



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:20 pm GMT

PDB ID : 1WZK  
Title : Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) mutatnt D465N  
Authors : Mizuno, M.; Ichikawa, K.; Tonozuka, T.; Ohtaki, A.; Shimura, Y.; Kamitori, S.; Nishikawa, A.; Sakano, Y.  
Deposited on : 2005-03-06  
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

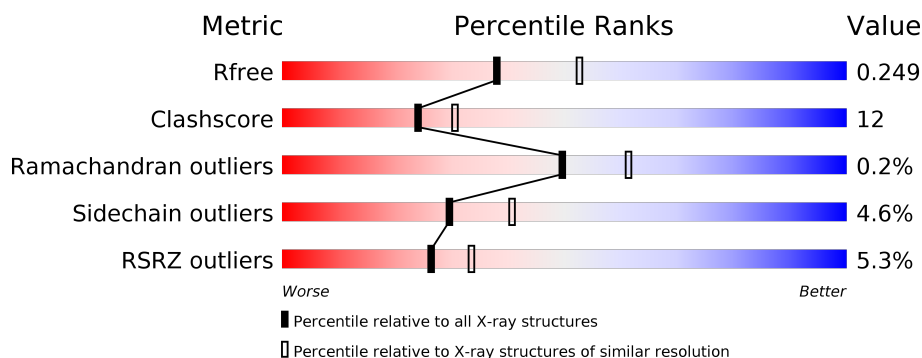
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (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 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>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	585	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10186 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
			4775	3056	832	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4775	3056	832	872	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	465	ASN	ASP	ENGINEERED	UNP Q08751
B	465	ASN	ASP	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	313	Total	O	0	0
			313	313		
3	B	321	Total	O	0	0
			321	321		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.39Å 117.66Å 112.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.21 – 2.30 32.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.21-2.30) 100.0 (32.21-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.74 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.248 0.203 , 0.249	Depositor DCC
$R_{free}$ test set	6795 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.012 for -k,-h,l 0.010 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

### 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	0.39	0/4905	0.59	0/6641
1	B	0.38	0/4905	0.59	1/6641 (0.0%)
All	All	0.38	0/9810	0.59	1/13282 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	TYR	N-CA-C	-5.48	96.20	111.00

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	4775	0	4609	123	0
1	B	4775	0	4609	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	313	0	0	8	0
3	B	321	0	0	8	0
All	All	10186	0	9218	224	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 (224) 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:277:LYS:HD3	1:A:278:THR:H	1.30	0.97
1:B:516:LEU:HD12	1:B:533:ASN:HA	1.48	0.95
1:A:441:LEU:HD21	1:A:580:ILE:HD11	1.58	0.85
1:B:465:ASN:HD22	1:B:466:PRO:HA	1.41	0.85
1:A:477:LYS:H	1:A:477:LYS:HD2	1.40	0.84
1:B:255:VAL:HG12	1:B:275:VAL:HG11	1.61	0.82
1:A:224:ARG:HA	1:A:224:ARG:HE	1.45	0.80
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.63	0.80
1:A:277:LYS:HD3	1:A:278:THR:N	1.98	0.78
