



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:31 pm BST

PDB ID : 2BS9
Title : Native crystal structure of a GH39 beta-xylosidase XynB1 from *Geobacillus stearothermophilus*
Authors : Czjzek, M.; Bravman, T.; Henrissat, B.; Shoham, Y.
Deposited on : 2005-05-19
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

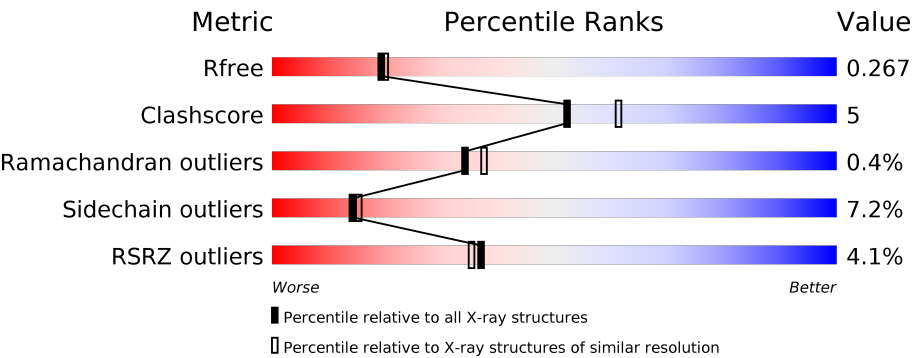
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	503	<div><div>4%</div><div><div></div><div>81%</div><div>16%</div><div>.</div></div></div>
1	B	503	<div><div>5%</div><div><div></div><div>83%</div><div>14%</div><div>.</div></div></div>
1	C	503	<div><div>5%</div><div><div></div><div>82%</div><div>16%</div><div>.</div></div></div>
1	D	503	<div><div>4%</div><div><div></div><div>79%</div><div>18%</div><div>.</div></div></div>
1	E	503	<div><div>2%</div><div><div></div><div>84%</div><div>12%</div><div>.</div></div></div>
1	F	503	<div><div>6%</div><div><div></div><div>81%</div><div>17%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	503	<div><div></div><div>4%</div><div>83%</div><div>14%</div><div></div></div>
1	H	503	<div><div></div><div>3%</div><div>83%</div><div>15%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34099 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-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	B	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	C	501	Total	C	N	O	S	0	0	0
			4088	2642	693	742	11			
1	D	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	E	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	F	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	G	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			
1	H	501	Total	C	N	O	S	0	0	0
			4091	2643	693	744	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	LYS	conflict	UNP Q9ZFM2
A	?	-	LEU	deletion	UNP Q9ZFM2
A	?	-	GLU	deletion	UNP Q9ZFM2
A	406	GLU	PHE	conflict	UNP Q9ZFM2
A	445	ARG	PRO	conflict	UNP Q9ZFM2
A	446	GLN	-	insertion	UNP Q9ZFM2
A	447	VAL	SER	conflict	UNP Q9ZFM2
B	2	GLY	LYS	conflict	UNP Q9ZFM2
B	?	-	LEU	deletion	UNP Q9ZFM2
B	?	-	GLU	deletion	UNP Q9ZFM2
B	406	GLU	PHE	conflict	UNP Q9ZFM2
B	445	ARG	PRO	conflict	UNP Q9ZFM2
B	446	GLN	-	insertion	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	447	VAL	SER	conflict	UNP Q9ZFM2
C	2	GLY	LYS	conflict	UNP Q9ZFM2
C	?	-	LEU	deletion	UNP Q9ZFM2
C	?	-	GLU	deletion	UNP Q9ZFM2
C	406	GLU	PHE	conflict	UNP Q9ZFM2
C	445	ARG	PRO	conflict	UNP Q9ZFM2
C	446	GLN	-	insertion	UNP Q9ZFM2
C	447	VAL	SER	conflict	UNP Q9ZFM2
D	2	GLY	LYS	conflict	UNP Q9ZFM2
D	?	-	LEU	deletion	UNP Q9ZFM2
D	?	-	GLU	deletion	UNP Q9ZFM2
D	406	GLU	PHE	conflict	UNP Q9ZFM2
D	445	ARG	PRO	conflict	UNP Q9ZFM2
D	446	GLN	-	insertion	UNP Q9ZFM2
D	447	VAL	SER	conflict	UNP Q9ZFM2
E	2	GLY	LYS	conflict	UNP Q9ZFM2
E	?	-	LEU	deletion	UNP Q9ZFM2
E	?	-	GLU	deletion	UNP Q9ZFM2
E	406	GLU	PHE	conflict	UNP Q9ZFM2
E	445	ARG	PRO	conflict	UNP Q9ZFM2
E	446	GLN	-	insertion	UNP Q9ZFM2
E	447	VAL	SER	conflict	UNP Q9ZFM2
F	2	GLY	LYS	conflict	UNP Q9ZFM2
F	?	-	LEU	deletion	UNP Q9ZFM2
F	?	-	GLU	deletion	UNP Q9ZFM2
F	406	GLU	PHE	conflict	UNP Q9ZFM2
F	445	ARG	PRO	conflict	UNP Q9ZFM2
F	446	GLN	-	insertion	UNP Q9ZFM2
F	447	VAL	SER	conflict	UNP Q9ZFM2
G	2	GLY	LYS	conflict	UNP Q9ZFM2
G	?	-	LEU	deletion	UNP Q9ZFM2
G	?	-	GLU	deletion	UNP Q9ZFM2
G	406	GLU	PHE	conflict	UNP Q9ZFM2
G	445	ARG	PRO	conflict	UNP Q9ZFM2
G	446	GLN	-	insertion	UNP Q9ZFM2
G	447	VAL	SER	conflict	UNP Q9ZFM2
H	2	GLY	LYS	conflict	UNP Q9ZFM2
H	?	-	LEU	deletion	UNP Q9ZFM2
H	?	-	GLU	deletion	UNP Q9ZFM2
H	406	GLU	PHE	conflict	UNP Q9ZFM2
H	445	ARG	PRO	conflict	UNP Q9ZFM2
H	446	GLN	-	insertion	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	447	VAL	SER	conflict	UNP Q9ZFM2

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

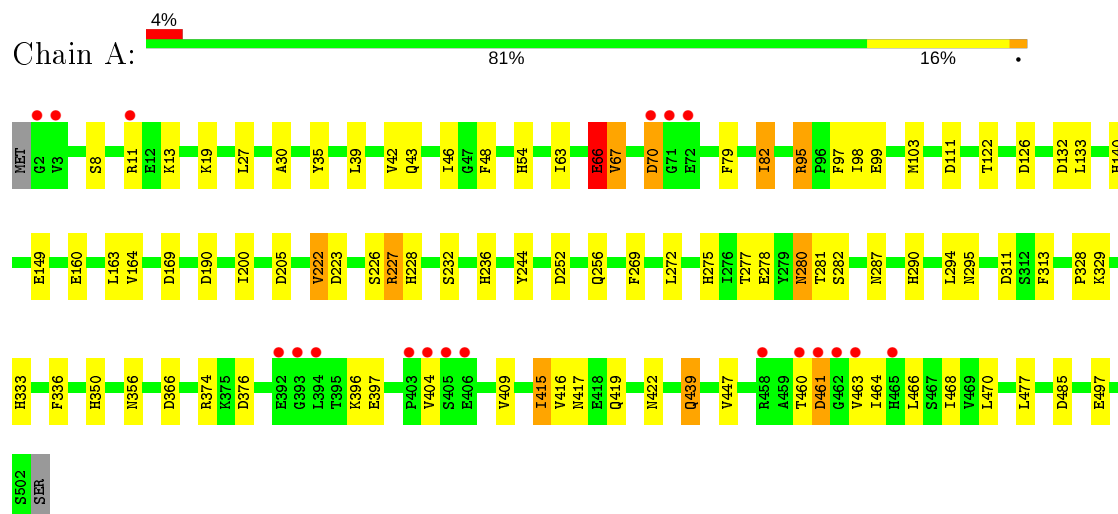
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	161	Total O 161 161	0	0
3	C	177	Total O 177 177	0	0
3	D	172	Total O 172 172	0	0
3	E	180	Total O 180 180	0	0
3	F	140	Total O 140 140	0	0
3	G	179	Total O 179 179	0	0
3	H	188	Total O 188 188	0	0

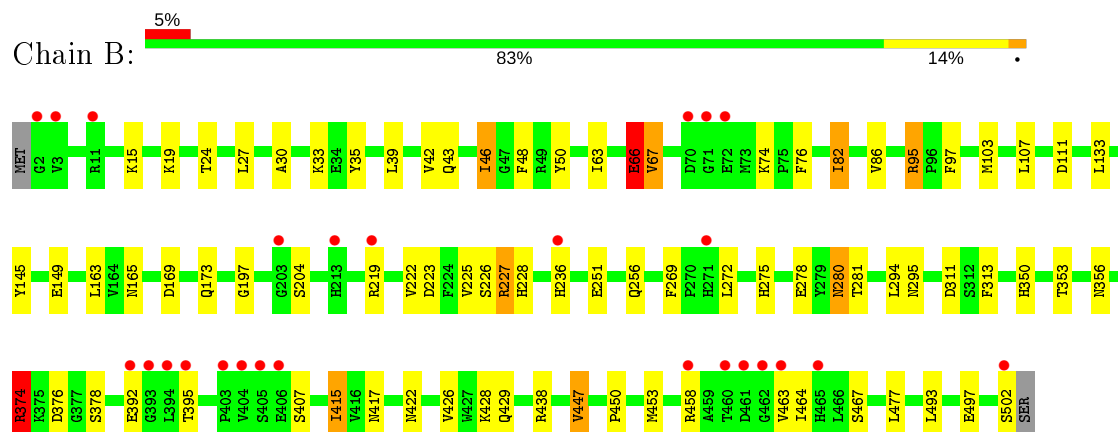
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

