



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:32 PM UTC

PDB ID : 4BCE / pdb_00004bce
Title : crystal structure of Ttb-gly N282T mutant
Authors : Teze, D.; Tran, V.; Tellier, C.; Dion, M.; Leroux, C.; Roncza, J.; Czjzek, M.
Deposited on : 2012-10-02
Resolution : 2.00 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

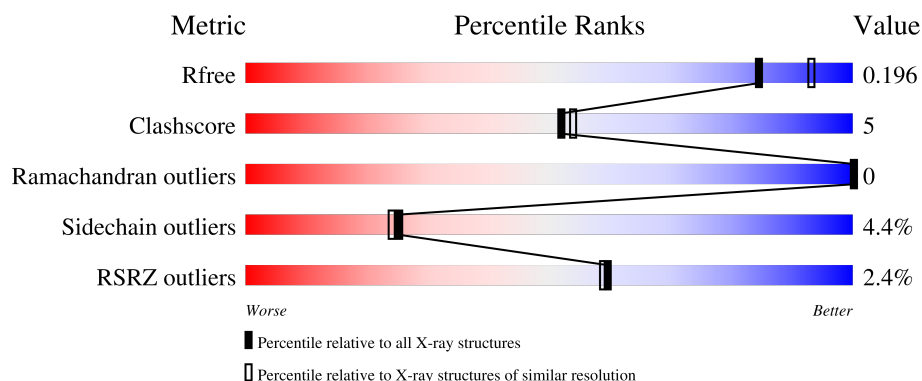
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	437	5% 80% 15% ..
1	B	437	84% 11% ..
1	C	437	5% 84% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10817 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-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	3	0
			3430	2209	617	599	5			
1	B	425	Total	C	N	O	S	0	1	0
			3427	2207	615	600	5			
1	C	424	Total	C	N	O	S	0	2	0
			3417	2202	610	600	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	HIS	-	expression tag	UNP Q53W75
A	433	HIS	-	expression tag	UNP Q53W75
A	434	HIS	-	expression tag	UNP Q53W75
A	435	HIS	-	expression tag	UNP Q53W75
A	436	HIS	-	expression tag	UNP Q53W75
A	437	HIS	-	expression tag	UNP Q53W75
A	282	THR	ASN	engineered mutation	UNP Q53W75
A	320	HIS	TYR	engineered mutation	UNP Q53W75
B	432	HIS	-	expression tag	UNP Q53W75
B	433	HIS	-	expression tag	UNP Q53W75
B	434	HIS	-	expression tag	UNP Q53W75
B	435	HIS	-	expression tag	UNP Q53W75
B	436	HIS	-	expression tag	UNP Q53W75
B	437	HIS	-	expression tag	UNP Q53W75
B	282	THR	ASN	engineered mutation	UNP Q53W75
B	320	HIS	TYR	engineered mutation	UNP Q53W75
C	432	HIS	-	expression tag	UNP Q53W75
C	433	HIS	-	expression tag	UNP Q53W75
C	434	HIS	-	expression tag	UNP Q53W75
C	435	HIS	-	expression tag	UNP Q53W75
C	436	HIS	-	expression tag	UNP Q53W75
C	437	HIS	-	expression tag	UNP Q53W75
C	282	THR	ASN	engineered mutation	UNP Q53W75

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Chain	Residue	Modelled	Actual	Comment	Reference
C	320	HIS	TYR	engineered mutation	UNP Q53W75

