



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:22 AM GMT

PDB ID : 2WVY
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

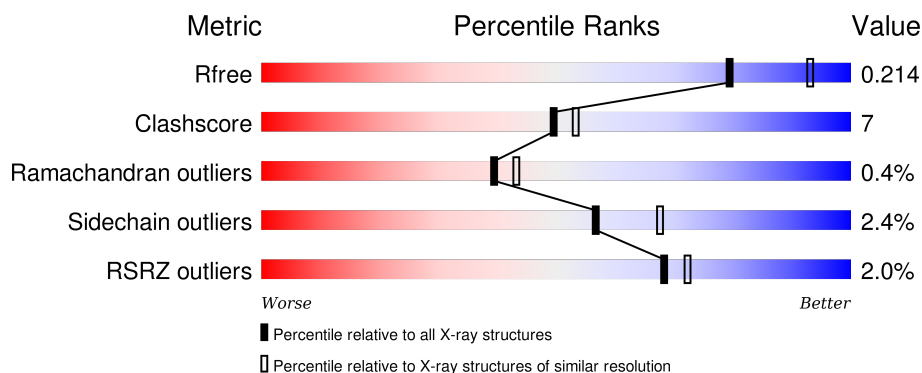
1 Overall quality at a glance

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	B	737	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	C	737	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>

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			

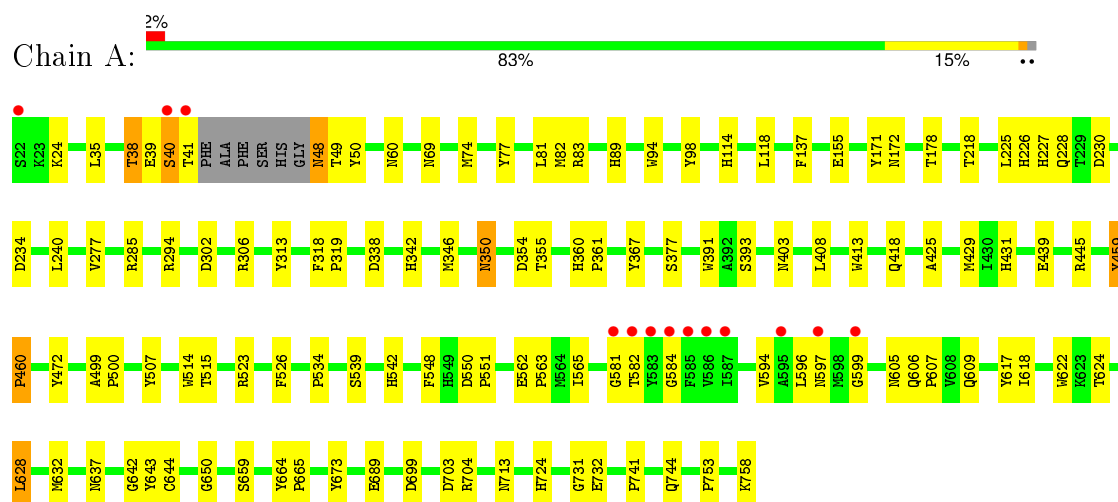
- Molecule 2 is water.

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		

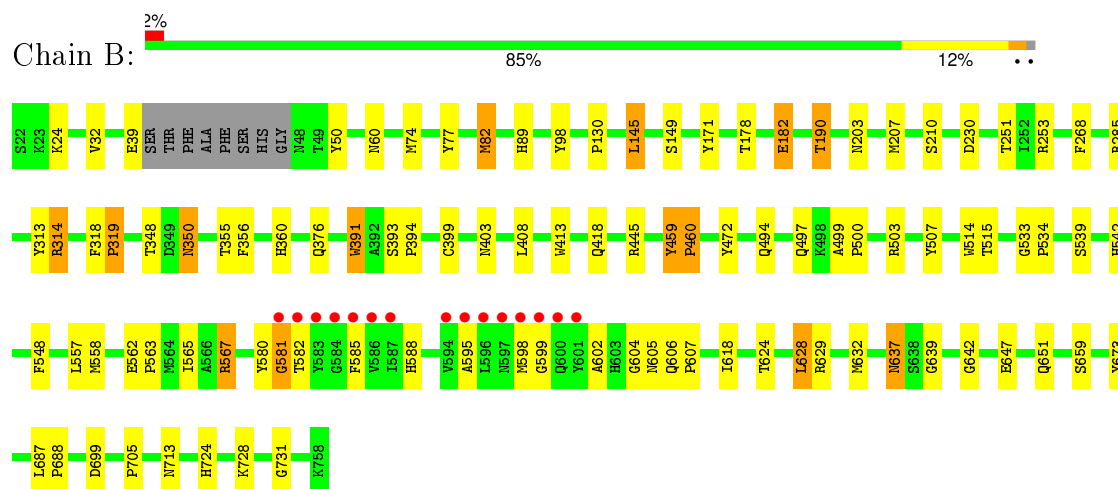
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

