



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:31 PM UTC

PDB ID : 5Z18 / pdb_00005z18
Title : The crystal structure of Ruminococcus gnavus beta-glucuronidase
Authors : Dashnyam, P.; Lin, H.Y.; Lin, C.H.
Deposited on : 2017-12-25
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

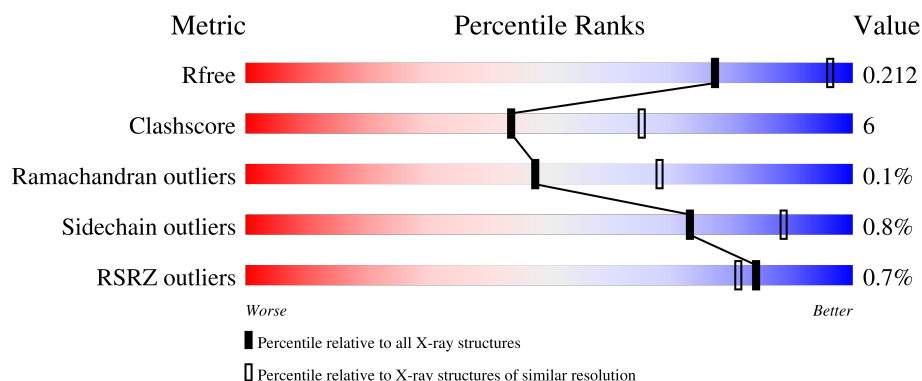
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	627	% 82% 11% 7%
1	B	627	% 82% 11% 7%
1	C	627	% 82% 11% 6%
1	D	627	% 82% 11% 6%
1	E	627	% 79% 14% 7%

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Mol	Chain	Length	Quality of chain
1	F	627	% 78% 14% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30433 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-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4811	3105	780	902	24			
1	B	586	Total	C	N	O	S	0	0	0
			4811	3105	780	902	24			
1	C	588	Total	C	N	O	S	0	0	0
			4829	3117	784	904	24			
1	D	591	Total	C	N	O	S	0	0	0
			4858	3137	788	909	24			
1	E	586	Total	C	N	O	S	0	0	0
			4810	3104	782	900	24			
1	F	582	Total	C	N	O	S	0	0	0
			4773	3079	776	894	24			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q6W7J7
A	-22	HIS	-	expression tag	UNP Q6W7J7
A	-21	HIS	-	expression tag	UNP Q6W7J7
A	-20	HIS	-	expression tag	UNP Q6W7J7
A	-19	HIS	-	expression tag	UNP Q6W7J7
A	-18	HIS	-	expression tag	UNP Q6W7J7
A	-17	HIS	-	expression tag	UNP Q6W7J7
A	-16	SER	-	expression tag	UNP Q6W7J7
A	-15	SER	-	expression tag	UNP Q6W7J7
A	-14	GLY	-	expression tag	UNP Q6W7J7
A	-13	VAL	-	expression tag	UNP Q6W7J7
A	-12	ASP	-	expression tag	UNP Q6W7J7
A	-11	LEU	-	expression tag	UNP Q6W7J7
A	-10	GLY	-	expression tag	UNP Q6W7J7
A	-9	THR	-	expression tag	UNP Q6W7J7
A	-8	GLU	-	expression tag	UNP Q6W7J7
A	-7	ASN	-	expression tag	UNP Q6W7J7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q6W7J7
A	-5	TYR	-	expression tag	UNP Q6W7J7
A	-4	PHE	-	expression tag	UNP Q6W7J7
A	-3	GLN	-	expression tag	UNP Q6W7J7
A	-2	SER	-	expression tag	UNP Q6W7J7
A	-1	ASN	-	expression tag	UNP Q6W7J7
A	0	GLY	-	expression tag	UNP Q6W7J7
A	1	MET	-	expression tag	UNP Q6W7J7
B	-23	MET	-	initiating methionine	UNP Q6W7J7
B	-22	HIS	-	expression tag	UNP Q6W7J7
B	-21	HIS	-	expression tag	UNP Q6W7J7
B	-20	HIS	-	expression tag	UNP Q6W7J7
B	-19	HIS	-	expression tag	UNP Q6W7J7
B	-18	HIS	-	expression tag	UNP Q6W7J7
B	-17	HIS	-	expression tag	UNP Q6W7J7
B	-16	SER	-	expression tag	UNP Q6W7J7
B	-15	SER	-	expression tag	UNP Q6W7J7
B	-14	GLY	-	expression tag	UNP Q6W7J7
B	-13	VAL	-	expression tag	UNP Q6W7J7
B	-12	ASP	-	expression tag	UNP Q6W7J7
B	-11	LEU	-	expression tag	UNP Q6W7J7
B	-10	GLY	-	expression tag	UNP Q6W7J7
B	-9	THR	-	expression tag	UNP Q6W7J7
B	-8	GLU	-	expression tag	UNP Q6W7J7
B	-7	ASN	-	expression tag	UNP Q6W7J7
B	-6	LEU	-	expression tag	UNP Q6W7J7
B	-5	TYR	-	expression tag	UNP Q6W7J7
B	-4	PHE	-	expression tag	UNP Q6W7J7
B	-3	GLN	-	expression tag	UNP Q6W7J7
B	-2	SER	-	expression tag	UNP Q6W7J7
B	-1	ASN	-	expression tag	UNP Q6W7J7
B	0	GLY	-	expression tag	UNP Q6W7J7
B	1	MET	-	expression tag	UNP Q6W7J7
C	-23	MET	-	initiating methionine	UNP Q6W7J7
C	-22	HIS	-	expression tag	UNP Q6W7J7
C	-21	HIS	-	expression tag	UNP Q6W7J7
C	-20	HIS	-	expression tag	UNP Q6W7J7
C	-19	HIS	-	expression tag	UNP Q6W7J7
C	-18	HIS	-	expression tag	UNP Q6W7J7
C	-17	HIS	-	expression tag	UNP Q6W7J7
C	-16	SER	-	expression tag	UNP Q6W7J7
C	-15	SER	-	expression tag	UNP Q6W7J7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLY	-	expression tag	UNP Q6W7J7
C	-13	VAL	-	expression tag	UNP Q6W7J7
C	-12	ASP	-	expression tag	UNP Q6W7J7
C	-11	LEU	-	expression tag	UNP Q6W7J7
C	-10	GLY	-	expression tag	UNP Q6W7J7
C	-9	THR	-	expression tag	UNP Q6W7J7
C	-8	GLU	-	expression tag	UNP Q6W7J7
C	-7	ASN	-	expression tag	UNP Q6W7J7
C	-6	LEU	-	expression tag	UNP Q6W7J7
C	-5	TYR	-	expression tag	UNP Q6W7J7
C	-4	PHE	-	expression tag	UNP Q6W7J7
C	-3	GLN	-	expression tag	UNP Q6W7J7
C	-2	SER	-	expression tag	UNP Q6W7J7
C	-1	ASN	-	expression tag	UNP Q6W7J7
C	0	GLY	-	expression tag	UNP Q6W7J7
C	1	MET	-	expression tag	UNP Q6W7J7
D	-23	MET	-	initiating methionine	UNP Q6W7J7
D	-22	HIS	-	expression tag	UNP Q6W7J7
D	-21	HIS	-	expression tag	UNP Q6W7J7
D	-20	HIS	-	expression tag	UNP Q6W7J7
D	-19	HIS	-	expression tag	UNP Q6W7J7
D	-18	HIS	-	expression tag	UNP Q6W7J7
D	-17	HIS	-	expression tag	UNP Q6W7J7
D	-16	SER	-	expression tag	UNP Q6W7J7
D	-15	SER	-	expression tag	UNP Q6W7J7
D	-14	GLY	-	expression tag	UNP Q6W7J7
D	-13	VAL	-	expression tag	UNP Q6W7J7
D	-12	ASP	-	expression tag	UNP Q6W7J7
D	-11	LEU	-	expression tag	UNP Q6W7J7
D	-10	GLY	-	expression tag	UNP Q6W7J7
D	-9	THR	-	expression tag	UNP Q6W7J7
D	-8	GLU	-	expression tag	UNP Q6W7J7
D	-7	ASN	-	expression tag	UNP Q6W7J7
D	-6	LEU	-	expression tag	UNP Q6W7J7
D	-5	TYR	-	expression tag	UNP Q6W7J7
D	-4	PHE	-	expression tag	UNP Q6W7J7
D	-3	GLN	-	expression tag	UNP Q6W7J7
D	-2	SER	-	expression tag	UNP Q6W7J7
D	-1	ASN	-	expression tag	UNP Q6W7J7
D	0	GLY	-	expression tag	UNP Q6W7J7
D	1	MET	-	expression tag	UNP Q6W7J7
E	-23	MET	-	initiating methionine	UNP Q6W7J7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	HIS	-	expression tag	UNP Q6W7J7
E	-21	HIS	-	expression tag	UNP Q6W7J7
E	-20	HIS	-	expression tag	UNP Q6W7J7
E	-19	HIS	-	expression tag	UNP Q6W7J7
E	-18	HIS	-	expression tag	UNP Q6W7J7
E	-17	HIS	-	expression tag	UNP Q6W7J7
E	-16	SER	-	expression tag	UNP Q6W7J7
E	-15	SER	-	expression tag	UNP Q6W7J7
E	-14	GLY	-	expression tag	UNP Q6W7J7
E	-13	VAL	-	expression tag	UNP Q6W7J7
E	-12	ASP	-	expression tag	UNP Q6W7J7
E	-11	LEU	-	expression tag	UNP Q6W7J7
E	-10	GLY	-	expression tag	UNP Q6W7J7
E	-9	THR	-	expression tag	UNP Q6W7J7
E	-8	GLU	-	expression tag	UNP Q6W7J7
E	-7	ASN	-	expression tag	UNP Q6W7J7
E	-6	LEU	-	expression tag	UNP Q6W7J7
E	-5	TYR	-	expression tag	UNP Q6W7J7
E	-4	PHE	-	expression tag	UNP Q6W7J7
E	-3	GLN	-	expression tag	UNP Q6W7J7
E	-2	SER	-	expression tag	UNP Q6W7J7
E	-1	ASN	-	expression tag	UNP Q6W7J7
E	0	GLY	-	expression tag	UNP Q6W7J7
E	1	MET	-	expression tag	UNP Q6W7J7
F	-23	MET	-	initiating methionine	UNP Q6W7J7
F	-22	HIS	-	expression tag	UNP Q6W7J7
F	-21	HIS	-	expression tag	UNP Q6W7J7
F	-20	HIS	-	expression tag	UNP Q6W7J7
F	-19	HIS	-	expression tag	UNP Q6W7J7
F	-18	HIS	-	expression tag	UNP Q6W7J7
F	-17	HIS	-	expression tag	UNP Q6W7J7
F	-16	SER	-	expression tag	UNP Q6W7J7
F	-15	SER	-	expression tag	UNP Q6W7J7
F	-14	GLY	-	expression tag	UNP Q6W7J7
F	-13	VAL	-	expression tag	UNP Q6W7J7
F	-12	ASP	-	expression tag	UNP Q6W7J7
F	-11	LEU	-	expression tag	UNP Q6W7J7
F	-10	GLY	-	expression tag	UNP Q6W7J7
F	-9	THR	-	expression tag	UNP Q6W7J7
F	-8	GLU	-	expression tag	UNP Q6W7J7
F	-7	ASN	-	expression tag	UNP Q6W7J7
F	-6	LEU	-	expression tag	UNP Q6W7J7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	TYR	-	expression tag	UNP Q6W7J7
F	-4	PHE	-	expression tag	UNP Q6W7J7
F	-3	GLN	-	expression tag	UNP Q6W7J7
F	-2	SER	-	expression tag	UNP Q6W7J7
F	-1	ASN	-	expression tag	UNP Q6W7J7
F	0	GLY	-	expression tag	UNP Q6W7J7
F	1	MET	-	expression tag	UNP Q6W7J7

