Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 07:46 pm GMT

PDB ID	:	1E1E
Title	:	Crystal structure of a Monocot (Maize ZMGlu1) beta-glucosidase
Authors	:	Czjzek, M.; Cicek, M.; Bevan, D.R.; Henrissat, B.; Esen, A.
Deposited on	:	2000-05-03
Resolution	:	2.50 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:

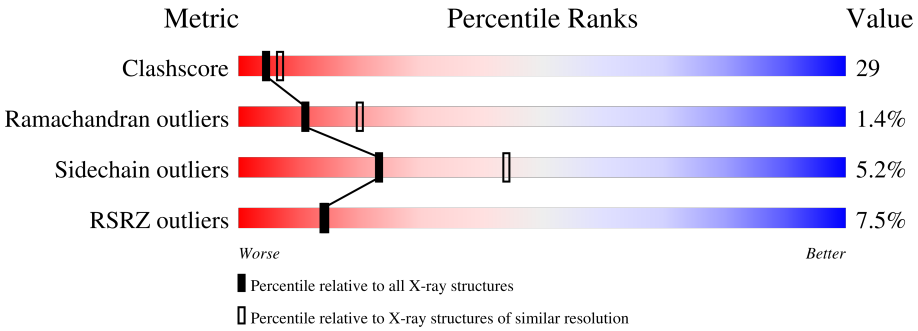
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	512	5% 58% 34%
1	B	512	9% 49% 43%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8302 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 BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3967	2544	656	749	18			
1	B	495	Total	C	N	O	S	0	0	0
			4004	2565	664	757	18			

- Molecule 2 is water.

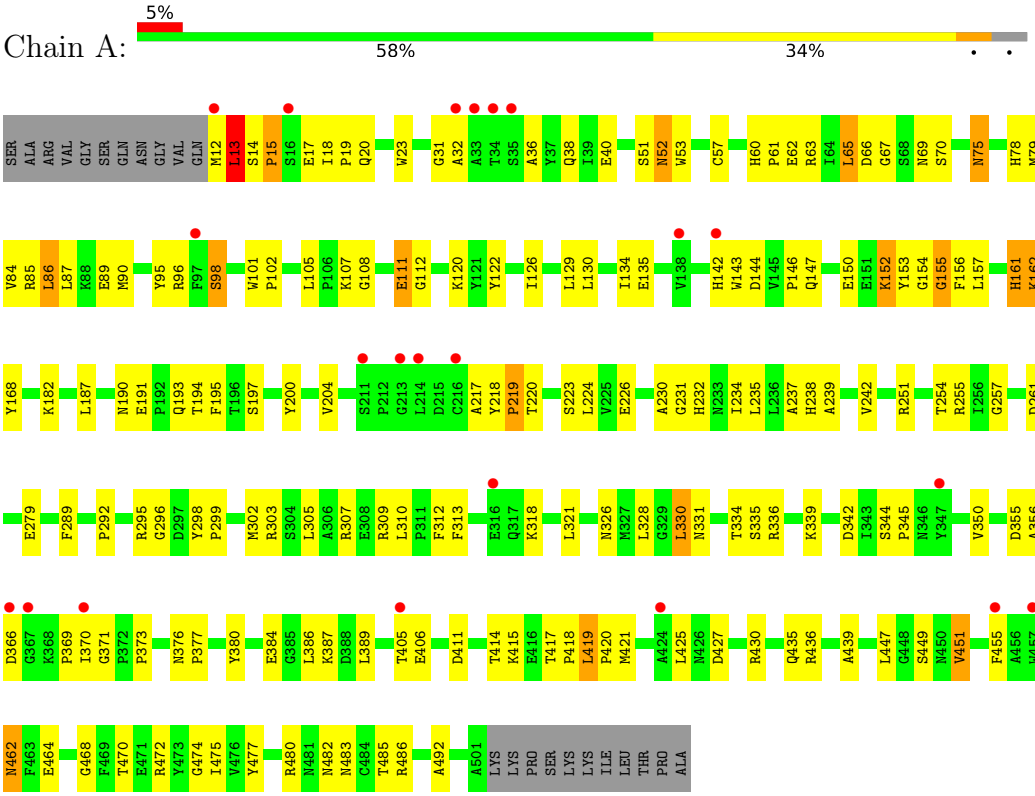
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	215	Total	O	0	0
			215	215		
2	B	116	Total	O	0	0
			116	116		

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.

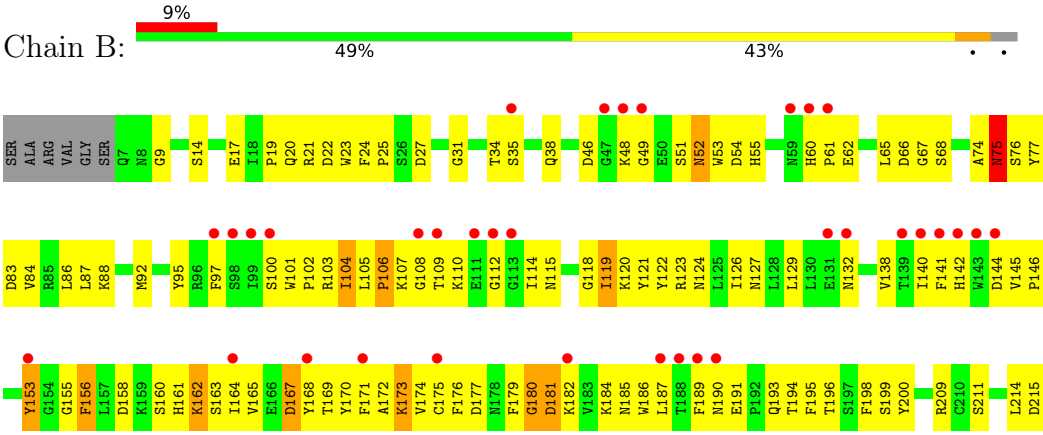
• Molecule 1: BETA-GLUCOSIDASE

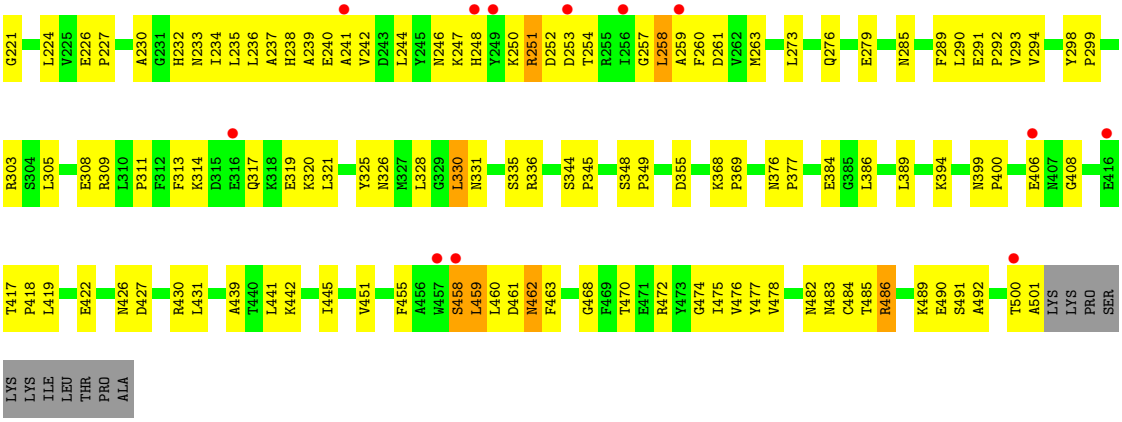
Chain A:



• Molecule 1: BETA-GLUCOSIDASE

Chain B:




G221 L224 V225 E226 P227 A230 G231 H232 N233 I234 L235 L236 A237 H238 A239 E240 A241 V242 D243 L244 Y245 N246 K247 H248 Y249 K250 R251 D252 D253 T254 R255 I256 G257 L258 A259 F260 D261 V262 M263 L273 Q276 E279 N285 F289 L290 E291 P292 V293 V294 Y298 P299
R303 S304 L305 E308 R309 L310 P311 F312 F313 K314 D315 E316 Q317 K318 E319 K320 L321 Y325 N326 M327 L328 G329 L330 N331 S335 R336 S344 P345 S348 P349 D355 K368 P369 N376 P377 E384 G385 L386 L389 K394 N399 P400 E406 N407 G408 E416
T417 P418 L419 E422 N426 D427 R430 L431 A439 T440 L441 K442 I445 V451 F455 A456 W457 S468 L459 L460 D461 N462 F463 G468 F469 T470 E471 R472 Y473 G474 I475 V476 Y477 V478 N482 N483 C484 T485 R486 K489 E490 S491 A492 T500 A501 LYS LYS PRO SER
LYS LYS ILE LEU THR PRO ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.88Å 118.34Å 77.10Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	27.00 – 2.50 29.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (27.00-2.50) 97.6 (29.17-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.322 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8302	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

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	0.45	0/4088	0.63	0/5550
1	B	0.47	0/4125	0.62	0/5600
All	All	0.46	0/8213	0.63	0/11150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3967	0	3759	175	0
1	B	4004	0	3793	273	0
2	A	215	0	0	33	0
2	B	116	0	0	36	0
All	All	8302	0	7552	443	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 29.

All (443) 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:376:ASN:HB2	1:A:377:PRO:HD2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TYR:HA	1:B:121:TYR:CZ	2.00	0.96
1:B:146:PRO:HG2	1:B:149:LEU:HG	1.48	0.94
1:A:461:ASP:HA	2:A:2198:HOH:O	1.67	0.94
1:B:49:GLY:O	1:B:102:PRO:HB2	1.65	0.94
1:B:236:LEU:HD12	2:B:2058:HOH:O	1.69	0.93
1:B:376:ASN:HB2	1:B:377:PRO:HD2	1.55	0.88
1:B:101:TRP:HA	1:B:171:PHE:CZ	2.10	0.86
1:A:436:ARG:CZ	2:A:2187:HOH:O	2.24	0.86
