



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:07 AM EDT

PDB ID : 4AEE / pdb_00004aee
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

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
Xtrriage (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

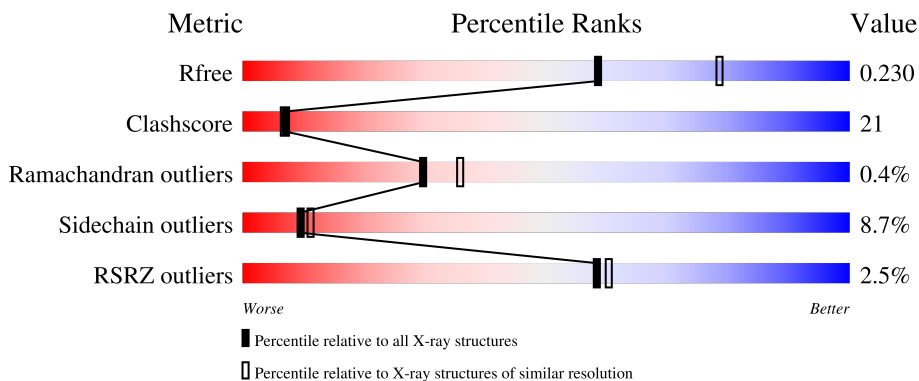
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 ≥ 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
			Total	C	N	O	S			
1	A	684	5735	3747	937	1028	23	0	0	0
1	B	684	5739	3750	938	1028	23	0	0	0

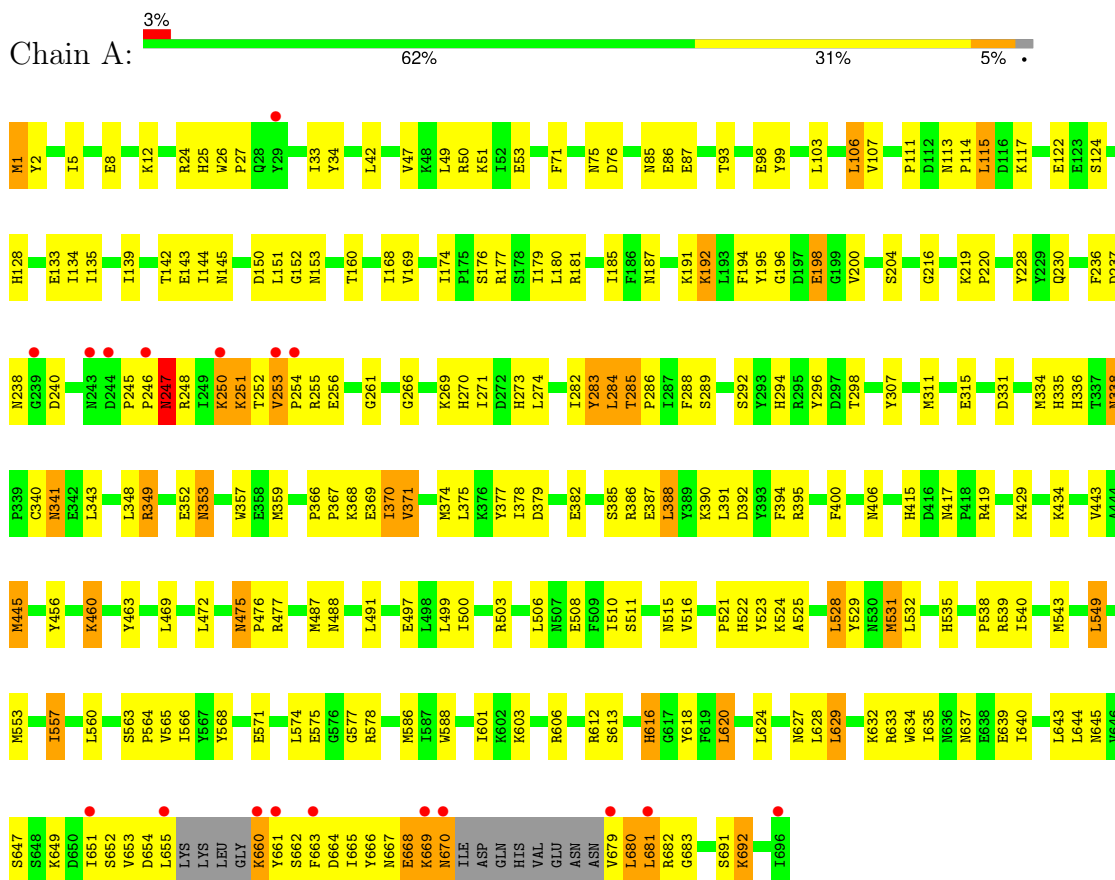
- Molecule 2 is water.

