



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:04 PM UTC

PDB ID : 2WVY / pdb_00002wvy
Title : STRUCTURE OF THE FAMILY GH92 INVERTING MANNOSIDASE
BT2199 FROM BACTEROIDES THETA IOTAOMICRON VPI-5482
Authors : Suits, M.D.L.; Zhu, Y.; Thompson, A.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-10-21
Resolution : 2.26 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

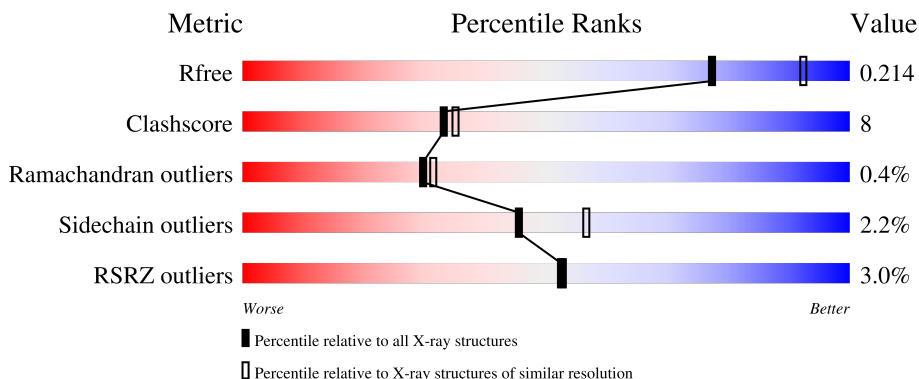
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	737	3% 82% 16% ..
1	B	737	4% 84% 13% ..
1	C	737	2% 84% 15% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18542 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 ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	731	Total	C	N	O	S	0	10	0
			5839	3723	968	1118	30			
1	B	729	Total	C	N	O	S	0	8	0
			5810	3706	964	1110	30			
1	C	730	Total	C	N	O	S	0	10	0
			5813	3709	967	1107	30			

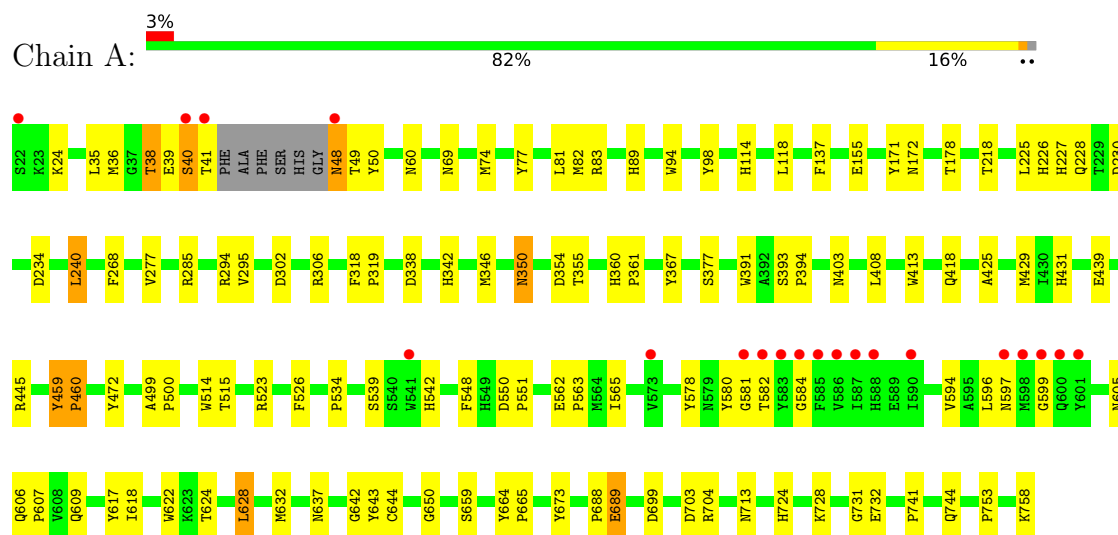
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	428	Total	O	0	0
			428	428		
2	B	311	Total	O	0	0
			311	311		
2	C	341	Total	O	0	0
			341	341		

