Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:53 PM EDT

PDB ID	:	5Z19
Title	:	The crystal structure of Ruminococcus gnavus beta-glucuronidase in complex with uronic isofagomine
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.

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:

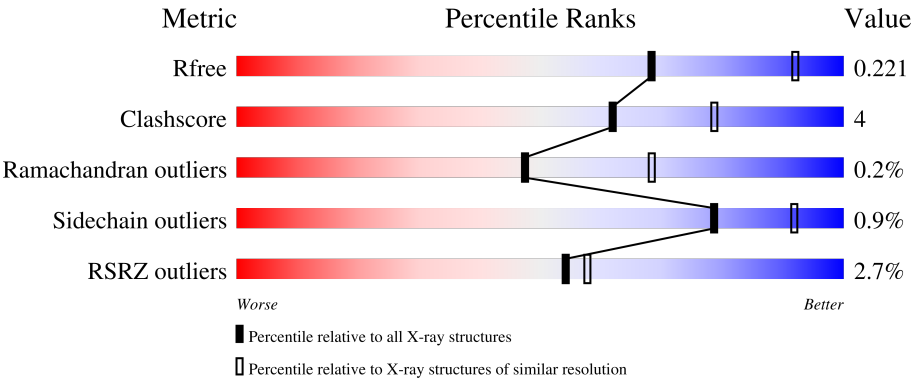
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	3% 84% 11% 5%
1	B	627	2% 83% 11%
1	C	627	3% 87% 9%
1	D	627	2% 83% 11% 5%
1	E	627	2% 85% 10% 5%

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Mol	Chain	Length	Quality of chain
1	F	627	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29830 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	593	Total	C	N	O	S	0	0	0
			4864	3138	791	911	24			
1	B	601	Total	C	N	O	S	0	0	0
			4923	3173	803	923	24			
1	C	600	Total	C	N	O	S	0	0	0
			4915	3167	802	922	24			
1	D	596	Total	C	N	O	S	0	0	0
			4880	3146	795	915	24			
1	E	597	Total	C	N	O	S	0	0	0
			4889	3152	797	916	24			
1	F	600	Total	C	N	O	S	0	0	0
			4915	3167	802	922	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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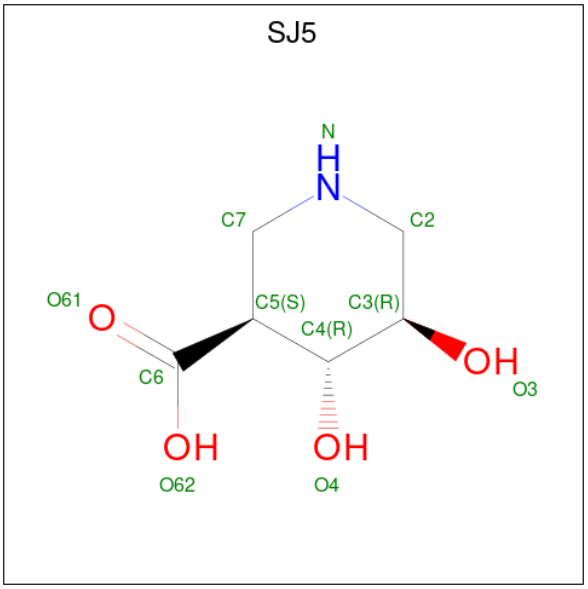
Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	TYR	-	expression tag	UNP Q6W7J7
F	-4	PHE	-	expression tag	UNP Q6W7J7
F	-3	GLN	-	expression tag	UNP Q6W7J7
F	-2	SER	-	expression tag	UNP Q6W7J7
F	-1	ASN	-	expression tag	UNP Q6W7J7
F	0	GLY	-	expression tag	UNP Q6W7J7
F	1	MET	-	expression tag	UNP Q6W7J7

- Molecule 2 is (3S,4R,5R)-4,5-dihydroxypiperidine-3-carboxylic acid (three-letter code: SJ5) (formula: $C_6H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	C	1	Total	C	N	O	0	0
			11	6	1	4		
2	D	1	Total	C	N	O	0	0
			11	6	1	4		
2	E	1	Total	C	N	O	0	0
			11	6	1	4		
2	F	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is water.

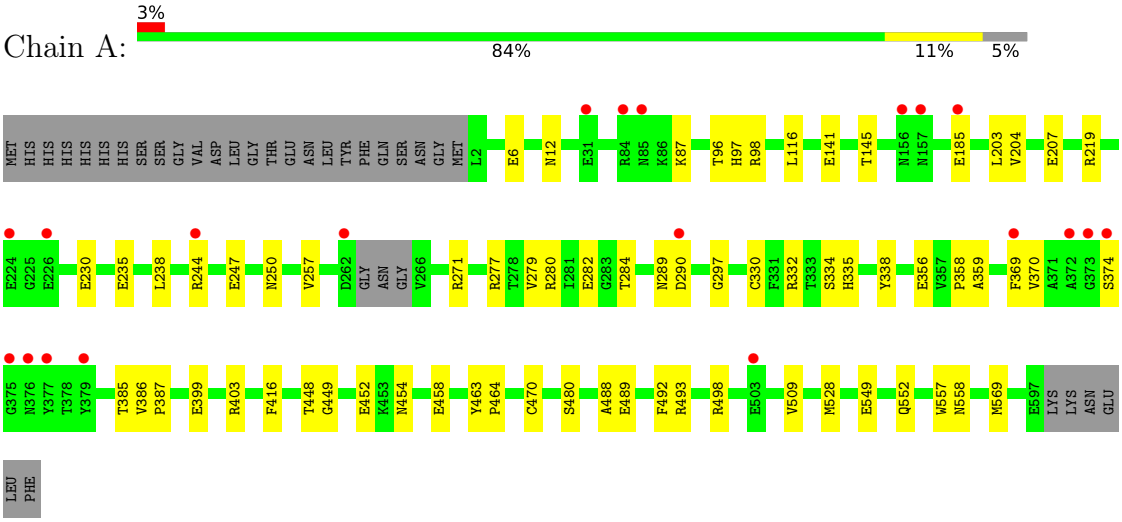
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	58	Total O 58 58	0	0
3	B	64	Total O 64 64	0	0
3	C	72	Total O 72 72	0	0
3	D	59	Total O 59 59	0	0
3	E	59	Total O 59 59	0	0
3	F	66	Total O 66 66	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