1:B:256:LEU:HA	1:B:275:VAL:HG21	1.68	0.75
1:B:256:LEU:HD23	1:B:275:VAL:HG23	1.69	0.74
1:B:465:ASN:HD22	1:B:466:PRO:CA	1.99	0.74
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.72	0.72
1:B:193:THR:HB	1:B:194:PRO:HD2	1.71	0.71
1:A:277:LYS:HB3	1:A:280:ARG:HB3	1.72	0.71
1:A:140:ARG:HG2	1:A:469:ARG:O	1.91	0.70
1:B:452:ILE:HD12	1:B:487:TYR:HE2	1.57	0.70
1:B:551:LYS:NZ	1:B:567:GLY:H	1.90	0.68
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.74	0.68
1:A:256:LEU:HD23	1:A:275:VAL:HG23	1.75	0.68
1:A:445:THR:HG21	1:A:580:ILE:HD12	1.76	0.67
1:A:477:LYS:HD2	1:A:477:LYS:N	2.08	0.67
1:A:229:ALA:HB3	1:A:236:ILE:HD11	1.76	0.67
1:B:499:SER:HB3	1:B:523:VAL:HG12	1.78	0.66
1:B:535:ARG:HD3	1:B:539:GLN:NE2	2.12	0.65
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.62	0.64
1:B:256:LEU:HA	1:B:275:VAL:CG2	2.28	0.64
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.80	0.64
1:B:328:ASN:HD22	1:B:328:ASN:N	1.95	0.63
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.79	0.63
1:A:133:ILE:HD13	1:A:414:TRP:CZ2	2.34	0.63
1:A:401:ALA:O	1:A:404:LEU:HB2	1.99	0.62
1:B:139:GLU:HB3	1:B:140:ARG:HH11	1.65	0.61
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.48	0.61
1:B:277:LYS:HG3	1:B:280:ARG:HB3	1.83	0.60
1:B:140:ARG:HG3	1:B:469:ARG:O	2.02	0.60
1:A:499:SER:HB3	1:A:523:VAL:HG12	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:VAL:HG11	1:A:351:ILE:HD11	1.83	0.59
1:A:504:ASN:HD21	1:A:522:THR:HB	1.68	0.59
1:A:390:HIS:HD2	1:A:393:ARG:H	1.50	0.59
1:A:504:ASN:HD22	1:A:504:ASN:C	2.05	0.59
1:B:551:LYS:HZ1	1:B:567:GLY:H	1.51	0.59
1:B:585:ARG:HB3	1:B:585:ARG:NH1	2.17	0.59
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.82	0.59
1:A:565:LYS:HD2	1:A:565:LYS:H	1.67	0.58
1:B:535:ARG:HD3	1:B:539:GLN:HE22	1.68	0.58
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.34	0.57
1:A:477:LYS:CD	1:A:477:LYS:H	2.15	0.57
1:A:224:ARG:NE	1:A:224:ARG:HA	2.19	0.57
1:A:441:LEU:CD2	1:A:580:ILE:HD11	2.33	0.56
1:B:470:ARG:HG3	3:B:1613:HOH:O	2.05	0.56
1:B:504:ASN:HD21	1:B:522:THR:HB	1.71	0.56
1:A:390:HIS:CD2	1:A:393:ARG:H	2.23	0.56
1:A:409:ALA:O	1:A:413:LEU:HD13	2.07	0.55
1:A:565:LYS:HD2	1:A:565:LYS:N	2.22	0.55
1:B:133:ILE:HB	1:B:451:LEU:HD23	1.89	0.55
1:A:275:VAL:HA	1:A:282:ASN:OD1	2.07	0.55
1:B:504:ASN:HD22	1:B:504:ASN:C	2.10	0.55
1:A:281:THR:HG21	1:A:291:PRO:HG3	1.89	0.55
1:B:281:THR:HG22	1:B:291:PRO:HB3	1.89	0.55
1:A:82:TYR:O	1:A:110:VAL:HG23	2.07	0.54
1:B:275:VAL:O	1:B:276:SER:HB2	2.08	0.54
1:A:346:ASN:ND2	1:A:348:ASP:H	2.05	0.54
1:A:416:LEU:HD23	1:A:416:LEU:H	1.72	0.54
1:B:475:GLU:HB2	1:B:478:GLU:HG2	1.89	0.54