1:B:147:GLN:HE21	1:B:147:GLN:HA	1.40	0.85
1:A:482:ASN:HD22	1:A:483:ASN:H	1.20	0.85
1:B:51:SER:O	2:B:2024:HOH:O	1.95	0.84
1:A:482:ASN:ND2	1:A:483:ASN:H	1.76	0.84
1:B:34:THR:HG21	2:B:2032:HOH:O	1.79	0.83
1:B:77:TYR:HA	1:B:121:TYR:OH	1.79	0.82
1:A:95:TYR:HD2	1:A:129:LEU:HD11	1.45	0.82
1:B:482:ASN:ND2	1:B:483:ASN:H	1.78	0.82
1:B:149:LEU:HB3	1:B:153:TYR:HE1	1.45	0.81
1:B:119:ILE:HD13	1:B:119:ILE:H	1.45	0.81
1:B:110:LYS:HG2	1:B:170:TYR:CZ	2.15	0.81
1:B:460:LEU:HD22	2:B:2108:HOH:O	1.80	0.81
1:A:194:THR:CB	2:A:2110:HOH:O	2.29	0.81
1:A:384:GLU:HB3	2:A:2167:HOH:O	1.80	0.80
1:B:48:LYS:HD2	1:B:103:ARG:HG3	1.62	0.80
1:B:87:LEU:HD21	1:B:459:LEU:HG	1.64	0.80
1:A:87:LEU:HD21	1:A:459:LEU:HG	1.64	0.79
1:A:194:THR:HB	2:A:2110:HOH:O	1.82	0.78
1:A:251:ARG:HB2	1:A:254:THR:HG23	1.65	0.78
1:B:9:GLY:O	2:B:2003:HOH:O	2.02	0.77
1:A:12:MET:C	1:A:13:LEU:HD23	2.05	0.77
1:B:171:PHE:HE2	2:B:2046:HOH:O	1.69	0.75
1:B:119:ILE:HD13	1:B:119:ILE:N	2.02	0.74
1:B:408:GLY:HA3	2:B:2107:HOH:O	1.88	0.74
1:B:177:ASP:HA	2:B:2050:HOH:O	1.87	0.74
1:B:19:PRO:HG3	1:B:439:ALA:HB2	1.68	0.74
1:B:54:ASP:HB2	2:B:2024:HOH:O	1.88	0.74
1:B:482:ASN:HD22	1:B:483:ASN:H	1.34	0.74
1:B:49:GLY:C	1:B:102:PRO:HB2	2.08	0.73
1:B:171:PHE:CE2	2:B:2046:HOH:O	2.42	0.73
1:A:298:TYR:O	2:A:2139:HOH:O	2.06	0.73
1:A:162:LYS:HD3	2:A:2095:HOH:O	1.88	0.73
1:B:232:HIS:CE1	1:B:311:PRO:HB2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HG2	2:A:2001:HOH:O	1.89	0.72
1:B:101:TRP:CG	1:B:146:PRO:HD3	2.25	0.72
1:A:120:LYS:HE3	2:A:2067:HOH:O	1.88	0.72
1:B:173:LYS:HA	1:B:176:PHE:CD2	2.24	0.72
1:B:460:LEU:HB3	2:B:2108:HOH:O	1.88	0.72
1:A:427:ASP:OD2	1:A:430:ARG:HD2	1.90	0.72
1:A:52:ASN:N	1:A:52:ASN:HD22	1.86	0.72
1:A:82:THR:O	1:A:86:LEU:HD22	1.89	0.71
1:B:84:VAL:HG13	1:B:129:LEU:HD23	1.71	0.71
1:A:157:LEU:HD11	1:A:200:TYR:CE1	2.26	0.71
1:B:140:ILE:HG23	2:B:2042:HOH:O	1.90	0.71
1:A:370:ILE:O	2:A:2162:HOH:O	2.09	0.71
1:B:52:ASN:N	1:B:52:ASN:HD22	1.88	0.71
1:B:104:ILE:O	1:B:105:LEU:HD23	1.91	0.71
1:A:239:ALA:HB2	1:A:321:LEU:HD23	1.72	0.70
1:B:232:HIS:CE1	1:B:313:PHE:CE2	2.79	0.70
1:B:101:TRP:HE1	1:B:108:GLY:CA	2.03	0.70
1:B:123:ARG:HH21	1:B:123:ARG:HG3	1.57	0.70
1:A:82:THR:HG22	1:A:85:ARG:NH2	2.06	0.69
1:B:240:GLU:OE2	1:B:240:GLU:HA	1.92	0.69
1:B:279:GLU:OE1	1:B:279:GLU:HA	1.92	0.69
1:B:55:HIS:N	2:B:2024:HOH:O	1.89	0.69
1:B:180:GLY:HA2	1:B:186:TRP:HZ2	1.56	0.69
1:B:244:LEU:HD12	1:B:248:HIS:HD2	1.57	0.69
1:A:107:LYS:HB2	1:A:112:GLY:HA3	1.75	0.69
1:B:149:LEU:HB3	1:B:153:TYR:CE1	2.26	0.68
1:A:130:LEU:HD11	1:A:182:LYS:HB3	1.74	0.68
1:B:147:GLN:HA	1:B:147:GLN:NE2	2.07	0.68
1:A:153:TYR:CE2	1:A:163:SER:HB3	2.28	0.68
1:A:279:GLU:HA	1:A:279:GLU:OE1	1.93	0.68
1:B:52:ASN:HD22	1:B:52:ASN:H	1.42	0.67
1:B:21:ARG:HB3	2:B:2011:HOH:O	1.94	0.67
1:B:114:ILE:CG2	1:B:119:ILE:HD11	2.24	0.67
1:B:88:LYS:HD3	1:B:132:ASN:HB3	1.77	0.67
1:B:101:TRP:HE1	1:B:108:GLY:HA2	1.60	0.67
1:B:442:LYS:O	1:B:442:LYS:HD3	1.95	0.66
1:B:107:LYS:HB2	1:B:112:GLY:HA3	1.77	0.66
1:B:150:GLU:OE2	1:B:155:GLY:HA3	1.95	0.66
1:A:156:PHE:O	1:A:230:ALA:HA	1.95	0.66
1:B:173:LYS:CB	1:B:244:LEU:HD21	2.24	0.66
