



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:54 PM UTC

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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

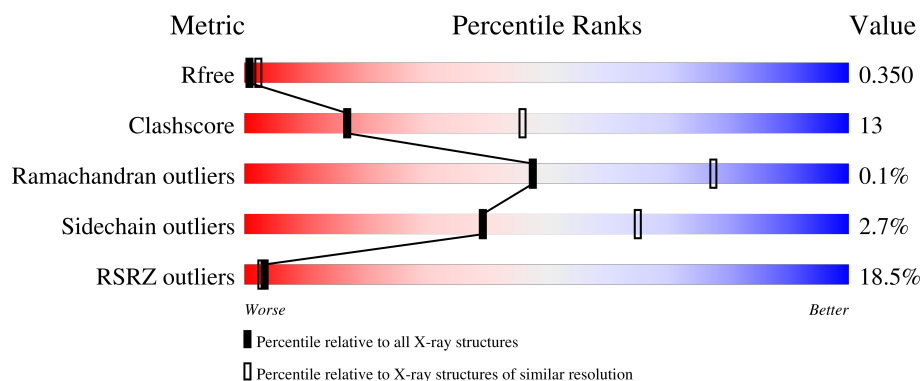
1 Overall quality at a glance

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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (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 $\leq 5\%$. 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	7% 67% 28% • 5%
1	B	577	28% 68% 24% • 6%

2 Entry composition

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			

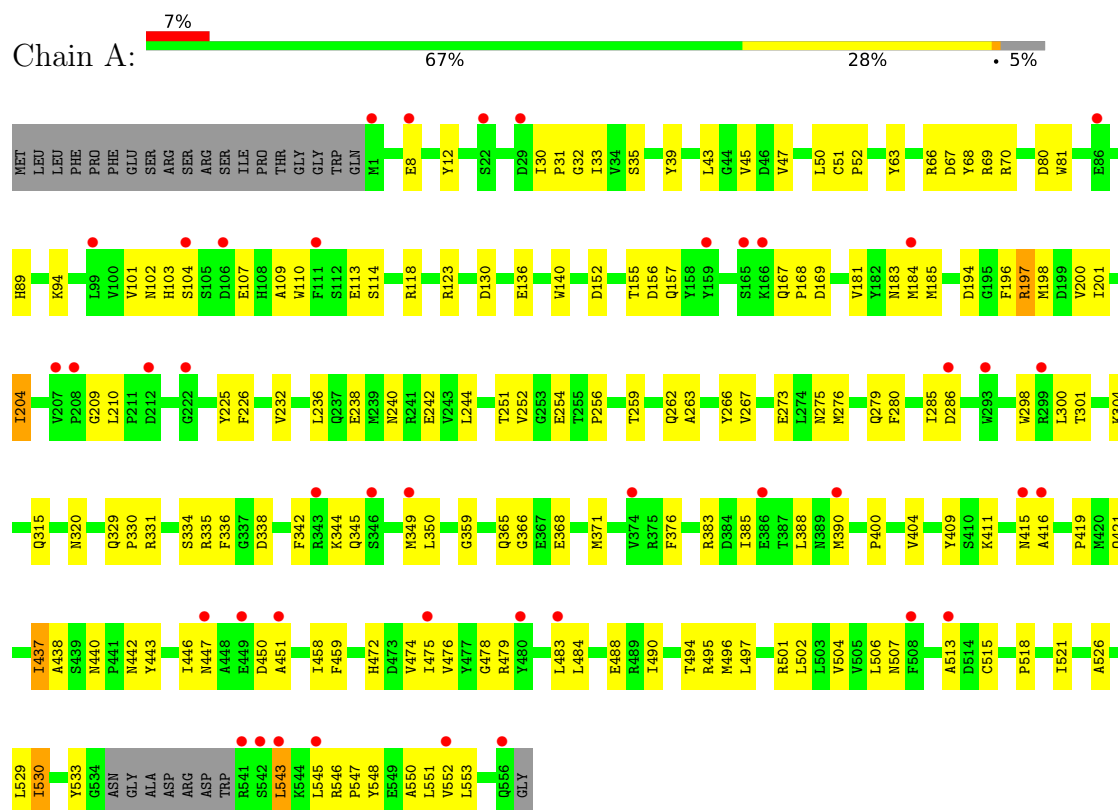
- Molecule 2 is water.

