



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:46 PM EDT

PDB ID : 7BWG / pdb_00007bwg
Title : A Glycoside Hydrolase Family 20 beta-N-Acetylglucosaminidase
Authors : Zhang, R.; Zhou, J.P.; Huang, Z.X.
Deposited on : 2020-04-14
Resolution : 2.85 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

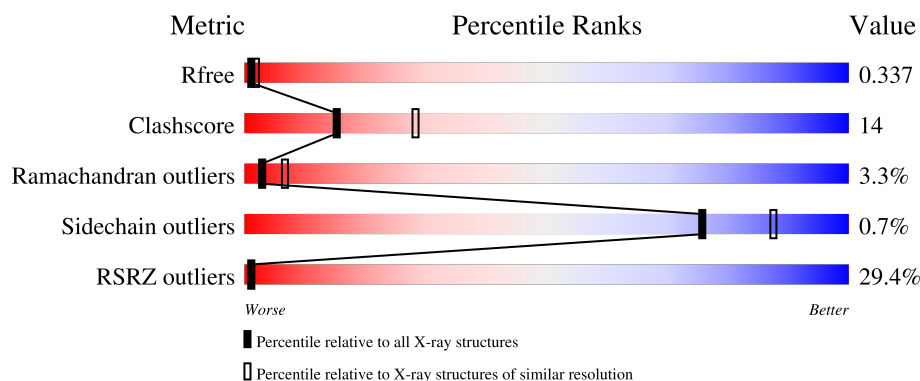
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	532	29% 67% 23% 9%
1	B	532	24% 62% 26% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6618 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-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3316	2113	565	631	7			
1	B	473	Total	C	N	O	S	0	0	0
			3284	2103	558	616	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A1W6AQA7
A	2	GLU	-	expression tag	UNP A0A1W6AQA7
A	3	LEU	-	expression tag	UNP A0A1W6AQA7
A	4	ALA	-	expression tag	UNP A0A1W6AQA7
A	5	LEU	-	expression tag	UNP A0A1W6AQA7
A	521	LYS	-	expression tag	UNP A0A1W6AQA7
A	522	GLY	-	expression tag	UNP A0A1W6AQA7
A	523	GLN	-	expression tag	UNP A0A1W6AQA7
A	524	PHE	-	expression tag	UNP A0A1W6AQA7
A	525	LEU	-	expression tag	UNP A0A1W6AQA7
A	526	GLU	-	expression tag	UNP A0A1W6AQA7
A	527	HIS	-	expression tag	UNP A0A1W6AQA7
A	528	HIS	-	expression tag	UNP A0A1W6AQA7
A	529	HIS	-	expression tag	UNP A0A1W6AQA7
A	530	HIS	-	expression tag	UNP A0A1W6AQA7
A	531	HIS	-	expression tag	UNP A0A1W6AQA7
A	532	HIS	-	expression tag	UNP A0A1W6AQA7
B	1	MET	-	initiating methionine	UNP A0A1W6AQA7
B	2	GLU	-	expression tag	UNP A0A1W6AQA7
B	3	LEU	-	expression tag	UNP A0A1W6AQA7
B	4	ALA	-	expression tag	UNP A0A1W6AQA7