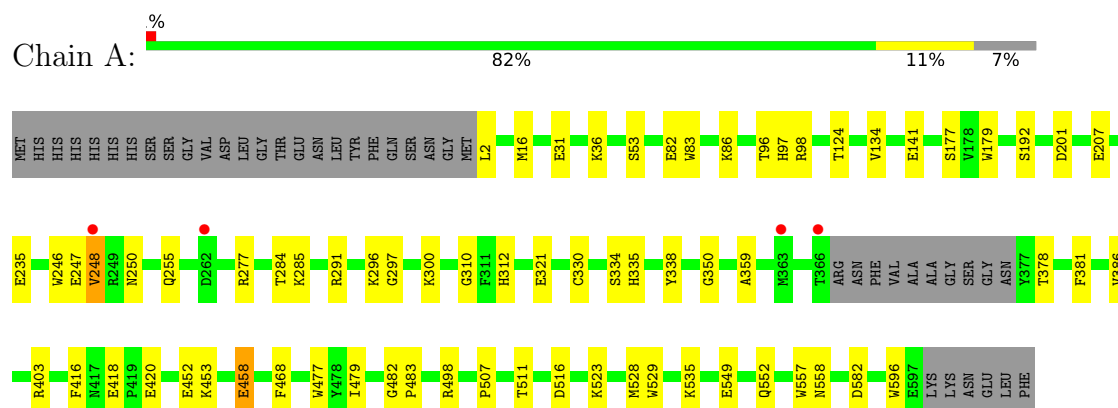
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	265	Total O 265 265	0	0
2	B	240	Total O 240 240	0	0
2	C	268	Total O 268 268	0	0
2	D	224	Total O 224 224	0	0
2	E	250	Total O 250 250	0	0
2	F	294	Total O 294 294	0	0

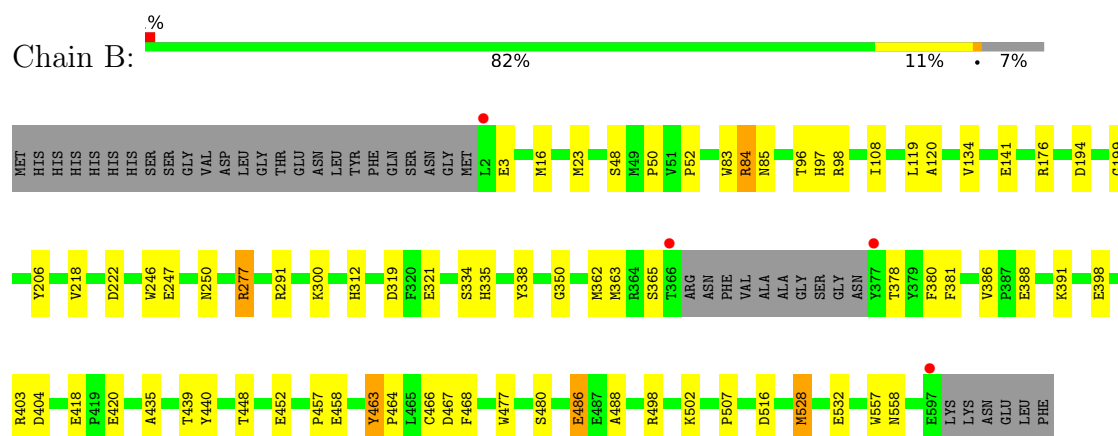
3 Residue-property plots

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.