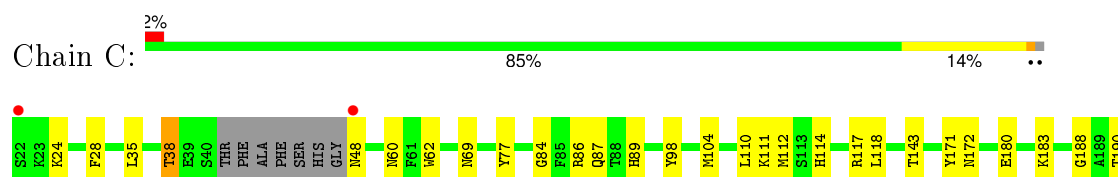
• Molecule 1: ALPHA-1,2-MANNOSIDASE

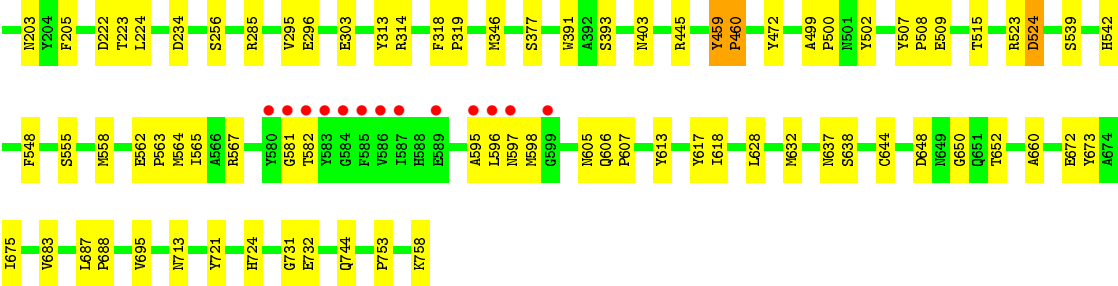


• Molecule 1: ALPHA-1,2-MANNOSIDASE



• Molecule 1: ALPHA-1,2-MANNOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	154.93 Å 163.76 Å 115.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 2.26 47.20 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.3 (115.47-2.26) 98.4 (47.20-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.27 Å)	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	6814 reflections (5.28%)	DCC
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 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 135971 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/6050	0.61	0/8239
1	B	0.43	0/6015	0.58	1/8193 (0.0%)
1	C	0.45	0/6024	0.59	0/8206
All	All	0.46	0/18089	0.59	1/24638 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ARG	NE-CZ-NH1	-5.20	117.70	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	PHE	Mainchain,Peptide
1	A	393	SER	Mainchain,Peptide
1	A	459	TYR	Mainchain,Peptide
1	B	318	PHE	Peptide
1	B	393	SER	Peptide
1	B	459	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	318	PHE	Peptide
1	C	393	SER	Mainchain,Peptide
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	85	0
1	B	5810	0	5346	76	0
1	C	5813	0	5350	78	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	238	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 7.