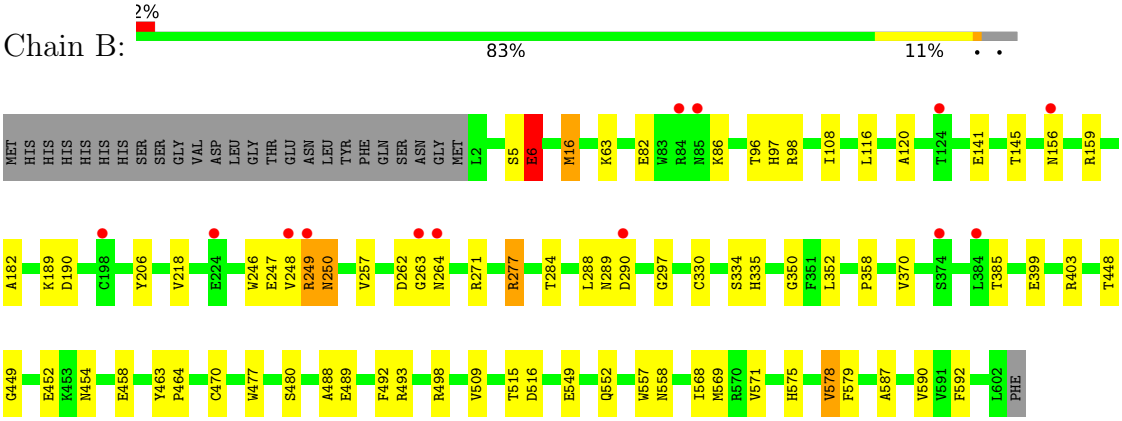
• Molecule 1: Beta-glucuronidase

Chain A:



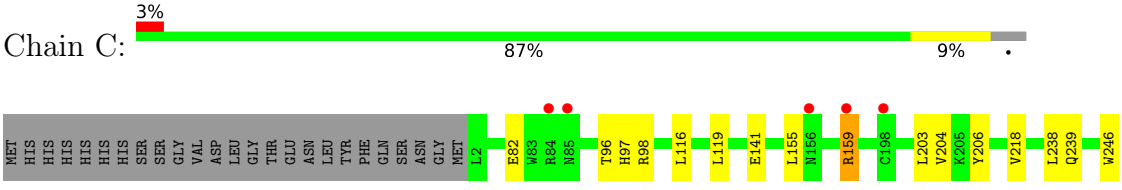
• Molecule 1: Beta-glucuronidase

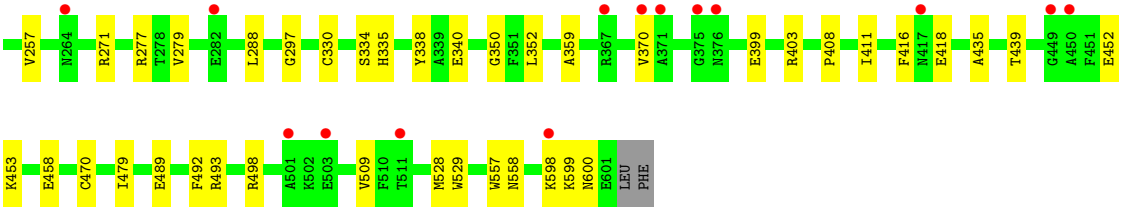
Chain B:



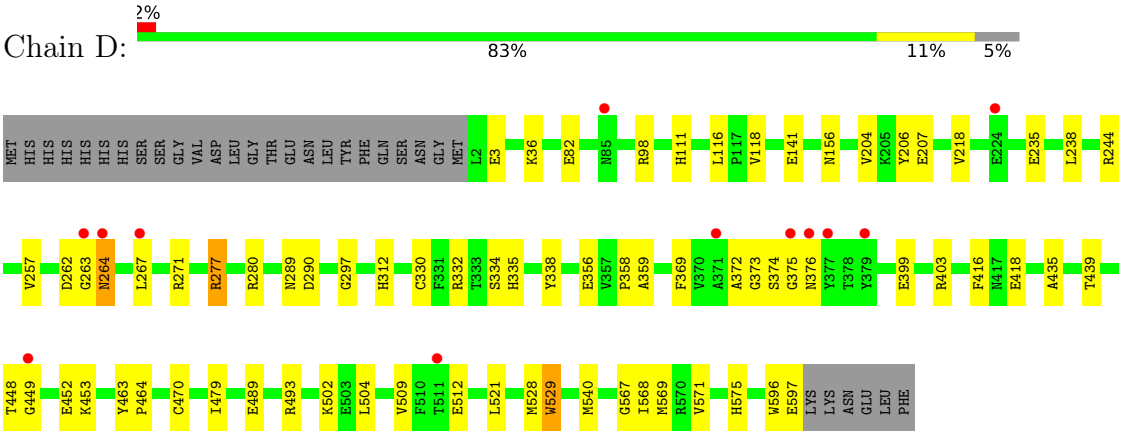
• Molecule 1: Beta-glucuronidase

Chain C:

