



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:34 AM UTC

PDB ID : 3V8U / pdb_00003v8u
Title : The crystal structure of transferrin binding protein B (TbpB) from *Neisseria meningitidis* serogroup B
Authors : Noinaj, N.; Easley, N.; Buchanan, S.K.
Deposited on : 2011-12-23
Resolution : 2.40 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

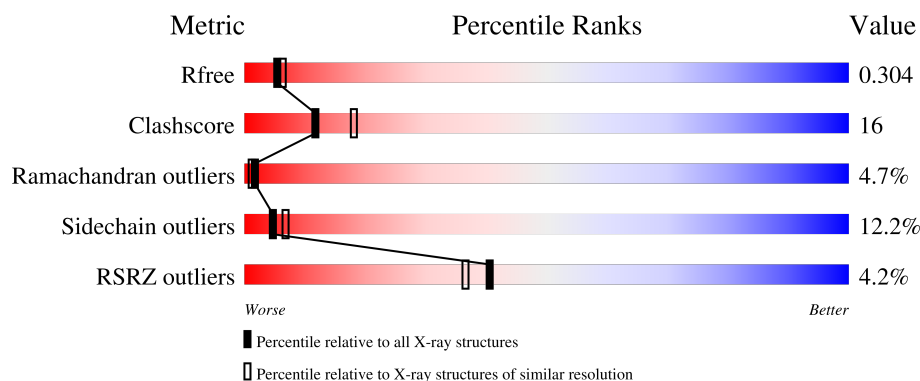
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	717	3% 44% 25% 5% 26%
1	B	717	3% 44% 24% 5% 26%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8366 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 Transferrin binding-protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4113	2586	707	814	6			
1	B	532	Total	C	N	O	S	0	0	0
			4106	2581	708	811	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q9JPI9
A	-24	SER	-	expression tag	UNP Q9JPI9
A	-23	TYR	-	expression tag	UNP Q9JPI9
A	-22	TYR	-	expression tag	UNP Q9JPI9
A	-21	HIS	-	expression tag	UNP Q9JPI9
A	-20	HIS	-	expression tag	UNP Q9JPI9
A	-19	HIS	-	expression tag	UNP Q9JPI9
A	-18	HIS	-	expression tag	UNP Q9JPI9
A	-17	HIS	-	expression tag	UNP Q9JPI9
A	-16	HIS	-	expression tag	UNP Q9JPI9
A	-15	ASP	-	expression tag	UNP Q9JPI9
A	-14	TYR	-	expression tag	UNP Q9JPI9
A	-13	ASP	-	expression tag	UNP Q9JPI9
A	-12	ILE	-	expression tag	UNP Q9JPI9
A	-11	PRO	-	expression tag	UNP Q9JPI9
A	-10	THR	-	expression tag	UNP Q9JPI9
A	-9	THR	-	expression tag	UNP Q9JPI9
A	-8	GLU	-	expression tag	UNP Q9JPI9
A	-7	ASN	-	expression tag	UNP Q9JPI9
A	-6	LEU	-	expression tag	UNP Q9JPI9
A	-5	TYR	-	expression tag	UNP Q9JPI9
A	-4	PHE	-	expression tag	UNP Q9JPI9
A	-3	GLN	-	expression tag	UNP Q9JPI9
A	-2	GLY	-	expression tag	UNP Q9JPI9
A	-1	ALA	-	expression tag	UNP Q9JPI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9JPI9
B	-25	MET	-	expression tag	UNP Q9JPI9
B	-24	SER	-	expression tag	UNP Q9JPI9
B	-23	TYR	-	expression tag	UNP Q9JPI9
B	-22	TYR	-	expression tag	UNP Q9JPI9
B	-21	HIS	-	expression tag	UNP Q9JPI9
B	-20	HIS	-	expression tag	UNP Q9JPI9
B	-19	HIS	-	expression tag	UNP Q9JPI9
B	-18	HIS	-	expression tag	UNP Q9JPI9
B	-17	HIS	-	expression tag	UNP Q9JPI9
B	-16	HIS	-	expression tag	UNP Q9JPI9
B	-15	ASP	-	expression tag	UNP Q9JPI9
B	-14	TYR	-	expression tag	UNP Q9JPI9
B	-13	ASP	-	expression tag	UNP Q9JPI9
B	-12	ILE	-	expression tag	UNP Q9JPI9
B	-11	PRO	-	expression tag	UNP Q9JPI9
B	-10	THR	-	expression tag	UNP Q9JPI9
B	-9	THR	-	expression tag	UNP Q9JPI9
B	-8	GLU	-	expression tag	UNP Q9JPI9
B	-7	ASN	-	expression tag	UNP Q9JPI9
B	-6	LEU	-	expression tag	UNP Q9JPI9
B	-5	TYR	-	expression tag	UNP Q9JPI9
B	-4	PHE	-	expression tag	UNP Q9JPI9
B	-3	GLN	-	expression tag	UNP Q9JPI9