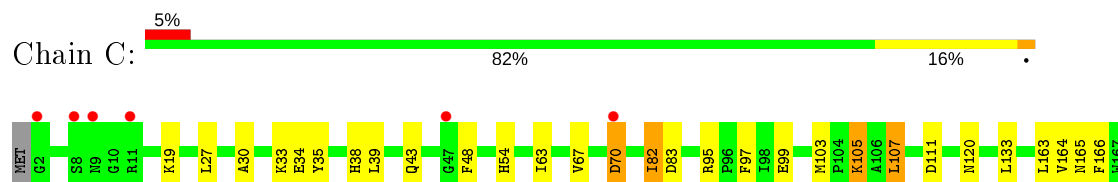
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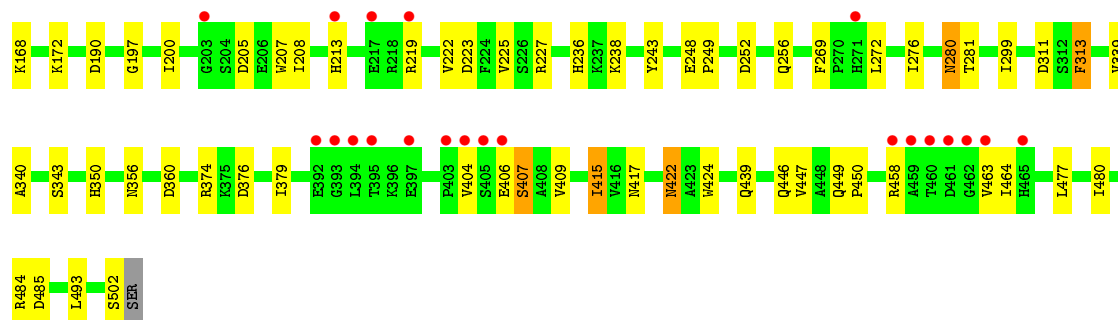


• Molecule 1: BETA-XYLOSIDASE

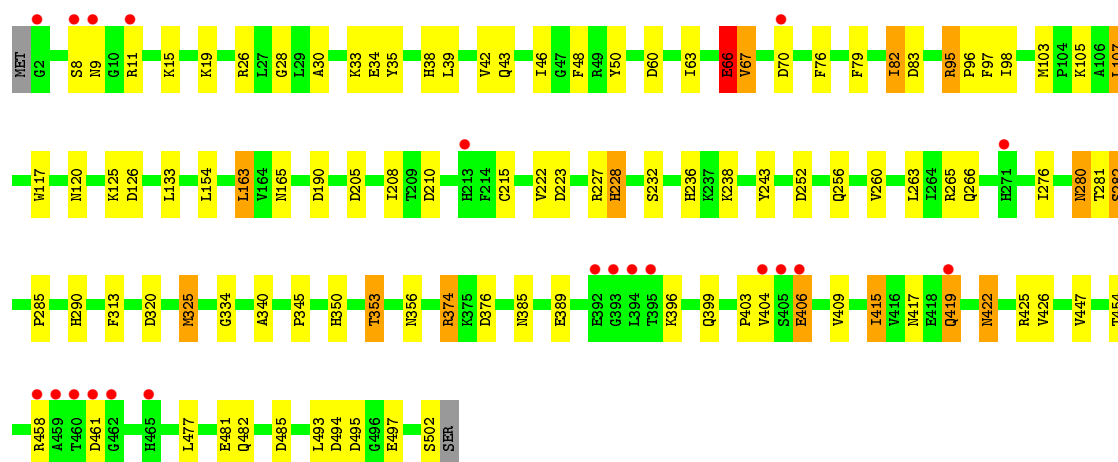
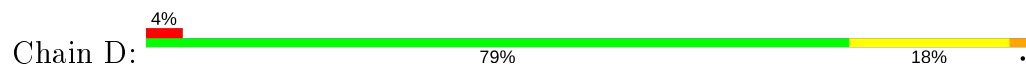


• Molecule 1: BETA-XYLOSIDASE

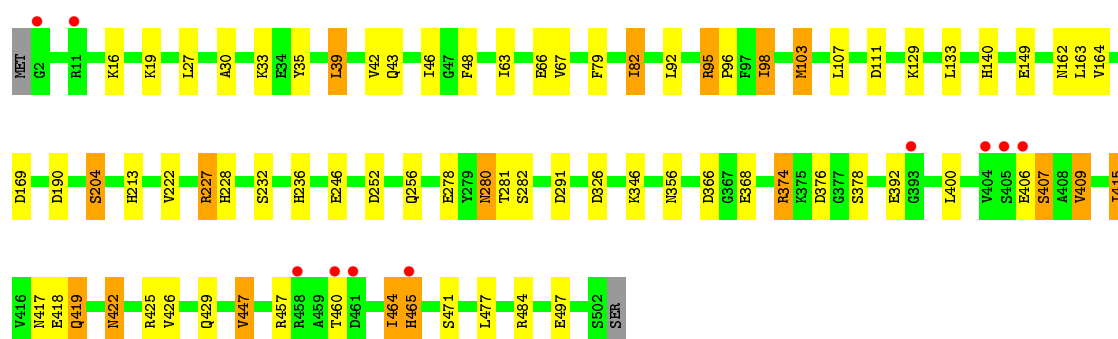
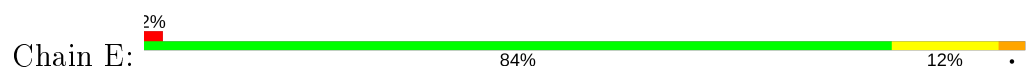




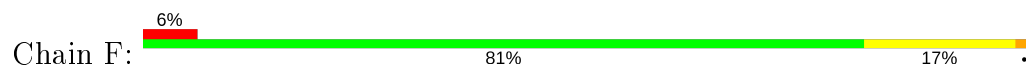
• Molecule 1: BETA-XYLOSIDASE

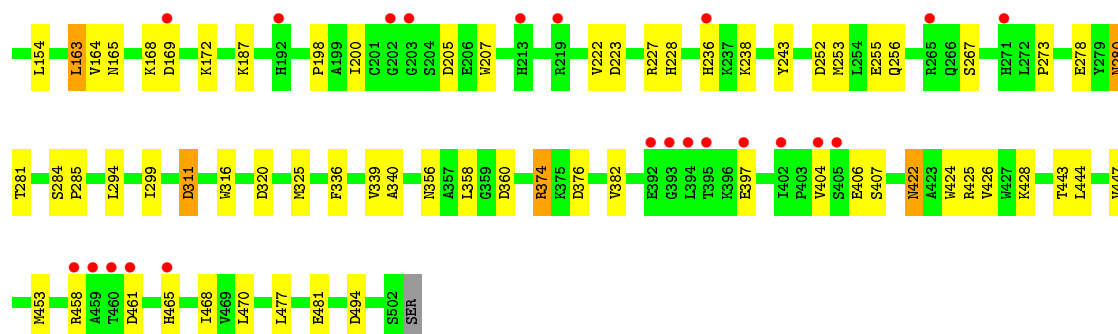


• Molecule 1: BETA-XYLOSIDASE

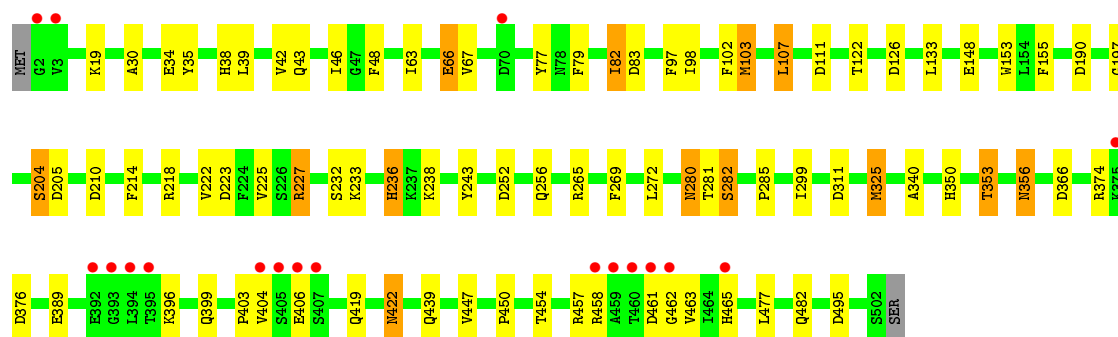
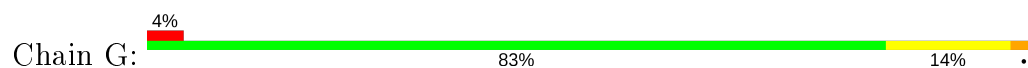


