Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2022 – 10:08 PM JST

PDB ID	:	7VMA
Title	:	The X-ray crystallographic structure of amylo-alpha-1,6-glucosidase from Thermococcus gammatolerans STB12
Authors	:	Li, Z.F.; Ban, X.F.; Wang, Y.M.; Li, C.M.; Gu, Z.B.
Deposited on	:	2021-10-08
Resolution	:	2.80 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:

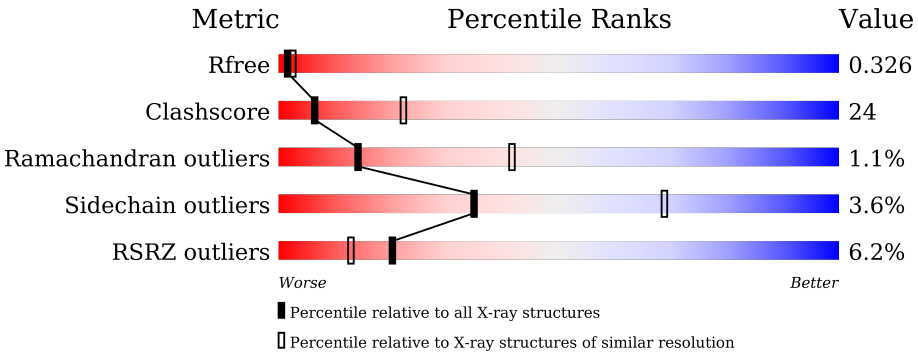
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	620	8% 54% 43% .
1	B	620	5% 60% 39% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9718 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 Amylo-alpha-1,6-glucosidase, putative archaeal type glycogen debranching enzyme (Gde).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4852	3116	831	895	10			
1	B	620	Total	C	N	O	S	0	0	0
			4852	3116	831	895	10			

- Molecule 2 is water.

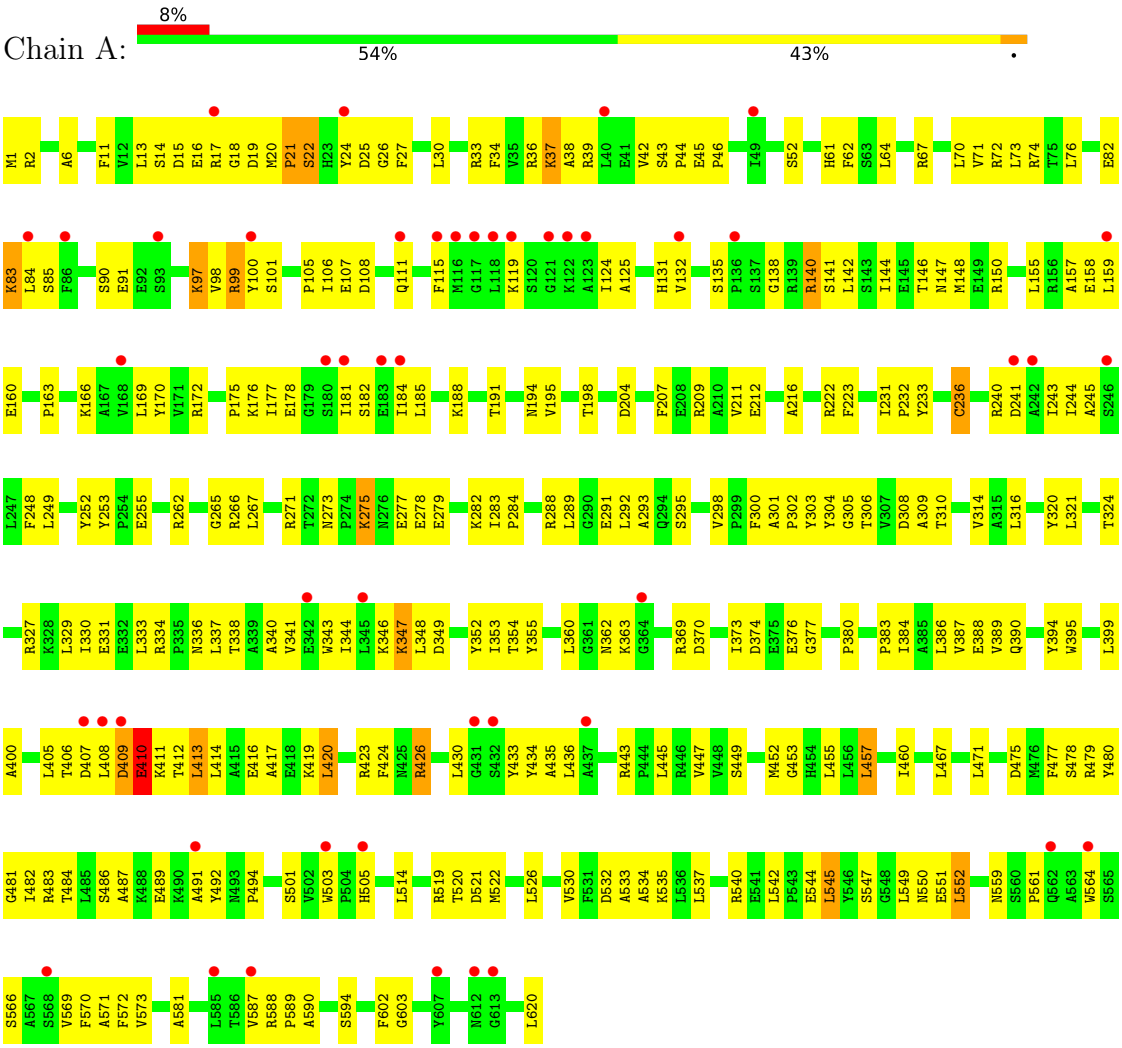
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	4	Total	O	0	0
			4	4		

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.