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:O	1:A:18:ILE:HG12	1.95	0.65
1:B:80:TYR:O	1:B:84:VAL:HG23	1.96	0.65
1:A:75:ASN:HD21	1:A:78:HIS:HD2	1.44	0.65
1:A:462:ASN:C	1:A:462:ASN:HD22	2.00	0.65
1:B:460:LEU:CB	2:B:2108:HOH:O	2.44	0.65
1:B:163:SER:O	1:B:167:ASP:OD2	2.15	0.64
1:A:303:ARG:HH22	1:A:312:PHE:HA	1.61	0.64
1:B:191:GLU:HG2	1:B:261:ASP:HB3	1.79	0.64
1:A:191:GLU:HG2	1:A:261:ASP:HB3	1.79	0.64
1:A:191:GLU:CG	1:A:261:ASP:HB3	2.28	0.64
1:B:101:TRP:HA	1:B:171:PHE:CE1	2.32	0.64
1:B:461:ASP:OD2	1:B:472:ARG:HB3	1.98	0.64
1:A:464:GLU:OE1	2:A:2201:HOH:O	2.15	0.63
1:B:460:LEU:CD2	2:B:2108:HOH:O	2.40	0.63
1:B:258:LEU:H	1:B:258:LEU:HD23	1.61	0.63
1:A:31:GLY:O	1:A:455:PHE:HA	1.99	0.62
1:A:193:GLN:HA	1:A:289:PHE:HE2	1.64	0.62
1:A:101:TRP:HB3	1:A:102:PRO:HD3	1.81	0.62
1:A:135:GLU:HG3	2:A:2025:HOH:O	2.00	0.61
1:A:312:PHE:CE2	1:B:345:PRO:HD3	2.34	0.61
1:B:289:PHE:C	1:B:292:PRO:HD2	2.21	0.61
1:A:13:LEU:O	1:A:14:SER:HB2	1.99	0.61
1:B:95:TYR:OH	2:B:2032:HOH:O	2.15	0.61
1:A:75:ASN:HB3	1:A:79:MET:CE	2.30	0.60
1:A:217:ALA:C	1:A:219:PRO:HD3	2.21	0.60
1:A:52:ASN:HD22	1:A:52:ASN:H	1.48	0.60
1:A:415:LYS:O	1:A:418:PRO:HD3	2.01	0.60
1:A:231:GLY:HA2	1:A:234:ILE:HD12	1.81	0.60
1:B:123:ARG:HH12	1:B:182:LYS:NZ	1.99	0.60
1:A:312:PHE:CE2	1:B:344:SER:HA	2.36	0.60
1:A:36:ALA:O	1:A:40:GLU:HB2	2.02	0.60
1:A:111:GLU:HG3	2:A:2064:HOH:O	2.00	0.60
1:B:211:SER:HA	1:B:221:GLY:O	2.02	0.60
1:B:52:ASN:N	1:B:145:VAL:O	2.34	0.60
1:B:250:LYS:HD3	1:B:251:ARG:H	1.66	0.59
1:A:373:PRO:HG3	1:A:380:TYR:CE2	2.36	0.59
1:B:22:ASP:N	2:B:2011:HOH:O	2.34	0.59
1:A:111:GLU:CG	2:A:2064:HOH:O	2.50	0.59
1:B:52:ASN:H	1:B:52:ASN:ND2	2.01	0.59
1:B:162:LYS:HA	1:B:165:VAL:HB	1.85	0.59
1:A:295:ARG:HD2	1:B:273:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASN:ND2	1:A:483:ASN:N	2.48	0.59
1:B:65:LEU:HD23	1:B:470:THR:HG21	1.84	0.59
1:B:179:PHE:C	1:B:181:ASP:H	2.06	0.59
1:B:478:VAL:CG2	2:B:2108:HOH:O	2.50	0.59
1:B:48:LYS:CD	1:B:103:ARG:HG3	2.30	0.58
1:B:174:VAL:O	1:B:177:ASP:HB2	2.03	0.58
1:B:124:ASN:HA	2:B:2038:HOH:O	2.03	0.58
1:B:123:ARG:HG3	1:B:123:ARG:NH2	2.18	0.58
1:B:20:GLN:O	1:B:23:TRP:HB2	2.03	0.57
1:B:459:LEU:HD13	1:B:460:LEU:HG	1.85	0.57
1:A:191:GLU:OE2	1:A:261:ASP:HB3	2.05	0.57
1:B:251:ARG:NH1	2:B:2062:HOH:O	2.37	0.57
1:B:145:VAL:HG13	1:B:146:PRO:HD2	1.86	0.57
1:A:472:ARG:HG2	2:A:2203:HOH:O	2.05	0.57
1:B:141:PHE:HD2	1:B:189:PHE:HD2	1.53	0.57
1:A:60:HIS:NE2	1:A:218:TYR:HE1	2.02	0.56
1:B:458:SER:O	1:B:474:GLY:HA2	2.04	0.56
1:B:173:LYS:HB2	1:B:244:LEU:HD21	1.86	0.56
1:B:251:ARG:HB3	2:B:2064:HOH:O	2.04	0.56
1:B:119:ILE:H	1:B:119:ILE:CD1	2.03	0.56
1:A:168:TYR:CD2	1:A:237:ALA:HB1	2.40	0.56
1:A:482:ASN:ND2	1:A:485:THR:OG1	2.38	0.56
1:B:101:TRP:HE1	1:B:108:GLY:HA3	1.70	0.56
1:B:250:LYS:O	1:B:251:ARG:HG2	2.05	0.56
1:A:449:SER:OG	1:A:451:VAL:HG22	2.05	0.56
1:A:459:LEU:HD13	1:A:460:LEU:HG	1.87	0.56
1:B:258:LEU:HD23	1:B:258:LEU:N	2.20	0.56
1:A:461:ASP:OD2	1:A:472:ARG:HB3	2.06	0.56
1:B:110:LYS:HG2	1:B:170:TYR:CE1	2.40	0.56
1:A:376:ASN:HB2	1:A:377:PRO:CD	2.26	0.56
1:B:51:SER:HB3	2:B:2023:HOH:O	2.05	0.55
1:B:21:ARG:C	1:B:23:TRP:H	2.10	0.55
