



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 03:19 am GMT

PDB ID : 4AEE  
Title : CRYSTAL STRUCTURE OF MALTOGENIC AMYLASE FROM S.MARINUS  
Authors : Jung, T.Y.; Park, C.H.; Yoon, S.M.; Park, S.H.; Park, K.H.; Woo, E.J.  
Deposited on : 2012-01-10  
Resolution : 2.28 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>.

---

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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

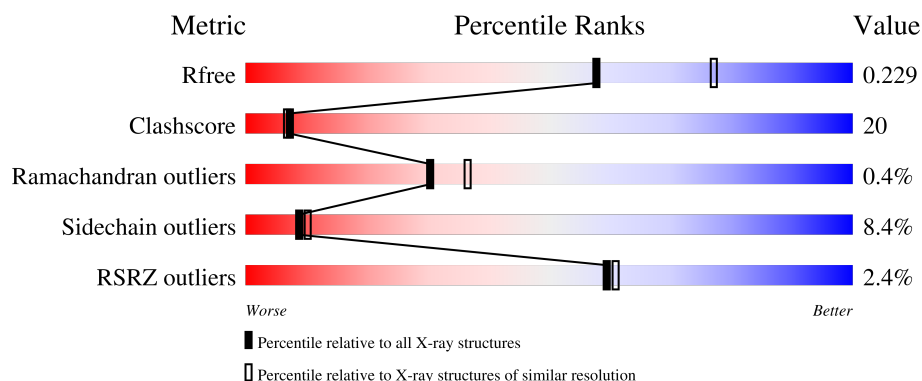
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

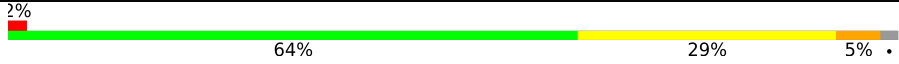

The reported resolution of this entry is 2.28 Å.

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))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	696	
1	B	696	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11772 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, CATALYTIC REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	0	0
			5735	3747	937	1028	23			
1	B	684	Total	C	N	O	S	0	0	0
			5739	3750	938	1028	23			

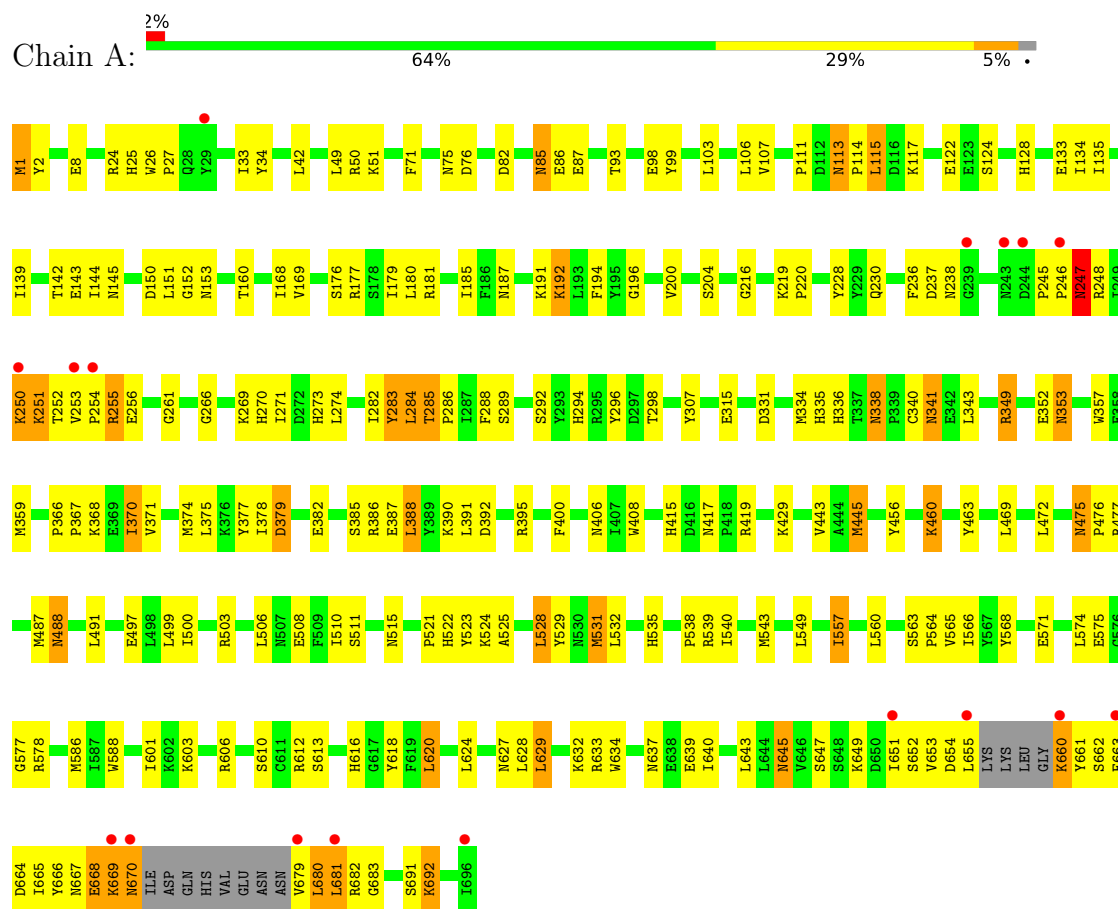
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	153	Total	O	0	0
			153	153		
2	B	145	Total	O	0	0
			145	145		

