Full wwPDB X-ray Structure Validation Report (i)

Jun 5, 2016 – 11:02 PM EDT

PDB ID	:	5C70
Title	:	The structure of Aspergillus oryzae beta-glucuronidase
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Deposited on	:	2015-06-24
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

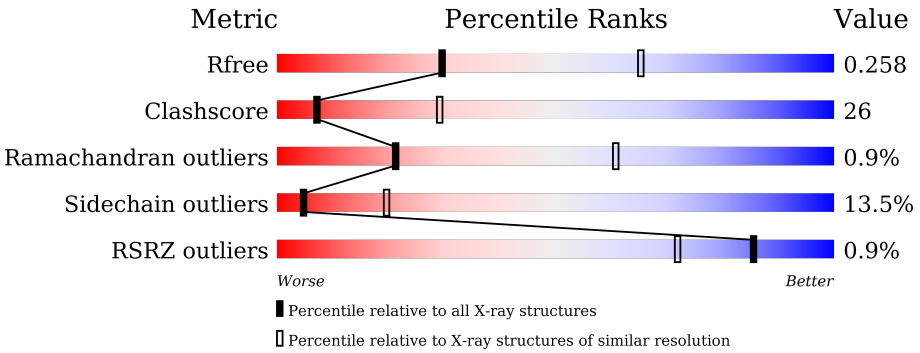
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	612	% 56% 34% 6% .
1	B	612	% 56% 33% 5% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9320 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 Glucuronidase.

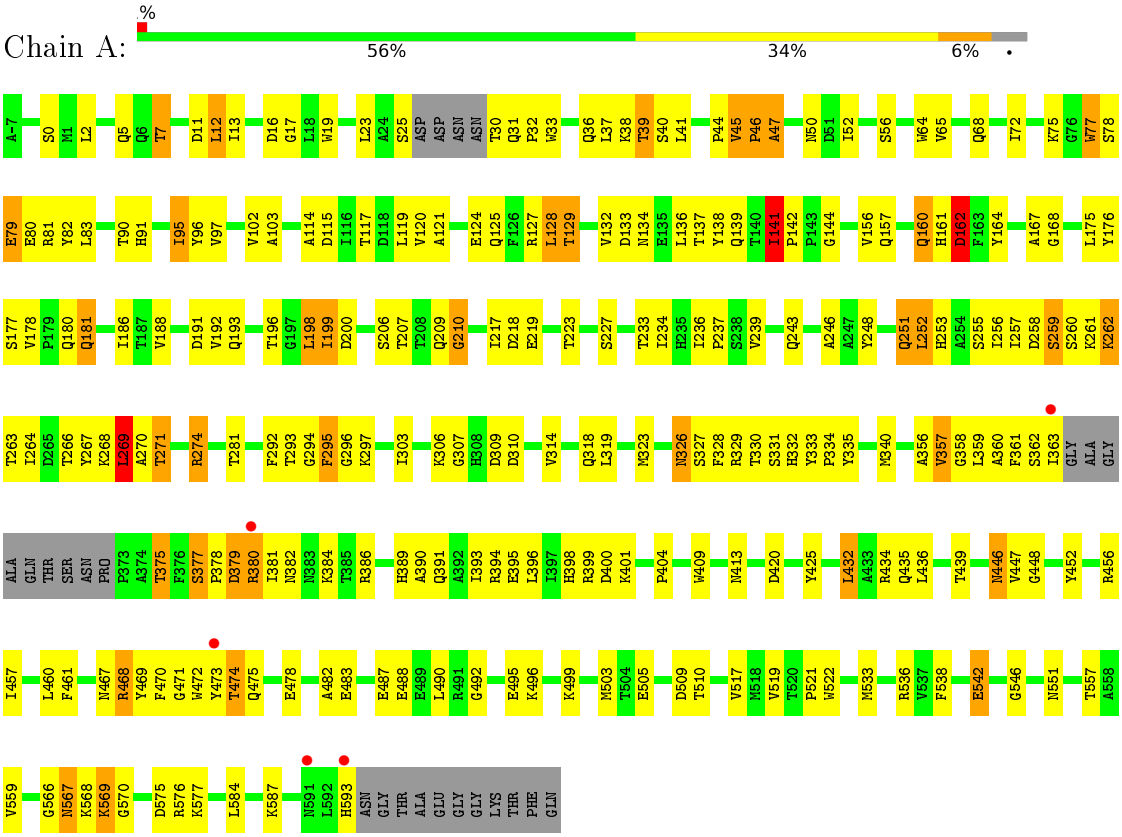
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4670	2965	806	886	13			
1	B	584	Total	C	N	O	S	0	0	0
			4650	2950	801	886	13			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

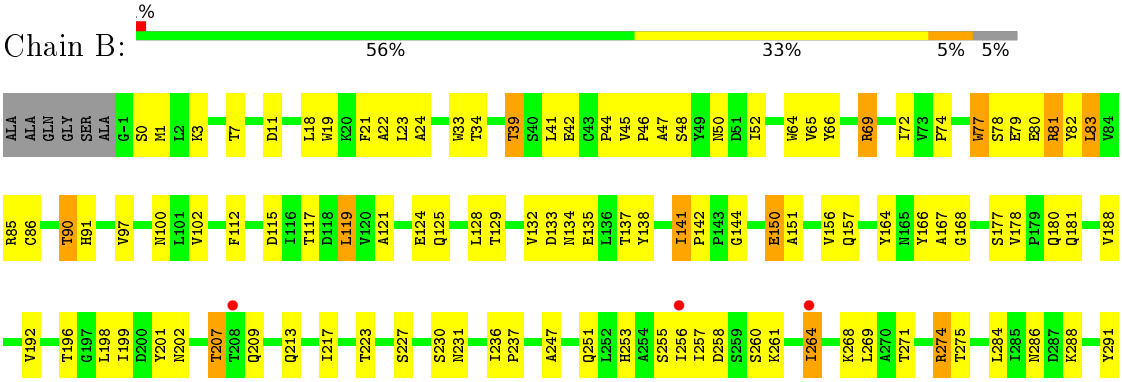
- Molecule 1: Glucuronidase

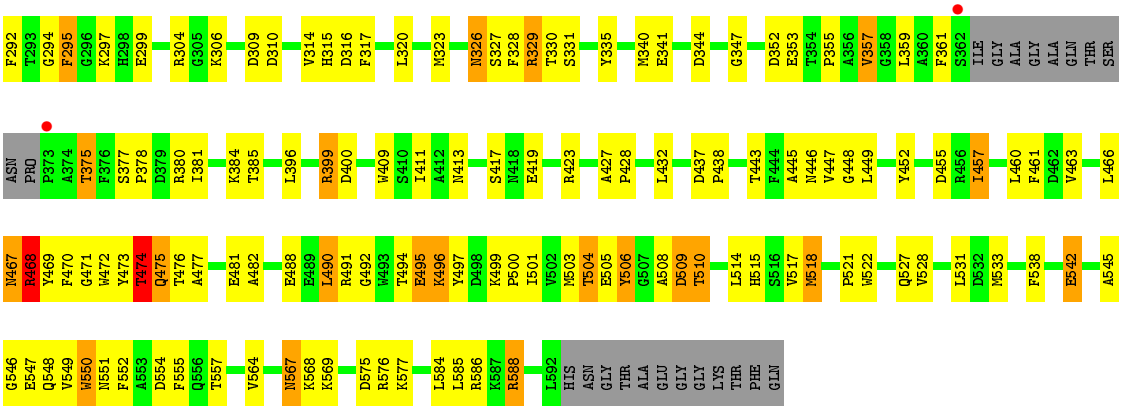
Chain A:



