Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 12:08 PM JST

PDB ID	:	9U7V / pdb_00009u7v
Title	:	The X-ray Crystallographic Structure of oligo-1,6-glucosidase from Paenibacillus sp. STB16
Authors	:	Li, Z.F.; Tian, Y.X.; Zhang, J.S.; Ban, X.F.
Deposited on	:	2025-03-25
Resolution	:	3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

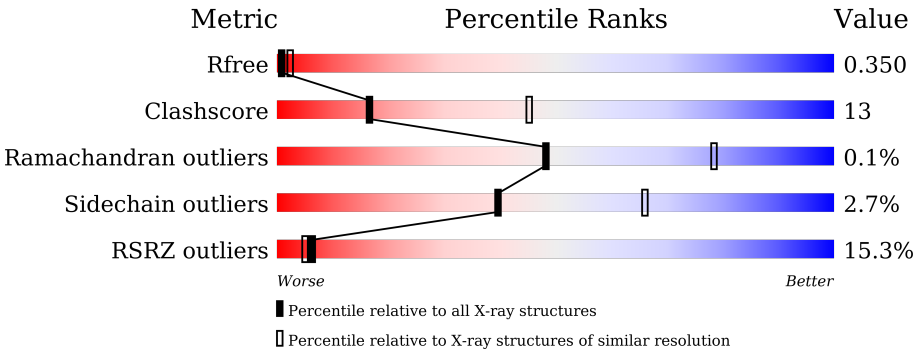
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	164625	1999 (3.28-3.20)
Clashscore	180529	2147 (3.28-3.20)
Ramachandran outliers	177936	2118 (3.28-3.20)
Sidechain outliers	177891	2117 (3.28-3.20)
RSRZ outliers	164620	2001 (3.28-3.20)

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	577	6% 67% 28% · 5%
1	B	577	23% 68% 24% · 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8992 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 oligo-1,6-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4503	2842	787	852	22			
1	B	540	Total	C	N	O	S	0	0	0
			4424	2797	766	839	22			

- Molecule 2 is water.

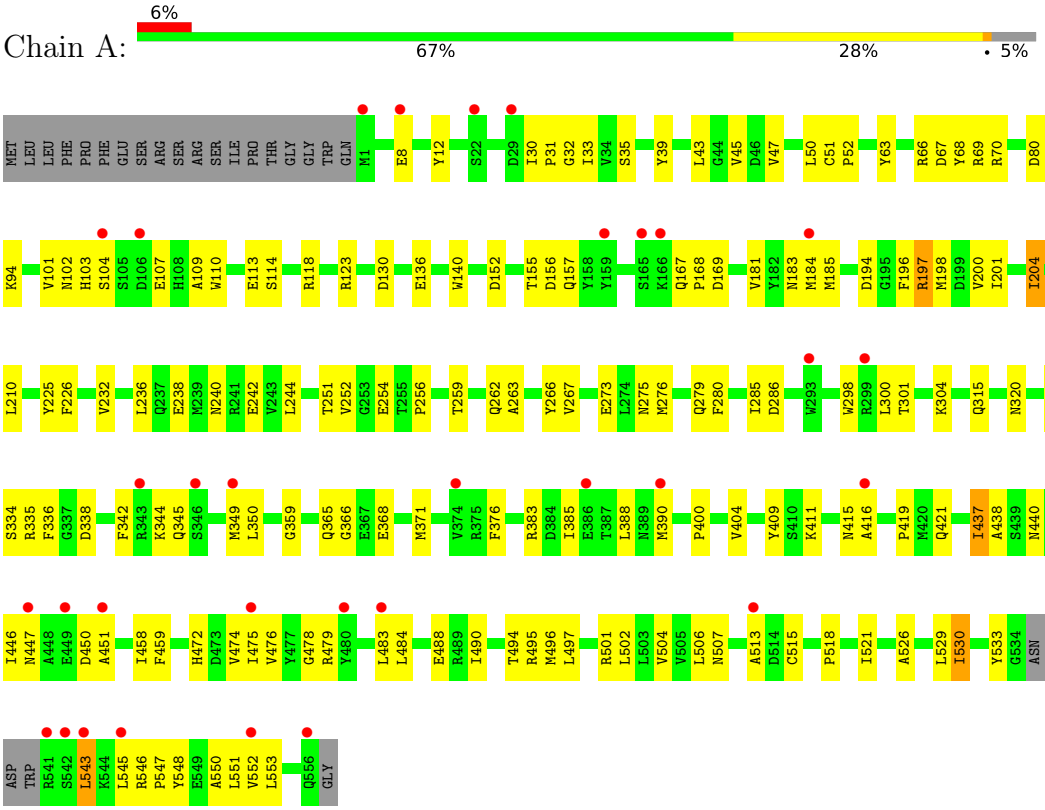
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	28	Total	O	0	0
			28	28		

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.

