



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 1YIF / pdb_00001yif
Title : CRYSTAL STRUCTURE OF beta-1,4-xylosidase FROM BACILLUS SUB-
TILIS, NEW YORK STRUCTURAL GENOMICS CONSORTIUM
Authors : Patskovsky, Y.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for
Structural Genomics (NYSGXRC)
Deposited on : 2005-01-11
Resolution : 1.80 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

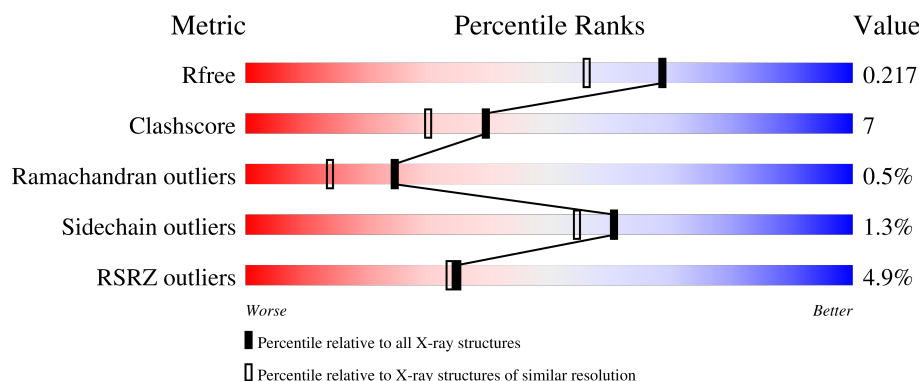
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	533	5% 85% 14%
1	B	533	5% 85% 14%
1	C	533	6% 83% 16%
1	D	533	4% 83% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20084 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-1,4-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4339	2785	728	815	11			
1	B	532	Total	C	N	O	S	0	0	0
			4339	2785	728	815	11			
1	C	532	Total	C	N	O	S	0	0	0
			4339	2785	728	815	11			
1	D	532	Total	C	N	O	S	0	0	0
			4339	2785	728	815	11			

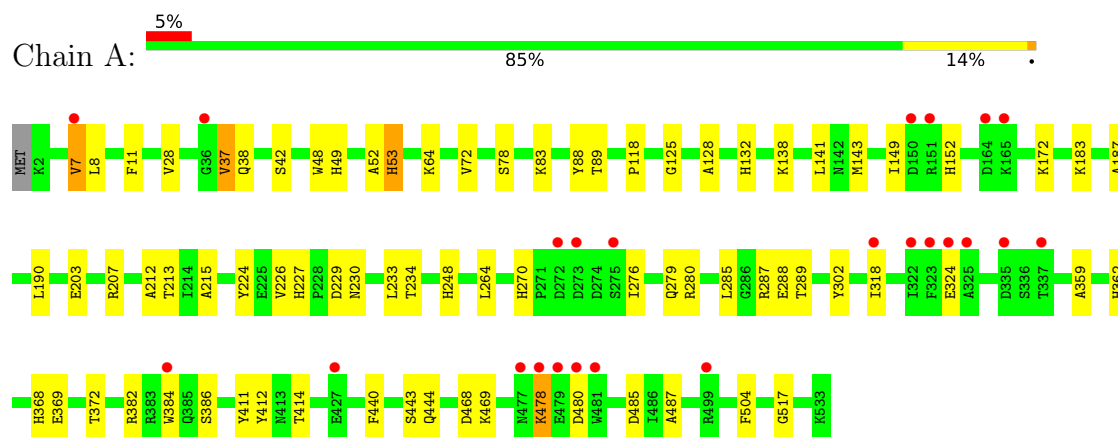
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	649	Total	O	0	0
			649	649		
2	B	671	Total	O	0	0
			671	671		
2	C	699	Total	O	0	0
			699	699		
2	D	709	Total	O	0	0
			709	709		

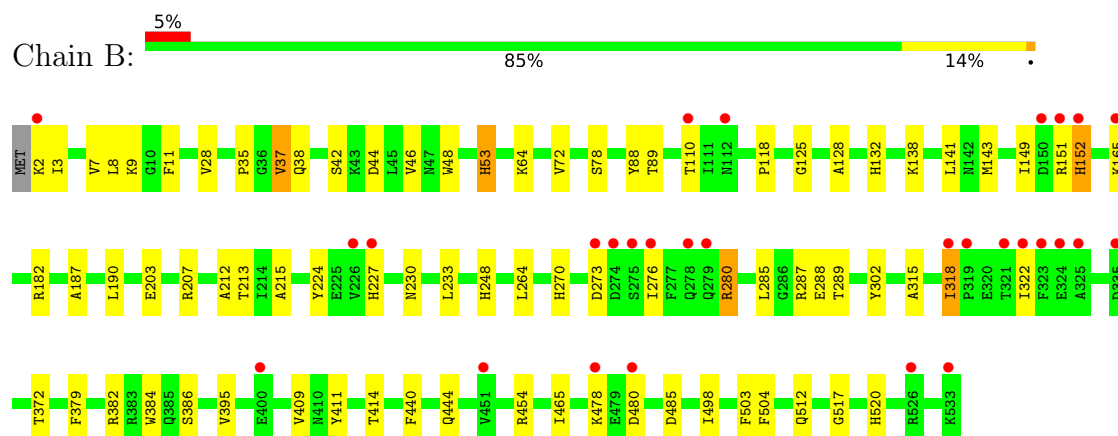
3 Residue-property plots [i](#)

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.