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

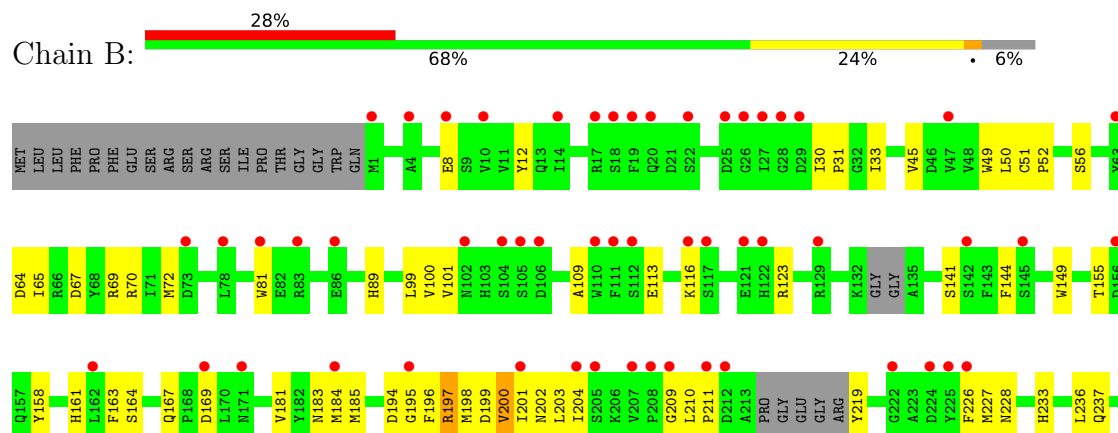
3 Residue-property plots [i](#)

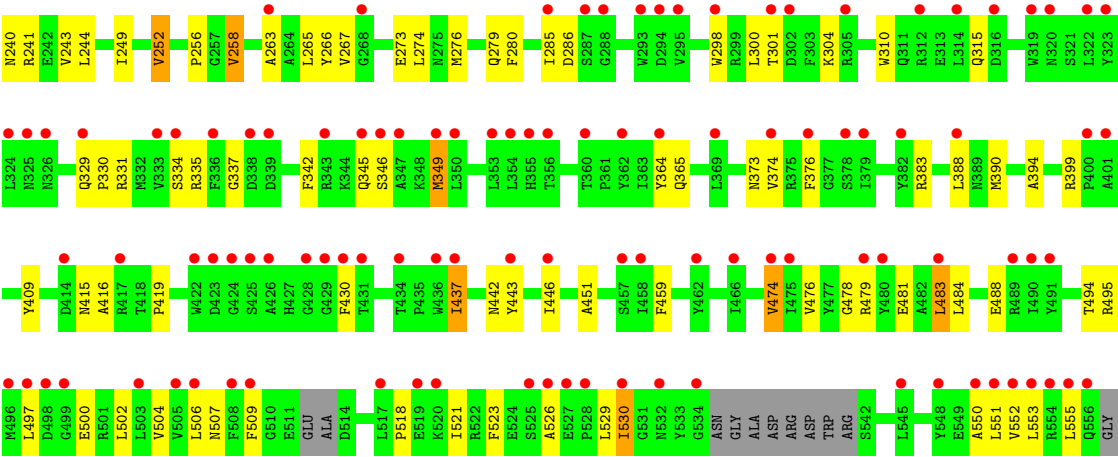
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



- Molecule 1: oligo-1,6-glucosidase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	1016 reflections (4.47%)	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 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	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(°)	Ideal(°)
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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%)	43	72
All	All	1076/1154 (93%)	1002 (93%)	73 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	VAL

5.3.2 Protein sidechains ⓘ

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%)	44	68
1	B	464/496 (94%)	450 (97%)	14 (3%)	36	63
All	All	935/992 (94%)	910 (97%)	25 (3%)	39	65