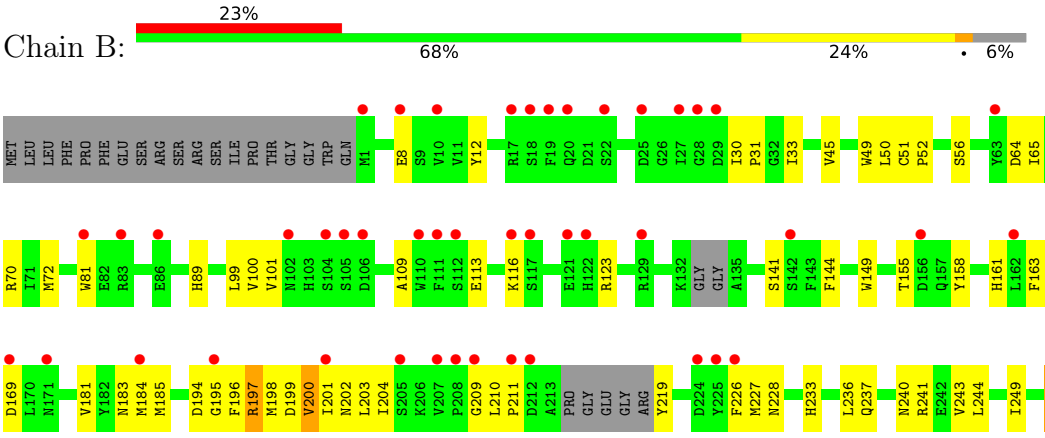
• Molecule 1: oligo-1,6-glucosidase

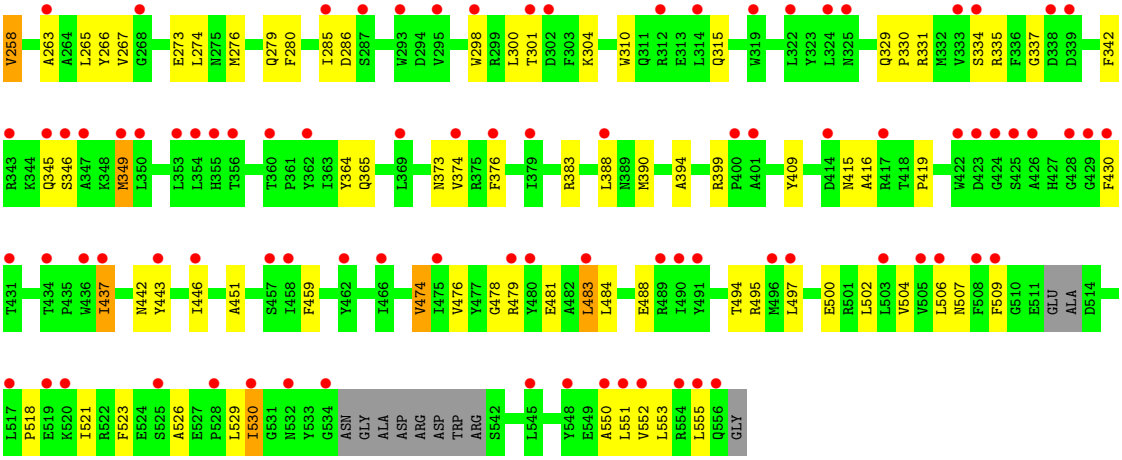
Chain A:



• Molecule 1: oligo-1,6-glucosidase

Chain B:




V258 A263 A264 L265 Y266 V267 G268 E273 L274 N275 M276 Q279 F280 I285 D286 S287 W293 D294 V295 W298 R299 L300 T301 D302 F303 K304 W310 Q311 R312 E313 L314 Q315 W319 L322 Y323 L324 N325 Q329 P330 R331 M332 V333 S334 R335 F336 G337 D338 D339 F342
R343 K344 Q345 S346 A347 K348 M349 L350 L353 L354 H355 T356 T360 P361 Y362 I363 Y364 Q365 L369 N373 V374 R375 F376 I379 R383 L388 N389 M390 A394 R399 P400 A401 Y409 D414 N415 A416 R417 T418 P419 W422 D423 G424 S425 A426 H427 G428 G429 F430
T431 T434 P435 W436 I437 N442 Y443 I446 A451 S457 I458 F459 Y462 I466 V474 I475 V476 Y477 G478 R479 Y480 E481 A482 L483 L484 E488 R489 I490 Y491 T494 R495 M496 L497 E500 R501 L502 L503 V504 V505 L506 N507 P508 F509 G510 E511 GLU ALA D514
L517 P518 E519 K520 I521 R522 F523 E524 S525 A526 E527 P528 L529 I530 G531 N532 Y533 G534 ASN GLY ALA ASP ARG ASP TRP ARG S542 L545 Y548 E549 A550 L551 V552 L553 R554 L555 Q556 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.57Å 154.57Å 115.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.44 – 3.24 31.44 – 3.24	Depositor EDS
% Data completeness (in resolution range)	86.9 (31.44-3.24) 86.9 (31.44-3.24)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.305 , 0.350 0.311 , 0.350	Depositor DCC
R_{free} test set	1155 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	8992	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.46	0/4622	0.90	1/6253 (0.0%)
1	B	0.46	0/4539	0.89	0/6139
All	All	0.46	0/9161	0.90	1/12392 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	PHE	CA-CB-CG	5.06	118.86	113.80

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	4503	0	4255	112	0
1	B	4424	0	4168	109	0
2	A	37	0	0	0	0
2	B	28	0	0	0	0
All	All	8992	0	8423	220	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 13.