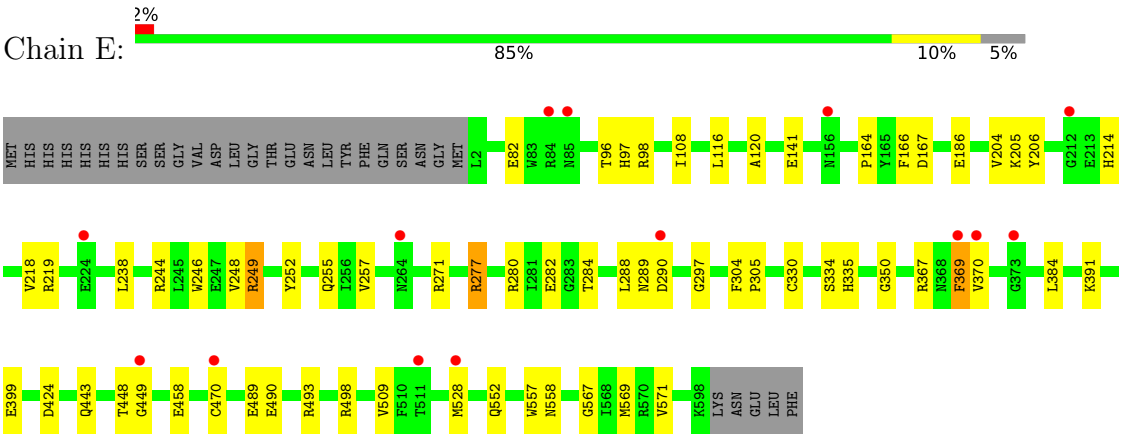




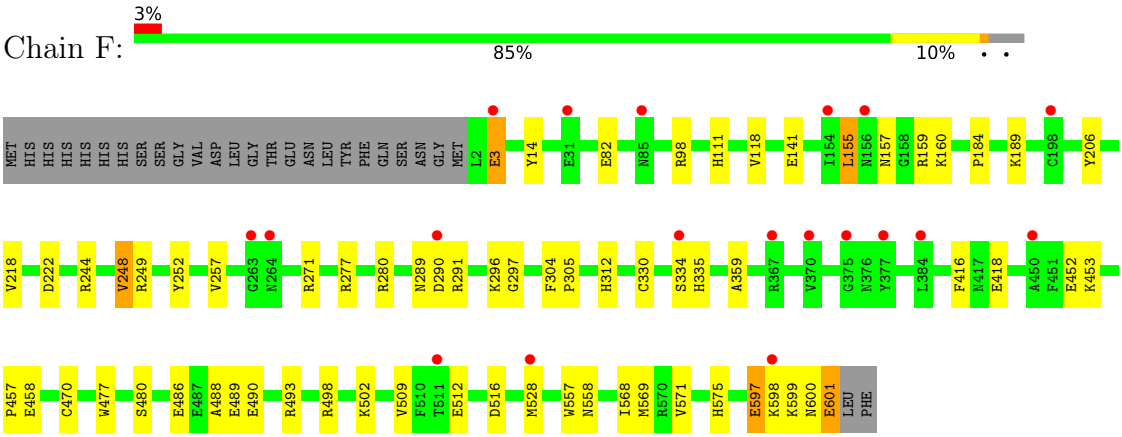
• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.28Å 112.36Å 209.79Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	29.92 – 2.50 29.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.92-2.50) 98.5 (29.92-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.209 0.189 , 0.221	Depositor DCC
R_{free} test set	7140 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29830	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SJ5

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	0.26	0/5003	0.46	0/6784
1	B	0.32	1/5063 (0.0%)	0.47	0/6864
1	C	0.30	0/5055	0.47	0/6853
1	D	0.31	0/5020	0.49	0/6808
1	E	0.27	0/5029	0.47	0/6819
1	F	0.27	0/5055	0.46	0/6853
All	All	0.29	1/30225 (0.0%)	0.47	0/40981

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	GLU	CD-OE1	-5.01	1.20	1.25

There are no bond angle outliers.

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	4864	0	4641	38	0
1	B	4923	0	4703	57	0
1	C	4915	0	4692	31	0
1	D	4880	0	4654	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4889	0	4667	40	0
1	F	4915	0	4692	42	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	11	0	0	1	0
2	E	11	0	0	1	0
2	F	11	0	0	1	0
3	A	58	0	0	2	0
3	B	64	0	0	1	0
3	C	72	0	0	1	0
3	D	59	0	0	1	0
3	E	59	0	0	3	0
3	F	66	0	0	1	0
All	All	29830	0	28049	254	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 4.