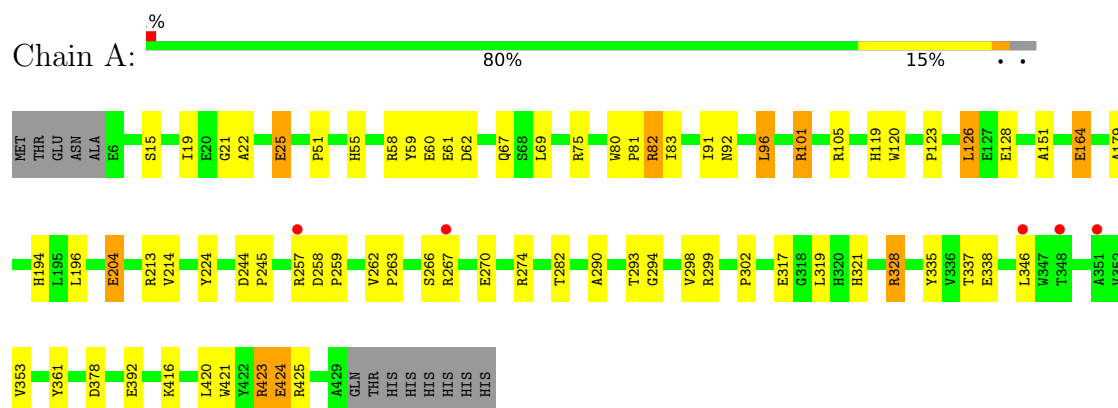
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	223	Total 224	O 224	0	1
2	B	187	Total 187	O 187	0	0
2	C	132	Total 132	O 132	0	0

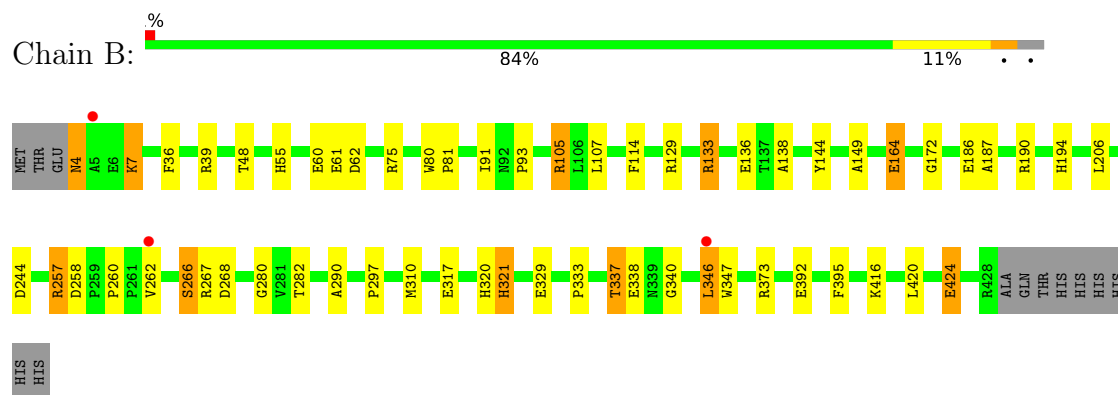
3 Residue-property plots [i](#)

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.