1:A:163:ARG:HH11	1:A:163:ARG:HB2	1.72	0.54
1:B:224:ARG:HA	1:B:224:ARG:HE	1.73	0.54
1:A:11:LYS:N	1:A:15:ALA:HB3	2.23	0.53
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.90	0.53
1:B:289:GLN:HG2	3:B:1794:HOH:O	2.09	0.53
1:A:276:SER:O	1:A:277:LYS:HB2	2.06	0.53
1:A:255:VAL:HA	1:A:262:SER:OG	2.09	0.53
1:A:27:LEU:C	1:A:27:LEU:HD23	2.29	0.53
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.44	0.52
1:B:183:GLU:CD	1:B:232:ARG:HG3	2.30	0.52
1:B:275:VAL:HA	1:B:282:ASN:HD21	1.73	0.52
1:A:271:GLU:HG3	1:A:272:ASP:N	2.25	0.52
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.91	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:H	1:A:195:ILE:HD13	1.75	0.52
1:B:273:PHE:HA	1:B:274:PRO:C	2.30	0.52
1:A:36:ARG:NH2	1:A:38:GLU:OE2	2.43	0.52
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.45	0.52
1:A:82:TYR:C	1:A:110:VAL:HG23	2.30	0.52
1:B:251:ALA:O	1:B:255:VAL:HG23	2.10	0.52
1:A:275:VAL:O	1:A:276:SER:HB2	2.11	0.51
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.92	0.51
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.90	0.51
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.40	0.51
1:A:140:ARG:HH21	1:A:162:PRO:HB3	1.74	0.51
1:A:6:ILE:HD13	1:A:86:LEU:HD13	1.91	0.51
1:B:256:LEU:HD23	1:B:275:VAL:CG2	2.40	0.51
1:B:444:MET:HG2	1:B:490:LEU:HB3	1.92	0.51
1:A:504:ASN:ND2	1:A:504:ASN:C	2.64	0.50
1:B:464:THR:HG22	3:B:1662:HOH:O	2.10	0.50
1:A:141:PHE:CZ	1:A:182:LEU:HD21	2.46	0.50
1:A:236:ILE:N	1:A:236:ILE:HD12	2.26	0.50
1:A:90:GLN:HG3	1:A:92:GLU:OE2	2.11	0.50
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.93	0.50
1:A:573:LEU:HD11	1:A:579:MET:HG3	1.94	0.50
1:B:390:HIS:CE1	1:B:392:GLU:HB2	2.47	0.49
1:B:276:SER:HA	1:B:282:ASN:OD1	2.12	0.49
1:B:467:ASP:OD1	1:B:470:ARG:HD3	2.12	0.49
1:B:195:ILE:HD13	1:B:195:ILE:H	1.77	0.49
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.93	0.49
1:B:229:ALA:HB3	1:B:236:ILE:HD11	1.94	0.49
1:A:523:VAL:HG13	1:A:523:VAL:O	2.12	0.49
1:B:27:LEU:HD23	1:B:27:LEU:C	2.31	0.49
1:B:328:ASN:ND2	1:B:328:ASN:H	2.11	0.49
1:A:278:THR:O	1:A:279:SER:HB2	2.13	0.49
1:A:57:ALA:CB	1:A:71:ALA:HB2	2.43	0.49
1:B:224:ARG:HA	1:B:224:ARG:NE	2.28	0.49
1:A:193:THR:HB	1:A:194:PRO:CD	2.43	0.48
1:B:229:ALA:CB	1:B:236:ILE:HD11	2.43	0.48
1:A:8:HIS:HD2	1:A:26:ARG:O	1.96	0.48
1:B:328:ASN:ND2	1:B:328:ASN:N	2.59	0.48
1:B:551:LYS:NZ	1:B:567:GLY:N	2.60	0.48
1:B:473:ILE:CG2	1:B:478:GLU:HB2	2.43	0.48
1:A:77:THR:O	1:A:78:LYS:HB2	2.14	0.47
1:B:400:ARG:HD3	3:B:1902:HOH:O	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:HD3	3:A:1646:HOH:O	2.14	0.47