B	-2	GLY	-	expression tag	UNP Q9JPI9
B	-1	ALA	-	expression tag	UNP Q9JPI9
B	0	MET	-	expression tag	UNP Q9JPI9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	78	Total O 78 78	0	0
2	B	69	Total O 69 69	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	75.03Å 82.13Å 111.31Å 90.00° 106.07° 90.00°	Depositor
Resolution (Å)	29.50 – 2.40 29.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.50-2.40) 95.2 (29.50-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.308 0.247 , 0.304	Depositor DCC
R_{free} test set	2001 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtrriage
Anisotropy	0.679	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8366	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8259e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.61	0/4200	1.01	15/5667 (0.3%)
1	B	0.61	0/4192	1.04	15/5655 (0.3%)
All	All	0.61	0/8392	1.02	30/11322 (0.3%)

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	6
All	All	0	12

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	625	LEU	N-CA-C	-16.97	90.61	113.18
1	B	649	GLY	CA-C-N	10.06	132.42	119.84
1	B	649	GLY	C-N-CA	10.06	132.42	119.84
1	B	347	THR	N-CA-C	-6.44	98.35	108.14
1	A	649	GLY	CA-C-N	6.37	127.80	119.84
1	A	649	GLY	C-N-CA	6.37	127.80	119.84
1	A	322	GLY	CA-C-N	6.32	127.74	119.84
1	A	322	GLY	C-N-CA	6.32	127.74	119.84
1	A	625	LEU	N-CA-C	-6.29	105.73	113.41
1	A	496	GLY	N-CA-C	6.19	118.22	110.29
1	A	205	GLN	CA-C-N	6.01	127.36	119.84
1	A	205	GLN	C-N-CA	6.01	127.36	119.84
1	B	205	GLN	CA-C-N	5.90	127.22	119.84
1	B	205	GLN	C-N-CA	5.90	127.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	THR	N-CA-C	-5.90	99.17	108.14
1	B	496	GLY	N-CA-C	5.75	117.65	110.29
1	B	221	ASP	N-CA-C	5.69	120.76	111.37
1	A	221	ASP	N-CA-C	5.68	120.74	111.37
1	B	322	GLY	CA-C-N	5.65	126.90	119.84
1	B	322	GLY	C-N-CA	5.65	126.90	119.84
1	B	129	TYR	CA-C-N	5.52	131.63	121.70
1	B	129	TYR	C-N-CA	5.52	131.63	121.70
1	A	129	TYR	CA-C-N	5.51	131.62	121.70
1	A	129	TYR	C-N-CA	5.51	131.62	121.70
1	A	295	THR	N-CA-C	5.35	117.53	111.11
1	B	93	ASP	N-CA-C	-5.11	99.92	110.80
1	B	211	GLY	N-CA-C	-5.09	108.63	114.69
1	B	204	ILE	CB-CA-C	-5.08	102.96	111.29
1	A	101	SER	CA-C-N	5.05	124.50	119.24
1	A	101	SER	C-N-CA	5.05	124.50	119.24

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	ASP	Peptide
1	A	633	THR	Peptide
1	A	634	PRO	Peptide
1	A	649	GLY	Peptide
1	A	90	VAL	Peptide
1	A	92	THR	Peptide
1	B	624	ASP	Peptide
1	B	633	THR	Peptide
1	B	634	PRO	Peptide
1	B	649	GLY	Peptide
1	B	90	VAL	Peptide
1	B	92	THR	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	4113	0	3871	131	0
1	B	4106	0	3871	122	0
2	A	78	0	0	4	0
2	B	69	0	0	3	0
All	All	8366	0	7742	253	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 16.