All (254) 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:248:VAL:HG23	1:B:288:LEU:HD22	1.37	1.03
1:B:248:VAL:HG23	1:B:288:LEU:CD2	1.98	0.92
1:D:82:GLU:HG2	1:F:82:GLU:HG2	1.51	0.89
1:D:263:GLY:HA3	1:D:264:ASN:HB2	1.57	0.87
1:B:16:MET:HE1	1:B:86:LYS:HE3	1.57	0.86
1:B:248:VAL:CG2	1:B:288:LEU:HD22	2.07	0.84
1:F:600:ASN:ND2	1:F:601:GLU:HG2	1.92	0.83
1:B:16:MET:HE2	1:B:182:ALA:HB3	1.63	0.81
1:B:262:ASP:HB2	1:B:264:ASN:H	1.48	0.79
1:D:374:SER:H	1:D:375:GLY:HA2	1.47	0.78
1:B:16:MET:HE1	1:B:86:LYS:CE	2.15	0.76
1:D:277:ARG:O	1:D:277:ARG:HD3	1.84	0.75
1:B:16:MET:HE1	1:B:86:LYS:CD	2.17	0.75
1:B:98:ARG:NH2	1:B:141:GLU:O	2.21	0.74
1:C:155:LEU:HD12	1:C:159:ARG:HG2	1.68	0.74
1:E:257:VAL:HG22	1:E:271:ARG:HG2	1.67	0.74
1:B:16:MET:CE	1:B:182:ALA:HB3	2.17	0.74
1:F:528:MET:O	3:F:801:HOH:O	2.04	0.74
1:D:257:VAL:HG22	1:D:271:ARG:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ARG:NH1	1:D:290:ASP:OD1	2.20	0.72
1:F:98:ARG:NH2	1:F:141:GLU:O	2.21	0.72
1:D:567:GLY:HA2	1:E:528:MET:SD	2.30	0.72
1:A:528:MET:O	3:A:801:HOH:O	2.08	0.71
1:A:98:ARG:NH2	1:A:141:GLU:O	2.23	0.71
1:D:156:ASN:ND2	1:E:490:GLU:OE1	2.22	0.71
1:E:98:ARG:NH2	1:E:141:GLU:O	2.22	0.70
1:C:98:ARG:NH2	1:C:141:GLU:O	2.26	0.68
1:D:98:ARG:NH2	1:D:141:GLU:O	2.25	0.68
1:D:373:GLY:H	1:D:374:SER:HB3	1.59	0.68
1:B:262:ASP:N	1:B:263:GLY:HA2	2.10	0.66
1:D:263:GLY:HA3	1:D:264:ASN:CB	2.27	0.65
1:E:205:LYS:NZ	3:E:802:HOH:O	2.25	0.65
1:C:277:ARG:HH11	1:C:279:VAL:HG23	1.62	0.65
1:D:277:ARG:HD3	1:D:277:ARG:C	2.17	0.64
1:A:277:ARG:HH11	1:A:279:VAL:HG23	1.62	0.64
1:D:567:GLY:CA	1:E:528:MET:SD	2.85	0.64
1:C:528:MET:O	1:C:529:TRP:HB2	1.98	0.63
1:D:569:MET:HG2	1:E:569:MET:HG2	1.81	0.63
1:A:257:VAL:HG22	1:A:271:ARG:HG2	1.81	0.62
1:F:257:VAL:HG22	1:F:271:ARG:HG2	1.81	0.62
1:A:549:GLU:H	1:A:549:GLU:CD	2.04	0.61
1:D:338:TYR:O	1:D:403:ARG:NH2	2.29	0.61
1:D:528:MET:O	1:D:529:TRP:HB2	2.00	0.61
1:B:289:ASN:O	1:B:290:ASP:HB2	2.01	0.61
1:B:284:THR:O	1:B:552:GLN:HG3	2.01	0.61
1:B:262:ASP:HB2	1:B:264:ASN:N	2.15	0.60
1:C:82:GLU:N	1:C:82:GLU:OE1	2.32	0.60
1:D:489:GLU:OE2	1:D:493:ARG:NH1	2.33	0.60
1:D:571:VAL:HG21	1:E:571:VAL:HG21	1.83	0.60
1:F:3:GLU:HA	1:F:189:LYS:NZ	2.17	0.59
1:D:263:GLY:CA	1:D:264:ASN:HB2	2.29	0.59
1:B:82:GLU:OE1	1:B:82:GLU:N	2.35	0.58
1:D:453:LYS:HD2	1:D:479:ILE:HD11	1.83	0.58
1:D:372:ALA:HB1	1:D:452:GLU:HG3	1.84	0.58
1:B:248:VAL:O	1:B:249:ARG:HB2	2.04	0.58
1:D:528:MET:SD	1:E:567:GLY:HA2	2.43	0.58
1:A:87:LYS:HE2	1:A:185:GLU:OE1	2.04	0.58
1:C:598:LYS:O	1:C:600:ASN:ND2	2.36	0.58
1:A:289:ASN:O	1:A:290:ASP:HB2	2.03	0.57
1:E:82:GLU:OE1	1:E:82:GLU:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLU:CD	1:B:549:GLU:H	2.07	0.57
1:B:480:SER:HB2	1:B:488:ALA:HB2	1.86	0.57
1:D:374:SER:H	1:D:375:GLY:CA	2.16	0.57
1:E:289:ASN:O	1:E:290:ASP:HB2	2.03	0.57
1:B:248:VAL:HG22	1:B:352:LEU:HD21	1.87	0.56
1:B:257:VAL:HG22	1:B:271:ARG:HG2	1.87	0.56
1:C:338:TYR:O	1:C:403:ARG:NH2	2.28	0.56
1:A:338:TYR:O	1:A:403:ARG:NH2	2.28	0.56
1:C:599:LYS:NZ	3:C:802:HOH:O	2.39	0.56
1:B:452:GLU:HG3	1:B:454:ASN:H	1.71	0.56
1:F:157:ASN:HD21	1:F:159:ARG:HD3	1.71	0.56
1:A:370:VAL:HG11	1:A:569:MET:CE	2.37	0.55
1:A:230:GLU:HG2	1:F:291:ARG:HD2	1.88	0.55
1:E:248:VAL:O	1:E:249:ARG:HB2	2.07	0.55
1:E:219:ARG:NH1	3:E:804:HOH:O	2.37	0.55
1:F:480:SER:HB2	1:F:488:ALA:HB2	1.89	0.54
1:F:280:ARG:NH1	1:F:290:ASP:OD1	2.41	0.53
1:C:340:GLU:HG3	1:C:403:ARG:HH21	1.73	0.53
1:A:116:LEU:HD13	1:A:399:GLU:HB2	1.90	0.53
1:A:359:ALA:HB3	1:A:416:PHE:HA	1.91	0.53
1:B:571:VAL:O	1:B:575:HIS:NE2	2.42	0.53
1:C:257:VAL:HG22	1:C:271:ARG:HG2	1.91	0.52
1:E:280:ARG:NH1	1:E:290:ASP:OD1	2.39	0.52
1:D:502:LYS:HB3	1:D:504:LEU:HD13	1.92	0.52
1:B:16:MET:CE	1:B:86:LYS:CD	2.86	0.52
1:D:596:TRP:O	1:D:597:GLU:HB2	2.09	0.52
1:B:16:MET:HB2	1:B:182:ALA:HB3	1.92	0.52
1:B:5:SER:OG	1:B:189:LYS:O	2.22	0.52