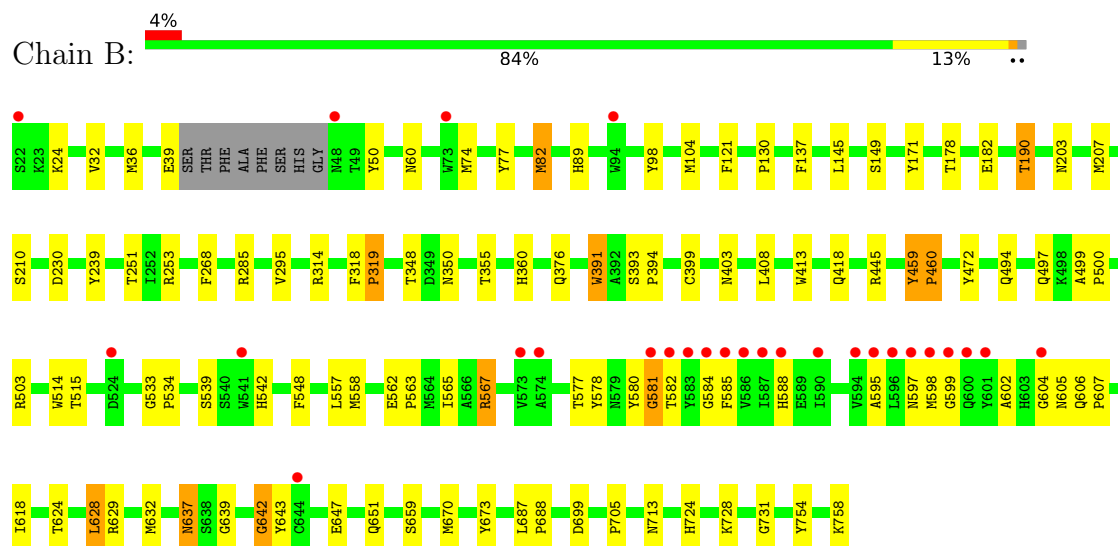
3 Residue-property plots [i](#)

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.

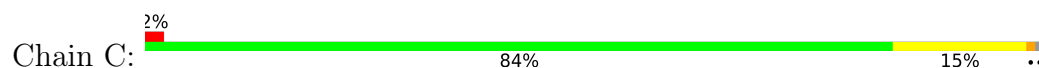
• Molecule 1: ALPHA-1,2-MANNOSIDASE

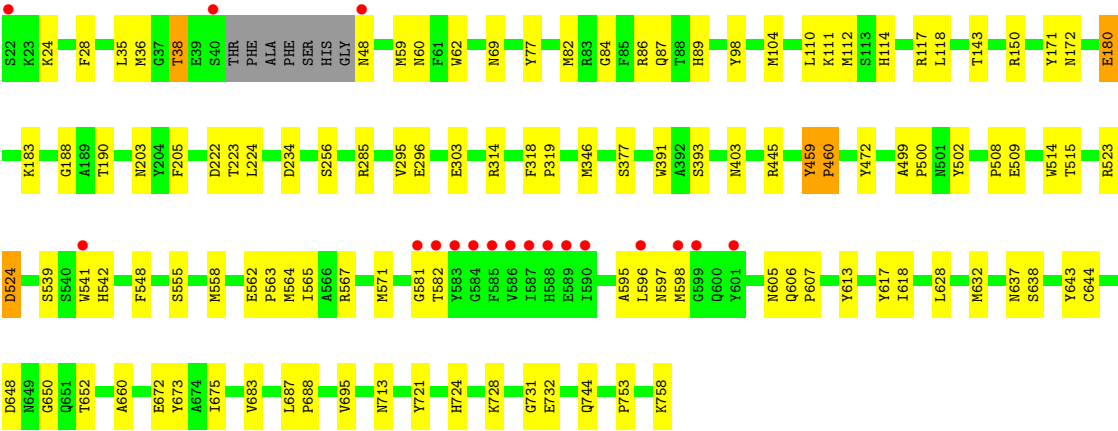


• Molecule 1: ALPHA-1,2-MANNOSIDASE



• Molecule 1: ALPHA-1,2-MANNOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.93Å 163.76Å 115.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 2.26 115.47 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.3 (115.47-2.26) 98.6 (115.47-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.169 , 0.207 0.177 , 0.214	Depositor DCC
R_{free} test set	6823 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18542	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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

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	0.58	0/6050	0.83	2/8239 (0.0%)
1	B	0.53	0/6015	0.81	4/8193 (0.0%)
1	C	0.55	0/6024	0.81	2/8206 (0.0%)
All	All	0.55	0/18089	0.81	8/24638 (0.0%)

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	6
1	B	0	3
1	C	0	4
All	All	0	13

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GLU	CA-C-N	6.02	125.73	119.05
1	C	180	GLU	C-N-CA	6.02	125.73	119.05
1	A	578	TYR	CB-CA-C	-5.68	110.05	116.63
1	B	584	GLY	N-CA-C	5.65	117.81	112.04
1	B	578	TYR	CB-CA-C	-5.24	110.55	116.63
1	A	394	PRO	N-CA-C	5.15	123.08	112.47
1	B	597	ASN	N-CA-C	-5.14	105.17	111.75
1	B	642	GLY	N-CA-C	5.00	118.93	112.83

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	PHE	Peptide,Mainchain
1	A	393	SER	Peptide,Mainchain
1	A	459	TYR	Peptide,Mainchain
1	B	318	PHE	Peptide
1	B	393	SER	Peptide
1	B	459	TYR	Peptide
1	C	318	PHE	Peptide
1	C	393	SER	Peptide,Mainchain
1	C	459	TYR	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	5839	0	5378	91	0
1	B	5810	0	5346	88	0
1	C	5813	0	5350	85	0
2	A	428	0	0	10	0
2	B	311	0	0	5	0
2	C	341	0	0	6	0
All	All	18542	0	16074	263	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 8.

