH12	1:A:302:GLU:CD	2.28	0.40
1:B:446:TYR:CG	1:B:447:LEU:N	2.90	0.40
1:A:36:ARG:NH2	1:A:38:GLU:OE2	2.44	0.40
1:A:382:ARG:HA	1:A:386:THR:OG1	2.21	0.40
1:B:522:THR:OG1	1:B:527:HIS:HD2	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	583/585 (100%)	558 (96%)	24 (4%)	1 (0%)	43 55
1	B	583/585 (100%)	565 (97%)	17 (3%)	1 (0%)	43 55
All	All	1166/1170 (100%)	1123 (96%)	41 (4%)	2 (0%)	43 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	GLU
1	A	277	LYS

### 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	493/493 (100%)	471 (96%)	22 (4%)	24	37
1	B	493/493 (100%)	474 (96%)	19 (4%)	28	43
All	All	986/986 (100%)	945 (96%)	41 (4%)	26	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	85	LEU
1	A	182	LEU
1	A	223	ARG
1	A	260	GLU
1	A	263	ARG
1	A	277	LYS
1	A	323	ARG
1	A	325	ASP
1	A	330	VAL
1	A	375	LEU
1	A	398	LEU
1	A	404	LEU
1	A	413	LEU
1	A	426	LEU
1	A	483	LEU
1	A	504	ASN
1	A	535	ARG
1	A	565	LYS
1	A	571	LEU
1	A	573	LEU
1	A	581	LEU
1	B	190	LEU
1	B	223	ARG
1	B	232	ARG
1	B	248	GLN
1	B	261	GLN

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Mol	Chain	Res	Type
1	B	323	ARG
1	B	325	ASP
1	B	328	ASN
1	B	364	MET
1	B	382	ARG
1	B	398	LEU
1	B	404	LEU
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	466	PRO
1	B	504	ASN
1	B	569	LEU
1	B	573	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	54	HIS
1	A	90	GLN
1	A	155	GLN
1	A	164	HIS
1	A	243	ASN
1	A	244	HIS
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS
1	A	539	GLN
1	A	544	GLN
1	B	135	GLN
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	261	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS

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Mol	Chain	Res	Type
1	B	367	GLN
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 [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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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

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%)	-0.15	8 (1%) 73 75	16, 26, 46, 73	0
1	B	585/585 (100%)	-0.17	15 (2%) 57 59	13, 26, 46, 75	0
All	All	1170/1170 (100%)	-0.16	23 (1%) 65 66	13, 26, 46, 75	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	SER	5.8
1	B	275	VAL	5.2
1	B	278	THR	4.9
1	A	278	THR	4.9
1	B	280	ARG	4.5
1	A	281	THR	4.5
1	B	279	SER	4.2
1	A	280	ARG	4.2
1	B	277	LYS	3.7
1	B	276	SER	3.7
1	A	275	VAL	3.6
1	B	274	PRO	3.2
1	B	272	ASP	3.0
1	A	277	LYS	3.0
1	B	551	LYS	2.9
1	B	273	PHE	2.4
1	A	155	GLN	2.3
1	B	164	HIS	2.2
1	B	281	THR	2.2
1	A	276	SER	2.2
1	B	513	GLN	2.1
1	B	282	ASN	2.1
1	B	167	PHE	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, 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	CA	A	1001	1/1	0.99	0.02	23,23,23,23	0
2	CA	B	1002	1/1	0.99	0.04	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.