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

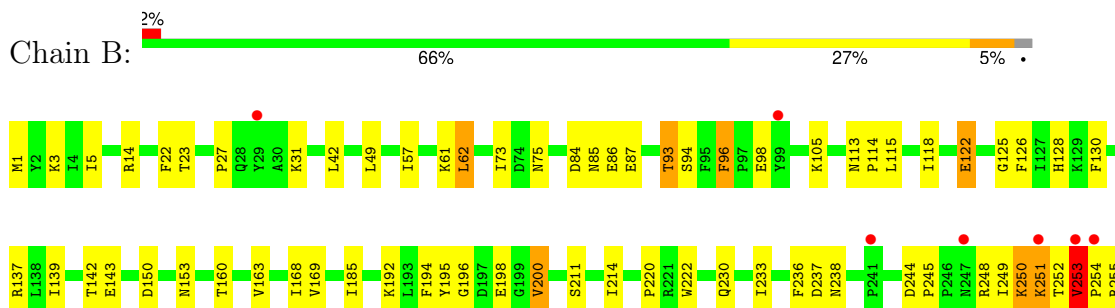
3 Residue-property plots

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.07 (at 2.27Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.238 0.185 , 0.230	Depositor DCC
R_{free} test set	3102 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.378	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage'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.*

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 i

5.1 Standard geometry i

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	0.52	0/5896	0.82	7/7972 (0.1%)
1	B	0.47	0/5900	0.81	8/7976 (0.1%)
All	All	0.50	0/11796	0.82	15/15948 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	HIS	N-CA-C	-7.78	98.94	110.46
1	B	253	VAL	N-CA-C	7.21	124.45	108.88
1	B	253	VAL	CB-CA-C	-6.86	98.88	111.36
1	B	96	PHE	CA-C-N	5.98	126.08	119.87
1	B	96	PHE	C-N-CA	5.98	126.08	119.87
1	B	616	HIS	N-CA-C	-5.78	101.90	110.46
1	B	695	ASN	N-CA-C	5.63	113.39	108.78
1	B	532	LEU	N-CA-C	-5.61	106.79	113.97
1	A	53	GLU	CB-CA-C	-5.56	110.18	116.63
1	A	240	ASP	CA-C-N	5.47	125.81	119.47
1	A	240	ASP	C-N-CA	5.47	125.81	119.47
1	B	233	ILE	N-CA-C	5.22	117.58	111.05
1	A	174	ILE	N-CA-C	5.17	114.65	108.45
1	A	47	VAL	N-CA-C	5.15	115.53	108.12
1	A	516	VAL	N-CA-C	-5.13	106.66	111.48

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	5735	0	5660	248	0
1	B	5739	0	5671	241	0
2	A	153	0	0	5	0
2	B	145	0	0	10	0
All	All	11772	0	11331	475	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 21.