B	5	LEU	-	expression tag	UNP A0A1W6AQA7
B	521	LYS	-	expression tag	UNP A0A1W6AQA7
B	522	GLY	-	expression tag	UNP A0A1W6AQA7
B	523	GLN	-	expression tag	UNP A0A1W6AQA7

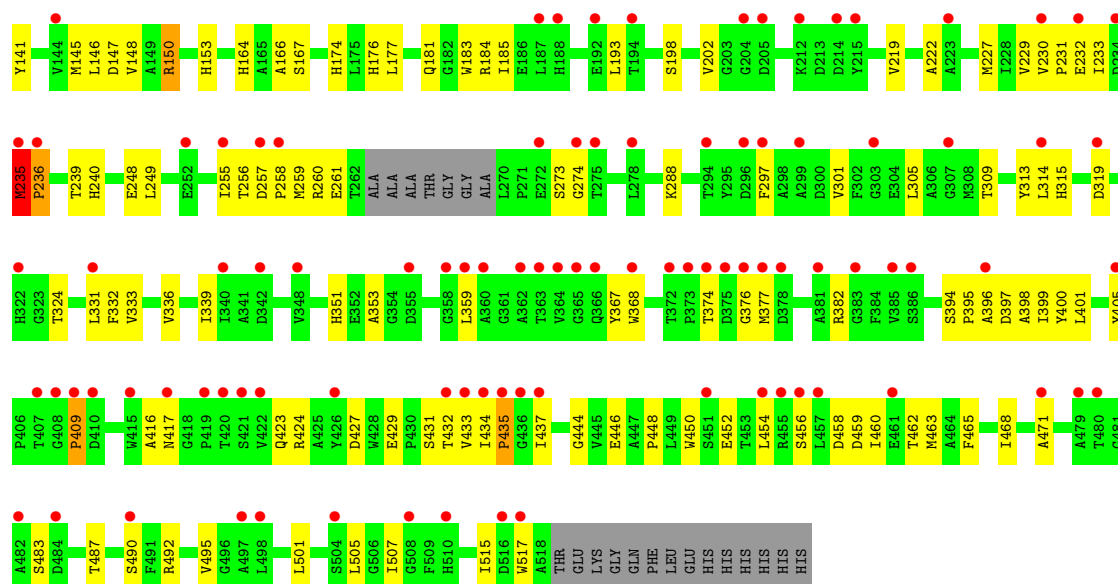
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Chain	Residue	Modelled	Actual	Comment	Reference
B	524	PHE	-	expression tag	UNP A0A1W6AQA7
B	525	LEU	-	expression tag	UNP A0A1W6AQA7
B	526	GLU	-	expression tag	UNP A0A1W6AQA7
B	527	HIS	-	expression tag	UNP A0A1W6AQA7
B	528	HIS	-	expression tag	UNP A0A1W6AQA7
B	529	HIS	-	expression tag	UNP A0A1W6AQA7
B	530	HIS	-	expression tag	UNP A0A1W6AQA7
B	531	HIS	-	expression tag	UNP A0A1W6AQA7
B	532	HIS	-	expression tag	UNP A0A1W6AQA7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	11	Total O 11 11	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.03Å 81.93Å 79.42Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	57.61 – 2.85 57.61 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (57.61-2.85) 99.7 (57.61-2.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.292 , 0.335 0.296 , 0.337	Depositor DCC
R_{free} test set	1190 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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	0.12	0/3400	0.37	0/4673
1	B	0.13	0/3372	0.38	0/4636
All	All	0.13	0/6772	0.38	0/9309

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	PHE	Peptide
1	B	235	MET	Peptide
1	B	257	ASP	Peptide
1	B	374	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3316	0	2976	75	0
1	B	3284	0	2995	96	0
2	A	7	0	0	0	0
2	B	11	0	0	0	0
All	All	6618	0	5971	171	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 14.