- Molecule 1: Glucuronidase

Chain B:




F292 T293 G294 F295 G296 K297 H298 E299 R304 G305 K306 D309 D310 V314 H315 D316 F317 L320 M323 N326 S327 F328 R329 T330 S331 Y335 M340 E341 D344 G347 D352 E353 T354 P355 A356 V357 G358 L359 A360 F361 S362 ILE GLY ALA GLY ALA GLN THR SER
ASN PRO P373 A374 T375 F376 S377 P378 D379 R380 I381 K384 T385 L396 R399 D400 W409 S410 I411 A412 N413 S417 N418 E419 R423 A427 P428 L432 D437 P438 T443 F444 A445 N446 V447 G448 L449 Y452 D455 R456 I457 L460 F461 D462 V463 L466
N467 R468 Y469 F470 G471 W472 Y473 T474 Q475 T476 A477 E481 A482 E488 E489 L490 R491 G492 W493 T494 E495 K496 Y497 D498 K499 P500 I501 V502 M503 T504 E505 Y506 G507 A508 D509 T510 L514 H515 S516 V517 M518 P521 W522 Q527 V528 L531 D532 M533 F538 E542 A545
G546 E547 Q548 V549 W550 N551 F552 A553 D554 F555 Q556 T557 V564 N567 K568 K569 D575 R576 K577 L584 L585 R586 K587 R588 L592 HIS ASN GLY THR ALA GLU GLY GLY LYS THR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.32Å 110.32Å 480.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 47.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.10) 99.1 (47.84-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.45 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.254 0.208 , 0.258	Depositor DCC
R_{free} test set	1641 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9320	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/4790	0.73	5/6521 (0.1%)
1	B	0.54	0/4770	0.70	4/6496 (0.1%)
All	All	0.54	0/9560	0.71	9/13017 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	474	THR	N-CA-C	7.04	130.00	111.00
1	A	162	ASP	CB-CA-C	-6.84	96.72	110.40
1	A	252	LEU	CA-CB-CG	6.63	130.56	115.30
1	B	468	ARG	CB-CA-C	-6.49	97.42	110.40
1	A	269	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	161	HIS	CB-CA-C	5.84	122.07	110.40
1	B	474	THR	CB-CA-C	-5.63	96.39	111.60
1	A	380	ARG	N-CA-C	5.44	125.69	111.00
1	B	475	GLN	N-CA-C	-5.37	96.49	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ILE	Peptide
1	A	295	PHE	Peptide
1	B	141	ILE	Peptide
1	B	295	PHE	Peptide
1	B	48	SER	Peptide
1	B	550	TRP	Peptide

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	4670	0	4505	240	0
1	B	4650	0	4477	246	0
All	All	9320	0	8982	479	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 26.