• Molecule 1: BETA-XYLOSIDASE

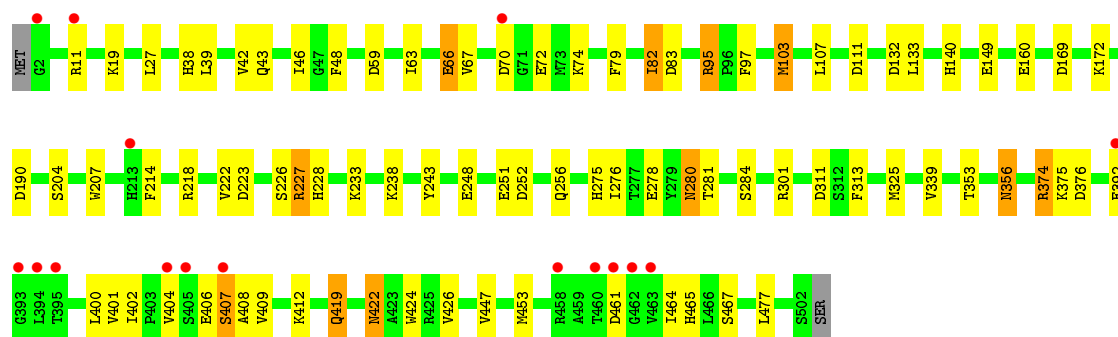
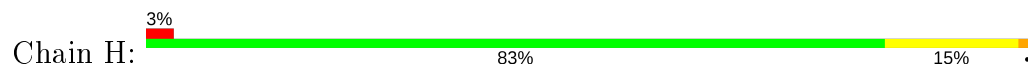




• Molecule 1: BETA-XYLOSIDASE



• Molecule 1: BETA-XYLOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 165.74Å 311.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 24.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 98.1 (24.96-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.259 0.223 , 0.267	Depositor DCC
R_{free} test set	13754 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34099	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.07 % 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 5.0212e-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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/4206	0.82	16/5710 (0.3%)
1	B	0.59	0/4206	0.80	9/5710 (0.2%)
1	C	0.58	0/4203	0.80	10/5706 (0.2%)
1	D	0.60	0/4206	0.81	16/5710 (0.3%)
1	E	0.60	1/4206 (0.0%)	0.80	6/5710 (0.1%)
1	F	0.55	0/4206	0.81	14/5710 (0.2%)
1	G	0.59	1/4206 (0.0%)	0.82	15/5710 (0.3%)
1	H	0.60	1/4206 (0.0%)	0.83	12/5710 (0.2%)
All	All	0.59	3/33645 (0.0%)	0.81	98/45676 (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	E	0	1
1	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	103	MET	SD-CE	-6.26	1.42	1.77
1	E	103	MET	SD-CE	-5.20	1.48	1.77
1	G	103	MET	SD-CE	-5.16	1.49	1.77