All (171) 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:78:LEU:HB3	1:A:108:LEU:HD21	1.73	0.69
1:B:147:ASP:HA	1:B:176:HIS:HB3	1.74	0.69
1:A:87:GLU:HG3	1:A:137:PRO:HG2	1.75	0.69
1:A:231:PRO:HG3	1:A:309:THR:HG21	1.72	0.69
1:B:454:LEU:HD23	1:B:460:ILE:HA	1.75	0.67
1:B:351:HIS:HE2	1:B:377:MET:HG2	1.60	0.67
1:B:32:ALA:HB3	1:B:130:ALA:HB1	1.78	0.66
1:A:466:PRO:HD3	1:A:509:PHE:HB2	1.76	0.65
1:B:91:LEU:HG	1:B:100:VAL:HG22	1.79	0.65
1:A:162:ILE:HG23	1:A:227:MET:HE2	1.79	0.64
1:B:145:MET:HB3	1:B:448:PRO:HA	1.79	0.63
1:A:364:VAL:HG21	1:A:384:PHE:CD2	2.32	0.63
1:B:492:ARG:HG3	1:B:515:ILE:HG22	1.80	0.63
1:B:145:MET:HE1	1:B:450:TRP:CZ2	2.34	0.63
1:A:145:MET:HB3	1:A:448:PRO:HA	1.81	0.62
1:B:78:LEU:HB3	1:B:108:LEU:HD21	1.83	0.61
1:A:417:ASN:HB2	1:A:424:ARG:NH2	2.16	0.60
1:A:465:PHE:O	1:A:467:ARG:N	2.35	0.60
1:A:465:PHE:HA	1:A:468:ILE:HG22	1.84	0.60
1:B:222:ALA:HB1	1:B:227:MET:HB3	1.83	0.59
1:A:76:ILE:HG23	1:A:98:VAL:HB	1.85	0.58
1:B:395:PRO:HB2	1:B:398:ALA:HB3	1.84	0.58
1:A:192:GLU:HG2	1:A:245:ALA:HB1	1.85	0.58
1:B:405:TYR:HB2	1:B:409:PRO:HD3	1.85	0.58
1:A:376:GLY:O	1:A:380:ARG:N	2.23	0.57
1:B:333:VAL:HG21	1:B:353:ALA:HB1	1.87	0.57
1:B:145:MET:HE3	1:B:448:PRO:HB3	1.87	0.56
1:B:454:LEU:HD11	1:B:463:MET:HG3	1.86	0.56
1:B:258:PRO:HA	1:B:260:ARG:H	1.71	0.56
1:B:116:GLY:HA2	1:B:119:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLU:HB3	1:B:432:THR:HG22	1.88	0.56
1:A:266:THR:HB	1:A:269:ALA:HB2	1.87	0.56
1:B:487:THR:HG23	1:B:490:SER:H	1.70	0.55
1:A:23:VAL:O	1:A:117:GLN:NE2	2.37	0.55
1:B:89:TYR:HA	1:B:102:GLY:HA2	1.88	0.55
1:B:231:PRO:HG3	1:B:309:THR:HG21	1.87	0.54
1:A:491:PHE:O	1:A:495:VAL:HG12	2.08	0.54
1:B:458:ASP:O	1:B:462:THR:OG1	2.24	0.54
1:A:364:VAL:HG21	1:A:384:PHE:CG	2.42	0.54
1:A:237:SER:OG	1:A:238:HIS:N	2.39	0.54
1:B:456:SER:HB3	1:B:459:ASP:H	1.71	0.54
1:A:366:GLN:OE1	1:A:381:ALA:CB	2.57	0.53
1:B:331:LEU:C	1:B:331:LEU:HD13	2.34	0.52
1:B:429:GLU:HG3	1:B:431:SER:H	1.73	0.52
1:B:495:VAL:HG13	1:B:515:ILE:HD13	1.91	0.52
1:B:37:PHE:HA	1:B:95:GLU:OE2	2.10	0.51
1:A:117:GLN:HA	1:A:501:LEU:HD22	1.93	0.51
1:B:93:ALA:HB3	1:B:131:VAL:HG12	1.92	0.50
1:B:181:GLN:HG2	1:B:202:VAL:HG22	1.93	0.50
1:B:146:LEU:HD11	1:B:153:HIS:CD2	2.46	0.50
1:B:396:ALA:O	1:B:400:TYR:HB2	2.12	0.49
1:B:515:ILE:HD11	1:B:517:TRP:CZ2	2.47	0.49