All (479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:CZ	1:A:380:ARG:HD2	1.71	1.25
1:A:90:THR:CG2	1:A:91:HIS:H	1.50	1.23
1:B:467:ASN:HB3	1:B:505:GLU:CG	1.73	1.18
1:B:21:PHE:O	1:B:39:THR:HG21	1.43	1.16
1:A:90:THR:OG1	1:A:167:ALA:HA	1.47	1.11
1:A:90:THR:HG23	1:A:91:HIS:N	1.65	1.11
1:B:90:THR:CG2	1:B:91:HIS:N	2.11	1.10
1:B:90:THR:HG23	1:B:91:HIS:H	1.17	1.08
1:B:467:ASN:HB3	1:B:505:GLU:HG3	1.37	1.07
1:B:82:TYR:H	1:B:117:THR:HG22	1.18	1.05
1:A:251:GLN:HG2	1:A:268:LYS:HE2	1.36	1.03
1:A:297:LYS:O	1:A:331:SER:HB2	1.58	1.02
1:B:39:THR:HG23	1:B:41:LEU:H	1.18	1.01
1:A:90:THR:HB	1:A:168:GLY:H	1.25	1.00
1:B:567:ASN:HD21	1:B:569:LYS:HB2	1.26	1.00
1:A:90:THR:CG2	1:A:91:HIS:N	2.19	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:CB	1:A:168:GLY:H	1.77	0.98
1:B:470:PHE:HA	1:B:474:THR:OG1	1.63	0.97
1:A:50:ASN:HD21	1:A:167:ALA:H	1.10	0.96
1:B:467:ASN:HB3	1:B:505:GLU:HG2	1.42	0.96
1:A:357:VAL:HG12	1:A:413:ASN:HB3	1.46	0.96
1:B:323:MET:HA	1:B:586:ARG:HG3	1.49	0.95
1:B:468:ARG:HG3	1:B:470:PHE:CE2	2.02	0.94
1:B:39:THR:CG2	1:B:41:LEU:H	1.80	0.94
1:A:90:THR:HG23	1:A:91:HIS:H	1.18	0.94
1:B:505:GLU:HB2	1:B:550:TRP:HB2	1.49	0.93
1:A:332:HIS:CG	1:A:357:VAL:HG11	2.02	0.93
1:A:81:ARG:HG3	1:A:117:THR:HG21	1.49	0.92
1:A:115:ASP:OD1	1:A:117:THR:HG23	1.70	0.92
1:A:361:PHE:HZ	1:A:380:ARG:HD2	1.30	0.92
1:A:332:HIS:HB3	1:A:357:VAL:HG21	1.50	0.92
1:A:162:ASP:O	1:A:557:THR:HB	1.70	0.92
1:A:361:PHE:CZ	1:A:380:ARG:CD	2.53	0.92
1:B:90:THR:HG22	1:B:91:HIS:N	1.82	0.92
1:A:181:GLN:HE22	1:A:207:THR:H	1.16	0.91
1:A:5:GLN:HE22	1:A:268:LYS:H	1.15	0.91
1:B:213:GLN:HG3	1:B:257:ILE:HG13	1.54	0.89
1:A:181:GLN:NE2	1:A:207:THR:H	1.71	0.89
1:B:503:MET:HG3	1:B:538:PHE:CZ	2.07	0.88
1:A:357:VAL:CG1	1:A:413:ASN:HB3	2.02	0.88
1:B:90:THR:CG2	1:B:91:HIS:H	1.79	0.88
1:B:474:THR:HB	1:B:475:GLN:NE2	1.89	0.88
1:B:467:ASN:CB	1:B:505:GLU:HG2	2.04	0.87
1:A:90:THR:HG22	1:A:91:HIS:H	1.37	0.86
1:B:474:THR:HB	1:B:475:GLN:CD	1.96	0.86
1:A:90:THR:OG1	1:A:167:ALA:CA	2.23	0.85
1:A:256:ILE:O	1:A:256:ILE:HG22	1.77	0.84
1:B:90:THR:HG23	1:B:91:HIS:N	1.84	0.84
1:B:474:THR:HB	1:B:475:GLN:OE1	1.78	0.84
1:B:326:ASN:C	1:B:326:ASN:HD22	1.82	0.83
1:B:503:MET:HG3	1:B:538:PHE:HZ	1.43	0.82
1:A:82:TYR:H	1:A:117:THR:HG22	1.45	0.82
1:B:547:GLU:OE1	1:B:588:ARG:NH1	2.12	0.81
1:B:81:ARG:HG3	1:B:117:THR:HG21	1.61	0.81
1:B:423:ARG:HA	1:B:457:ILE:HD11	1.63	0.81
1:A:567:ASN:ND2	1:A:569:LYS:H	1.80	0.80
1:A:5:GLN:NE2	1:A:268:LYS:H	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:HG12	1:B:223:THR:HG22	1.63	0.80
1:B:213:GLN:HG3	1:B:257:ILE:CG1	2.12	0.80
1:A:474:THR:HB	1:A:475:GLN:NE2	1.96	0.79
1:B:11:ASP:HB3	1:B:77:TRP:CH2	2.18	0.79
1:B:468:ARG:HG3	1:B:470:PHE:HE2	1.44	0.79
1:A:64:TRP:CD2	1:A:133:ASP:HB2	2.18	0.79
1:B:50:ASN:HD21	1:B:167:ALA:H	1.32	0.78
1:A:83:LEU:HB2	1:A:114:ALA:O	1.83	0.77
1:B:567:ASN:ND2	1:B:569:LYS:HB2	1.99	0.77
1:A:470:PHE:HA	1:A:474:THR:OG1	1.83	0.77
1:B:82:TYR:H	1:B:117:THR:CG2	1.97	0.77
1:A:332:HIS:HB3	1:A:357:VAL:CG2	2.13	0.77
1:B:90:THR:HB	1:B:132:VAL:CG1	2.15	0.76
1:B:256:ILE:O	1:B:264:ILE:HG22	1.84	0.76
1:B:457:ILE:HG23	1:B:461:PHE:HE2	1.50	0.76
1:B:467:ASN:CB	1:B:505:GLU:CG	2.59	0.75
1:A:474:THR:HB	1:A:475:GLN:CD	2.07	0.75
1:A:188:VAL:HG11	1:A:271:THR:HG21	1.69	0.75
1:B:90:THR:OG1	1:B:167:ALA:HA	1.86	0.75
1:B:201:TYR:O	1:B:231:ASN:HB2	1.86	0.74
1:B:141:ILE:HG23	1:B:142:PRO:HD3	1.69	0.74
1:A:567:ASN:HD21	1:A:569:LYS:HB2	1.52	0.74
1:A:11:ASP:HB3	1:A:77:TRP:CH2	2.24	0.73
1:A:217:ILE:HG12	1:A:223:THR:HG22	1.71	0.73
1:A:326:ASN:HD22	1:A:327:SER:N	1.87	0.73
1:B:467:ASN:CG	1:B:505:GLU:HG2	2.10	0.72
1:A:446:ASN:ND2	1:A:468:ARG:HH12	1.88	0.72
1:B:470:PHE:CA	1:B:474:THR:OG1	2.38	0.71
1:A:474:THR:HB	1:A:475:GLN:OE1	1.91	0.71
1:B:11:ASP:CB	1:B:77:TRP:CH2	2.73	0.71
1:B:39:THR:HG23	1:B:41:LEU:N	2.02	0.71
1:B:470:PHE:CA	1:B:474:THR:HG1	2.04	0.71
1:B:457:ILE:HG23	1:B:461:PHE:CE2	2.27	0.70
1:B:357:VAL:HG13	1:B:413:ASN:HB3	1.74	0.70
1:A:399:ARG:HD2	1:A:400:ASP:OD1	1.92	0.69
1:B:21:PHE:O	1:B:39:THR:CG2	2.34	0.69
1:A:256:ILE:O	1:A:264:ILE:HG22	1.92	0.69
1:A:469:TYR:OH	1:A:505:GLU:HB3	1.91	0.69
1:A:17:GLY:H	1:A:45:VAL:HG23	1.58	0.69
1:B:188:VAL:HG11	1:B:271:THR:HG21	1.74	0.69
1:A:332:HIS:HB3	1:A:357:VAL:HG11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TYR:HB3	1:B:380:ARG:O	1.93	0.68
1:B:100:ASN:HD22	1:B:119:LEU:HD11	1.59	0.68
1:B:474:THR:CB	1:B:475:GLN:OE1	2.41	0.68
1:A:90:THR:HG22	1:A:132:VAL:HG12	1.76	0.68
1:B:474:THR:HB	1:B:475:GLN:HE22	1.58	0.68
1:B:470:PHE:HB3	1:B:475:GLN:OE1	1.94	0.68
1:A:90:THR:CG2	1:A:132:VAL:HG12	2.23	0.68
1:A:90:THR:HG22	1:A:132:VAL:CG1	2.24	0.68
1:B:83:LEU:HB3	1:B:115:ASP:HA	1.77	0.67
1:B:45:VAL:O	1:B:46:PRO:C	2.32	0.67
1:B:510:THR:HG21	1:B:527:GLN:HB2	1.76	0.67
1:A:332:HIS:CB	1:A:357:VAL:HG11	2.24	0.67
1:B:503:MET:CG	1:B:538:PHE:CZ	2.78	0.66
1:B:82:TYR:N	1:B:117:THR:HG22	2.02	0.66
1:A:446:ASN:HD22	1:A:468:ARG:HH12	1.44	0.66
1:A:102:VAL:HG12	1:A:114:ALA:HB1	1.77	0.66
1:B:256:ILE:O	1:B:264:ILE:CG2	2.43	0.66
1:A:162:ASP:O	1:A:557:THR:CB	2.45	0.65
1:A:326:ASN:HD22	1:A:326:ASN:C	2.00	0.64
1:A:357:VAL:CG1	1:A:413:ASN:CB	2.76	0.64
1:B:141:ILE:HG21	1:B:355:PRO:HG2	1.79	0.64
1:B:181:GLN:HG3	1:B:207:THR:HG23	1.80	0.64