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	376	ASP	CB-CG-OD2	7.59	125.13	118.30
1	D	190	ASP	CB-CG-OD2	7.33	124.90	118.30
1	B	376	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	70	ASP	CB-CG-OD2	7.10	124.69	118.30
1	G	111	ASP	CB-CG-OD2	7.08	124.67	118.30
1	G	223	ASP	CB-CG-OD2	6.97	124.57	118.30
1	F	374	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	H	132	ASP	CB-CG-OD2	6.89	124.50	118.30
1	D	70	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	111	ASP	CB-CG-OD2	6.59	124.23	118.30
1	G	205	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	223	ASP	CB-CG-OD2	6.52	124.17	118.30
1	H	169	ASP	CB-CG-OD2	6.50	124.15	118.30
1	F	376	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	252	ASP	CB-CG-OD2	6.39	124.05	118.30
1	H	376	ASP	CB-CG-OD2	6.33	124.00	118.30
1	H	70	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	169	ASP	CB-CG-OD2	6.32	123.99	118.30
1	F	360	ASP	CB-CG-OD2	6.15	123.83	118.30
1	G	461	ASP	CB-CG-OD2	6.14	123.82	118.30
1	G	66	GLU	C-N-CA	6.09	136.93	121.70
1	C	376	ASP	CB-CG-OD2	6.06	123.75	118.30
1	F	494	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	223	ASP	CB-CG-OD2	6.05	123.75	118.30
1	F	223	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	374	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	83	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	311	ASP	CB-CG-OD2	5.98	123.68	118.30
1	E	190	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	169	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	70	ASP	CB-CG-OD2	5.86	123.57	118.30
1	E	111	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	376	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	252	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	320	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	252	ASP	CB-CG-OD2	5.76	123.48	118.30
1	H	190	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	485	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	461	ASP	CB-CG-OD2	5.74	123.46	118.30
1	D	494	ASP	CB-CG-OD2	5.72	123.45	118.30
1	G	190	ASP	CB-CG-OD2	5.72	123.45	118.30
1	G	83	ASP	CB-CG-OD2	5.68	123.41	118.30
1	H	66	GLU	C-N-CA	5.67	135.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	376	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	111	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	223	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	205	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	59	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	126	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	66	GLU	C-N-CA	5.48	135.40	121.70
1	E	252	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	132	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	205	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	311	ASP	CB-CG-OD2	5.44	123.20	118.30
1	F	374	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	205	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	252	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	223	ASP	CB-CG-OD2	5.43	123.19	118.30
1	H	252	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	366	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	46	ILE	N-CA-C	-5.42	96.37	111.00
1	F	66	GLU	C-N-CA	5.41	135.22	121.70
1	G	126	ASP	CB-CG-OD2	5.39	123.15	118.30
1	G	376	ASP	CB-CG-OD2	5.39	123.15	118.30
1	G	311	ASP	CB-CG-OD2	5.38	123.15	118.30
1	H	461	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	66	GLU	C-N-CA	5.35	135.09	121.70
1	G	366	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	126	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	461	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	366	ASP	CB-CG-OD2	5.32	123.09	118.30
1	H	374	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	374	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	190	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	169	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	190	ASP	CB-CG-OD2	5.27	123.04	118.30
1	H	59	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	111	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	485	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	374	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	485	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	210	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	169	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	252	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ASP	CB-CG-OD2	5.17	122.96	118.30
1	G	66	GLU	CA-C-N	5.16	128.55	117.20
1	B	311	ASP	CB-CG-OD2	5.15	122.93	118.30
1	G	210	ASP	CB-CG-OD2	5.15	122.93	118.30
1	G	495	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	320	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	311	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	311	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	205	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	461	ASP	CB-CG-OD2	5.07	122.87	118.30
1	H	223	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	222	VAL	CB-CA-C	-5.03	101.84	111.40
1	A	66	GLU	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	66	GLU	Peptide
1	H	66	GLU	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	4091	0	4001	44	0
1	B	4091	0	4001	45	0
1	C	4088	0	3999	44	0
1	D	4091	0	4001	54	0
1	E	4091	0	4001	41	0
1	F	4091	0	4001	49	0
1	G	4091	0	4001	37	0
1	H	4091	0	4001	50	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	170	0	0	4	0
3	B	161	0	0	2	0
3	C	177	0	0	3	0
3	D	172	0	0	5	0
3	E	180	0	0	5	0
3	F	140	0	0	2	0
3	G	179	0	0	4	0
3	H	188	0	0	8	0
All	All	34099	0	32006	354	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 (354) 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:D:227:ARG:HH12	1:D:256:GLN:HE21	1.12	0.93
1:F:426:VAL:HG21	1:F:447:VAL:HG11	1.51	0.91
1:B:227:ARG:HH12	1:B:256:GLN:HE21	1.09	0.91
1:B:42:VAL:O	1:B:46:ILE:O	1.89	0.90
1:D:280:ASN:HD22	1:D:281:THR:H	1.19	0.88
1:C:280:ASN:HD22	1:C:281:THR:H	1.18	0.87
1:A:227:ARG:HH12	1:A:256:GLN:HE21	1.16	0.87
1:E:103:MET:SD	3:E:2062:HOH:O	2.31	0.86
1:C:227:ARG:HH12	1:C:256:GLN:HE21	1.25	0.85
1:H:280:ASN:HD22	1:H:281:THR:H	1.23	0.85
1:H:19:LYS:NZ	1:H:356:ASN:HD21	1.73	0.84
1:G:227:ARG:HH12	1:G:256:GLN:HE21	1.26	0.84
1:F:19:LYS:NZ	1:F:356:ASN:HD21	1.78	0.81
1:D:426:VAL:HG21	1:D:447:VAL:HG11	1.61	0.81
1:D:353:THR:HG21	3:D:2131:HOH:O	1.81	0.80
1:H:19:LYS:HZ2	1:H:356:ASN:HD21	1.24	0.80
1:G:465:HIS:HB2	3:G:2161:HOH:O	1.81	0.80
1:H:233:LYS:NZ	1:H:248:GLU:OE2	2.15	0.79
1:H:426:VAL:HG21	1:H:447:VAL:HG11	1.65	0.79
1:G:353:THR:HG21	3:G:2125:HOH:O	1.83	0.78
1:E:280:ASN:HD22	1:E:281:THR:H	1.28	0.78
1:E:227:ARG:HH12	1:E:256:GLN:HE21	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:ASN:HD22	1:G:281:THR:H	1.30	0.78
1:H:227:ARG:HH12	1:H:256:GLN:HE21	1.29	0.78
1:H:227:ARG:HH12	1:H:256:GLN:NE2	1.82	0.77
1:B:280:ASN:HD22	1:B:281:THR:H	1.31	0.76
1:E:422:ASN:ND2	3:E:2148:HOH:O	2.19	0.75
1:B:502:SER:C	3:B:2160:HOH:O	2.23	0.75
1:B:103:MET:HE1	1:B:107:LEU:HB3	1.68	0.75
1:D:227:ARG:NH1	1:D:256:GLN:HE21	1.83	0.75
1:F:103:MET:HG3	1:F:122:THR:O	1.87	0.75
1:H:111:ASP:HB2	3:H:2064:HOH:O	1.87	0.74
1:A:287:ASN:O	1:A:290:HIS:HD2	1.69	0.74
1:F:280:ASN:HD22	1:F:281:THR:H	1.37	0.73