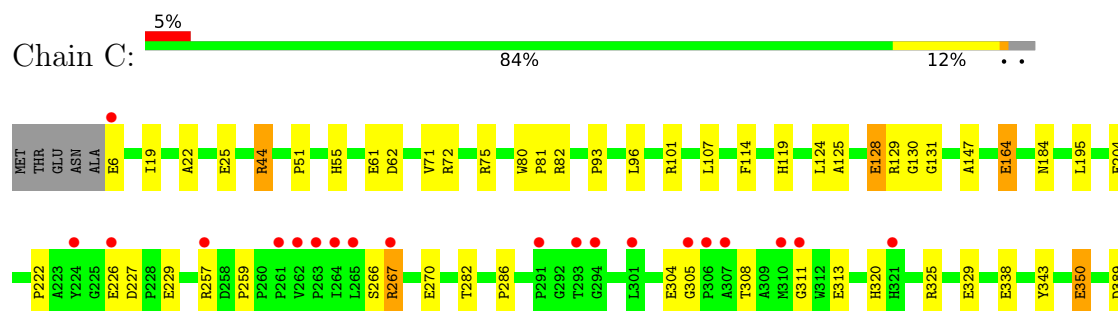
• Molecule 1: BETA-GLUCOSIDASE

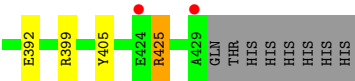


• Molecule 1: BETA-GLUCOSIDASE



• Molecule 1: BETA-GLUCOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.17Å 77.67Å 122.02Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	39.97 – 2.00 39.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.97-2.00) 99.3 (39.97-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.190 0.173 , 0.196	Depositor DCC
R_{free} test set	4465 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10817	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	1.59	23/3542 (0.6%)	1.24	9/4831 (0.2%)
1	B	1.54	15/3539 (0.4%)	1.24	12/4828 (0.2%)
1	C	1.43	11/3529 (0.3%)	1.16	11/4815 (0.2%)
All	All	1.52	49/10610 (0.5%)	1.22	32/14474 (0.2%)