All (253) 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:261:ARG:NH1	1:A:263:ASN:OD1	2.11	0.84
1:B:611:GLY:HA2	1:B:646:GLY:HA2	1.58	0.83
1:B:202:GLU:HB3	1:B:261:ARG:HH21	1.44	0.83
1:A:611:GLY:HA2	1:A:646:GLY:HA2	1.60	0.82
1:A:87:ILE:HD11	1:A:163:GLY:HA2	1.62	0.81
1:A:202:GLU:HB3	1:A:261:ARG:HH21	1.46	0.81
1:B:205:GLN:O	1:B:207:SER:N	2.13	0.80
1:A:205:GLN:O	1:A:207:SER:N	2.14	0.80
1:B:87:ILE:HD11	1:B:163:GLY:HA2	1.63	0.80
1:B:261:ARG:NH1	1:B:263:ASN:OD1	2.19	0.76
1:B:412:ASP:OD2	1:B:500:ARG:NH2	2.19	0.76
1:A:53:PRO:O	1:A:55:ALA:N	2.19	0.75
1:A:412:ASP:OD2	1:A:500:ARG:NH2	2.19	0.75
1:A:613:GLU:OE2	1:A:642:LYS:NZ	2.21	0.74
1:B:613:GLU:OE2	1:B:642:LYS:NZ	2.21	0.74
1:A:209:SER:HB3	1:A:212:ASP:HB3	1.71	0.73
1:B:53:PRO:O	1:B:55:ALA:N	2.22	0.72
1:B:209:SER:HB3	1:B:212:ASP:HB3	1.73	0.71
1:B:91:GLU:N	1:B:92:THR:HA	2.10	0.67
1:B:81:LYS:H	1:B:81:LYS:HD2	1.60	0.66
1:B:481:TYR:N	2:B:719:HOH:O	2.28	0.66
1:B:44:MET:HE1	1:B:62:LEU:HB3	1.78	0.66
1:A:621:SER:O	1:A:635:LYS:NZ	2.29	0.65
1:A:173:SER:OG	1:A:322:GLY:O	2.12	0.65
1:B:596:ARG:HH11	1:B:596:ARG:HG3	1.61	0.65
1:B:203:ILE:HD13	1:B:223:GLU:HB2	1.79	0.64
1:B:202:GLU:O	1:B:223:GLU:HG2	1.96	0.64
1:A:44:MET:HE1	1:A:62:LEU:HB3	1.79	0.64
1:A:596:ARG:HG3	1:A:596:ARG:HH11	1.62	0.64
1:B:173:SER:OG	1:B:322:GLY:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HD13	1:A:223:GLU:HB2	1.79	0.63
1:A:82:ARG:NH1	2:A:774:HOH:O	2.31	0.62
1:B:236:GLY:HA3	1:B:272:THR:HG21	1.79	0.62
1:A:201:ARG:HH11	1:A:307:HIS:HD2	1.46	0.62
1:A:202:GLU:O	1:A:223:GLU:HG2	1.98	0.62
1:A:236:GLY:HA3	1:A:272:THR:HG21	1.81	0.62
1:A:81:LYS:H	1:A:81:LYS:HD2	1.63	0.62
1:B:44:MET:HE2	1:B:62:LEU:HD22	1.81	0.61
1:A:83:GLN:HA	1:A:86:VAL:HG23	1.83	0.60
1:B:83:GLN:HA	1:B:86:VAL:HG23	1.84	0.60
1:A:346:LYS:NZ	1:A:347:THR:O	2.28	0.60
1:A:44:MET:HE2	1:A:62:LEU:HD22	1.84	0.60
1:B:201:ARG:HH11	1:B:307:HIS:HD2	1.48	0.60
1:A:596:ARG:HH11	1:A:596:ARG:CG	2.15	0.59
1:B:596:ARG:HH11	1:B:596:ARG:CG	2.15	0.58
1:A:557:ASN:HB3	1:A:560:SER:HB3	1.87	0.57
1:B:346:LYS:NZ	1:B:347:THR:O	2.33	0.57
1:A:560:SER:OG	1:A:561:THR:N	2.37	0.57
1:A:294:ALA:N	1:A:312:ASP:OD1	2.27	0.56
1:A:204:ILE:HG12	1:A:224:GLU:HG2	1.88	0.55
1:B:129:TYR:CA	1:B:130:GLU:HB2	2.36	0.55
1:B:129:TYR:HA	1:B:130:GLU:HB2	1.89	0.55
1:A:129:TYR:HA	1:A:130:GLU:HB2	1.89	0.55
1:A:401:ASP:O	1:A:410:VAL:HB	2.07	0.55
1:B:184:TYR:OH	1:B:325:GLY:O	2.23	0.55
1:B:623:PHE:HB3	1:B:636:ALA:HB3	1.89	0.55
