Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 05:19 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

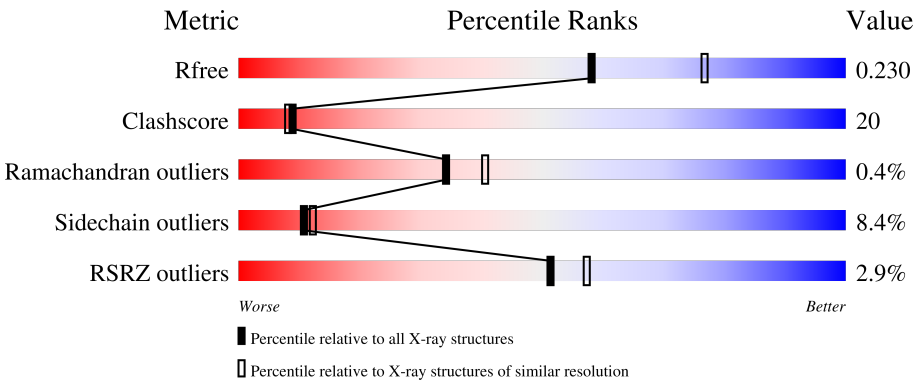
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	3% 64% 29% 5% •
1	B	696	3% 67% 26% 5% •

2 Entry composition (i)

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.

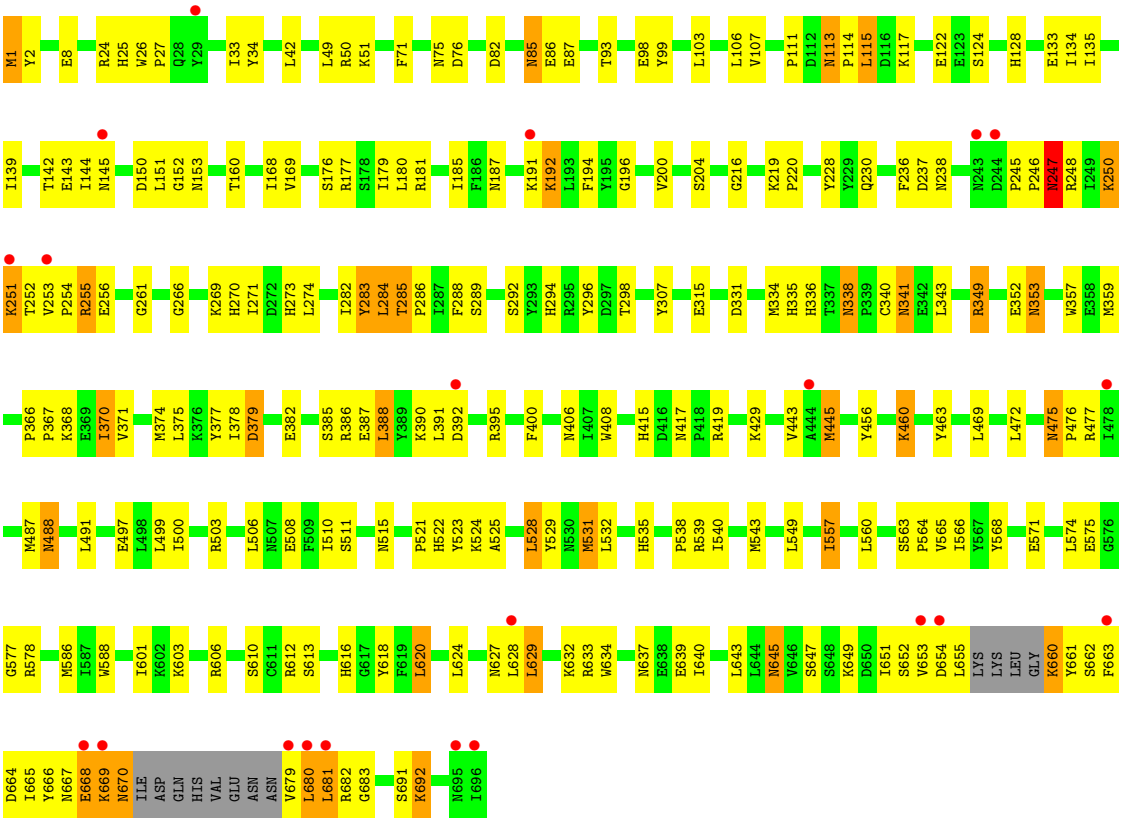
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	153	153	153	0	0
2	B	145	145	145	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

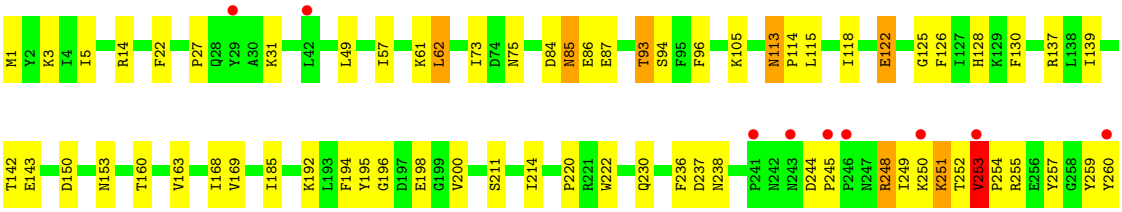
• Molecule 1: ALPHA AMYLASE, CATALYTIC REGION