1:B:494:THR:HG22	1:B:501:ILE:CD1	2.27	0.64
1:A:83:LEU:HB3	1:A:115:ASP:HA	1.79	0.64
1:A:386:ARG:HB2	1:A:425:TYR:CE1	2.33	0.64
1:A:467:ASN:O	1:A:468:ARG:HD3	1.98	0.64
1:B:470:PHE:CB	1:B:474:THR:HG1	2.11	0.63
1:A:11:ASP:CB	1:A:77:TRP:CH2	2.80	0.63
1:B:567:ASN:ND2	1:B:569:LYS:H	1.95	0.63
1:B:475:GLN:HG2	1:B:482:ALA:HA	1.78	0.63
1:A:293:THR:H	1:A:326:ASN:HD21	1.44	0.63
1:A:457:ILE:HG23	1:A:461:PHE:HE2	1.62	0.63
1:A:474:THR:CB	1:A:475:GLN:OE1	2.47	0.63
1:A:39:THR:HB	1:A:41:LEU:H	1.64	0.62
1:B:166:TYR:HB2	1:B:306:LYS:HG3	1.81	0.62
1:B:77:TRP:O	1:B:80:GLU:CB	2.48	0.62
1:A:314:VAL:O	1:A:318:GLN:HG2	1.99	0.62
1:B:90:THR:OG1	1:B:167:ALA:CA	2.47	0.62
1:A:258:ASP:OD1	1:A:260:SER:N	2.30	0.62
1:A:468:ARG:HG3	1:A:470:PHE:CE2	2.34	0.62
1:A:45:VAL:O	1:A:47:ALA:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:TRP:CE3	1:B:508:ALA:HB1	2.35	0.62
1:A:16:ASP:HA	1:A:45:VAL:HG21	1.82	0.62
1:A:82:TYR:H	1:A:117:THR:CG2	2.11	0.62
1:B:423:ARG:HA	1:B:457:ILE:CD1	2.29	0.62
1:B:467:ASN:HA	1:B:505:GLU:O	2.00	0.62
1:A:138:TYR:HB3	1:A:380:ARG:O	2.00	0.62
1:B:466:LEU:C	1:B:467:ASN:OD1	2.38	0.62
1:B:317:PHE:HA	1:B:320:LEU:HD12	1.80	0.61
1:A:7:THR:HG21	1:A:266:THR:HG23	1.82	0.61
1:B:297:LYS:O	1:B:331:SER:HB2	2.01	0.61
1:B:375:THR:HG23	1:B:419:GLU:OE1	2.01	0.61
1:B:90:THR:HG1	1:B:167:ALA:HA	1.64	0.61
1:A:319:LEU:O	1:A:323:MET:HG2	2.01	0.61
1:A:50:ASN:HD21	1:A:167:ALA:N	1.92	0.60
1:B:64:TRP:CD2	1:B:133:ASP:HB2	2.37	0.60
1:B:359:LEU:HD23	1:B:381:ILE:HG12	1.83	0.60
1:A:19:TRP:CD1	1:A:45:VAL:HG22	2.37	0.60
1:A:90:THR:HB	1:A:132:VAL:HG11	1.83	0.60
1:A:521:PRO:O	1:A:522:TRP:HB2	2.00	0.60
1:B:472:TRP:CZ3	1:B:508:ALA:HB1	2.35	0.60
1:A:78:SER:O	1:A:79:GLU:HB2	2.00	0.60
1:A:332:HIS:HB3	1:A:357:VAL:CG1	2.31	0.60
1:A:45:VAL:HB	1:A:46:PRO:HD3	1.84	0.60
1:B:45:VAL:O	1:B:47:ALA:N	2.35	0.60
1:A:470:PHE:C	1:A:472:TRP:H	2.06	0.59
1:A:5:GLN:HE22	1:A:268:LYS:N	1.95	0.59
1:B:476:THR:O	1:B:477:ALA:HB3	2.01	0.59
1:A:139:GLN:NE2	1:A:382:ASN:HD21	2.00	0.59
1:A:258:ASP:C	1:A:258:ASP:OD1	2.40	0.59
1:A:296:GLY:O	1:A:551:ASN:OD1	2.21	0.59
1:B:331:SER:HG	1:B:550:TRP:HZ3	1.50	0.59
1:A:474:THR:HB	1:A:475:GLN:HE22	1.63	0.59
1:B:39:THR:CG2	1:B:41:LEU:N	2.60	0.59
1:B:567:ASN:HD22	1:B:569:LYS:H	1.50	0.59
1:A:470:PHE:HA	1:A:474:THR:HG1	1.67	0.59
1:A:256:ILE:O	1:A:256:ILE:CG2	2.50	0.59
1:A:90:THR:HB	1:A:168:GLY:N	2.06	0.59
1:B:100:ASN:O	1:B:102:VAL:HG23	2.03	0.59
1:B:361:PHE:H	1:B:375:THR:HG21	1.68	0.58
1:B:274:ARG:HA	1:B:286:ASN:OD1	2.03	0.58
1:A:50:ASN:ND2	1:A:167:ALA:H	1.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:N	1:A:379:ASP:OD1	2.30	0.58
1:B:256:ILE:O	1:B:256:ILE:HG22	2.02	0.58
1:B:475:GLN:HG2	1:B:482:ALA:CA	2.33	0.58
1:B:470:PHE:O	1:B:472:TRP:N	2.37	0.57
1:A:2:LEU:HD11	1:A:186:ILE:HG13	1.84	0.57
1:A:12:LEU:HD12	1:A:13:ILE:H	1.70	0.57
1:B:326:ASN:HD22	1:B:327:SER:N	2.02	0.57
1:B:470:PHE:HB3	1:B:474:THR:HG1	1.69	0.57
1:B:521:PRO:O	1:B:522:TRP:HB2	2.04	0.57
1:A:334:PRO:HG3	1:A:396:LEU:HD12	1.86	0.57
1:A:475:GLN:N	1:A:475:GLN:CD	2.58	0.57
1:A:567:ASN:C	1:A:567:ASN:HD22	2.08	0.57
1:A:64:TRP:CE2	1:A:133:ASP:HB2	2.40	0.57
1:A:90:THR:CG2	1:A:132:VAL:CG1	2.83	0.56
1:A:293:THR:H	1:A:326:ASN:ND2	2.03	0.56
1:A:483:GLU:O	1:A:487:GLU:HG2	2.05	0.56
1:B:475:GLN:HB2	1:B:482:ALA:HB2	1.88	0.56
1:A:452:TYR:CE1	1:A:492:GLY:HA3	2.41	0.56
1:B:357:VAL:CG1	1:B:413:ASN:HB3	2.35	0.56
1:B:475:GLN:N	1:B:475:GLN:CD	2.59	0.56
1:B:81:ARG:CG	1:B:117:THR:HG21	2.35	0.56
1:A:399:ARG:CD	1:A:400:ASP:OD1	2.53	0.56
1:B:166:TYR:CB	1:B:306:LYS:HG3	2.36	0.56
1:A:45:VAL:HB	1:A:46:PRO:CD	2.37	0.55
1:B:475:GLN:HG3	1:B:481:GLU:HG3	1.86	0.55
1:A:452:TYR:CD1	1:A:492:GLY:HA3	2.40	0.55
1:A:309:ASP:CG	1:B:304:ARG:HH21	2.09	0.55
1:A:12:LEU:HD13	1:A:176:TYR:HB3	1.89	0.55
1:B:551:ASN:ND2	1:B:555:PHE:CD2	2.73	0.55
1:B:326:ASN:C	1:B:326:ASN:ND2	2.55	0.55
1:A:164:TYR:N	1:A:557:THR:HA	2.21	0.55
1:B:417:SER:HB2	1:B:455:ASP:OD1	2.07	0.55
1:A:357:VAL:HG13	1:A:413:ASN:CB	2.37	0.55
1:A:420:ASP:OD1	1:A:456:ARG:NH1	2.39	0.55
1:B:260:SER:OG	1:B:261:LYS:N	2.40	0.54
1:B:490:LEU:O	1:B:494:THR:HG23	2.07	0.54
1:A:475:GLN:N	1:A:475:GLN:OE1	2.40	0.54
1:A:199:ILE:O	1:A:199:ILE:HG12	2.06	0.54
1:B:547:GLU:CD	1:B:588:ARG:NH1	2.61	0.54
1:A:251:GLN:HG2	1:A:268:LYS:CE	2.25	0.54
1:A:33:TRP:O	1:A:127:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:HB2	1:A:473:TYR:HD2	1.73	0.54
1:B:446:ASN:HD21	1:B:468:ARG:HH22	1.56	0.53
1:B:77:TRP:O	1:B:80:GLU:HB3	2.08	0.53
1:A:31:GLN:N	1:A:32:PRO:HD3	2.23	0.53
1:B:141:ILE:CG2	1:B:142:PRO:HD3	2.37	0.53
1:B:423:ARG:NH2	1:B:460:LEU:HD21	2.23	0.53
1:A:11:ASP:HB3	1:A:77:TRP:HH2	1.72	0.53
1:A:134:ASN:HB3	1:A:167:ALA:CB	2.39	0.53
1:A:141:ILE:HD13	1:A:141:ILE:O	2.09	0.53
1:B:202:ASN:HA	1:B:231:ASN:HB3	1.90	0.53
1:A:96:TYR:HB2	1:A:129:THR:HG23	1.91	0.52
1:B:377:SER:HB2	1:B:378:PRO:HD2	1.91	0.52
1:A:519:VAL:HG12	1:A:519:VAL:O	2.09	0.52
1:B:137:THR:HA	1:B:144:GLY:O	2.09	0.52
1:B:340:MET:HE2	1:B:340:MET:HA	1.91	0.52
1:B:469:TYR:OH	1:B:550:TRP:CB	2.58	0.52
1:B:81:ARG:HA	1:B:117:THR:HG21	1.91	0.52
1:A:68:GLN:HE21	1:A:129:THR:HB	1.74	0.52
1:B:466:LEU:O	1:B:504:THR:N	2.42	0.52
1:A:309:ASP:OD2	1:B:304:ARG:NH2	2.38	0.52