1:B:25:PRO:HB2	1:B:27:ASP:OD1	2.07	0.55
1:B:49:GLY:O	1:B:102:PRO:CB	2.47	0.55
1:A:52:ASN:H	1:A:52:ASN:ND2	2.05	0.55
1:A:90:MET:HE1	1:A:475:ILE:HD12	1.88	0.55
1:A:52:ASN:N	1:A:52:ASN:ND2	2.55	0.55
1:B:247:LYS:HA	2:B:2060:HOH:O	2.07	0.55
1:B:179:PHE:O	1:B:181:ASP:N	2.40	0.55
1:B:224:LEU:O	1:B:309:ARG:HD2	2.06	0.55
1:B:239:ALA:HB1	1:B:320:LYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:O	1:A:87:LEU:HG	2.06	0.54
1:A:142:HIS:NE2	1:A:190:ASN:ND2	2.55	0.54
1:B:173:LYS:HE2	1:B:174:VAL:CG2	2.37	0.54
1:B:160:SER:O	1:B:161:HIS:HB2	2.07	0.54
1:B:462:ASN:HD22	1:B:462:ASN:C	2.09	0.54
1:A:344:SER:HB2	1:A:345:PRO:HD2	1.89	0.54
1:A:419:LEU:HD23	1:A:420:PRO:HD2	1.89	0.54
1:B:209:ARG:HG2	1:B:209:ARG:NH1	2.23	0.54
1:B:290:LEU:O	1:B:294:VAL:HG23	2.08	0.54
1:A:60:HIS:HE2	1:A:218:TYR:HE1	1.54	0.54
1:A:130:LEU:CD1	1:A:182:LYS:HB3	2.38	0.54
1:A:86:LEU:HD21	1:A:486:ARG:HD3	1.88	0.54
1:A:421:MET:O	1:A:425:LEU:HG	2.08	0.54
1:B:184:LYS:C	1:B:185:ASN:HD22	2.11	0.54
1:B:19:PRO:CG	1:B:439:ALA:HB2	2.36	0.54
1:B:226:GLU:HB2	1:B:227:PRO:HD3	1.91	0.54
1:B:427:ASP:HB2	1:B:430:ARG:HB3	1.89	0.54
1:A:373:PRO:HG3	1:A:380:TYR:HE2	1.73	0.53
1:B:49:GLY:N	1:B:102:PRO:O	2.40	0.53
1:B:46:ASP:O	1:B:115:ASN:OD1	2.26	0.53
1:B:77:TYR:CA	1:B:121:TYR:OH	2.54	0.53
1:A:312:PHE:CD2	1:B:345:PRO:HD3	2.44	0.53
1:A:191:GLU:OE1	2:A:2107:HOH:O	2.19	0.53
1:B:232:HIS:ND1	1:B:311:PRO:HB2	2.23	0.52
1:B:52:ASN:N	1:B:52:ASN:ND2	2.56	0.52
1:B:426:ASN:HA	1:B:490:GLU:HG2	1.92	0.52
1:B:459:LEU:HD13	1:B:460:LEU:CD2	2.39	0.52
1:A:387:LYS:HD2	1:A:447:LEU:HD12	1.91	0.52
1:A:14:SER:HB3	1:A:17:GLU:HB2	1.91	0.52
1:A:414:THR:HG22	1:A:470:THR:HB	1.91	0.52
1:B:75:ASN:HD21	1:B:78:HIS:CD2	2.28	0.52
1:B:122:TYR:O	1:B:126:ILE:HG13	2.10	0.52
1:B:196:THR:HG22	1:B:230:ALA:HB3	1.90	0.52
1:B:97:PHE:CZ	1:B:138:VAL:HG22	2.44	0.52
1:A:330:LEU:HG	1:A:389:LEU:HD21	1.91	0.52
1:A:135:GLU:CG	2:A:2025:HOH:O	2.56	0.52
1:B:172:ALA:O	1:B:175:CYS:HB2	2.10	0.52
1:B:123:ARG:HH12	1:B:182:LYS:HZ2	1.58	0.52
1:A:147:GLN:NE2	1:A:150:GLU:HB3	2.24	0.51
1:A:200:TYR:HB3	1:A:226:GLU:HB3	1.93	0.51
1:A:326:ASN:HA	2:A:2151:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PHE:HD2	1:B:189:PHE:CD2	2.28	0.51
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.74	0.51
1:B:478:VAL:HG23	2:B:2108:HOH:O	2.11	0.51
1:A:477:TYR:O	1:A:486:ARG:HA	2.11	0.51
1:B:60:HIS:HA	1:B:62:GLU:OE1	2.11	0.51
1:B:427:ASP:OD1	1:B:427:ASP:N	2.42	0.51
1:A:218:TYR:O	1:A:220:THR:N	2.36	0.51
1:A:342:ASP:HB3	2:A:2155:HOH:O	2.10	0.51
1:B:24:PHE:CD1	1:B:24:PHE:N	2.78	0.51
1:B:173:LYS:HA	1:B:176:PHE:HD2	1.72	0.51
1:B:101:TRP:HB3	1:B:102:PRO:HD3	1.93	0.51
1:B:119:ILE:O	1:B:123:ARG:HB2	2.10	0.51
1:B:173:LYS:HE2	1:B:174:VAL:HG23	1.93	0.51
1:A:194:THR:O	1:A:195:PHE:C	2.48	0.51
1:A:235:LEU:HD21	1:A:289:PHE:HD1	1.76	0.51
1:B:252:ASP:N	2:B:2064:HOH:O	2.38	0.51
1:B:303:ARG:HG2	1:B:303:ARG:NH1	2.24	0.51
1:B:431:LEU:HD13	1:B:491:SER:HA	1.92	0.51
1:A:371:GLY:HA2	2:A:2079:HOH:O	2.09	0.50
1:B:173:LYS:HG3	1:B:174:VAL:N	2.26	0.50
1:A:51:SER:HB3	1:A:102:PRO:HG2	1.93	0.50
1:A:61:PRO:O	1:A:67:GLY:HA2	2.11	0.50
1:A:251:ARG:HB2	1:A:254:THR:CG2	2.39	0.50