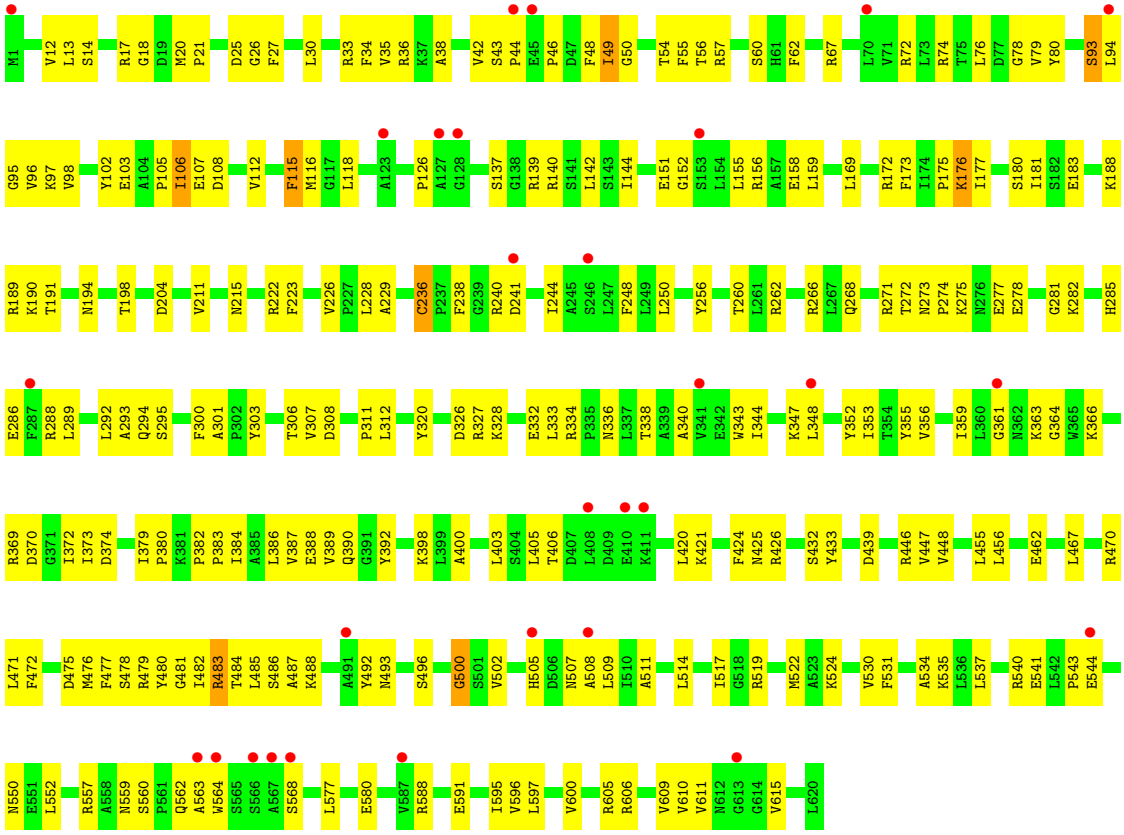
• Molecule 1: Amylo-alpha-1,6-glucosidase, putative archaeal type glycogen debranching enzyme (Gde)

Chain A:



• Molecule 1: Amylo-alpha-1,6-glucosidase, putative archaeal type glycogen debranching enzyme (Gde)

Chain B:


M1 V12 L13 S14 R17 G18 D19 M20 P21 D25 G26 F27 L30 R33 F34 V35 R36 K37 A38 V42 S43 P44 E45 P46 D47 F48 I49 G50 T54 F55 T56 R57 S60 H61 F62 R67 L70 V71 R72 L73 R74 T75 L76 D77 G78 V79 Y80 S93 L94
G95 V96 K97 V98 Y102 E103 A104 P105 I106 E107 D108 V112 F115 M116 G117 L118 A123 P126 A127 G128 S137 G138 R139 R140 S141 L142 S143 I144 E151 G152 S153 L154 L155 R156 A157 E158 L159 L169 R172 F173 I174 P175 K176 I177 S180 I181 S182 E183 K188
R189 K190 T191 N194 T198 D204 V211 N215 R222 F223 V226 P227 L228 A229 C236 P237 F238 G239 R240 D241 I244 A245 S246 L247 F248 L249 L250 Y256 T260 L261 R262 R266 L267 Q268 R271 T272 N273 P274 K275 N276 E277 E278 G281 K282 H285
E286 F287 R288 L289 L292 A293 Q294 S295 F300 A301 P302 Y303 T306 V307 D308 P311 L312 Y320 D326 R327 K328 E332 L333 R334 P335 N336 L337 T338 A339 A340 V341 E342 W343 I344 K347 L348 Y352 I353 T354 Y355 V356 I359 L360 G361 N362 K363 G364 W365 K366
R369 D370 G371 I372 I373 D374 I379 P380 K381 P382 P383 I384 A385 L386 V387 E388 V389 Q390 G391 Y392 K398 L399 A400 L403 S404 L405 T406 D407 L408 D409 E410 K411 L420 K421 F424 N425 R426 S432 Y433 D439 R446 V447 V448 L455 L456 E462 L467 R470
L471 F472 D475 M476 F477 S478 R479 Y480 G481 I482 R483 T484 L485 S486 A487 K488 A491 Y492 N493 S496 G500 S501 V502 H505 D506 N507 A508 L509 I510 A511 L514 I517 G518 R519 M522 A523 K524 V530 F531 A534 K535 L536 L537 R540 E541 L542 P543 E544
N550 E551 L552 R557 A558 N559 S560 P561 Q562 A563 W564 S565 S566 A567 S568 L577 E580 V587 R588 E591 I595 V596 L597 V600 R605 R606 V609 V610 V611 N612 G613 G614 V615 L620

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	108.09Å 108.09Å 225.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.80 38.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.00-2.80) 99.9 (38.99-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.244 , 0.328 0.247 , 0.326	Depositor DCC
R_{free} test set	1563 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9718	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8849e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.53	1/4967 (0.0%)	0.75	5/6727 (0.1%)
1	B	0.50	0/4967	0.67	0/6727
All	All	0.51	1/9934 (0.0%)	0.71	5/13454 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLU	CG-CD	5.47	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	LYS	CD-CE-NZ	-6.46	96.85	111.70
1	A	42	VAL	C-N-CA	-6.05	106.57	121.70
1	A	552	LEU	CA-CB-CG	-5.84	101.87	115.30
1	A	426	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	413	LEU	CA-CB-CG	5.25	127.37	115.30

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	4852	0	4874	272	2
1	B	4852	0	4873	197	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	4	0
2	B	4	0	0	4	0
All	All	9718	0	9747	466	2

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 24.