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 ⓘ

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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	550/577 (95%)	0.88	42 (7%) 20 14	18, 31, 52, 87	0
1	B	540/577 (93%)	1.61	160 (29%) 1 1	26, 59, 89, 106	0
All	All	1090/1154 (94%)	1.24	202 (18%) 3 3	18, 42, 81, 106	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	ALA	4.9
1	B	496	MET	4.7
1	B	295	VAL	4.5
1	B	28	GLY	4.4
1	B	106	ASP	4.3
1	B	425	SER	4.3
1	B	422	TRP	4.2
1	B	532	ASN	4.0
1	A	416	ALA	3.9
1	B	426	ALA	3.8
1	B	346	SER	3.8
1	B	81	TRP	3.7
1	B	19	PHE	3.7
1	B	414	ASP	3.7
1	B	505	VAL	3.6
1	B	121	GLU	3.6
1	A	374	VAL	3.6
1	B	224	ASP	3.5
1	B	314	LEU	3.5
1	B	388	LEU	3.5
1	B	268	GLY	3.5
1	B	550	ALA	3.5
1	B	225	TYR	3.4
1	B	436	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	302	ASP	3.4
1	A	513	ALA	3.4
1	B	18	SER	3.4
1	B	169	ASP	3.4
1	B	343	ARG	3.3
1	A	447	ASN	3.3
1	B	355	HIS	3.2
1	B	312	ARG	3.2
1	B	552	VAL	3.2
1	B	437	ILE	3.2
1	A	104	SER	3.2
1	B	104	SER	3.2
1	B	424	GLY	3.1
1	B	483	LEU	3.1
1	B	263	ALA	3.0
1	B	22	SER	3.0
1	B	545	LEU	3.0
1	B	334	SER	3.0
1	B	319	TRP	3.0
1	B	520	LYS	3.0
1	B	209	GLY	3.0
1	B	356	THR	3.0
1	B	105	SER	2.9
1	B	534	GLY	2.9
1	B	212	ASP	2.9
1	B	345	GLN	2.9
1	A	299	ARG	2.9
1	B	324	LEU	2.9
1	B	353	LEU	2.9
1	A	208	PRO	2.9
1	B	205	SER	2.9
1	B	457	SER	2.9
1	A	480	TYR	2.9
1	B	184	MET	2.9
1	B	360	THR	2.8
1	B	431	THR	2.8
1	B	491	TYR	2.8
1	A	29	ASP	2.8
1	A	386	GLU	2.8
1	B	434	THR	2.8
1	A	541	ARG	2.8
1	B	339	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	369	LEU	2.8
1	B	401	ALA	2.8
1	B	285	ILE	2.8
1	B	430	PHE	2.7
1	B	226	PHE	2.7
1	B	301	THR	2.7
1	B	156	ASP	2.7
1	B	10	VAL	2.7
1	B	506	LEU	2.7
1	B	551	LEU	2.7
1	B	350	LEU	2.7
1	B	490	ILE	2.7
1	B	122	HIS	2.7
1	B	102	ASN	2.7
1	B	129	ARG	2.7
1	B	428	GLY	2.7
1	A	390	MET	2.6
1	A	22	SER	2.6
1	A	166	LYS	2.6
1	B	400	PRO	2.6
1	B	528	PRO	2.6
1	B	338	ASP	2.6
1	B	142	SER	2.6
1	B	443	TYR	2.6
1	B	525	SER	2.6
1	B	63	TYR	2.6
1	B	207	VAL	2.6
1	B	556	GLN	2.5
1	B	379	ILE	2.5
1	B	20	GLN	2.5
1	B	111	PHE	2.5
1	B	354	LEU	2.5
1	B	508	PHE	2.5
1	B	211	PRO	2.5
1	B	480	TYR	2.5
1	B	201	ILE	2.5
1	A	349	MET	2.5
1	B	503	LEU	2.5
1	B	117	SER	2.4
1	A	8	GLU	2.4
1	A	184	MET	2.4
1	B	462	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	429	GLY	2.4
1	A	556	GLN	2.4
1	A	165	SER	2.4
1	A	542	SER	2.4
1	B	519	GLU	2.4
1	B	376	PHE	2.4
1	B	298	TRP	2.4
1	B	17	ARG	2.4
1	B	116	LYS	2.4
1	B	349	MET	2.4
1	B	509	PHE	2.4
1	B	287	SER	2.4
1	B	25	ASP	2.4
1	B	423	ASP	2.4
1	B	347	ALA	2.4
1	B	548	TYR	2.4
1	B	86	GLU	2.4
1	B	112	SER	2.4
1	A	207	VAL	2.4
1	B	195	GLY	2.3
1	B	489	ARG	2.3
1	B	1	MET	2.3
1	A	449	GLU	2.3
1	B	208	PRO	2.3
1	A	159	TYR	2.3
1	A	545	LEU	2.3
1	A	346	SER	2.3
1	B	293	TRP	2.3
1	B	171	ASN	2.3
1	B	29	ASP	2.3
1	B	333	VAL	2.3
1	B	458	ILE	2.3
1	B	83	ARG	2.3
1	B	479	ARG	2.3
1	B	530	ILE	2.3
1	A	293	TRP	2.3
1	B	110	TRP	2.3
1	B	322	LEU	2.3
1	B	325	ASN	2.3
1	B	374	VAL	2.3
1	B	555	LEU	2.2
1	B	362	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	552	VAL	2.2
1	B	27	ILE	2.2
1	B	466	ILE	2.2
1	A	1	MET	2.2
1	A	106	ASP	2.2
1	B	497	LEU	2.2
1	B	417	ARG	2.2
1	B	517	LEU	2.2
1	B	554	ARG	2.2
1	B	378	SER	2.2
1	A	483	LEU	2.2
1	A	543	LEU	2.2
1	B	162	LEU	2.2
1	A	343	ARG	2.2
1	A	111	PHE	2.2
1	A	475	ILE	2.1
1	B	446	ILE	2.1
1	B	475	ILE	2.1
1	B	8	GLU	2.1
1	B	222	GLY	2.1
1	A	415	ASN	2.1
1	B	326	ASN	2.1
1	B	294	ASP	2.1
1	B	474	VAL	2.1
1	B	204	ILE	2.1
1	B	323	TYR	2.1
1	A	99	LEU	2.1
1	B	145	SER	2.1
1	B	320	ASN	2.1
1	B	336	PHE	2.1
1	B	47	VAL	2.1
1	B	73	ASP	2.1
1	B	553	LEU	2.1
1	B	526	ALA	2.1
1	B	26	GLY	2.1
1	B	288	GLY	2.1
1	A	508	PHE	2.1
1	B	316	ASP	2.1
1	B	498	ASP	2.1
1	B	329	GLN	2.1
1	B	499	GLY	2.1
1	B	364	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	ILE	2.0
1	A	212	ASP	2.0
1	B	4	ALA	2.0
1	B	382	TYR	2.0
1	A	222	GLY	2.0
1	A	86	GLU	2.0
1	B	527	GLU	2.0
1	A	286	ASP	2.0
1	B	305	ARG	2.0
1	B	78	LEU	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 oligosaccharides 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.