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	B	0	1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	PRO	N-CA	9.36	1.54	1.47
1	C	320	HIS	C-N	-8.34	1.23	1.33
1	A	294	GLY	N-CA	8.07	1.57	1.45
1	A	164	GLU	C-O	7.59	1.27	1.23
1	B	244	ASP	N-CA	7.53	1.53	1.46
1	A	258	ASP	N-CA	7.38	1.51	1.46
1	A	424	GLU	CG-CD	7.00	1.69	1.52
1	C	164	GLU	C-O	-6.99	1.20	1.23
1	C	343	TYR	N-CA	6.98	1.51	1.45
1	B	290	ALA	C-O	6.82	1.30	1.24
1	C	222	PRO	N-CA	-6.53	1.39	1.47
1	A	421	TRP	CA-C	6.29	1.60	1.52
1	A	259	PRO	CA-C	6.29	1.55	1.51
1	B	340	GLY	N-CA	6.21	1.52	1.45
1	C	125	ALA	CA-CB	6.20	1.63	1.53
1	A	424	GLU	CD-OE1	6.00	1.36	1.25
1	B	258	ASP	C-O	-5.87	1.21	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	LEU	C-O	-5.84	1.17	1.24
1	A	378	ASP	CA-C	5.84	1.59	1.53
1	B	164	GLU	N-CA	5.84	1.50	1.46
1	A	263	PRO	CA-C	5.75	1.58	1.52
1	C	204	GLU	CG-CD	5.59	1.66	1.52
1	C	204	GLU	CD-OE1	5.56	1.35	1.25
1	A	294	GLY	CA-C	5.54	1.59	1.51
1	A	123	PRO	CA-C	5.51	1.59	1.52
1	A	319	LEU	C-N	-5.50	1.26	1.33
1	B	424	GLU	CD-OE1	5.50	1.35	1.25
1	B	164	GLU	C-O	5.50	1.26	1.23
1	A	67	GLN	C-O	-5.44	1.17	1.24
1	A	214	VAL	N-CA	-5.43	1.40	1.46
1	A	196	LEU	N-CA	-5.41	1.40	1.46
1	A	328	ARG	C-O	-5.40	1.17	1.24
1	A	179	ALA	C-O	-5.37	1.17	1.24
1	B	186	GLU	C-O	-5.32	1.17	1.24
1	B	172	GLY	C-O	5.30	1.30	1.23
1	C	195	LEU	C-O	5.26	1.30	1.24
1	A	120	TRP	N-CA	5.26	1.52	1.46
1	B	280	GLY	C-O	5.25	1.29	1.24
1	B	320	HIS	N-CA	5.21	1.52	1.46
1	B	321	HIS	N-CA	5.18	1.52	1.46
1	A	179	ALA	CA-CB	5.17	1.60	1.53
1	A	204	GLU	CD-OE1	5.16	1.35	1.25
1	B	333	PRO	C-O	5.16	1.29	1.23
1	A	126	LEU	CA-C	5.15	1.59	1.52
1	C	147	ALA	CA-CB	-5.12	1.45	1.53
1	B	424	GLU	CG-CD	5.08	1.64	1.52
1	A	259	PRO	C-O	-5.05	1.20	1.25
1	C	222	PRO	CA-C	5.05	1.58	1.52
1	A	290	ALA	N-CA	-5.00	1.42	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	THR	CA-C-N	-11.13	99.60	121.41
1	A	293	THR	C-N-CA	-11.13	99.60	121.41
1	B	260	PRO	CA-C-N	6.82	126.58	119.76
1	B	260	PRO	C-N-CA	6.82	126.58	119.76
1	B	262	VAL	CB-CA-C	-6.47	103.44	110.37
1	B	4	ASN	CA-C-N	6.26	132.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASN	C-N-CA	6.26	132.98	121.70
1	C	259	PRO	CA-C-N	-6.22	115.18	119.66
1	C	259	PRO	C-N-CA	-6.22	115.18	119.66
1	A	425	ARG	NE-CZ-NH2	-6.13	113.69	119.20
1	A	293	THR	O-C-N	-6.05	114.54	122.59
1	B	373	ARG	CG-CD-NE	-5.96	98.88	112.00
1	C	305	GLY	CA-C-N	5.70	126.97	119.84
1	C	305	GLY	C-N-CA	5.70	126.97	119.84
1	A	128	GLU	CA-CB-CG	-5.55	103.00	114.10
1	B	138	ALA	N-CA-C	-5.53	105.33	111.36
1	A	335	TYR	N-CA-C	-5.42	99.59	108.76
1	A	213	ARG	CB-CA-C	-5.40	101.82	110.14
1	C	227	ASP	CA-C-N	5.39	125.47	119.32
1	C	227	ASP	C-N-CA	5.39	125.47	119.32
1	C	19	ILE	N-CA-C	5.30	120.37	109.34
1	B	190	ARG	N-CA-C	-5.20	105.69	111.36
1	A	302	PRO	O-C-N	5.18	123.69	121.31
1	C	329	GLU	N-CA-CB	-5.17	103.71	110.59
1	C	343	TYR	CA-C-N	-5.08	113.50	119.84
1	C	343	TYR	C-N-CA	-5.08	113.50	119.84
1	B	416	LYS	N-CA-C	-5.07	102.96	110.46
1	C	19	ILE	CB-CA-C	-5.06	103.00	111.29
1	B	268	ASP	N-CA-CB	5.05	117.33	110.01
1	B	329	GLU	N-CA-C	5.04	119.70	113.50
1	B	48	THR	N-CA-C	-5.02	101.78	108.86
1	A	262	VAL	N-CA-CB	-5.00	107.07	112.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3321	47	0
1	B	3427	0	3316	27	0
1	C	3417	0	3302	30	0
2	A	224	0	0	6	0
2	B	187	0	0	5	0
2	C	132	0	0	6	0
All	All	10817	0	9939	103	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 5.