All (466) 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:20:MET:CE	1:A:26:GLY:HA2	1.14	1.58
1:A:20:MET:CE	1:A:26:GLY:CA	1.91	1.46
1:A:20:MET:HE2	1:A:26:GLY:CA	1.44	1.42
1:A:15:ASP:OD2	1:A:19:ASP:CB	1.71	1.35
1:A:409:ASP:O	1:A:413:LEU:HD23	1.22	1.30
1:A:409:ASP:HB3	1:A:412:THR:OG1	1.19	1.30
1:A:15:ASP:CG	1:A:19:ASP:HB2	1.61	1.20
1:A:20:MET:HE3	1:A:26:GLY:HA2	1.30	1.13
1:B:34:PHE:HB3	1:B:142:LEU:HD13	1.35	1.04
1:A:20:MET:HE3	1:A:26:GLY:CA	1.78	1.03
1:A:409:ASP:O	1:A:413:LEU:CD2	2.07	1.01
1:A:15:ASP:OD1	1:A:19:ASP:N	1.94	0.99
1:A:409:ASP:CB	1:A:412:THR:OG1	2.11	0.97
1:A:241:ASP:CG	1:A:564:TRP:CZ3	2.39	0.97
1:A:241:ASP:OD2	1:A:564:TRP:HZ3	1.47	0.95
1:A:400:ALA:HA	1:A:405:LEU:CD1	1.96	0.95
1:A:15:ASP:OD2	1:A:19:ASP:HB2	0.76	0.94
1:A:20:MET:CE	1:A:26:GLY:C	2.34	0.94
1:B:277:GLU:OE1	1:B:363:LYS:NZ	2.02	0.92
1:A:231:ILE:HG22	1:A:232:PRO:HD3	1.52	0.91
1:A:241:ASP:OD1	1:A:564:TRP:CZ3	2.23	0.91
1:A:241:ASP:CG	1:A:564:TRP:HZ3	1.75	0.90
1:A:400:ALA:HA	1:A:405:LEU:HD13	1.55	0.89
1:A:409:ASP:HB3	1:A:412:THR:CB	2.00	0.88
1:B:30:LEU:HD22	1:B:289:LEU:HD12	1.55	0.87
1:B:190:LYS:HD2	1:B:191:THR:H	1.40	0.87
1:B:505:HIS:HB3	1:B:564:TRP:HD1	1.40	0.86
1:A:13:LEU:CD2	1:A:25:ASP:OD1	2.25	0.84
1:A:150:ARG:HB3	1:A:155:LEU:HD23	1.59	0.83
1:A:38:ALA:O	2:A:701:HOH:O	1.97	0.83
1:A:74:ARG:HG2	1:A:82:GLU:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HD11	1:B:294:GLN:HG3	1.60	0.82
1:A:241:ASP:OD2	1:A:564:TRP:CZ3	2.31	0.82
1:A:36:ARG:HE	1:A:105:PRO:HG3	1.42	0.81
1:A:34:PHE:HZ	1:A:177:ILE:HD11	1.45	0.81
1:A:13:LEU:HD23	1:A:25:ASP:OD1	1.81	0.81
1:A:223:PHE:HB3	1:A:262:ARG:HB3	1.62	0.80
1:A:14:SER:OG	1:A:15:ASP:O	2.00	0.80
1:B:190:LYS:HD2	1:B:191:THR:N	1.97	0.80
1:A:293:ALA:HB1	1:A:301:ALA:HB2	1.65	0.79
1:B:229:ALA:O	1:B:562:GLN:NE2	2.16	0.78
1:A:170:TYR:OH	1:B:275:LYS:HD2	1.84	0.77
1:B:479:ARG:N	1:B:550:ASN:OD1	2.17	0.77
1:B:447:VAL:HG12	1:B:485:LEU:HD11	1.68	0.76
1:A:400:ALA:HA	1:A:405:LEU:HD12	1.68	0.76
1:A:34:PHE:CZ	1:A:177:ILE:HD11	2.22	0.75
1:A:62:PHE:HB2	1:A:70:LEU:HB3	1.67	0.75
1:A:241:ASP:CG	1:A:564:TRP:CE3	2.59	0.75
1:B:27:PHE:CZ	1:B:175:PRO:HG3	2.22	0.74
1:A:19:ASP:C	1:A:21:PRO:HD2	2.08	0.74
1:B:353:ILE:HD11	1:B:389:VAL:HG12	1.70	0.74
1:A:559:ASN:ND2	2:A:702:HOH:O	2.01	0.73
1:A:20:MET:HE1	1:A:26:GLY:C	2.09	0.73
1:B:17:ARG:HH22	1:B:46:PRO:HG2	1.53	0.73
1:B:596:VAL:HG22	1:B:610:VAL:HG13	1.71	0.72
1:A:142:LEU:HD12	1:A:144:ILE:HD11	1.72	0.71
1:B:42:VAL:HG22	1:B:98:VAL:HG23	1.72	0.71
1:A:265:GLY:O	1:A:336:ASN:ND2	2.24	0.71
1:B:334:ARG:O	1:B:338:THR:HG23	1.89	0.71
1:B:541:GLU:OE1	1:B:560:SER:OG	2.09	0.71
1:B:266:ARG:NH2	2:B:701:HOH:O	2.23	0.71
1:B:543:PRO:HB3	1:B:560:SER:HB2	1.70	0.71
1:A:73:LEU:HB3	1:A:83:LYS:HE3	1.73	0.71
1:B:140:ARG:HG2	1:B:177:ILE:HG12	1.71	0.71
1:B:505:HIS:HB3	1:B:564:TRP:CD1	2.26	0.70
1:A:20:MET:HE3	1:A:26:GLY:N	2.05	0.70
1:B:332:GLU:OE1	2:B:701:HOH:O	2.09	0.70
1:B:356:VAL:HG12	1:B:382:PRO:HB2	1.74	0.69
1:B:190:LYS:NZ	1:B:191:THR:OG1	2.19	0.69
1:A:20:MET:N	1:A:21:PRO:CD	2.55	0.69
1:A:241:ASP:OD1	1:A:564:TRP:CE3	2.44	0.69
1:A:306:THR:HA	1:A:363:LYS:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:N	1:A:157:ALA:O	2.23	0.69
1:A:334:ARG:O	1:A:338:THR:HG23	1.93	0.68
1:B:355:TYR:HE2	1:B:386:LEU:HG	1.58	0.68
1:A:91:GLU:HA	1:A:163:PRO:HB3	1.74	0.67
1:B:34:PHE:CB	1:B:142:LEU:HD13	2.18	0.67
1:B:34:PHE:HZ	1:B:177:ILE:HD11	1.59	0.67
1:A:532:ASP:HA	1:A:535:LYS:HE3	1.77	0.67
1:A:347:LYS:HE3	1:A:353:ILE:HG23	1.76	0.66
1:A:30:LEU:HD22	1:A:289:LEU:HD12	1.78	0.66
1:A:240:ARG:HG3	1:A:244:ILE:HD12	1.78	0.66
1:A:374:ASP:OD1	1:A:376:GLU:N	2.26	0.66
1:B:605:ARG:HG2	1:B:606:ARG:H	1.61	0.65
1:A:341:VAL:HG21	1:A:406:THR:HG21	1.79	0.65
1:B:373:ILE:HD12	1:B:373:ILE:C	2.16	0.65
1:A:386:LEU:HB2	1:A:389:VAL:HG12	1.79	0.65
1:B:307:VAL:HG23	1:B:389:VAL:HG11	1.78	0.65
1:A:39:ARG:HB3	1:A:101:SER:OG	1.97	0.65
1:A:482:ILE:HG13	1:A:526:LEU:HD11	1.79	0.64
1:A:67:ARG:HG2	1:A:90:SER:HB3	1.77	0.64
1:A:275:LYS:N	1:A:275:LYS:HD3	2.13	0.63
1:A:387:VAL:HG22	1:A:455:LEU:HD11	1.81	0.63
1:A:191:THR:HG22	2:A:707:HOH:O	1.98	0.63
1:A:17:ARG:O	1:A:72:ARG:NH1	2.32	0.62
1:A:124:ILE:HG23	1:A:131:HIS:ND1	2.14	0.62
1:B:476:MET:HE3	1:B:486:SER:HB2	1.81	0.62
1:A:20:MET:HE2	1:A:26:GLY:HA2	0.62	0.62
1:A:71:VAL:HG12	1:A:85:SER:HB2	1.81	0.61
1:A:6:ALA:HB3	1:A:216:ALA:HB1	1.82	0.61
1:B:244:ILE:HD13	1:B:509:LEU:HD11	1.82	0.61
1:B:105:PRO:O	1:B:107:GLU:N	2.32	0.61
1:A:146:THR:HG21	1:A:155:LEU:HD22	1.82	0.61
1:B:478:SER:HB3	1:B:483:ARG:HE	1.65	0.61
1:B:159:LEU:HD21	1:B:169:LEU:HD11	1.82	0.61
1:A:354:THR:OG1	1:A:383:PRO:HB2	2.01	0.61
1:A:252:TYR:OH	1:A:573:VAL:HG13	2.01	0.61
1:B:478:SER:HB3	1:B:483:ARG:NE	2.16	0.61
1:A:380:PRO:HG2	1:A:384:ILE:HD11	1.82	0.60
1:B:605:ARG:HG2	1:B:606:ARG:N	2.16	0.60
1:A:284:PRO:HB3	1:A:302:PRO:HB2	1.82	0.60
1:A:17:ARG:HB2	1:A:19:ASP:OD2	2.01	0.60
1:A:331:GLU:HG2	1:A:334:ARG:HE	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLU:HG3	1:B:588:ARG:HH21	1.66	0.60
1:B:591:GLU:CD	1:B:591:GLU:H	2.05	0.60
1:B:20:MET:SD	1:B:26:GLY:HA2	2.41	0.60
1:A:321:LEU:HD11	1:A:327:ARG:HG2	1.84	0.60
