



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:13 PM EDT

PDB ID : 8J53 / pdb\_00008j53  
Title : Crystal structure of Bacteroides salyersiae GH31 alpha-galactosidase  
Authors : Ikegaya, M.; Miyazaki, T.  
Deposited on : 2023-04-21  
Resolution : 3.50 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](mailto: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>.

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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

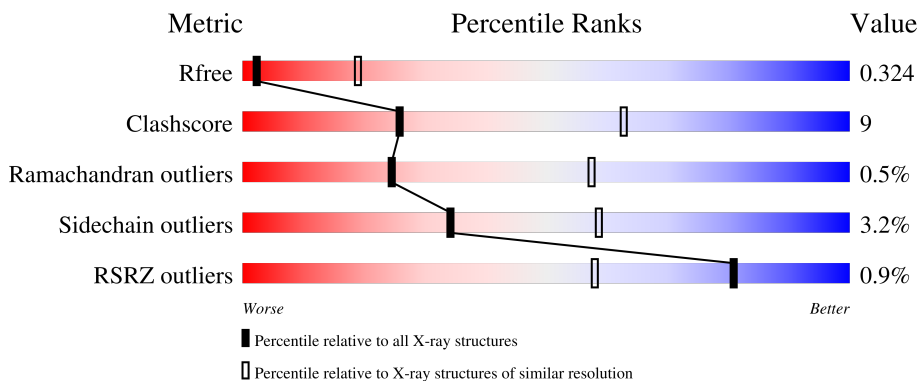
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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  $\geq 3$ , 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	532	 71% 23% • 5%
1	B	532	 75% 19% • 5%
1	C	532	 72% 22% • 5%
1	D	532	 73% 21% • •
1	E	532	 73% 20% • •

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 40710 atoms, of which 20099 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 GH31 alpha-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	507	8136	2654	4019	686	748	29	96	0	0
1	B	503	8064	2632	3980	681	742	29	96	0	0
1	C	508	8150	2658	4025	688	750	29	96	0	0
1	D	510	8178	2666	4038	691	754	29	97	0	0
1	E	511	8182	2668	4037	692	755	30	100	0	0