All (263) 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:B:602:ALA:CB	1:B:647:GLU:OE1	1.74	1.32
1:B:602:ALA:HB1	1:B:647:GLU:OE1	0.97	1.13
1:C:314[A]:ARG:HH22	1:C:650:GLY:HA3	1.10	1.12
1:B:350:ASN:HD21	1:B:355:THR:HG21	1.18	1.08
1:A:60:ASN:ND2	1:A:89:HIS:HE1	1.58	1.00
1:A:60:ASN:HD22	1:A:89:HIS:CE1	1.80	1.00
1:A:539:SER:H	1:A:542:HIS:HD2	1.07	1.00
1:C:539:SER:H	1:C:542:HIS:HD2	1.04	0.98
1:B:60:ASN:HD22	1:B:89:HIS:HE1	1.05	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:HG23	1:A:77:TYR:HB2	1.51	0.93
1:C:60:ASN:HD22	1:C:89:HIS:CE1	1.86	0.93
1:A:60:ASN:HD22	1:A:89:HIS:HE1	0.95	0.93
1:C:60:ASN:HD22	1:C:89:HIS:HE1	1.03	0.91
1:B:60:ASN:ND2	1:B:89:HIS:HE1	1.67	0.91
1:B:60:ASN:HD22	1:B:89:HIS:CE1	1.88	0.91
1:B:350:ASN:HD21	1:B:355:THR:CG2	1.85	0.89
1:A:48:ASN:N	2:A:2015:HOH:O	2.06	0.89
1:B:539:SER:H	1:B:542:HIS:HD2	1.21	0.86
1:C:555:SER:HA	1:C:564:MET:HE3	1.59	0.85
1:B:178[B]:THR:HG22	1:B:230:ASP:OD2	1.75	0.85
1:A:178[B]:THR:HG22	1:A:230:ASP:OD1	1.78	0.84
1:C:60:ASN:ND2	1:C:89:HIS:HE1	1.74	0.84
1:C:314[A]:ARG:HH22	1:C:650:GLY:CA	1.90	0.80
1:C:314[A]:ARG:NH2	1:C:650:GLY:HA3	1.94	0.80
1:B:637:ASN:OD1	2:B:2265:HOH:O	2.00	0.80
1:A:354[B]:ASP:OD2	1:A:606:GLN:NE2	2.15	0.80
1:C:758:LYS:CD	2:C:2337:HOH:O	2.29	0.79
1:B:350:ASN:ND2	1:B:355:THR:HG21	1.97	0.79
1:C:35:LEU:O	1:C:38:THR:HB	1.83	0.78
1:B:403:ASN:HD21	1:B:445:ARG:HE	1.31	0.76
1:A:403:ASN:HD21	1:A:445:ARG:HE	1.30	0.76
1:A:637:ASN:ND2	2:A:2357:HOH:O	2.10	0.76
1:A:60:ASN:ND2	1:A:89:HIS:CE1	2.47	0.75
1:C:38:THR:CG2	1:C:77:TYR:HB2	2.15	0.75
1:A:758:LYS:CD	2:A:2425:HOH:O	2.34	0.75
1:B:628:LEU:O	1:B:632[B]:MET:HG2	1.87	0.74
1:C:38:THR:HG22	1:C:77:TYR:HB2	1.70	0.73
1:A:38:THR:CG2	1:A:77:TYR:HB2	2.19	0.72
1:A:94:TRP:NE1	2:A:2043:HOH:O	2.24	0.71
1:C:539:SER:H	1:C:542:HIS:CD2	1.97	0.70
1:A:539:SER:H	1:A:542:HIS:CD2	2.00	0.70
1:C:509:GLU:OE1	1:C:509:GLU:N	2.24	0.70
1:B:605:ASN:ND2	1:B:607:PRO:HD2	2.06	0.70
1:A:403:ASN:ND2	1:A:445:ARG:HE	1.90	0.69
1:A:403:ASN:HD22	1:A:445:ARG:HH21	1.41	0.68
1:B:580:TYR:C	1:B:582:THR:N	2.50	0.68
1:C:403:ASN:HD21	1:C:445:ARG:HE	1.42	0.68
1:A:41:THR:CB	1:A:48:ASN:OD1	2.42	0.68
1:B:637:ASN:HD22	1:B:639:GLY:H	1.41	0.66
1:B:628:LEU:HD11	1:B:659:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASN:ND2	1:B:445:ARG:HE	1.93	0.65
1:A:628:LEU:O	1:A:632[B]:MET:HG2	1.96	0.65
1:B:624:THR:O	1:B:628:LEU:HB2	1.97	0.65
1:B:82[A]:MET:HE3	1:B:137:PHE:CE1	2.30	0.65
1:B:403:ASN:HD22	1:B:445:ARG:HH21	1.45	0.65
1:B:89:HIS:HD2	1:B:98:TYR:O	1.81	0.64
1:B:604:GLY:O	1:B:651:GLN:NE2	2.28	0.64
1:C:555:SER:CA	1:C:564:MET:HE3	2.28	0.64
1:C:672:GLU:OE2	2:C:2290:HOH:O	2.15	0.64
1:B:580:TYR:C	1:B:582:THR:H	2.05	0.63
1:C:637:ASN:ND2	2:C:2276:HOH:O	2.11	0.63
1:B:595:ALA:O	1:B:598:MET:CB	2.46	0.63
1:C:403:ASN:ND2	1:C:445:ARG:HE	1.97	0.62
1:C:524:ASP:OD1	1:C:524:ASP:N	2.28	0.62
1:A:50:TYR:CG	1:A:74:MET:HE3	2.36	0.61
1:C:36:MET:HE2	1:C:643:TYR:CZ	2.35	0.61