1:B:373:ILE:HD12	1:B:373:ILE:O	2.02	0.60
1:B:241:ASP:OD2	1:B:564:TRP:CZ3	2.55	0.59
1:A:334:ARG:HA	1:A:337:LEU:HB2	1.83	0.59
1:A:303:TYR:CE2	1:A:305:GLY:HA3	2.37	0.59
1:B:54:THR:HG22	1:B:55:PHE:H	1.68	0.59
1:B:228:LEU:O	1:B:563:ALA:HB2	2.02	0.59
1:B:241:ASP:HB3	1:B:564:TRP:CE3	2.36	0.59
1:B:400:ALA:HA	1:B:405:LEU:HD12	1.83	0.59
1:A:100:TYR:HD2	1:A:155:LEU:HD12	1.68	0.59
1:A:380:PRO:HG3	1:A:445:LEU:HD11	1.85	0.59
1:A:198:THR:HG22	1:A:204:ASP:OD1	2.02	0.58
1:B:17:ARG:HB2	1:B:62:PHE:HZ	1.67	0.58
1:A:587:VAL:HG12	1:A:589:PRO:HD3	1.85	0.58
1:B:27:PHE:HZ	1:B:175:PRO:HG3	1.65	0.58
1:A:300:PHE:HA	1:A:303:TYR:HB2	1.84	0.58
1:A:15:ASP:CG	1:A:19:ASP:CB	2.48	0.58
1:B:17:ARG:NH2	1:B:46:PRO:HG2	2.19	0.58
1:B:256:TYR:O	1:B:260:THR:HG23	2.04	0.58
1:A:20:MET:N	1:A:21:PRO:HD2	2.19	0.57
1:A:148:MET:HB2	1:A:155:LEU:HB3	1.85	0.57
1:B:13:LEU:HB3	1:B:25:ASP:HA	1.85	0.57
1:B:470:ARG:NH2	1:B:475:ASP:OD2	2.24	0.57
1:A:36:ARG:NE	1:A:105:PRO:HG3	2.17	0.57
1:A:535:LYS:NZ	2:A:703:HOH:O	2.38	0.57
1:B:79:VAL:HG21	1:B:172:ARG:NH2	2.19	0.57
1:B:241:ASP:HB3	1:B:564:TRP:HE3	1.69	0.57
1:A:142:LEU:CD1	1:A:144:ILE:HD11	2.34	0.57
1:B:223:PHE:HB3	1:B:262:ARG:HB3	1.87	0.57
1:B:476:MET:HG2	1:B:482:ILE:HG23	1.87	0.57
1:B:514:LEU:HD22	1:B:522:MET:HE3	1.86	0.57
1:B:347:LYS:HB2	1:B:353:ILE:HG22	1.85	0.57
1:A:338:THR:HG22	1:A:407:ASP:H	1.70	0.57
1:A:521:ASP:N	1:A:521:ASP:OD1	2.37	0.57
1:A:282:LYS:HD3	1:A:304:TYR:HB3	1.87	0.57
1:B:493:ASN:HB3	1:B:496:SER:HB3	1.87	0.57
1:B:12:VAL:HG23	1:B:76:LEU:HD22	1.87	0.56
1:B:379:ILE:HD12	1:B:380:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:SER:OG	1:A:481:GLY:O	2.24	0.56
1:B:20:MET:HG3	1:B:38:ALA:HB3	1.87	0.56
1:A:266:ARG:HD3	1:A:267:LEU:HD12	1.87	0.56
1:B:240:ARG:NH1	1:B:306:THR:OG1	2.39	0.56
1:A:447:VAL:HG12	1:A:489:GLU:OE2	2.06	0.55
1:B:359:ILE:HD12	1:B:359:ILE:H	1.71	0.55
1:A:147:ASN:HD21	1:A:169:LEU:HA	1.72	0.55
1:A:505:HIS:CG	1:A:564:TRP:CD1	2.95	0.55
1:A:172:ARG:NH2	1:B:272:THR:O	2.39	0.55
1:A:395:TRP:CH2	1:A:457:LEU:HD21	2.41	0.55
1:A:13:LEU:HD22	1:A:25:ASP:OD1	2.03	0.55
1:B:102:TYR:OH	1:B:144:ILE:HG13	2.07	0.55
1:B:115:PHE:CD1	1:B:116:MET:HG2	2.41	0.55
1:A:409:ASP:HB3	1:A:412:THR:HG1	1.59	0.55
1:A:343:TRP:CH2	1:A:347:LYS:HD3	2.41	0.55
1:B:340:ALA:O	1:B:344:ILE:HG13	2.05	0.55
1:B:597:LEU:HB2	1:B:609:VAL:CG1	2.37	0.55
1:A:36:ARG:HE	1:A:105:PRO:CG	2.14	0.55
1:A:519:ARG:HB3	1:A:522:MET:HE2	1.90	0.54
1:B:176:LYS:O	1:B:177:ILE:HG13	2.07	0.54
1:B:370:ASP:OD1	1:B:370:ASP:N	2.39	0.54
1:A:373:ILE:HD13	1:A:491:ALA:HB3	1.89	0.54
1:B:446:ARG:HH11	1:B:446:ARG:HG2	1.72	0.54
1:A:537:LEU:HD21	1:A:552:LEU:HD21	1.90	0.54
1:B:17:ARG:HB2	1:B:62:PHE:CZ	2.42	0.54
1:B:597:LEU:HB2	1:B:609:VAL:HG12	1.90	0.54
1:B:273:ASN:HB3	1:B:278:GLU:HB3	1.90	0.54
1:A:18:GLY:HA2	1:A:74:ARG:NH1	2.22	0.53
1:B:348:LEU:HD21	1:B:420:LEU:HD13	1.90	0.53
1:A:46:PRO:HB3	1:A:64:LEU:HD11	1.89	0.53
1:B:108:ASP:HB2	1:B:292:LEU:HD13	1.89	0.53
1:A:314:VAL:HG23	1:A:337:LEU:HD22	1.90	0.53
1:A:140:ARG:HD2	1:A:177:ILE:HG23	1.90	0.53
1:A:252:TYR:CE2	1:A:570:PHE:HB3	2.43	0.53
1:B:328:LYS:NZ	1:B:332:GLU:OE2	2.32	0.53
1:B:432:SER:HB3	1:B:433:TYR:HD1	1.73	0.53
1:A:194:ASN:HA	1:A:211:VAL:HG21	1.89	0.53
1:B:386:LEU:HB3	1:B:388:GLU:OE2	2.09	0.53
1:B:537:LEU:HG	1:B:552:LEU:HD21	1.91	0.53
1:A:20:MET:CE	1:A:27:PHE:N	2.72	0.53
1:B:229:ALA:HB2	1:B:238:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:MET:HE3	1:B:486:SER:CB	2.39	0.53
1:B:487:ALA:HA	1:B:492:TYR:CG	2.44	0.52
1:B:190:LYS:CD	1:B:191:THR:H	2.16	0.52
1:B:241:ASP:OD2	1:B:564:TRP:HZ3	1.92	0.52
1:B:386:LEU:O	1:B:390:GLN:HG2	2.09	0.52
1:B:300:PHE:HD1	1:B:303:TYR:HB2	1.74	0.52
1:A:386:LEU:O	1:A:390:GLN:HG2	2.10	0.52
1:A:20:MET:HE1	1:A:27:PHE:N	2.23	0.52
1:A:387:VAL:CG2	1:A:455:LEU:HD11	2.40	0.52
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.74	0.52
1:B:140:ARG:HG2	1:B:177:ILE:CG1	2.38	0.52
1:A:146:THR:HG21	1:A:155:LEU:CD2	2.40	0.52
1:B:33:ARG:CZ	1:B:36:ARG:HD3	2.41	0.52
1:A:380:PRO:HG2	1:A:384:ILE:CD1	2.40	0.51
1:B:531:PHE:O	1:B:535:LYS:HG3	2.09	0.51
1:A:108:ASP:HB2	1:A:292:LEU:HD13	1.91	0.51
1:B:557:ARG:HH11	1:B:557:ARG:HG2	1.76	0.51
1:A:21:PRO:O	1:A:22:SER:O	2.28	0.51
1:B:34:PHE:CZ	1:B:177:ILE:HD11	2.44	0.51
1:B:35:VAL:HG21	1:B:173:PHE:CD2	2.46	0.51
1:B:421:LYS:HG3	1:B:425:ASN:ND2	2.26	0.51
1:B:238:PHE:CE2	1:B:286:GLU:HB3	2.46	0.51
1:B:248:PHE:CD2	1:B:568:SER:HA	2.45	0.51
1:B:236:CYS:SG	1:B:288:ARG:HD3	2.51	0.51
1:A:308:ASP:OD1	1:A:309:ALA:N	2.44	0.51
1:B:268:GLN:OE1	1:B:336:ASN:HB3	2.11	0.51
1:B:600:VAL:O	1:B:606:ARG:HA	2.11	0.50
1:A:72:ARG:HH21	1:A:82:GLU:CD	2.15	0.50
1:B:56:THR:O	1:B:57:ARG:HG3	2.10	0.50
1:A:520:THR:HB	1:A:590:ALA:HB2	1.93	0.50
1:A:232:PRO:HD2	1:A:559:ASN:HB3	1.93	0.50
1:B:43:SER:HA	1:B:44:PRO:C	2.32	0.50
1:A:248:PHE:CG	1:A:571:ALA:HB2	2.46	0.50
1:A:449:SER:O	1:A:452:MET:HG2	2.12	0.50
1:A:505:HIS:HB3	1:A:564:TRP:HD1	1.75	0.50
1:B:471:LEU:HB3	1:B:482:ILE:HD13	1.94	0.50
1:A:1:MET:HG3	1:A:2:ARG:N	2.25	0.50
1:B:106:ILE:HD12	1:B:106:ILE:H	1.77	0.50
1:B:142:LEU:HD23	1:B:144:ILE:HD11	1.94	0.50
1:B:338:THR:HG22	1:B:406:THR:OG1	2.12	0.50