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7J4XIY8
A	2	GLY	-	expression tag	UNP A0A7J4XIY8
A	3	SER	-	expression tag	UNP A0A7J4XIY8
A	4	SER	-	expression tag	UNP A0A7J4XIY8
A	5	HIS	-	expression tag	UNP A0A7J4XIY8
A	6	HIS	-	expression tag	UNP A0A7J4XIY8
A	7	HIS	-	expression tag	UNP A0A7J4XIY8
A	8	HIS	-	expression tag	UNP A0A7J4XIY8
A	9	HIS	-	expression tag	UNP A0A7J4XIY8
A	10	HIS	-	expression tag	UNP A0A7J4XIY8
A	11	SER	-	expression tag	UNP A0A7J4XIY8
A	12	SER	-	expression tag	UNP A0A7J4XIY8
A	13	GLY	-	expression tag	UNP A0A7J4XIY8
A	14	LEU	-	expression tag	UNP A0A7J4XIY8
A	15	VAL	-	expression tag	UNP A0A7J4XIY8
A	16	PRO	-	expression tag	UNP A0A7J4XIY8
A	17	ARG	-	expression tag	UNP A0A7J4XIY8
A	18	GLY	-	expression tag	UNP A0A7J4XIY8
A	19	SER	-	expression tag	UNP A0A7J4XIY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	HIS	-	expression tag	UNP A0A7J4XIY8
A	21	MET	-	expression tag	UNP A0A7J4XIY8
A	22	ALA	-	expression tag	UNP A0A7J4XIY8
A	23	SER	-	expression tag	UNP A0A7J4XIY8
A	24	GLN	-	expression tag	UNP A0A7J4XIY8
A	25	ASN	-	expression tag	UNP A0A7J4XIY8
A	26	VAL	-	expression tag	UNP A0A7J4XIY8
A	27	PHE	-	expression tag	UNP A0A7J4XIY8
A	28	THR	-	expression tag	UNP A0A7J4XIY8
B	1	MET	-	initiating methionine	UNP A0A7J4XIY8
B	2	GLY	-	expression tag	UNP A0A7J4XIY8
B	3	SER	-	expression tag	UNP A0A7J4XIY8
B	4	SER	-	expression tag	UNP A0A7J4XIY8
B	5	HIS	-	expression tag	UNP A0A7J4XIY8
B	6	HIS	-	expression tag	UNP A0A7J4XIY8
B	7	HIS	-	expression tag	UNP A0A7J4XIY8
B	8	HIS	-	expression tag	UNP A0A7J4XIY8
B	9	HIS	-	expression tag	UNP A0A7J4XIY8
B	10	HIS	-	expression tag	UNP A0A7J4XIY8
B	11	SER	-	expression tag	UNP A0A7J4XIY8
B	12	SER	-	expression tag	UNP A0A7J4XIY8
B	13	GLY	-	expression tag	UNP A0A7J4XIY8
B	14	LEU	-	expression tag	UNP A0A7J4XIY8
B	15	VAL	-	expression tag	UNP A0A7J4XIY8
B	16	PRO	-	expression tag	UNP A0A7J4XIY8
B	17	ARG	-	expression tag	UNP A0A7J4XIY8
B	18	GLY	-	expression tag	UNP A0A7J4XIY8
B	19	SER	-	expression tag	UNP A0A7J4XIY8
B	20	HIS	-	expression tag	UNP A0A7J4XIY8
B	21	MET	-	expression tag	UNP A0A7J4XIY8
B	22	ALA	-	expression tag	UNP A0A7J4XIY8
B	23	SER	-	expression tag	UNP A0A7J4XIY8
B	24	GLN	-	expression tag	UNP A0A7J4XIY8
B	25	ASN	-	expression tag	UNP A0A7J4XIY8
B	26	VAL	-	expression tag	UNP A0A7J4XIY8
B	27	PHE	-	expression tag	UNP A0A7J4XIY8
B	28	THR	-	expression tag	UNP A0A7J4XIY8
C	1	MET	-	initiating methionine	UNP A0A7J4XIY8
C	2	GLY	-	expression tag	UNP A0A7J4XIY8
C	3	SER	-	expression tag	UNP A0A7J4XIY8
C	4	SER	-	expression tag	UNP A0A7J4XIY8
C	5	HIS	-	expression tag	UNP A0A7J4XIY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP A0A7J4XIY8
C	7	HIS	-	expression tag	UNP A0A7J4XIY8
C	8	HIS	-	expression tag	UNP A0A7J4XIY8
C	9	HIS	-	expression tag	UNP A0A7J4XIY8
C	10	HIS	-	expression tag	UNP A0A7J4XIY8
C	11	SER	-	expression tag	UNP A0A7J4XIY8
C	12	SER	-	expression tag	UNP A0A7J4XIY8
C	13	GLY	-	expression tag	UNP A0A7J4XIY8
C	14	LEU	-	expression tag	UNP A0A7J4XIY8
C	15	VAL	-	expression tag	UNP A0A7J4XIY8
C	16	PRO	-	expression tag	UNP A0A7J4XIY8
C	17	ARG	-	expression tag	UNP A0A7J4XIY8
C	18	GLY	-	expression tag	UNP A0A7J4XIY8
C	19	SER	-	expression tag	UNP A0A7J4XIY8
C	20	HIS	-	expression tag	UNP A0A7J4XIY8
C	21	MET	-	expression tag	UNP A0A7J4XIY8
C	22	ALA	-	expression tag	UNP A0A7J4XIY8
C	23	SER	-	expression tag	UNP A0A7J4XIY8
C	24	GLN	-	expression tag	UNP A0A7J4XIY8
C	25	ASN	-	expression tag	UNP A0A7J4XIY8
C	26	VAL	-	expression tag	UNP A0A7J4XIY8
C	27	PHE	-	expression tag	UNP A0A7J4XIY8
C	28	THR	-	expression tag	UNP A0A7J4XIY8
D	1	MET	-	initiating methionine	UNP A0A7J4XIY8
D	2	GLY	-	expression tag	UNP A0A7J4XIY8
D	3	SER	-	expression tag	UNP A0A7J4XIY8
D	4	SER	-	expression tag	UNP A0A7J4XIY8
D	5	HIS	-	expression tag	UNP A0A7J4XIY8
D	6	HIS	-	expression tag	UNP A0A7J4XIY8
D	7	HIS	-	expression tag	UNP A0A7J4XIY8
D	8	HIS	-	expression tag	UNP A0A7J4XIY8
D	9	HIS	-	expression tag	UNP A0A7J4XIY8
D	10	HIS	-	expression tag	UNP A0A7J4XIY8
D	11	SER	-	expression tag	UNP A0A7J4XIY8
D	12	SER	-	expression tag	UNP A0A7J4XIY8
D	13	GLY	-	expression tag	UNP A0A7J4XIY8
D	14	LEU	-	expression tag	UNP A0A7J4XIY8
D	15	VAL	-	expression tag	UNP A0A7J4XIY8
D	16	PRO	-	expression tag	UNP A0A7J4XIY8
D	17	ARG	-	expression tag	UNP A0A7J4XIY8
D	18	GLY	-	expression tag	UNP A0A7J4XIY8
D	19	SER	-	expression tag	UNP A0A7J4XIY8