1:B:227:ARG:HH12	1:B:256:GLN:NE2	1.85	0.72
1:D:215:CYS:SG	1:D:222:VAL:HG21	2.30	0.72
1:A:280:ASN:HD22	1:A:281:THR:H	1.35	0.72
1:B:236:HIS:NE2	1:D:497:GLU:OE1	2.20	0.72
1:E:406:GLU:O	1:E:407:SER:HB3	1.90	0.72
1:E:419:GLN:HG2	3:E:2147:HOH:O	1.90	0.71
1:A:227:ARG:HH12	1:A:256:GLN:NE2	1.89	0.70
1:A:287:ASN:O	1:A:290:HIS:CD2	2.44	0.70
1:C:34:GLU:O	1:C:38:HIS:HD2	1.74	0.70
1:D:38:HIS:HE1	1:D:340:ALA:O	1.75	0.70
1:H:103:MET:HE3	1:H:107:LEU:HB2	1.72	0.70
1:F:38:HIS:HE1	1:F:340:ALA:O	1.75	0.69
1:B:103:MET:CE	1:B:107:LEU:HB3	2.22	0.69
1:B:227:ARG:NH1	1:B:256:GLN:HE21	1.89	0.69
1:F:34:GLU:O	1:F:38:HIS:HD2	1.77	0.68
1:A:290:HIS:CG	3:A:2109:HOH:O	2.45	0.68
1:C:54:HIS:ND1	1:C:99:GLU:OE2	2.24	0.68
1:A:63:ILE:HD11	1:A:82:ILE:HG12	1.75	0.67
1:D:103:MET:HE3	1:D:107:LEU:HB3	1.77	0.67
1:A:439:GLN:HE21	1:A:439:GLN:H	1.42	0.67
1:G:42:VAL:O	1:G:46:ILE:O	2.12	0.67
1:B:228:HIS:CE1	1:B:278:GLU:CD	2.68	0.67
1:F:227:ARG:NH1	1:F:256:GLN:HE21	1.93	0.67
1:C:422:ASN:C	1:C:422:ASN:HD22	1.98	0.66
1:H:280:ASN:ND2	1:H:281:THR:H	1.93	0.66
1:A:103:MET:HG3	1:A:122:THR:O	1.95	0.66
1:B:353:THR:HG21	3:B:2120:HOH:O	1.95	0.66
1:B:43:GLN:HE22	1:B:48:PHE:H	1.44	0.66
1:F:34:GLU:O	1:F:38:HIS:CD2	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASN:HD22	1:C:281:THR:N	1.92	0.65
1:E:103:MET:CE	1:E:107:LEU:HB3	2.26	0.65
1:H:19:LYS:NZ	1:H:356:ASN:ND2	2.44	0.65
1:H:95:ARG:NH2	3:H:2056:HOH:O	2.29	0.65
1:E:429:GLN:NE2	1:G:454:THR:OG1	2.25	0.64
1:H:419:GLN:HG2	3:H:2151:HOH:O	1.97	0.64
1:F:227:ARG:HH12	1:F:256:GLN:HE21	1.46	0.64
1:F:19:LYS:HZ3	1:F:356:ASN:HD21	1.45	0.63
1:H:280:ASN:HD22	1:H:281:THR:N	1.96	0.63
1:E:497:GLU:OE1	1:G:236:HIS:NE2	2.30	0.63
1:A:328:PRO:HG3	1:A:333:HIS:CE1	2.33	0.63
1:A:497:GLU:OE1	1:C:236:HIS:HE1	1.82	0.63
1:G:280:ASN:ND2	1:G:281:THR:H	1.97	0.63
1:E:63:ILE:HD11	1:E:82:ILE:HG12	1.80	0.62
1:E:426:VAL:HG21	1:E:447:VAL:HG11	1.81	0.62
1:H:19:LYS:HZ2	1:H:356:ASN:ND2	1.95	0.62
1:D:103:MET:CE	1:D:107:LEU:HB3	2.30	0.62
1:H:43:GLN:HE22	1:H:48:PHE:H	1.48	0.61
1:E:236:HIS:HD2	3:E:2089:HOH:O	1.83	0.61
1:G:350:HIS:ND1	1:G:450:PRO:HG3	2.16	0.61
1:D:502:SER:C	3:D:2171:HOH:O	2.39	0.61
1:D:422:ASN:ND2	3:D:2144:HOH:O	2.34	0.61
1:H:63:ILE:HD11	1:H:82:ILE:HG12	1.82	0.60
1:H:103:MET:CE	1:H:107:LEU:HB2	2.31	0.60
1:F:19:LYS:HZ2	1:F:356:ASN:HD21	1.48	0.60
1:A:54:HIS:HD2	1:A:99:GLU:OE2	1.84	0.59
1:B:95:ARG:HD3	1:B:149:GLU:OE2	2.02	0.59
1:D:426:VAL:CG2	1:D:447:VAL:HG11	2.32	0.59
1:B:19:LYS:NZ	1:B:356:ASN:HD21	2.01	0.59
1:B:63:ILE:HD11	1:B:82:ILE:HG12	1.84	0.59
1:G:63:ILE:HD11	1:G:82:ILE:HG12	1.83	0.59
1:C:34:GLU:O	1:C:38:HIS:CD2	2.54	0.58
1:A:290:HIS:ND1	1:A:336:PHE:HA	2.18	0.58
1:H:140:HIS:HE1	3:H:2048:HOH:O	1.87	0.58
1:A:42:VAL:O	1:A:46:ILE:O	2.21	0.58
1:C:38:HIS:HE1	1:C:340:ALA:O	1.86	0.58
1:D:43:GLN:HE22	1:D:48:PHE:H	1.52	0.58
1:C:63:ILE:HD11	1:C:82:ILE:HG12	1.86	0.58
1:D:105:LYS:NZ	1:D:120:ASN:HD22	2.01	0.58
1:G:34:GLU:O	1:G:38:HIS:HD2	1.86	0.57
1:H:227:ARG:NH1	1:H:256:GLN:HE21	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:MET:HE1	1:G:107:LEU:HB3	1.87	0.57
1:H:406:GLU:O	1:H:408:ALA:N	2.37	0.56
1:A:95:ARG:HD3	1:A:149:GLU:OE2	2.05	0.56
1:F:19:LYS:NZ	1:F:356:ASN:ND2	2.51	0.56
1:B:426:VAL:HG21	1:B:447:VAL:HG21	1.86	0.56
1:D:63:ILE:HD11	1:D:82:ILE:HG12	1.88	0.56
1:H:422:ASN:C	1:H:422:ASN:HD22	2.08	0.56
1:G:422:ASN:ND2	3:G:2139:HOH:O	2.38	0.56
1:G:19:LYS:NZ	1:G:356:ASN:HD21	2.03	0.56
1:A:160:GLU:OE2	1:A:228:HIS:HD2	1.89	0.56
1:B:66:GLU:HA	1:B:67:VAL:HB	1.88	0.56
1:D:34:GLU:O	1:D:38:HIS:HD2	1.89	0.56
1:D:280:ASN:HD22	1:D:281:THR:N	1.97	0.56
1:C:38:HIS:CE1	1:C:339:VAL:HG12	2.41	0.56
1:D:419:GLN:HB3	3:D:2142:HOH:O	2.05	0.55
1:H:228:HIS:CE1	1:H:278:GLU:HG3	2.41	0.55
1:H:42:VAL:O	1:H:46:ILE:O	2.25	0.55
1:F:103:MET:HE1	1:F:107:LEU:HB3	1.89	0.55
1:F:468:ILE:HG22	1:F:470:LEU:HD12	1.89	0.55
1:H:160:GLU:HG2	1:H:228:HIS:HD2	1.71	0.54
1:F:228:HIS:CE1	1:F:278:GLU:HG3	2.43	0.54
1:A:280:ASN:ND2	1:A:281:THR:H	2.05	0.54
1:D:227:ARG:HH12	1:D:256:GLN:NE2	1.94	0.54
1:G:34:GLU:O	1:G:38:HIS:CD2	2.61	0.54
1:G:43:GLN:HE22	1:G:48:PHE:H	1.55	0.54
1:F:106:ALA:O	1:F:125:LYS:NZ	2.40	0.54
1:E:42:VAL:O	1:E:46:ILE:O	2.24	0.54
1:B:228:HIS:HE1	1:B:278:GLU:OE2	1.91	0.54
1:D:345:PRO:HB2	1:D:350:HIS:CE1	2.43	0.54
1:B:228:HIS:CE1	1:B:278:GLU:OE2	2.61	0.53
1:E:232:SER:HB3	1:E:282:SER:HA	1.91	0.53
1:G:285:PRO:HG2	1:G:325:MET:HG3	1.89	0.53
1:C:38:HIS:ND1	1:C:339:VAL:CG1	2.72	0.53
1:B:350:HIS:CE1	1:B:450:PRO:HD3	2.43	0.53
1:C:238:LYS:HE2	1:C:243:TYR:CZ	2.44	0.53
1:D:34:GLU:O	1:D:38:HIS:CD2	2.61	0.53
1:A:43:GLN:HE22	1:A:48:PHE:H	1.57	0.53
1:C:269:PHE:HB3	1:C:272:LEU:HG	1.91	0.53
1:C:406:GLU:O	1:C:407:SER:CB	2.56	0.52
1:D:263:LEU:HA	1:D:266:GLN:HE21	1.75	0.52
1:E:43:GLN:HE22	1:E:48:PHE:H	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:VAL:CG2	1:H:447:VAL:HG11	2.37	0.52
1:G:227:ARG:HH12	1:G:256:GLN:NE2	2.02	0.52
1:H:79:PHE:CD2	1:H:140:HIS:CD2	2.97	0.52
1:H:301:ARG:HB2	3:H:2112:HOH:O	2.09	0.52
1:D:285:PRO:HG2	1:D:325:MET:HG3	1.92	0.52
1:F:172:LYS:HA	1:F:207:TRP:CH2	2.45	0.52
1:G:38:HIS:HE1	1:G:340:ALA:O	1.92	0.52
1:G:269:PHE:HB3	1:G:272:LEU:HG	1.92	0.51
1:B:33:LYS:HG3	1:C:33:LYS:HG3	1.92	0.51
1:A:66:GLU:HA	1:A:67:VAL:HB	1.93	0.51
1:F:422:ASN:C	1:F:422:ASN:HD22	2.14	0.51
1:B:280:ASN:HD22	1:B:281:THR:N	2.03	0.50
1:A:228:HIS:CE1	1:A:278:GLU:HG3	2.46	0.50
1:E:103:MET:HE2	1:E:107:LEU:HB3	1.91	0.50
1:G:280:ASN:HD22	1:G:281:THR:N	2.03	0.50
1:B:228:HIS:CE1	1:B:278:GLU:CG	2.95	0.50
1:D:493:LEU:C	1:D:493:LEU:HD23	2.32	0.50
1:E:415:ILE:HD11	1:E:417:ASN:ND2	2.26	0.50
1:H:238:LYS:HE2	1:H:243:TYR:CZ	2.47	0.50
1:D:215:CYS:SG	1:D:222:VAL:CG2	2.98	0.50
1:D:415:ILE:CD1	1:D:417:ASN:ND2	2.75	0.50
1:A:200:ILE:HD12	3:A:2084:HOH:O	2.12	0.49
1:G:98:ILE:HD13	1:G:155:PHE:CE2	2.46	0.49
1:E:280:ASN:HD22	1:E:281:THR:N	2.04	0.49
1:E:374:ARG:HD3	1:E:378:SER:OG	2.11	0.49
1:F:103:MET:CE	1:F:107:LEU:HB3	2.42	0.49
1:G:79:PHE:HA	1:G:82:ILE:HD11	1.94	0.49
1:H:227:ARG:O	1:H:276:ILE:HA	2.12	0.49
1:C:19:LYS:NZ	1:C:356:ASN:HD21	2.10	0.49
1:C:280:ASN:ND2	1:C:281:THR:H	1.99	0.49
1:D:26:ARG:HD3	1:D:117:TRP:CD2	2.48	0.49
1:D:30:ALA:HA	1:D:35:TYR:CG	2.48	0.49
1:D:30:ALA:HA	1:D:35:TYR:CD2	2.47	0.49
1:A:350:HIS:CG	1:A:416:VAL:HG11	2.48	0.49
1:D:79:PHE:HD2	1:D:82:ILE:HD11	1.78	0.49
1:B:350:HIS:HE1	1:B:450:PRO:HD3	1.77	0.49
1:F:30:ALA:HA	1:F:35:TYR:CD2	2.48	0.49
1:D:227:ARG:O	1:D:276:ILE:HA	2.13	0.49
1:B:493:LEU:HD23	1:B:493:LEU:C	2.33	0.48
1:C:197:GLY:O	1:C:225:VAL:HA	2.13	0.48
1:A:329:LYS:HB3	1:D:76:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:HD3	1:B:378:SER:OG	2.13	0.48
1:D:208:ILE:HD13	1:D:260:VAL:HG13	1.94	0.48
1:D:96:PRO:HB2	1:D:98:ILE:HG13	1.94	0.48
1:H:228:HIS:CE1	1:H:278:GLU:CD	2.87	0.48
1:B:43:GLN:HE22	1:B:48:PHE:N	2.08	0.48
1:C:43:GLN:HE22	1:C:48:PHE:HB2	1.79	0.48
1:H:79:PHE:CG	1:H:140:HIS:CD2	3.01	0.48
1:G:98:ILE:HD11	1:G:153:TRP:CE3	2.48	0.48
1:B:226:SER:HA	1:B:275:HIS:O	2.14	0.48
1:F:406:GLU:O	1:F:407:SER:HB3	2.12	0.48
1:C:38:HIS:CE1	1:C:343:SER:H	2.31	0.48
1:G:103:MET:HG3	1:G:122:THR:O	2.13	0.48
1:H:79:PHE:HD2	1:H:82:ILE:HD11	1.79	0.48
1:B:228:HIS:ND1	1:B:278:GLU:CD	2.67	0.48
1:E:19:LYS:NZ	1:E:356:ASN:HD21	2.12	0.47