All (220) 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:102:ASN:HB3	1:A:204:ILE:HD12	1.55	0.87
1:A:315:GLN:HE22	1:A:479:ARG:HG3	1.40	0.84
1:B:315:GLN:HE22	1:B:479:ARG:HG3	1.43	0.83
1:A:530:ILE:HG22	1:A:552:VAL:HG12	1.58	0.83
1:B:530:ILE:HG22	1:B:552:VAL:HG12	1.61	0.81
1:A:256:PRO:HA	1:A:280:PHE:CD1	2.18	0.78
1:A:419:PRO:HD3	1:A:437:ILE:HG23	1.67	0.77
1:A:240:ASN:HA	1:A:244:LEU:HB2	1.65	0.76
1:B:240:ASN:HA	1:B:244:LEU:HB2	1.66	0.76
1:B:419:PRO:HD3	1:B:437:ILE:HG23	1.72	0.72
1:A:504:VAL:HG22	1:A:552:VAL:HG23	1.74	0.69
1:A:349:MET:HB2	1:A:550:ALA:HB2	1.74	0.69
1:B:99:LEU:HD23	1:B:198:MET:HG2	1.74	0.69
1:B:329:GLN:HE21	1:B:330:PRO:HD2	1.60	0.67
1:B:504:VAL:HG22	1:B:552:VAL:HG23	1.75	0.67
1:A:349:MET:CB	1:A:550:ALA:HB2	2.24	0.67
1:A:507:ASN:HB2	1:A:545:LEU:HD13	1.78	0.66
1:B:526:ALA:HA	1:B:553:LEU:HD11	1.78	0.66
1:B:197:ARG:HG2	1:B:252:VAL:HG13	1.78	0.66
1:B:164:SER:HB3	1:B:167:GLN:HE21	1.61	0.65
1:A:336:PHE:HB2	1:A:350:LEU:HD21	1.79	0.64
1:A:513:ALA:HB3	1:A:545:LEU:HD11	1.79	0.64
1:A:104:SER:O	1:A:168:PRO:HD2	1.99	0.63
1:A:197:ARG:HG2	1:A:252:VAL:HG13	1.80	0.63
1:B:237:GLN:O	1:B:241:ARG:HG3	1.98	0.63
1:B:285:ILE:HG22	1:B:298:TRP:HB2	1.81	0.63
1:B:483:LEU:HD13	1:B:521:ILE:HG13	1.82	0.62
1:A:526:ALA:HA	1:A:553:LEU:HD11	1.81	0.61
1:A:285:ILE:HG22	1:A:298:TRP:HB2	1.82	0.61
1:A:109:ALA:O	1:A:113:GLU:HG2	2.01	0.60
1:A:200:VAL:HA	1:A:254:GLU:O	2.02	0.60
1:A:198:MET:HB3	1:A:201:ILE:CG2	2.32	0.59
1:B:267:VAL:HG13	1:B:276:MET:HA	1.84	0.59
1:A:550:ALA:C	1:A:551:LEU:HD12	2.28	0.59
1:A:552:VAL:HG13	1:A:552:VAL:O	2.02	0.59
1:A:483:LEU:HD13	1:A:521:ILE:HG13	1.85	0.59
1:B:228:ASN:HD21	1:B:258:VAL:HG23	1.67	0.58
1:A:232:VAL:HG11	1:A:266:TYR:OH	2.03	0.58
1:B:502:LEU:HD22	1:B:552:VAL:HG22	1.84	0.58
1:A:8:GLU:HB3	1:A:476:VAL:HG11	1.85	0.58
1:B:483:LEU:HD11	1:B:494:THR:HG23	1.86	0.58
1:B:67:ASP:OD2	1:B:70:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:LEU:HD12	1:B:555:LEU:HD23	1.84	0.58
1:A:502:LEU:HD22	1:A:552:VAL:HG22	1.85	0.58
1:B:89:HIS:NE2	1:B:194:ASP:OD2	2.37	0.57
1:B:243:VAL:HG23	1:B:244:LEU:HD13	1.86	0.57
1:A:329:GLN:HE21	1:A:330:PRO:HD2	1.70	0.56
1:B:256:PRO:HA	1:B:280:PHE:CD1	2.41	0.56
1:B:394:ALA:HB1	1:B:399:ARG:HB2	1.88	0.56
1:A:533:TYR:CG	1:A:546:ARG:HD2	2.41	0.55
1:B:198:MET:HB3	1:B:201:ILE:CG2	2.36	0.55