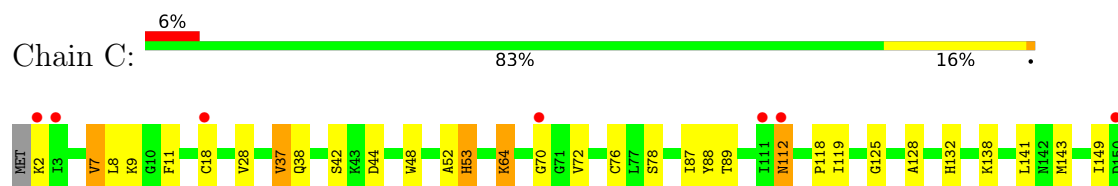
• Molecule 1: BETA-1,4-XYLOSIDASE

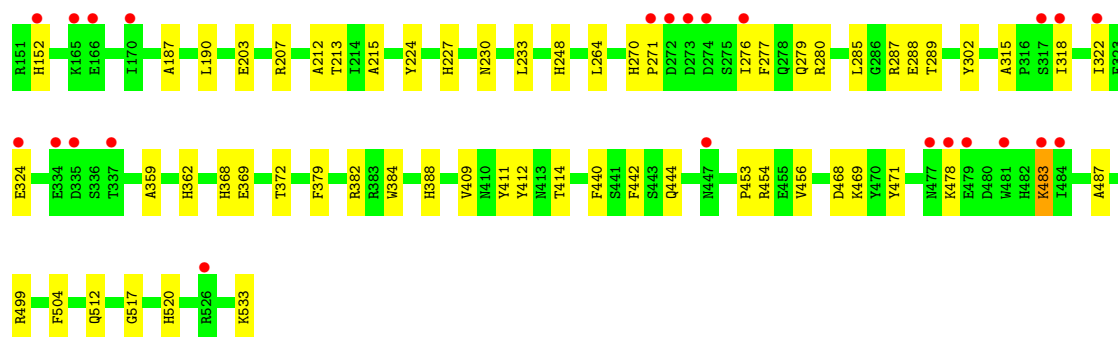


• Molecule 1: BETA-1,4-XYLOSIDASE

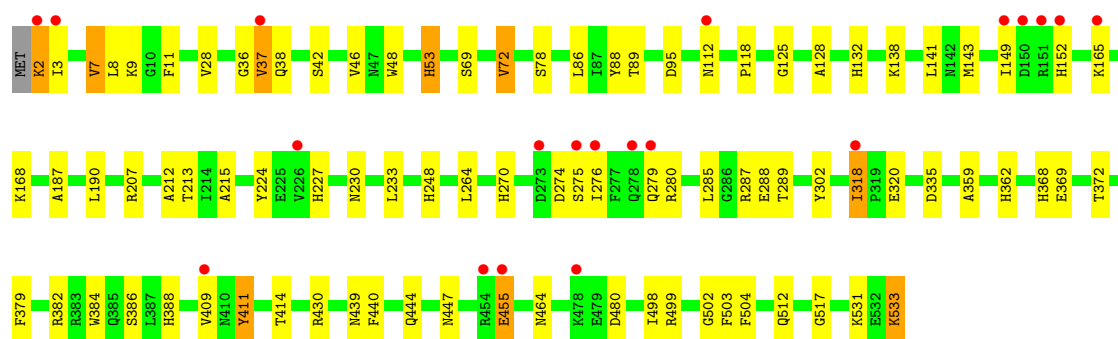
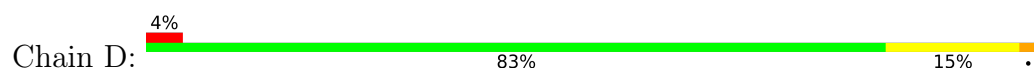