1:B:195:ILE:HD13	3:B:1845:HOH:O	2.14	0.47
1:B:535:ARG:HG3	1:B:535:ARG:HH11	1.80	0.47
1:A:1:MET:HB2	1:A:33:ASP:OD2	2.14	0.47
1:A:47:SER:OG	1:A:48:PRO:HD2	2.14	0.47
1:B:77:THR:O	1:B:78:LYS:HB2	2.14	0.47
1:B:504:ASN:ND2	1:B:504:ASN:C	2.68	0.47
1:B:160:ALA:O	1:B:162:PRO:HD3	2.15	0.46
1:A:573:LEU:CD1	1:A:579:MET:HG3	2.46	0.46
1:A:256:LEU:CD2	1:A:275:VAL:HG23	2.45	0.46
1:A:84:PHE:O	1:A:95:TYR:HA	2.15	0.46
1:A:565:LYS:O	1:A:565:LYS:HG2	2.15	0.46
1:B:127:TRP:CG	1:B:235:LYS:HE3	2.51	0.46
1:B:255:VAL:HG11	1:B:270:ILE:HD11	1.98	0.46
1:B:401:ALA:O	1:B:404:LEU:HB2	2.16	0.46
1:B:275:VAL:CA	1:B:282:ASN:HD21	2.29	0.46
1:B:355:ILE:HG23	1:B:357:HIS:CE1	2.51	0.46
1:A:199:PRO:HG3	1:A:248:GLN:HG3	1.97	0.45
1:A:271:GLU:HG2	1:A:282:ASN:O	2.16	0.45
1:B:248:GLN:HB2	3:B:1691:HOH:O	2.16	0.45
1:A:195:ILE:HD12	3:A:1639:HOH:O	2.17	0.45
1:A:195:ILE:HD13	3:A:1795:HOH:O	2.17	0.45
1:A:488:LYS:O	1:A:492:ARG:HG3	2.16	0.45
1:A:508:TRP:HB2	1:A:520:VAL:HG23	1.98	0.45
1:B:250:PHE:CG	1:B:251:ALA:N	2.85	0.45
1:A:516:LEU:C	1:A:516:LEU:HD23	2.38	0.45
1:B:438:LEU:HD23	1:B:438:LEU:HA	1.81	0.45
1:A:260:GLU:HG2	3:A:1798:HOH:O	2.17	0.45
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.82	0.45
1:B:118:ARG:HG3	1:B:119:SER:N	2.31	0.44
1:B:163:ARG:HG3	1:B:163:ARG:HH11	1.81	0.44
1:A:289:GLN:O	1:A:291:PRO:HD3	2.17	0.44
1:B:136:ILE:HD12	1:B:190:LEU:HG	2.00	0.44
1:A:445:THR:HG21	1:A:580:ILE:CD1	2.46	0.44
1:A:504:ASN:O	1:A:521:ARG:HA	2.17	0.44
1:B:275:VAL:C	1:B:282:ASN:HD21	2.21	0.44
1:A:149:ASP:HB3	1:A:153:THR:OG1	2.18	0.44
1:A:277:LYS:HB3	1:A:280:ARG:CB	2.45	0.44
1:B:533:ASN:O	1:B:576:TYR:HA	2.18	0.44
1:A:224:ARG:CA	1:A:224:ARG:HE	2.24	0.43
1:B:475:GLU:HB2	1:B:478:GLU:CG	2.47	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HB2	1:A:262:SER:OG	2.18	0.43
1:A:411:GLN:NE2	3:A:1912:HOH:O	2.50	0.43
1:A:82:TYR:N	1:A:110:VAL:CG2	2.81	0.43
1:B:313:PHE:O	1:B:317:GLN:HG2	2.19	0.43
1:A:163:ARG:NH1	1:A:163:ARG:HB2	2.34	0.43
1:B:386:THR:OG1	1:B:388:GLU:HG3	2.18	0.43
1:A:229:ALA:CB	1:A:236:ILE:HD11	2.46	0.43
1:A:519:PHE:CE1	1:A:530:VAL:HB	2.54	0.43
1:B:263:ARG:HH21	1:B:263:ARG:HG3	1.83	0.43
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.54	0.43
1:A:518:ALA:HA	1:A:530:VAL:O	2.18	0.43
1:B:491:ILE:HG23	1:B:495:HIS:CE1	2.54	0.43
1:A:465:ASN:HA	1:A:466:PRO:HA	1.84	0.43
1:A:426:LEU:HB2	3:A:1737:HOH:O	2.17	0.43
1:A:504:ASN:ND2	1:A:522:THR:HB	2.32	0.42
1:A:533:ASN:O	1:A:576:TYR:HA	2.19	0.42
1:A:544:GLN:O	1:A:545:VAL:HG13	2.19	0.42
1:B:451:LEU:HD13	3:B:1885:HOH:O	2.18	0.42
1:B:551:LYS:HZ1	1:B:567:GLY:N	2.17	0.42