1:B:109:ALA:O	1:B:113:GLU:HG2	2.07	0.55
1:A:181:VAL:O	1:A:185:MET:HG3	2.07	0.55
1:B:144:PHE:CD2	1:B:163:PHE:O	2.59	0.55
1:B:201:ILE:O	1:B:204:ILE:HG12	2.06	0.55
1:A:200:VAL:HG23	1:A:200:VAL:O	2.06	0.55
1:A:130:ASP:HA	1:A:157:GLN:HG2	1.89	0.55
1:A:267:VAL:HG13	1:A:276:MET:HA	1.88	0.55
1:B:185:MET:HE1	1:B:244:LEU:HD11	1.88	0.55
1:B:228:ASN:ND2	1:B:258:VAL:HG23	2.22	0.54
1:A:101:VAL:HG21	1:A:181:VAL:CG1	2.38	0.54
1:A:259:THR:HG23	1:A:262:GLN:H	1.73	0.54
1:A:483:LEU:HD11	1:A:494:THR:HG23	1.90	0.53
1:A:225:TYR:HE1	1:B:211:PRO:HG3	1.73	0.53
1:A:483:LEU:O	1:A:484:LEU:C	2.51	0.53
1:B:550:ALA:C	1:B:551:LEU:HD12	2.33	0.53
1:A:101:VAL:HG13	1:A:204:ILE:HD11	1.91	0.53
1:B:8:GLU:HB3	1:B:476:VAL:HG11	1.90	0.53
1:B:419:PRO:HB3	1:B:430:PHE:CD2	2.43	0.53
1:B:181:VAL:O	1:B:185:MET:HG3	2.09	0.53
1:B:99:LEU:HD22	1:B:185:MET:HE3	1.91	0.52
1:B:552:VAL:O	1:B:552:VAL:HG13	2.09	0.52
1:A:198:MET:CB	1:A:201:ILE:CG2	2.87	0.52
1:B:30:ILE:N	1:B:31:PRO:HD2	2.25	0.51
1:A:300:LEU:HG	1:A:304:LYS:HD2	1.94	0.50
1:B:64:ASP:N	1:B:64:ASP:OD1	2.44	0.50
1:B:236:LEU:HD13	1:B:274:LEU:HD13	1.94	0.50
1:A:366:GLY:HA3	1:A:371:MET:SD	2.52	0.50
1:A:494:THR:HA	1:A:502:LEU:O	2.11	0.50
1:B:198:MET:CB	1:B:201:ILE:CG2	2.91	0.49
1:A:279:GLN:OE1	1:A:279:GLN:N	2.37	0.49
1:A:490:ILE:HD11	1:A:513:ALA:HB1	1.95	0.49
1:B:141:SER:HB3	1:B:219:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:HA	1:A:388:LEU:HD11	1.95	0.49
1:B:233:HIS:NE2	1:B:265:LEU:HB2	2.28	0.49
1:B:374:VAL:HG21	1:B:376:PHE:CZ	2.47	0.49
1:B:451:ALA:HB1	1:B:459:PHE:HB3	1.95	0.49
1:B:494:THR:HA	1:B:502:LEU:O	2.13	0.48
1:A:530:ILE:HG22	1:A:552:VAL:CG1	2.38	0.48
1:A:409:TYR:O	1:A:415:ASN:ND2	2.47	0.48
1:B:263:ALA:O	1:B:266:TYR:N	2.42	0.48
1:A:33:ILE:HD13	1:A:50:LEU:HD22	1.96	0.48
1:A:66:ARG:HD3	1:A:107:GLU:OE1	2.14	0.48
1:B:241:ARG:NH2	1:B:241:ARG:HB3	2.29	0.48
1:A:101:VAL:HG21	1:A:181:VAL:HG13	1.95	0.47
1:B:301:THR:HG23	1:B:488:GLU:HG2	1.96	0.47
1:B:331:ARG:NH1	1:B:365:GLN:O	2.45	0.47
1:B:383:ARG:HA	1:B:388:LEU:HD11	1.95	0.47
1:A:31:PRO:HD3	1:A:80:ASP:HB3	1.96	0.47
1:B:337:GLY:HA3	1:B:346:SER:HB3	1.97	0.47
1:B:195:GLY:HA2	1:B:249:ILE:HB	1.96	0.47
1:A:263:ALA:O	1:A:266:TYR:N	2.44	0.47
1:A:301:THR:HG23	1:A:488:GLU:HG2	1.95	0.47
1:A:383:ARG:HD2	1:A:437:ILE:HD12	1.97	0.47
1:B:237:GLN:HG3	1:B:273:GLU:HG3	1.96	0.47