1:A:396:LEU:CD2	1:A:409:TRP:CZ3	2.92	0.52
1:A:274:ARG:NH1	1:A:404:PRO:HA	2.25	0.52
1:B:503:MET:HE2	1:B:506:TYR:HB3	1.90	0.52
1:A:188:VAL:CG1	1:A:271:THR:HG21	2.39	0.52
1:A:357:VAL:HG13	1:A:413:ASN:HB3	1.88	0.52
1:A:483:GLU:OE1	1:A:536:ARG:NH2	2.41	0.52
1:A:567:ASN:HD22	1:A:569:LYS:H	1.57	0.51
1:B:491:ARG:O	1:B:495:GLU:HB2	2.10	0.51
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.75	0.51
1:A:470:PHE:O	1:A:472:TRP:N	2.43	0.51
1:A:567:ASN:HD21	1:A:569:LYS:CB	2.21	0.51
1:A:136:LEU:HD22	1:A:142:PRO:O	2.11	0.51
1:A:358:GLY:C	1:A:360:ALA:H	2.13	0.51
1:A:377:SER:HB2	1:A:378:PRO:CD	2.41	0.51
1:B:329:ARG:HH21	1:B:413:ASN:ND2	2.08	0.51
1:B:549:VAL:HG21	1:B:585:LEU:HD11	1.93	0.51
1:A:36:GLN:HE21	1:A:127:ARG:HD3	1.76	0.51
1:B:100:ASN:ND2	1:B:119:LEU:HD11	2.25	0.51
1:B:496:LYS:HG2	1:B:497:TYR:CD2	2.46	0.51
1:B:19:TRP:CZ2	1:B:69:ARG:HD3	2.46	0.51
1:B:551:ASN:ND2	1:B:555:PHE:CE2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:O	1:A:542:GLU:HG2	2.10	0.51
1:B:470:PHE:C	1:B:472:TRP:H	2.14	0.51
1:B:550:TRP:O	1:B:550:TRP:CG	2.62	0.51
1:B:33:TRP:CD1	1:B:34:THR:HG23	2.45	0.51
1:B:494:THR:HG22	1:B:501:ILE:HD12	1.91	0.51
1:A:134:ASN:HB3	1:A:167:ALA:HB2	1.93	0.50
1:B:472:TRP:CZ2	1:B:509:ASP:HB2	2.47	0.50
1:B:510:THR:CG2	1:B:527:GLN:HB2	2.42	0.50
1:B:11:ASP:HB3	1:B:77:TRP:CZ2	2.46	0.50
1:A:509:ASP:O	1:A:522:TRP:HA	2.12	0.50
1:B:448:GLY:HA2	1:B:468:ARG:NH1	2.26	0.50
1:B:463:VAL:HG22	1:B:500:PRO:HG2	1.93	0.50
1:A:44:PRO:HB3	1:B:310:ASP:HB3	1.94	0.50
1:B:475:GLN:HG2	1:B:482:ALA:N	2.26	0.50
1:B:230:SER:O	1:B:231:ASN:HB3	2.11	0.49
1:A:434:ARG:NH2	1:A:460:LEU:O	2.43	0.49
1:A:90:THR:OG1	1:A:168:GLY:N	2.44	0.49
1:B:150:GLU:HG3	1:B:151:ALA:N	2.27	0.49
1:B:340:MET:CE	1:B:340:MET:HA	2.42	0.49
1:A:90:THR:HG1	1:A:167:ALA:HA	1.67	0.49
1:B:72:ILE:CG1	1:B:125:GLN:HG3	2.41	0.49
1:B:201:TYR:CE1	1:B:231:ASN:HA	2.47	0.49
1:A:95:ILE:HG13	1:A:103:ALA:HB3	1.94	0.49
1:A:469:TYR:HB2	1:A:473:TYR:CD2	2.46	0.49
1:B:90:THR:HB	1:B:132:VAL:HG11	1.90	0.49
1:B:291:TYR:HA	1:B:545:ALA:O	2.13	0.49
1:B:467:ASN:HA	1:B:503:MET:HE3	1.94	0.49
1:A:0:SER:O	1:A:398:HIS:HE1	1.94	0.49
1:B:361:PHE:HD2	1:B:375:THR:HB	1.77	0.49
1:B:427:ALA:HB3	1:B:428:PRO:HD3	1.94	0.49
1:B:446:ASN:HB3	1:B:466:LEU:HD23	1.95	0.49
1:B:1:MET:O	1:B:85:ARG:NH2	2.43	0.49
1:A:475:GLN:HG2	1:A:482:ALA:HA	1.94	0.49
1:B:135:GLU:HA	1:B:157:GLN:HE22	1.78	0.49
1:A:457:ILE:HG23	1:A:461:PHE:CE2	2.47	0.48
1:A:210:GLY:HA3	1:A:257:ILE:O	2.14	0.48
1:A:389:HIS:O	1:A:393:ILE:HG13	2.13	0.48
1:A:120:VAL:HG12	1:A:121:ALA:N	2.28	0.48
1:A:12:LEU:HD12	1:A:13:ILE:N	2.27	0.48
1:A:19:TRP:CH2	1:A:128:LEU:HD13	2.48	0.48
1:B:470:PHE:C	1:B:472:TRP:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LEU:HD23	1:B:515:HIS:N	2.29	0.48
1:B:503:MET:CE	1:B:505:GLU:O	2.62	0.48
1:B:50:ASN:ND2	1:B:50:ASN:H	2.12	0.48
1:B:466:LEU:O	1:B:467:ASN:OD1	2.30	0.48
1:B:213:GLN:HG3	1:B:257:ILE:HG12	1.94	0.48
1:A:568:LYS:C	1:A:570:GLY:H	2.15	0.48
1:B:509:ASP:O	1:B:510:THR:HG23	2.14	0.48
1:B:575:ASP:O	1:B:576:ARG:HB2	2.12	0.48
1:A:432:LEU:HD22	1:A:436:LEU:CD1	2.44	0.47
1:A:377:SER:CB	1:A:378:PRO:CD	2.92	0.47
1:B:213:GLN:CG	1:B:257:ILE:CG1	2.90	0.47
1:B:475:GLN:N	1:B:475:GLN:OE1	2.48	0.47
1:B:90:THR:HG21	1:B:134:ASN:HA	1.97	0.47
1:A:475:GLN:HB2	1:A:482:ALA:HB2	1.96	0.47
1:A:467:ASN:CB	1:A:505:GLU:HB2	2.45	0.47
1:B:78:SER:C	1:B:80:GLU:H	2.16	0.47
1:B:83:LEU:HD23	1:B:83:LEU:N	2.29	0.47
1:A:575:ASP:O	1:A:576:ARG:HB2	2.13	0.47
1:A:198:LEU:HA	1:A:234:ILE:O	2.14	0.47
1:B:547:GLU:OE2	1:B:588:ARG:NH1	2.48	0.47
1:B:78:SER:O	1:B:79:GLU:HB2	2.15	0.47
1:A:434:ARG:HG3	1:A:434:ARG:NH1	2.29	0.47
1:B:473:TYR:O	1:B:476:THR:OG1	2.32	0.47
1:A:470:PHE:C	1:A:472:TRP:N	2.67	0.47
1:B:550:TRP:O	1:B:551:ASN:HB2	2.14	0.47
1:A:361:PHE:CE2	1:A:380:ARG:HD2	2.38	0.47
1:A:16:ASP:HA	1:A:45:VAL:CG2	2.44	0.47
1:B:236:ILE:HA	1:B:237:PRO:HD2	1.75	0.47
1:A:72:ILE:HG12	1:A:125:GLN:HE21	1.80	0.47
1:A:219:GLU:HG3	1:A:248:TYR:CE1	2.50	0.47
1:A:377:SER:HB2	1:A:378:PRO:HD2	1.96	0.47
1:B:77:TRP:O	1:B:80:GLU:HB2	2.13	0.46
1:A:136:LEU:H	1:A:157:GLN:NE2	2.11	0.46
1:A:181:GLN:HA	1:A:206:SER:OG	2.15	0.46
1:A:391:GLN:O	1:A:395:GLU:HG3	2.15	0.46
1:A:340:MET:HA	1:A:340:MET:CE	2.46	0.46
1:A:474:THR:OG1	1:A:475:GLN:OE1	2.30	0.46
1:B:11:ASP:CB	1:B:77:TRP:CZ2	2.99	0.46
1:B:64:TRP:CE3	1:B:133:ASP:HB2	2.50	0.46
1:B:18:LEU:HB3	1:B:42:GLU:HB3	1.97	0.46
1:B:253:HIS:CE1	1:B:268:LYS:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB2	1:B:378:PRO:CD	2.44	0.46
1:B:396:LEU:CD2	1:B:409:TRP:CZ3	2.98	0.46
1:B:509:ASP:HA	1:B:569:LYS:HA	1.98	0.46
1:A:46:PRO:O	1:A:47:ALA:HB2	2.15	0.46
1:B:437:ASP:HA	1:B:438:PRO:HD2	1.77	0.46
1:B:164:TYR:N	1:B:557:THR:HA	2.31	0.46
1:A:97:VAL:HG23	1:A:102:VAL:HG21	1.97	0.46
1:B:554:ASP:OD1	1:B:568:LYS:HA	2.16	0.46
1:A:390:ALA:O	1:A:394:ARG:HG3	2.16	0.45
1:A:256:ILE:O	1:A:264:ILE:CG2	2.64	0.45
1:B:141:ILE:CG2	1:B:355:PRO:HG2	2.45	0.45
1:A:191:ASP:OD2	1:A:192:VAL:N	2.44	0.45
1:A:218:ASP:HB2	1:A:248:TYR:OH	2.15	0.45
1:B:503:MET:CE	1:B:506:TYR:HB3	2.47	0.45
1:B:192:VAL:HG23	1:B:275:THR:HG23	1.98	0.45
1:B:445:ALA:HB1	1:B:467:ASN:HD21	1.80	0.45
1:A:309:ASP:CG	1:B:304:ARG:NH2	2.70	0.45
1:B:518:MET:HB3	1:B:518:MET:HE3	1.89	0.45