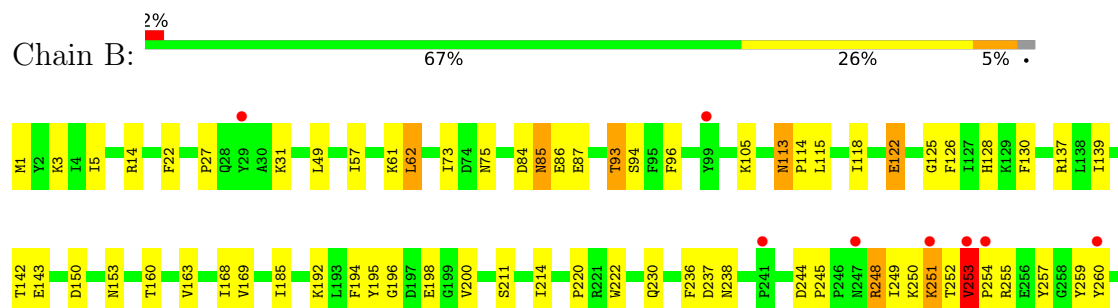
### 3 Residue-property plots

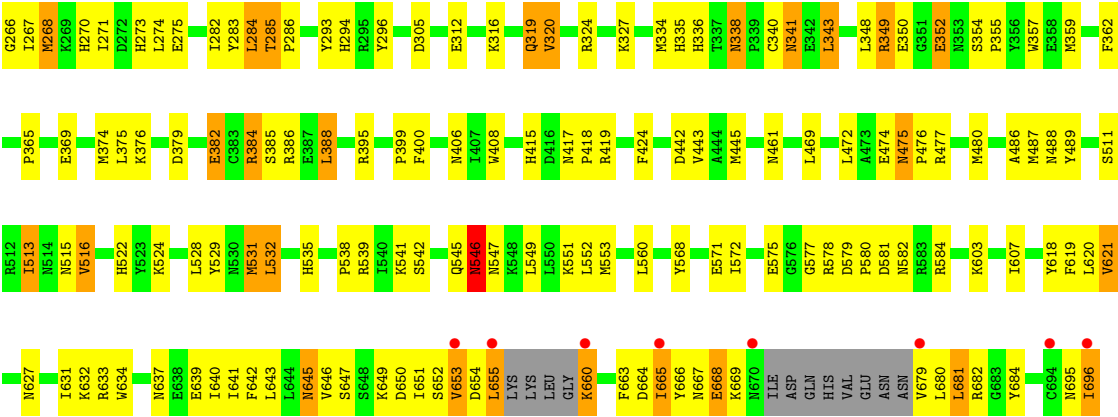
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, CATALYTIC REGION



#### • Molecule 1: ALPHA AMYLASE, CATALYTIC REGION





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.39Å 117.51Å 199.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.28 49.55 – 2.28	Depositor EDS
% Data completeness (in resolution range)	85.6 (49.55-2.28) 85.6 (49.55-2.28)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.07 (at 2.27Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.238 0.184 , 0.229	Depositor DCC
$R_{free}$ test set	3087 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

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	0.44	0/5896	0.56	0/7972
1	B	0.41	0/5900	0.56	1/7976 (0.0%)
All	All	0.42	0/11796	0.56	1/15948 (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	253	VAL	CB-CA-C	-6.59	98.88	111.40

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	5735	0	5660	241	0
1	B	5739	0	5671	234	0
2	A	153	0	0	4	0
2	B	145	0	0	9	0
All	All	11772	0	11331	462	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 20.

All (462) 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:253:VAL:CB	1:B:254:PRO:HD3	1.68	1.22
1:B:253:VAL:HB	1:B:254:PRO:HD3	1.16	1.14
1:A:253:VAL:HG22	1:A:254:PRO:HD3	1.19	1.13
1:B:349:ARG:NH1	1:B:379:ASP:OD2	1.84	1.11
1:A:368:LYS:H	1:A:368:LYS:HD2	1.20	1.06
1:B:253:VAL:CG2	1:B:254:PRO:HD3	1.86	1.04
1:B:653:VAL:CG2	1:B:679:VAL:O	2.06	1.03
1:B:253:VAL:HG23	1:B:254:PRO:CD	1.89	1.01
1:B:253:VAL:HG23	1:B:254:PRO:HD2	1.41	1.01
1:B:653:VAL:HG22	1:B:679:VAL:O	1.61	1.00
1:B:338:ASN:HD22	1:B:340:CYS:H	1.08	1.00
1:A:645:ASN:HB2	1:A:681:LEU:CD1	1.92	1.00
1:A:645:ASN:HB2	1:A:681:LEU:HD11	1.39	0.99
1:B:255:ARG:HG2	1:B:580:PRO:O	1.63	0.99
1:A:645:ASN:CB	1:A:681:LEU:HD11	1.91	0.98
1:A:253:VAL:HG22	1:A:254:PRO:CD	1.92	0.98
1:A:367:PRO:HG2	1:A:370:ILE:HG12	1.45	0.98
1:B:253:VAL:CB	1:B:254:PRO:CD	2.42	0.97
1:A:654:ASP:O	1:A:655:LEU:HB2	1.64	0.96
1:A:613:SER:OG	1:A:640:ILE:HD13	1.66	0.94
1:B:253:VAL:HB	1:B:254:PRO:CD	1.97	0.94
1:A:632:LYS:HZ2	1:A:639:GLU:HG2	1.29	0.94
1:A:253:VAL:CG2	1:A:254:PRO:HD3	1.97	0.94
1:B:250:LYS:O	1:B:252:THR:HG23	1.68	0.93
1:A:338:ASN:HD22	1:A:340:CYS:H	1.16	0.91
1:B:253:VAL:CG2	1:B:254:PRO:CD	2.47	0.90
1:A:578:ARG:NH2	1:B:252:THR:CG2	2.37	0.87
1:A:632:LYS:NZ	1:A:639:GLU:HG2	1.89	0.87
1:B:655:LEU:HD13	1:B:660:LYS:NZ	1.88	0.87
1:A:253:VAL:CG2	1:A:254:PRO:CD	2.54	0.86
1:B:255:ARG:HB3	1:B:581:ASP:HA	1.56	0.86
1:A:368:LYS:H	1:A:368:LYS:CD	1.88	0.85
1:A:578:ARG:NH2	1:B:252:THR:HG21	1.92	0.84
1:A:627:ASN:HD22	1:A:649:LYS:NZ	1.75	0.83
1:A:274:LEU:HD13	1:A:282:ILE:HD11	1.59	0.83
1:B:352:GLU:OE2	1:B:365:PRO:HG3	1.79	0.82
1:A:603:LYS:HG3	1:A:606:ARG:NH2	1.95	0.81
1:B:577:GLY:O	1:B:582:ASN:HB3	1.82	0.80
1:B:250:LYS:O	1:B:252:THR:CG2	2.30	0.80
1:B:653:VAL:HG23	1:B:679:VAL:O	1.78	0.80
1:A:645:ASN:CB	1:A:681:LEU:CD1	2.56	0.80
1:B:294:HIS:HD2	1:B:296:TYR:H	1.27	0.80