• Molecule 1: BETA-1,4-XYLOSIDASE





● Molecule 1: BETA-1,4-XYLOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.23Å 104.61Å 114.60Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-1.80) 94.5 (20.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.218 0.205 , 0.217	Depositor DCC
R_{free} test set	6434 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.6	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	0.94	EDS
Total number of atoms	20084	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	0.36	0/4475	0.88	11/6090 (0.2%)
1	B	0.35	0/4475	0.87	13/6090 (0.2%)
1	C	0.36	0/4475	0.87	14/6090 (0.2%)
1	D	0.36	0/4475	0.89	12/6090 (0.2%)
All	All	0.36	0/17900	0.88	50/24360 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	GLN	CA-C-N	9.16	128.90	119.56
1	A	444	GLN	C-N-CA	9.16	128.90	119.56
1	D	444	GLN	CA-C-N	9.11	128.85	119.56
1	D	444	GLN	C-N-CA	9.11	128.85	119.56
1	C	444	GLN	CA-C-N	8.56	128.29	119.56
1	C	444	GLN	C-N-CA	8.56	128.29	119.56
1	B	444	GLN	CA-C-N	7.91	127.63	119.56
1	B	444	GLN	C-N-CA	7.91	127.63	119.56
1	B	35	PRO	CA-C-N	7.38	127.35	120.34
1	B	35	PRO	C-N-CA	7.38	127.35	120.34
1	B	149	ILE	N-CA-C	7.33	118.05	110.36
1	C	149	ILE	N-CA-C	7.23	117.95	110.36
1	B	409	VAL	N-CA-C	7.11	118.37	107.78
1	A	149	ILE	N-CA-C	6.96	117.67	110.36
1	D	149	ILE	N-CA-C	6.95	117.65	110.36
1	D	409	VAL	N-CA-C	6.74	117.82	107.78
1	D	72	VAL	N-CA-C	6.31	116.57	108.12
1	A	480	ASP	N-CA-C	5.93	117.96	108.41
1	C	409	VAL	N-CA-C	5.89	116.77	108.17
1	D	36	GLY	N-CA-C	5.84	119.67	112.14
1	C	53	HIS	CA-C-N	5.78	125.25	119.24
1	C	53	HIS	C-N-CA	5.78	125.25	119.24
1	B	480	ASP	N-CA-C	5.67	117.47	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	480	ASP	N-CA-C	5.67	117.46	108.67
1	D	411	TYR	N-CA-C	5.67	118.01	109.23
1	A	52	ALA	N-CA-C	5.60	117.05	108.42
1	C	411	TYR	N-CA-C	5.57	118.30	109.50
1	D	53	HIS	CA-C-N	5.54	125.01	119.24
1	D	53	HIS	C-N-CA	5.54	125.01	119.24
1	C	412	TYR	N-CA-C	-5.50	104.75	112.12
1	B	411	TYR	N-CA-C	5.41	117.61	109.23
1	A	53	HIS	CA-C-N	5.38	124.83	119.24
1	A	53	HIS	C-N-CA	5.38	124.83	119.24
1	C	52	ALA	CA-C-N	5.37	127.80	122.00
1	C	52	ALA	C-N-CA	5.37	127.80	122.00
1	A	411	TYR	N-CA-C	5.28	117.42	109.23
1	D	447	ASN	CA-CB-CG	5.26	117.86	112.60
1	C	483	LYS	N-CA-C	5.22	117.26	108.96
1	C	52	ALA	N-CA-C	5.21	116.20	108.60
1	C	70	GLY	N-CA-C	-5.19	105.17	112.13
1	C	442	PHE	N-CA-C	5.16	118.11	110.48
1	B	53	HIS	CA-C-N	5.15	124.60	119.24
1	B	53	HIS	C-N-CA	5.15	124.60	119.24
1	B	395	VAL	N-CA-C	5.12	115.28	108.11
1	A	412	TYR	N-CA-C	-5.11	105.27	112.12
1	A	443	SER	CA-C-N	5.04	128.39	122.85
1	A	443	SER	C-N-CA	5.04	128.39	122.85
1	D	274	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	280	ARG	N-CA-C	5.02	118.51	112.38
1	B	409	VAL	CB-CA-C	-5.02	103.30	110.12

There are no chirality outliers.

There are no planarity outliers.