1:B:177:LEU:HD22	1:B:185:ILE:HB	1.95	0.49
1:A:186:GLU:HA	1:A:194:THR:HG21	1.94	0.49
1:B:235:MET:SD	1:B:336:VAL:HG11	2.52	0.49
1:B:183:TRP:O	1:B:198:SER:HB3	2.12	0.49
1:A:458:ASP:O	1:A:462:THR:OG1	2.29	0.49
1:B:150:ARG:HG2	1:B:452:GLU:HG3	1.95	0.49
1:A:445:VAL:HB	1:A:475:ALA:HB2	1.95	0.48
1:B:117:GLN:HA	1:B:501:LEU:HD22	1.94	0.48
1:A:405:TYR:HB2	1:A:409:PRO:CD	2.43	0.48
1:B:505:LEU:HB2	1:B:507:ILE:HD13	1.94	0.48
1:A:183:TRP:O	1:A:198:SER:HB3	2.14	0.48
1:B:240:HIS:NE2	1:B:273:SER:O	2.40	0.48
1:B:183:TRP:NE1	1:B:185:ILE:O	2.47	0.47
1:B:248:GLU:HG2	1:B:249:LEU:CD1	2.44	0.47
1:B:397:ASP:O	1:B:424:ARG:HD3	2.13	0.47
1:B:164:HIS:O	1:B:167:SER:OG	2.29	0.47
1:B:236:PRO:HB2	1:B:319:ASP:O	2.13	0.47
1:B:109:PHE:HA	1:B:112:VAL:HG12	1.96	0.47
1:A:395:PRO:HB2	1:A:398:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:O	1:B:133:ILE:N	2.30	0.47
1:B:417:ASN:HB2	1:B:424:ARG:HH22	1.79	0.47
1:B:305:LEU:HD23	1:B:314:LEU:HD11	1.96	0.47
1:B:400:TYR:CE1	1:B:448:PRO:HG2	2.50	0.47
1:B:515:ILE:HD11	1:B:517:TRP:CE2	2.50	0.47
1:B:456:SER:H	1:B:459:ASP:HB2	1.79	0.47
1:B:109:PHE:O	1:B:113:GLN:HG2	2.15	0.46
1:B:55:LEU:HA	1:B:58:LEU:HB2	1.97	0.46
1:A:24:PRO:HG3	1:A:472:ALA:HB1	1.96	0.46
1:A:147:ASP:HA	1:A:176:HIS:HB3	1.98	0.46
1:A:487:THR:HG23	1:A:490:SER:H	1.80	0.46
1:B:37:PHE:HB3	1:B:128:VAL:HB	1.97	0.46
1:A:91:LEU:HB3	1:A:133:ILE:HB	1.98	0.46
1:A:138:ARG:NH2	1:A:431:SER:OG	2.49	0.46
1:B:174:HIS:NE2	1:B:232:GLU:HB2	2.31	0.46
1:B:181:GLN:N	1:B:181:GLN:OE1	2.49	0.46
1:A:242:ILE:HD13	1:A:297:PHE:CZ	2.51	0.45
1:A:305:LEU:O	1:A:309:THR:HG23	2.17	0.45
1:B:331:LEU:HD13	1:B:331:LEU:O	2.16	0.45
1:A:145:MET:HE2	1:A:174:HIS:CE1	2.51	0.45
1:A:202:VAL:HG21	1:A:280:ILE:HG22	1.99	0.45
1:B:258:PRO:HA	1:B:260:ARG:N	2.31	0.45
1:A:43:THR:HG22	1:A:74:ALA:HB3	1.99	0.45
1:A:141:TYR:HB2	1:A:443:LEU:HG	1.98	0.45
1:A:417:ASN:HB2	1:A:424:ARG:HH22	1.80	0.45
1:B:258:PRO:HB3	1:B:261:GLU:H	1.81	0.45
1:A:77:ALA:HB3	1:A:99:THR:HG23	1.98	0.45
1:A:183:TRP:NE1	1:A:185:ILE:O	2.50	0.45
1:A:366:GLN:OE1	1:A:381:ALA:HB2	2.17	0.45
1:A:454:LEU:HD23	1:A:460:ILE:HA	1.99	0.44
1:B:164:HIS:ND1	1:B:507:ILE:HD11	2.32	0.44
1:A:400:TYR:HE1	1:A:448:PRO:HG2	1.81	0.44
1:A:465:PHE:CZ	1:A:507:ILE:HD13	2.52	0.44
1:A:146:LEU:HD11	1:A:460:ILE:HD13	1.98	0.44