1:B:319:PRO:HB3	1:B:350:ASN:HB2	1.83	0.61
1:C:605:ASN:HD21	1:C:607:PRO:HG2	1.66	0.60
1:C:403:ASN:HD22	1:C:445:ARG:HH21	1.49	0.60
1:B:565:ILE:HG13	1:B:618:ILE:HD12	1.84	0.59
1:C:28:PHE:HZ	1:C:296:GLU:HG2	1.66	0.59
1:C:581:GLY:O	1:C:582:THR:C	2.45	0.59
1:C:539:SER:N	1:C:542:HIS:HD2	1.88	0.59
1:A:581:GLY:O	1:A:584:GLY:N	2.26	0.58
1:B:32:VAL:HG11	1:B:130:PRO:HG3	1.86	0.58
1:A:155:GLU:HG2	1:A:277:VAL:HG11	1.84	0.57
1:A:713:ASN:ND2	1:A:732:GLU:H	2.01	0.57
1:A:413:TRP:CE3	1:A:418:GLN:HG2	2.39	0.57
1:B:60:ASN:ND2	1:B:89:HIS:CE1	2.57	0.57
1:B:628:LEU:HD13	1:B:632[A]:MET:HE2	1.87	0.56
1:A:50:TYR:CD2	1:A:74:MET:CE	2.89	0.56
1:A:713:ASN:HD21	1:A:731:GLY:HA3	1.70	0.56
1:A:459:TYR:CG	1:A:460:PRO:HA	2.41	0.56
1:B:514:TRP:CG	1:B:515:THR:H	2.24	0.56
1:B:580:TYR:O	1:B:582:THR:N	2.39	0.55
1:C:558:MET:HG2	1:C:567:ARG:NH1	2.21	0.55
1:B:687:LEU:HB3	1:B:688:PRO:HD2	1.88	0.55
1:B:494:GLN:O	1:B:497:GLN:HB2	2.07	0.55
1:A:226:HIS:O	1:A:227:HIS:HB2	2.07	0.54
1:B:562:GLU:HB3	1:B:563:PRO:HD3	1.89	0.54
1:C:628:LEU:O	1:C:632[B]:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:ASN:HD21	1:B:731:GLY:HA3	1.73	0.54
1:B:628:LEU:CD1	1:B:632[A]:MET:HE2	2.38	0.54
1:B:687:LEU:HB3	1:B:688:PRO:CD	2.38	0.54
1:C:60:ASN:ND2	1:C:89:HIS:CE1	2.60	0.54
1:C:596:LEU:O	1:C:597:ASN:C	2.49	0.54
1:A:350:ASN:HD21	1:A:355:THR:HG21	1.72	0.53
1:A:594:VAL:HA	1:A:597:ASN:HB2	1.90	0.53
1:A:606:GLN:HG3	1:A:609:GLN:NE2	2.24	0.53
1:A:89:HIS:HD2	1:A:98:TYR:O	1.92	0.53
1:A:562:GLU:HB3	1:A:563:PRO:CD	2.39	0.53
1:A:605:ASN:ND2	1:A:607:PRO:HD2	2.23	0.53
1:B:637:ASN:ND2	1:B:642:GLY:HA2	2.24	0.53
1:A:306:ARG:HD2	2:A:2007:HOH:O	2.09	0.52
1:C:648:ASP:OD2	1:C:652:THR:OG1	2.23	0.52
1:B:637:ASN:ND2	1:B:639:GLY:H	2.08	0.52
1:C:314[A]:ARG:NH2	1:C:650:GLY:CA	2.64	0.52
1:C:713:ASN:ND2	1:C:732:GLU:H	2.07	0.52
1:A:69:ASN:H	1:A:114:HIS:CD2	2.28	0.52
1:C:180:GLU:OE2	1:C:183:LYS:NZ	2.43	0.52
1:C:28:PHE:CZ	1:C:296:GLU:HG2	2.44	0.52
1:B:558:MET:HG2	1:B:567:ARG:NH1	2.24	0.51
1:B:190:THR:HG23	1:B:203:ASN:HB3	1.93	0.51
1:A:606:GLN:HA	1:A:609:GLN:NE2	2.25	0.51
1:C:459:TYR:CG	1:C:460:PRO:HA	2.46	0.51
1:B:637:ASN:HD22	1:B:637:ASN:C	2.19	0.51
1:B:50:TYR:CG	1:B:74:MET:HE3	2.46	0.50
1:B:580:TYR:O	1:B:581:GLY:C	2.55	0.50
1:C:117:ARG:C	1:C:118:LEU:HD22	2.36	0.50
1:A:294:ARG:HD2	1:A:367:TYR:CE1	2.47	0.50
1:C:562:GLU:HB3	1:C:563:PRO:HD3	1.94	0.50
1:C:285:ARG:HD3	2:C:2110:HOH:O	2.12	0.49
1:A:624:THR:O	1:A:628:LEU:HB2	2.12	0.49
1:A:413:TRP:CD2	1:A:418:GLN:HG2	2.47	0.49
1:B:606:GLN:HB2	1:B:607:PRO:HD3	1.95	0.49
1:A:673:TYR:OH	1:A:724:HIS:HD2	1.94	0.49
1:A:82[B]:MET:HE3	1:A:137:PHE:CE1	2.48	0.48
1:A:582:THR:C	1:A:584:GLY:H	2.21	0.48
1:C:112:MET:HG3	1:C:224:LEU:HD13	1.94	0.48
1:B:82[A]:MET:HE3	1:B:137:PHE:HE1	1.78	0.48
1:B:562:GLU:HB3	1:B:563:PRO:CD	2.44	0.48
1:A:637:ASN:OD1	1:A:642:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:TYR:OH	1:B:724:HIS:HD2	1.97	0.48
1:C:595:ALA:O	1:C:598:MET:CB	2.62	0.48