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	4339	0	4106	53	0
1	B	4339	0	4106	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4339	0	4106	61	0
1	D	4339	0	4106	58	0
2	A	649	0	0	23	0
2	B	671	0	0	14	0
2	C	699	0	0	24	0
2	D	709	0	0	21	0
All	All	20084	0	16424	225	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 (225) 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:152:HIS:CD2	1:B:152:HIS:H	1.77	0.96
1:B:152:HIS:H	1:B:152:HIS:HD2	1.18	0.90
1:B:64:LYS:HD2	2:B:1117:HOH:O	1.74	0.87
1:A:468:ASP:HB3	2:A:998:HOH:O	1.77	0.83
1:A:64:LYS:HD2	2:A:946:HOH:O	1.79	0.83
1:D:464:ASN:HB3	2:D:1193:HOH:O	1.81	0.79
1:B:322:ILE:HG13	2:B:1021:HOH:O	1.84	0.77
1:D:335:ASP:HB3	2:D:1221:HOH:O	1.85	0.75
1:C:471:TYR:HB3	2:C:1212:HOH:O	1.88	0.72
1:A:478:LYS:HA	2:A:949:HOH:O	1.89	0.72
1:B:165:LYS:HG2	2:B:938:HOH:O	1.90	0.70
1:C:285:LEU:HD22	1:C:384:TRP:O	1.91	0.70
1:B:110:THR:HB	2:B:783:HOH:O	1.90	0.70
1:D:517:GLY:HA3	2:D:675:HOH:O	1.92	0.69
1:A:226:VAL:HB	2:A:1159:HOH:O	1.93	0.69
1:B:285:LEU:HD22	1:B:384:TRP:O	1.93	0.68
1:C:270:HIS:HD2	2:C:672:HOH:O	1.75	0.68
1:B:9:LYS:HE2	2:B:1080:HOH:O	1.93	0.68
1:C:2:LYS:HE2	1:C:315:ALA:H	1.59	0.67
1:A:141:LEU:HD11	1:A:190:LEU:HB2	1.76	0.67
1:B:141:LEU:HD11	1:B:190:LEU:HB2	1.76	0.67
1:A:270:HIS:HD2	2:A:762:HOH:O	1.75	0.67
1:B:318:ILE:HG21	2:B:1186:HOH:O	1.95	0.67
1:C:141:LEU:HD11	1:C:190:LEU:HB2	1.77	0.67
1:D:112:ASN:HB2	2:D:943:HOH:O	1.95	0.66
1:B:2:LYS:HE2	1:B:315:ALA:H	1.61	0.66
1:D:287:ARG:NH2	1:D:504:PHE:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD22	1:A:384:TRP:O	1.95	0.65
1:C:287:ARG:NH2	1:C:504:PHE:HB3	2.12	0.65
1:D:141:LEU:HD11	1:D:190:LEU:HB2	1.79	0.64
1:B:287:ARG:NH2	1:B:504:PHE:HB3	2.13	0.64
1:B:152:HIS:CD2	1:B:152:HIS:N	2.56	0.63
1:A:287:ARG:NH2	1:A:504:PHE:HB3	2.13	0.63
1:A:276:ILE:O	1:A:280:ARG:HD2	2.00	0.62
1:C:533:LYS:HG2	2:C:1211:HOH:O	1.98	0.61
1:C:454:ARG:HG3	2:C:992:HOH:O	1.99	0.61
1:D:270:HIS:HD2	2:D:615:HOH:O	1.84	0.61
1:A:83:LYS:HE2	2:A:939:HOH:O	2.01	0.60
1:D:455:GLU:H	1:D:455:GLU:CD	2.08	0.60
1:C:276:ILE:O	1:C:280:ARG:HD2	2.01	0.60
1:C:324:GLU:HG2	2:C:1001:HOH:O	2.02	0.60
1:B:44:ASP:HB2	2:B:963:HOH:O	2.02	0.60
1:C:382:ARG:HD2	2:C:577:HOH:O	2.01	0.60
1:C:112:ASN:HB3	2:C:883:HOH:O	2.02	0.59
1:C:64:LYS:HD2	2:C:818:HOH:O	2.02	0.59
1:C:322:ILE:HG13	2:C:945:HOH:O	2.03	0.59
1:C:388:HIS:HD2	2:C:994:HOH:O	1.85	0.59
1:D:37:VAL:HG11	1:D:86:LEU:HD21	1.86	0.58
1:C:483:LYS:HG3	2:C:1212:HOH:O	2.03	0.58
1:D:285:LEU:HD22	1:D:384:TRP:O	2.03	0.57
1:D:165:LYS:HG3	2:D:891:HOH:O	2.04	0.57
1:D:276:ILE:O	1:D:280:ARG:HD2	2.05	0.57
1:B:270:HIS:HD2	2:B:557:HOH:O	1.88	0.57
1:B:227:HIS:CE1	1:B:302:TYR:CZ	2.93	0.56
1:D:165:LYS:HG2	2:D:823:HOH:O	2.05	0.56
1:D:78:SER:OG	1:D:132:HIS:HE1	1.89	0.56
1:A:517:GLY:HA3	2:A:1135:HOH:O	2.04	0.56
1:D:531:LYS:HE2	2:D:922:HOH:O	2.06	0.56
1:B:182:ARG:HD3	1:C:277:PHE:CD2	2.42	0.55
1:B:273:ASP:O	1:C:152:HIS:CE1	2.60	0.54
1:C:517:GLY:HA3	2:C:1014:HOH:O	2.08	0.54
1:B:276:ILE:O	1:B:280:ARG:HD2	2.08	0.54
1:B:187:ALA:HB2	1:B:248:HIS:CE1	2.43	0.53
1:A:226:VAL:HG22	2:A:660:HOH:O	2.08	0.53
1:C:78:SER:OG	1:C:132:HIS:HE1	1.91	0.53
1:A:152:HIS:HB3	2:A:721:HOH:O	2.09	0.53
1:C:499:ARG:HG3	2:C:942:HOH:O	2.09	0.53
1:D:9:LYS:HE2	2:D:899:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:CB	2:A:1159:HOH:O	2.57	0.52
1:C:227:HIS:HE1	1:C:302:TYR:CE1	2.27	0.52
1:C:280:ARG:HD3	2:C:762:HOH:O	2.08	0.52
1:D:187:ALA:HB2	1:D:248:HIS:CE1	2.45	0.52