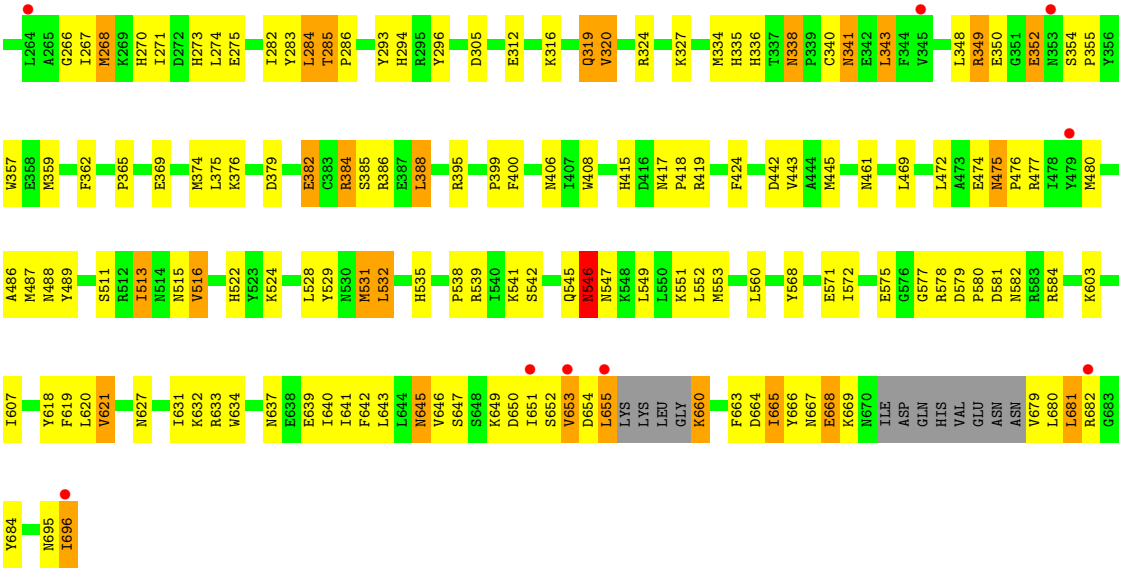
Chain A:



• Molecule 1: ALPHA AMYLASE, CATALYTIC REGION

Chain B:




L264 A265 G266 I267 M268 K269 H270 I271 D272 H273 L274 E275 I282 Y283 L284 T285 P286 Y293 H294 R295 Y296 D305 E312 K316 Q319 V320 R324 K327 M334 H335 H336 T337 N338 P339 C340 N341 E342 L343 F344 V345 L348 R349 E350 G351 E352 N353 S354 P355 Y356
W357 E358 M359 F362 P365 E369 M374 L375 K376 D379 E382 C383 R384 S385 R386 E387 L388 R395 P399 F400 M406 I407 W408 H415 D416 N417 P418 R419 F424 D442 V443 A444 M445 N461 L469 L472 A473 E474 M475 P476 R477 I478 Y479 M480
A486 M487 N488 Y489 S511 R512 I513 N514 N515 V516 H522 Y523 K524 L528 Y529 N530 M531 L532 H535 P538 R539 I540 K541 S542 Q545 N546 N547 K548 L549 L550 K551 L552 M553 L560 Y568 E571 I572 E575 G576 G577 R578 D579 P580 D581 N582 R583 R584 K603
I607 Y618 F619 L620 V621 N627 I631 K632 R633 W634 N637 E638 E639 I640 I641 F642 L643 L644 N645 V646 S647 S648 K649 D650 I651 S652 V653 D654 L655 LYS LYS LEU GLY K660 F663 D664 I665 Y666 N667 E668 K669 N670 ILE ASP GLN HIS VAL GLU ASN ASN V679 L680 L681 R682 G683
Y684 N695 I696

4 Data and refinement statistics (i)

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) 85.5 (49.55-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 2.27Å)	Xtriage
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	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	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(^{o})	Ideal(^{o})
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 (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	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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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 (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%)	34	40
1	B	678/696 (97%)	643 (95%)	33 (5%)	2 (0%)	41	49
All	All	1356/1392 (97%)	1282 (94%)	69 (5%)	5 (0%)	34	40

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%)	10	11
1	B	628/639 (98%)	577 (92%)	51 (8%)	11	13
All	All	1255/1278 (98%)	1149 (92%)	106 (8%)	11	12

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

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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

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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

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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

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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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.14	21 (3%)	49	54	22, 37, 64, 99	0
1	B	684/696 (98%)	-0.05	18 (2%)	56	62	22, 38, 63, 91	0
All	All	1368/1392 (98%)	-0.09	39 (2%)	51	57	22, 38, 64, 99	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	696	ILE	4.4
1	B	253	VAL	4.3
1	A	679	VAL	4.0
1	B	260	TYR	3.7
1	B	653	VAL	3.4
1	A	653	VAL	3.1
1	A	696	ILE	2.9
1	A	243	ASN	2.8
1	A	244	ASP	2.7
1	B	682	ARG	2.7
1	A	663	PHE	2.7
1	A	668	GLU	2.7
1	A	695	ASN	2.7
1	B	29	TYR	2.6
1	A	669	LYS	2.6
1	B	246	PRO	2.5
1	A	253	VAL	2.5
1	B	651	ILE	2.5
1	B	250	LYS	2.4
1	B	353	ASN	2.4
1	A	29	TYR	2.4
1	B	264	LEU	2.4
1	A	145	ASN	2.4
1	B	655	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	654	ASP	2.3
1	A	681	LEU	2.3
1	A	478	ILE	2.3
1	A	191	LYS	2.2
1	A	251	LYS	2.2
1	A	628	LEU	2.2
1	B	42	LEU	2.2
1	A	392	ASP	2.1
1	B	245	PRO	2.1
1	B	243	ASN	2.1
1	B	241	PRO	2.1
1	B	479	TYR	2.1
1	B	345	VAL	2.0
1	A	680	LEU	2.0
1	A	444	ALA	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.