All (475) 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:632:LYS:HZ2	1:A:639:GLU:HG2	1.26	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: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:A:359:MET:HE1	1:A:419:ARG:HB2	1.53	0.91
1:B:253:VAL:CG2	1:B:254:PRO:CD	2.47	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:374:MET:HE1	1:B:400:PHE:HE2	1.40	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:A:374:MET:HE1	1:A:400:PHE:HE2	1.44	0.83
1:B:352:GLU:OE2	1:B:365:PRO:HG3	1.79	0.82
1:A:374:MET:HE1	1:A:400:PHE:CE2	2.15	0.81
1:A:639:GLU:C	1:A:640:ILE:HD12	2.06	0.81
1:A:603:LYS:HG3	1:A:606:ARG:NH2	1.95	0.81
1:A:645:ASN:CG	1:A:681:LEU:HD11	2.06	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
1:A:160:THR:HG21	1:A:634:TRP:HH2	1.46	0.79
1:A:253:VAL:HG23	1:A:254:PRO:N	1.95	0.79
1:B:654:ASP:CG	1:B:655:LEU:H	1.91	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:681:LEU:C	1:A:681:LEU:HD12	2.09	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:680:LEU:O	1:A:680:LEU:HG	1.84	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:653:VAL:CG2	1:B:679:VAL:C	2.60	0.74
1:B:237:ASP:OD2	1:B:270:HIS:HE1	1.71	0.74
1:B:667:ASN:C	1:B:668:GLU:HG2	2.12	0.74
1:B:374:MET:HE1	1:B:400:PHE:CE2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:ASN:HB3	1:B:669:LYS:HE3	1.68	0.74
1:B:655:LEU:HD13	1:B:660:LYS:HZ2	1.52	0.73
1:A:645:ASN:OD1	1:A:681:LEU:HD11	1.88	0.72
1:A:475:ASN:C	1:A:475:ASN:HD22	1.97	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:359:MET:HE2	1:A:359:MET:HA	1.72	0.70
1:A:529:TYR:CE1	1:A:531:MET:HG2	2.27	0.70
1:A:417:ASN:HD21	1:A:419:ARG:NH1	1.89	0.69
1:A:539:ARG:HG3	1:A:575:GLU:C	2.17	0.69
1:B:250:LYS:O	1:B:251:LYS:C	2.36	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:475:ASN:C	1:B:475:ASN:HD22	2.01	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:250:LYS:C	1:A:252:THR:H	2.01	0.68
1:A:578:ARG:HH21	1:B:252:THR:HB	1.58	0.68
1:A:128:HIS:CE1	1:A:522:HIS:H	2.11	0.68
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:B:642:PHE:C	1:B:643:LEU:HD12	2.19	0.67
1:B:254:PRO:O	1:B:255:ARG:C	2.38	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ASN:HD22	1:A:649:LYS:HZ1	1.43	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: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: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: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:B:359:MET:HE1	1:B:419:ARG:HB3	1.79	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
1:B:27:PRO:HG2	1:B:73:ILE:HD13	1.81	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:546:ASN:HD22	1:B:546:ASN:C	2.09	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:B:653:VAL:HG23	1:B:679:VAL:C	2.22	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:B:113:ASN:HD22	1:B:113:ASN:C	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PRO:HG3	1:A:307:TYR:CD1	2.36	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:359:MET:HE3	1:A:417:ASN:ND2	2.18	0.58
1:B:654:ASP:CG	1:B:655:LEU:N	2.61	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:664:ASP:OD1	1:B:664:ASP:C	2.47	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:A:250:LYS:C	1:A:252:THR:N	2.62	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
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:A:341:ASN:HD22	1:A:343:LEU:H	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:251:LYS:O	1:A:252:THR:C	2.46	0.54
1:B:270:HIS:HD2	2:B:2070:HOH:O	1.89	0.54
1:A:359:MET:CE	1:A:419:ARG:HB2	2.33	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:A:682:ARG:O	1:A:683:GLY:C	2.51	0.54
1:B:545:GLN:HA	1:B:545:GLN:HE21	1.73	0.54
1:A:133:GLU:C	1:A:134:ILE:HD12	2.33	0.53
1:A:578:ARG:CZ	1:B:252:THR:HG21	2.38	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: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:B:653:VAL:HG22	1:B:679:VAL:C	2.26	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
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:379:ASP:C	1:A:379:ASP:OD1	2.52	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:645:ASN:HD22	1:B:645:ASN:C	2.17	0.52
1:B:654:ASP:O	1:B:655:LEU:C	2.52	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:A:374:MET:HE2	1:A:394:PHE:HE1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:681:LEU:CD1	1:A:681:LEU:C	2.81	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:HD12	1:A:134:ILE:N	2.26	0.51
1:B:513:ILE:HD13	1:B:513:ILE:N	2.26	0.51
1:A:238:ASN:OD1	1:A:261:GLY:C	2.54	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: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:113:ASN:C	1:A:113:ASN:HD22	2.20	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:283:TYR:CD1	1:A:283:TYR:C	2.90	0.50