All (238) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:178[B]:THR:HG22	1:B:230:ASP:OD2	1.75	0.85
1:C:555:SER:HA	1:C:564:MET:HE3	1.59	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: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
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: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:C:672:GLU:OE2	2:C:2290:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:GLY:O	1:B:651:GLN:NE2	2.28	0.64
1:B:580:TYR:C	1:B:582:THR:N	2.50	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:555:SER:CA	1:C:564:MET:HE3	2.29	0.63
1:C:403:ASN:ND2	1:C:445:ARG:HE	1.97	0.62
1:C:524:ASP:N	1:C:524:ASP:OD1	2.28	0.62
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:539:SER:N	1:C:542:HIS:HD2	1.88	0.59
1:B:580:TYR:C	1:B:582:THR:H	2.05	0.59
1:B:32:VAL:HG11	1:B:130:PRO:HG3	1.86	0.58
1:A:581:GLY:O	1:A:584:GLY:N	2.26	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:A:713:ASN:HD21	1:A:731:GLY:HA3	1.70	0.56
1:A:50:TYR:CD2	1:A:74:MET:CE	2.89	0.56
1:A:459:TYR:CG	1:A:460:PRO:HA	2.41	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:C:581:GLY:O	1:C:582:THR:C	2.45	0.54
1:A:226:HIS:O	1:A:227:HIS:HB2	2.07	0.54
1:C:628:LEU:O	1:C:632[B]:MET:HG2	2.08	0.54
1:B:562:GLU:HB3	1:B:563:PRO:HD3	1.89	0.54
1:B:713:ASN:HD21	1:B:731:GLY:HA3	1.73	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: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:B:637:ASN:ND2	1:B:642:GLY:HA2	2.24	0.53
1:A:605:ASN:ND2	1:A:607:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:606:GLN:HB2	1:B:607:PRO:HD3	1.95	0.49
1:A:413:TRP:CD2	1:A:418:GLN:HG2	2.47	0.49
1:A:50:TYR:CG	1:A:74:MET:HE3	2.47	0.49
1:C:555:SER:N	1:C:564:MET:HE1	2.28	0.49
1:C:596:LEU:O	1:C:597:ASN:C	2.49	0.49
1:A:673:TYR:OH	1:A:724:HIS:HD2	1.94	0.49
1:C:112:MET:HG3	1:C:224:LEU:HD13	1.94	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
1:C:595:ALA:O	1:C:598:MET:CB	2.62	0.48
1:B:673:TYR:OH	1:B:724:HIS:HD2	1.97	0.48
1:B:602:ALA:HB2	1:B:647:GLU:OE1	1.96	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: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:C:713:ASN:HD21	1:C:732:GLU:H	1.62	0.47
1:A:346:MET:HA	1:A:377[A]:SER:HB2	1.97	0.47
1:C:69:ASN:H	1:C:114:HIS:CD2	2.33	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:HE3	1:C:24:LYS:HB2	1.78	0.46
1:B:637:ASN:C	1:B:637:ASN:HD22	2.19	0.46
1:C:110:LEU:O	1:C:111:LYS:HD3	2.16	0.46
1:B:376:GLN:NE2	2:B:2180:HOH:O	2.49	0.46
1:A:82[B]:MET:HE3	1:A:137:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HB2	1:B:77:TYR:HB3	1.98	0.46
1:C:713:ASN:HD21	1:C:731:GLY:HA3	1.81	0.46
1:A:664:TYR:CG	1:A:665:PRO:HD2	2.50	0.46
1:C:180:GLU:OE2	1:C:183:LYS:NZ	2.43	0.46
1:A:172:ASN:HA	1:A:234:ASP:O	2.16	0.46
1:C:62:TRP:HA	1:C:86:ARG:O	2.16	0.46
1:C:673:TYR:OH	1:C:724:HIS:HD2	1.98	0.46
1:C:617:TYR:CZ	1:C:753:PRO:HG2	2.51	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:360:HIS:CD2	1:B:408:LEU:HD21	2.51	0.45
1:B:580:TYR:O	1:B:581:GLY:C	2.55	0.45
1:C:632[B]:MET:HE1	1:C:660:ALA:HB2	1.97	0.45
1:C:188:GLY:HA3	1:C:205:PHE:CZ	2.52	0.45