1:G:419:GLN:HG2	3:G:2137:HOH:O	2.12	0.47
1:H:103:MET:CE	1:H:107:LEU:CB	2.92	0.47
1:C:406:GLU:O	1:C:407:SER:HB3	2.14	0.47
1:F:422:ASN:ND2	1:F:425:ARG:H	2.12	0.47
1:F:19:LYS:HZ3	1:F:356:ASN:ND2	2.12	0.47
1:C:422:ASN:HD21	1:C:424:TRP:HB3	1.80	0.47
1:E:418:GLU:O	1:E:425:ARG:HD2	2.15	0.47
1:E:39:LEU:HD12	1:E:92:LEU:HD12	1.96	0.47
1:H:228:HIS:CE1	1:H:278:GLU:CG	2.97	0.47
1:B:95:ARG:CD	1:B:149:GLU:OE2	2.61	0.47
1:G:238:LYS:HE2	1:G:243:TYR:CZ	2.50	0.47
1:B:19:LYS:HZ3	1:B:356:ASN:HD21	1.62	0.47
1:A:280:ASN:HD22	1:A:281:THR:N	2.10	0.47
1:C:165:ASN:HB2	3:C:2080:HOH:O	2.15	0.47
1:C:415:ILE:CD1	1:C:417:ASN:ND2	2.78	0.47
1:D:232:SER:HB3	1:D:282:SER:HA	1.96	0.47
1:D:38:HIS:CE1	1:D:340:ALA:O	2.61	0.47
1:E:107:LEU:HD21	1:E:129:LYS:HB3	1.97	0.47
1:F:426:VAL:CG2	1:F:447:VAL:HG11	2.35	0.47
1:A:281:THR:OG1	1:A:295:ASN:ND2	2.47	0.46
1:F:316:TRP:O	1:F:336:PHE:HB3	2.14	0.46
1:A:95:ARG:CD	1:A:149:GLU:OE2	2.63	0.46
1:G:406:GLU:HG2	1:G:482:GLN:HE21	1.81	0.46
1:C:407:SER:O	1:C:458:ARG:HG2	2.15	0.46
1:A:290:HIS:HE1	1:A:336:PHE:CD2	2.34	0.46
1:A:328:PRO:HB3	1:A:333:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ALA:HA	1:E:35:TYR:CD2	2.50	0.46
1:C:30:ALA:HA	1:C:35:TYR:CD2	2.51	0.46
1:B:228:HIS:CE1	1:B:278:GLU:HG3	2.51	0.46
1:E:228:HIS:CE1	1:E:278:GLU:OE2	2.69	0.46
1:C:38:HIS:CE1	1:C:343:SER:HA	2.51	0.45
1:E:422:ASN:C	1:E:422:ASN:HD22	2.19	0.45
1:F:165:ASN:HD22	1:F:165:ASN:H	1.63	0.45
1:F:30:ALA:HA	1:F:35:TYR:CG	2.52	0.45
1:F:66:GLU:HA	1:F:67:VAL:HB	1.98	0.45
1:G:19:LYS:HZ1	1:G:356:ASN:HD21	1.65	0.45
1:F:253:MET:O	1:F:256:GLN:HB2	2.16	0.45
1:F:38:HIS:CE1	1:F:339:VAL:HG12	2.52	0.45
1:A:30:ALA:HA	1:A:35:TYR:CD2	2.52	0.45
1:G:197:GLY:O	1:G:225:VAL:HA	2.16	0.45
1:H:422:ASN:HD21	1:H:424:TRP:HB3	1.80	0.45
1:E:16:LYS:HD3	3:E:2007:HOH:O	2.17	0.45
1:F:43:GLN:HE22	1:F:48:PHE:H	1.64	0.45
1:A:269:PHE:HB3	1:A:272:LEU:HG	1.99	0.45
1:B:415:ILE:CD1	1:B:417:ASN:ND2	2.80	0.45
1:B:428:LYS:HE3	1:D:495:ASP:OD2	2.16	0.45
1:D:238:LYS:NZ	1:D:243:TYR:CZ	2.76	0.45
1:F:228:HIS:ND1	1:F:278:GLU:HB2	2.32	0.45
1:F:54:HIS:HD2	3:F:2089:HOH:O	2.00	0.45
1:H:172:LYS:HA	1:H:207:TRP:CH2	2.52	0.45
1:B:30:ALA:HA	1:B:35:TYR:CG	2.52	0.45
1:C:236:HIS:HD2	3:C:2088:HOH:O	2.00	0.45
1:E:415:ILE:CD1	1:E:417:ASN:ND2	2.80	0.45
1:E:409:VAL:HG11	1:E:464:ILE:HD13	1.99	0.45
1:C:63:ILE:HD11	1:C:82:ILE:CG1	2.47	0.44
1:F:358:LEU:HD21	1:F:382:VAL:HG23	1.99	0.44
1:G:79:PHE:HD2	1:G:82:ILE:HD11	1.81	0.44
1:A:30:ALA:HA	1:A:35:TYR:CG	2.52	0.44
1:C:350:HIS:CE1	1:C:450:PRO:HD3	2.53	0.44
1:D:66:GLU:HA	1:D:67:VAL:HB	1.99	0.44
1:C:103:MET:HE3	1:C:107:LEU:HB3	1.99	0.44
1:A:19:LYS:NZ	1:A:356:ASN:HD21	2.16	0.44
1:A:290:HIS:H	1:A:290:HIS:CD2	2.36	0.44
1:B:86:VAL:HB	1:B:145:TYR:OH	2.17	0.44
1:C:103:MET:CE	1:C:107:LEU:HB3	2.47	0.44
1:C:163:LEU:HD23	1:C:166:PHE:CD1	2.53	0.44
1:C:276:ILE:HB	1:C:313:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:ASP:OD1	1:H:140:HIS:NE2	2.36	0.43
1:H:19:LYS:HZ3	1:H:356:ASN:ND2	2.16	0.43
1:F:443:THR:HG23	1:H:412:LYS:HE3	2.00	0.43
1:B:415:ILE:HD11	1:B:417:ASN:ND2	2.33	0.43
1:G:19:LYS:NZ	1:G:356:ASN:ND2	2.65	0.43
1:C:172:LYS:HA	1:C:207:TRP:CH2	2.53	0.43
1:B:497:GLU:OE1	1:D:236:HIS:HE1	2.01	0.43
1:F:285:PRO:CG	1:F:325:MET:HG3	2.49	0.43
1:A:236:HIS:CE1	1:A:244:TYR:HB3	2.54	0.43
1:E:43:GLN:HE22	1:E:48:PHE:N	2.16	0.43
1:A:103:MET:HB3	1:A:103:MET:HE2	1.76	0.43
1:F:28:GLY:HA3	1:F:60:ASP:OD2	2.18	0.43
1:E:228:HIS:CE1	1:E:278:GLU:CD	2.92	0.43
1:B:269:PHE:HB3	1:B:272:LEU:HG	2.00	0.43
1:E:96:PRO:HB2	1:E:98:ILE:HG13	2.01	0.43
1:A:232:SER:HB3	1:A:282:SER:HA	2.01	0.42
1:D:163:LEU:HD22	1:D:165:ASN:HD22	1.83	0.42
1:F:273:PRO:HA	1:F:311:ASP:OD2	2.19	0.42
1:D:19:LYS:NZ	1:D:356:ASN:HD21	2.16	0.42
1:F:51:ILE:O	1:F:51:ILE:HG23	2.19	0.42
1:A:350:HIS:CD2	1:A:416:VAL:HG11	2.54	0.42
1:B:50:TYR:HA	1:B:95:ARG:O	2.20	0.42
1:D:103:MET:HE1	1:D:107:LEU:HD13	2.00	0.42
1:B:163:LEU:HD22	1:B:165:ASN:ND2	2.35	0.42
1:H:400:LEU:HD23	1:H:402:ILE:HD11	2.02	0.42
1:E:140:HIS:HE1	3:H:2154:HOH:O	2.02	0.42
1:F:444:LEU:HA	1:F:444:LEU:HD23	1.92	0.42
1:C:493:LEU:C	1:C:493:LEU:HD23	2.40	0.42
1:D:50:TYR:HA	1:D:95:ARG:O	2.19	0.42
1:D:28:GLY:HA3	1:D:60:ASP:OD2	2.19	0.42
1:E:426:VAL:CG2	1:E:447:VAL:HG11	2.48	0.42
1:E:79:PHE:CG	1:E:140:HIS:CD2	3.07	0.42
1:F:163:LEU:HD22	1:F:165:ASN:HD22	1.85	0.42
1:A:468:ILE:HG22	1:A:470:LEU:HD23	2.02	0.42
1:B:281:THR:OG1	1:B:295:ASN:ND2	2.52	0.42
1:C:200:ILE:HD11	1:C:208:ILE:CD1	2.50	0.42
1:E:162:ASN:HD22	1:E:204:SER:HB3	1.84	0.42
1:F:79:PHE:HD2	1:F:82:ILE:HD11	1.85	0.42
1:G:232:SER:HB3	1:G:282:SER:HA	2.01	0.42
1:C:227:ARG:NH1	1:C:256:GLN:HE21	2.05	0.42
1:C:379:ILE:HB	1:C:480:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:VAL:HG21	1:E:447:VAL:HG21	2.01	0.42
1:E:460:THR:HG1	1:E:465:HIS:CE1	2.38	0.42
1:F:198:PRO:HG2	1:F:200:ILE:HG12	2.02	0.42
1:F:447:VAL:CG1	3:F:2109:HOH:O	2.67	0.42
1:G:30:ALA:HA	1:G:35:TYR:CG	2.55	0.42
1:H:401:VAL:HG22	1:H:465:HIS:CE1	2.54	0.42
1:A:415:ILE:CD1	1:A:417:ASN:ND2	2.83	0.41
1:D:425:ARG:NE	3:D:2145:HOH:O	2.52	0.41
1:F:238:LYS:HG2	1:F:243:TYR:CD2	2.55	0.41
1:F:422:ASN:HD21	1:F:424:TRP:HB3	1.85	0.41
1:H:95:ARG:CD	1:H:149:GLU:OE2	2.68	0.41
1:C:449:GLN:NE2	3:C:2156:HOH:O	2.48	0.41
1:H:228:HIS:ND1	1:H:278:GLU:HB2	2.34	0.41
1:H:38:HIS:CE1	1:H:339:VAL:HG12	2.54	0.41
1:D:227:ARG:HD3	1:D:228:HIS:O	2.20	0.41
1:E:291:ASP:HA	1:E:346:LYS:HD3	2.02	0.41
1:H:214:PHE:CE1	1:H:218:ARG:HD3	2.55	0.41
1:A:236:HIS:HD2	3:A:2090:HOH:O	2.04	0.41
1:C:248:GLU:HB3	1:C:249:PRO:HD2	2.02	0.41
1:F:38:HIS:ND1	1:F:339:VAL:CG1	2.84	0.41
1:D:290:HIS:HD2	1:D:334:GLY:O	2.04	0.41
1:D:8:SER:HA	1:D:403:PRO:HG2	2.02	0.41
1:G:403:PRO:HA	1:G:462:GLY:O	2.21	0.41
1:H:251:GLU:HB2	3:H:2103:HOH:O	2.20	0.41
1:B:67:VAL:HG21	1:B:76:PHE:CB	2.50	0.41
1:H:353:THR:HG21	3:H:2140:HOH:O	2.19	0.41
1:B:197:GLY:O	1:B:225:VAL:HA	2.21	0.41
1:D:385:ASN:HD22	1:D:396:LYS:NZ	2.18	0.41
1:D:42:VAL:O	1:D:46:ILE:O	2.38	0.41
1:F:280:ASN:HD22	1:F:281:THR:N	2.11	0.41
1:H:226:SER:HA	1:H:275:HIS:O	2.21	0.41
1:C:38:HIS:ND1	1:C:339:VAL:HG12	2.34	0.41
1:G:214:PHE:CE1	1:G:218:ARG:HD3	2.56	0.41
1:F:187:LYS:HD3	1:F:187:LYS:HA	1.94	0.41
1:B:429:GLN:NE2	1:D:454:THR:OG1	2.48	0.40
1:G:63:ILE:O	1:G:77:TYR:HA	2.21	0.40
1:A:290:HIS:CE1	3:A:2109:HOH:O	2.75	0.40
1:D:406:GLU:OE1	1:D:482:GLN:HB2	2.21	0.40
1:A:226:SER:HA	1:A:275:HIS:O	2.22	0.40
1:A:79:PHE:CD1	1:A:140:HIS:ND1	2.90	0.40
1:E:95:ARG:HD2	1:E:149:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ALA:HA	1:E:35:TYR:CG	2.57	0.40
1:A:43:GLN:HE22	1:A:48:PHE:N	2.18	0.40
1:C:105:LYS:NZ	1:C:120:ASN:HD22	2.19	0.40
1:H:160:GLU:CG	1:H:228:HIS:CD2	3.05	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	499/503 (99%)	473 (95%)	24 (5%)	2 (0%)	34	37
1	B	499/503 (99%)	476 (95%)	21 (4%)	2 (0%)	34	37
1	C	499/503 (99%)	477 (96%)	21 (4%)	1 (0%)	47	55
1	D	499/503 (99%)	474 (95%)	23 (5%)	2 (0%)	34	37
1	E	499/503 (99%)	476 (95%)	19 (4%)	4 (1%)	19	19
1	F	499/503 (99%)	476 (95%)	22 (4%)	1 (0%)	47	55
1	G	499/503 (99%)	476 (95%)	20 (4%)	3 (1%)	25	26
1	H	499/503 (99%)	473 (95%)	24 (5%)	2 (0%)	34	37
All	All	3992/4024 (99%)	3801 (95%)	174 (4%)	17 (0%)	34	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	B	407	SER
1	D	67	VAL
1	E	67	VAL
1	E	407	SER
1	F	67	VAL