1:B:146:PRO:O	1:B:148:ALA:N	2.45	0.50
1:A:164:ILE:HG23	1:A:165:VAL:N	2.26	0.50
1:B:31:GLY:HA2	1:B:92:MET:SD	2.51	0.50
1:B:100:SER:HB2	2:B:2018:HOH:O	2.11	0.50
1:B:235:LEU:O	1:B:321:LEU:HD21	2.12	0.50
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.77	0.50
1:A:364:GLY:HA3	2:A:2160:HOH:O	2.12	0.50
1:B:105:LEU:C	1:B:107:LYS:H	2.14	0.50
1:B:251:ARG:HG3	1:B:251:ARG:HH11	1.75	0.50
1:B:263:MET:HE1	2:B:2065:HOH:O	2.11	0.50
1:A:89:GLU:HB3	2:A:2211:HOH:O	2.11	0.50
1:B:246:ASN:HA	1:B:250:LYS:HG2	1.94	0.50
1:B:251:ARG:HB2	1:B:254:THR:HG23	1.93	0.50
1:B:35:SER:HB3	1:B:38:GLN:OE1	2.11	0.49
1:B:48:LYS:CG	1:B:103:ARG:HG3	2.42	0.49
1:B:291:GLU:OE2	1:B:299:PRO:HA	2.12	0.49
1:B:293:VAL:O	1:B:325:TYR:HE2	1.95	0.49
1:B:241:ALA:O	1:B:244:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:THR:HG22	1:A:417:THR:O	2.13	0.49
1:B:305:LEU:HD13	1:B:355:ASP:O	2.12	0.49
1:A:152:LYS:HD2	1:A:153:TYR:CD2	2.47	0.49
1:B:20:GLN:HB2	1:B:23:TRP:CD1	2.48	0.49
1:B:107:LYS:CB	1:B:112:GLY:HA3	2.43	0.49
1:A:57:CYS:HB3	1:A:69:ASN:HB3	1.94	0.48
1:A:60:HIS:HB3	1:A:62:GLU:OE2	2.13	0.48
1:B:195:PHE:O	1:B:199:SER:HB2	2.13	0.48
1:B:232:HIS:CE1	1:B:313:PHE:HE2	2.31	0.48
1:B:54:ASP:CB	2:B:2024:HOH:O	2.56	0.48
1:B:173:LYS:HB3	1:B:244:LEU:HD21	1.95	0.48
1:B:184:LYS:C	1:B:185:ASN:ND2	2.66	0.48
1:B:187:LEU:HA	1:B:257:GLY:O	2.13	0.48
1:A:480:ARG:NH1	2:A:2207:HOH:O	2.47	0.48
1:B:149:LEU:N	1:B:149:LEU:HD23	2.27	0.48
1:B:191:GLU:CG	1:B:261:ASP:HB3	2.43	0.48
1:B:482:ASN:ND2	1:B:485:THR:OG1	2.46	0.48
1:A:20:GLN:O	1:A:23:TRP:HB2	2.13	0.48
1:A:289:PHE:C	1:A:292:PRO:HD2	2.33	0.48
1:B:54:ASP:N	2:B:2024:HOH:O	2.45	0.48
1:B:477:TYR:O	1:B:486:ARG:HA	2.12	0.48
1:B:83:ASP:OD1	1:B:460:LEU:HD11	2.13	0.48
1:B:107:LYS:O	1:B:149:LEU:HD21	2.14	0.48
1:B:482:ASN:ND2	1:B:483:ASN:N	2.55	0.48
1:B:101:TRP:CD2	1:B:146:PRO:HD3	2.47	0.48
1:B:101:TRP:HB3	1:B:102:PRO:CD	2.43	0.48
1:B:190:ASN:HA	1:B:259:ALA:HB3	1.94	0.48
1:A:411:ASP:HA	2:A:2178:HOH:O	2.13	0.48
1:B:66:ASP:OD1	1:B:468:GLY:HA3	2.14	0.48
1:B:173:LYS:HG3	1:B:174:VAL:H	1.78	0.48
1:A:60:HIS:NE2	1:A:218:TYR:CE1	2.81	0.47
1:B:142:HIS:NE2	1:B:190:ASN:ND2	2.62	0.47
1:A:82:THR:HG22	1:A:85:ARG:HH22	1.77	0.47
1:A:193:GLN:HA	1:A:289:PHE:CE2	2.48	0.47
1:B:77:TYR:O	1:B:121:TYR:CE1	2.68	0.47
1:A:38:GLN:O	1:A:462:ASN:HB2	2.14	0.47
1:B:368:LYS:HB3	1:B:369:PRO:HD2	1.97	0.47
1:B:258:LEU:N	1:B:258:LEU:CD2	2.78	0.47
1:B:399:ASN:N	1:B:400:PRO:CD	2.78	0.47
1:A:52:ASN:HD22	1:A:53:TRP:H	1.63	0.47
1:A:96:ARG:NH1	1:A:405:THR:HB	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TYR:C	1:B:170:TYR:N	2.68	0.47
1:A:356:ALA:O	1:A:357:TYR:C	2.53	0.47
1:B:105:LEU:HD11	1:B:171:PHE:HA	1.96	0.47
1:B:114:ILE:HG22	1:B:119:ILE:HD11	1.97	0.47
1:B:153:TYR:CD2	1:B:163:SER:HB3	2.49	0.47
1:B:230:ALA:O	1:B:234:ILE:HG13	2.14	0.47
1:A:312:PHE:HE2	1:B:344:SER:HA	1.79	0.47
1:A:339:LYS:HE3	2:A:2153:HOH:O	2.15	0.47
1:B:105:LEU:HD12	1:B:108:GLY:HA2	1.97	0.46
1:A:266:VAL:HG13	1:A:267:PRO:HD2	1.97	0.46
1:A:80:TYR:O	1:A:84:VAL:HG23	2.15	0.46
1:B:54:ASP:CA	2:B:2024:HOH:O	2.64	0.46
1:A:191:GLU:HB3	2:A:2110:HOH:O	2.15	0.46
1:B:49:GLY:HA3	1:B:106:PRO:HA	1.98	0.46