1:B:6:GLU:HG2	1:B:403:ARG:HB2	1.91	0.51
1:D:528:MET:O	1:D:529:TRP:CB	2.58	0.51
1:B:63:LYS:HG3	1:B:159:ARG:HH12	1.75	0.51
1:B:249:ARG:O	1:B:250:ASN:HB2	2.11	0.51
1:D:116:LEU:HD13	1:D:399:GLU:HB2	1.92	0.51
1:C:297:GLY:HA3	1:C:330:CYS:O	2.11	0.51
1:A:207:GLU:HG2	1:A:235:GLU:HG2	1.94	0.50
1:D:262:ASP:HB3	1:D:267:LEU:HD11	1.92	0.50
1:C:203:LEU:HD22	1:C:239:GLN:HG2	1.94	0.50
1:D:568:ILE:HG13	1:D:569:MET:HG3	1.93	0.50
1:F:296:LYS:NZ	1:F:599:LYS:O	2.38	0.50
1:D:418:GLU:HG2	1:D:452:GLU:HB2	1.93	0.49
1:C:204:VAL:HB	1:C:238:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD21	1:F:244:ARG:HD3	1.94	0.49
1:B:458:GLU:OE2	1:B:498:ARG:HD2	2.12	0.49
1:D:289:ASN:O	1:D:290:ASP:HB2	2.11	0.49
1:B:568:ILE:HG13	1:B:569:MET:HG3	1.95	0.49
1:A:6:GLU:HG2	1:A:403:ARG:HB2	1.95	0.49
1:A:480:SER:HB2	1:A:488:ALA:HB2	1.93	0.49
1:D:334:SER:HA	1:D:335:HIS:HA	1.68	0.48
1:E:186:GLU:OE1	1:E:214:HIS:ND1	2.37	0.48
1:A:145:THR:HG22	1:A:385:THR:HB	1.95	0.48
1:B:246:TRP:CZ2	1:B:350:GLY:HA2	2.49	0.48
1:D:374:SER:N	1:D:375:GLY:HA2	2.17	0.48
1:E:282:GLU:OE1	3:E:801:HOH:O	2.20	0.48
1:C:246:TRP:CZ2	1:C:350:GLY:HA2	2.48	0.48
1:B:16:MET:CE	1:B:182:ALA:CB	2.91	0.47
1:B:247:GLU:HB3	1:B:250:ASN:HB3	1.96	0.47
1:E:297:GLY:HA3	1:E:330:CYS:O	2.15	0.47
1:C:96:THR:HA	1:C:97:HIS:HA	1.69	0.47
1:C:277:ARG:HG3	1:C:288:LEU:HD11	1.96	0.47
1:C:489:GLU:O	1:C:493:ARG:HG3	2.15	0.47
1:D:204:VAL:HB	1:D:238:LEU:HB2	1.97	0.47
1:D:332:ARG:NH1	1:D:356:GLU:OE2	2.46	0.47
1:F:418:GLU:HG2	1:F:452:GLU:HB2	1.97	0.47
1:A:297:GLY:HA3	1:A:330:CYS:O	2.14	0.47
1:F:477:TRP:CZ2	1:F:516:ASP:HB2	2.50	0.47
1:F:141:GLU:OE1	1:F:160:LYS:NZ	2.45	0.47
1:F:489:GLU:O	1:F:493:ARG:HG3	2.14	0.47
1:C:458:GLU:OE2	1:C:498:ARG:HD2	2.14	0.46
1:D:369:PHE:HE1	1:D:569:MET:HE2	1.80	0.46
1:D:448:THR:OG1	1:D:449:GLY:N	2.47	0.46
1:F:248:VAL:O	1:F:249:ARG:HB2	2.16	0.46
1:A:96:THR:HA	1:A:97:HIS:HA	1.71	0.46
1:A:219:ARG:NH2	1:F:600:ASN:HD21	2.14	0.46
1:C:557:TRP:HA	1:C:558:ASN:HA	1.70	0.46
1:E:489:GLU:O	1:E:493:ARG:HG3	2.14	0.46
1:E:448:THR:OG1	1:E:449:GLY:N	2.48	0.46
1:E:369:PHE:N	1:E:369:PHE:CD1	2.81	0.46
1:E:82:GLU:H	1:E:82:GLU:CD	2.14	0.46
1:B:448:THR:OG1	1:B:449:GLY:N	2.48	0.46
1:D:493:ARG:NH2	3:D:804:HOH:O	2.48	0.46
1:E:458:GLU:OE2	1:E:498:ARG:HD2	2.15	0.46
1:E:334:SER:HA	1:E:335:HIS:HA	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:THR:OG1	1:A:449:GLY:N	2.48	0.46
1:D:435:ALA:O	1:D:439:THR:HG23	2.16	0.46
1:A:277:ARG:NH1	1:A:279:VAL:HG23	2.31	0.45
1:B:16:MET:HE2	1:B:16:MET:HB2	1.70	0.45
1:E:116:LEU:HD13	1:E:399:GLU:HB2	1.98	0.45
1:B:578:VAL:HG12	1:B:579:PHE:CD2	2.50	0.45
1:E:96:THR:HA	1:E:97:HIS:HA	1.71	0.45
1:F:206:TYR:CE1	1:F:218:VAL:HG21	2.50	0.45
1:A:458:GLU:OE2	1:A:498:ARG:HD2	2.17	0.45
1:F:297:GLY:HA3	1:F:330:CYS:O	2.17	0.45
1:A:369:PHE:CD1	1:A:370:VAL:HG13	2.52	0.45
1:B:477:TRP:CZ2	1:B:516:ASP:HB2	2.52	0.45
1:C:119:LEU:HA	1:C:119:LEU:HD23	1.77	0.45
1:C:453:LYS:HD2	1:C:479:ILE:HD11	1.97	0.45
1:F:571:VAL:O	1:F:575:HIS:NE2	2.49	0.45
1:C:277:ARG:HE	1:C:408:PRO:HA	1.82	0.45
1:C:418:GLU:HG2	1:C:452:GLU:HB2	1.99	0.45
1:D:312:HIS:CD2	1:F:312:HIS:HD2	2.35	0.45
1:A:386:VAL:HG22	1:A:387:PRO:HD3	1.97	0.45
1:B:470:CYS:HA	1:B:509:VAL:O	2.18	0.44
1:C:352:LEU:HB3	1:C:411:ILE:HD13	1.97	0.44
1:C:334:SER:HA	1:C:335:HIS:HA	1.67	0.44
1:D:453:LYS:HD2	1:D:479:ILE:CD1	2.47	0.44
1:E:204:VAL:HB	1:E:238:LEU:HB2	2.00	0.44
1:E:167:ASP:OD2	2:E:701:SJ5:O4	2.35	0.44
1:B:96:THR:HA	1:B:97:HIS:HA	1.66	0.44
1:F:155:LEU:HD23	1:F:159:ARG:HG2	2.00	0.44
1:F:457:PRO:O	1:F:502:LYS:NZ	2.47	0.44
1:A:470:CYS:HA	1:A:509:VAL:O	2.17	0.44
1:A:204:VAL:HB	1:A:238:LEU:HB2	2.00	0.44
1:A:284:THR:O	1:A:552:GLN:HG3	2.18	0.44
1:D:528:MET:O	1:D:529:TRP:CD1	2.71	0.44
1:F:334:SER:HA	1:F:335:HIS:HA	1.63	0.44
1:B:16:MET:HE1	1:B:86:LYS:HD3	1.98	0.44
1:C:116:LEU:HD13	1:C:399:GLU:HB2	1.99	0.44