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Mol	Chain	Res	Type
1	G	67	VAL
1	H	67	VAL
1	H	407	SER
1	B	67	VAL
1	C	407	SER
1	A	70	ASP
1	D	406	GLU
1	E	326	ASP
1	G	204	SER
1	E	204	SER
1	G	102	PHE

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	440/442 (100%)	405 (92%)	35 (8%)	12	12
1	B	440/442 (100%)	408 (93%)	32 (7%)	14	15
1	C	439/442 (99%)	407 (93%)	32 (7%)	14	15
1	D	440/442 (100%)	408 (93%)	32 (7%)	14	15
1	E	440/442 (100%)	411 (93%)	29 (7%)	16	19
1	F	440/442 (100%)	407 (92%)	33 (8%)	13	14
1	G	440/442 (100%)	409 (93%)	31 (7%)	15	16
1	H	440/442 (100%)	411 (93%)	29 (7%)	16	19
All	All	3519/3536 (100%)	3266 (93%)	253 (7%)	14	15

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	11	ARG
1	A	13	LYS
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	66	GLU
1	A	82	ILE
1	A	95	ARG
1	A	97	PHE
1	A	98	ILE
1	A	133	LEU
1	A	163	LEU
1	A	164	VAL
1	A	222	VAL
1	A	227	ARG
1	A	277	THR
1	A	280	ASN
1	A	294	LEU
1	A	313	PHE
1	A	374	ARG
1	A	396	LYS
1	A	397	GLU
1	A	404	VAL
1	A	409	VAL
1	A	415	ILE
1	A	419	GLN
1	A	422	ASN
1	A	439	GLN
1	A	447	VAL
1	A	460	THR
1	A	461	ASP
1	A	463	VAL
1	A	464	ILE
1	A	466	LEU
1	A	477	LEU
1	B	15	LYS
1	B	24	THR
1	B	27	LEU
1	B	39	LEU
1	B	66	GLU
1	B	74	LYS
1	B	82	ILE
1	B	95	ARG
1	B	97	PHE
1	B	133	LEU
1	B	173	GLN

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Mol	Chain	Res	Type
1	B	204	SER
1	B	219	ARG
1	B	222	VAL
1	B	227	ARG
1	B	251	GLU
1	B	280	ASN
1	B	294	LEU
1	B	313	PHE
1	B	374	ARG
1	B	392	GLU
1	B	395	THR
1	B	415	ILE
1	B	422	ASN
1	B	438	ARG
1	B	447	VAL
1	B	453	MET
1	B	458	ARG
1	B	463	VAL
1	B	464	ILE
1	B	467	SER
1	B	477	LEU
1	C	27	LEU
1	C	39	LEU
1	C	67	VAL
1	C	70	ASP
1	C	82	ILE
1	C	95	ARG
1	C	97	PHE
1	C	105	LYS
1	C	107	LEU
1	C	133	LEU
1	C	164	VAL
1	C	168	LYS
1	C	213	HIS
1	C	219	ARG
1	C	222	VAL
1	C	280	ASN
1	C	299	ILE
1	C	313	PHE
1	C	360	ASP
1	C	374	ARG
1	C	404	VAL

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Mol	Chain	Res	Type
1	C	409	VAL
1	C	415	ILE
1	C	422	ASN
1	C	439	GLN
1	C	446	GLN
1	C	447	VAL
1	C	463	VAL
1	C	464	ILE
1	C	477	LEU
1	C	484	ARG
1	C	502	SER
1	D	9	ASN
1	D	11	ARG
1	D	15	LYS
1	D	33	LYS
1	D	39	LEU
1	D	66	GLU
1	D	82	ILE
1	D	95	ARG
1	D	97	PHE
1	D	107	LEU
1	D	125	LYS
1	D	133	LEU
1	D	154	LEU
1	D	163	LEU
1	D	228	HIS
1	D	265	ARG
1	D	280	ASN
1	D	282	SER
1	D	313	PHE
1	D	325	MET
1	D	353	THR
1	D	374	ARG
1	D	389	GLU
1	D	399	GLN
1	D	404	VAL
1	D	409	VAL
1	D	415	ILE
1	D	419	GLN
1	D	422	ASN
1	D	458	ARG
1	D	477	LEU

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Mol	Chain	Res	Type
1	D	481	GLU
1	E	27	LEU
1	E	33	LYS
1	E	39	LEU
1	E	82	ILE
1	E	95	ARG
1	E	98	ILE
1	E	133	LEU
1	E	163	LEU
1	E	164	VAL
1	E	213	HIS
1	E	222	VAL
1	E	227	ARG
1	E	246	GLU
1	E	280	ASN
1	E	368	GLU
1	E	374	ARG
1	E	392	GLU
1	E	400	LEU
1	E	409	VAL
1	E	415	ILE
1	E	419	GLN
1	E	422	ASN
1	E	447	VAL
1	E	457	ARG
1	E	464	ILE
1	E	465	HIS
1	E	471	SER
1	E	477	LEU
1	E	484	ARG
1	F	3	VAL
1	F	8	SER
1	F	24	THR
1	F	39	LEU
1	F	82	ILE
1	F	95	ARG
1	F	97	PHE
1	F	98	ILE
1	F	107	LEU
1	F	125	LYS
1	F	133	LEU
1	F	154	LEU

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Mol	Chain	Res	Type
1	F	163	LEU
1	F	164	VAL
1	F	168	LYS
1	F	222	VAL
1	F	236	HIS
1	F	255	GLU
1	F	267	SER
1	F	280	ASN
1	F	284	SER
1	F	294	LEU
1	F	299	ILE
1	F	374	ARG
1	F	397	GLU
1	F	404	VAL
1	F	422	ASN
1	F	428	LYS
1	F	453	MET
1	F	458	ARG
1	F	465	HIS
1	F	477	LEU
1	F	481	GLU
1	G	39	LEU
1	G	66	GLU
1	G	82	ILE
1	G	97	PHE
1	G	107	LEU
1	G	133	LEU
1	G	148	GLU
1	G	204	SER
1	G	222	VAL
1	G	227	ARG
1	G	233	LYS
1	G	236	HIS
1	G	265	ARG
1	G	280	ASN
1	G	282	SER
1	G	299	ILE
1	G	325	MET
1	G	353	THR
1	G	356	ASN
1	G	374	ARG
1	G	389	GLU

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Mol	Chain	Res	Type
1	G	396	LYS
1	G	399	GLN
1	G	404	VAL
1	G	422	ASN
1	G	439	GLN
1	G	447	VAL
1	G	457	ARG
1	G	458	ARG
1	G	463	VAL
1	G	477	LEU
1	H	11	ARG
1	H	27	LEU
1	H	39	LEU
1	H	72	GLU
1	H	74	LYS
1	H	82	ILE
1	H	95	ARG
1	H	97	PHE
1	H	133	LEU
1	H	204	SER
1	H	222	VAL
1	H	227	ARG
1	H	280	ASN
1	H	284	SER
1	H	313	PHE
1	H	325	MET
1	H	356	ASN
1	H	374	ARG
1	H	375	LYS
1	H	392	GLU
1	H	404	VAL
1	H	407	SER
1	H	409	VAL
1	H	419	GLN
1	H	422	ASN
1	H	453	MET
1	H	464	ILE
1	H	467	SER
1	H	477	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	54	HIS
1	A	165	ASN
1	A	228	HIS
1	A	236	HIS
1	A	256	GLN
1	A	280	ASN
1	A	290	HIS
1	A	295	ASN
1	A	333	HIS
1	A	356	ASN
1	A	422	ASN
1	A	429	GLN
1	A	439	GLN
1	B	43	GLN
1	B	165	ASN
1	B	192	HIS
1	B	256	GLN
1	B	266	GLN
1	B	280	ASN
1	B	295	ASN
1	B	356	ASN
1	B	385	ASN
1	B	422	ASN
1	B	429	GLN
1	B	439	GLN
1	B	449	GLN
1	C	38	HIS
1	C	43	GLN
1	C	165	ASN
1	C	236	HIS
1	C	256	GLN
1	C	280	ASN
1	C	290	HIS
1	C	295	ASN
1	C	356	ASN
1	C	385	ASN
1	C	399	GLN
1	C	422	ASN
1	C	429	GLN
1	C	439	GLN
1	C	446	GLN
1	C	449	GLN