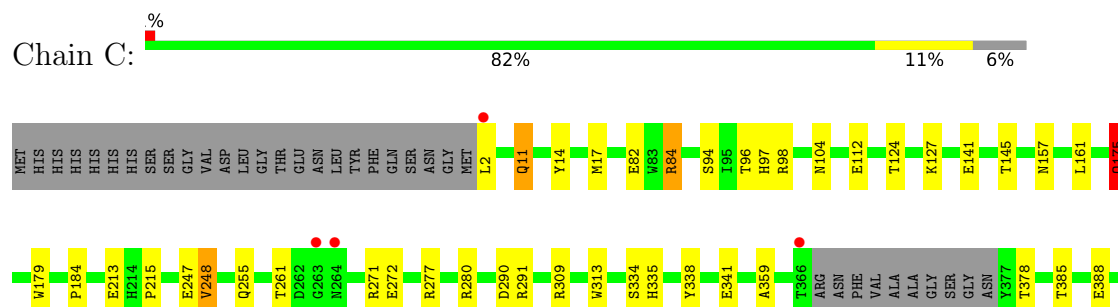
• Molecule 1: Beta-glucuronidase

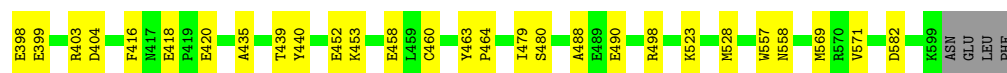


• Molecule 1: Beta-glucuronidase

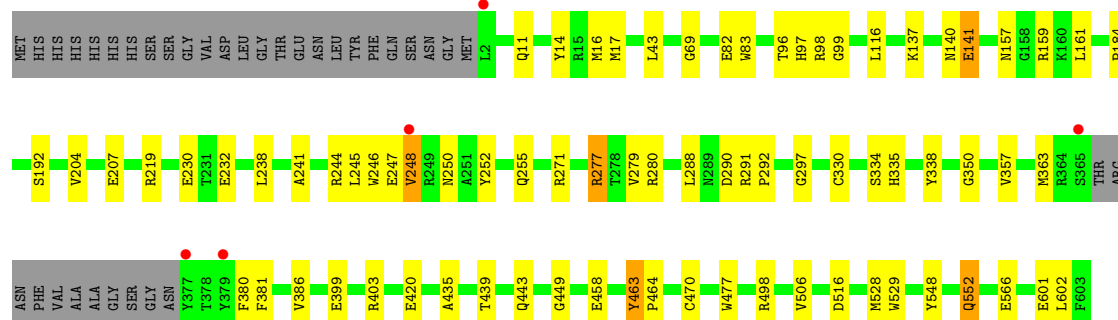
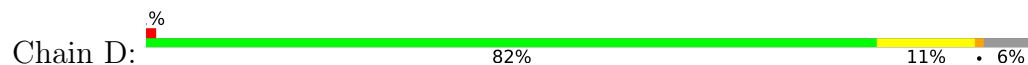


• Molecule 1: Beta-glucuronidase

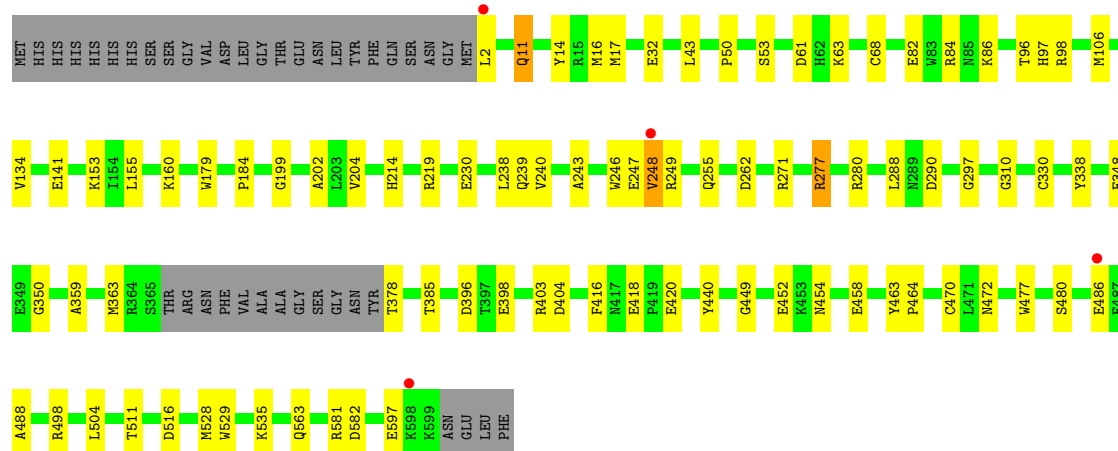
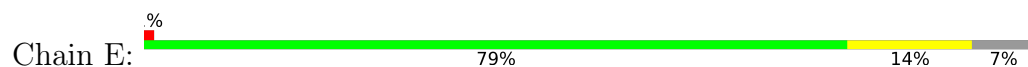