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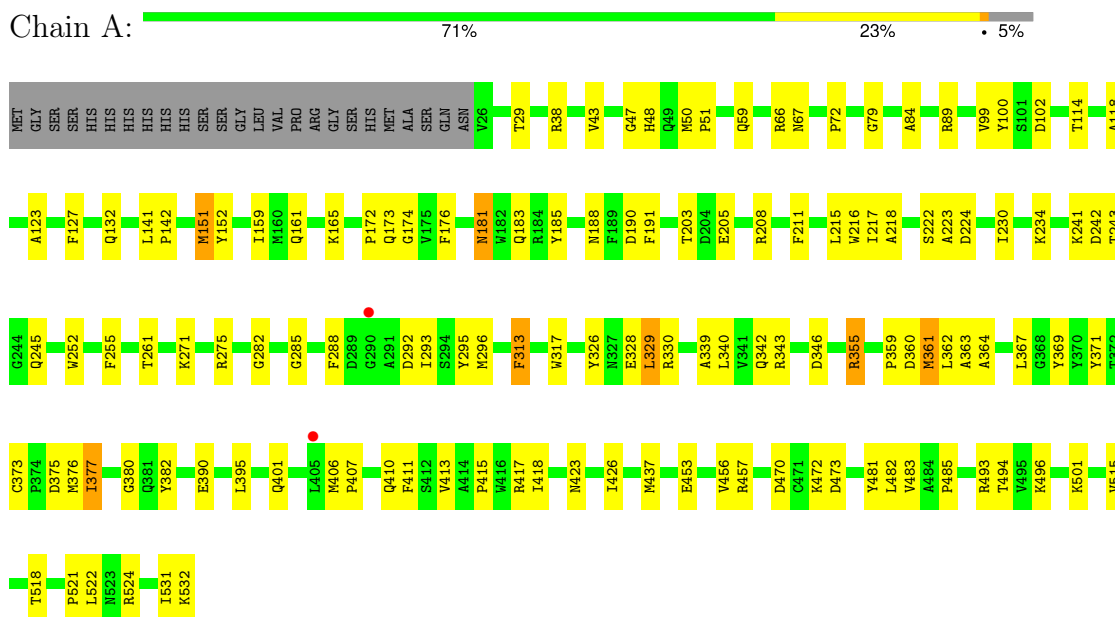
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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP A0A7J4XIY8
D	21	MET	-	expression tag	UNP A0A7J4XIY8
D	22	ALA	-	expression tag	UNP A0A7J4XIY8
D	23	SER	-	expression tag	UNP A0A7J4XIY8
D	24	GLN	-	expression tag	UNP A0A7J4XIY8
D	25	ASN	-	expression tag	UNP A0A7J4XIY8
D	26	VAL	-	expression tag	UNP A0A7J4XIY8
D	27	PHE	-	expression tag	UNP A0A7J4XIY8
D	28	THR	-	expression tag	UNP A0A7J4XIY8
E	1	MET	-	initiating methionine	UNP A0A7J4XIY8
E	2	GLY	-	expression tag	UNP A0A7J4XIY8
E	3	SER	-	expression tag	UNP A0A7J4XIY8
E	4	SER	-	expression tag	UNP A0A7J4XIY8
E	5	HIS	-	expression tag	UNP A0A7J4XIY8
E	6	HIS	-	expression tag	UNP A0A7J4XIY8
E	7	HIS	-	expression tag	UNP A0A7J4XIY8
E	8	HIS	-	expression tag	UNP A0A7J4XIY8
E	9	HIS	-	expression tag	UNP A0A7J4XIY8
E	10	HIS	-	expression tag	UNP A0A7J4XIY8
E	11	SER	-	expression tag	UNP A0A7J4XIY8
E	12	SER	-	expression tag	UNP A0A7J4XIY8
E	13	GLY	-	expression tag	UNP A0A7J4XIY8
E	14	LEU	-	expression tag	UNP A0A7J4XIY8
E	15	VAL	-	expression tag	UNP A0A7J4XIY8
E	16	PRO	-	expression tag	UNP A0A7J4XIY8
E	17	ARG	-	expression tag	UNP A0A7J4XIY8
E	18	GLY	-	expression tag	UNP A0A7J4XIY8
E	19	SER	-	expression tag	UNP A0A7J4XIY8
E	20	HIS	-	expression tag	UNP A0A7J4XIY8
E	21	MET	-	expression tag	UNP A0A7J4XIY8
E	22	ALA	-	expression tag	UNP A0A7J4XIY8
E	23	SER	-	expression tag	UNP A0A7J4XIY8
E	24	GLN	-	expression tag	UNP A0A7J4XIY8
E	25	ASN	-	expression tag	UNP A0A7J4XIY8
E	26	VAL	-	expression tag	UNP A0A7J4XIY8
E	27	PHE	-	expression tag	UNP A0A7J4XIY8
E	28	THR	-	expression tag	UNP A0A7J4XIY8