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG21	1:A:634:TRP:HH2	1.46	0.79
1:A:359:MET:HE2	1:A:359:MET:HA	1.62	0.79
1:A:253:VAL:HG23	1:A:254:PRO:N	1.95	0.79
1:B:251:LYS:CG	1:B:251:LYS:O	2.31	0.78
1:B:285:THR:HG23	1:B:286:PRO:HD2	1.66	0.77
1:A:368:LYS:HD2	1:A:368:LYS:N	1.97	0.77
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.50	0.77
1:A:292:SER:HB3	1:A:386:ARG:NH2	2.00	0.76
1:A:639:GLU:C	1:A:640:ILE:HD12	2.06	0.76
1:A:680:LEU:O	1:A:680:LEU:HG	1.84	0.76
1:A:645:ASN:CG	1:A:681:LEU:HD11	2.06	0.76
1:B:338:ASN:ND2	1:B:340:CYS:H	1.84	0.76
1:A:245:PRO:HG3	1:A:307:TYR:CG	2.21	0.76
1:A:253:VAL:CG2	1:A:254:PRO:N	2.48	0.76
1:A:664:ASP:O	1:A:668:GLU:N	2.19	0.75
1:B:352:GLU:OE2	1:B:365:PRO:CG	2.33	0.75
1:B:603:LYS:HD2	1:B:666:TYR:CE1	2.22	0.74
1:B:654:ASP:CG	1:B:655:LEU:H	1.91	0.74
1:B:237:ASP:OD2	1:B:270:HIS:HE1	1.71	0.74
1:B:667:ASN:HB3	1:B:669:LYS:HE3	1.68	0.74
1:A:645:ASN:OD1	1:A:681:LEU:HD11	1.88	0.73
1:B:655:LEU:HD13	1:B:660:LYS:HZ2	1.52	0.73
1:A:681:LEU:C	1:A:681:LEU:HD12	2.09	0.72
1:A:539:ARG:HD3	2:A:2129:HOH:O	1.89	0.71
1:B:579:ASP:OD1	1:B:580:PRO:HB3	1.91	0.71
1:B:529:TYR:CE1	1:B:531:MET:HG3	2.25	0.70
1:A:529:TYR:CE1	1:A:531:MET:HG2	2.27	0.70
1:B:653:VAL:CG2	1:B:679:VAL:C	2.60	0.70
1:A:417:ASN:HD21	1:A:419:ARG:NH1	1.89	0.69
1:B:341:ASN:HD22	1:B:343:LEU:H	1.40	0.69
1:A:487:MET:HA	1:A:529:TYR:HB3	1.73	0.69
1:B:255:ARG:CG	1:B:580:PRO:O	2.40	0.69
1:B:294:HIS:CD2	1:B:296:TYR:H	2.11	0.69
1:A:237:ASP:OD2	1:A:270:HIS:HE1	1.75	0.69
1:A:335:HIS:ND1	1:A:336:HIS:HD2	1.91	0.69
1:A:628:LEU:HD11	1:A:643:LEU:HD22	1.75	0.69
1:B:126:PHE:HE2	1:B:139:ILE:HD13	1.58	0.69
1:B:113:ASN:ND2	1:B:115:LEU:H	1.91	0.69
1:A:578:ARG:HH21	1:B:252:THR:HB	1.58	0.68
1:B:667:ASN:C	1:B:668:GLU:HG2	2.12	0.68
1:A:128:HIS:CE1	1:A:522:HIS:H	2.11	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASN:ND2	1:A:477:ARG:H	1.91	0.68
1:B:128:HIS:CE1	1:B:522:HIS:H	2.12	0.68
1:B:350:GLU:HB3	1:B:354:SER:HB3	1.74	0.68
1:A:294:HIS:HD2	1:A:296:TYR:H	1.41	0.68
1:A:177:ARG:HD2	1:A:180:LEU:HD12	1.74	0.67
1:A:529:TYR:HE1	1:A:531:MET:HG2	1.59	0.67
1:A:385:SER:O	1:A:388:LEU:HB2	1.94	0.67
1:A:475:ASN:C	1:A:475:ASN:HD22	1.97	0.67
1:B:274:LEU:HD13	1:B:282:ILE:HD11	1.77	0.66
1:A:603:LYS:HG3	1:A:606:ARG:HH21	1.60	0.66
1:B:579:ASP:OD1	1:B:580:PRO:CA	2.44	0.66
1:B:475:ASN:ND2	1:B:477:ARG:H	1.93	0.65
1:A:142:THR:HG22	1:A:168:ILE:HD11	1.78	0.65
1:B:113:ASN:HD22	1:B:115:LEU:H	1.43	0.65
1:A:85:ASN:ND2	1:A:87:GLU:H	1.95	0.65
1:A:627:ASN:HD22	1:A:649:LYS:HZ1	1.43	0.65
1:A:539:ARG:HG3	1:A:575:GLU:C	2.17	0.65
1:A:651:ILE:HD11	1:A:681:LEU:HD21	1.79	0.65
1:B:237:ASP:O	1:B:266:GLY:HA3	1.97	0.65
1:B:87:GLU:CG	1:B:105:LYS:HE2	2.28	0.65
1:B:250:LYS:O	1:B:251:LYS:C	2.36	0.65
1:A:113:ASN:ND2	1:A:115:LEU:HB2	2.12	0.64
1:A:660:LYS:N	1:A:660:LYS:CD	2.59	0.64
1:A:613:SER:HG	1:A:640:ILE:HD13	1.60	0.64
1:B:273:HIS:HE1	1:B:571:GLU:OE2	1.79	0.64
1:A:627:ASN:HD22	1:A:649:LYS:HZ3	1.45	0.64
1:A:113:ASN:HD21	1:A:115:LEU:HB2	1.62	0.64
1:A:352:GLU:HA	1:A:357:TRP:CG	2.32	0.64
1:A:349:ARG:HH11	1:A:349:ARG:CG	2.09	0.64
1:B:475:ASN:C	1:B:475:ASN:HD22	2.01	0.64
1:A:250:LYS:C	1:A:252:THR:H	2.01	0.64
1:B:382:GLU:CG	1:B:384:ARG:HD3	2.27	0.64
1:A:628:LEU:HD23	1:A:651:ILE:HD11	1.80	0.63
1:A:228:TYR:HB2	1:A:565:VAL:HG22	1.80	0.63
1:A:639:GLU:O	1:A:640:ILE:HD12	1.99	0.63
1:B:222:TRP:CE3	1:B:327:LYS:HD2	2.34	0.63
1:B:653:VAL:HG23	1:B:679:VAL:N	2.12	0.63
1:A:250:LYS:O	1:A:252:THR:N	2.32	0.63
1:A:475:ASN:HD22	1:A:476:PRO:N	1.96	0.63
1:A:2:TYR:CE1	1:A:106:LEU:HD12	2.33	0.63
1:A:679:VAL:HG22	1:A:680:LEU:N	2.14	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:HG2	1:B:73:ILE:HD13	1.81	0.62
1:B:642:PHE:C	1:B:643:LEU:HD12	2.19	0.62
1:A:24:ARG:HD2	1:A:71:PHE:CD2	2.35	0.61
1:A:662:SER:O	1:A:670:ASN:HB3	2.00	0.61
1:B:254:PRO:O	1:B:255:ARG:C	2.38	0.61
1:A:292:SER:HB3	1:A:386:ARG:HH21	1.65	0.61
1:A:338:ASN:ND2	1:A:340:CYS:H	1.94	0.61
1:A:247:ASN:HD21	1:B:395:ARG:HH12	1.48	0.61
1:A:352:GLU:O	1:A:353:ASN:ND2	2.34	0.61
1:A:664:ASP:O	1:A:668:GLU:CA	2.48	0.60
1:B:650:ASP:OD1	1:B:682:ARG:HA	2.01	0.60
1:B:271:ILE:CD1	1:B:320:VAL:CG2	2.78	0.60
1:B:579:ASP:OD1	1:B:580:PRO:CB	2.49	0.60
1:B:653:VAL:N	1:B:679:VAL:O	2.31	0.60
1:A:285:THR:HG23	1:A:286:PRO:HD2	1.84	0.60
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.67	0.60
1:A:538:PRO:HA	1:A:577:GLY:O	2.01	0.60
1:B:61:LYS:O	1:B:62:LEU:HD13	2.02	0.59
1:A:245:PRO:HG3	1:A:307:TYR:CD1	2.36	0.59
1:A:359:MET:CE	1:A:419:ARG:HB2	2.33	0.59
1:B:87:GLU:HG2	1:B:105:LYS:HE2	1.84	0.59
1:B:285:THR:HG23	1:B:286:PRO:CD	2.32	0.59
1:B:627:ASN:HB3	1:B:646:VAL:HG22	1.85	0.59
1:B:251:LYS:O	1:B:251:LYS:HG2	2.03	0.59