1:C:117:ARG:C	1:C:118:LEU:HD22	2.36	0.45
1:B:459:TYR:CD1	1:B:460:PRO:HA	2.51	0.45
1:B:595:ALA:O	1:B:599:GLY:N	2.45	0.45
1:A:81:LEU:HD11	1:C:744:GLN:HG3	1.99	0.45
1:B:699:ASP:HB2	2:B:2303:HOH:O	2.16	0.45
1:C:605:ASN:ND2	1:C:607:PRO:HG2	2.30	0.45
1:B:24:LYS:HB2	1:B:24:LYS:HE3	1.60	0.45
1:A:50:TYR:CG	1:A:74:MET:CE	2.99	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:C:445:ARG:HG3	1:C:472:TYR:CZ	2.52	0.44
1:B:595:ALA:O	1:B:598:MET:N	2.50	0.44
1:C:606:GLN:N	1:C:607:PRO:HD2	2.32	0.44
1:B:145:LEU:N	1:B:145:LEU:HD23	2.32	0.44
1:A:744:GLN:HG3	2:A:2418:HOH:O	2.16	0.44
1:C:508:PRO:HD2	1:C:509:GLU:OE1	2.18	0.44
1:B:210:SER:HB3	1:B:251:THR:HB	1.99	0.44
1:A:431:HIS:HE1	2:A:2271:HOH:O	2.00	0.44
1:B:82[A]:MET:HB2	1:B:82[A]:MET:HE2	1.85	0.43
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:582:THR:C	1:A:584:GLY:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:TYR:CG	1:B:460:PRO:HA	2.53	0.43
1:B:50:TYR:CG	1:B:74:MET:CE	3.02	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:A:605:ASN:ND2	1:A:607:PRO:HG2	2.34	0.43
1:C:459:TYR:HB3	1:C:515:THR:OG1	2.18	0.43
1:A:24:LYS:HB2	1:A:24:LYS:HE3	1.84	0.43
1:B:268:PHE:C	1:B:268:PHE:CD2	2.92	0.43
1:B:585:PHE:O	1:B:588:HIS:N	2.50	0.43
1:A:699:ASP:HB2	2:A:2396:HOH:O	2.17	0.43
1:A:514:TRP:CZ2	1:A:526:PHE:HA	2.54	0.43
1:B:629:ARG:HD2	1:B:632[A]:MET:HE3	2.00	0.42
1:C:223:THR:HG22	1:C:224:LEU:O	2.19	0.42
1:B:503:ARG:HG2	1:B:557:LEU:HD21	2.02	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
1:A:581:GLY:O	1:A:582:THR:C	2.58	0.42
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: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:50:TYR:CG	1:B:74:MET:HE3	2.55	0.42
1:A:360:HIS:CD2	1:A:408:LEU:HD21	2.54	0.42
1:C:675:ILE:HD12	1:C:721:TYR:N	2.35	0.41
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:60:ASN:HB2	2:C:2057:HOH:O	2.21	0.41
1:C:596:LEU:C	1:C:598:MET:N	2.70	0.41
1:A:617:TYR:CE1	1:A:753:PRO:HB2	2.55	0.41
1:C:555:SER:N	1:C:564:MET:CE	2.83	0.41
1:C:346:MET:HA	1:C:377[A]:SER:HB2	2.01	0.41
1:C:190:THR:HG23	1:C:203:ASN:HB3	2.03	0.41
1:A:582:THR:C	1:A:584:GLY:N	2.74	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:703:ASP:OD1	1:A:704:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLY:HA3	1:B:534:PRO:HD2	1.91	0.41
1:C:84:GLY:HA2	1:C:104:MET:SD	2.61	0.41
1:A:285:ARG:HD3	2:A:2184:HOH:O	2.20	0.41
1:A:445:ARG:HG3	1:A:472:TYR:CZ	2.56	0.41
1:A:360:HIS:N	1:A:361:PRO:CD	2.83	0.41
1:A:240:LEU:N	1:A:240:LEU:HD22	2.35	0.41
1:B:413:TRP:CZ3	1:B:418:GLN:HB3	2.56	0.41
1:B:595:ALA:O	1:B:598:MET:CA	2.69	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:445:ARG:HG3	1:B:472:TYR:CZ	2.57	0.40
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
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:B:182:GLU:CD	1:B:182:GLU:H	2.24	0.40
1:B:606:GLN:N	1:B:607:PRO:CD	2.84	0.40
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.58	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%)	39	43
1	B	733/737 (100%)	707 (96%)	23 (3%)	3 (0%)	39	43
1	C	736/737 (100%)	704 (96%)	30 (4%)	2 (0%)	46	52
All	All	2206/2211 (100%)	2115 (96%)	83 (4%)	8 (0%)	39	43