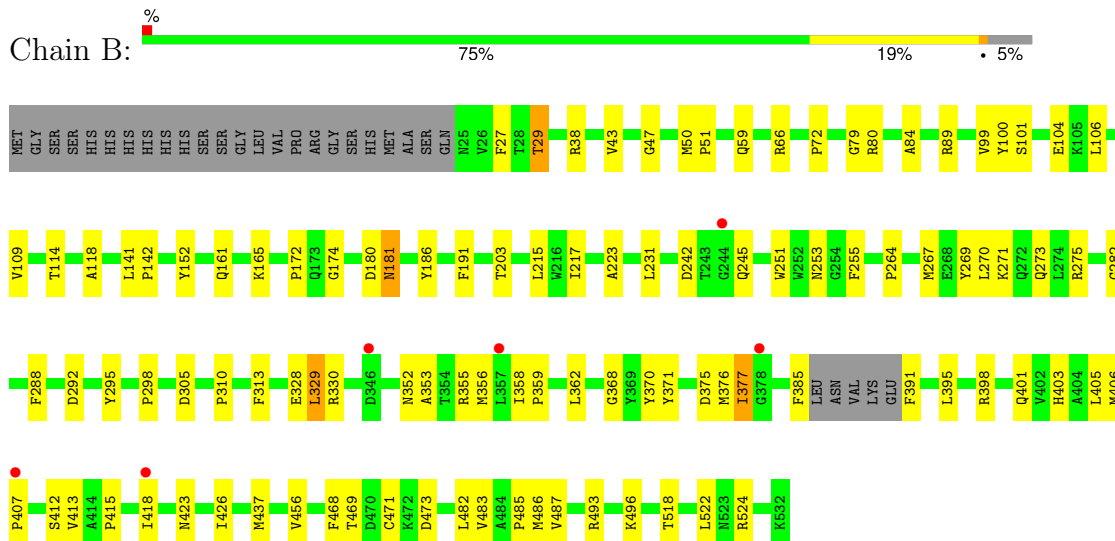
### 3 Residue-property plots

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.