1:B:78:SER:OG	1:B:132:HIS:HE1	1.93	0.52
1:B:212:ALA:HB3	1:B:233:LEU:HB3	1.92	0.51
1:B:227:HIS:CE1	1:B:302:TYR:CE1	2.98	0.51
1:A:212:ALA:HB3	1:A:233:LEU:HB3	1.92	0.51
1:B:382:ARG:HD2	2:B:612:HOH:O	2.10	0.51
1:A:213:THR:CG2	1:A:230:ASN:HD21	2.22	0.51
1:C:8:LEU:HB2	1:C:289:THR:HB	1.91	0.51
1:A:229:ASP:HB2	2:A:1001:HOH:O	2.10	0.51
1:D:382:ARG:HD2	2:D:634:HOH:O	2.09	0.51
1:A:172:LYS:HD3	2:A:1170:HOH:O	2.10	0.51
1:C:212:ALA:HB3	1:C:233:LEU:HB3	1.93	0.51
1:C:213:THR:CG2	1:C:230:ASN:HD21	2.24	0.51
1:D:212:ALA:HB3	1:D:233:LEU:HB3	1.93	0.51
1:A:324:GLU:HB2	2:A:1040:HOH:O	2.10	0.51
1:D:213:THR:CG2	1:D:230:ASN:HD21	2.23	0.51
1:A:8:LEU:HB2	1:A:289:THR:HB	1.92	0.50
1:B:227:HIS:HE1	1:B:302:TYR:CE1	2.29	0.50
1:B:125:GLY:HA3	1:B:143:MET:O	2.10	0.50
1:A:280:ARG:HD3	2:A:763:HOH:O	2.12	0.50
1:C:119:ILE:HG13	2:C:937:HOH:O	2.12	0.50
1:A:187:ALA:HB2	1:A:248:HIS:CE1	2.47	0.50
1:A:78:SER:OG	1:A:132:HIS:HE1	1.94	0.49
1:B:8:LEU:HB2	1:B:289:THR:HB	1.94	0.49
1:C:44:ASP:HB2	2:C:946:HOH:O	2.11	0.49
1:A:207:ARG:HB2	2:A:591:HOH:O	2.12	0.49
1:A:132:HIS:HD2	1:A:138:LYS:NZ	2.11	0.49
1:B:213:THR:CG2	1:B:230:ASN:HD21	2.25	0.49
1:D:168:LYS:HE3	2:D:1222:HOH:O	2.11	0.49
1:D:8:LEU:HB2	1:D:289:THR:HB	1.95	0.49
1:D:95:ASP:HB2	2:D:996:HOH:O	2.13	0.48
1:B:38:GLN:HG2	1:B:53:HIS:NE2	2.29	0.48
1:A:230:ASN:CG	2:A:1159:HOH:O	2.57	0.48
1:D:279:GLN:HB3	2:D:1237:HOH:O	2.13	0.48
1:A:215:ALA:HB1	1:A:224:TYR:HB3	1.96	0.48
1:C:2:LYS:HE2	1:C:315:ALA:N	2.27	0.48
1:D:320:GLU:HG3	2:D:884:HOH:O	2.14	0.48
1:B:88:TYR:OH	1:B:118:PRO:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:HIS:HA	2:A:880:HOH:O	2.13	0.47
1:A:42:SER:HB2	1:A:48:TRP:CD2	2.50	0.47
1:D:533:LYS:HB3	1:D:533:LYS:NZ	2.29	0.47
1:A:37:VAL:O	1:A:53:HIS:HA	2.14	0.47
1:A:382:ARG:HD2	2:A:699:HOH:O	2.13	0.47
1:D:132:HIS:HD2	1:D:138:LYS:NZ	2.12	0.47
1:C:42:SER:HB2	1:C:48:TRP:CD2	2.50	0.47
1:C:279:GLN:HB3	2:C:619:HOH:O	2.13	0.47
1:B:182:ARG:HD3	1:C:277:PHE:CE2	2.49	0.47
1:C:128:ALA:HA	1:C:141:LEU:O	2.15	0.47
1:D:227:HIS:HE1	1:D:302:TYR:CE1	2.33	0.47
1:C:187:ALA:HB2	1:C:248:HIS:CE1	2.49	0.47
1:D:125:GLY:HA3	1:D:143:MET:O	2.14	0.47
1:C:125:GLY:HA3	1:C:143:MET:O	2.15	0.47
1:B:517:GLY:HA3	2:B:556:HOH:O	2.14	0.46
1:B:3:ILE:HG12	1:B:46:VAL:HG22	1.96	0.46
1:B:454:ARG:O	1:B:454:ARG:HG3	2.15	0.46
1:B:478:LYS:O	1:B:478:LYS:HG2	2.14	0.46
1:D:42:SER:HB2	1:D:48:TRP:CD2	2.51	0.46
1:D:388:HIS:HD2	2:D:1153:HOH:O	1.96	0.46
1:D:7:VAL:HG12	1:D:8:LEU:HG	1.98	0.46
1:B:143:MET:C	1:B:143:MET:SD	2.99	0.46
1:B:273:ASP:O	1:C:152:HIS:HE1	1.98	0.46
1:C:28:VAL:CG2	1:C:38:GLN:HB2	2.46	0.46
1:C:37:VAL:O	1:C:53:HIS:HA	2.16	0.46
1:D:88:TYR:OH	1:D:118:PRO:HB3	2.16	0.46
1:B:2:LYS:HE2	1:B:315:ALA:N	2.30	0.46
1:D:207:ARG:HB2	2:D:586:HOH:O	2.16	0.45
1:A:203:GLU:OE1	1:A:213:THR:HG21	2.16	0.45
1:A:226:VAL:HG23	2:A:1021:HOH:O	2.16	0.45
1:A:227:HIS:CE1	1:A:302:TYR:CE1	3.03	0.45
1:C:207:ARG:HB2	2:C:665:HOH:O	2.17	0.45
1:A:227:HIS:HE1	1:A:302:TYR:CE1	2.34	0.45
1:D:128:ALA:HA	1:D:141:LEU:O	2.17	0.45
1:A:38:GLN:HG2	1:A:53:HIS:HE2	1.82	0.45
1:B:215:ALA:HB1	1:B:224:TYR:HB3	1.99	0.45
1:C:533:LYS:HE3	2:C:722:HOH:O	2.17	0.45
1:A:28:VAL:CG2	1:A:38:GLN:HB2	2.47	0.45
1:A:88:TYR:OH	1:A:118:PRO:HB3	2.17	0.45
1:C:264:LEU:HA	1:C:288:GLU:O	2.17	0.45
1:A:125:GLY:HA3	1:A:143:MET:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:HG12	1:C:8:LEU:HG	2.00	0.44
1:C:203:GLU:OE1	1:C:213:THR:HG21	2.18	0.44
1:C:215:ALA:HB1	1:C:224:TYR:HB3	1.99	0.44
1:A:38:GLN:HG2	1:A:53:HIS:NE2	2.32	0.44