1:A:36:MET:HE2	1:A:643:TYR:CZ	2.49	0.48
1:B:602:ALA:HB2	1:B:647:GLU:OE1	1.96	0.48
1:C:555:SER:N	1:C:564:MET:HE1	2.29	0.48
1:C:499:ALA:N	1:C:500:PRO:CD	2.77	0.47
1:C:523:ARG:HD2	2:C:2237:HOH:O	2.13	0.47
1:B:268:PHE:C	1:B:268:PHE:CD2	2.92	0.47
1:C:172:ASN:HA	1:C:234:ASP:O	2.14	0.47
1:A:565:ILE:HG13	1:A:618:ILE:HD12	1.97	0.47
1:A:346:MET:HA	1:A:377[A]:SER:HB2	1.97	0.47
1:C:713:ASN:HD21	1:C:732:GLU:H	1.62	0.47
1:A:581:GLY:O	1:A:582:THR:C	2.58	0.47
1:B:82[B]:MET:HG2	1:B:104:MET:HE1	1.97	0.47
1:C:69:ASN:H	1:C:114:HIS:CD2	2.33	0.47
1:C:541:TRP:NE1	1:C:571:MET:HE3	2.30	0.47
1:C:38:THR:HG23	1:C:77:TYR:HB2	1.92	0.47
1:C:303:GLU:OE2	1:C:638:SER:N	2.45	0.47
1:C:24:LYS:HB2	1:C:24:LYS:HE3	1.78	0.46
1:C:110:LEU:O	1:C:111:LYS:HD3	2.16	0.46
1:B:39:GLU:HB2	1:B:77:TYR:HB3	1.98	0.46
1:B:376:GLN:NE2	2:B:2180:HOH:O	2.49	0.46
1:C:596:LEU:C	1:C:598:MET:N	2.70	0.46
1:A:172:ASN:HA	1:A:234:ASP:O	2.16	0.46
1:A:664:TYR:CG	1:A:665:PRO:HD2	2.50	0.46
1:C:62:TRP:HA	1:C:86:ARG:O	2.16	0.46
1:C:713:ASN:HD21	1:C:731:GLY:HA3	1.81	0.46
1:C:617:TYR:CZ	1:C:753:PRO:HG2	2.51	0.46
1:C:673:TYR:OH	1:C:724:HIS:HD2	1.98	0.46
1:A:515:THR:HG21	1:A:534:PRO:HG3	1.99	0.45
1:A:459:TYR:CD1	1:A:460:PRO:HA	2.51	0.45
1:A:562:GLU:HB3	1:A:563:PRO:HD3	1.98	0.45
1:B:670:MET:HE3	1:B:754:TYR:CG	2.52	0.45
1:B:360:HIS:CD2	1:B:408:LEU:HD21	2.51	0.45
1:C:188:GLY:HA3	1:C:205:PHE:CZ	2.52	0.45
1:B:459:TYR:CD1	1:B:460:PRO:HA	2.51	0.45
1:A:81:LEU:HD11	1:C:744:GLN:HG3	1.99	0.45
1:B:182:GLU:CD	1:B:182:GLU:H	2.24	0.45
1:B:595:ALA:O	1:B:599:GLY:N	2.45	0.45
1:B:699:ASP:HB2	2:B:2303:HOH:O	2.16	0.45
1:B:24:LYS:HB2	1:B:24:LYS:HE3	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HE2	1:C:643:TYR:CE2	2.51	0.45
1:C:605:ASN:ND2	1:C:607:PRO:HG2	2.30	0.45
1:A:50:TYR:CG	1:A:74:MET:CE	2.99	0.45
1:B:239:TYR:CD1	1:B:239:TYR:C	2.95	0.45
1:C:59:MET:HE2	1:C:150:ARG:HG2	1.99	0.45
1:A:622:TRP:HB2	1:A:741:PRO:HB3	1.98	0.45
1:B:207:MET:HA	1:B:253:ARG:O	2.17	0.45
1:B:285:ARG:HD3	2:B:2138:HOH:O	2.17	0.44
1:C:687:LEU:HB3	1:C:688:PRO:HD2	1.99	0.44
1:B:595:ALA:O	1:B:598:MET:N	2.50	0.44
1:C:445:ARG:HG3	1:C:472:TYR:CZ	2.52	0.44
1:A:268:PHE:CD2	1:A:268:PHE:C	2.96	0.44
1:B:145:LEU:N	1:B:145:LEU:HD23	2.32	0.44
1:C:606:GLN:N	1:C:607:PRO:HD2	2.32	0.44
1:A:744:GLN:HG3	2:A:2418:HOH:O	2.16	0.44
1:A:431:HIS:HE1	2:A:2271:HOH:O	2.00	0.44
1:B:210:SER:HB3	1:B:251:THR:HB	1.99	0.44
1:C:508:PRO:HD2	1:C:509:GLU:OE1	2.18	0.44
1:A:499:ALA:N	1:A:500:PRO:CD	2.80	0.43
1:B:391:TRP:CD1	1:B:399:CYS:HB3	2.52	0.43
1:A:459:TYR:HB3	1:A:515:THR:OG1	2.18	0.43
1:C:500:PRO:HA	1:C:502:TYR:CE2	2.53	0.43
1:A:580:TYR:O	1:A:581:GLY:C	2.59	0.43
1:A:582:THR:C	1:A:584:GLY:N	2.74	0.43
1:B:50:TYR:CG	1:B:74:MET:CE	3.02	0.43
1:B:459:TYR:CG	1:B:460:PRO:HA	2.53	0.43
1:C:89:HIS:HD2	1:C:98:TYR:O	2.02	0.43
1:C:683:VAL:CG2	1:C:695:VAL:HB	2.49	0.43
1:A:431:HIS:HD2	2:A:2272:HOH:O	2.01	0.43
1:C:82[B]:MET:HE2	1:C:82[B]:MET:HB2	1.92	0.43
1:A:24:LYS:HB2	1:A:24:LYS:HE3	1.84	0.43