1:B:164:HIS:CE1	1:B:507:ILE:HD11	2.53	0.44
1:B:305:LEU:O	1:B:309:THR:HG23	2.18	0.44
1:A:466:PRO:CD	1:A:509:PHE:HB2	2.47	0.44
1:A:94:ASP:OD1	1:A:96:ALA:N	2.50	0.44
1:B:55:LEU:HB2	1:B:112:VAL:HG23	2.00	0.44
1:B:336:VAL:HA	1:B:339:ILE:HD12	1.99	0.44
1:B:219:VAL:HA	1:B:229:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:HD11	1:B:305:LEU:HD22	2.00	0.44
1:A:434:ILE:O	1:A:435:PRO:C	2.61	0.43
1:B:145:MET:HB2	1:B:446:GLU:CD	2.42	0.43
1:B:399:ILE:HD11	1:B:471:ALA:HA	2.00	0.43
1:B:248:GLU:HG2	1:B:249:LEU:HD13	2.01	0.43
1:B:401:LEU:HD11	1:B:468:ILE:HD13	2.00	0.43
1:B:432:THR:C	1:B:434:ILE:H	2.26	0.43
1:A:179:ASP:OD1	1:A:238:HIS:ND1	2.36	0.43
1:B:82:GLY:HA2	1:B:103:ALA:HA	2.01	0.43
1:A:174:HIS:NE2	1:A:232:GLU:HB2	2.34	0.43
1:A:287:LEU:HD13	1:A:294:THR:HG23	1.99	0.43
1:A:145:MET:HG3	1:A:174:HIS:CG	2.53	0.43
1:B:434:ILE:O	1:B:435:PRO:C	2.61	0.43
1:B:141:TYR:O	1:B:444:GLY:HA3	2.18	0.43
1:B:423:GLN:O	1:B:427:ASP:N	2.52	0.43
1:A:89:TYR:HA	1:A:102:GLY:HA2	2.00	0.43
1:A:396:ALA:O	1:A:400:TYR:HB2	2.19	0.43
1:B:148:VAL:HG23	1:B:184:ARG:HG3	2.00	0.43
1:B:227:MET:HE3	1:B:227:MET:HB2	1.88	0.43
1:B:109:PHE:HE2	1:B:166:ALA:HB1	1.83	0.42
1:B:55:LEU:HB2	1:B:112:VAL:CG2	2.48	0.42
1:A:183:TRP:CH2	1:A:233:ILE:HD12	2.54	0.42
1:B:450:TRP:HB3	1:B:452:GLU:OE2	2.20	0.42
1:A:137:PRO:HG3	1:A:476:TRP:CZ3	2.55	0.42
1:B:273:SER:HB3	1:B:274:GLY:H	1.72	0.42
1:A:348:VAL:HG13	1:A:363:THR:HG22	2.01	0.42
1:A:429:GLU:HG3	1:A:432:THR:H	1.84	0.42
1:A:492:ARG:O	1:A:515:ILE:HG13	2.20	0.42
1:A:183:TRP:HH2	1:A:301:VAL:HG11	1.84	0.41
1:A:399:ILE:HD11	1:A:471:ALA:HB2	2.02	0.41
1:B:235:MET:HA	1:B:239:THR:HG23	2.02	0.41
1:A:429:GLU:HG3	1:A:431:SER:H	1.85	0.41
1:B:183:TRP:CZ2	1:B:193:LEU:HD13	2.56	0.41
1:B:332:PHE:O	1:B:336:VAL:HG23	2.20	0.41
1:A:366:GLN:HB3	1:A:393:LEU:HD12	2.02	0.41
1:A:435:PRO:HB2	1:A:436:GLY:H	1.75	0.41
1:B:139:PHE:HB3	1:B:444:GLY:HA2	2.02	0.41
1:A:349:ALA:O	1:A:364:VAL:HA	2.20	0.41
1:A:393:LEU:HD21	1:A:442:ILE:HG12	2.03	0.41
1:A:422:VAL:HG22	1:A:467:ARG:HG2	2.03	0.41
1:A:511:PRO:HA	1:A:517:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HG3	1:B:315:HIS:CG	2.56	0.41
1:B:230:VAL:HG22	1:B:313:TYR:HB2	2.02	0.41
1:A:473:GLU:HG3	1:A:491:PHE:CE1	2.56	0.41
1:A:478:PRO:O	1:A:486:ARG:HD3	2.21	0.41
1:B:58:LEU:C	1:B:60:GLU:H	2.28	0.41