1:A:324:GLU:CB	2:A:1040:HOH:O	2.66	0.44
1:D:38:GLN:HG2	1:D:53:HIS:NE2	2.32	0.44
1:D:318:ILE:HD11	2:D:837:HOH:O	2.17	0.44
1:D:379:PHE:CD1	1:D:512:GLN:HB2	2.52	0.44
1:C:469:LYS:HD3	1:C:487:ALA:HB1	2.00	0.44
1:D:215:ALA:HB1	1:D:224:TYR:HB3	2.00	0.44
1:A:7:VAL:HG12	1:A:8:LEU:HG	1.99	0.44
1:B:132:HIS:HD2	1:B:138:LYS:NZ	2.16	0.44
1:D:28:VAL:O	1:D:37:VAL:HG23	2.17	0.44
1:A:279:GLN:HB3	2:A:592:HOH:O	2.17	0.44
1:A:469:LYS:HD3	1:A:487:ALA:HB1	2.00	0.44
1:B:285:LEU:CD2	1:B:384:TRP:O	2.65	0.44
1:D:270:HIS:HE1	2:D:995:HOH:O	2.01	0.44
1:C:76:CYS:HB3	1:C:87:ILE:HB	2.00	0.43
1:C:132:HIS:HD2	1:C:138:LYS:NZ	2.16	0.43
1:D:498:ILE:HD11	1:D:503:PHE:HA	1.99	0.43
1:B:151:ARG:HG3	2:B:861:HOH:O	2.17	0.43
1:B:128:ALA:HA	1:B:141:LEU:O	2.18	0.43
1:B:227:HIS:HE1	1:B:302:TYR:CZ	2.34	0.43
1:B:379:PHE:CD1	1:B:512:GLN:HB2	2.54	0.43
1:A:128:ALA:HA	1:A:141:LEU:O	2.17	0.42
1:B:42:SER:HB2	1:B:48:TRP:CD2	2.54	0.42
1:C:112:ASN:CB	2:C:883:HOH:O	2.63	0.42
1:C:9:LYS:HE2	2:C:1054:HOH:O	2.18	0.42
1:A:359:ALA:O	1:A:362:HIS:HB2	2.19	0.42
1:D:69:SER:HB2	1:D:502:GLY:HA3	2.01	0.42
1:C:271:PRO:HB3	2:C:980:HOH:O	2.19	0.42
1:A:49:HIS:HA	2:A:620:HOH:O	2.19	0.42
1:D:3:ILE:HG12	1:D:46:VAL:HG22	2.02	0.42
1:D:72:VAL:HA	1:D:89:THR:O	2.19	0.42
1:D:411:TYR:HE2	2:D:901:HOH:O	2.03	0.42
1:B:454:ARG:HA	2:B:551:HOH:O	2.19	0.42
1:D:38:GLN:HG2	1:D:53:HIS:CD2	2.54	0.42
1:D:227:HIS:CE1	1:D:302:TYR:CE1	3.08	0.42
1:B:38:GLN:HG2	1:B:53:HIS:CD2	2.54	0.42
1:B:498:ILE:HD11	1:B:503:PHE:HA	2.02	0.42
1:C:359:ALA:O	1:C:362:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:THR:HA	1:D:414:THR:HB	2.02	0.42
1:C:72:VAL:HA	1:C:89:THR:O	2.20	0.41
1:B:203:GLU:OE1	1:B:213:THR:HG21	2.21	0.41
1:B:372:THR:HA	1:B:414:THR:HB	2.01	0.41
1:B:465:ILE:N	1:B:465:ILE:HD12	2.35	0.41
1:C:478:LYS:HG2	1:C:478:LYS:O	2.20	0.41
1:C:520:HIS:HE1	2:C:579:HOH:O	2.03	0.41
1:D:143:MET:SD	1:D:143:MET:C	3.02	0.41
1:A:264:LEU:HA	1:A:288:GLU:O	2.21	0.41
1:B:273:ASP:CG	1:C:152:HIS:CE1	2.98	0.41
1:C:468:ASP:HB3	2:C:980:HOH:O	2.20	0.41
1:D:359:ALA:O	1:D:362:HIS:HB2	2.21	0.41
1:D:439:ASN:CG	1:D:499:ARG:HG3	2.46	0.41
1:A:372:THR:HA	1:A:414:THR:HB	2.01	0.41
1:C:372:THR:HA	1:C:414:THR:HB	2.02	0.41
1:B:37:VAL:O	1:B:53:HIS:HA	2.21	0.41
1:B:520:HIS:HE1	2:B:604:HOH:O	2.02	0.41
1:C:88:TYR:OH	1:C:118:PRO:HB3	2.21	0.41
1:D:2:LYS:HA	2:D:1087:HOH:O	2.21	0.41
1:A:368:HIS:HB3	1:A:369:GLU:H	1.65	0.41
1:D:368:HIS:HB3	1:D:369:GLU:H	1.62	0.41
1:D:430:ARG:HB2	2:D:640:HOH:O	2.21	0.41
1:B:264:LEU:HA	1:B:288:GLU:O	2.20	0.41
1:C:368:HIS:HB3	1:C:369:GLU:H	1.66	0.41
1:B:28:VAL:CG2	1:B:38:GLN:HB2	2.51	0.41
1:A:183:LYS:HB2	1:D:275:SER:HB2	2.02	0.40
1:A:183:LYS:HB3	2:A:633:HOH:O	2.21	0.40
1:D:28:VAL:CG2	1:D:38:GLN:HB2	2.52	0.40
1:B:72:VAL:HA	1:B:89:THR:O	2.22	0.40
1:C:379:PHE:CD1	1:C:512:GLN:HB2	2.56	0.40
1:A:72:VAL:HA	1:A:89:THR:O	2.21	0.40
1:B:207:ARG:HB2	2:B:617:HOH:O	2.21	0.40
1:C:453:PRO:HB2	1:C:456:VAL:HG23	2.03	0.40
1:D:264:LEU:HA	1:D:288:GLU:O	2.22	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	530/533 (99%)	498 (94%)	28 (5%)	4 (1%)	16	6
1	B	530/533 (99%)	500 (94%)	27 (5%)	3 (1%)	21	11
1	C	530/533 (99%)	500 (94%)	28 (5%)	2 (0%)	30	19
1	D	530/533 (99%)	498 (94%)	30 (6%)	2 (0%)	30	19
All	All	2120/2132 (99%)	1996 (94%)	113 (5%)	11 (0%)	24	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	ASP
1	B	485	ASP
1	A	11	PHE
1	B	11	PHE
1	B	37	VAL
1	C	11	PHE
1	D	11	PHE
1	D	37	VAL
1	A	37	VAL
1	C	37	VAL
1	A	234	THR