1:B:271:ILE:CD1	1:B:320:VAL:HG21	2.32	0.59
1:B:85:ASN:ND2	1:B:87:GLU:H	2.01	0.59
1:A:115:LEU:HG	1:A:200:VAL:HG11	1.85	0.59
1:B:385:SER:O	1:B:388:LEU:HB2	2.03	0.58
1:B:695:ASN:O	1:B:696:ILE:HG23	2.03	0.58
1:A:475:ASN:HD22	1:A:477:ARG:H	1.51	0.58
1:A:663:PHE:CE1	1:A:668:GLU:O	2.56	0.58
1:A:681:LEU:HD12	1:A:681:LEU:O	2.02	0.58
1:B:382:GLU:HG3	1:B:384:ARG:HD3	1.84	0.58
1:B:645:ASN:HD22	1:B:647:SER:H	1.48	0.58
1:B:665:ILE:HD12	1:B:665:ILE:O	2.03	0.58
1:B:645:ASN:ND2	1:B:647:SER:H	2.03	0.57
1:A:274:LEU:HD13	1:A:282:ILE:CD1	2.32	0.57
1:B:475:ASN:HD22	1:B:477:ARG:H	1.50	0.57
1:B:160:THR:HG21	1:B:634:TRP:HH2	1.68	0.57
1:B:480:MET:O	1:B:524:LYS:HE3	2.05	0.57
1:A:578:ARG:HH21	1:B:252:THR:CB	2.17	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:OD1	1:A:654:ASP:N	2.34	0.57
1:B:251:LYS:O	1:B:251:LYS:HG3	2.05	0.57
1:B:619:PHE:CZ	1:B:621:VAL:HG22	2.40	0.57
1:A:499:LEU:O	1:A:500:ILE:HD13	2.05	0.57
1:A:679:VAL:HG22	1:A:680:LEU:H	1.70	0.57
1:A:2:TYR:CZ	1:A:106:LEU:HD12	2.39	0.57
1:A:497:GLU:OE2	1:A:503:ARG:NH1	2.38	0.57
1:B:552:LEU:HD22	1:B:684:TYR:HA	1.87	0.57
1:A:488:ASN:ND2	1:A:491:LEU:H	2.03	0.56
1:A:645:ASN:HB2	1:A:681:LEU:HD13	1.86	0.56
1:B:571:GLU:HG2	1:B:572:ILE:HG23	1.87	0.56
1:B:653:VAL:HG23	1:B:679:VAL:C	2.22	0.56
1:B:546:ASN:HD22	1:B:546:ASN:C	2.09	0.56
1:A:341:ASN:HD22	1:A:343:LEU:H	1.54	0.55
1:A:374:MET:HE1	1:A:400:PHE:HE2	1.72	0.55
1:B:545:GLN:HA	1:B:545:GLN:NE2	2.20	0.55
1:B:607:ILE:HD13	1:B:665:ILE:HD11	1.88	0.55
1:A:670:ASN:N	1:A:670:ASN:OD1	2.39	0.55
1:B:113:ASN:HD22	1:B:113:ASN:C	2.10	0.55
1:B:354:SER:HB2	1:B:355:PRO:HD2	1.89	0.55
1:A:98:GLU:OE2	1:B:253:VAL:HG22	2.07	0.55
1:A:349:ARG:CG	1:A:349:ARG:NH1	2.66	0.55
1:A:160:THR:HB	1:A:620:LEU:HD12	1.87	0.55
1:B:270:HIS:HD2	2:B:2070:HOH:O	1.89	0.54
1:B:480:MET:HB3	1:B:524:LYS:HG2	1.88	0.54
1:A:387:GLU:HG2	1:A:390:LYS:NZ	2.22	0.54
1:B:305:ASP:OD1	2:B:2069:HOH:O	2.18	0.54
1:A:506:LEU:O	1:A:510:ILE:HG13	2.08	0.54
1:A:578:ARG:HH21	1:B:252:THR:CG2	2.18	0.54
1:B:545:GLN:HA	1:B:545:GLN:HE21	1.73	0.54
1:A:578:ARG:CZ	1:B:252:THR:HG21	2.38	0.53
1:A:359:MET:HE3	1:A:419:ARG:HB2	1.91	0.53
1:B:654:ASP:CG	1:B:655:LEU:N	2.61	0.53
1:B:655:LEU:HD13	1:B:660:LYS:CE	2.37	0.53
1:A:160:THR:CG2	1:A:634:TRP:HH2	2.19	0.53
1:B:664:ASP:OD1	1:B:664:ASP:C	2.47	0.53
1:A:134:ILE:HD13	1:A:176:SER:HA	1.90	0.53
1:A:245:PRO:HB3	1:A:246:PRO:HD2	1.90	0.53
1:B:541:LYS:HG2	1:B:575:GLU:HG2	1.90	0.53
1:A:660:LYS:N	1:A:660:LYS:HD2	2.22	0.53
1:A:177:ARG:HD2	1:A:180:LEU:CD1	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PHE:HZ	1:B:578:ARG:HG2	1.73	0.53
1:B:125:GLY:O	1:B:137:ARG:HD2	2.09	0.53
1:A:250:LYS:C	1:A:252:THR:N	2.62	0.52
1:A:618:TYR:O	1:A:633:ARG:HA	2.09	0.52
1:B:75:ASN:HB2	1:B:406:ASN:OD1	2.08	0.52
1:B:316:LYS:O	1:B:320:VAL:HG13	2.08	0.52
1:B:542:SER:OG	1:B:575:GLU:HB3	2.09	0.52
1:B:268:MET:SD	1:B:316:LYS:HG3	2.49	0.52
1:A:135:ILE:HD12	1:A:135:ILE:N	2.23	0.52
1:A:139:ILE:HG12	1:A:169:VAL:HG22	1.90	0.52
1:A:443:VAL:HG12	1:A:443:VAL:O	2.10	0.52
1:B:579:ASP:OD1	1:B:580:PRO:HA	2.09	0.52
1:A:76:ASP:HB3	2:A:2031:HOH:O	2.09	0.52
1:A:667:ASN:O	1:A:668:GLU:CB	2.58	0.52
1:A:75:ASN:HB2	1:A:406:ASN:OD1	2.10	0.52
1:A:177:ARG:HG3	1:A:179:ILE:O	2.10	0.52
1:B:475:ASN:HD22	1:B:476:PRO:N	2.07	0.52
1:B:442:ASP:OD2	1:B:443:VAL:HG23	2.09	0.52
1:B:681:LEU:O	1:B:681:LEU:HD23	2.10	0.52
1:B:3:LYS:HE2	1:B:5:ILE:CD1	2.40	0.51
1:B:529:TYR:CD1	1:B:531:MET:HG3	2.45	0.51
1:B:621:VAL:CG1	1:B:631:ILE:HG12	2.40	0.51
1:A:85:ASN:HD22	1:A:87:GLU:H	1.57	0.51
1:B:639:GLU:O	1:B:640:ILE:HD12	2.11	0.51
1:A:113:ASN:ND2	1:A:115:LEU:H	2.08	0.51
1:A:236:PHE:O	1:A:237:ASP:HB2	2.10	0.51
1:A:134:ILE:N	1:A:134:ILE:HD12	2.26	0.51
1:A:374:MET:HE1	1:A:408:TRP:HZ3	1.76	0.51
1:B:513:ILE:HD13	1:B:513:ILE:N	2.26	0.51
1:B:621:VAL:HG13	1:B:631:ILE:HG12	1.91	0.51
1:A:230:GLN:OE1	1:A:535:HIS:HD2	1.94	0.50
1:A:653:VAL:O	1:A:679:VAL:HG12	2.12	0.50
1:B:350:GLU:HB2	1:B:354:SER:OG	2.11	0.50
1:A:374:MET:HE1	1:A:400:PHE:CE2	2.46	0.50
1:B:268:MET:O	1:B:271:ILE:HG13	2.11	0.50
1:B:139:ILE:HD12	1:B:139:ILE:N	2.27	0.50
1:A:374:MET:CE	1:A:400:PHE:HE2	2.24	0.50
1:A:506:LEU:HD11	1:A:629:LEU:HG	1.92	0.50
1:B:649:LYS:HD2	1:B:649:LYS:N	2.26	0.50
1:A:99:TYR:HE2	1:A:578:ARG:HH12	1.60	0.50
1:A:251:LYS:O	1:A:252:THR:C	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:THR:OG1	1:A:256:GLU:OE2	2.29	0.49
1:A:391:LEU:O	1:A:395:ARG:HG2	2.12	0.49
1:A:230:GLN:OE1	1:A:535:HIS:CD2	2.65	0.49
1:A:379:ASP:OD1	1:A:379:ASP:O	2.30	0.49
1:A:668:GLU:O	1:A:669:LYS:O	2.30	0.49
1:B:192:LYS:HE2	1:B:194:PHE:CE1	2.47	0.49
1:B:319:GLN:OE1	1:B:319:GLN:N	2.45	0.49
1:B:655:LEU:CD1	1:B:660:LYS:NZ	2.70	0.49