1:A:399:LEU:O	1:A:405:LEU:CD1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:HIS:HB3	1:A:564:TRP:CD1	2.47	0.49
1:B:188:LYS:NZ	2:B:702:HOH:O	2.42	0.49
1:A:99:ARG:HA	1:A:155:LEU:O	2.11	0.49
1:A:243:ILE:HG23	1:A:316:LEU:HD22	1.93	0.49
1:B:544:GLU:HG3	1:B:564:TRP:HZ2	1.77	0.49
1:B:271:ARG:NH1	1:B:278:GLU:OE1	2.43	0.49
1:B:352:TYR:HB3	1:B:390:GLN:OE1	2.13	0.49
1:A:279:GLU:HB2	1:A:343:TRP:HE1	1.77	0.49
1:A:341:VAL:CG2	1:A:406:THR:HG21	2.43	0.49
1:B:115:PHE:O	1:B:118:LEU:HG	2.13	0.49
1:A:142:LEU:C	1:A:142:LEU:HD13	2.33	0.49
1:A:172:ARG:HD2	1:B:274:PRO:HD2	1.95	0.49
1:A:282:LYS:HG3	1:A:343:TRP:CZ2	2.48	0.49
1:A:105:PRO:C	1:A:107:GLU:H	2.14	0.49
1:A:194:ASN:OD1	1:A:195:VAL:N	2.46	0.49
1:B:282:LYS:HG3	1:B:343:TRP:CE2	2.48	0.49
1:A:343:TRP:CZ2	1:A:347:LYS:HD3	2.48	0.49
1:B:366:LYS:HB2	1:B:372:ILE:HD11	1.95	0.48
1:B:343:TRP:CZ2	1:B:347:LYS:HD2	2.48	0.48
1:A:33:ARG:HD2	1:A:36:ARG:HB3	1.95	0.48
1:A:399:LEU:O	1:A:405:LEU:HD12	2.13	0.48
1:B:14:SER:OG	1:B:74:ARG:NH2	2.46	0.48
1:A:370:ASP:OD1	1:A:370:ASP:N	2.44	0.48
1:B:384:ILE:HD13	1:B:439:ASP:HA	1.96	0.48
1:B:534:ALA:O	1:B:540:ARG:HA	2.14	0.48
1:B:611:VAL:HG22	1:B:615:VAL:HG12	1.95	0.48
1:B:190:LYS:CD	1:B:191:THR:N	2.72	0.48
1:A:62:PHE:HD2	1:A:70:LEU:HG	1.79	0.48
1:A:240:ARG:NH1	1:A:306:THR:OG1	2.46	0.48
1:A:303:TYR:CZ	1:A:305:GLY:HA3	2.49	0.48
1:A:327:ARG:HA	1:A:330:ILE:HG13	1.96	0.48
1:A:21:PRO:O	1:A:22:SER:C	2.53	0.48
1:B:54:THR:HG22	1:B:55:PHE:N	2.28	0.48
1:A:231:ILE:HG21	1:A:561:PRO:HD2	1.95	0.48
1:A:581:ALA:HB1	1:A:602:PHE:HE1	1.79	0.48
1:B:95:GLY:HA2	1:B:159:LEU:O	2.14	0.48
1:B:559:ASN:HB2	1:B:562:GLN:OE1	2.14	0.48
1:A:480:TYR:HB3	1:A:533:ALA:HB2	1.95	0.47
1:B:44:PRO:HD2	1:B:96:VAL:HG23	1.95	0.47
1:A:61:HIS:ND1	1:A:71:VAL:HG23	2.30	0.47
1:A:338:THR:CG2	1:A:407:ASP:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:TYR:HD2	1:A:434:TYR:O	1.97	0.47
1:A:19:ASP:HB3	1:A:21:PRO:HD3	1.95	0.47
1:B:126:PRO:HG3	1:B:152:GLY:O	2.14	0.47
1:A:97:LYS:HB3	1:A:158:GLU:HB3	1.97	0.47
1:A:514:LEU:HD22	1:A:522:MET:HE3	1.97	0.47
1:A:105:PRO:O	1:A:107:GLU:N	2.42	0.47
1:A:207:PHE:CE1	1:A:569:VAL:HG12	2.49	0.47
1:A:305:GLY:O	1:A:363:LYS:HG2	2.14	0.47
1:A:374:ASP:OD1	1:A:377:GLY:N	2.47	0.47
1:A:503:TRP:HZ3	1:A:564:TRP:HZ2	1.62	0.47
1:B:387:VAL:CG2	1:B:455:LEU:HD11	2.45	0.47
1:B:472:PHE:HA	1:B:477:PHE:HB2	1.96	0.47
1:A:124:ILE:HD11	1:A:132:VAL:O	2.14	0.47
1:B:49:ILE:HG22	1:B:50:GLY:N	2.29	0.47
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.77	0.47
1:A:39:ARG:N	1:A:101:SER:O	2.42	0.47
1:A:492:TYR:CZ	1:A:494:PRO:HD3	2.50	0.47
1:A:232:PRO:HD2	1:A:559:ASN:CB	2.45	0.46
1:A:331:GLU:OE2	1:A:334:ARG:NE	2.48	0.46
1:B:483:ARG:HG3	1:B:502:VAL:CG2	2.45	0.46
1:A:24:TYR:CZ	1:A:233:TYR:HE1	2.32	0.46
1:A:233:TYR:H	1:A:559:ASN:ND2	2.12	0.46
1:B:478:SER:OG	1:B:481:GLY:O	2.26	0.46
1:A:13:LEU:HD23	1:A:25:ASP:CG	2.36	0.46
1:A:231:ILE:CG2	1:A:232:PRO:HD3	2.35	0.46
1:A:331:GLU:OE2	1:A:334:ARG:CZ	2.63	0.46
1:A:337:LEU:HD13	1:A:405:LEU:HB3	1.98	0.46
1:B:190:LYS:HZ2	1:B:191:THR:HG1	1.56	0.46
1:A:14:SER:HA	1:A:19:ASP:O	2.15	0.46
1:A:340:ALA:O	1:A:344:ILE:HG13	2.14	0.46
1:B:12:VAL:HG21	1:B:80:TYR:CE1	2.51	0.46
1:A:13:LEU:HD22	1:A:24:TYR:O	2.16	0.46
1:A:273:ASN:ND2	1:A:275:LYS:HG2	2.30	0.46
1:B:97:LYS:HD3	1:B:158:GLU:HG2	1.96	0.46
1:B:300:PHE:CD1	1:B:303:TYR:HB2	2.50	0.46
1:A:73:LEU:HD23	1:A:83:LYS:HE3	1.97	0.46
1:B:36:ARG:NE	1:B:105:PRO:HG3	2.30	0.46
1:B:356:VAL:HG12	1:B:383:PRO:HA	1.97	0.46
1:A:487:ALA:HA	1:A:492:TYR:CG	2.52	0.46
1:B:380:PRO:HB2	1:B:384:ILE:HD11	1.97	0.46
1:A:20:MET:O	1:A:37:LYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:C	1:A:21:PRO:CD	2.81	0.45
1:A:400:ALA:CA	1:A:405:LEU:CD1	2.83	0.45
1:A:420:LEU:O	1:A:424:PHE:N	2.47	0.45
1:B:17:ARG:HA	1:B:60:SER:OG	2.15	0.45
1:B:194:ASN:HB2	1:B:211:VAL:HG21	1.97	0.45
1:B:361:GLY:HA3	1:B:369:ARG:HA	1.97	0.45
1:B:562:GLN:NE2	1:B:564:TRP:CZ3	2.84	0.45
1:A:271:ARG:HH11	1:A:271:ARG:HG2	1.81	0.45
1:A:400:ALA:CA	1:A:405:LEU:HD13	2.38	0.45
1:B:508:ALA:HA	1:B:511:ALA:HB3	1.98	0.45
1:A:426:ARG:HH21	1:A:426:ARG:HD2	1.59	0.45
1:B:108:ASP:O	1:B:112:VAL:HG23	2.17	0.45
1:A:38:ALA:HA	1:A:101:SER:O	2.16	0.45
1:A:303:TYR:HE2	1:A:360:LEU:HD12	1.81	0.45
1:A:346:LYS:O	1:A:349:ASP:HB2	2.17	0.45
1:B:190:LYS:HD2	1:B:190:LYS:HA	1.62	0.45
1:A:503:TRP:HZ3	1:A:564:TRP:CZ2	2.35	0.45
1:A:15:ASP:OD1	1:A:19:ASP:CB	2.64	0.45
1:B:475:ASP:O	1:B:483:ARG:NH1	2.49	0.45
1:A:352:TYR:OH	1:A:423:ARG:HG2	2.17	0.45
1:A:84:LEU:N	1:A:84:LEU:HD22	2.32	0.45
1:B:151:GLU:HG3	1:B:156:ARG:NH1	2.31	0.45
1:B:268:GLN:HE21	1:B:281:GLY:HA2	1.82	0.45
1:B:544:GLU:HG3	1:B:564:TRP:CZ2	2.52	0.45
1:B:194:ASN:HA	1:B:211:VAL:HG21	1.97	0.44
1:B:238:PHE:HE2	1:B:285:HIS:CE1	2.35	0.44
1:B:352:TYR:HB3	1:B:390:GLN:CD	2.37	0.44
1:B:190:LYS:HD2	2:B:704:HOH:O	2.17	0.44
1:B:456:LEU:HD22	1:B:517:ILE:HD13	1.99	0.44
1:A:430:LEU:HD12	1:A:433:TYR:CE2	2.51	0.44
1:A:475:ASP:OD2	1:A:486:SER:HB2	2.17	0.44
1:A:15:ASP:OD1	1:A:19:ASP:HB2	2.13	0.44
1:A:416:GLU:O	1:A:419:LYS:HB2	2.17	0.44
1:A:138:GLY:HA3	1:A:178:GLU:O	2.17	0.44
1:A:283:ILE:HD12	1:A:310:THR:HG23	1.98	0.44