1:B:149:LEU:CB	1:B:153:TYR:HE1	2.23	0.46
1:B:34:THR:CG2	2:B:2032:HOH:O	2.52	0.46
1:B:38:GLN:O	1:B:462:ASN:HB2	2.16	0.46
1:B:52:ASN:HD22	1:B:53:TRP:H	1.64	0.46
1:A:142:HIS:O	1:A:143:TRP:HB2	2.16	0.46
1:B:146:PRO:C	1:B:148:ALA:N	2.66	0.46
1:B:165:VAL:HG13	1:B:237:ALA:HA	1.98	0.45
1:A:95:TYR:CD2	1:A:129:LEU:HD11	2.37	0.45
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.79	0.45
1:A:105:LEU:O	1:A:108:GLY:N	2.45	0.45
1:B:115:ASN:O	1:B:119:ILE:HD11	2.16	0.45
1:B:298:TYR:HB3	1:B:299:PRO:HD2	1.99	0.45
1:B:317:GLN:C	1:B:319:GLU:H	2.19	0.45
1:B:417:THR:N	1:B:418:PRO:HD3	2.32	0.45
1:B:106:PRO:O	1:B:107:LYS:HD3	2.16	0.45
1:B:194:THR:O	1:B:198:PHE:HB2	2.17	0.45
1:A:66:ASP:OD1	1:A:468:GLY:HA3	2.15	0.45
1:A:144:ASP:OD2	1:A:144:ASP:N	2.48	0.45
1:A:96:ARG:HH12	1:A:406:GLU:HG3	1.81	0.45
1:A:436:ARG:NE	2:A:2187:HOH:O	2.44	0.45
1:B:442:LYS:HD3	1:B:442:LYS:C	2.36	0.45
1:A:98:SER:HB3	2:A:2081:HOH:O	2.17	0.45
1:B:335:SER:O	1:B:336:ARG:HG2	2.17	0.45
1:B:251:ARG:HB2	1:B:254:THR:CG2	2.47	0.45
1:A:18:ILE:HD12	1:A:435:GLN:NE2	2.32	0.45
1:A:475:ILE:O	1:A:492:ALA:HB2	2.17	0.45
1:B:459:LEU:CD1	1:B:460:LEU:HG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:CD2	1:A:339:LYS:HD2	2.52	0.44
1:B:172:ALA:O	1:B:175:CYS:N	2.46	0.44
1:A:255:ARG:HD3	2:A:2129:HOH:O	2.16	0.44
1:B:118:GLY:C	1:B:120:LYS:H	2.20	0.44
1:B:156:PHE:O	1:B:233:ASN:ND2	2.41	0.44
1:B:168:TYR:O	1:B:170:TYR:N	2.50	0.44
1:B:161:HIS:O	1:B:165:VAL:HG21	2.17	0.44
1:B:289:PHE:O	1:B:292:PRO:HD2	2.18	0.44
1:B:105:LEU:HD23	1:B:114:ILE:HG12	2.00	0.44
1:B:115:ASN:O	1:B:119:ILE:CD1	2.66	0.44
1:B:123:ARG:NH2	1:B:127:ASN:HD21	2.15	0.44
1:A:239:ALA:HB2	1:A:321:LEU:CD2	2.45	0.44
1:A:303:ARG:NH2	1:A:312:PHE:HA	2.28	0.44
1:A:459:LEU:O	1:A:459:LEU:HD22	2.18	0.44
1:A:194:THR:O	1:A:197:SER:N	2.51	0.44
1:A:299:PRO:HD2	1:A:302:MET:SD	2.58	0.44
1:B:384:GLU:OE2	2:B:2094:HOH:O	2.21	0.44
1:A:200:TYR:O	1:A:223:SER:HA	2.18	0.44
1:A:472:ARG:HA	2:A:2203:HOH:O	2.18	0.43
1:B:114:ILE:CG2	1:B:119:ILE:CD1	2.94	0.43
1:B:147:GLN:NE2	1:B:147:GLN:CA	2.74	0.43
1:A:60:HIS:C	1:A:62:GLU:H	2.21	0.43
1:A:369:PRO:C	1:A:371:GLY:H	2.21	0.43
1:A:19:PRO:HA	1:A:23:TRP:CZ3	2.53	0.43
1:B:200:TYR:HA	1:B:209:ARG:O	2.19	0.43
1:B:394:LYS:HA	1:B:399:ASN:HA	2.01	0.43
1:A:19:PRO:HG3	1:A:439:ALA:HB2	2.00	0.43
1:A:65:LEU:HD23	1:A:470:THR:HG21	1.99	0.43
1:A:101:TRP:N	1:A:102:PRO:CD	2.81	0.43
1:A:309:ARG:CB	1:A:309:ARG:HH11	2.32	0.43
1:B:308:GLU:HG2	1:B:309:ARG:N	2.32	0.43
1:B:331:ASN:CG	1:B:406:GLU:HB2	2.39	0.43
1:A:161:HIS:O	1:A:162:LYS:HB2	2.18	0.43
1:A:331:ASN:CG	1:A:406:GLU:HB2	2.39	0.43
1:B:31:GLY:O	1:B:455:PHE:HA	2.19	0.43
1:B:158:ASP:HB3	1:B:164:ILE:HG22	2.01	0.43
1:B:169:THR:O	1:B:173:LYS:HB3	2.17	0.43
1:B:215:ASP:CG	1:B:215:ASP:O	2.56	0.43
1:B:459:LEU:HD22	1:B:459:LEU:O	2.19	0.43
1:A:232:HIS:CE1	1:A:313:PHE:CE2	3.06	0.43
1:B:276:GLN:NE2	2:B:2071:HOH:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:SER:HA	1:B:349:PRO:HD3	1.84	0.43
1:A:63:ARG:HH21	1:A:217:ALA:HA	1.83	0.43
1:B:123:ARG:HH22	1:B:127:ASN:HD21	1.66	0.43
1:B:149:LEU:HD22	1:B:153:TYR:OH	2.19	0.43
1:B:335:SER:O	1:B:336:ARG:NH1	2.52	0.43