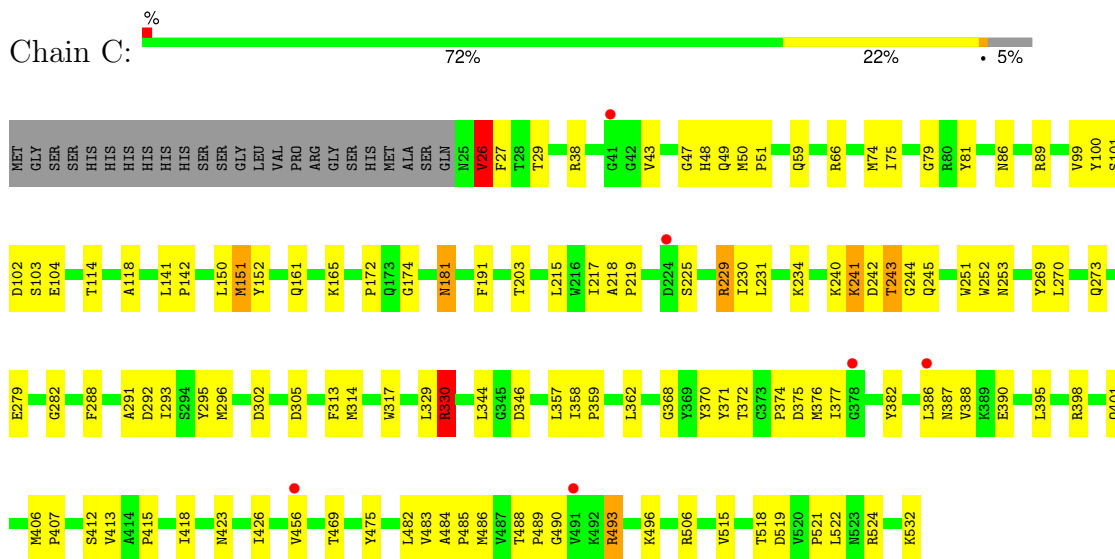
- Molecule 1: GH31 alpha-galactosidase



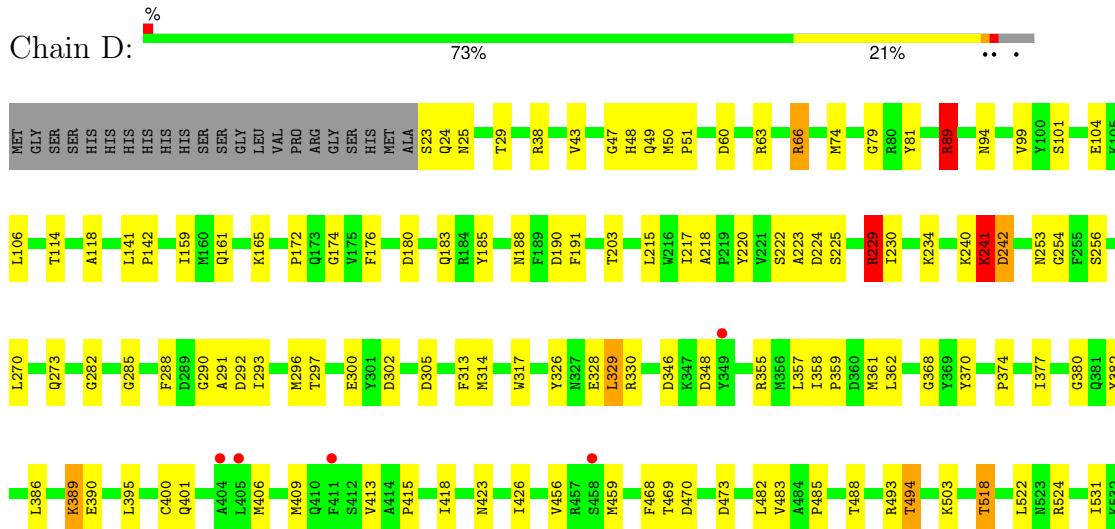
- Molecule 1: GH31 alpha-galactosidase



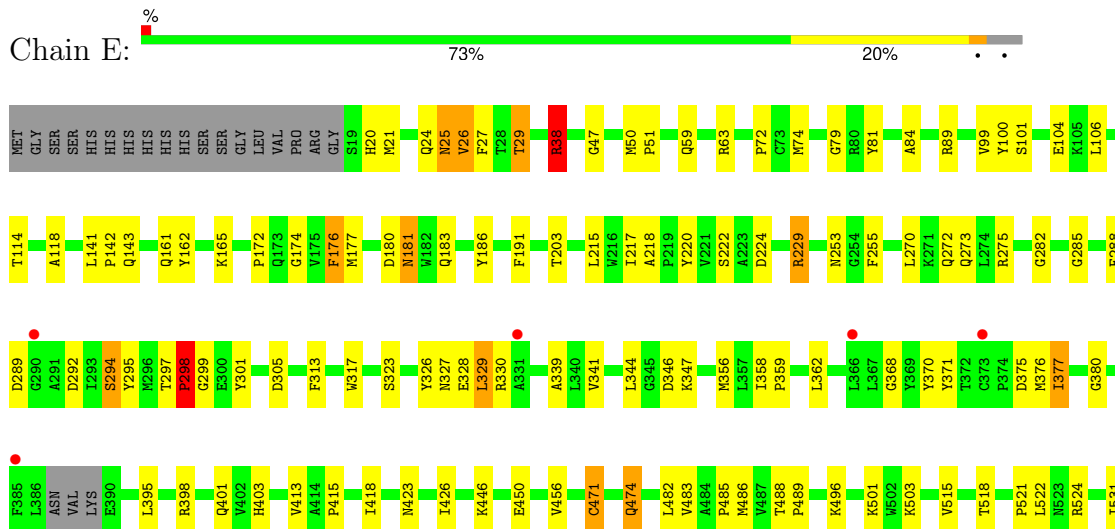
- Molecule 1: GH31 alpha-galactosidase



• Molecule 1: GH31 alpha-galactosidase



• Molecule 1: GH31 alpha-galactosidase



K532

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.52Å 157.53Å 131.41Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	48.63 – 3.50 48.63 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-3.50) 99.9 (48.63-3.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, $R_{free}$	0.257 , 0.313 0.265 , 0.324	Depositor DCC
$R_{free}$ test set	2223 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	40710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.65	0/4237	1.15	3/5733 (0.1%)
1	B	0.62	0/4203	1.10	1/5686 (0.0%)
1	C	0.62	0/4245	1.10	4/5744 (0.1%)
1	D	0.61	0/4260	1.10	4/5764 (0.1%)
1	E	0.64	0/4265	1.12	7/5769 (0.1%)
All	All	0.63	0/21210	1.11	19/28696 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	2
1	D	0	3
1	E	0	2
All	All	0	11