1:A:605:ASN:ND2	1:A:607:PRO:HG2	2.34	0.43
1:A:699:ASP:HB2	2:A:2396:HOH:O	2.17	0.43
1:B:585:PHE:O	1:B:588:HIS:N	2.50	0.43
1:C:459:TYR:HB3	1:C:515:THR:OG1	2.18	0.43
1:A:514:TRP:CZ2	1:A:526:PHE:HA	2.54	0.43
1:A:580:TYR:C	1:A:582:THR:N	2.77	0.42
1:B:503:ARG:HG2	1:B:557:LEU:HD21	2.02	0.42
1:C:223:THR:HG22	1:C:224:LEU:O	2.19	0.42
1:A:550:ASP:N	1:A:551:PRO:HD3	2.34	0.42
1:A:218:THR:HG23	1:A:228:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:LEU:HB3	1:C:688:PRO:CD	2.50	0.42
1:B:629:ARG:NH1	1:B:705:PRO:HA	2.34	0.42
1:B:82[A]:MET:HE2	1:B:121:PHE:CD2	2.55	0.42
1:B:499:ALA:N	1:B:500:PRO:CD	2.83	0.42
1:A:35:LEU:O	1:A:38:THR:HB	2.18	0.42
1:B:36:MET:HE2	1:B:643:TYR:CZ	2.54	0.42
1:C:514:TRP:CG	1:C:515:THR:H	2.37	0.42
1:C:632[B]:MET:HE1	1:C:660:ALA:HB2	2.02	0.42
1:A:360:HIS:CD2	1:A:408:LEU:HD21	2.54	0.42
1:B:670:MET:HE3	1:B:754:TYR:CD1	2.54	0.42
1:A:338:ASP:OD1	1:A:342:HIS:HE1	2.03	0.41
1:A:643:TYR:CE1	1:A:650:GLY:HA2	2.54	0.41
1:C:675:ILE:HD12	1:C:721:TYR:N	2.35	0.41
1:A:617:TYR:CE1	1:A:753:PRO:HB2	2.55	0.41
1:C:60:ASN:HB2	2:C:2057:HOH:O	2.21	0.41
1:B:514:TRP:CD1	1:B:515:THR:H	2.38	0.41
1:C:190:THR:HG23	1:C:203:ASN:HB3	2.03	0.41
1:C:346:MET:HA	1:C:377[A]:SER:HB2	2.01	0.41
1:C:555:SER:N	1:C:564:MET:CE	2.83	0.41
1:A:350:ASN:HD22	1:A:350:ASN:HA	1.60	0.41
1:A:425:ALA:O	1:A:429:MET:HG3	2.20	0.41
1:B:514:TRP:CG	1:B:515:THR:N	2.88	0.41
1:A:39:GLU:O	1:A:40:SER:HB2	2.19	0.41
1:C:613:TYR:CE1	1:C:628:LEU:HD11	2.56	0.41
1:A:83:ARG:HG2	1:A:118:LEU:HD13	2.02	0.41
1:A:514:TRP:CG	1:A:515:THR:H	2.38	0.41
1:A:703:ASP:OD1	1:A:704:ARG:HG3	2.20	0.41
1:B:533:GLY:HA3	1:B:534:PRO:HD2	1.91	0.41
1:B:558:MET:HE2	1:B:567:ARG:CZ	2.50	0.41
1:A:285:ARG:HD3	2:A:2184:HOH:O	2.20	0.41
1:A:688:PRO:C	1:A:689:GLU:CG	2.93	0.41
1:C:84:GLY:HA2	1:C:104:MET:SD	2.61	0.41
1:A:240:LEU:N	1:A:240:LEU:HD22	2.35	0.41
1:A:360:HIS:N	1:A:361:PRO:CD	2.83	0.41
1:A:445:ARG:HG3	1:A:472:TYR:CZ	2.56	0.41
1:B:413:TRP:CZ3	1:B:418:GLN:HB3	2.56	0.41
1:B:149:SER:HB3	2:B:2155:HOH:O	2.20	0.41
1:B:348:THR:OG1	1:B:394:PRO:HA	2.21	0.41
1:B:595:ALA:O	1:B:598:MET:CA	2.69	0.41
1:A:302:ASP:O	1:A:306:ARG:HG3	2.22	0.40
1:A:596:LEU:O	1:A:599:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ARG:HG3	1:B:472:TYR:CZ	2.57	0.40
1:C:541:TRP:CD1	1:C:571:MET:HE3	2.55	0.40
1:C:87:GLN:HE22	1:C:256:SER:HB3	1.86	0.40
1:A:628:LEU:HD11	1:A:659:SER:HB3	2.03	0.40
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.58	0.40
1:B:606:GLN:N	1:B:607:PRO:CD	2.84	0.40
1:C:565:ILE:HG13	1:C:618:ILE:HD12	2.04	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	737/737 (100%)	704 (96%)	30 (4%)	3 (0%)	30	31
1	B	733/737 (100%)	707 (96%)	23 (3%)	3 (0%)	30	31
1	C	736/737 (100%)	704 (96%)	30 (4%)	2 (0%)	36	40
All	All	2206/2211 (100%)	2115 (96%)	83 (4%)	8 (0%)	30	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PRO
1	A	40	SER
1	A	460	PRO
1	B	460	PRO
1	C	460	PRO
1	B	319	PRO
1	C	319	PRO
1	B	581	GLY