1:A:20:GLN:HB2	1:A:23:TRP:CD1	2.54	0.42
1:A:122:TYR:O	1:A:126:ILE:HD12	2.19	0.42
1:B:55:HIS:ND1	1:B:147:GLN:OE1	2.52	0.42
1:B:74:ALA:O	1:B:75:ASN:C	2.57	0.42
1:B:330:LEU:HG	1:B:389:LEU:HD21	1.99	0.42
1:B:260:PHE:CZ	1:B:290:LEU:HA	2.55	0.42
1:B:164:ILE:HA	1:B:167:ASP:OD2	2.19	0.42
1:A:305:LEU:HD13	1:A:355:ASP:O	2.19	0.42
1:A:376:ASN:CB	1:A:377:PRO:HD2	2.28	0.42
1:B:38:GLN:HG2	1:B:463:PHE:O	2.20	0.42
1:B:142:HIS:CE1	1:B:190:ASN:ND2	2.87	0.42
1:A:32:ALA:CB	1:A:459:LEU:HB2	2.50	0.42
1:B:251:ARG:NH2	1:B:253:ASP:OD1	2.52	0.42
1:A:155:GLY:N	2:A:2086:HOH:O	2.52	0.42
1:B:19:PRO:HA	1:B:23:TRP:CZ3	2.55	0.42
1:B:51:SER:HB3	1:B:102:PRO:HG3	2.02	0.42
1:B:52:ASN:ND2	1:B:145:VAL:H	2.17	0.42
1:A:298:TYR:CD2	1:A:310:LEU:HD21	2.54	0.42
1:B:61:PRO:O	1:B:67:GLY:HA2	2.19	0.42
1:B:376:ASN:CB	1:B:377:PRO:HD2	2.36	0.42
1:A:101:TRP:CD1	1:A:146:PRO:HG2	2.55	0.42
1:A:462:ASN:C	1:A:462:ASN:ND2	2.72	0.42
1:B:173:LYS:CG	1:B:174:VAL:N	2.82	0.42
1:B:200:TYR:C	1:B:227:PRO:HG3	2.41	0.41
1:B:217:ALA:C	1:B:218:TYR:HD1	2.23	0.41
1:B:14:SER:HB2	1:B:17:GLU:HG3	2.02	0.41
1:B:238:HIS:O	1:B:242:VAL:HG23	2.20	0.41
1:A:63:ARG:NH1	2:A:2038:HOH:O	2.53	0.41
1:A:96:ARG:NH1	1:A:406:GLU:HG3	2.35	0.41
1:B:263:MET:CE	2:B:2065:HOH:O	2.66	0.41
1:B:314:LYS:HG3	1:B:317:GLN:OE1	2.20	0.41
1:B:486:ARG:H	1:B:486:ARG:HG2	1.55	0.41
1:B:60:HIS:NE2	1:B:218:TYR:HE1	2.18	0.41
1:B:76:SER:O	1:B:121:TYR:OH	2.34	0.41
1:B:103:ARG:O	1:B:104:ILE:HD13	2.20	0.41
1:B:179:PHE:C	1:B:181:ASP:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HA	1:A:257:GLY:O	2.21	0.41
1:A:335:SER:O	1:A:336:ARG:NH1	2.53	0.41
1:B:80:TYR:HD1	1:B:80:TYR:H	1.67	0.41
1:A:193:GLN:HB3	1:A:261:ASP:OD2	2.21	0.41
1:A:154:GLY:O	1:A:155:GLY:C	2.59	0.41
1:A:217:ALA:O	1:A:219:PRO:HD3	2.20	0.41
1:A:296:GLY:O	1:A:318:LYS:HG2	2.21	0.41
1:A:334:THR:OG1	1:A:335:SER:N	2.54	0.41
1:A:335:SER:O	1:A:336:ARG:HG2	2.21	0.41
1:A:458:SER:O	1:A:474:GLY:HA2	2.21	0.41
1:B:123:ARG:HD2	1:B:123:ARG:HA	1.91	0.41
1:B:170:TYR:HD1	1:B:173:LYS:HZ3	1.64	0.41
1:B:483:ASN:O	1:B:484:CYS:HB2	2.21	0.41
1:A:129:LEU:HD23	1:A:134:ILE:HD12	2.03	0.41
1:A:224:LEU:HD13	1:A:350:VAL:O	2.21	0.41
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.82	0.41
1:B:263:MET:HE2	2:B:2028:HOH:O	2.21	0.41
1:A:238:HIS:CE1	1:A:242:VAL:HG21	2.55	0.40
1:B:165:VAL:O	1:B:165:VAL:HG12	2.21	0.40
1:B:459:LEU:O	1:B:476:VAL:HB	2.22	0.40
1:B:500:THR:O	1:B:501:ALA:C	2.58	0.40
1:B:475:ILE:O	1:B:492:ALA:HB2	2.22	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.95	0.40
1:B:153:TYR:CD1	1:B:153:TYR:N	2.69	0.40
1:B:246:ASN:HA	1:B:250:LYS:CG	2.51	0.40
1:B:474:GLY:O	1:B:489:LYS:HD2	2.22	0.40
1:A:32:ALA:HB1	1:A:459:LEU:HB2	2.03	0.40
1:A:81:LYS:HB2	2:A:2049:HOH:O	2.22	0.40
1:A:152:LYS:HD2	1:A:153:TYR:HD2	1.87	0.40
1:B:193:GLN:HA	1:B:289:PHE:HE2	1.85	0.40
1:B:441:LEU:O	1:B:445:ILE:HG13	2.22	0.40
1:B:458:SER:C	1:B:460:LEU:N	2.74	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	488/512 (95%)	430 (88%)	50 (10%)	8 (2%)	9 17
1	B	493/512 (96%)	425 (86%)	62 (13%)	6 (1%)	13 24
All	All	981/1024 (96%)	855 (87%)	112 (11%)	14 (1%)	11 20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	A	162	LYS