1:A:492:TYR:CE2	1:A:494:PRO:HD3	2.53	0.44
1:A:544:GLU:HB3	1:A:545:LEU:HD23	1.99	0.44
1:B:18:GLY:HA3	1:B:72:ARG:CZ	2.47	0.44
1:B:308:ASP:O	1:B:312:LEU:HG	2.18	0.44
1:A:295:SER:O	1:A:295:SER:OG	2.34	0.44
1:A:320:TYR:CE2	1:A:324:THR:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HA	1:A:426:ARG:HE	1.82	0.43
1:A:209:ARG:HA	1:A:212:GLU:HG2	2.00	0.43
1:A:453:GLY:HA2	1:A:471:LEU:HD11	2.00	0.43
1:B:467:LEU:O	1:B:467:LEU:HD12	2.18	0.43
1:A:394:TYR:CD1	1:A:417:ALA:HB1	2.54	0.43
1:B:507:ASN:O	1:B:511:ALA:N	2.49	0.43
1:B:94:LEU:HD13	1:B:94:LEU:O	2.18	0.43
1:A:43:SER:OG	1:A:44:PRO:HA	2.19	0.43
1:A:236:CYS:SG	1:A:288:ARG:HD3	2.58	0.43
1:A:266:ARG:HH11	1:A:267:LEU:HD11	1.82	0.43
1:A:410:GLU:HB3	1:A:411:LYS:H	1.63	0.43
1:A:534:ALA:O	1:A:540:ARG:HA	2.18	0.43
1:B:352:TYR:OH	1:B:424:PHE:HA	2.19	0.43
1:A:184:ILE:O	1:A:222:ARG:N	2.44	0.43
1:A:355:TYR:CE1	1:A:362:ASN:HA	2.54	0.43
1:B:448:VAL:HG12	1:B:476:MET:CE	2.49	0.43
1:A:324:THR:O	1:A:603:GLY:HA2	2.19	0.43
1:B:36:ARG:CZ	1:B:105:PRO:HG3	2.48	0.43
1:B:470:ARG:HD2	1:B:470:ARG:HA	1.80	0.43
1:A:16:GLU:C	1:A:18:GLY:H	2.21	0.43
1:A:159:LEU:HD12	1:A:160:GLU:H	1.84	0.43
1:B:311:PRO:HB2	1:B:392:TYR:O	2.19	0.43
1:A:176:LYS:O	1:A:177:ILE:HD13	2.19	0.43
1:A:241:ASP:CG	1:A:564:TRP:HE3	2.21	0.43
1:A:475:ASP:O	1:A:483:ARG:NH1	2.52	0.43
1:A:111:GLN:HB3	1:A:119:LYS:O	2.19	0.42
1:A:479:ARG:HD3	1:A:480:TYR:CZ	2.54	0.42
1:A:486:SER:OG	1:A:489:GLU:HG2	2.19	0.42
1:A:46:PRO:HB3	1:A:64:LEU:CD1	2.48	0.42
1:A:73:LEU:CD2	1:A:83:LYS:HE3	2.49	0.42
1:A:282:LYS:HG3	1:A:343:TRP:CE2	2.54	0.42
1:B:102:TYR:HE2	1:B:155:LEU:HD11	1.84	0.42
1:B:137:SER:OG	1:B:295:SER:HB2	2.19	0.42
1:B:191:THR:HB	1:B:215:ASN:ND2	2.34	0.42
1:A:98:VAL:CG1	1:A:148:MET:HE3	2.50	0.42
1:A:248:PHE:CD1	1:A:571:ALA:HB2	2.54	0.42
1:B:480:TYR:O	1:B:530:VAL:HG12	2.19	0.42
1:A:108:ASP:CB	1:A:292:LEU:HD13	2.49	0.42
1:A:245:ALA:O	1:A:249:LEU:HG	2.19	0.42
1:B:373:ILE:CD1	1:B:374:ASP:O	2.68	0.42
1:A:147:ASN:HD21	1:A:170:TYR:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HA	1:A:414:LEU:HG	2.00	0.42
1:B:266:ARG:NH1	1:B:333:LEU:HD21	2.35	0.42
1:B:198:THR:HG22	1:B:204:ASP:OD1	2.20	0.42
1:B:484:THR:OG1	1:B:500:GLY:N	2.53	0.42
1:A:181:ILE:HD12	1:A:182:SER:N	2.35	0.42
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.47	0.42
1:A:410:GLU:O	1:A:413:LEU:N	2.53	0.42
1:A:430:LEU:HD11	1:A:435:ALA:HB2	2.01	0.42
1:A:484:THR:HG23	1:A:501:SER:O	2.20	0.42
1:A:72:ARG:NE	1:A:82:GLU:OE2	2.50	0.42
1:A:195:VAL:HG23	1:A:253:TYR:OH	2.20	0.42
1:A:452:MET:HG3	1:A:467:LEU:HD11	2.01	0.42
1:B:300:PHE:HD1	1:B:303:TYR:CB	2.33	0.42
1:B:373:ILE:C	1:B:373:ILE:CD1	2.86	0.42
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.35	0.42
1:A:530:VAL:O	1:A:533:ALA:HB3	2.20	0.42
1:B:432:SER:HB3	1:B:433:TYR:CD1	2.55	0.42
1:A:184:ILE:HG13	1:A:185:LEU:HD23	2.02	0.42
1:A:292:LEU:HB3	1:A:298:VAL:HG22	2.02	0.42
1:B:223:PHE:CE1	1:B:266:ARG:HG2	2.55	0.42
1:A:542:LEU:HD23	1:A:542:LEU:HA	1.75	0.41
1:B:355:TYR:HB2	1:B:363:LYS:HD2	2.01	0.41
1:B:373:ILE:HD13	1:B:374:ASP:O	2.19	0.41
1:A:333:LEU:O	1:A:336:ASN:HB2	2.19	0.41
1:A:147:ASN:HB3	1:A:170:TYR:CE2	2.55	0.41
1:A:321:LEU:CD1	1:A:327:ARG:HG2	2.50	0.41
1:A:420:LEU:CD2	1:A:460:ILE:HD11	2.50	0.41
1:A:142:LEU:CD1	1:A:144:ILE:CD1	2.98	0.41
1:A:416:GLU:HA	1:A:419:LYS:HB2	2.02	0.41
1:B:115:PHE:HD1	1:B:116:MET:N	2.19	0.41
1:B:293:ALA:HB1	1:B:301:ALA:HB2	2.02	0.41
1:B:425:ASN:OD1	1:B:462:GLU:HG2	2.21	0.41
1:B:36:ARG:NH1	1:B:103:GLU:OE1	2.54	0.41
1:A:97:LYS:HB3	1:A:158:GLU:CB	2.50	0.41
1:A:140:ARG:NH2	1:A:289:LEU:O	2.43	0.41
1:A:262:ARG:HG3	1:A:329:LEU:HD11	2.01	0.41
1:B:519:ARG:HD2	1:B:519:ARG:HA	1.78	0.41
1:A:188:LYS:HE2	1:A:188:LYS:HB3	1.86	0.41
1:A:6:ALA:HA	1:A:11:PHE:HA	2.01	0.41
1:A:334:ARG:O	1:A:334:ARG:HG2	2.20	0.41
1:B:12:VAL:HA	1:B:26:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLU:O	1:B:222:ARG:HG3	2.20	0.41
1:B:320:TYR:HE1	1:B:326:ASP:HB3	1.86	0.41
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.82	0.41
1:A:45:GLU:OE2	1:A:46:PRO:HD2	2.21	0.40
1:A:388:GLU:HG2	1:A:389:VAL:N	2.35	0.40
1:B:446:ARG:HG2	1:B:446:ARG:NH1	2.35	0.40
1:B:577:LEU:HD11	1:B:595:ILE:HG21	2.03	0.40
1:A:570:PHE:O	1:A:573:VAL:HG12	2.20	0.40
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.85	0.40
1:A:338:THR:HG22	1:A:406:THR:HA	2.02	0.40
1:A:387:VAL:HG12	1:A:436:LEU:O	2.21	0.40
1:A:530:VAL:HG21	1:A:572:PHE:CE2	2.56	0.40
1:A:549:LEU:HD12	1:A:550:ASN:H	1.87	0.40
1:B:306:THR:OG1	1:B:308:ASP:OD1	2.38	0.40
1:B:320:TYR:CE1	1:B:326:ASP:HB3	2.57	0.40
1:B:327:ARG:NH2	1:B:403:LEU:O	2.43	0.40
1:B:364:GLY:HA3	1:B:386:LEU:CD1	2.51	0.40
1:A:100:TYR:CD2	1:A:155:LEU:HD12	2.54	0.40
1:B:483:ARG:HG3	1:B:502:VAL:HG22	2.02	0.40
1:A:27:PHE:CZ	1:A:175:PRO:HG3	2.56	0.40
1:A:67:ARG:HG3	1:A:67:ARG:HH11	1.86	0.40
1:A:147:ASN:HB3	1:A:170:TYR:CZ	2.56	0.40
1:A:271:ARG:O	1:A:278:GLU:HG2	2.21	0.40
1:A:503:TRP:CZ3	1:A:564:TRP:HZ2	2.39	0.40
1:B:226:VAL:HG13	1:B:260:THR:HG22	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ARG:NH2	1:B:93:SER:OG[7_544]	1.87	0.33
1:A:166:LYS:NZ	1:A:551:GLU:OE1[6_555]	2.12	0.08