1:B:139:TRP:NE1	2:B:764:HOH:O	2.32	0.54
1:A:129:TYR:CA	1:A:130:GLU:HB2	2.37	0.54
1:A:199:LYS:HB3	1:A:307:HIS:HA	1.89	0.54
1:B:204:ILE:O	1:B:205:GLN:C	2.50	0.54
1:B:557:ASN:HB3	1:B:560:SER:HB3	1.90	0.54
1:B:527:MET:HE1	1:B:680:THR:C	2.33	0.53
1:A:93:ASP:O	1:A:95:ASP:N	2.41	0.53
1:B:199:LYS:HB3	1:B:307:HIS:HA	1.90	0.53
1:A:204:ILE:O	1:A:205:GLN:C	2.51	0.53
1:B:183:THR:HG22	1:B:247:GLU:OE1	2.09	0.53
1:A:184:TYR:CD1	1:A:328:LEU:HD23	2.43	0.53
1:B:202:GLU:HA	1:B:225:TYR:HD2	1.74	0.53
1:A:186:GLY:HA3	1:A:344:SER:O	2.09	0.53
1:B:202:GLU:OE2	1:B:308:PRO:HD3	2.09	0.53
1:B:401:ASP:O	1:B:410:VAL:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PRO:HA	1:A:81:LYS:HE3	1.91	0.52
1:A:80:PRO:HB2	1:A:83:GLN:HG2	1.92	0.52
1:B:80:PRO:HB2	1:B:83:GLN:HG2	1.91	0.52
1:B:271:ALA:O	1:B:272:THR:HB	2.08	0.52
1:A:634:PRO:HB2	1:A:635:LYS:HA	1.91	0.52
1:B:44:MET:HE3	1:B:66:ASP:HB2	1.90	0.52
1:B:186:GLY:HA3	1:B:344:SER:O	2.08	0.52
1:A:527:MET:HE1	1:A:680:THR:C	2.34	0.52
1:B:248:VAL:HG22	1:B:255:LEU:HD13	1.91	0.52
1:A:44:MET:HE3	1:A:66:ASP:HB2	1.91	0.52
1:A:545:ILE:HD12	1:A:582:PHE:HE2	1.75	0.51
1:A:256:THR:HA	1:A:279:LEU:O	2.10	0.51
1:B:93:ASP:O	1:B:95:ASP:N	2.43	0.51
1:A:202:GLU:HA	1:A:225:TYR:HD2	1.75	0.51
1:A:93:ASP:H	1:A:145:LYS:HB2	1.76	0.51
1:B:95:ASP:OD1	1:B:96:ASN:N	2.44	0.51
1:A:623:PHE:HB3	1:A:636:ALA:HB3	1.93	0.51
1:B:542:GLU:HG3	1:B:545:ILE:HD11	1.93	0.51
1:A:248:VAL:HG22	1:A:255:LEU:HD13	1.92	0.50
1:A:184:TYR:OH	1:A:325:GLY:O	2.25	0.50
1:B:545:ILE:HD12	1:B:582:PHE:HE2	1.76	0.50
1:B:578:PHE:CD1	1:B:589:GLY:HA3	2.45	0.50
1:A:72:LEU:HD12	1:A:73:PRO:HD2	1.93	0.50
1:A:271:ALA:O	1:A:272:THR:HB	2.11	0.50
1:A:599:ALA:N	2:A:764:HOH:O	2.37	0.50
1:A:303:GLU:HB2	2:A:771:HOH:O	2.11	0.49
1:A:542:GLU:HG3	1:A:545:ILE:HD11	1.95	0.49
1:B:643:VAL:HA	1:B:659:PHE:HB3	1.94	0.49
1:B:73:PRO:HA	1:B:81:LYS:HE3	1.93	0.49
1:A:275:GLN:HG2	1:A:295:THR:HG21	1.94	0.49
1:B:653:GLU:HG3	1:B:654:GLU:HG3	1.95	0.49
1:A:391:LYS:O	1:A:394:ASP:N	2.42	0.48
1:A:618:THR:HG23	1:A:638:ILE:HB	1.96	0.48
1:B:391:LYS:O	1:B:394:ASP:N	2.42	0.48
1:A:95:ASP:OD1	1:A:96:ASN:N	2.47	0.48
1:A:122:PRO:HB3	1:A:228:LYS:HG3	1.95	0.48
1:A:259:LEU:HB2	1:A:277:TYR:HB2	1.96	0.48
1:A:50:ASN:OD1	1:A:157:ALA:N	2.41	0.48
1:B:560:SER:OG	1:B:561:THR:N	2.44	0.48
1:A:320:PHE:HB3	1:A:325:GLY:CA	2.44	0.48
1:A:572:SER:O	1:A:575:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:VAL:HA	1:A:659:PHE:HB3	1.94	0.48
1:A:653:GLU:HG3	1:A:654:GLU:HG3	1.96	0.48