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	298	PRO	N-CA-CB	-8.45	94.37	103.25
1	E	305	ASP	CA-CB-CG	7.82	120.42	112.60
1	C	305	ASP	CA-CB-CG	7.71	120.31	112.60
1	D	305	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	305	ASP	CA-CB-CG	7.70	120.30	112.60
1	E	289	ASP	CB-CA-C	6.38	120.35	110.14
1	C	279	GLU	CB-CA-C	-6.37	100.84	110.90
1	E	297	THR	CA-C-N	6.06	127.42	119.84
1	E	297	THR	C-N-CA	6.06	127.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	ILE	N-CA-C	-5.76	105.51	113.00
1	A	293	ILE	N-CA-C	-5.75	105.52	113.00
1	C	372	THR	CA-CB-OG1	5.41	117.72	109.60
1	E	298	PRO	CA-N-CD	5.41	119.57	112.00
1	A	261	THR	CA-CB-OG1	-5.38	101.52	109.60
1	A	205	GLU	CB-CG-CD	5.28	121.58	112.60
1	C	293	ILE	N-CA-C	-5.24	106.18	113.00
1	D	254	GLY	N-CA-C	5.10	116.72	111.56
1	E	220	TYR	CB-CA-C	5.07	118.10	109.53
1	D	220	TYR	CB-CA-C	5.01	118.00	109.53

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	417	ARG	Sidechain
1	C	229	ARG	Sidechain
1	C	330	ARG	Sidechain
1	D	229	ARG	Sidechain
1	D	66	ARG	Sidechain
1	D	89	ARG	Sidechain
1	E	229	ARG	Sidechain
1	E	38	ARG	Sidechain