1:B:72:ILE:HG13	1:B:125:GLN:HG3	1.99	0.45
1:A:19:TRP:NE1	1:A:45:VAL:HG22	2.32	0.45
1:A:330:THR:HA	1:A:335:TYR:CZ	2.52	0.45
1:A:361:PHE:HE2	1:A:380:ARG:HB3	1.82	0.45
1:B:11:ASP:HB3	1:B:77:TRP:HH2	1.77	0.45
1:B:257:ILE:HG22	1:B:258:ASP:N	2.32	0.45
1:A:141:ILE:HG13	1:A:389:HIS:HA	1.99	0.44
1:A:37:LEU:HD12	1:A:38:LYS:H	1.81	0.44
1:B:505:GLU:O	1:B:506:TYR:HB3	2.16	0.44
1:A:251:GLN:OE1	1:A:270:ALA:HB2	2.17	0.44
1:A:503:MET:HG3	1:A:538:PHE:CZ	2.52	0.44
1:B:97:VAL:HB	1:B:102:VAL:HG21	1.99	0.44
1:A:23:LEU:HD23	1:A:65:VAL:HG12	1.99	0.44
1:A:258:ASP:O	1:A:259:SER:C	2.56	0.44
1:A:306:LYS:CE	1:A:333:TYR:CZ	3.00	0.44
1:A:90:THR:CB	1:A:168:GLY:N	2.61	0.44
1:B:564:VAL:O	1:B:564:VAL:HG12	2.18	0.44
1:A:236:ILE:HA	1:A:237:PRO:HD2	1.75	0.44
1:A:306:LYS:HE2	1:A:333:TYR:CZ	2.53	0.44
1:A:340:MET:HE2	1:A:340:MET:HA	1.99	0.44
1:A:467:ASN:HB3	1:A:505:GLU:HB2	1.98	0.44
1:A:294:GLY:HA3	1:A:327:SER:O	2.18	0.44
1:A:377:SER:HB2	1:A:379:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:HB2	1:A:546:GLY:HA3	2.00	0.44
1:A:521:PRO:O	1:A:522:TRP:CB	2.65	0.44
1:B:503:MET:HE3	1:B:505:GLU:O	2.18	0.44
1:B:141:ILE:HD12	1:B:141:ILE:HA	1.60	0.43
1:B:381:ILE:HG13	1:B:385:THR:HG21	2.00	0.43
1:A:267:TYR:HE1	1:A:269:LEU:HB2	1.83	0.43
1:B:381:ILE:O	1:B:381:ILE:HG22	2.17	0.43
1:B:399:ARG:HD3	1:B:400:ASP:OD1	2.17	0.43
1:B:353:GLU:OE2	1:B:413:ASN:HB2	2.18	0.43
1:B:247:ALA:HB2	1:B:347:GLY:N	2.32	0.43
1:A:82:TYR:O	1:A:117:THR:HG22	2.18	0.43
1:A:380:ARG:C	1:A:381:ILE:HD12	2.38	0.43
1:B:528:VAL:HG13	1:B:584:LEU:HD13	1.99	0.43
1:A:377:SER:CB	1:A:379:ASP:OD1	2.66	0.43
1:B:121:ALA:O	1:B:124:GLU:HB2	2.18	0.43
1:B:411:ILE:HG12	1:B:443:THR:O	2.18	0.43
1:A:295:PHE:O	1:A:328:PHE:HA	2.19	0.43
1:A:45:VAL:O	1:A:46:PRO:C	2.55	0.43
1:B:469:TYR:HH	1:B:550:TRP:CB	2.31	0.43
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.33	0.43
1:A:137:THR:C	1:A:144:GLY:O	2.56	0.43
1:A:47:ALA:HA	1:A:307:GLY:HA3	2.01	0.43
1:B:82:TYR:N	1:B:117:THR:CG2	2.71	0.43
1:A:303:ILE:HD13	1:B:315:HIS:CG	2.53	0.43
1:A:120:VAL:CG1	1:A:124:GLU:HB3	2.49	0.43
1:A:83:LEU:HD23	1:A:83:LEU:N	2.34	0.43
1:B:24:ALA:HB2	1:B:66:TYR:HE2	1.84	0.43
1:B:292:PHE:HB2	1:B:546:GLY:HA3	1.99	0.43
1:A:326:ASN:C	1:A:326:ASN:ND2	2.71	0.42
1:B:112:PHE:CD1	1:B:112:PHE:N	2.86	0.42
1:A:120:VAL:CG1	1:A:121:ALA:N	2.82	0.42
1:A:361:PHE:CE2	1:A:380:ARG:HB3	2.54	0.42
1:A:447:VAL:HG22	1:A:448:GLY:N	2.34	0.42
1:B:341:GLU:O	1:B:344:ASP:HB2	2.19	0.42
1:A:386:ARG:HD3	1:A:425:TYR:O	2.19	0.42
1:B:309:ASP:C	1:B:309:ASP:OD1	2.57	0.42
1:A:160:GLN:HG3	1:A:358:GLY:O	2.19	0.42
1:A:396:LEU:CD2	1:A:409:TRP:HZ3	2.30	0.42
1:A:39:THR:HB	1:A:41:LEU:HB2	2.02	0.42
1:B:396:LEU:HD23	1:B:396:LEU:C	2.40	0.42
1:A:557:THR:OG1	1:A:566:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLN:HG3	1:B:481:GLU:CG	2.50	0.42
1:B:468:ARG:H	1:B:503:MET:HE3	1.85	0.42
1:A:509:ASP:HB3	1:A:522:TRP:CZ3	2.55	0.42
1:B:294:GLY:O	1:B:548:GLN:HA	2.20	0.42
1:A:310:ASP:HB3	1:B:44:PRO:HB3	2.02	0.42
1:A:219:GLU:HG3	1:A:248:TYR:CZ	2.55	0.42
1:A:78:SER:O	1:A:79:GLU:CB	2.66	0.42
1:A:68:GLN:HG3	1:A:129:THR:HB	2.01	0.41
1:B:213:GLN:CG	1:B:257:ILE:HG12	2.50	0.41
1:B:295:PHE:O	1:B:328:PHE:HB2	2.20	0.41
1:B:299:GLU:HG3	1:B:335:TYR:CD1	2.55	0.41
1:B:496:LYS:HG2	1:B:497:TYR:CE2	2.55	0.41
1:A:141:ILE:HD11	1:A:356:ALA:HB2	2.01	0.41
1:B:550:TRP:O	1:B:550:TRP:CD1	2.73	0.41
1:B:22:ALA:HB2	1:B:39:THR:HB	2.03	0.41
1:B:11:ASP:HB2	1:B:77:TRP:CH2	2.55	0.41
1:A:120:VAL:HG13	1:A:124:GLU:HB3	2.02	0.41
1:A:267:TYR:CE1	1:A:269:LEU:HB2	2.56	0.41
1:B:90:THR:OG1	1:B:168:GLY:N	2.50	0.41
1:A:260:SER:O	1:A:262:LYS:N	2.48	0.41
1:A:50:ASN:H	1:A:50:ASN:ND2	2.19	0.41
1:A:567:ASN:ND2	1:A:569:LYS:N	2.58	0.41
1:B:361:PHE:HB2	1:B:375:THR:HG22	2.02	0.41
1:B:476:THR:O	1:B:477:ALA:CB	2.66	0.41
1:A:243:GLN:HB2	1:A:246:ALA:HB3	2.03	0.41
1:A:257:ILE:HD13	1:A:257:ILE:N	2.34	0.41
1:A:258:ASP:OD2	1:A:262:LYS:HD2	2.20	0.41
1:B:413:ASN:HD22	1:B:445:ALA:HB3	1.86	0.41
1:A:181:GLN:HE21	1:A:181:GLN:HA	1.86	0.41
1:B:542:GLU:O	1:B:542:GLU:HG2	2.21	0.41
1:A:361:PHE:HD2	1:A:375:THR:HB	1.86	0.41
1:B:0:SER:HB3	1:B:1:MET:H	1.65	0.41
1:B:509:ASP:OD2	1:B:569:LYS:NZ	2.37	0.41
1:B:74:PRO:HG2	1:B:77:TRP:CE2	2.56	0.41
1:B:90:THR:OG1	1:B:167:ALA:CB	2.69	0.41
1:A:503:MET:CE	1:A:505:GLU:O	2.69	0.41
1:B:468:ARG:HD3	1:B:468:ARG:HA	1.70	0.41
1:B:85:ARG:HG2	1:B:86:CYS:N	2.36	0.41
1:B:274:ARG:HG2	1:B:275:THR:N	2.36	0.40
1:B:361:PHE:H	1:B:375:THR:CG2	2.34	0.40
1:B:19:TRP:CE2	1:B:45:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:N	1:A:117:THR:HG22	2.23	0.40
1:A:475:GLN:HB3	1:A:478:GLU:HB2	2.03	0.40
1:B:81:ARG:CG	1:B:81:ARG:HH11	2.34	0.40
1:B:264:ILE:HG13	1:B:264:ILE:O	2.20	0.40
1:A:193:GLN:HB2	1:A:198:LEU:HD21	2.04	0.40
1:B:330:THR:HA	1:B:335:TYR:CZ	2.56	0.40
1:B:23:LEU:HA	1:B:65:VAL:HA	2.02	0.40
1:A:134:ASN:CB	1:A:167:ALA:HB2	2.51	0.40
1:A:253:HIS:CE1	1:A:268:LYS:HG3	2.56	0.40
1:A:44:PRO:HD3	1:B:314:VAL:HG21	2.04	0.40
1:B:316:ASP:OD1	1:B:552:PHE:HE2	2.04	0.40
1:B:452:TYR:CE1	1:B:492:GLY:HA3	2.56	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	582/612 (95%)	527 (90%)	46 (8%)	9 (2%)	13 46
1	B	580/612 (95%)	514 (89%)	64 (11%)	2 (0%)	46 80
All	All	1162/1224 (95%)	1041 (90%)	110 (10%)	11 (1%)	21 61