1:D:207:GLU:HG2	1:D:235:GLU:HG2	2.00	0.44
1:B:116:LEU:HD13	1:B:399:GLU:HB2	2.00	0.43
1:B:334:SER:HA	1:B:335:HIS:HA	1.67	0.43
1:B:489:GLU:O	1:B:493:ARG:HG3	2.18	0.43
1:B:206:TYR:CE1	1:B:218:VAL:HG21	2.53	0.43
1:B:477:TRP:HB2	1:B:515:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:TRP:HA	1:B:558:ASN:HA	1.72	0.43
1:C:435:ALA:O	1:C:439:THR:HG23	2.18	0.43
1:A:334:SER:HA	1:A:335:HIS:HA	1.60	0.43
1:A:452:GLU:HG3	1:A:454:ASN:H	1.82	0.43
1:D:3:GLU:O	1:D:3:GLU:HG2	2.18	0.43
1:A:557:TRP:HA	1:A:558:ASN:HA	1.72	0.43
1:C:359:ALA:HB3	1:C:416:PHE:HA	2.00	0.43
1:D:297:GLY:HA3	1:D:330:CYS:O	2.18	0.43
1:A:247:GLU:HB2	1:A:250:ASN:HB3	2.00	0.43
1:F:568:ILE:HG13	1:F:569:MET:HG3	2.00	0.43
1:B:297:GLY:HA3	1:B:330:CYS:O	2.19	0.43
1:E:277:ARG:HG3	1:E:288:LEU:HD11	2.01	0.43
1:B:190:ASP:OD1	3:B:801:HOH:O	2.22	0.42
1:D:359:ALA:HB3	1:D:416:PHE:HA	2.00	0.42
1:B:145:THR:HG22	1:B:385:THR:HB	2.00	0.42
1:B:463:TYR:CG	1:B:464:PRO:HD3	2.54	0.42
1:C:206:TYR:CE1	1:C:218:VAL:HG21	2.53	0.42
1:F:222:ASP:HB2	1:F:252:TYR:OH	2.19	0.42
1:F:359:ALA:HB3	1:F:416:PHE:HA	2.02	0.42
1:B:578:VAL:HG21	1:B:592:PHE:CE2	2.53	0.42
1:A:332:ARG:NH1	1:A:356:GLU:OE2	2.52	0.42
1:A:489:GLU:O	1:A:493:ARG:HG3	2.18	0.42
1:D:373:GLY:N	1:D:374:SER:HB3	2.32	0.42
1:B:587:ALA:O	1:B:590:VAL:HG22	2.19	0.42
1:E:164:PRO:HB3	1:E:166:PHE:CZ	2.55	0.42
1:E:284:THR:O	1:E:552:GLN:HG3	2.20	0.42
1:F:289:ASN:O	1:F:290:ASP:HB2	2.20	0.42
1:C:470:CYS:HA	1:C:509:VAL:O	2.19	0.42
1:D:36:LYS:HB3	1:D:36:LYS:HE2	1.96	0.42
1:F:486:GLU:O	1:F:490:GLU:HG2	2.19	0.42
1:C:334:SER:HB3	1:C:335:HIS:CE1	2.54	0.42
1:D:335:HIS:O	1:D:358:PRO:HA	2.20	0.42
1:F:557:TRP:HA	1:F:558:ASN:HA	1.71	0.42
1:F:600:ASN:C	1:F:601:GLU:CG	2.88	0.42
1:F:600:ASN:CG	1:F:601:GLU:N	2.73	0.42
1:E:244:ARG:HB3	1:E:252:TYR:CD2	2.55	0.42
1:A:335:HIS:O	1:A:358:PRO:HA	2.20	0.42
1:E:557:TRP:HA	1:E:558:ASN:HA	1.72	0.42
1:E:470:CYS:HA	1:E:509:VAL:O	2.20	0.41
1:B:16:MET:HE3	1:B:182:ALA:HB3	1.98	0.41
1:D:512:GLU:OE1	2:D:701:SJ5:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:TYR:CE1	1:D:218:VAL:HG21	2.55	0.41
1:B:335:HIS:O	1:B:358:PRO:HA	2.20	0.41
1:E:304:PHE:CG	1:E:305:PRO:HD2	2.56	0.41
1:A:463:TYR:CG	1:A:464:PRO:HD3	2.56	0.41
1:B:82:GLU:H	1:B:82:GLU:CD	2.15	0.41
1:D:82:GLU:HG2	1:F:82:GLU:CG	2.38	0.41
1:F:111:HIS:CG	1:F:118:VAL:HG22	2.55	0.41
1:A:12:ASN:HB2	3:A:843:HOH:O	2.21	0.41
1:D:528:MET:O	1:D:529:TRP:HD1	2.04	0.41
1:E:367:ARG:O	1:E:367:ARG:HG3	2.21	0.41
1:F:597:GLU:HG2	1:F:598:LYS:HG3	2.03	0.41
1:B:108:ILE:HG21	1:B:120:ALA:HB1	2.03	0.41
1:D:418:GLU:CG	1:D:452:GLU:HB2	2.51	0.41
1:E:108:ILE:HG21	1:E:120:ALA:HB1	2.03	0.41
1:F:14:TYR:O	1:F:184:PRO:HD3	2.21	0.41
1:A:280:ARG:NH1	1:A:282:GLU:OE2	2.53	0.40
1:E:246:TRP:CZ2	1:E:350:GLY:HA2	2.56	0.40
1:E:255:GLN:OE1	1:E:271:ARG:HD3	2.20	0.40
1:F:304:PHE:CG	1:F:305:PRO:HD2	2.56	0.40
1:E:206:TYR:CE1	1:E:218:VAL:HG21	2.56	0.40
1:D:463:TYR:CG	1:D:464:PRO:HD3	2.56	0.40
1:D:470:CYS:HA	1:D:509:VAL:O	2.21	0.40
1:E:277:ARG:NH2	1:E:443:GLN:OE1	2.51	0.40
1:F:470:CYS:HA	1:F:509:VAL:O	2.21	0.40
1:F:512:GLU:OE1	2:F:701:SJ5:N	2.54	0.40
1:B:277:ARG:HG3	1:B:288:LEU:HD11	2.04	0.40
1:D:111:HIS:CG	1:D:118:VAL:HG22	2.57	0.40
1:F:452:GLU:HG2	1:F:453:LYS:H	1.86	0.40
1:D:571:VAL:O	1:D:575:HIS:NE2	2.55	0.40
1:F:458:GLU:OE2	1:F:498:ARG:HD2	2.20	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	589/627 (94%)	571 (97%)	17 (3%)	1 (0%)	47 68
1	B	599/627 (96%)	577 (96%)	20 (3%)	2 (0%)	41 61
1	C	598/627 (95%)	578 (97%)	20 (3%)	0	100 100
1	D	594/627 (95%)	570 (96%)	21 (4%)	3 (0%)	29 48
1	E	595/627 (95%)	575 (97%)	19 (3%)	1 (0%)	47 68
1	F	598/627 (95%)	578 (97%)	20 (3%)	0	100 100
All	All	3573/3762 (95%)	3449 (96%)	117 (3%)	7 (0%)	47 68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER
1	D	264	ASN
1	D	529	TRP
1	B	249	ARG
1	B	250	ASN
1	D	376	ASN
1	E	249	ARG