1:B:383:ARG:HD2	1:B:437:ILE:HD12	1.97	0.46
1:A:550:ALA:O	1:A:551:LEU:HD12	2.15	0.46
1:B:443:TYR:HA	1:B:446:ILE:O	2.15	0.46
1:A:12:TYR:HB2	1:A:45:VAL:HG21	1.97	0.46
1:A:30:ILE:N	1:A:31:PRO:HD2	2.30	0.46
1:A:345:GLN:HG2	1:A:533:TYR:CZ	2.50	0.46
1:B:478:GLY:HA2	1:B:497:LEU:HB2	1.98	0.46
1:B:300:LEU:HG	1:B:304:LYS:HD2	1.97	0.46
1:A:484:LEU:HD11	1:A:518:PRO:HD3	1.98	0.46
1:A:251:THR:OG1	1:A:275:ASN:ND2	2.49	0.45
1:A:376:PHE:CE1	1:A:438:ALA:HB3	2.51	0.45
1:A:478:GLY:HA2	1:A:497:LEU:HB2	1.98	0.45
1:A:39:TYR:OH	1:A:368:GLU:HG3	2.17	0.45
1:A:338:ASP:HB3	1:A:342:PHE:H	1.82	0.45
1:A:390:MET:SD	1:A:404:VAL:HG13	2.57	0.45
1:A:344:LYS:HA	1:A:458:ILE:HD11	1.98	0.45
1:A:349:MET:HE3	1:A:506:LEU:HB3	1.98	0.45
1:B:241:ARG:HB3	1:B:241:ARG:HH21	1.80	0.45
1:B:301:THR:CG2	1:B:488:GLU:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:MET:HE2	1:B:390:MET:HB3	1.85	0.45
1:B:506:LEU:CD2	1:B:550:ALA:HB1	2.47	0.45
1:A:102:ASN:OD1	1:A:103:HIS:ND1	2.50	0.45
1:B:523:PHE:HB3	1:B:555:LEU:HD22	1.99	0.45
1:A:502:LEU:HD21	1:A:529:LEU:HD22	1.98	0.44
1:B:258:VAL:HG12	1:B:310:TRP:HH2	1.82	0.44
1:B:502:LEU:HD21	1:B:529:LEU:HD22	1.98	0.44
1:A:331:ARG:NH2	1:A:416:ALA:O	2.51	0.44
1:B:185:MET:CE	1:B:244:LEU:HD11	2.47	0.44
1:B:484:LEU:HD11	1:B:518:PRO:HD3	1.98	0.44
1:A:32:GLY:O	1:A:35:SER:OG	2.32	0.44
1:B:99:LEU:HB3	1:B:198:MET:HA	1.99	0.44
1:A:67:ASP:OD2	1:A:70:ARG:NH1	2.51	0.44
1:A:506:LEU:CD2	1:A:550:ALA:HB1	2.48	0.44
1:B:99:LEU:CD1	1:B:101:VAL:HG13	2.48	0.44
1:A:236:LEU:HB2	1:A:273:GLU:OE1	2.17	0.44
1:B:226:PHE:HE1	1:B:227:MET:HE3	1.82	0.44
1:A:443:TYR:HA	1:A:446:ILE:O	2.18	0.44
1:B:113:GLU:HA	1:B:116:LYS:HD2	2.00	0.44
1:B:349:MET:HB2	1:B:550:ALA:HB2	1.99	0.44
1:B:451:ALA:HB1	1:B:459:PHE:CB	2.48	0.43
1:A:238:GLU:O	1:A:242:GLU:N	2.44	0.43
1:B:209:GLY:O	1:B:210:LEU:C	2.62	0.43
1:B:479:ARG:O	1:B:495:ARG:HA	2.18	0.43
1:A:30:ILE:HG21	1:A:81:TRP:HA	1.99	0.43
1:B:33:ILE:HD13	1:B:50:LEU:HD22	2.01	0.43
1:B:184:MET:HG3	1:B:185:MET:N	2.32	0.43
1:B:483:LEU:O	1:B:484:LEU:C	2.61	0.43
1:A:301:THR:CG2	1:A:488:GLU:HG2	2.48	0.43
1:A:263:ALA:O	1:A:267:VAL:HG23	2.19	0.43
1:B:100:VAL:HA	1:B:199:ASP:HB3	2.00	0.43
1:A:421:GLN:O	1:A:447:ASN:HA	2.19	0.43
1:B:161:HIS:O	1:B:161:HIS:CD2	2.71	0.43
1:B:200:VAL:HG23	1:B:200:VAL:O	2.17	0.43
1:A:140:TRP:CZ2	1:A:225:TYR:HB2	2.54	0.43