1:B:217:PHE:O	1:B:219:GLY:N	2.46	0.48
1:A:651:LYS:N	2:A:742:HOH:O	2.28	0.48
1:B:547:TYR:CE1	1:B:687:ARG:HB2	2.49	0.47
1:B:572:SER:O	1:B:575:ARG:NH1	2.47	0.47
1:A:233:LEU:O	1:A:235:ASP:N	2.46	0.47
1:B:130:GLU:HB3	1:B:131:ASN:H	1.27	0.47
1:B:596:ARG:HH12	1:B:623:PHE:HZ	1.63	0.47
1:B:612:PHE:CZ	1:B:645:GLY:HA3	2.50	0.47
1:B:623:PHE:CG	1:B:624:ASP:N	2.82	0.47
1:A:40:TYR:CE1	1:A:72:LEU:HD13	2.49	0.47
1:A:217:PHE:O	1:A:219:GLY:N	2.48	0.47
1:A:254:LYS:HA	1:A:254:LYS:HD3	1.61	0.47
1:A:400:LEU:HD22	1:A:411:VAL:HG12	1.97	0.47
1:B:122:PRO:HB3	1:B:228:LYS:HG3	1.95	0.47
1:B:187:VAL:HA	1:B:243:THR:HA	1.95	0.47
1:B:275:GLN:HG2	1:B:295:THR:HG21	1.95	0.47
1:A:183:THR:HG22	1:A:247:GLU:OE1	2.15	0.47
1:A:600:THR:HG23	1:A:623:PHE:CD1	2.50	0.47
1:A:292:ALA:HB3	1:A:313:SER:HB3	1.97	0.47
1:B:400:LEU:HD22	1:B:411:VAL:HG12	1.97	0.47
1:B:527:MET:HE1	1:B:680:THR:O	2.15	0.46
1:B:270:GLN:CB	1:B:271:ALA:HB2	2.46	0.46
1:A:612:PHE:CZ	1:A:645:GLY:HA3	2.51	0.46
1:B:147:GLU:HB3	1:B:158:LYS:HB2	1.96	0.46
1:B:300:GLN:C	1:B:302:SER:H	2.24	0.46
1:A:657:GLY:HA3	1:A:683:PHE:CZ	2.50	0.46
1:B:195:LYS:O	1:B:196:LYS:HD2	2.16	0.46
1:B:320:PHE:HB3	1:B:325:GLY:CA	2.45	0.46
1:B:602:THR:HG22	1:B:617:LYS:HG2	1.98	0.46
1:A:151:LYS:HB3	1:A:151:LYS:HE2	1.70	0.46
1:A:175:GLN:HG3	1:A:381:LEU:HD23	1.97	0.45
1:A:578:PHE:CD1	1:A:589:GLY:HA3	2.50	0.45
1:A:596:ARG:HH12	1:A:623:PHE:HZ	1.64	0.45
1:B:618:THR:HG23	1:B:638:ILE:HB	1.98	0.45
1:A:263:ASN:HD21	1:A:274:THR:HG22	1.80	0.45
1:A:300:GLN:C	1:A:302:SER:H	2.24	0.45
1:B:50:ASN:OD1	1:B:157:ALA:N	2.42	0.45
1:B:72:LEU:HD12	1:B:73:PRO:HD2	1.97	0.45
1:B:151:LYS:HB3	1:B:151:LYS:HE2	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:MET:HE3	1:A:66:ASP:CB	2.46	0.45
1:A:414:ILE:HD12	1:A:414:ILE:HA	1.79	0.45
1:B:315:SER:HB3	2:B:724:HOH:O	2.16	0.45
1:A:129:TYR:CG	1:A:185:LYS:HB2	2.51	0.45
1:A:187:VAL:HA	1:A:243:THR:HA	1.98	0.45
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.56	0.45
1:B:175:GLN:HG3	1:B:381:LEU:HD23	1.98	0.45
1:B:139:TRP:HA	1:B:164:TYR:O	2.16	0.45
1:A:209:SER:HB2	1:A:213:ARG:HD2	1.97	0.45
1:A:57:GLU:O	1:A:59:GLU:N	2.49	0.44
1:A:602:THR:HG22	1:A:617:LYS:HG2	1.98	0.44
1:B:40:TYR:CE1	1:B:72:LEU:HD13	2.53	0.44
1:A:202:GLU:OE2	1:A:308:PRO:HD3	2.17	0.44
1:A:221:ASP:N	1:A:222:GLY:HA3	2.33	0.44
1:A:591:LEU:HB2	1:A:601:PHE:HB2	1.98	0.44
1:B:44:MET:HE3	1:B:66:ASP:CB	2.47	0.44
1:B:316:LEU:HA	1:B:332:PHE:HB3	2.00	0.44
1:B:596:ARG:HE	1:B:627:GLN:HG3	1.82	0.44