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 [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	604/620 (97%)	589 (98%)	15 (2%)	55	66
1	B	599/620 (97%)	582 (97%)	17 (3%)	51	62
1	C	598/620 (96%)	586 (98%)	12 (2%)	63	73
All	All	1801/1860 (97%)	1757 (98%)	44 (2%)	57	67

All (44) 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	313	TYR
1	A	350	ASN
1	A	391	TRP
1	A	439	GLU
1	A	507	TYR
1	A	523	ARG
1	A	548	PHE
1	A	628	LEU
1	A	644	CYS
1	A	689	GLU

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Mol	Chain	Res	Type
1	B	82[A]	MET
1	B	82[B]	MET
1	B	145	LEU
1	B	171	TYR
1	B	182	GLU
1	B	190	THR
1	B	313	TYR
1	B	314	ARG
1	B	350	ASN
1	B	356	PHE
1	B	391	TRP
1	B	507	TYR
1	B	548	PHE
1	B	567	ARG
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	313	TYR
1	C	391	TRP
1	C	507	TYR
1	C	524	ASP
1	C	548	PHE
1	C	644	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) 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	340	ASN
1	A	342	HIS
1	A	350	ASN

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Mol	Chain	Res	Type
1	A	403	ASN
1	A	431	HIS
1	A	494	GLN
1	A	542	HIS
1	A	605	ASN
1	A	713	ASN
1	A	724	HIS
1	B	60	ASN
1	B	87	GLN
1	B	89	HIS
1	B	114	HIS
1	B	132	ASN
1	B	203	ASN
1	B	228	GLN
1	B	350	ASN
1	B	376	GLN
1	B	403	ASN
1	B	404	ASN
1	B	431	HIS
1	B	494	GLN
1	B	542	HIS
1	B	605	ASN
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	340	ASN
1	C	342	HIS
1	C	403	ASN
1	C	404	ASN
1	C	431	HIS
1	C	510	HIS
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 carbohydrates 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%)	-0.40	13 (1%) 71 75	5, 11, 31, 54	0
1	B	729/737 (98%)	-0.27	15 (2%) 67 71	8, 17, 35, 54	0
1	C	730/737 (99%)	-0.40	15 (2%) 67 71	8, 14, 33, 56	0
All	All	2190/2211 (99%)	-0.36	43 (1%) 68 72	5, 15, 33, 56	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	GLY	7.4
1	C	584	GLY	7.2
1	B	586	VAL	7.1
1	B	585	PHE	7.1
1	B	583	TYR	7.0
1	A	583	TYR	7.0
1	A	585	PHE	6.8
1	A	586	VAL	6.7
1	B	582	THR	6.6
1	A	582	THR	6.6
1	C	585	PHE	5.9
1	C	582	THR	5.8
1	C	599	GLY	5.4
1	B	584	GLY	5.2
1	C	581	GLY	5.0
1	C	583	TYR	4.8
1	B	599	GLY	4.5
1	B	581	GLY	4.3
1	C	586	VAL	4.2
1	A	599	GLY	4.1
1	A	587	ILE	3.5
1	B	587	ILE	3.4
1	A	581	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	601	TYR	3.2
1	B	598	MET	3.1
1	B	596	LEU	3.1
1	A	595	ALA	2.8
1	B	595	ALA	2.7
1	B	594	VAL	2.6
1	B	600	GLN	2.6
1	C	580	TYR	2.5
1	C	22	SER	2.4
1	A	41	THR	2.4
1	C	595	ALA	2.3
1	A	597	ASN	2.3
1	C	587	ILE	2.2
1	A	40	SER	2.2
1	C	48	ASN	2.2
1	C	589	GLU	2.1
1	A	22	SER	2.1
1	B	597	ASN	2.1
1	C	597	ASN	2.1
1	C	596	LEU	2.1

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 carbohydrates 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.