1:A:682:ARG:O	1:A:683:GLY:C	2.51	0.49
1:B:334:MET:O	1:B:415:HIS:HE1	1.95	0.49
1:B:382:GLU:HG2	1:B:384:ARG:HD3	1.93	0.49
1:B:581:ASP:O	1:B:584:ARG:HG3	2.12	0.49
1:B:312:GLU:OE1	1:B:312:GLU:N	2.44	0.49
1:B:352:GLU:HA	1:B:357:TRP:CG	2.47	0.49
1:A:352:GLU:O	1:A:353:ASN:CB	2.61	0.49
1:A:603:LYS:HE2	1:A:666:TYR:CE1	2.48	0.49
1:B:248:ARG:HG2	1:B:248:ARG:HH11	1.77	0.49
1:A:133:GLU:C	1:A:134:ILE:HD12	2.33	0.49
1:B:96:PHE:CZ	1:B:578:ARG:HG2	2.47	0.49
1:B:374:MET:HE1	1:B:400:PHE:HE2	1.77	0.49
1:A:85:ASN:HD22	1:A:86:GLU:N	2.10	0.49
1:B:222:TRP:CG	1:B:327:LYS:HE3	2.48	0.49
1:A:627:ASN:ND2	1:A:649:LYS:NZ	2.54	0.48
1:A:247:ASN:ND2	1:B:395:ARG:HH12	2.11	0.48
1:A:578:ARG:NH2	1:B:252:THR:HG22	2.28	0.48
1:B:150:ASP:HB2	1:B:185:ILE:HD11	1.95	0.48
1:A:653:VAL:O	1:A:679:VAL:CG1	2.62	0.48
1:A:566:ILE:HD11	1:A:601:ILE:CG2	2.43	0.48
1:A:647:SER:OG	1:A:649:LYS:HG2	2.12	0.48
1:A:359:MET:CE	1:A:417:ASN:ND2	2.76	0.48
1:A:645:ASN:CB	1:A:681:LEU:HD13	2.41	0.48
1:B:653:VAL:HG22	1:B:679:VAL:C	2.26	0.48
1:B:532:LEU:HD21	1:B:553:MET:HB3	1.95	0.48
1:B:643:LEU:HD12	1:B:643:LEU:N	2.28	0.48
1:B:118:ILE:HA	1:B:139:ILE:O	2.14	0.48
1:B:645:ASN:HD22	1:B:645:ASN:C	2.17	0.48
1:A:379:ASP:OD1	1:A:379:ASP:C	2.52	0.48
1:B:14:ARG:HD3	1:B:196:GLY:O	2.14	0.48
1:B:654:ASP:O	1:B:655:LEU:C	2.52	0.48
1:A:294:HIS:CD2	1:A:296:TYR:H	2.27	0.48
1:A:460:LYS:HE2	1:A:460:LYS:HA	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:LYS:HD3	1:A:661:TYR:H	1.78	0.48
1:B:238:ASN:ND2	2:B:2067:HOH:O	2.47	0.48
1:A:284:LEU:O	1:A:331:ASP:HB2	2.14	0.47
1:B:350:GLU:HB3	1:B:354:SER:CB	2.43	0.47
1:A:160:THR:HG21	1:A:634:TRP:CH2	2.36	0.47
1:A:663:PHE:CE2	1:A:665:ILE:HD13	2.49	0.47
1:B:85:ASN:HD22	1:B:86:GLU:N	2.11	0.47
1:A:273:HIS:HE1	1:A:571:GLU:OE2	1.97	0.47
1:B:619:PHE:CZ	1:B:621:VAL:CG2	2.97	0.47
1:A:370:ILE:N	1:A:370:ILE:HD13	2.29	0.47
1:A:529:TYR:CE1	1:A:531:MET:CG	2.97	0.47
1:A:691:SER:O	1:A:692:LYS:HB3	2.14	0.47
1:A:681:LEU:CD1	1:A:681:LEU:C	2.81	0.47
1:A:682:ARG:NH2	1:B:649:LYS:NZ	2.62	0.47
1:B:93:THR:HG23	1:B:96:PHE:O	2.15	0.47
1:B:341:ASN:ND2	1:B:343:LEU:H	2.08	0.47
1:A:632:LYS:NZ	1:A:639:GLU:CG	2.72	0.47
1:B:271:ILE:CD1	1:B:320:VAL:HG23	2.43	0.47
1:B:271:ILE:HD13	1:B:320:VAL:HG23	1.96	0.47
1:A:540:ILE:HA	1:A:543:MET:HE2	1.97	0.47
1:B:249:ILE:HD11	1:B:260:TYR:HB2	1.97	0.47
1:B:195:TYR:HD1	1:B:200:VAL:HG12	1.79	0.47
1:B:511:SER:O	1:B:515:ASN:HB2	2.15	0.47
1:A:288:PHE:HB2	2:A:2082:HOH:O	2.16	0.46
1:B:194:PHE:O	1:B:200:VAL:HA	2.16	0.46
1:B:211:SER:HA	1:B:214:ILE:HD12	1.97	0.46
1:A:230:GLN:NE2	2:A:2070:HOH:O	2.47	0.46
1:B:568:TYR:CG	1:B:568:TYR:O	2.67	0.46
1:A:377:TYR:CE2	1:A:391:LEU:HD11	2.51	0.46
1:A:667:ASN:O	1:A:668:GLU:HB3	2.14	0.46
1:A:124:SER:HB2	1:A:521:PRO:HG3	1.96	0.46
1:B:96:PHE:CZ	1:B:538:PRO:HD3	2.50	0.46
1:A:238:ASN:OD1	1:A:261:GLY:C	2.54	0.46
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.15	0.46
1:B:22:PHE:O	1:B:57:ILE:HA	2.16	0.46
1:B:143:GLU:OE1	1:B:143:GLU:N	2.49	0.46
1:B:399:PRO:HA	1:B:408:TRP:CH2	2.51	0.46
1:A:25:HIS:O	1:A:27:PRO:HD3	2.16	0.46
1:B:352:GLU:OE2	1:B:365:PRO:HG2	2.15	0.46
1:A:429:LYS:HG2	1:A:463:TYR:OH	2.16	0.45
1:B:667:ASN:CB	1:B:669:LYS:HE3	2.43	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD21	1:A:103:LEU:HD11	1.97	0.45
1:A:366:PRO:HG3	1:A:400:PHE:CG	2.51	0.45
1:A:682:ARG:HH22	1:B:649:LYS:NZ	2.14	0.45
1:B:335:HIS:ND1	1:B:336:HIS:HD2	2.14	0.45
1:B:369:GLU:OE2	2:B:2093:HOH:O	2.21	0.45
1:B:85:ASN:HD22	1:B:87:GLU:H	1.65	0.45
1:B:275:GLU:OE1	1:B:324:ARG:NH1	2.50	0.45
1:B:579:ASP:HA	1:B:580:PRO:HA	1.60	0.45
1:B:618:TYR:O	1:B:633:ARG:HA	2.16	0.45
1:A:113:ASN:C	1:A:113:ASN:HD22	2.20	0.45
1:A:341:ASN:ND2	1:A:343:LEU:H	2.14	0.45
1:A:283:TYR:CD1	1:A:283:TYR:C	2.90	0.45
1:B:359:MET:HE2	1:B:359:MET:HA	1.97	0.45
1:B:603:LYS:HD2	1:B:666:TYR:CZ	2.51	0.45
1:B:607:ILE:CD1	1:B:665:ILE:HD11	2.45	0.45
1:A:387:GLU:HG2	1:A:390:LYS:HZ2	1.82	0.45
1:B:359:MET:CE	1:B:419:ARG:HB3	2.47	0.45
1:A:359:MET:HE2	1:A:359:MET:CA	2.40	0.45
1:B:31:LYS:HE3	1:B:362:PHE:O	2.17	0.45
1:A:152:GLY:HA3	1:A:181:ARG:HE	1.82	0.45
1:A:586:MET:HG2	1:A:588:TRP:CZ2	2.52	0.45
1:A:253:VAL:N	1:A:254:PRO:HD2	2.31	0.44
1:A:511:SER:O	1:A:515:ASN:HB2	2.17	0.44
1:A:557:ILE:HA	1:A:557:ILE:HD13	1.67	0.44
1:A:664:ASP:O	1:A:668:GLU:HA	2.17	0.44
1:B:472:LEU:HD12	1:B:486:ALA:CB	2.47	0.44
1:B:153:ASN:OD1	1:B:153:ASN:N	2.50	0.44
1:B:350:GLU:CB	1:B:354:SER:CB	2.96	0.44
1:B:651:ILE:HG22	1:B:652:SER:N	2.32	0.44
1:A:24:ARG:HD2	1:A:71:PHE:CG	2.52	0.44
1:A:185:ILE:CG2	1:A:192:LYS:HE3	2.48	0.44
1:A:392:ASP:CG	1:A:395:ARG:NH2	2.71	0.44
1:B:1:MET:HB2	1:B:84:ASP:OD2	2.18	0.44
1:B:271:ILE:HD11	1:B:320:VAL:HG21	1.98	0.44