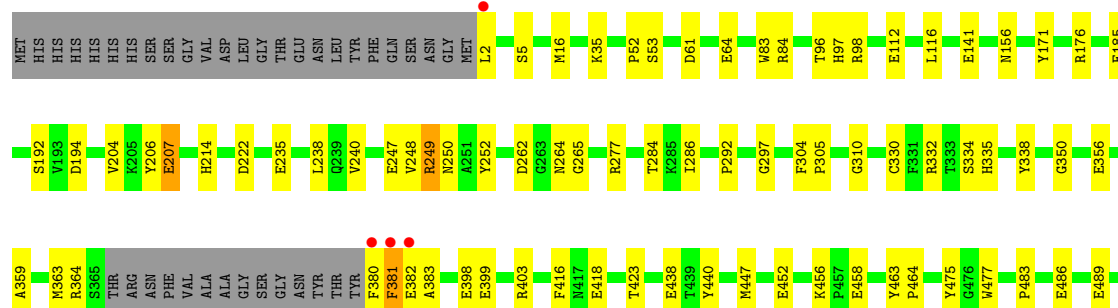
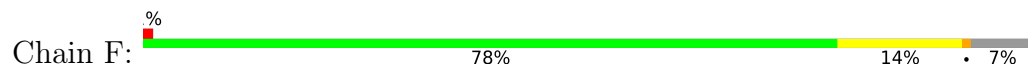
• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.87Å 118.18Å 210.35Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	29.03 – 2.50 29.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.03-2.50) 93.9 (29.03-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.167 , 0.209 0.172 , 0.212	Depositor DCC
R_{free} test set	2000 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30433	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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	0.56	0/4949	0.84	2/6711 (0.0%)
1	B	0.56	0/4949	0.84	3/6711 (0.0%)
1	C	0.56	0/4967	0.83	2/6733 (0.0%)
1	D	0.52	0/4997	0.84	10/6773 (0.1%)
1	E	0.55	0/4947	0.83	5/6705 (0.1%)
1	F	0.57	0/4909	0.86	4/6655 (0.1%)
All	All	0.55	0/29718	0.84	26/40288 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	528	MET	N-CA-C	7.04	119.85	111.33
1	D	380	PHE	N-CA-C	-7.03	101.76	110.41
1	E	248	VAL	CB-CA-C	-6.89	101.99	112.05
1	D	248	VAL	N-CA-C	6.53	118.06	110.62
1	F	249	ARG	N-CA-C	-6.35	102.92	110.41
1	A	248	VAL	N-CA-C	6.31	119.88	111.17
1	D	248	VAL	CB-CA-C	-6.21	103.90	112.04
1	B	528	MET	N-CA-C	6.16	118.78	111.33
1	D	463	TYR	CA-C-N	-5.96	113.48	119.56
1	D	463	TYR	C-N-CA	-5.96	113.48	119.56
1	D	43	LEU	CA-C-N	5.84	125.22	118.85
1	D	43	LEU	C-N-CA	5.84	125.22	118.85
1	F	240	VAL	N-CA-C	5.68	115.78	107.37
1	B	463	TYR	CA-C-N	-5.47	113.98	119.56
1	B	463	TYR	C-N-CA	-5.47	113.98	119.56
1	E	248	VAL	N-CA-C	5.29	118.48	111.17
1	E	43	LEU	CA-C-N	5.28	124.60	118.85
1	E	43	LEU	C-N-CA	5.28	124.60	118.85
1	D	506	VAL	CA-C-N	-5.27	114.53	119.85
1	D	506	VAL	C-N-CA	-5.27	114.53	119.85
1	A	248	VAL	CB-CA-C	-5.21	104.45	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	GLN	CA-CB-CG	5.18	124.45	114.10
1	D	141	GLU	N-CA-C	5.13	117.30	110.53
1	F	381	PHE	CA-C-N	5.12	130.92	121.70
1	F	381	PHE	C-N-CA	5.12	130.92	121.70
1	E	249	ARG	N-CA-C	-5.08	105.37	112.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4811	0	4589	55	0
1	B	4811	0	4589	53	0
1	C	4829	0	4615	56	0
1	D	4858	0	4640	49	1
1	E	4810	0	4599	68	1
1	F	4773	0	4557	74	0
2	A	265	0	0	15	2
2	B	240	0	0	12	4
2	C	268	0	0	14	0
2	D	224	0	0	8	0
2	E	250	0	0	21	0
2	F	294	0	0	24	2
All	All	30433	0	27589	342	5