1:B:409:TYR:O	1:B:415:ASN:ND2	2.52	0.43
1:B:30:ILE:HG21	1:B:81:TRP:HA	2.01	0.43
1:B:101:VAL:HG11	1:B:181:VAL:HG13	2.01	0.43
1:A:331:ARG:NH1	1:A:365:GLN:O	2.46	0.42
1:B:163:PHE:CZ	1:B:200:VAL:HG11	2.54	0.42
1:B:364:TYR:CE2	1:B:416:ALA:HB1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:OD2	1:A:335:ARG:NE	2.53	0.42
1:A:315:GLN:NE2	1:A:479:ARG:HG3	2.22	0.42
1:A:43:LEU:HD23	1:A:45:VAL:HG23	2.01	0.42
1:A:400:PRO:O	1:A:404:VAL:HG23	2.19	0.42
1:B:51:CYS:HB3	1:B:52:PRO:HD2	2.02	0.42
1:B:123:ARG:NH1	1:B:155:THR:HG21	2.34	0.42
1:A:110:TRP:O	1:A:114:SER:N	2.45	0.42
1:A:184:MET:HG3	1:A:185:MET:N	2.35	0.42
1:A:52:PRO:HG2	1:A:63:TYR:CE1	2.55	0.42
1:B:203:LEU:HD11	1:B:227:MET:HE2	2.01	0.42
1:A:152:ASP:O	1:A:156:ASP:N	2.49	0.42
1:A:447:ASN:HD21	1:A:450:ASP:HB2	1.85	0.42
1:A:547:PRO:O	1:A:548:TYR:C	2.63	0.42
1:A:156:ASP:O	1:A:157:GLN:HG3	2.19	0.42
1:B:233:HIS:NE2	1:B:265:LEU:CB	2.83	0.42
1:B:507:ASN:ND2	1:B:509:PHE:O	2.53	0.42
1:B:201:ILE:CD1	1:B:274:LEU:HD22	2.50	0.41
1:B:530:ILE:HG22	1:B:552:VAL:CG1	2.41	0.41
1:A:118:ARG:NH2	1:A:155:THR:O	2.46	0.41
1:A:123:ARG:NH1	1:A:155:THR:HG21	2.35	0.41
1:A:252:VAL:HA	1:A:276:MET:O	2.20	0.41
1:B:12:TYR:HB2	1:B:45:VAL:HG21	2.02	0.41
1:B:49:TRP:CE2	1:B:197:ARG:HG3	2.55	0.41
1:B:69:ARG:NH2	1:B:183:ASN:OD1	2.53	0.41
1:A:440:ASN:C	1:A:442:ASN:H	2.28	0.41
1:B:200:VAL:HB	1:B:203:LEU:HB2	2.01	0.41
1:B:342:PHE:HB3	1:B:345:GLN:HB2	2.01	0.41
1:A:104:SER:O	1:A:167:GLN:HA	2.20	0.41
1:A:12:TYR:HB2	1:A:45:VAL:CG2	2.50	0.41
1:A:68:TYR:CD1	1:A:184:MET:HE1	2.55	0.41
1:A:472:HIS:HB2	1:A:475:ILE:HD12	2.02	0.41
1:B:99:LEU:CD2	1:B:185:MET:HE3	2.51	0.41
1:B:202:ASN:OD1	1:B:256:PRO:HD2	2.21	0.41
1:A:451:ALA:HB1	1:A:459:PHE:HB3	2.01	0.41
1:A:515:CYS:HB3	1:A:543:LEU:HA	2.01	0.41
1:B:51:CYS:HB3	1:B:52:PRO:CD	2.50	0.41
1:B:149:TRP:HB3	1:B:158:TYR:HB3	2.03	0.41
1:B:198:MET:HB3	1:B:201:ILE:HG22	2.03	0.41
1:B:202:ASN:OD1	1:B:202:ASN:N	2.54	0.41
1:B:373:ASN:HB3	1:B:415:ASN:HD22	1.86	0.41
1:A:259:THR:HG22	1:A:262:GLN:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:HG21	1:B:500:GLU:HB3	2.03	0.41
1:A:89:HIS:NE2	1:A:194:ASP:OD2	2.54	0.40
1:B:56:SER:HB3	1:B:72:MET:HE2	2.03	0.40
1:A:47:VAL:HG22	1:A:94:LYS:HD2	2.04	0.40
1:A:69:ARG:NH2	1:A:183:ASN:OD1	2.53	0.40
1:A:496:MET:HG3	1:A:501:ARG:HG2	2.03	0.40
1:A:209:GLY:O	1:A:210:LEU:C	2.64	0.40