All (103) 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:C:129:ARG:NH1	2:C:2059:HOH:O	1.74	1.18
1:A:266:SER:O	1:A:267[B]:ARG:HB2	1.51	1.07
1:A:423:ARG:HH11	1:A:423:ARG:HG2	0.99	1.07
1:A:423:ARG:HG2	1:A:423:ARG:NH1	1.75	0.97
1:C:101[B]:ARG:HH11	1:C:101[B]:ARG:HG2	1.24	0.97
1:C:257:ARG:HD2	2:C:2096:HOH:O	1.67	0.92
1:B:129:ARG:NH1	1:B:136:GLU:OE1	2.05	0.90
1:C:101[B]:ARG:HH11	1:C:101[B]:ARG:CG	1.86	0.88
1:C:101[B]:ARG:CG	1:C:101[B]:ARG:NH1	2.42	0.79
1:A:224:TYR:OH	1:A:321:HIS:HD2	1.65	0.78
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.48	0.78
1:B:392:GLU:OE1	2:B:2185:HOH:O	2.06	0.73
1:C:101[B]:ARG:CZ	2:C:2051:HOH:O	2.37	0.73
1:A:266:SER:O	1:A:267[B]:ARG:CB	2.27	0.71
1:C:101[B]:ARG:HG2	1:C:101[B]:ARG:NH1	2.02	0.70
1:C:425:ARG:NH1	2:C:2116:HOH:O	2.17	0.70
1:B:133:ARG:HD2	1:B:187:ALA:HB1	1.72	0.70
1:B:55:HIS:HD2	1:B:62:ASP:OD2	1.76	0.68
1:B:164:GLU:OE2	1:B:282:THR:HG21	1.94	0.68
1:C:55:HIS:HD2	1:C:62:ASP:OD2	1.76	0.67
1:B:194:HIS:HE1	2:B:2076:HOH:O	1.79	0.64
1:A:392:GLU:OE1	2:A:2221:HOH:O	2.16	0.61
1:A:224:TYR:OH	1:A:321:HIS:CD2	2.52	0.59
1:C:350:GLU:H	1:C:350:GLU:CD	2.11	0.59
1:A:59:TYR:OH	1:A:101[A]:ARG:NE	2.36	0.59
1:A:59:TYR:OH	1:A:101[B]:ARG:NE	2.36	0.59
1:C:80:TRP:HB3	1:C:81:PRO:HD3	1.86	0.57
1:A:164:GLU:OE2	1:A:282:THR:HG21	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:CD	1:A:101[A]:ARG:HH21	2.14	0.56
1:A:194:HIS:HE1	2:A:2092:HOH:O	1.89	0.56
1:A:60:GLU:CD	1:A:101[B]:ARG:HH21	2.14	0.55
1:C:164:GLU:OE2	1:C:282:THR:HG21	2.07	0.55
1:A:266:SER:O	1:A:267[A]:ARG:HB2	2.01	0.54
1:C:44:ARG:NH2	1:C:399:ARG:HH12	2.05	0.53
1:A:101[A]:ARG:NH2	1:A:105:ARG:HD3	2.23	0.53
1:A:101[B]:ARG:NH2	1:A:105:ARG:HD3	2.23	0.53
1:C:22:ALA:HA	1:C:25:GLU:HG3	1.90	0.53
1:C:282:THR:HG23	1:C:338:GLU:HB2	1.89	0.53
1:A:55:HIS:HD2	1:A:62:ASP:OD2	1.93	0.52
1:A:59:TYR:OH	1:A:101[A]:ARG:HD3	2.10	0.51
1:A:59:TYR:OH	1:A:101[B]:ARG:HD3	2.10	0.50
1:A:22:ALA:HB1	1:A:25:GLU:HG3	1.94	0.49
1:B:60:GLU:HG2	1:B:105:ARG:HD2	1.94	0.49
1:B:7:LYS:O	2:B:2003:HOH:O	2.20	0.49
1:C:101[B]:ARG:NH1	1:C:101[B]:ARG:HG3	2.26	0.49
1:A:59:TYR:OH	1:A:101[A]:ARG:CD	2.61	0.48
1:A:59:TYR:OH	1:A:101[B]:ARG:CD	2.61	0.48
1:A:83:ILE:HG23	1:A:96:LEU:HD13	1.95	0.48
1:A:257[A]:ARG:HD3	1:A:257[A]:ARG:HA	1.59	0.48
1:C:124:LEU:O	1:C:128:GLU:HG2	2.13	0.48
1:C:389:ASP:OD2	1:C:405:TYR:HA	2.13	0.48
1:B:149:ALA:HB2	1:B:206:LEU:HD23	1.95	0.48
1:A:69:LEU:HA	1:A:423:ARG:HD3	1.94	0.48
1:C:130:GLY:O	1:C:131:GLY:C	2.56	0.47
1:A:58:ARG:NH1	2:A:2048:HOH:O	2.47	0.47
1:B:257:ARG:HH11	1:B:257:ARG:CG	2.22	0.47