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	517/546 (95%)	515 (100%)	2 (0%)	91 97
1	B	523/546 (96%)	516 (99%)	7 (1%)	69 87
1	C	522/546 (96%)	519 (99%)	3 (1%)	86 95
1	D	518/546 (95%)	514 (99%)	4 (1%)	81 93
1	E	519/546 (95%)	513 (99%)	6 (1%)	71 88
1	F	522/546 (96%)	516 (99%)	6 (1%)	73 89
All	All	3121/3276 (95%)	3093 (99%)	28 (1%)	78 92

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	ARG
1	A	492	PHE
1	B	6	GLU
1	B	16	MET
1	B	156	ASN
1	B	277	ARG
1	B	370	VAL
1	B	492	PHE
1	B	578	VAL
1	C	159	ARG
1	C	370	VAL
1	C	492	PHE
1	D	244	ARG
1	D	277	ARG
1	D	521	LEU
1	D	540	MET
1	E	277	ARG
1	E	369	PHE
1	E	370	VAL
1	E	384	LEU
1	E	391	LYS
1	E	424	ASP
1	F	3	GLU
1	F	155	LEU
1	F	248	VAL
1	F	277	ARG
1	F	597	GLU
1	F	601	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	F	600	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SJ5	E	701	-	11,11,11	0.62	0	11,15,15	3.16	3 (27%)
2	SJ5	F	701	-	11,11,11	0.58	0	11,15,15	2.80	3 (27%)
2	SJ5	C	701	-	11,11,11	0.57	0	11,15,15	2.94	3 (27%)
2	SJ5	B	701	-	11,11,11	0.59	0	11,15,15	2.92	3 (27%)
2	SJ5	A	701	-	11,11,11	0.61	0	11,15,15	3.45	3 (27%)
2	SJ5	D	701	-	11,11,11	0.63	0	11,15,15	2.94	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SJ5	E	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	F	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	C	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	B	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	A	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	D	701	-	-	2/4/18/18	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	SJ5	C7-N-C2	10.94	123.71	111.70
2	E	701	SJ5	C7-N-C2	9.89	122.55	111.70
2	C	701	SJ5	C7-N-C2	9.16	121.76	111.70
2	D	701	SJ5	C7-N-C2	9.07	121.65	111.70
2	B	701	SJ5	C7-N-C2	9.06	121.65	111.70
2	F	701	SJ5	C7-N-C2	8.54	121.08	111.70
2	D	701	SJ5	O62-C6-C5	2.36	120.52	114.03
2	F	701	SJ5	O62-C6-C5	2.32	120.40	114.03
2	B	701	SJ5	O62-C6-C5	2.31	120.40	114.03
2	B	701	SJ5	O62-C6-O61	-2.24	119.01	124.09
2	A	701	SJ5	O62-C6-C5	2.23	120.17	114.03
2	D	701	SJ5	O62-C6-O61	-2.23	119.02	124.09
2	E	701	SJ5	O62-C6-O61	-2.22	119.06	124.09
2	C	701	SJ5	O62-C6-C5	2.19	120.07	114.03
2	C	701	SJ5	O62-C6-O61	-2.19	119.11	124.09
2	E	701	SJ5	O62-C6-C5	2.19	120.05	114.03
2	A	701	SJ5	O62-C6-O61	-2.16	119.17	124.09
2	F	701	SJ5	O62-C6-O61	-2.14	119.23	124.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	SJ5	C4-C5-C6-O62
2	B	701	SJ5	C4-C5-C6-O61
2	C	701	SJ5	C4-C5-C6-O61
2	A	701	SJ5	C4-C5-C6-O61
2	D	701	SJ5	C4-C5-C6-O61
2	E	701	SJ5	C4-C5-C6-O62
2	F	701	SJ5	C4-C5-C6-O62
2	F	701	SJ5	C4-C5-C6-O61
2	A	701	SJ5	C4-C5-C6-O62
2	C	701	SJ5	C4-C5-C6-O62
2	D	701	SJ5	C4-C5-C6-O62
2	E	701	SJ5	C4-C5-C6-O61