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 6.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LEU:N	2:C:702:HOH:O	1.82	1.12
1:F:563:GLN:NE2	2:F:702:HOH:O	1.87	1.06
1:C:213:GLU:OE2	2:C:701:HOH:O	1.82	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:552:GLN:NE2	2:F:704:HOH:O	1.99	0.95
1:F:262:ASP:OD1	2:F:701:HOH:O	1.85	0.94
1:D:255:GLN:OE1	2:D:701:HOH:O	1.86	0.93
1:A:201:ASP:OD1	2:A:701:HOH:O	1.87	0.92
1:E:396:ASP:OD1	2:E:702:HOH:O	1.88	0.91
1:F:364:ARG:HH22	1:F:381:PHE:HB2	1.36	0.89
1:E:472:ASN:O	2:E:703:HOH:O	1.89	0.89
1:E:240:VAL:O	2:E:704:HOH:O	1.91	0.88
1:D:16:MET:SD	2:D:845:HOH:O	2.30	0.88
1:F:222:ASP:OD2	2:F:703:HOH:O	1.89	0.88
1:C:175:GLN:HE21	1:C:309:ARG:HB2	1.41	0.85
1:B:16:MET:SD	2:B:887:HOH:O	2.34	0.85
1:C:272:GLU:OE2	2:C:703:HOH:O	1.95	0.84
1:C:338:TYR:O	1:C:403:ARG:NH2	2.11	0.84
1:E:504:LEU:O	2:E:705:HOH:O	1.98	0.82
1:D:363:MET:SD	2:D:734:HOH:O	2.36	0.82
1:C:490:GLU:OE1	1:F:156:ASN:ND2	2.13	0.81
1:E:202:ALA:N	2:E:704:HOH:O	2.10	0.81
1:A:338:TYR:O	1:A:403:ARG:NH2	2.14	0.80
1:B:321:GLU:OE2	2:B:701:HOH:O	1.98	0.80
1:F:16:MET:SD	2:F:883:HOH:O	2.38	0.80
1:C:112:GLU:OE2	2:C:705:HOH:O	1.99	0.80
1:E:348:GLU:OE2	2:E:706:HOH:O	2.00	0.79
1:C:11:GLN:NE2	2:C:704:HOH:O	1.99	0.79
1:C:523:LYS:NZ	2:C:711:HOH:O	2.16	0.79
1:E:516:ASP:OD2	2:E:707:HOH:O	2.00	0.78
1:B:338:TYR:O	1:B:403:ARG:NH2	2.15	0.77
1:E:199:GLY:O	2:E:708:HOH:O	2.01	0.77
1:C:11:GLN:HG2	1:C:17:MET:HG2	1.68	0.76
1:A:82:GLU:OE2	2:A:703:HOH:O	2.04	0.76
1:A:321:GLU:OE2	2:A:702:HOH:O	2.03	0.75
1:B:528:MET:O	2:B:702:HOH:O	2.03	0.75
1:F:438:GLU:O	2:F:705:HOH:O	2.05	0.75
1:E:239:GLN:OE1	2:E:709:HOH:O	2.04	0.74
1:E:214:HIS:CD2	1:E:262:ASP:HB3	2.23	0.74
1:E:363:MET:SD	2:E:929:HOH:O	2.46	0.72
1:F:489:GLU:OE2	2:F:706:HOH:O	2.07	0.72
1:F:363:MET:SD	2:F:770:HOH:O	2.46	0.72
1:E:247:GLU:OE1	2:E:710:HOH:O	2.08	0.71
1:B:98:ARG:NH2	1:B:141:GLU:O	2.23	0.71
1:E:2:LEU:N	2:E:715:HOH:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ARG:NH1	1:D:290:ASP:OD1	2.24	0.71
1:B:250:ASN:O	2:B:703:HOH:O	2.08	0.70
1:C:582:ASP:OD2	2:C:707:HOH:O	2.09	0.70
1:C:247:GLU:OE1	1:C:291:ARG:NH2	2.24	0.70
1:E:338:TYR:O	1:E:403:ARG:NH2	2.22	0.69
1:D:552:GLN:NE2	1:D:601:GLU:OE2	2.25	0.69
1:B:391:LYS:HD2	2:B:791:HOH:O	1.93	0.69
1:D:548:TYR:O	2:D:702:HOH:O	2.11	0.69
1:F:207:GLU:HG3	1:F:235:GLU:HG2	1.75	0.69
1:F:486:GLU:OE1	2:F:709:HOH:O	2.10	0.69
1:E:63:LYS:O	2:E:711:HOH:O	2.10	0.69
1:F:380:PHE:HZ	1:F:423:THR:HG21	1.58	0.68
1:E:98:ARG:NH2	1:E:141:GLU:O	2.26	0.68
1:E:243:ALA:HB2	2:E:704:HOH:O	1.94	0.68
1:F:5:SER:O	2:F:708:HOH:O	2.10	0.68
1:A:98:ARG:NH2	1:A:141:GLU:O	2.26	0.68
1:F:277:ARG:HG3	1:F:277:ARG:HH11	1.58	0.67
1:F:185:GLU:OE2	2:F:710:HOH:O	2.13	0.67
1:E:11:GLN:HE21	1:E:17:MET:HG2	1.58	0.67
1:F:53:SER:O	2:F:711:HOH:O	2.13	0.67
1:C:94:SER:O	2:C:708:HOH:O	2.13	0.66
1:A:582:ASP:OD2	2:A:704:HOH:O	2.13	0.65
1:B:247:GLU:OE1	2:B:704:HOH:O	2.13	0.65
1:F:194:ASP:OD1	2:F:712:HOH:O	2.14	0.65
1:C:82:GLU:HG2	1:E:82:GLU:HG2	1.77	0.65
1:F:517:THR:OG1	1:F:534:GLN:HG3	1.96	0.65
1:E:247:GLU:OE2	1:E:248:VAL:HG23	1.98	0.64
1:B:199:GLY:O	2:B:705:HOH:O	2.14	0.64
1:B:222:ASP:OD2	2:B:706:HOH:O	2.14	0.64
1:F:98:ARG:NH2	1:F:141:GLU:O	2.28	0.64
1:F:247:GLU:HB2	1:F:250:ASN:HB3	1.80	0.63
1:D:11:GLN:HB2	1:D:17:MET:HE2	1.81	0.63
1:A:285:LYS:NZ	1:A:549:GLU:OE2	2.32	0.63
1:C:175:GLN:HE21	1:C:309:ARG:CB	2.12	0.63
1:C:277:ARG:HG2	1:C:277:ARG:HH11	1.65	0.62
1:C:378:THR:OG1	1:C:420:GLU:OE2	2.14	0.61
1:A:523:LYS:O	2:A:705:HOH:O	2.16	0.61
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.65	0.61
1:C:399:GLU:OE1	2:C:709:HOH:O	2.16	0.60
1:F:112:GLU:OE2	2:F:713:HOH:O	2.16	0.60
1:F:265:GLY:N	2:F:701:HOH:O	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.66	0.60
1:C:460:CYS:O	2:C:712:HOH:O	2.16	0.60
1:C:435:ALA:O	1:C:439:THR:HG23	2.02	0.59
1:F:580:THR:OG1	1:F:582:ASP:OD1	2.11	0.59
1:E:277:ARG:O	1:E:277:ARG:HG2	2.01	0.58
1:B:435:ALA:O	1:B:439:THR:HG23	2.04	0.58
1:B:458:GLU:OE2	1:B:498:ARG:HD2	2.03	0.58
1:D:247:GLU:HB2	1:D:250:ASN:HB3	1.85	0.58
1:E:378:THR:N	1:E:420:GLU:OE2	2.35	0.58
1:A:255:GLN:NE2	2:A:722:HOH:O	2.33	0.58
1:C:480:SER:HB2	1:C:488:ALA:HB2	1.86	0.57
1:E:535:LYS:NZ	2:E:712:HOH:O	2.11	0.57
1:F:214:HIS:CD2	1:F:262:ASP:HB3	2.40	0.57
1:A:453:LYS:HD2	1:A:479:ILE:HD11	1.86	0.56
1:A:418:GLU:HG2	1:A:452:GLU:HB2	1.86	0.56
1:B:300:LYS:NZ	1:B:319:ASP:OD2	2.35	0.56
1:E:297:GLY:HA3	1:E:330:CYS:O	2.06	0.56
1:F:84:ARG:HD3	2:F:744:HOH:O	2.05	0.56
1:E:418:GLU:HG2	1:E:452:GLU:HB2	1.87	0.55
1:E:582:ASP:OD1	2:E:713:HOH:O	2.18	0.55
1:E:597:GLU:O	2:E:714:HOH:O	2.18	0.55
1:F:2:LEU:HD11	1:F:440:TYR:HE1	1.70	0.55
1:F:534:GLN:OE1	2:F:714:HOH:O	2.18	0.54
1:D:98:ARG:NH2	1:D:141:GLU:O	2.29	0.54
1:A:16:MET:HG3	2:A:871:HOH:O	2.08	0.54
1:F:363:MET:HE2	2:F:967:HOH:O	2.06	0.54
1:F:452:GLU:OE2	2:F:715:HOH:O	2.19	0.54
1:C:104:ASN:ND2	1:C:127:LYS:HE2	2.23	0.53
1:E:11:GLN:HE21	1:E:17:MET:CG	2.21	0.53
1:C:280:ARG:NH1	1:C:290:ASP:OD1	2.42	0.53
1:A:468:PHE:HB3	1:A:507:PRO:HG2	1.90	0.53
1:F:53:SER:HA	1:F:310:GLY:HA3	1.90	0.53
1:C:175:GLN:NE2	1:C:309:ARG:HB2	2.17	0.53
1:C:458:GLU:OE2	1:C:498:ARG:HD2	2.08	0.53
1:A:549:GLU:OE1	2:A:706:HOH:O	2.18	0.53
1:B:477:TRP:CZ2	1:B:516:ASP:HB2	2.44	0.53
1:A:277:ARG:HG3	1:A:277:ARG:O	2.09	0.53
1:A:296:LYS:NZ	1:A:596:TRP:O	2.39	0.53
1:C:388:GLU:HG3	1:D:232:GLU:OE1	2.09	0.53
1:A:458:GLU:OE1	1:A:498:ARG:NH1	2.42	0.52
1:A:516:ASP:O	1:A:529:TRP:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:VAL:HB	1:F:238:LEU:HB2	1.90	0.52
1:A:124:THR:OG1	2:A:707:HOH:O	2.19	0.52
1:C:277:ARG:HG2	1:C:277:ARG:NH1	2.24	0.52
1:C:248:VAL:HG12	2:C:857:HOH:O	2.07	0.52
1:E:486:GLU:OE1	1:E:486:GLU:N	2.30	0.52
1:E:32:GLU:OE2	1:E:160:LYS:NZ	2.34	0.52
1:D:458:GLU:OE2	1:D:498:ARG:HD2	2.10	0.52
1:C:98:ARG:NH2	1:C:141:GLU:O	2.33	0.52
1:D:255:GLN:NE2	1:D:271:ARG:HD3	2.25	0.51
1:A:16:MET:HE2	1:A:83:TRP:CD1	2.45	0.51
1:B:486:GLU:CD	1:B:486:GLU:H	2.18	0.51
1:D:11:GLN:NE2	2:D:726:HOH:O	2.43	0.51
1:F:380:PHE:CZ	1:F:423:THR:HG21	2.42	0.51
1:C:582:ASP:OD1	2:C:713:HOH:O	2.19	0.51
1:A:248:VAL:HG23	2:A:772:HOH:O	2.09	0.51
1:C:161:LEU:HD21	1:F:483:PRO:HB2	1.93	0.51
1:D:277:ARG:NH1	1:D:279:VAL:HG23	2.25	0.51
1:F:284:THR:O	1:F:552:GLN:HG3	2.11	0.51
1:F:297:GLY:HA3	1:F:330:CYS:O	2.10	0.51
1:C:255:GLN:OE1	1:C:271:ARG:HD3	2.11	0.51
1:D:381:PHE:HA	1:D:386:VAL:HG21	1.92	0.50
1:E:246:TRP:CZ2	1:E:350:GLY:HA2	2.46	0.50
1:D:16:MET:HE2	1:D:83:TRP:CD1	2.45	0.50
1:E:14:TYR:O	1:E:184:PRO:HD3	2.10	0.50
1:D:420:GLU:OE1	2:D:705:HOH:O	2.19	0.50
1:B:277:ARG:HG2	1:B:277:ARG:NH1	2.27	0.50
1:B:362:MET:HB2	2:B:829:HOH:O	2.11	0.50
1:F:498:ARG:NH1	2:F:707:HOH:O	2.08	0.50
1:B:84:ARG:HH11	1:B:84:ARG:HG2	1.75	0.50
1:D:477:TRP:CZ2	1:D:516:ASP:HB2	2.47	0.50
1:C:569:MET:HG2	1:F:569:MET:HG2	1.94	0.50
1:B:468:PHE:HB3	1:B:507:PRO:HG2	1.94	0.49
1:C:571:VAL:HG21	1:F:571:VAL:HG21	1.95	0.49
1:E:477:TRP:CZ2	1:E:516:ASP:HB2	2.48	0.49
1:B:194:ASP:OD1	2:B:708:HOH:O	2.20	0.49
1:E:458:GLU:OE2	1:E:498:ARG:HD2	2.13	0.49
1:B:467:ASP:O	2:B:709:HOH:O	2.20	0.49
1:D:449:GLY:O	1:D:470:CYS:HB2	2.13	0.49
1:E:255:GLN:OE1	1:E:271:ARG:HD3	2.13	0.49
1:B:480:SER:HB2	1:B:488:ALA:HB2	1.95	0.48
1:A:246:TRP:CZ2	1:A:350:GLY:HA2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:THR:HG23	2:E:808:HOH:O	2.13	0.48
1:F:398:GLU:HG2	1:F:440:TYR:CD2	2.48	0.48
1:D:116:LEU:HD13	1:D:399:GLU:HB2	1.94	0.48
1:A:31:GLU:CD	2:A:713:HOH:O	2.56	0.48
1:A:334:SER:HA	1:A:335:HIS:HA	1.68	0.48
1:A:378:THR:OG1	1:A:420:GLU:OE2	2.23	0.48