1:B:522:THR:HG23	1:B:527:HIS:CD2	2.54	0.42
1:A:179:LEU:N	1:A:180:PRO:CD	2.82	0.42
1:A:339:ARG:O	1:A:343:LYS:HG2	2.19	0.42
1:B:364:MET:HB2	3:B:1646:HOH:O	2.19	0.42
1:B:465:ASN:HA	1:B:466:PRO:HA	1.82	0.42
1:B:179:LEU:N	1:B:180:PRO:CD	2.82	0.42
1:A:416:LEU:H	1:A:416:LEU:CD2	2.32	0.42
1:A:260:GLU:H	1:A:260:GLU:HG2	1.50	0.42
1:A:581:LEU:HD22	1:A:581:LEU:N	2.34	0.42
1:A:223:ARG:HD2	1:A:223:ARG:HA	1.88	0.42
1:A:290:VAL:HG11	1:A:293:MET:CE	2.50	0.42
1:A:332:HIS:HD2	1:A:367:GLN:OE1	2.02	0.41
1:B:326:VAL:O	1:B:326:VAL:HG12	2.19	0.41
1:B:328:ASN:HD22	1:B:328:ASN:H	1.62	0.41
1:B:464:THR:O	1:B:465:ASN:C	2.58	0.41
1:B:467:ASP:O	1:B:470:ARG:HG3	2.19	0.41
1:A:251:ALA:O	1:A:255:VAL:HG23	2.20	0.41
1:A:554:LEU:HD12	1:A:560:GLU:O	2.20	0.41
1:B:458:ILE:HD12	1:B:473:ILE:HB	2.02	0.41
1:B:133:ILE:HD13	1:B:189:ALA:HB3	2.02	0.41
1:A:264:TYR:O	1:A:267:TRP:HB2	2.21	0.41
1:A:441:LEU:HD21	1:A:580:ILE:CD1	2.37	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:OE1	1:A:54:HIS:HD2	2.04	0.41
1:A:1:MET:HA	3:A:1886:HOH:O	2.20	0.41
1:A:444:MET:O	1:A:494:ARG:NH1	2.50	0.41
1:B:183:GLU:OE2	1:B:232:ARG:HG3	2.20	0.41
1:B:524:GLN:HB3	1:B:525:ASP:H	1.56	0.41
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.95	0.41
1:B:377:ARG:HA	1:B:380:VAL:HG22	2.03	0.41
1:A:235:LYS:C	1:A:236:ILE:HD12	2.41	0.41
1:A:63:ASP:HB2	3:A:1728:HOH:O	2.20	0.41
1:B:6:ILE:HA	1:B:28:ARG:O	2.21	0.41
1:B:573:LEU:CD1	1:B:579:MET:HG3	2.51	0.40
1:A:110:VAL:HG22	1:A:111:PHE:O	2.21	0.40
1:A:281:THR:CG2	1:A:291:PRO:HG3	2.51	0.40
1:A:346:ASN:HD22	1:A:346:ASN:C	2.24	0.40
1:A:411:GLN:HB3	1:A:411:GLN:HE21	1.70	0.40
1:A:583:ASN:ND2	1:A:585:ARG:HB2	2.36	0.40
1:B:585:ARG:HH11	1:B:585:ARG:HB3	1.83	0.40
1:A:381:ILE:O	1:A:385:ALA:HB3	2.22	0.40
1:A:141:PHE:HZ	1:A:182:LEU:HD21	1.85	0.40
1:A:219:LEU:HB2	1:A:220:PRO:HD3	2.04	0.40
1:A:88:GLY:HA3	1:A:92:GLU:OE1	2.22	0.40
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.56	0.40
1:A:410:ALA:HA	1:A:413:LEU:HD22	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%)	559 (96%)	23 (4%)	1 (0%)	49 61
1	B	583/585 (100%)	555 (95%)	27 (5%)	1 (0%)	49 61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1166/1170 (100%)	1114 (96%)	50 (4%)	2 (0%)	49	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	275	VAL
1	A	277	LYS

### 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%)	472 (96%)	21 (4%)	32	43
1	B	493/493 (100%)	469 (95%)	24 (5%)	27	38
All	All	986/986 (100%)	941 (95%)	45 (5%)	29	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	85	LEU
1	A	122	PHE
1	A	195	ILE
1	A	260	GLU
1	A	323	ARG
1	A	325	ASP
1	A	346	ASN