1:A:286:ASP:CG	1:A:411:LYS:HE2	2.46	0.40
1:A:320:ASN:O	1:A:359:GLY:HA3	2.21	0.40
1:B:286:ASP:OD2	1:B:335:ARG:NE	2.53	0.40
1:A:51:CYS:HB3	1:A:52:PRO:CD	2.51	0.40
1:A:479:ARG:O	1:A:495:ARG:HA	2.21	0.40
1:B:550:ALA:O	1:B:551:LEU:HD12	2.22	0.40
1:B:279:GLN:OE1	1:B:279:GLN:N	2.40	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	546/577 (95%)	508 (93%)	38 (7%)	0	100	100
1	B	530/577 (92%)	494 (93%)	35 (7%)	1 (0%)	44	73
All	All	1076/1154 (93%)	1002 (93%)	73 (7%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	VAL

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	471/496 (95%)	460 (98%)	11 (2%)	45 69
1	B	464/496 (94%)	450 (97%)	14 (3%)	36 63
All	All	935/992 (94%)	910 (97%)	25 (3%)	40 66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	169	ASP
1	A	196	PHE
1	A	197	ARG
1	A	204	ILE
1	A	334	SER
1	A	385	ILE
1	A	437	ILE
1	A	474	VAL
1	A	530	ILE
1	A	543	LEU
1	B	65	ILE
1	B	169	ASP
1	B	196	PHE
1	B	197	ARG
1	B	252	VAL
1	B	258	VAL
1	B	334	SER
1	B	349	MET
1	B	437	ILE
1	B	442	ASN
1	B	474	VAL
1	B	481	GLU
1	B	483	LEU
1	B	530	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	161	HIS
1	A	167	GLN
1	A	237	GLN
1	A	275	ASN
1	A	315	GLN
1	A	329	GLN
1	A	389	ASN
1	A	427	HIS
1	A	442	ASN
1	B	13	GLN
1	B	61	ASN
1	B	102	ASN
1	B	161	HIS
1	B	167	GLN
1	B	228	ASN
1	B	237	GLN
1	B	315	GLN
1	B	320	ASN
1	B	329	GLN
1	B	345	GLN
1	B	358	GLN
1	B	365	GLN
1	B	442	ASN
1	B	460	HIS
1	B	507	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	550/577 (95%)	0.73	34 (6%) 28 20	18, 31, 52, 87	0
1	B	540/577 (93%)	1.46	133 (24%) 2 2	26, 59, 89, 106	0
All	All	1090/1154 (94%)	1.09	167 (15%) 6 5	18, 42, 81, 106	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	ALA	4.8
1	B	496	MET	4.5
1	B	295	VAL	4.4
1	B	28	GLY	4.2
1	B	106	ASP	4.2
1	B	425	SER	4.1
1	B	422	TRP	3.9
1	B	532	ASN	3.8
1	A	416	ALA	3.7
1	B	426	ALA	3.6
1	B	346	SER	3.6
1	B	19	PHE	3.5
1	B	414	ASP	3.5
1	B	121	GLU	3.5
1	B	81	TRP	3.5
1	B	505	VAL	3.5
1	A	374	VAL	3.4
1	B	314	LEU	3.3
1	B	388	LEU	3.3
1	B	550	ALA	3.3
1	B	224	ASP	3.3
1	B	268	GLY	3.3
1	A	513	ALA	3.3
1	B	225	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	302	ASP	3.2
1	B	169	ASP	3.2
1	B	18	SER	3.2
1	B	436	TRP	3.2
1	B	343	ARG	3.2
1	A	447	ASN	3.1
1	B	312	ARG	3.1
1	B	355	HIS	3.1
1	B	552	VAL	3.1
1	B	437	ILE	3.0
1	A	104	SER	3.0