1:B:296:TYR:OH	1:B:535:HIS:CE1	2.70	0.44
1:B:382:GLU:HG2	1:B:382:GLU:O	2.17	0.44
1:B:539:ARG:HG3	1:B:575:GLU:C	2.38	0.44
1:B:85:ASN:HD22	1:B:85:ASN:C	2.21	0.43
1:B:130:PHE:CZ	1:B:220:PRO:HG3	2.53	0.43
1:B:230:GLN:NE2	2:B:2065:HOH:O	2.51	0.43
1:B:236:PHE:HB3	2:B:2066:HOH:O	2.17	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PRO:HG2	1:A:117:LYS:CG	2.48	0.43
1:B:273:HIS:CE1	1:B:571:GLU:OE2	2.66	0.43
1:A:368:LYS:CD	1:A:368:LYS:N	2.64	0.43
1:A:113:ASN:HA	1:A:114:PRO:HD2	1.87	0.43
1:A:352:GLU:O	1:A:353:ASN:HB3	2.18	0.43
1:B:87:GLU:HG3	1:B:105:LYS:HE2	1.99	0.43
1:B:539:ARG:HD3	2:B:2132:HOH:O	2.18	0.43
1:B:334:MET:HA	1:B:424:PHE:CZ	2.53	0.43
1:B:113:ASN:HD22	1:B:114:PRO:N	2.16	0.43
1:B:257:TYR:CD1	1:B:257:TYR:C	2.92	0.43
1:B:334:MET:HG2	1:B:424:PHE:CD1	2.53	0.43
1:B:603:LYS:O	1:B:607:ILE:HG13	2.18	0.43
1:A:359:MET:HE1	1:A:419:ARG:HB2	2.00	0.43
1:B:461:ASN:ND2	2:B:2114:HOH:O	2.51	0.43
1:B:259:TYR:CE1	1:B:293:TYR:HA	2.54	0.43
1:A:245:PRO:CB	1:A:246:PRO:HD2	2.49	0.43
1:A:538:PRO:HG2	1:A:543:MET:SD	2.58	0.43
1:B:529:TYR:CE1	1:B:531:MET:CG	3.00	0.43
1:B:320:VAL:O	1:B:324:ARG:HG2	2.19	0.42
1:A:1:MET:HG3	1:A:2:TYR:N	2.34	0.42
1:A:282:ILE:HG22	1:A:284:LEU:HD13	2.01	0.42
1:A:563:SER:HA	1:A:564:PRO:HD2	1.88	0.42
1:B:14:ARG:HH22	1:B:122:GLU:CD	2.23	0.42
1:A:445:MET:HG3	1:A:472:LEU:HA	2.02	0.42
1:B:475:ASN:ND2	1:B:475:ASN:C	2.72	0.42
1:A:185:ILE:HG12	1:A:194:PHE:CE2	2.54	0.42
1:A:368:LYS:O	1:A:371:VAL:HG22	2.19	0.42
1:A:627:ASN:ND2	1:A:649:LYS:HZ1	2.14	0.42
1:B:250:LYS:HD3	1:B:250:LYS:N	2.35	0.42
1:A:1:MET:N	1:A:82:ASP:OD2	2.39	0.42
1:A:254:PRO:O	1:A:255:ARG:C	2.57	0.42
1:A:655:LEU:HB3	1:A:660:LYS:HE2	2.02	0.42
1:B:139:ILE:HG13	1:B:169:VAL:HG22	2.00	0.42
1:A:34:TYR:O	1:A:71:PHE:HA	2.20	0.42
1:A:196:GLY:HA3	1:A:204:SER:HB3	2.01	0.42
1:A:266:GLY:O	1:A:269:LYS:HG2	2.20	0.42
1:B:637:ASN:HD22	1:B:637:ASN:HA	1.64	0.42
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.78	0.42
1:A:219:LYS:HA	1:A:220:PRO:HD3	1.95	0.42
1:A:366:PRO:HG3	1:A:400:PHE:CD2	2.55	0.42
1:B:475:ASN:HD21	1:B:516:VAL:HB	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLY:HA2	1:A:523:TYR:CZ	2.54	0.42
1:A:612:ARG:O	1:A:616:HIS:O	2.37	0.42
1:A:251:LYS:C	1:A:252:THR:O	2.53	0.41
1:B:62:LEU:HD12	2:B:2024:HOH:O	2.19	0.41
1:B:244:ASP:HA	1:B:245:PRO:HD3	1.91	0.41
1:B:126:PHE:CE2	1:B:139:ILE:HD13	2.46	0.41
1:B:577:GLY:H	1:B:581:ASP:HB3	1.84	0.41
1:B:663:PHE:CD1	1:B:669:LYS:O	2.72	0.41
1:A:285:THR:HG23	1:A:286:PRO:CD	2.50	0.41
1:A:679:VAL:CG2	1:A:680:LEU:N	2.82	0.41
1:A:33:ILE:HG22	1:A:49:LEU:HD22	2.02	0.41
1:A:144:ILE:HG22	1:A:145:ASN:O	2.20	0.41
1:B:254:PRO:O	1:B:255:ARG:O	2.38	0.41
1:B:237:ASP:OD2	1:B:270:HIS:CE1	2.62	0.41
1:B:275:GLU:CD	1:B:324:ARG:HH11	2.23	0.41
1:A:187:ASN:HA	1:A:191:LYS:O	2.21	0.41
1:A:382:GLU:O	1:A:382:GLU:HG3	2.21	0.41
1:A:26:TRP:CD1	1:A:51:LYS:HD2	2.56	0.41
1:B:142:THR:HG22	1:B:168:ILE:HD11	2.03	0.41
1:B:267:ILE:HD13	1:B:284:LEU:HD11	2.03	0.41
1:B:384:ARG:HG3	1:B:384:ARG:HH11	1.86	0.41
1:B:620:LEU:HD23	1:B:632:LYS:HE2	2.02	0.41
1:A:566:ILE:HD11	1:A:601:ILE:HG21	2.02	0.41
1:A:667:ASN:O	1:A:668:GLU:HG2	2.21	0.41
1:B:250:LYS:O	1:B:252:THR:HG22	2.16	0.41
1:B:417:ASN:HA	1:B:418:PRO:HD2	1.91	0.41
1:A:359:MET:HE3	1:A:417:ASN:ND2	2.34	0.41
1:A:456:TYR:CE1	1:A:460:LYS:HD3	2.56	0.41
1:A:488:ASN:C	1:A:488:ASN:HD22	2.24	0.41
1:A:628:LEU:HD23	1:A:651:ILE:CD1	2.49	0.41
1:A:655:LEU:HD13	1:A:660:LYS:HZ1	1.85	0.41
1:A:663:PHE:HE2	1:A:665:ILE:HD13	1.86	0.41
1:A:568:TYR:O	1:A:568:TYR:CG	2.73	0.41
1:A:375:LEU:HA	1:A:378:ILE:HG12	2.03	0.40
1:A:566:ILE:CD1	1:A:601:ILE:HG21	2.52	0.40
1:B:248:ARG:HG2	1:B:248:ARG:NH1	2.36	0.40
1:B:352:GLU:HA	1:B:357:TRP:CD2	2.56	0.40
1:B:374:MET:HB2	1:B:374:MET:HE2	1.70	0.40
1:B:487:MET:HA	1:B:529:TYR:HB3	2.02	0.40
1:B:547:ASN:O	1:B:551:LYS:HG3	2.21	0.40
1:A:150:ASP:OD1	1:A:151:LEU:O	2.38	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:MET:O	1:A:415:HIS:HE1	2.04	0.40
1:A:628:LEU:HD11	1:A:643:LEU:CD2	2.48	0.40
1:A:525:ALA:HA	1:A:528:LEU:HD22	2.03	0.40
1:B:268:MET:HE2	1:B:268:MET:HB2	1.86	0.40
1:B:374:MET:CE	1:B:400:PHE:HE2	2.34	0.40
1:B:94:SER:OG	1:B:489:TYR:HB3	2.22	0.40
1:B:160:THR:HG21	1:B:634:TRP:CH2	2.53	0.40
1:A:247:ASN:HD21	1:B:395:ARG:NH1	2.16	0.40
1:A:624:LEU:HD12	1:A:628:LEU:HD12	2.03	0.40
1:B:641:ILE:HD12	1:B:643:LEU:HD11	2.03	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	678/696 (97%)	639 (94%)	36 (5%)	3 (0%)	30	36
1	B	678/696 (97%)	643 (95%)	33 (5%)	2 (0%)	37	45
All	All	1356/1392 (97%)	1282 (94%)	69 (5%)	5 (0%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	669	LYS
1	A	251	LYS
1	B	251	LYS
1	B	546	ASN
1	A	247	ASN