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
1	A	471	GLY
1	B	471	GLY
1	A	47	ALA
1	A	359	LEU
1	A	401	LYS

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Mol	Chain	Res	Type
1	A	45	VAL
1	A	261	LYS
1	A	569	LYS
1	B	506	TYR
1	A	46	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	493/509 (97%)	420 (85%)	73 (15%)	4 16
1	B	493/509 (97%)	433 (88%)	60 (12%)	6 24
All	All	986/1018 (97%)	853 (86%)	133 (14%)	5 20

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	12	LEU
1	A	25	SER
1	A	30	THR
1	A	39	THR
1	A	40	SER
1	A	52	ILE
1	A	56	SER
1	A	75	LYS
1	A	77	TRP
1	A	79	GLU
1	A	80	GLU
1	A	95	ILE
1	A	119	LEU
1	A	128	LEU
1	A	129	THR
1	A	141	ILE
1	A	156	VAL

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	162	ASP
1	A	175	LEU
1	A	177	SER
1	A	178	VAL
1	A	180	GLN
1	A	181	GLN
1	A	196	THR
1	A	198	LEU
1	A	199	ILE
1	A	200	ASP
1	A	209	GLN
1	A	227	SER
1	A	233	THR
1	A	239	VAL
1	A	251	GLN
1	A	252	LEU
1	A	255	SER
1	A	259	SER
1	A	262	LYS
1	A	263	THR
1	A	269	LEU
1	A	271	THR
1	A	274	ARG
1	A	281	THR
1	A	326	ASN
1	A	329	ARG
1	A	357	VAL
1	A	362	SER
1	A	363	ILE
1	A	375	THR
1	A	377	SER
1	A	379	ASP
1	A	384	LYS
1	A	432	LEU
1	A	435	GLN
1	A	439	THR
1	A	446	ASN
1	A	468	ARG
1	A	474	THR
1	A	488	GLU
1	A	490	LEU