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	466/467 (100%)	461 (99%)	5 (1%)	65	60
1	B	466/467 (100%)	461 (99%)	5 (1%)	65	60
1	C	466/467 (100%)	460 (99%)	6 (1%)	61	54
1	D	466/467 (100%)	458 (98%)	8 (2%)	53	45
All	All	1864/1868 (100%)	1840 (99%)	24 (1%)	61	54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	318	ILE
1	A	386	SER
1	A	440	PHE
1	A	478	LYS
1	B	7	VAL
1	B	152	HIS
1	B	318	ILE
1	B	386	SER
1	B	440	PHE
1	C	7	VAL
1	C	18	CYS
1	C	64	LYS
1	C	112	ASN
1	C	318	ILE
1	C	440	PHE
1	D	2	LYS
1	D	7	VAL
1	D	152	HIS
1	D	318	ILE
1	D	386	SER
1	D	440	PHE
1	D	455	GLU
1	D	533	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	132	HIS
1	A	270	HIS

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	424	HIS
1	A	448	ASN
1	B	132	HIS
1	B	152	HIS
1	B	270	HIS
1	B	388	HIS
1	B	448	ASN
1	C	132	HIS
1	C	152	HIS
1	C	270	HIS
1	C	341	ASN
1	C	424	HIS
1	C	448	ASN
1	C	482	HIS
1	D	56	GLN
1	D	132	HIS
1	D	270	HIS
1	D	341	ASN
1	D	388	HIS
1	D	447	ASN
1	D	448	ASN
1	D	464	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