1:C:75:ARG:HA	1:C:114:PHE:O	2.15	0.47
1:C:308:THR:O	1:C:311:GLY:N	2.42	0.47
1:A:353:VAL:HB	1:A:416:LYS:HG2	1.97	0.46
1:A:151:ALA:HB1	1:C:93:PRO:HG3	1.98	0.45
1:B:317:GLU:HG3	1:B:321:HIS:CE1	2.50	0.45
1:A:119:HIS:HE1	2:A:2014:HOH:O	2.00	0.45
1:A:321:HIS:HE1	2:A:2184:HOH:O	1.99	0.45
1:B:282:THR:OG1	2:B:2088:HOH:O	2.13	0.45
1:C:80:TRP:N	1:C:81:PRO:HD2	2.31	0.45
1:B:91:ILE:O	1:B:93:PRO:HD3	2.17	0.44
1:B:75:ARG:HA	1:B:114:PHE:O	2.17	0.44
1:B:80:TRP:HB3	1:B:81:PRO:HD3	1.99	0.44
1:B:337:THR:O	1:B:338:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:CB	1:A:25:GLU:HG3	2.48	0.43
1:B:282:THR:HG21	2:B:2088:HOH:O	2.17	0.43
1:C:101[B]:ARG:NH2	2:C:2051:HOH:O	2.49	0.43
1:A:75:ARG:NH1	1:A:338:GLU:HG3	2.34	0.43
1:C:392[B]:GLU:HA	1:C:392[B]:GLU:OE1	2.19	0.43
1:A:361:TYR:CD1	1:A:361:TYR:C	2.97	0.43
1:C:119:HIS:HD2	2:C:2006:HOH:O	2.02	0.43
1:C:80:TRP:N	1:C:81:PRO:CD	2.82	0.42
1:A:60:GLU:CD	1:A:101[A]:ARG:NH2	2.76	0.42
1:B:75:ARG:NH1	1:B:338:GLU:HG3	2.33	0.42
1:A:60:GLU:CD	1:A:101[B]:ARG:NH2	2.76	0.42
1:A:22:ALA:HA	1:A:25:GLU:HG3	2.02	0.42
1:C:286:PRO:HD2	1:C:313:GLU:HB3	2.02	0.42
1:B:266:SER:O	1:B:267[B]:ARG:HB2	2.19	0.42
1:A:282:THR:HG21	2:A:2104:HOH:O	2.19	0.41
1:B:80:TRP:HA	1:B:144:TYR:CE1	2.55	0.41
1:B:266:SER:O	1:B:267[A]:ARG:HB2	2.20	0.41
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.93	0.41
1:C:267:ARG:NH1	1:C:270:GLU:OE1	2.54	0.41
1:A:204:GLU:HB2	1:A:274:ARG:NH1	2.35	0.41
1:A:244:ASP:HB2	1:A:245:PRO:HD3	2.02	0.41
1:B:80:TRP:N	1:B:81:PRO:CD	2.83	0.41
1:A:80:TRP:HB3	1:A:81:PRO:HD3	2.02	0.41
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.59	0.41
1:B:36:PHE:O	1:B:39:ARG:HB2	2.20	0.41
1:B:310:MET:HE1	1:B:395:PHE:CE1	2.56	0.41
1:A:80:TRP:N	1:A:81:PRO:HD2	2.36	0.41
1:A:82:ARG:O	1:A:92:ASN:HB3	2.21	0.41
1:B:133:ARG:HH11	1:B:133:ARG:HD3	1.66	0.41
1:B:346:LEU:HD12	1:B:347:TRP:H	1.86	0.41
1:A:317:GLU:HG3	1:A:321:HIS:CE1	2.56	0.40
1:A:21:GLY:O	1:A:22:ALA:C	2.61	0.40
1:C:184:ASN:OD1	1:C:184:ASN:C	2.64	0.40
1:A:15:SER:O	1:A:19:ILE:HG12	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	425/437 (97%)	414 (97%)	11 (3%)	0	100	100
1	B	425/437 (97%)	410 (96%)	15 (4%)	0	100	100
1	C	424/437 (97%)	407 (96%)	17 (4%)	0	100	100
All	All	1274/1311 (97%)	1231 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	336/345 (97%)	319 (95%)	17 (5%)	21	19
1	B	336/345 (97%)	325 (97%)	11 (3%)	33	34
1	C	335/345 (97%)	318 (95%)	17 (5%)	21	19
All	All	1007/1035 (97%)	962 (96%)	45 (4%)	25	23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	51	PRO
1	A	61	GLU
1	A	82	ARG
1	A	91	ILE