1	A	307	ARG
1	B	180	GLY
1	A	15	PRO
1	B	75	ASN
1	B	147	GLN
1	A	13	LEU
1	A	161	HIS
1	A	219	PRO
1	A	65	LEU
1	B	68	SER
1	B	104	ILE
1	B	106	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	423/441 (96%)	405 (96%)	18 (4%)	29 53
1	B	427/441 (97%)	401 (94%)	26 (6%)	18 36
All	All	850/882 (96%)	806 (95%)	44 (5%)	23 44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	52	ASN
1	A	70	SER
1	A	75	ASN
1	A	86	LEU
1	A	98	SER
1	A	111	GLU
1	A	152	LYS
1	A	204	VAL
1	A	328	LEU
1	A	330	LEU
1	A	366	ASP
1	A	386	LEU
1	A	419	LEU
1	A	451	VAL
1	A	458	SER
1	A	459	LEU
1	A	462	ASN
1	B	52	ASN
1	B	75	ASN
1	B	86	LEU
1	B	109	THR
1	B	119	ILE
1	B	144	ASP
1	B	153	TYR
1	B	156	PHE
1	B	162	LYS
1	B	167	ASP
1	B	173	LYS
1	B	181	ASP
1	B	251	ARG
1	B	258	LEU
1	B	285	ASN
1	B	326	ASN
1	B	328	LEU
1	B	330	LEU
1	B	386	LEU
1	B	419	LEU
1	B	422	GLU
1	B	451	VAL
1	B	458	SER
1	B	459	LEU
1	B	462	ASN

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Mol	Chain	Res	Type
1	B	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	75	ASN
1	A	124	ASN
1	A	132	ASN
1	A	246	ASN
1	A	276	GLN
1	A	435	GLN
1	A	450	ASN
1	A	452	GLN
1	A	462	ASN
1	A	481	ASN
1	A	482	ASN
1	A	499	ASN
1	B	52	ASN
1	B	75	ASN
1	B	78	HIS
1	B	115	ASN
1	B	127	ASN
1	B	190	ASN
1	B	193	GLN
1	B	232	HIS
1	B	248	HIS
1	B	276	GLN
1	B	450	ASN
1	B	452	GLN
1	B	462	ASN
1	B	481	ASN
1	B	482	ASN
1	B	499	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 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

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	490/512 (95%)	0.30	26 (5%)	26	28	7, 45, 75, 94	1 (0%)
1	B	495/512 (96%)	0.54	48 (9%)	7	7	8, 52, 86, 99	1 (0%)
All	All	985/1024 (96%)	0.42	74 (7%)	14	14	7, 48, 83, 99	2 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	SER	7.8
1	B	141	PHE	4.3
1	B	458	SER	4.3
1	A	457	TRP	3.8
1	A	459	LEU	3.7
1	B	153	TYR	3.5
1	A	97	PHE	3.5
1	B	148	ALA	3.5
1	B	316	GLU	3.4
1	A	213	GLY	3.4
1	B	98	SER	3.4
1	B	35	SER	3.3
1	B	99	ILE	3.2
1	B	113	GLY	3.2
1	B	142	HIS	3.1
1	B	109	THR	3.1
1	A	35	SER	3.0
1	A	211	SER	2.9
1	B	112	GLY	2.8
1	B	164	ILE	2.8
1	B	49	GLY	2.8
1	A	32	ALA	2.8
1	A	34	THR	2.7
1	B	47	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.6
1	A	33	ALA	2.6
1	A	370	ILE	2.5
1	B	500	THR	2.5
1	B	59	ASN	2.5
1	B	406	GLU	2.5
1	A	366	ASP	2.5
1	B	140	ILE	2.5
1	B	111	GLU	2.5
1	B	60	HIS	2.4
1	A	367	GLY	2.4
1	A	12	MET	2.4
1	A	364	GLY	2.4
1	B	144	ASP	2.4
1	B	416	GLU	2.4
1	B	241	ALA	2.4
1	A	142	HIS	2.4
1	B	182	LYS	2.4
1	A	16	SER	2.4
1	B	189	PHE	2.3
1	B	139	THR	2.3
1	B	190	ASN	2.3
1	A	316	GLU	2.3
1	A	405	THR	2.3
1	B	132	ASN	2.3
1	B	171	PHE	2.3
1	B	259	ALA	2.3
1	B	168	TYR	2.3
1	B	216	CYS	2.3
1	B	48	LYS	2.2
1	A	216	CYS	2.2
1	B	108	GLY	2.2
1	B	175	CYS	2.2
1	B	256	ILE	2.2
1	B	61	PRO	2.2
1	A	424	ALA	2.2
1	A	365	PRO	2.2
1	A	138	VAL	2.1
1	B	143	TRP	2.1
1	B	248	HIS	2.1
1	B	253	ASP	2.1
1	B	457	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	455	PHE	2.1
1	B	131	GLU	2.1
1	A	347	TYR	2.0
1	B	97	PHE	2.0
1	B	188	THR	2.0
1	B	187	LEU	2.0
1	B	100	SER	2.0
1	B	249	TYR	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.