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Mol	Chain	Res	Type
1	A	495	GLU
1	A	496	LYS
1	A	499	LYS
1	A	510	THR
1	A	517	VAL
1	A	533	MET
1	A	542	GLU
1	A	559	VAL
1	A	567	ASN
1	A	577	LYS
1	A	584	LEU
1	A	587	LYS
1	A	593	HIS
1	B	3	LYS
1	B	7	THR
1	B	39	THR
1	B	52	ILE
1	B	69	ARG
1	B	77	TRP
1	B	81	ARG
1	B	83	LEU
1	B	90	THR
1	B	119	LEU
1	B	128	LEU
1	B	129	THR
1	B	150	GLU
1	B	156	VAL
1	B	177	SER
1	B	178	VAL
1	B	180	GLN
1	B	196	THR
1	B	198	LEU
1	B	199	ILE
1	B	207	THR
1	B	209	GLN
1	B	227	SER
1	B	251	GLN
1	B	255	SER
1	B	264	ILE
1	B	269	LEU
1	B	274	ARG
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	288	LYS
1	B	326	ASN
1	B	329	ARG
1	B	352	ASP
1	B	357	VAL
1	B	375	THR
1	B	384	LYS
1	B	399	ARG
1	B	432	LEU
1	B	447	VAL
1	B	449	LEU
1	B	457	ILE
1	B	467	ASN
1	B	468	ARG
1	B	474	THR
1	B	488	GLU
1	B	490	LEU
1	B	495	GLU
1	B	496	LYS
1	B	499	LYS
1	B	504	THR
1	B	509	ASP
1	B	510	THR
1	B	517	VAL
1	B	518	MET
1	B	531	LEU
1	B	533	MET
1	B	542	GLU
1	B	567	ASN
1	B	577	LYS
1	B	588	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	36	GLN
1	A	50	ASN
1	A	125	GLN
1	A	139	GLN
1	A	157	GLN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	332	HIS
1	A	389	HIS
1	A	398	HIS
1	A	413	ASN
1	A	446	ASN
1	A	548	GLN
1	A	567	ASN
1	B	50	ASN
1	B	100	ASN
1	B	157	GLN
1	B	165	ASN
1	B	184	GLN
1	B	251	GLN
1	B	326	ASN
1	B	389	HIS
1	B	413	ASN
1	B	446	ASN
1	B	556	GLN
1	B	567	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	588/612 (96%)	-0.44	5 (0%) 85 72	30, 45, 63, 96	0
1	B	584/612 (95%)	-0.34	5 (0%) 85 72	29, 47, 64, 79	0
All	All	1172/1224 (95%)	-0.39	10 (0%) 85 72	29, 46, 64, 96	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	593	HIS	3.0
1	B	362	SER	2.8
1	A	591	ASN	2.5
1	B	373	PRO	2.4
1	B	264	ILE	2.4
1	A	380	ARG	2.1
1	B	256	ILE	2.1
1	A	473	TYR	2.1
1	A	363	ILE	2.0
1	B	208	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.