1:A:99:TYR:HE2	1:A:578:ARG:HH12	1.60	0.50
1:A:311:MET:HE2	1:A:434:LYS:HD2	1.94	0.50
1:A:252:THR:OG1	1:A:256:GLU:OE2	2.29	0.49
1:A:387:GLU:HG2	1:A:390:LYS:HZ2	1.77	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:B:374:MET:HE2	1:B:394:PHE:HE1	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:96:PHE:CZ	1:B:578:ARG:HG2	2.47	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:392:ASP:CG	1:A:395:ARG:NH2	2.71	0.48
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:B:539:ARG:HG3	1:B:575:GLU:C	2.38	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:B:85:ASN:C	1:B:85:ASN:HD22	2.21	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: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:14:ARG:HD3	1:B:196:GLY:O	2.14	0.48
1:B:257:TYR:CD1	1:B:257:TYR:C	2.92	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
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:682:ARG:NH2	1:B:649:LYS:NZ	2.62	0.47
1:B:14:ARG:HH22	1:B:122:GLU:CD	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:254:PRO:O	1:A:255:ARG:C	2.57	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:251:LYS:C	1:A:252:THR:O	2.53	0.46
1:A:230:GLN:NE2	2:A:2070:HOH:O	2.47	0.46
1:B:568:TYR:O	1:B:568:TYR:CG	2.67	0.46
1:A:195:TYR:OH	2:A:2009:HOH:O	2.01	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: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:A:540:ILE:HA	1:A:543:MET:HE2	1.98	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:A:488:ASN:C	1:A:488:ASN:HD22	2.24	0.46
1:B:275:GLU:CD	1:B:324:ARG:HH11	2.23	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
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:341:ASN:ND2	1:A:343:LEU:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:359:MET:CE	1:B:419:ARG:HB3	2.47	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:B:364:SER:O	1:B:365:PRO:C	2.59	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:130:PHE:CZ	1:B:220:PRO:HG3	2.53	0.43
1:B:150:ASP:OD1	1:B:150:ASP:C	2.61	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
1:A:111:PRO:HG2	1:A:117:LYS:CG	2.48	0.43
1:A:475:ASN:C	1:A:475:ASN:ND2	2.68	0.43
1:A:682:ARG:NH2	1:B:649:LYS:HZ1	2.16	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:643:LEU:C	1:A:644:LEU:HD12	2.43	0.43
1:A:113:ASN:HA	1:A:114:PRO:HD2	1.87	0.43
1:A:341:ASN:HD22	1:A:341:ASN:C	2.26	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: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:B:268:MET:HB2	1:B:268:MET:HE2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:ND2	2:B:2114:HOH:O	2.51	0.43
1:A:353:ASN:ND2	1:A:353:ASN:C	2.76	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:B:341:ASN:HD22	1:B:341:ASN:C	2.26	0.42
1:A:549:LEU:HD13	1:A:553:MET:HE3	2.01	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:A:445:MET:HG3	1:A:472:LEU:HA	2.02	0.42
1:A:85:ASN:HD22	1:A:85:ASN:C	2.26	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:369:GLU:H	1:A:369:GLU:CD	2.27	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: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:12:LYS:C	1:A:198:GLU:HA	2.45	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
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: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:546:ASN:C	1:B:546:ASN:ND2	2.78	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:645:ASN:C	1:A:645:ASN:HD22	2.28	0.41
1:A:679:VAL:CG2	1:A:680:LEU:N	2.82	0.41
1:B:643:LEU:C	1:B:644:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:655:LEU:HD13	1:A:660:LYS:HZ1	1.85	0.41
1:B:305:ASP:CG	2:B:2069:HOH:O	2.63	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:456:TYR:CE1	1:A:460:LYS:HD3	2.56	0.41
1:A:628:LEU:HD23	1:A:651:ILE:CD1	2.49	0.41
1:A:663:PHE:HE2	1:A:665:ILE:HD13	1.86	0.41
1:A:1:MET:HG3	1:A:2:TYR:N	2.34	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:1:MET:HE2	1:B:23:THR:HB	2.03	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: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
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:A:568:TYR:O	1:A:568:TYR:CG	2.73	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 [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	678/696 (97%)	639 (94%)	36 (5%)	3 (0%)	30	36
1	B	678/696 (97%)	643 (95%)	33 (5%)	2 (0%)	36	44
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 [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	627/639 (98%)	572 (91%)	55 (9%)	9	11
1	B	628/639 (98%)	574 (91%)	54 (9%)	10	11
All	All	1255/1278 (98%)	1146 (91%)	109 (9%)	9	11