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	604/620 (97%)	588 (97%)	16 (3%)	40	50
1	B	599/620 (97%)	586 (98%)	13 (2%)	45	56
1	C	598/620 (96%)	587 (98%)	11 (2%)	51	63
All	All	1801/1860 (97%)	1761 (98%)	40 (2%)	45	56

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	48	ASN
1	A	49	THR
1	A	171	TYR
1	A	225	LEU
1	A	240	LEU
1	A	295	VAL
1	A	350	ASN
1	A	391	TRP
1	A	439	GLU
1	A	523	ARG
1	A	548	PHE
1	A	628	LEU
1	A	644	CYS
1	A	689	GLU
1	A	728	LYS
1	B	82[A]	MET
1	B	82[B]	MET
1	B	171	TYR
1	B	190	THR
1	B	295	VAL
1	B	314	ARG
1	B	391	TRP
1	B	548	PHE
1	B	567	ARG
1	B	577	THR

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Mol	Chain	Res	Type
1	B	628	LEU
1	B	637	ASN
1	B	728	LYS
1	C	38	THR
1	C	48	ASN
1	C	143	THR
1	C	171	TYR
1	C	222	ASP
1	C	295	VAL
1	C	391	TRP
1	C	524	ASP
1	C	548	PHE
1	C	644	CYS
1	C	728	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	87	GLN
1	A	89	HIS
1	A	114	HIS
1	A	203	ASN
1	A	228	GLN
1	A	287	GLN
1	A	340	ASN
1	A	342	HIS
1	A	350	ASN
1	A	376	GLN
1	A	403	ASN
1	A	404	ASN
1	A	431	HIS
1	A	434	GLN
1	A	489	GLN
1	A	494	GLN
1	A	542	HIS
1	A	605	ASN
1	A	649	ASN
1	A	713	ASN
1	A	720	ASN
1	A	724	HIS
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	87	GLN
1	B	89	HIS
1	B	114	HIS
1	B	124	GLN
1	B	132	ASN
1	B	203	ASN
1	B	228	GLN
1	B	287	GLN
1	B	340	ASN
1	B	342	HIS
1	B	350	ASN
1	B	376	GLN
1	B	403	ASN
1	B	431	HIS
1	B	434	GLN
1	B	494	GLN
1	B	542	HIS
1	B	637	ASN
1	B	713	ASN
1	B	724	HIS
1	C	60	ASN
1	C	87	GLN
1	C	89	HIS
1	C	114	HIS
1	C	125	GLN
1	C	203	ASN
1	C	287	GLN
1	C	340	ASN
1	C	342	HIS
1	C	376	GLN
1	C	403	ASN
1	C	404	ASN
1	C	431	HIS
1	C	434	GLN
1	C	494	GLN
1	C	510	HIS
1	C	521	ASN
1	C	542	HIS
1	C	605	ASN
1	C	713	ASN
1	C	724	HIS