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	618/620 (100%)	560 (91%)	50 (8%)	8 (1%)	12	36
1	B	618/620 (100%)	573 (93%)	39 (6%)	6 (1%)	15	44
All	All	1236/1240 (100%)	1133 (92%)	89 (7%)	14 (1%)	14	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	106	ILE
1	A	125	ALA
1	A	21	PRO
1	A	22	SER
1	B	106	ILE
1	A	410	GLU
1	B	78	GLY
1	A	408	LEU
1	B	180	SER
1	A	255	GLU
1	B	500	GLY
1	B	21	PRO
1	B	49	ILE

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	507/507 (100%)	483 (95%)	24 (5%)	26	59
1	B	507/507 (100%)	495 (98%)	12 (2%)	49	81
All	All	1014/1014 (100%)	978 (96%)	36 (4%)	35	69

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	76	LEU
1	A	83	LYS
1	A	97	LYS
1	A	99	ARG
1	A	115	PHE
1	A	135	SER
1	A	140	ARG
1	A	141	SER
1	A	236	CYS
1	A	291	GLU
1	A	347	LYS
1	A	369	ARG
1	A	409	ASP
1	A	410	GLU
1	A	420	LEU
1	A	443	ARG
1	A	457	LEU
1	A	477	PHE
1	A	545	LEU
1	A	547	SER
1	A	566	SER
1	A	594	SER
1	A	620	LEU
1	B	48	PHE
1	B	93	SER
1	B	115	PHE
1	B	139	ARG
1	B	176	LYS
1	B	189	ARG
1	B	236	CYS
1	B	398	LYS
1	B	426	ARG
1	B	483	ARG
1	B	488	LYS
1	B	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	HIS