1	A	375	LEU
1	A	398	LEU
1	A	404	LEU
1	A	411	GLN
1	A	413	LEU
1	A	426	LEU
1	A	444	MET
1	A	466	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	483	LEU
1	A	504	ASN
1	A	535	ARG
1	A	565	LYS
1	A	571	LEU
1	B	49	GLU
1	B	94	VAL
1	B	122	PHE
1	B	155	GLN
1	B	190	LEU
1	B	195	ILE
1	B	223	ARG
1	B	232	ARG
1	B	248	GLN
1	B	323	ARG
1	B	325	ASP
1	B	328	ASN
1	B	364	MET
1	B	404	LEU
1	B	411	GLN
1	B	438	LEU
1	B	444	MET
1	B	451	LEU
1	B	465	ASN
1	B	466	PRO
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 (30) 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	244	HIS
1	A	261	GLN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	390	HIS
1	A	411	GLN
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS
1	A	563	HIS
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	465	ASN
1	B	504	ASN
1	B	527	HIS
1	B	539	GLN
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 carbohydrates 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

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	30 (5%) 28 35	14, 25, 47, 51	0
1	B	585/585 (100%)	0.15	32 (5%) 25 32	12, 25, 47, 51	0
All	All	1170/1170 (100%)	0.15	62 (5%) 26 33	12, 25, 47, 51	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	THR	14.6
1	A	279	SER	12.3
1	A	278	THR	10.7
1	B	279	SER	7.7
1	B	275	VAL	7.6
1	B	280	ARG	7.2
1	A	280	ARG	6.0
1	B	274	PRO	5.2
1	B	277	LYS	5.1
1	B	273	PHE	4.9
1	B	548	SER	4.8
1	A	277	LYS	3.9
1	B	551	LYS	3.9
1	B	546	PRO	3.9
1	B	276	SER	3.7
1	B	513	GLN	3.7
1	B	547	GLU	3.7
1	A	565	LYS	3.6
1	B	136	ILE	3.5
1	A	547	GLU	3.3
1	A	90	GLN	3.2
1	A	192	PHE	3.2
1	A	477	LYS	3.1
1	B	159	ASP	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	164	HIS	3.1
1	A	550	GLY	2.9
1	A	191	TYR	2.9
1	A	549	GLY	2.9
1	A	475	GLU	2.9
1	A	548	SER	2.8
1	B	550	GLY	2.8
1	A	566	GLN	2.7
1	A	263	ARG	2.7
1	B	49	GLU	2.6
1	A	275	VAL	2.5
1	B	192	PHE	2.5
1	B	155	GLN	2.5
1	B	566	GLN	2.5
1	A	93	ALA	2.4
1	B	524	GLN	2.4
1	A	106	SER	2.3
1	A	190	LEU	2.3
1	A	89	PRO	2.3
1	B	167	PHE	2.3
1	B	261	GLN	2.3
1	B	585	ARG	2.3
1	A	451	LEU	2.2
1	A	136	ILE	2.2
1	B	281	THR	2.2
1	B	477	LYS	2.2
1	A	238	LEU	2.2
1	A	240	ALA	2.1
1	A	546	PRO	2.1
1	B	164	HIS	2.1
1	B	478	GLU	2.1
1	B	48	PRO	2.1
1	A	237	ILE	2.1
1	A	159	ASP	2.1
1	B	193	THR	2.1
1	B	237	ILE	2.1
1	B	190	LEU	2.0
1	A	276	SER	2.0

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

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. 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	1601	1/1	0.98	0.07	24,24,24,24	0
2	CA	B	1602	1/1	0.98	0.04	30,30,30,30	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.