1:B:193:LEU:HD11	1:B:297:PHE:CE1	2.56	0.41
1:A:164:HIS:O	1:A:167:SER:OG	2.36	0.41
1:A:315:HIS:HA	1:A:348:VAL:HB	2.03	0.41
1:B:465:PHE:HA	1:B:468:ILE:HG22	2.02	0.41
1:A:348:VAL:HA	1:A:363:THR:O	2.21	0.40
1:A:405:TYR:HB2	1:A:409:PRO:HD3	2.03	0.40
1:A:450:TRP:O	1:A:454:LEU:HD13	2.20	0.40
1:B:255:ILE:O	1:B:256:THR:OG1	2.30	0.40
1:B:382:ARG:HD3	1:B:435:PRO:HB2	2.03	0.40
1:B:145:MET:HA	1:B:174:HIS:HB3	2.03	0.40
1:B:233:ILE:HD13	1:B:301:VAL:CG1	2.52	0.40
1:B:367:TYR:HA	1:B:394:SER:O	2.22	0.40
1:B:368:TRP:O	1:B:395:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	477/532 (90%)	426 (89%)	33 (7%)	18 (4%)	2	5
1	B	463/532 (87%)	420 (91%)	30 (6%)	13 (3%)	4	9
All	All	940/1064 (88%)	846 (90%)	63 (7%)	31 (3%)	3	7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ARG
1	A	373	PRO
1	A	375	ASP
1	A	416	ALA
1	A	435	PRO
1	A	465	PHE
1	A	466	PRO
1	B	235	MET
1	B	236	PRO
1	B	416	ALA
1	B	435	PRO
1	A	45	ILE
1	A	75	VAL
1	A	236	PRO
1	A	263	ALA
1	A	374	THR
1	A	410	ASP
1	B	259	MET
1	B	288	LYS
1	B	483	SER
1	A	268	GLY
1	A	270	LEU
1	A	437	ILE
1	B	75	VAL
1	B	437	ILE
1	B	359	LEU
1	A	409	PRO
1	B	376	GLY
1	B	433	VAL
1	A	408	GLY
1	B	409	PRO

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	279/393 (71%)	277 (99%)	2 (1%)	76 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	286/393 (73%)	284 (99%)	2 (1%)	76	87
All	All	565/786 (72%)	561 (99%)	4 (1%)	76	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	324	THR
1	B	150	ARG
1	B	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	B	390	GLN

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 [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 ⓘ

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	485/532 (91%)	1.72	155 (31%)  	15, 27, 43, 57	0
1	B	473/532 (88%)	1.60	127 (26%)  	15, 26, 42, 62	0
All	All	958/1064 (90%)	1.66	282 (29%)  	15, 27, 43, 62	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	GLY	7.0
1	B	435	PRO	6.6
1	B	375	ASP	5.9
1	A	434	ILE	5.5
1	A	364	VAL	5.3
1	A	275	THR	4.9
1	A	269	ALA	4.9
1	B	434	ILE	4.9
1	A	518	ALA	4.8
1	B	364	VAL	4.8
1	A	268	GLY	4.8
1	B	374	THR	4.7
1	A	235	MET	4.5
1	A	356	ALA	4.5
1	B	373	PRO	4.5
1	A	355	ASP	4.5
1	A	365	GLY	4.4
1	B	408	GLY	4.4
1	A	435	PRO	4.4
1	A	386	SER	4.2
1	B	355	ASP	4.1
1	A	33	THR	4.0