## 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	4117	4019	4008	90	0
1	B	4084	3980	3968	72	0
1	C	4125	4025	4014	75	0
1	D	4140	4038	4027	86	0
1	E	4145	4037	4024	79	0
All	All	20611	20099	20041	384	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 9.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:MET:HE1	1:A:313:PHE:CE1	2.12	0.85
1:B:355:ARG:HG2	1:B:487:VAL:CG1	2.13	0.78
1:C:296:MET:HE1	1:C:313:PHE:CE1	2.19	0.78
1:A:493:ARG:NH1	1:A:494:THR:O	2.18	0.77
1:D:29:THR:CG2	1:D:99:VAL:HB	2.14	0.77
1:D:473:ASP:O	1:D:493:ARG:NH2	2.19	0.75
1:A:355:ARG:HH21	1:A:355:ARG:HB2	1.52	0.74
1:A:29:THR:CG2	1:A:99:VAL:HB	2.20	0.72
1:D:413:VAL:O	1:D:415:PRO:HD3	1.91	0.71
1:E:376:MET:SD	1:E:380:GLY:HA2	2.30	0.71
1:C:413:VAL:O	1:C:415:PRO:HD3	1.91	0.70
1:A:473:ASP:O	1:A:493:ARG:NH2	2.23	0.70
1:B:413:VAL:O	1:B:415:PRO:HD3	1.92	0.69
1:B:264:PRO:HG3	1:D:348:ASP:OD2	1.94	0.68
1:C:29:THR:CG2	1:C:99:VAL:HB	2.24	0.67
1:B:355:ARG:HG2	1:B:487:VAL:HG13	1.75	0.67
1:D:296:MET:HE1	1:D:313:PHE:CE1	2.31	0.66
1:E:531:ILE:O	1:E:532:LYS:HG3	1.96	0.66
1:E:413:VAL:O	1:E:415:PRO:HD3	1.95	0.65
1:A:29:THR:HG23	1:A:29:THR:O	1.95	0.65
1:A:342:GLN:HG3	1:A:369:TYR:HB3	1.79	0.65
1:A:413:VAL:O	1:A:415:PRO:HD3	1.96	0.65
1:A:531:ILE:O	1:A:532:LYS:HB3	1.97	0.65
1:C:243:THR:C	1:C:245:GLN:H	2.04	0.64
1:B:29:THR:HG23	1:B:99:VAL:HB	1.80	0.64
1:D:413:VAL:HG21	1:D:418:ILE:HD13	1.80	0.63
1:D:296:MET:HE1	1:D:313:PHE:CD1	2.34	0.63
1:B:355:ARG:HG2	1:B:487:VAL:HG12	1.80	0.63
1:D:222:SER:HA	1:E:224:ASP:OD2	1.99	0.62
1:A:161:GLN:HE21	1:A:165:LYS:HE3	1.62	0.62
1:A:255:PHE:O	1:B:223:ALA:HB3	2.00	0.62
1:E:162:TYR:CD1	1:E:176:PHE:HZ	2.19	0.61
1:D:297:THR:HB	1:D:300:GLU:OE1	2.01	0.60
1:C:152:TYR:O	1:C:181:ASN:HB3	2.01	0.60
1:B:375:ASP:CG	1:B:376:MET:H	2.10	0.60
1:E:518:THR:OG1	1:E:524:ARG:NH1	2.33	0.60
1:D:29:THR:HG23	1:D:99:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:MET:HG2	1:C:412:SER:HB2	1.84	0.60
1:C:518:THR:OG1	1:C:524:ARG:NH1	2.35	0.60
1:B:518:THR:OG1	1:B:524:ARG:NH1	2.34	0.59
1:D:159:ILE:HG23	1:D:176:PHE:CE2	2.37	0.59
1:A:328:GLU:C	1:A:329:LEU:HD23	2.28	0.58
1:C:29:THR:O	1:C:29:THR:HG23	2.03	0.58
1:A:413:VAL:HG21	1:A:418:ILE:HD13	1.85	0.58
1:C:296:MET:HE1	1:C:313:PHE:CD1	2.39	0.58
1:E:99:VAL:CG1	1:E:106:LEU:HD12	2.34	0.58
1:E:191:PHE:CZ	1:E:215:LEU:HD11	2.39	0.58
1:A:296:MET:HE1	1:A:313:PHE:CD1	2.39	0.57
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.70	0.57
1:D:518:THR:OG1	1:D:524:ARG:NH1	2.38	0.56
1:B:292:ASP:OD1	1:B:330:ARG:NH1	2.38	0.56
1:E:186:TYR:OH	1:E:253:ASN:ND2	2.38	0.56
1:D:29:THR:HG23	1:D:29:THR:O	2.05	0.56
1:D:361:MET:HE2	1:D:406:MET:SD	2.46	0.56
1:C:413:VAL:HG21	1:C:418:ILE:HD13	1.88	0.56
1:C:142:PRO:HG3	1:C:172:PRO:HG2	1.88	0.56
1:E:63:ARG:O	1:E:294:SER:HA	2.05	0.55
1:D:292:ASP:OD1	1:D:330:ARG:NH1	2.39	0.55
1:A:242:ASP:OD1	1:A:243:THR:HG23	2.07	0.55
1:D:101:SER:HB3	1:D:104:GLU:O	2.05	0.55
1:D:224:ASP:C	1:D:229:ARG:HH22	2.15	0.55
1:A:518:THR:OG1	1:A:524:ARG:NH1	2.37	0.55
1:D:230:ILE:O	1:D:234:LYS:HG3	2.07	0.55
1:A:243:THR:C	1:A:245:GLN:H	2.16	0.54
1:C:483:VAL:HG12	1:C:485:PRO:HD3	1.89	0.54