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	532/533 (99%)	0.21	24 (4%) 38 37	9, 15, 29, 45	0
1	B	532/533 (99%)	0.25	29 (5%) 30 29	8, 15, 28, 43	0
1	C	532/533 (99%)	0.23	31 (5%) 29 27	8, 14, 27, 42	0
1	D	532/533 (99%)	0.15	20 (3%) 44 44	8, 14, 27, 40	0
All	All	2128/2132 (99%)	0.21	104 (4%) 35 33	8, 14, 28, 45	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	ILE	7.3
1	C	478	LYS	7.0
1	B	276	ILE	5.7
1	D	152	HIS	5.3
1	D	273	ASP	5.3
1	A	478	LYS	5.2
1	D	150	ASP	4.7
1	C	165	LYS	4.7
1	A	164	ASP	4.7
1	A	322	ILE	4.6
1	B	152	HIS	4.6
1	B	273	ASP	4.6
1	A	325	ALA	4.5
1	C	150	ASP	4.4
1	A	324	GLU	4.1
1	C	272	ASP	4.1
1	B	325	ALA	4.0
1	C	111	ILE	4.0
1	C	479	GLU	4.0
1	D	275	SER	3.9
1	B	318	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	321	THR	3.8
1	A	477	ASN	3.8
1	B	150	ASP	3.8
1	B	478	LYS	3.6
1	D	478	LYS	3.6
1	D	37	VAL	3.5
1	D	276	ILE	3.4
1	D	455	GLU	3.2
1	A	150	ASP	3.2
1	A	273	ASP	3.2
1	B	2	LYS	3.1
1	B	324	GLU	3.1
1	C	2	LYS	3.1
1	C	477	ASN	3.1
1	C	526	ARG	3.0
1	A	481	TRP	3.0
1	A	337	THR	3.0
1	D	454	ARG	3.0
1	C	273	ASP	2.9
1	B	227	HIS	2.9
1	D	2	LYS	2.9
1	C	335	ASP	2.9
1	C	334	GLU	2.9
1	D	278	GLN	2.9
1	C	481	TRP	2.9
1	B	112	ASN	2.8
1	C	170	ILE	2.8
1	A	165	LYS	2.8
1	B	319	PRO	2.8
1	A	318	ILE	2.8
1	B	451	VAL	2.8
1	B	335	ASP	2.7
1	B	278	GLN	2.7
1	B	165	LYS	2.7
1	C	70	GLY	2.6
1	C	166	GLU	2.6
1	C	322	ILE	2.6
1	A	427	GLU	2.6
1	B	526	ARG	2.6
1	B	279	GLN	2.6
1	C	483	LYS	2.6
1	B	275	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	323	PHE	2.5
1	D	318	ILE	2.5
1	C	18	CYS	2.5
1	A	480	ASP	2.5
1	B	274	ASP	2.5
1	A	36	GLY	2.5
1	C	112	ASN	2.5
1	D	165	LYS	2.4
1	D	409	VAL	2.4
1	C	152	HIS	2.4
1	B	323	PHE	2.4
1	C	447	ASN	2.4
1	C	318	ILE	2.4
1	D	151	ARG	2.4
1	C	337	THR	2.3
1	C	484	ILE	2.3
1	C	324	GLU	2.3
1	C	271	PRO	2.3
1	A	384	TRP	2.3
1	A	272	ASP	2.3
1	B	533	LYS	2.2
1	B	110	THR	2.2
1	D	3	ILE	2.2
1	D	149	ILE	2.2
1	B	226	VAL	2.2
1	C	3	ILE	2.1
1	B	151	ARG	2.1
1	A	479	GLU	2.1
1	C	276	ILE	2.1
1	A	275	SER	2.1
1	A	7	VAL	2.1
1	D	279	GLN	2.1
1	D	226	VAL	2.1
1	A	335	ASP	2.1
1	B	480	ASP	2.1
1	C	274	ASP	2.1
1	C	317	SER	2.0
1	D	112	ASN	2.0
1	B	400	GLU	2.0
1	A	151	ARG	2.0
1	A	499	ARG	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.