1	B	436	GLY	3.9
1	A	274	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	74	ALA	3.9
1	A	61	ALA	3.8
1	A	187	LEU	3.8
1	B	359	LEU	3.8
1	A	250	ALA	3.8
1	A	363	THR	3.8
1	A	261	GLU	3.7
1	A	211	THR	3.7
1	B	61	ALA	3.7
1	A	411	LEU	3.7
1	A	516	ASP	3.6
1	A	384	PHE	3.6
1	B	274	GLY	3.6
1	A	506	GLY	3.6
1	B	368	TRP	3.6
1	A	366	GLN	3.6
1	B	358	GLY	3.6
1	B	409	PRO	3.6
1	A	59	LEU	3.6
1	A	309	THR	3.6
1	B	378	ASP	3.5
1	A	265	ALA	3.5
1	A	94	ASP	3.5
1	A	511	PRO	3.4
1	B	96	ALA	3.4
1	A	378	ASP	3.4
1	A	84	GLY	3.4
1	A	267	GLY	3.4
1	A	432	THR	3.4
1	A	46	GLU	3.4
1	B	517	TRP	3.4
1	A	358	GLY	3.3
1	A	479	ALA	3.3
1	A	40	ASP	3.3
1	A	73	GLY	3.3
1	A	375	ASP	3.3
1	A	273	SER	3.3
1	B	482	ALA	3.2
1	B	433	VAL	3.2
1	B	257	ASP	3.2
1	A	47	GLY	3.2
1	A	374	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	186	GLU	3.2
1	A	373	PRO	3.2
1	B	258	PRO	3.2
1	B	437	ILE	3.2
1	B	294	THR	3.2
1	A	484	ASP	3.1
1	B	480	THR	3.1
1	B	50	ASP	3.1
1	B	98	VAL	3.1
1	B	415	TRP	3.1
1	A	362	ALA	3.1
1	A	410	ASP	3.1
1	B	35	ALA	3.1
1	B	497	ALA	3.1
1	A	439	ASP	3.1
1	B	377	MET	3.1
1	A	270	LEU	3.1
1	B	471	ALA	3.0
1	A	354	GLY	3.0
1	A	359	LEU	3.0
1	A	257	ASP	3.0
1	A	512	SER	3.0
1	B	73	GLY	3.0
1	B	212	LYS	3.0
1	A	63	THR	3.0
1	B	303	GLY	3.0
1	A	291	ASP	3.0
1	A	62	ARG	2.9
1	A	368	TRP	2.9
1	A	147	ASP	2.9
1	A	158	VAL	2.9
1	B	63	THR	2.9
1	B	383	GLY	2.9
1	A	214	ASP	2.9
1	B	362	ALA	2.9
1	A	262	THR	2.9
1	B	49	ALA	2.9
1	B	132	SER	2.9
1	A	35	ALA	2.9
1	A	281	GLU	2.8
1	A	85	PRO	2.8
1	B	252	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	417	ASN	2.8
1	B	194	THR	2.8
1	A	75	VAL	2.8
1	A	21	ALA	2.8
1	A	109	PHE	2.8
1	A	416	ALA	2.8
1	B	235	MET	2.8
1	B	516	ASP	2.8
1	A	336	VAL	2.7
1	A	497	ALA	2.7
1	A	517	TRP	2.7
1	A	213	ASP	2.7
1	B	419	PRO	2.7
1	B	348	VAL	2.7
1	A	96	ALA	2.7
1	A	370	TYR	2.7
1	A	104	ASP	2.7
1	A	178	SER	2.7
1	A	216	ARG	2.7
1	A	453	THR	2.7
1	A	337	SER	2.7
1	B	100	VAL	2.7
1	A	376	GLY	2.7
1	A	514	GLU	2.7
1	A	172	ALA	2.6
1	A	360	ALA	2.6
1	B	381	ALA	2.6
1	A	276	PRO	2.6
1	B	454	LEU	2.6
1	A	42	SER	2.6
1	B	307	GLY	2.6
1	B	365	GLY	2.6
1	B	457	LEU	2.6
1	B	255	ILE	2.6
1	A	79	ARG	2.6
1	A	162	ILE	2.6
1	A	255	ILE	2.6
1	A	515	ILE	2.6
1	B	385	VAL	2.6
1	A	28	ALA	2.6
1	B	234	ASP	2.6
1	B	376	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	59	LEU	2.6
1	B	422	VAL	2.6
1	A	77	ALA	2.6