### 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	627/639 (98%)	572 (91%)	55 (9%)	8	9
1	B	628/639 (98%)	577 (92%)	51 (8%)	9	11
All	All	1255/1278 (98%)	1149 (92%)	106 (8%)	9	10

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	GLU
1	A	50	ARG
1	A	85	ASN
1	A	93	THR
1	A	107	VAL
1	A	113	ASN
1	A	115	LEU
1	A	122	GLU
1	A	143	GLU
1	A	153	ASN
1	A	192	LYS
1	A	247	ASN
1	A	248	ARG
1	A	250	LYS
1	A	255	ARG
1	A	271	ILE
1	A	283	TYR
1	A	284	LEU
1	A	285	THR
1	A	289	SER
1	A	298	THR
1	A	338	ASN
1	A	341	ASN
1	A	349	ARG
1	A	353	ASN
1	A	370	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	379	ASP
1	A	388	LEU
1	A	445	MET
1	A	460	LYS
1	A	469	LEU
1	A	475	ASN
1	A	488	ASN
1	A	508	GLU
1	A	524	LYS
1	A	528	LEU
1	A	531	MET
1	A	532	LEU
1	A	549	LEU
1	A	557	ILE
1	A	560	LEU
1	A	574	LEU
1	A	610	SER
1	A	620	LEU
1	A	629	LEU
1	A	637	ASN
1	A	645	ASN
1	A	652	SER
1	A	660	LYS
1	A	668	GLU
1	A	670	ASN
1	A	680	LEU
1	A	681	LEU
1	A	692	LYS
1	B	49	LEU
1	B	62	LEU
1	B	85	ASN
1	B	93	THR
1	B	113	ASN
1	B	122	GLU
1	B	163	VAL
1	B	198	GLU
1	B	248	ARG
1	B	253	VAL
1	B	268	MET
1	B	283	TYR
1	B	284	LEU
1	B	285	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	319	GLN
1	B	320	VAL
1	B	338	ASN
1	B	341	ASN
1	B	343	LEU
1	B	348	LEU
1	B	349	ARG
1	B	352	GLU
1	B	375	LEU
1	B	376	LYS
1	B	382	GLU
1	B	384	ARG
1	B	386	ARG
1	B	388	LEU
1	B	445	MET
1	B	469	LEU
1	B	474	GLU
1	B	475	ASN
1	B	488	ASN
1	B	513	ILE
1	B	516	VAL
1	B	528	LEU
1	B	531	MET
1	B	532	LEU
1	B	546	ASN
1	B	549	LEU
1	B	560	LEU
1	B	621	VAL
1	B	645	ASN
1	B	653	VAL
1	B	655	LEU
1	B	660	LYS
1	B	665	ILE
1	B	668	GLU
1	B	680	LEU
1	B	681	LEU
1	B	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	85	ASN
1	A	113	ASN
1	A	128	HIS
1	A	162	HIS
1	A	189	ASN
1	A	230	GLN
1	A	247	ASN
1	A	270	HIS
1	A	273	HIS
1	A	294	HIS
1	A	336	HIS
1	A	338	ASN
1	A	341	ASN
1	A	415	HIS
1	A	461	ASN
1	A	475	ASN
1	A	488	ASN
1	A	514	ASN
1	A	535	HIS
1	A	545	GLN
1	A	627	ASN
1	B	55	GLN
1	B	85	ASN
1	B	113	ASN
1	B	128	HIS
1	B	162	HIS
1	B	189	ASN
1	B	230	GLN
1	B	270	HIS
1	B	273	HIS
1	B	294	HIS
1	B	336	HIS
1	B	338	ASN
1	B	341	ASN
1	B	415	HIS
1	B	461	ASN
1	B	475	ASN
1	B	488	ASN
1	B	514	ASN
1	B	535	HIS
1	B	545	GLN
1	B	546	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	637	ASN
1	B	645	ASN