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	SJ5	1	0
2	F	701	SJ5	1	0
2	D	701	SJ5	1	0

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, 95^{th} 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	593/627 (94%)	-0.16	20 (3%)	45	48	27, 39, 63, 100	0
1	B	601/627 (95%)	-0.13	13 (2%)	62	65	27, 40, 62, 95	0
1	C	600/627 (95%)	-0.16	19 (3%)	47	51	27, 41, 64, 92	0
1	D	596/627 (95%)	-0.22	12 (2%)	65	68	26, 38, 63, 100	0
1	E	597/627 (95%)	-0.19	14 (2%)	60	63	28, 39, 65, 95	0
1	F	600/627 (95%)	-0.17	19 (3%)	47	51	27, 40, 62, 93	0
All	All	3587/3762 (95%)	-0.17	97 (2%)	54	58	26, 39, 64, 100	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ASN	4.2
1	E	369	PHE	4.0
1	D	264	ASN	4.0
1	F	375	GLY	4.0
1	E	290	ASP	3.9
1	A	373	GLY	3.9
1	E	156	ASN	3.9
1	F	264	ASN	3.8
1	D	511	THR	3.8
1	A	374	SER	3.7
1	B	249	ARG	3.6
1	E	264	ASN	3.5
1	A	379	TYR	3.5
1	F	450	ALA	3.5
1	C	264	ASN	3.5
1	A	369	PHE	3.4
1	D	371	ALA	3.4
1	A	375	GLY	3.4
1	E	224	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	185	GLU	3.4
1	E	370	VAL	3.3
1	C	156	ASN	3.3
1	D	376	ASN	3.3
1	C	159	ARG	3.2
1	E	528	MET	3.1
1	B	198	CYS	3.1
1	C	375	GLY	3.1
1	B	224	GLU	3.0
1	D	379	TYR	3.0
1	F	528	MET	3.0
1	F	367	ARG	3.0
1	F	511	THR	2.9
1	C	84	ARG	2.9
1	B	290	ASP	2.9
1	C	198	CYS	2.8
1	E	85	ASN	2.7
1	C	503	GLU	2.7
1	F	370	VAL	2.7
1	C	85	ASN	2.7
1	C	282	GLU	2.7
1	C	598	LYS	2.7
1	B	384	LEU	2.7
1	F	85	ASN	2.6
1	B	124	THR	2.6
1	C	501	ALA	2.5
1	A	290	ASP	2.5
1	F	384	LEU	2.5
1	A	156	ASN	2.5
1	C	376	ASN	2.5
1	E	84	ARG	2.5
1	D	375	GLY	2.5
1	D	224	GLU	2.5
1	B	156	ASN	2.4
1	D	85	ASN	2.4
1	C	370	VAL	2.4
1	A	376	ASN	2.4
1	C	417	ASN	2.4
1	B	374	SER	2.4
1	A	226	GLU	2.4
1	F	290	ASP	2.4
1	A	244	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	377	TYR	2.4
1	A	224	GLU	2.3
1	C	449	GLY	2.3
1	B	84	ARG	2.3
1	C	367	ARG	2.3
1	E	511	THR	2.3
1	A	262	ASP	2.3
1	F	3	GLU	2.3
1	D	263	GLY	2.3
1	E	470	CYS	2.3
1	A	85	ASN	2.3
1	B	85	ASN	2.2
1	F	263	GLY	2.2
1	F	156	ASN	2.2
1	E	373	GLY	2.2
1	E	449	GLY	2.2
1	F	154	ILE	2.2
1	E	212	GLY	2.2
1	A	84	ARG	2.2
1	D	267	LEU	2.1
1	C	511	THR	2.1
1	F	598	LYS	2.1
1	A	157	ASN	2.1
1	A	372	ALA	2.1
1	B	263	GLY	2.1
1	C	371	ALA	2.1
1	F	377	TYR	2.1
1	D	377	TYR	2.1
1	A	31	GLU	2.1
1	F	198	CYS	2.1
1	A	503	GLU	2.0
1	F	334	SER	2.0
1	C	450	ALA	2.0
1	B	248	VAL	2.0
1	D	449	GLY	2.0
1	F	31	GLU	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 monosaccharides 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, 95^{th} 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SJ5	B	701	11/11	0.95	0.17	34,38,50,54	0
2	SJ5	C	701	11/11	0.95	0.17	31,35,38,40	0
2	SJ5	E	701	11/11	0.96	0.14	32,34,38,43	0
2	SJ5	F	701	11/11	0.96	0.24	35,39,42,43	0
2	SJ5	A	701	11/11	0.97	0.12	31,37,40,43	0
2	SJ5	D	701	11/11	0.97	0.19	35,37,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.