1	B	104	SER	3.0
1	B	424	GLY	2.9
1	B	483	LEU	2.9
1	B	263	ALA	2.9
1	B	545	LEU	2.9
1	B	22	SER	2.9
1	B	520	LYS	2.9
1	B	334	SER	2.8
1	A	299	ARG	2.8
1	B	356	THR	2.8
1	B	209	GLY	2.8
1	B	345	GLN	2.8
1	B	324	LEU	2.8
1	B	353	LEU	2.8
1	B	534	GLY	2.8
1	B	319	TRP	2.7
1	B	105	SER	2.7
1	B	212	ASP	2.7
1	A	208	PRO	2.7
1	B	205	SER	2.7
1	B	457	SER	2.7
1	A	386	GLU	2.7
1	A	541	ARG	2.7
1	A	480	TYR	2.7
1	B	360	THR	2.7
1	B	431	THR	2.7
1	B	184	MET	2.7
1	B	434	THR	2.7
1	B	491	TYR	2.7
1	A	29	ASP	2.6
1	B	339	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	369	LEU	2.6
1	B	401	ALA	2.6
1	B	285	ILE	2.6
1	B	10	VAL	2.6
1	B	301	THR	2.6
1	B	430	PHE	2.6
1	B	506	LEU	2.6
1	B	551	LEU	2.6
1	B	129	ARG	2.6
1	B	156	ASP	2.6
1	B	102	ASN	2.6
1	B	490	ILE	2.5
1	B	226	PHE	2.5
1	B	350	LEU	2.5
1	A	166	LYS	2.5
1	B	122	HIS	2.5
1	B	428	GLY	2.5
1	A	390	MET	2.5
1	A	22	SER	2.5
1	B	338	ASP	2.4
1	B	400	PRO	2.4
1	B	528	PRO	2.4
1	B	142	SER	2.4
1	B	207	VAL	2.4
1	B	443	TYR	2.4
1	B	525	SER	2.4
1	B	556	GLN	2.4
1	B	63	TYR	2.4
1	B	379	ILE	2.4
1	B	20	GLN	2.4
1	B	354	LEU	2.3
1	B	201	ILE	2.3
1	B	111	PHE	2.3
1	A	8	GLU	2.3
1	B	503	LEU	2.3
1	B	211	PRO	2.3
1	B	480	TYR	2.3
1	B	508	PHE	2.3
1	A	349	MET	2.3
1	B	519	GLU	2.3
1	A	556	GLN	2.3
1	A	184	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	17	ARG	2.3
1	B	117	SER	2.3
1	B	116	LYS	2.3
1	B	429	GLY	2.3
1	B	462	TYR	2.3
1	A	165	SER	2.3
1	A	542	SER	2.3
1	B	376	PHE	2.2
1	B	489	ARG	2.2
1	B	347	ALA	2.2
1	B	86	GLU	2.2
1	B	349	MET	2.2
1	A	207	VAL	2.2
1	A	449	GLU	2.2
1	B	112	SER	2.2
1	B	287	SER	2.2
1	B	298	TRP	2.2
1	B	25	ASP	2.2
1	B	423	ASP	2.2
1	B	509	PHE	2.2
1	B	548	TYR	2.2
1	B	195	GLY	2.2
1	B	1	MET	2.2
1	A	545	LEU	2.2
1	B	83	ARG	2.2
1	B	479	ARG	2.2
1	B	208	PRO	2.2
1	B	171	ASN	2.2
1	B	333	VAL	2.2
1	A	159	TYR	2.2
1	B	458	ILE	2.1
1	A	346	SER	2.1
1	B	29	ASP	2.1
1	B	530	ILE	2.1
1	B	322	LEU	2.1
1	B	374	VAL	2.1
1	B	325	ASN	2.1
1	A	552	VAL	2.1
1	B	293	TRP	2.1
1	B	555	LEU	2.1
1	B	417	ARG	2.1
1	B	27	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	2.1
1	B	554	ARG	2.1
1	B	362	TYR	2.1
1	B	497	LEU	2.1
1	A	293	TRP	2.0
1	B	110	TRP	2.0
1	A	343	ARG	2.0
1	A	106	ASP	2.0
1	B	517	LEU	2.0
1	A	1	MET	2.0
1	A	483	LEU	2.0
1	A	543	LEU	2.0
1	B	162	LEU	2.0
1	A	475	ILE	2.0
1	B	8	GLU	2.0
1	B	446	ILE	2.0
1	B	475	ILE	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.