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 monosaccharides 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	620/620 (100%)	0.54	48 (7%)	13 7	65, 96, 119, 133	0
1	B	620/620 (100%)	0.31	29 (4%)	31 22	68, 92, 111, 125	0
All	All	1240/1240 (100%)	0.42	77 (6%)	20 13	65, 93, 116, 133	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	5.8
1	A	409	ASP	5.7
1	A	180	SER	5.0
1	A	408	LEU	4.9
1	A	111	GLN	4.7
1	A	613	GLY	4.5
1	A	40	LEU	4.0
1	A	159	LEU	3.9
1	A	136	PRO	3.8
1	A	121	GLY	3.7
1	A	168	VAL	3.6
1	A	24	TYR	3.6
1	A	116	MET	3.5
1	A	100	TYR	3.4
1	A	181	ILE	3.4
1	A	568	SER	3.3
1	A	132	VAL	3.3
1	B	241	ASP	3.2
1	B	564	TRP	3.2
1	B	505	HIS	3.2
1	B	348	LEU	3.2
1	B	45	GLU	3.2
1	A	123	ALA	3.2
1	B	94	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	568	SER	3.1
1	A	119	LYS	3.1
1	B	563	ALA	3.1
1	A	345	LEU	3.1
1	B	123	ALA	3.0
1	A	364	GLY	3.0
1	A	607	TYR	2.9
1	A	241	ASP	2.9
1	B	491	ALA	2.9
1	A	122	LYS	2.8
1	B	567	ALA	2.8
1	A	183	GLU	2.8
1	A	86	PHE	2.8
1	B	411	LYS	2.7
1	B	408	LEU	2.7
1	A	49	ILE	2.7
1	A	437	ALA	2.7
1	A	407	ASP	2.6
1	B	508	ALA	2.6
1	A	117	GLY	2.6
1	A	93	SER	2.6
1	B	153	SER	2.6
1	B	613	GLY	2.5
1	A	564	TRP	2.5
1	B	287	PHE	2.4
1	B	341	VAL	2.4
1	A	17	ARG	2.4
1	A	503	TRP	2.4
1	A	118	LEU	2.4
1	B	127	ALA	2.4
1	A	585	LEU	2.4
1	A	184	ILE	2.4
1	A	342	GLU	2.3
1	A	431	GLY	2.3
1	A	505	HIS	2.3
1	A	246	SER	2.3
1	B	128	GLY	2.2
1	A	587	VAL	2.2
1	B	587	VAL	2.2
1	B	410	GLU	2.2
1	A	491	ALA	2.2
1	B	246	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	44	PRO	2.1
1	B	70	LEU	2.1
1	A	432	SER	2.1
1	B	361	GLY	2.1
1	A	84	LEU	2.1
1	A	242	ALA	2.1
1	A	115	PHE	2.1
1	A	562	GLN	2.1
1	B	544	GLU	2.0
1	B	566	SER	2.0
1	A	612	ASN	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.