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Mol	Chain	Res	Type
1	C	465	HIS
1	C	482	GLN
1	D	38	HIS
1	D	43	GLN
1	D	120	ASN
1	D	165	ASN
1	D	236	HIS
1	D	256	GLN
1	D	266	GLN
1	D	280	ASN
1	D	290	HIS
1	D	295	ASN
1	D	356	ASN
1	D	385	ASN
1	D	419	GLN
1	D	422	ASN
1	D	429	GLN
1	D	449	GLN
1	E	43	GLN
1	E	236	HIS
1	E	256	GLN
1	E	280	ASN
1	E	295	ASN
1	E	356	ASN
1	E	385	ASN
1	E	419	GLN
1	E	422	ASN
1	E	429	GLN
1	E	449	GLN
1	F	43	GLN
1	F	54	HIS
1	F	165	ASN
1	F	256	GLN
1	F	266	GLN
1	F	280	ASN
1	F	290	HIS
1	F	295	ASN
1	F	356	ASN
1	F	385	ASN
1	F	422	ASN
1	F	429	GLN
1	F	449	GLN

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Mol	Chain	Res	Type
1	F	451	HIS
1	F	456	GLN
1	G	43	GLN
1	G	54	HIS
1	G	173	GLN
1	G	256	GLN
1	G	266	GLN
1	G	280	ASN
1	G	290	HIS
1	G	295	ASN
1	G	356	ASN
1	G	385	ASN
1	G	422	ASN
1	G	429	GLN
1	G	439	GLN
1	H	43	GLN
1	H	165	ASN
1	H	228	HIS
1	H	256	GLN
1	H	280	ASN
1	H	290	HIS
1	H	295	ASN
1	H	356	ASN
1	H	385	ASN
1	H	422	ASN
1	H	429	GLN
1	H	451	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	501/503 (99%)	-0.00	19 (3%)	40	38	10, 16, 39, 45	0
1	B	501/503 (99%)	0.03	26 (5%)	27	26	7, 16, 40, 46	0
1	C	501/503 (99%)	0.05	27 (5%)	25	24	8, 16, 39, 44	0
1	D	501/503 (99%)	0.07	21 (4%)	36	34	11, 17, 39, 45	0
1	E	501/503 (99%)	-0.07	10 (1%)	65	63	8, 16, 38, 44	0
1	F	501/503 (99%)	0.14	28 (5%)	24	23	9, 16, 39, 44	0
1	G	501/503 (99%)	-0.08	18 (3%)	42	41	10, 16, 38, 45	0
1	H	501/503 (99%)	-0.07	16 (3%)	47	45	8, 16, 38, 45	0
All	All	4008/4024 (99%)	0.01	165 (4%)	37	35	7, 16, 40, 46	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	GLY	7.6
1	F	405	SER	7.0
1	D	405	SER	6.3
1	H	2	GLY	6.3
1	H	11	ARG	5.9
1	D	393	GLY	5.9
1	B	405	SER	5.9
1	F	393	GLY	5.8
1	G	405	SER	5.6
1	C	405	SER	5.5
1	B	404	VAL	5.4
1	C	393	GLY	4.9
1	G	462	GLY	4.8
1	H	393	GLY	4.8
1	E	2	GLY	4.8
1	C	11	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	2	GLY	4.6
1	C	2	GLY	4.6
1	B	70	ASP	4.6
1	A	404	VAL	4.6
1	C	404	VAL	4.5
1	A	394	LEU	4.5
1	A	2	GLY	4.4
1	H	462	GLY	4.3
1	F	458	ARG	4.3
1	F	395	THR	4.2
1	A	460	THR	4.2
1	B	11	ARG	4.2
1	F	404	VAL	4.2
1	B	465	HIS	4.1
1	G	404	VAL	4.1
1	A	461	ASP	4.1
1	A	405	SER	4.1
1	F	394	LEU	4.0
1	D	459	ALA	4.0
1	B	460	THR	4.0
1	D	11	ARG	4.0
1	B	395	THR	3.9
1	E	461	ASP	3.9
1	H	461	ASP	3.8
1	C	458	ARG	3.8
1	A	70	ASP	3.7
1	C	213	HIS	3.7
1	H	394	LEU	3.7
1	G	393	GLY	3.7
1	D	404	VAL	3.7
1	F	465	HIS	3.6
1	G	461	ASP	3.6
1	G	465	HIS	3.6
1	B	213	HIS	3.6
1	F	203	GLY	3.6
1	G	458	ARG	3.6
1	E	458	ARG	3.5
1	C	395	THR	3.5
1	D	213	HIS	3.5
1	E	465	HIS	3.5
1	F	213	HIS	3.5
1	G	392	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	3.5
1	A	465	HIS	3.5
1	B	271	HIS	3.4
1	A	392	GLU	3.4
1	B	2	GLY	3.4
1	F	459	ALA	3.4
1	D	395	THR	3.3
1	E	11	ARG	3.3
1	D	460	THR	3.3
1	F	392	GLU	3.3
1	G	394	LEU	3.3
1	B	458	ARG	3.3
1	F	72	GLU	3.3
1	E	405	SER	3.2
1	C	392	GLU	3.2
1	H	404	VAL	3.2
1	G	460	THR	3.2
1	B	406	GLU	3.2
1	H	460	THR	3.2
1	D	465	HIS	3.2
1	B	393	GLY	3.2
1	A	393	GLY	3.2
1	C	465	HIS	3.2
1	D	392	GLU	3.1
1	H	405	SER	3.1
1	G	459	ALA	3.1
1	F	219	ARG	3.1
1	C	461	ASP	3.1
1	C	460	THR	3.1
1	C	403	PRO	3.1
1	D	458	ARG	3.1
1	B	403	PRO	3.1
1	A	406	GLU	3.0
1	A	462	GLY	3.0
1	G	70	ASP	3.0
1	C	271	HIS	3.0
1	F	461	ASP	2.9
1	F	11	ARG	2.9
1	D	70	ASP	2.9
1	B	392	GLU	2.9
1	C	459	ALA	2.9
1	B	72	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	461	ASP	2.8
1	D	8	SER	2.8
1	A	3	VAL	2.8
1	G	375	LYS	2.8
1	G	395	THR	2.8
1	G	407	SER	2.8
1	H	213	HIS	2.8
1	A	458	ARG	2.8
1	C	462	GLY	2.7
1	B	461	ASP	2.7
1	E	404	VAL	2.7
1	G	406	GLU	2.7
1	H	392	GLU	2.7
1	D	9	ASN	2.7
1	H	395	THR	2.7
1	C	9	ASN	2.7
1	D	394	LEU	2.7
1	C	203	GLY	2.7
1	F	460	THR	2.6
1	H	458	ARG	2.6
1	C	394	LEU	2.6
1	F	271	HIS	2.6
1	E	393	GLY	2.6
1	D	462	GLY	2.6
1	E	406	GLU	2.6
1	C	70	ASP	2.5
1	B	394	LEU	2.5
1	B	502	SER	2.5
1	H	407	SER	2.4
1	A	72	GLU	2.4
1	D	406	GLU	2.4
1	C	8	SER	2.4
1	F	9	ASN	2.4
1	C	406	GLU	2.4
1	A	403	PRO	2.4
1	H	463	VAL	2.3
1	B	203	GLY	2.3
1	F	70	ASP	2.3
1	B	463	VAL	2.3
1	C	397	GLU	2.3
1	F	236	HIS	2.3
1	C	463	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	47	GLY	2.2
1	D	271	HIS	2.2
1	F	265	ARG	2.2
1	G	3	VAL	2.2
1	A	463	VAL	2.2
1	F	71	GLY	2.2
1	F	192	HIS	2.2
1	A	71	GLY	2.2
1	H	70	ASP	2.2
1	B	236	HIS	2.2
1	C	219	ARG	2.2
1	C	217	GLU	2.2
1	B	462	GLY	2.2
1	D	419	GLN	2.2
1	F	2	GLY	2.1
1	F	169	ASP	2.1
1	B	219	ARG	2.1
1	F	397	GLU	2.1
1	E	460	THR	2.1
1	F	202	GLY	2.0
1	A	11	ARG	2.0
1	F	402	ILE	2.0
1	B	71	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	F	1503	1/1	0.97	0.10	29,29,29,29	0
2	CA	D	1503	1/1	0.98	0.16	24,24,24,24	0
2	CA	E	1503	1/1	0.99	0.15	24,24,24,24	0
2	CA	C	1503	1/1	0.99	0.11	24,24,24,24	0
2	CA	G	1503	1/1	0.99	0.12	22,22,22,22	0
2	CA	H	1503	1/1	0.99	0.10	22,22,22,22	0
2	CA	A	1503	1/1	1.00	0.10	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.