1:F:381:PHE:HB3	1:F:383:ALA:N	2.28	0.48
1:C:17:MET:HE2	1:C:179:TRP:CZ3	2.48	0.48
1:A:177:SER:HB2	1:A:179:TRP:CH2	2.49	0.48
1:F:2:LEU:HD11	1:F:440:TYR:CE1	2.49	0.48
1:F:418:GLU:HG2	1:F:452:GLU:HB2	1.95	0.48
1:A:82:GLU:OE1	1:A:82:GLU:N	2.38	0.48
1:E:449:GLY:O	1:E:470:CYS:HB2	2.14	0.48
1:D:244:ARG:NH1	1:D:245:LEU:O	2.47	0.47
1:D:248:VAL:HG22	1:D:288:LEU:HD23	1.95	0.47
1:D:248:VAL:O	1:D:350:GLY:O	2.31	0.47
1:E:563:GLN:NE2	2:E:739:HOH:O	2.47	0.47
1:F:61:ASP:OD2	1:F:64:GLU:HG3	2.15	0.47
1:B:23:MET:CE	1:B:48:SER:HB3	2.45	0.47
1:D:297:GLY:HA3	1:D:330:CYS:O	2.14	0.47
1:E:248:VAL:HG22	1:E:288:LEU:HD23	1.96	0.47
1:F:248:VAL:O	1:F:350:GLY:O	2.32	0.47
1:A:312:HIS:CD2	1:B:312:HIS:CD2	3.03	0.47
1:E:277:ARG:HG2	1:E:277:ARG:HH11	1.78	0.47
1:A:277:ARG:HG3	1:A:277:ARG:NH1	2.29	0.47
1:E:528:MET:O	1:E:529:TRP:HB2	2.15	0.47
1:F:463:TYR:CG	1:F:464:PRO:HD3	2.50	0.47
1:D:338:TYR:O	1:D:403:ARG:NH2	2.28	0.46
1:E:463:TYR:CG	1:E:464:PRO:HD3	2.50	0.46
1:D:69:GLY:H	1:D:140:ASN:HB2	1.80	0.46
1:A:312:HIS:CD2	1:B:312:HIS:HD2	2.34	0.46
1:E:581:ARG:HD2	2:E:930:HOH:O	2.14	0.46
1:F:338:TYR:O	1:F:403:ARG:NH2	2.32	0.46
1:C:175:GLN:HB2	2:C:768:HOH:O	2.16	0.46
1:F:475:TYR:N	2:F:739:HOH:O	2.48	0.46
1:A:300:LYS:HE2	1:A:300:LYS:HB3	1.50	0.46
1:D:516:ASP:O	1:D:529:TRP:HA	2.16	0.46
1:B:108:ILE:HG21	1:B:120:ALA:HB1	1.97	0.46
1:C:215:PRO:HG2	1:C:261:THR:HG23	1.97	0.46
1:C:96:THR:HA	1:C:97:HIS:HA	1.74	0.46
1:C:145:THR:HG22	1:C:385:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:HA3	1:A:330:CYS:O	2.15	0.46
1:B:418:GLU:HG2	1:B:452:GLU:HB2	1.98	0.46
1:F:248:VAL:O	1:F:249:ARG:HG2	2.16	0.45
1:B:247:GLU:CD	1:B:291:ARG:HH22	2.23	0.45
1:E:204:VAL:HB	1:E:238:LEU:HB2	1.97	0.45
1:E:359:ALA:HB3	1:E:416:PHE:HA	1.99	0.45
1:A:248:VAL:O	1:A:350:GLY:O	2.33	0.45
1:A:516:ASP:HB3	1:A:529:TRP:CZ3	2.52	0.45
1:B:532:GLU:OE2	2:B:711:HOH:O	2.20	0.45
1:D:566:GLU:HG2	2:D:762:HOH:O	2.14	0.45
1:D:244:ARG:HG3	1:D:252:TYR:CG	2.52	0.45
1:E:96:THR:HA	1:E:97:HIS:HA	1.67	0.45
1:F:222:ASP:HB2	1:F:252:TYR:OH	2.17	0.45
1:F:380:PHE:O	1:F:381:PHE:HD1	1.99	0.45
1:F:264:ASN:N	2:F:701:HOH:O	2.50	0.45
1:F:456:LYS:HB3	2:F:707:HOH:O	2.15	0.45
1:A:458:GLU:CD	1:A:458:GLU:H	2.25	0.45
1:C:463:TYR:CG	1:C:464:PRO:HD3	2.52	0.45
1:F:116:LEU:HD13	1:F:399:GLU:HB2	1.98	0.45
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.77	0.45
1:A:381:PHE:HA	1:A:386:VAL:HG21	1.99	0.45
1:A:535:LYS:NZ	2:A:724:HOH:O	2.35	0.45
1:B:448:THR:HG22	1:B:468:PHE:O	2.17	0.45
1:E:280:ARG:NH1	1:E:290:ASP:OD1	2.47	0.45
1:B:363:MET:HE3	1:B:365:SER:HB3	1.99	0.45
1:C:334:SER:HA	1:C:335:HIS:HA	1.66	0.45
1:D:277:ARG:HH11	1:D:279:VAL:HG23	1.82	0.45
1:E:248:VAL:O	1:E:350:GLY:O	2.35	0.44
1:B:398:GLU:HB2	1:B:440:TYR:CE1	2.53	0.44
1:F:458:GLU:OE2	1:F:498:ARG:HD2	2.18	0.44
1:C:403:ARG:NH1	1:C:404:ASP:OD2	2.51	0.44
1:D:528:MET:O	1:D:529:TRP:HB2	2.18	0.44
1:F:418:GLU:CG	1:F:452:GLU:HB2	2.47	0.44
1:A:53:SER:HA	1:A:310:GLY:HA3	2.00	0.44
1:D:246:TRP:CZ2	1:D:350:GLY:HA2	2.52	0.44
1:B:463:TYR:CG	1:B:464:PRO:HD3	2.53	0.44
1:B:52:PRO:HB3	1:B:176:ARG:C	2.43	0.44
1:C:453:LYS:HD2	1:C:479:ILE:HD11	2.00	0.44
1:E:363:MET:HE2	1:E:363:MET:HB3	1.77	0.44
1:A:312:HIS:HD2	1:B:312:HIS:CD2	2.36	0.44
1:E:219:ARG:HG2	1:E:230:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:O	1:A:552:GLN:HG3	2.17	0.43
1:C:157:ASN:N	2:C:739:HOH:O	2.51	0.43
1:B:96:THR:HA	1:B:97:HIS:HA	1.79	0.43
1:A:192:SER:HB2	1:A:207:GLU:HG2	2.00	0.43
1:A:247:GLU:HB2	1:A:250:ASN:HB3	1.99	0.43
1:E:17:MET:HE2	1:E:179:TRP:CZ3	2.54	0.43
1:B:381:PHE:HA	1:B:386:VAL:HG21	2.00	0.43
1:E:61:ASP:OD2	1:E:63:LYS:HE2	2.19	0.43
1:F:334:SER:HA	1:F:335:HIS:HA	1.71	0.43
1:A:235:GLU:O	2:A:708:HOH:O	2.21	0.43
1:B:16:MET:HE2	1:B:83:TRP:CD1	2.53	0.43
1:D:96:THR:HA	1:D:97:HIS:HA	1.76	0.43
1:A:359:ALA:HB3	1:A:416:PHE:HA	1.99	0.43
1:A:482:GLY:HA3	1:A:483:PRO:HD3	1.84	0.43
1:B:457:PRO:O	1:B:502:LYS:HE3	2.18	0.43
1:D:241:ALA:O	2:D:706:HOH:O	2.20	0.43
1:C:175:GLN:HE21	1:C:309:ARG:CG	2.31	0.43
1:C:453:LYS:HD2	1:C:479:ILE:CD1	2.48	0.43
1:D:14:TYR:O	1:D:184:PRO:HD3	2.18	0.43
1:E:106:MET:HE3	1:E:106:MET:HB3	1.93	0.43
1:F:84:ARG:NH1	2:F:744:HOH:O	2.51	0.43
1:F:96:THR:HA	1:F:97:HIS:HA	1.80	0.43
1:F:381:PHE:HA	1:F:382:GLU:CB	2.49	0.43
1:D:204:VAL:HB	1:D:238:LEU:HB2	2.01	0.43
1:D:334:SER:HA	1:D:335:HIS:HA	1.64	0.43
1:A:247:GLU:OE1	1:A:291:ARG:NH2	2.52	0.43
1:B:300:LYS:HE2	1:B:300:LYS:HB3	1.53	0.43
1:E:418:GLU:CG	1:E:452:GLU:HB2	2.49	0.43
1:B:403:ARG:NH1	1:B:404:ASP:OD2	2.52	0.43
1:A:477:TRP:CZ2	1:A:516:ASP:HB2	2.53	0.42
1:A:528:MET:O	1:A:529:TRP:HB2	2.20	0.42
1:C:313:TRP:CH2	1:C:341:GLU:HB3	2.55	0.42
1:D:277:ARG:NH2	1:D:443:GLN:OE1	2.37	0.42
1:F:16:MET:HE2	1:F:83:TRP:CD1	2.54	0.42
1:F:359:ALA:HB3	1:F:416:PHE:HA	2.02	0.42
1:A:16:MET:SD	1:A:86:LYS:HE3	2.58	0.42
1:C:14:TYR:O	1:C:184:PRO:HD3	2.20	0.42
1:C:418:GLU:HG2	1:C:452:GLU:HB2	2.02	0.42
1:D:192:SER:HB2	1:D:207:GLU:HG2	2.00	0.42
1:D:435:ALA:O	1:D:439:THR:HG23	2.19	0.42
1:E:11:GLN:HG3	1:E:17:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:SER:HA	1:E:310:GLY:HA3	2.01	0.42
1:E:277:ARG:HG2	1:E:277:ARG:NH1	2.34	0.42
1:F:35:LYS:HD2	1:F:35:LYS:HA	1.79	0.42
1:B:3:GLU:O	1:B:3:GLU:HG2	2.19	0.42
1:B:380:PHE:O	1:B:381:PHE:HB2	2.20	0.42
1:A:96:THR:HA	1:A:97:HIS:HA	1.75	0.42
1:B:246:TRP:CZ2	1:B:350:GLY:HA2	2.55	0.42
1:F:192:SER:O	1:F:206:TYR:HA	2.20	0.42
1:B:334:SER:HA	1:B:335:HIS:HA	1.71	0.42
1:B:378:THR:OG1	1:B:420:GLU:OE2	2.27	0.42
1:B:557:TRP:HA	1:B:558:ASN:HA	1.88	0.42
1:F:304:PHE:CG	1:F:305:PRO:HD2	2.55	0.42
1:E:363:MET:HE1	2:E:929:HOH:O	2.20	0.41
2:A:703:HOH:O	1:B:16:MET:HE3	2.19	0.41
1:D:277:ARG:HH11	1:D:277:ARG:HG2	1.85	0.41
1:F:286:ILE:O	1:F:292:PRO:HA	2.20	0.41
1:D:463:TYR:CG	1:D:464:PRO:HD3	2.56	0.41
1:E:68:CYS:O	1:E:160:LYS:HB2	2.20	0.41
1:E:153:LYS:HE3	1:E:155:LEU:HD23	2.02	0.41
1:A:2:LEU:N	2:A:753:HOH:O	2.53	0.41
1:E:452:GLU:CD	1:E:454:ASN:H	2.29	0.41
1:F:52:PRO:HB3	1:F:176:ARG:C	2.46	0.41
1:F:171:TYR:OH	1:F:563:GLN:HG2	2.20	0.41
1:B:466:CYS:HB3	1:B:468:PHE:O	2.21	0.41
1:C:124:THR:HG21	1:D:435:ALA:CB	2.50	0.41
1:C:398:GLU:HG2	1:C:440:TYR:CE2	2.55	0.41
1:E:16:MET:SD	1:E:86:LYS:HE3	2.61	0.41
1:F:447:MET:HE3	1:F:447:MET:HB2	1.88	0.41
1:A:418:GLU:CG	1:A:452:GLU:HB2	2.50	0.41
1:B:23:MET:HE1	1:B:50:PRO:HD3	2.02	0.41
1:C:359:ALA:HB3	1:C:416:PHE:HA	2.03	0.41
1:C:557:TRP:HA	1:C:558:ASN:HA	1.84	0.41
1:D:291:ARG:HA	1:D:292:PRO:HD3	1.95	0.41
1:E:248:VAL:HG22	1:E:288:LEU:CD2	2.51	0.41
1:B:391:LYS:HD3	1:B:391:LYS:HA	1.77	0.41
1:E:398:GLU:HG3	1:E:440:TYR:CE1	2.56	0.41
1:E:480:SER:HB2	1:E:488:ALA:HB2	2.03	0.41
1:D:82:GLU:H	1:D:82:GLU:CD	2.29	0.40
1:E:378:THR:OG1	1:E:420:GLU:OE2	2.36	0.40
1:F:398:GLU:HG2	1:F:440:TYR:CE2	2.56	0.40
1:C:124:THR:HG21	1:D:435:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLY:HA2	1:D:137:LYS:O	2.21	0.40
1:A:557:TRP:HA	1:A:558:ASN:HA	1.87	0.40
1:B:206:TYR:CE1	1:B:218:VAL:HG21	2.57	0.40
1:D:157:ASN:HD21	1:D:159:ARG:HE	1.69	0.40
1:D:219:ARG:HG2	1:D:230:GLU:HG3	2.03	0.40
1:F:381:PHE:HA	1:F:382:GLU:HG3	2.03	0.40
1:F:477:TRP:CZ2	1:F:516:ASP:HB2	2.56	0.40
1:C:569:MET:SD	1:F:569:MET:HE2	2.60	0.40
1:F:332:ARG:NH1	1:F:356:GLU:OE2	2.53	0.40
1:C:313:TRP:HB3	1:E:50:PRO:HB3	2.03	0.40
1:E:403:ARG:NH1	1:E:404:ASP:OD2	2.54	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:HOH:O	2:F:731:HOH:O[4_1413]	1.89	0.31
2:B:777:HOH:O	2:F:887:HOH:O[4_1413]	2.00	0.20
2:A:962:HOH:O	2:B:939:HOH:O[4_1413]	2.05	0.15
1:D:159:ARG:NH2	1:E:486:GLU:OE2[3_445]	2.18	0.02
2:A:760:HOH:O	2:B:907:HOH:O[4_1413]	2.19	0.01