1:B:414:ILE:HD12	1:B:414:ILE:HA	1.80	0.44
1:A:195:LYS:O	1:A:196:LYS:HD2	2.18	0.44
1:A:227:ASN:ND2	1:A:234:THR:HG23	2.32	0.44
1:A:81:LYS:H	1:A:81:LYS:CD	2.30	0.44
1:B:227:ASN:ND2	1:B:234:THR:HG23	2.32	0.44
1:A:288:PHE:HZ	1:A:328:LEU:HD13	1.81	0.44
1:B:539:ILE:HG13	1:B:539:ILE:O	2.18	0.44
1:B:600:THR:HG23	1:B:623:PHE:CD1	2.53	0.44
1:B:221:ASP:N	1:B:222:GLY:HA3	2.33	0.44
1:B:254:LYS:HA	1:B:254:LYS:HD3	1.63	0.44
1:A:255:LEU:N	1:A:281:ALA:O	2.38	0.44
1:B:205:GLN:HA	1:B:206:PRO:HD2	1.76	0.44
1:B:346:LYS:HB3	1:B:347:THR:H	1.60	0.44
1:A:147:GLU:HB3	1:A:158:LYS:HB2	1.99	0.43
1:B:204:ILE:HG13	1:B:222:GLY:C	2.43	0.43
1:B:236:GLY:HA3	1:B:272:THR:CG2	2.47	0.43
1:B:392:LEU:HA	1:B:393:GLY:HA2	1.68	0.43
1:A:91:GLU:N	1:A:92:THR:HA	2.33	0.43
1:B:184:TYR:CD1	1:B:328:LEU:HD23	2.52	0.43
1:A:547:TYR:CE1	1:A:687:ARG:HB2	2.53	0.43
1:A:129:TYR:HB3	1:A:185:LYS:O	2.18	0.43
1:A:347:THR:HG22	1:A:348:LYS:H	1.83	0.43
1:A:99:TYR:HB2	1:A:141:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:HA	1:B:279:LEU:O	2.18	0.43
1:B:263:ASN:HD21	1:B:274:THR:HG22	1.82	0.43
1:A:316:LEU:HA	1:A:332:PHE:HB3	2.00	0.43
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.56	0.43
1:A:307:HIS:C	1:A:307:HIS:HD1	2.27	0.43
1:B:99:TYR:HB2	1:B:141:TYR:CE2	2.54	0.43
1:B:292:ALA:HB3	1:B:313:SER:HB3	2.01	0.43
1:A:139:TRP:HA	1:A:164:TYR:O	2.18	0.43
1:B:43:ALA:HA	1:B:165:ILE:O	2.19	0.43
1:B:83:GLN:HB2	1:B:164:TYR:CE2	2.54	0.43
1:B:625:LEU:HD13	1:B:625:LEU:HA	1.92	0.43
1:A:130:GLU:HB3	1:A:131:ASN:H	1.26	0.43
1:A:132:PHE:CD1	1:A:346:LYS:HG3	2.54	0.43
1:A:539:ILE:O	1:A:539:ILE:HG13	2.18	0.43
1:B:129:TYR:CG	1:B:185:LYS:HB2	2.54	0.42
1:B:129:TYR:HB3	1:B:185:LYS:O	2.18	0.42
1:A:204:ILE:HG13	1:A:222:GLY:C	2.44	0.42
1:B:57:GLU:O	1:B:59:GLU:N	2.51	0.42
1:B:81:LYS:H	1:B:81:LYS:CD	2.25	0.42
1:A:634:PRO:HB2	1:A:635:LYS:CA	2.49	0.42
1:B:50:ASN:HA	1:B:157:ALA:O	2.19	0.42
1:B:198:GLN:HB2	1:B:206:PRO:HG3	2.01	0.42
1:B:205:GLN:C	1:B:207:SER:N	2.76	0.42
1:B:209:SER:HB2	1:B:213:ARG:HD2	2.01	0.42
1:A:538:GLU:HG3	1:A:651:LYS:HG3	2.01	0.42
1:B:657:GLY:HA3	1:B:683:PHE:CZ	2.54	0.42
1:A:248:VAL:HG11	1:A:250:PHE:CZ	2.54	0.42
1:B:181:LYS:HA	1:B:248:VAL:O	2.20	0.42
1:A:246:LEU:HD21	1:A:279:LEU:HD12	2.01	0.42
1:B:259:LEU:HB2	1:B:277:TYR:HB2	2.02	0.42
1:A:270:GLN:CB	1:A:271:ALA:HB2	2.50	0.41
1:A:386:ASP:O	1:A:530:GLN:HA	2.20	0.41
1:A:418:LEU:O	1:A:419:LEU:HD13	2.19	0.41
1:B:658:TRP:HA	1:B:681:VAL:O	2.20	0.41