### 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](#)

There are no ligands in this entry.

### 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	684/696 (98%)	-0.13	17 (2%) 58 59	22, 37, 64, 99	0
1	B	684/696 (98%)	-0.08	16 (2%) 61 62	22, 38, 63, 91	0
All	All	1368/1392 (98%)	-0.11	33 (2%) 59 61	22, 38, 64, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	655	LEU	6.8
1	A	655	LEU	6.4
1	B	253	VAL	5.7
1	A	696	ILE	4.3
1	B	660	LYS	4.1
1	B	696	ILE	3.6
1	A	660	LYS	3.5
1	A	253	VAL	3.4
1	A	243	ASN	3.3
1	B	260	TYR	2.9
1	B	254	PRO	2.8
1	A	670	ASN	2.8
1	B	670	ASN	2.6
1	A	246	PRO	2.6
1	A	254	PRO	2.6
1	A	681	LEU	2.4
1	A	244	ASP	2.4
1	A	651	ILE	2.4
1	B	665	ILE	2.4
1	B	679	VAL	2.3
1	B	694	CYS	2.3
1	B	29	TYR	2.2
1	B	99	TYR	2.2
1	B	653	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	2.2
1	A	29	TYR	2.2
1	A	239	GLY	2.2
1	A	663	PHE	2.1
1	A	250	LYS	2.1
1	A	669	LYS	2.1
1	B	251	LYS	2.1
1	B	241	PRO	2.1
1	A	679	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.