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	582/627 (93%)	563 (97%)	19 (3%)	0	100	100
1	B	582/627 (93%)	566 (97%)	15 (3%)	1 (0%)	43	63
1	C	584/627 (93%)	565 (97%)	18 (3%)	1 (0%)	43	63
1	D	587/627 (94%)	570 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	582/627 (93%)	561 (96%)	20 (3%)	1 (0%)	43	63
1	F	578/627 (92%)	559 (97%)	19 (3%)	0	100	100
All	All	3495/3762 (93%)	3384 (97%)	108 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ARG
1	E	84	ARG
1	C	84	ARG

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	512/546 (94%)	509 (99%)	3 (1%)	78	91
1	B	512/546 (94%)	506 (99%)	6 (1%)	63	83
1	C	514/546 (94%)	510 (99%)	4 (1%)	73	88
1	D	517/546 (95%)	512 (99%)	5 (1%)	68	86
1	E	512/546 (94%)	508 (99%)	4 (1%)	73	88
1	F	508/546 (93%)	505 (99%)	3 (1%)	78	91
All	All	3075/3276 (94%)	3050 (99%)	25 (1%)	73	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
1	A	458	GLU
1	A	511	THR
1	B	85	ASN
1	B	119	LEU
1	B	134	VAL
1	B	277	ARG