1:A:220:ASP:OD1	1:A:222:GLY:HA3	2.21	0.41
1:A:661:TYR:HA	1:A:662:PRO:HA	1.81	0.41
1:A:236:GLY:HA3	1:A:272:THR:CG2	2.48	0.41
1:A:276:TYR:HE1	1:A:307:HIS:CD2	2.39	0.41
1:B:390:LEU:O	1:B:526:SER:HB2	2.20	0.41
1:A:50:ASN:OD1	1:A:156:SER:HA	2.21	0.41
1:A:57:GLU:C	1:A:59:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	1:A:142:LYS:HD2	2.03	0.41
1:B:141:TYR:HE1	1:B:143:HIS:CE1	2.39	0.41
1:A:496:GLY:HA2	1:A:552:TYR:CE2	2.56	0.41
1:A:623:PHE:CG	1:A:624:ASP:N	2.88	0.41
1:B:57:GLU:C	1:B:59:GLU:H	2.28	0.41
1:A:205:GLN:C	1:A:207:SER:N	2.77	0.41
1:B:418:LEU:O	1:B:419:LEU:HD13	2.21	0.41
1:B:190:PHE:HA	1:B:340:ALA:O	2.21	0.41
1:A:198:GLN:HB2	1:A:206:PRO:HG3	2.02	0.40
1:A:255:LEU:HD23	1:A:281:ALA:HB3	2.03	0.40
1:B:90:VAL:HG12	1:B:142:LYS:HD2	2.03	0.40
1:B:409:LEU:HA	1:B:530:GLN:HE22	1.86	0.40
1:B:50:ASN:OD1	1:B:156:SER:HA	2.21	0.40
1:B:132:PHE:CD1	1:B:346:LYS:HG3	2.56	0.40
1:A:72:LEU:HD12	1:A:73:PRO:CD	2.51	0.40
1:A:294:ALA:O	1:A:297:LYS:HG3	2.22	0.40
1:A:655:LEU:HD12	1:A:655:LEU:C	2.46	0.40
1:B:248:VAL:HG11	1:B:250:PHE:CZ	2.56	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	518/717 (72%)	446 (86%)	47 (9%)	25 (5%)	2	1
1	B	518/717 (72%)	449 (87%)	45 (9%)	24 (5%)	2	1
All	All	1036/1434 (72%)	895 (86%)	92 (9%)	49 (5%)	2	1

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	93	ASP
1	A	94	SER
1	A	130	GLU
1	A	155	LYS
1	A	206	PRO
1	A	218	SER
1	A	234	THR
1	A	348	LYS
1	A	634	PRO
1	A	635	LYS
1	A	650	PRO
1	B	54	GLN
1	B	94	SER
1	B	130	GLU
1	B	155	LYS
1	B	206	PRO
1	B	218	SER
1	B	348	LYS
1	B	634	PRO
1	B	635	LYS
1	A	272	THR
1	A	633	THR
1	A	639	THR
1	B	234	THR
1	B	271	ALA
1	B	272	THR
1	B	633	THR
1	B	639	THR
1	B	649	GLY
1	A	53	PRO
1	A	92	THR
1	A	267	ASP
1	A	271	ALA
1	B	53	PRO
1	B	267	ASP
1	B	544	ASN
1	A	268	ASN
1	A	349	ASP
1	B	127	LYS
1	B	268	ASN
1	B	349	ASP
1	A	205	GLN

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Mol	Chain	Res	Type
1	B	205	GLN
1	A	127	LYS
1	A	544	ASN
1	B	216	GLY
1	B	154	PRO
1	A	154	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	423/586 (72%)	373 (88%)	50 (12%)	5	7
1	B	422/586 (72%)	369 (87%)	53 (13%)	4	6
All	All	845/1172 (72%)	742 (88%)	103 (12%)	5	7

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	65	SER
1	A	81	LYS
1	A	83	GLN
1	A	84	LYS
1	A	87	ILE
1	A	90	VAL
1	A	101	SER
1	A	131	ASN
1	A	135	VAL
1	A	152	VAL
1	A	187	VAL
1	A	192	THR
1	A	196	LYS
1	A	198	GLN
1	A	202	GLU
1	A	204	ILE

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Mol	Chain	Res	Type