1	A	106	ALA	2.6
1	A	125	ALA	2.6
1	A	513	GLY	2.5
1	B	18	PRO	2.5
1	A	144	VAL	2.5
1	A	192	GLU	2.5
1	B	410	ASP	2.5
1	B	451	SER	2.5
1	B	498	LEU	2.5
1	A	31	GLN	2.5
1	B	372	THR	2.5
1	B	342	ASP	2.5
1	A	258	PRO	2.5
1	A	307	GLY	2.5
1	B	84	GLY	2.5
1	A	215	TYR	2.5
1	B	223	ALA	2.5
1	B	319	ASP	2.5
1	A	466	PRO	2.5
1	B	204	GLY	2.5
1	B	23	VAL	2.5
1	B	297	PHE	2.5
1	B	25	ALA	2.5
1	B	90	ALA	2.5
1	B	407	THR	2.5
1	B	21	ALA	2.4
1	A	407	THR	2.4
1	B	363	THR	2.4
1	B	432	THR	2.4
1	B	188	HIS	2.4
1	A	115	LEU	2.4
1	B	187	LEU	2.4
1	A	32	ALA	2.4
1	A	191	PRO	2.4
1	B	144	VAL	2.4
1	B	230	VAL	2.4
1	B	53	SER	2.4
1	B	232	GLU	2.4
1	B	479	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	131	VAL	2.4
1	A	48	GLU	2.4
1	A	263	ALA	2.4
1	A	464	ALA	2.4
1	A	372	THR	2.4
1	B	360	ALA	2.3
1	A	157	THR	2.3
1	B	19	LEU	2.3
1	A	371	VAL	2.3
1	B	75	VAL	2.3
1	A	509	PHE	2.3
1	B	192	GLU	2.3
1	A	43	THR	2.3
1	A	236	PRO	2.3
1	A	166	ALA	2.3
1	B	106	ALA	2.3
1	A	397	ASP	2.3
1	B	278	LEU	2.3
1	A	415	TRP	2.3
1	B	133	ILE	2.3
1	A	256	THR	2.3
1	A	266	THR	2.3
1	A	436	GLY	2.3
1	A	290	HIS	2.3
1	B	405	TYR	2.3
1	A	74	ALA	2.2
1	B	331	LEU	2.2
1	B	62	ARG	2.2
1	B	322	HIS	2.2
1	A	30	GLU	2.2
1	B	314	LEU	2.2
1	B	124	ASP	2.2
1	B	236	PRO	2.2
1	A	97	SER	2.2
1	B	215	TYR	2.2
1	A	452	GLU	2.2
1	B	54	ALA	2.2
1	A	41	ALA	2.2
1	B	134	GLU	2.2
1	B	299	ALA	2.2
1	A	348	VAL	2.2
1	A	379	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	495	VAL	2.2
1	A	200	THR	2.2
1	B	275	THR	2.2
1	B	490	SER	2.2
1	A	86	ALA	2.2
1	B	136	ALA	2.2
1	B	366	GLN	2.1
1	A	440	ALA	2.1
1	B	97	SER	2.1
1	A	380	ARG	2.1
1	B	461	GLU	2.1
1	A	409	PRO	2.1
1	A	418	GLY	2.1
1	B	420	THR	2.1
1	A	331	LEU	2.1
1	A	29	ILE	2.1
1	A	237	SER	2.1
1	B	504	SER	2.1
1	B	510	HIS	2.1
1	A	219	VAL	2.1
1	A	342	ASP	2.1
1	B	214	ASP	2.1
1	A	165	ALA	2.1
1	A	460	ILE	2.1
1	B	272	GLU	2.1
1	B	340	ILE	2.1
1	B	386	SER	2.1
1	A	322	HIS	2.1
1	A	142	ARG	2.1
1	A	194	THR	2.1
1	B	205	ASP	2.1
1	B	455	ARG	2.1
1	B	484	ASP	2.1
1	A	218	ILE	2.1
1	B	396	ALA	2.1
1	B	426	TYR	2.1
1	A	189	SER	2.0
1	B	456	SER	2.0
1	A	417	ASN	2.0
1	B	118	LEU	2.0
1	A	465	PHE	2.0
1	A	353	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	445	VAL	2.0
1	B	421	SER	2.0
1	A	177	LEU	2.0
1	B	107	GLY	2.0
1	A	507	ILE	2.0
1	B	296	ASP	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.