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Mol	Chain	Res	Type
1	B	388	GLU
1	B	486	GLU
1	C	11	GLN
1	C	84	ARG
1	C	175	GLN
1	C	248	VAL
1	D	161	LEU
1	D	277	ARG
1	D	357	VAL
1	D	552	GLN
1	D	602	LEU
1	E	11	GLN
1	E	134	VAL
1	E	277	ARG
1	E	511	THR
1	F	207	GLU
1	F	534	GLN
1	F	549	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	62	HIS
1	A	85	ASN
1	A	130	GLN
1	A	312	HIS
1	A	552	GLN
1	A	563	GLN
1	A	584	GLN
1	B	11	GLN
1	B	41	ASN
1	B	584	GLN
1	C	175	GLN
1	C	505	ASN
1	D	41	ASN
1	D	255	GLN
1	D	327	ASN
1	E	11	GLN
1	E	41	ASN
1	E	239	GLN
1	E	242	ASN

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Mol	Chain	Res	Type
1	F	41	ASN
1	F	534	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	586/627 (93%)	-0.31	4 (0%) 84 81	25, 33, 49, 76	0
1	B	586/627 (93%)	-0.29	4 (0%) 84 81	26, 34, 52, 73	0
1	C	588/627 (93%)	-0.29	4 (0%) 84 81	26, 33, 50, 74	0
1	D	591/627 (94%)	-0.25	5 (0%) 82 80	27, 36, 55, 76	0
1	E	586/627 (93%)	-0.25	4 (0%) 84 81	27, 35, 53, 79	0
1	F	582/627 (92%)	-0.29	4 (0%) 84 81	25, 33, 51, 84	0
All	All	3519/3762 (93%)	-0.28	25 (0%) 84 81	25, 34, 52, 84	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	GLY	4.3
1	F	381	PHE	3.6
1	F	380	PHE	3.4
1	E	2	LEU	3.0
1	F	2	LEU	3.0
1	D	365	SER	3.0
1	A	366	THR	2.9
1	D	2	LEU	2.7
1	C	366	THR	2.7
1	B	377	TYR	2.7
1	F	382	GLU	2.7
1	B	366	THR	2.7
1	C	2	LEU	2.4
1	C	264	ASN	2.4
1	D	377	TYR	2.4
1	D	248	VAL	2.4
1	A	262	ASP	2.4
1	B	597	GLU	2.4
1	A	248	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	363	MET	2.3
1	E	248	VAL	2.2
1	B	2	LEU	2.2
1	D	379	TYR	2.2
1	E	486	GLU	2.1
1	E	598	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.