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Mol	Chain	Res	Type
1	A	96	LEU
1	A	101[A]	ARG
1	A	101[B]	ARG
1	A	270	GLU
1	A	298	VAL
1	A	299	ARG
1	A	328	ARG
1	A	337	THR
1	A	346	LEU
1	A	420	LEU
1	A	423	ARG
1	A	424	GLU
1	B	7	LYS
1	B	61	GLU
1	B	105	ARG
1	B	107	LEU
1	B	133	ARG
1	B	257	ARG
1	B	266	SER
1	B	337	THR
1	B	346	LEU
1	B	420	LEU
1	B	424	GLU
1	C	6	GLU
1	C	44	ARG
1	C	51	PRO
1	C	61	GLU
1	C	71	VAL
1	C	72	ARG
1	C	82	ARG
1	C	96	LEU
1	C	128	GLU
1	C	226	GLU
1	C	229	GLU
1	C	266	SER
1	C	267	ARG
1	C	304	GLU
1	C	325	ARG
1	C	350	GLU
1	C	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	119	HIS
1	A	194	HIS
1	A	321	HIS
1	B	4	ASN
1	B	55	HIS
1	B	67	GLN
1	B	119	HIS
1	B	194	HIS
1	B	320	HIS
1	B	321	HIS
1	C	55	HIS
1	C	119	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	424/437 (97%)	-0.39	5 (1%) 76 76	14, 26, 46, 67	3 (0%)
1	B	425/437 (97%)	-0.28	3 (0%) 84 84	13, 29, 51, 72	1 (0%)
1	C	424/437 (97%)	0.33	22 (5%) 33 31	18, 38, 67, 84	2 (0%)
All	All	1273/1311 (97%)	-0.11	30 (2%) 59 59	13, 31, 58, 84	6 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	429	ALA	4.9
1	B	5	ALA	3.9
1	A	346	LEU	3.6
1	C	262	VAL	3.5
1	C	257	ARG	3.5
1	A	267[A]	ARG	3.2
1	C	306	PRO	3.0
1	A	257[A]	ARG	2.8
1	C	321	HIS	2.8
1	C	305	GLY	2.7
1	C	263	PRO	2.6
1	C	226	GLU	2.6
1	C	261	PRO	2.5
1	C	424	GLU	2.3
1	C	267	ARG	2.3
1	C	293	THR	2.3
1	A	348	THR	2.3
1	C	294	GLY	2.3
1	C	301	LEU	2.3
1	C	291	PRO	2.2
1	A	351	ALA	2.2
1	B	346	LEU	2.2
1	C	311	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	307	ALA	2.2
1	C	224	TYR	2.2
1	C	310	MET	2.1
1	B	262	VAL	2.1
1	C	265	LEU	2.1
1	C	6	GLU	2.1
1	C	264	ILE	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 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.