1	A	221	ASP
1	A	228	LYS
1	A	254	LYS
1	A	260	ILE
1	A	272	THR
1	A	273	THR
1	A	275	GLN
1	A	284	THR
1	A	299	GLN
1	A	331	ARG
1	A	346	LYS
1	A	348	LYS
1	A	383	THR
1	A	392	LEU
1	A	414	ILE
1	A	419	LEU
1	A	479	LYS
1	A	483	VAL
1	A	494	LYS
1	A	499	THR
1	A	555	ILE
1	A	571	THR
1	A	580	VAL
1	A	585	LYS
1	A	590	THR
1	A	591	LEU
1	A	596	ARG
1	A	602	THR
1	A	625	LEU
1	A	635	LYS
1	A	640	ASP
1	A	643	VAL
1	A	681	VAL
1	B	61	LYS
1	B	65	SER
1	B	81	LYS
1	B	83	GLN
1	B	84	LYS
1	B	87	ILE
1	B	89	LYS
1	B	90	VAL
1	B	131	ASN

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Mol	Chain	Res	Type
1	B	135	VAL
1	B	152	VAL
1	B	187	VAL
1	B	192	THR
1	B	196	LYS
1	B	198	GLN
1	B	202	GLU
1	B	204	ILE
1	B	221	ASP
1	B	228	LYS
1	B	254	LYS
1	B	260	ILE
1	B	272	THR
1	B	273	THR
1	B	275	GLN
1	B	284	THR
1	B	299	GLN
1	B	323	PRO
1	B	331	ARG
1	B	346	LYS
1	B	348	LYS
1	B	382	THR
1	B	383	THR
1	B	392	LEU
1	B	414	ILE
1	B	419	LEU
1	B	479	LYS
1	B	483	VAL
1	B	494	LYS
1	B	499	THR
1	B	555	ILE
1	B	571	THR
1	B	579	THR
1	B	580	VAL
1	B	585	LYS
1	B	590	THR
1	B	591	LEU
1	B	596	ARG
1	B	602	THR
1	B	625	LEU
1	B	635	LYS
1	B	640	ASP

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Mol	Chain	Res	Type
1	B	643	VAL
1	B	681	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	307	HIS
1	A	489	ASN
1	A	629	ASN
1	A	676	ASN
1	B	96	ASN
1	B	307	HIS
1	B	489	ASN
1	B	629	ASN

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	532/717 (74%)	0.54	20 (3%)	44 40	28, 62, 101, 140	0
1	B	532/717 (74%)	0.53	25 (4%)	36 32	30, 61, 101, 141	0
All	All	1064/1434 (74%)	0.54	45 (4%)	40 36	28, 62, 101, 141	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ASN	4.6
1	B	269	ASN	4.2
1	B	302	SER	3.6
1	B	268	ASN	3.5
1	A	634	PRO	3.4
1	B	238	GLU	3.2
1	A	88	GLU	3.1
1	A	221	ASP	3.1
1	B	106	PRO	3.0
1	B	204	ILE	3.0
1	A	268	ASN	3.0
1	B	622	GLY	3.0
1	B	420	PRO	2.8
1	A	302	SER	2.7
1	B	92	THR	2.6
1	A	232	THR	2.6
1	A	624	ASP	2.6
1	B	634	PRO	2.6
1	B	502	ASN	2.4
1	B	630	THR	2.4
1	B	37	GLN	2.4
1	A	633	THR	2.4
1	B	633	THR	2.4
1	A	649	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLN	2.4
1	A	635	LYS	2.3
1	B	674	SER	2.3
1	B	381	LEU	2.3
1	B	91	GLU	2.2
1	B	480	THR	2.2
1	B	81	LYS	2.1
1	B	206	PRO	2.1
1	A	37	GLN	2.1
1	A	558	ASP	2.1
1	A	674	SER	2.1
1	B	415	MET	2.1
1	A	301	ASN	2.1
1	A	625	LEU	2.1
1	B	604	ASP	2.1
1	A	392	LEU	2.0
1	A	151	LYS	2.0
1	B	304	THR	2.0
1	A	497	MET	2.0
1	B	198	GLN	2.0
1	B	270	GLN	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.