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	GLU
1	A	50	ARG
1	A	93	THR
1	A	106	LEU
1	A	107	VAL
1	A	115	LEU
1	A	122	GLU
1	A	143	GLU
1	A	153	ASN
1	A	192	LYS
1	A	198	GLU
1	A	247	ASN
1	A	248	ARG
1	A	250	LYS
1	A	253	VAL
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	348	LEU
1	A	349	ARG
1	A	353	ASN
1	A	370	ILE
1	A	371	VAL
1	A	388	LEU
1	A	445	MET
1	A	460	LYS
1	A	469	LEU
1	A	475	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

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Mol	Chain	Res	Type
1	A	574	LEU
1	A	620	LEU
1	A	629	LEU
1	A	635	ILE
1	A	637	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	42	LEU
1	B	49	LEU
1	B	62	LEU
1	B	93	THR
1	B	98	GLU
1	B	122	GLU
1	B	163	VAL
1	B	198	GLU
1	B	200	VAL
1	B	250	LYS
1	B	253	VAL
1	B	268	MET
1	B	283	TYR
1	B	284	LEU
1	B	285	THR
1	B	319	GLN
1	B	320	VAL
1	B	341	ASN
1	B	343	LEU
1	B	348	LEU
1	B	349	ARG
1	B	350	GLU
1	B	352	GLU
1	B	353	ASN
1	B	359	MET
1	B	369	GLU
1	B	375	LEU
1	B	376	LYS
1	B	386	ARG
1	B	388	LEU

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Mol	Chain	Res	Type
1	B	419	ARG
1	B	445	MET
1	B	469	LEU
1	B	474	GLU
1	B	475	ASN
1	B	513	ILE
1	B	516	VAL
1	B	524	LYS
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	640	ILE
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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
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	319	GLN
1	A	336	HIS
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	397	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	167	ASN
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	397	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
1	B	637	ASN
1	B	645	ASN

5.3.3 RNA

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, 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	684/696 (98%)	-0.03	18 (2%) 57 59	22, 37, 64, 99	0
1	B	684/696 (98%)	0.02	16 (2%) 61 63	22, 38, 63, 91	0
All	All	1368/1392 (98%)	-0.01	34 (2%) 58 60	22, 38, 64, 99	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	655	LEU	7.0
1	A	655	LEU	6.6
1	B	253	VAL	5.8
1	A	696	ILE	4.4
1	B	660	LYS	4.1
1	B	696	ILE	3.7
1	A	253	VAL	3.6
1	A	660	LYS	3.5
1	A	243	ASN	3.4
1	B	260	TYR	3.0
1	B	254	PRO	2.9
1	A	670	ASN	2.8
1	A	246	PRO	2.7
1	A	254	PRO	2.7
1	B	670	ASN	2.7
1	A	681	LEU	2.5
1	A	651	ILE	2.5
1	B	665	ILE	2.5
1	A	244	ASP	2.5
1	B	679	VAL	2.5
1	B	29	TYR	2.4
1	B	694	CYS	2.4
1	B	99	TYR	2.3
1	B	653	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	29	TYR	2.3
1	A	239	GLY	2.3
1	B	247	ASN	2.3
1	A	663	PHE	2.2
1	A	679	VAL	2.2
1	B	241	PRO	2.2
1	A	250	LYS	2.1
1	A	669	LYS	2.1
1	B	251	LYS	2.1
1	A	661	TYR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.