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	731/737 (99%)	-0.44	20 (2%) 56 57	5, 11, 31, 54	10 (1%)
1	B	729/737 (98%)	-0.31	27 (3%) 45 45	8, 17, 35, 54	8 (1%)
1	C	730/737 (99%)	-0.43	18 (2%) 58 59	8, 14, 33, 56	10 (1%)
All	All	2190/2211 (99%)	-0.39	65 (2%) 52 53	5, 15, 33, 56	28 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	THR	7.4
1	B	585	PHE	6.3
1	B	582	THR	6.3
1	A	584	GLY	5.8
1	A	583	TYR	5.7
1	C	583	TYR	5.2
1	A	586	VAL	5.0
1	C	585	PHE	4.9
1	B	583	TYR	4.8
1	C	584	GLY	4.8
1	B	586	VAL	4.6
1	A	585	PHE	4.4
1	B	600	GLN	4.4
1	B	599	GLY	4.1
1	B	581	GLY	4.0
1	C	582	THR	4.0
1	B	601	TYR	4.0
1	A	40	SER	3.9
1	A	599	GLY	3.8
1	C	599	GLY	3.5
1	A	41	THR	3.5
1	C	48	ASN	3.5
1	A	22	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	581	GLY	3.4
1	C	586	VAL	3.2
1	B	598	MET	3.2
1	B	595	ALA	3.2
1	B	584	GLY	3.1
1	B	588	HIS	3.1
1	B	587	ILE	3.0
1	C	598	MET	3.0
1	C	22	SER	3.0
1	A	48	ASN	3.0
1	A	573	VAL	2.9
1	B	590	ILE	2.8
1	B	73	TRP	2.7
1	A	600	GLN	2.6
1	B	48	ASN	2.5
1	C	588	HIS	2.5
1	C	590	ILE	2.5
1	B	604	GLY	2.5
1	A	587	ILE	2.4
1	A	598	MET	2.4
1	B	573	VAL	2.4
1	B	574	ALA	2.3
1	B	596	LEU	2.3
1	B	594	VAL	2.3
1	B	644	CYS	2.3
1	A	588	HIS	2.3
1	B	524	ASP	2.3
1	A	581	GLY	2.3
1	B	541	TRP	2.3
1	A	590	ILE	2.3
1	A	597	ASN	2.2
1	C	40	SER	2.2
1	B	597	ASN	2.2
1	C	601	TYR	2.2
1	B	22	SER	2.2
1	A	601	TYR	2.1
1	A	541	TRP	2.1
1	C	589	GLU	2.1
1	C	596	LEU	2.0
1	C	587	ILE	2.0
1	B	94	TRP	2.0
1	C	541	TRP	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.