1:E:180:ASP:O	1:E:181:ASN:HB2	2.06	0.54
1:B:413:VAL:HG21	1:B:418:ILE:HD13	1.88	0.54
1:A:390:GLU:OE2	1:E:275:ARG:HD3	2.07	0.54
1:C:346:ASP:HA	1:C:375:ASP:OD1	2.07	0.54
1:A:47:GLY:HA3	1:A:360:ASP:HA	1.88	0.54
1:D:142:PRO:HG3	1:D:172:PRO:HG2	1.90	0.54
1:A:313:PHE:CD1	1:A:313:PHE:C	2.85	0.54
1:B:99:VAL:CG1	1:B:106:LEU:HD12	2.37	0.54
1:C:29:THR:HG23	1:C:99:VAL:HB	1.89	0.54
1:C:161:GLN:O	1:C:165:LYS:HG2	2.08	0.53
1:A:48:HIS:HA	1:A:359:PRO:HB2	1.90	0.53
1:A:329:LEU:HD23	1:A:329:LEU:N	2.23	0.53
1:A:230:ILE:O	1:A:234:LYS:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:PHE:CD1	1:D:313:PHE:C	2.86	0.53
1:E:101:SER:HB3	1:E:104:GLU:O	2.09	0.53
1:A:223:ALA:HB3	1:B:255:PHE:O	2.08	0.53
1:B:483:VAL:HG12	1:B:485:PRO:HD3	1.91	0.53
1:B:328:GLU:C	1:B:329:LEU:HD23	2.33	0.53
1:D:222:SER:HB3	1:D:225:SER:HB3	1.90	0.53
1:B:43:VAL:HG11	1:B:66:ARG:HD2	1.89	0.53
1:E:358:ILE:HB	1:E:359:PRO:HD3	1.90	0.53
1:A:355:ARG:HH21	1:A:355:ARG:CB	2.20	0.53
1:D:159:ILE:HG23	1:D:176:PHE:HE2	1.73	0.53
1:B:329:LEU:HD23	1:B:329:LEU:N	2.23	0.52
1:C:48:HIS:CD2	1:C:49:GLN:HG3	2.44	0.52
1:D:224:ASP:C	1:D:224:ASP:OD1	2.52	0.52
1:E:501:LYS:HD3	1:E:532:LYS:HD2	1.92	0.52
1:B:368:GLY:HA2	1:B:370:TYR:CZ	2.44	0.52
1:D:329:LEU:N	1:D:329:LEU:HD23	2.25	0.52
1:A:59:GLN:O	1:A:89:ARG:HA	2.10	0.52
1:A:29:THR:HG22	1:A:99:VAL:HB	1.90	0.52
1:B:142:PRO:HG3	1:B:172:PRO:HG2	1.92	0.52
1:B:405:LEU:HD22	1:B:437:MET:HE2	1.90	0.52
1:E:142:PRO:HG3	1:E:172:PRO:HG2	1.90	0.52
1:A:373:CYS:SG	1:A:410:GLN:HB2	2.50	0.52
1:D:241:LYS:O	1:D:242:ASP:C	2.52	0.52
1:A:296:MET:HE1	1:A:313:PHE:CZ	2.45	0.52
1:C:313:PHE:CD1	1:C:313:PHE:C	2.88	0.52
1:E:329:LEU:N	1:E:329:LEU:HD23	2.24	0.52
1:C:151:MET:HG2	1:C:382:TYR:CD2	2.45	0.52
1:D:328:GLU:C	1:D:329:LEU:HD23	2.35	0.52
1:B:101:SER:HB3	1:B:104:GLU:O	2.08	0.51
1:C:251:TRP:CH2	1:C:253:ASN:HB2	2.45	0.51
1:E:272:GLN:HG2	1:E:275:ARG:NH1	2.25	0.51
1:B:313:PHE:CD1	1:B:313:PHE:C	2.88	0.51
1:C:43:VAL:HG11	1:C:66:ARG:HD2	1.92	0.51
1:A:142:PRO:HG3	1:A:172:PRO:HG2	1.92	0.51
1:E:346:ASP:HA	1:E:375:ASP:OD1	2.10	0.51
1:E:141:LEU:HD13	1:E:174:GLY:HA2	1.92	0.51
1:C:368:GLY:HA2	1:C:370:TYR:CE1	2.45	0.51
1:C:423:ASN:HA	1:C:426:ILE:HD12	1.93	0.51
1:E:313:PHE:CD1	1:E:313:PHE:C	2.88	0.51
1:B:358:ILE:O	1:B:362:LEU:HG	2.10	0.51
1:A:423:ASN:HA	1:A:426:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ALA:HA	1:B:356:MET:HE2	1.93	0.51
1:B:423:ASN:HA	1:B:426:ILE:HD12	1.93	0.51
1:C:89:ARG:HB2	1:C:100:TYR:HB2	1.93	0.51
1:E:446:LYS:O	1:E:450:GLU:HG3	2.11	0.51
1:E:483:VAL:HG12	1:E:485:PRO:HD3	1.92	0.51
1:A:47:GLY:O	1:A:50:MET:HB2	2.11	0.50
1:D:368:GLY:HA2	1:D:370:TYR:CE1	2.46	0.50
1:A:141:LEU:HD13	1:A:174:GLY:HA2	1.92	0.50
1:D:229:ARG:HH21	1:D:229:ARG:HG3	1.76	0.50
1:E:423:ASN:HA	1:E:426:ILE:HD12	1.92	0.50
1:C:230:ILE:O	1:C:234:LYS:HG3	2.11	0.50
1:C:362:LEU:HD23	1:C:456:VAL:HG12	1.93	0.50
1:A:159:ILE:HG23	1:A:176:PHE:CE1	2.47	0.50
1:E:368:GLY:HA2	1:E:370:TYR:CZ	2.47	0.50
1:C:101:SER:HB3	1:C:104:GLU:O	2.11	0.50
1:B:89:ARG:HB2	1:B:100:TYR:HB2	1.92	0.50
1:B:473:ASP:HB2	1:B:487:VAL:HG21	1.93	0.50
1:C:368:GLY:HA2	1:C:370:TYR:CZ	2.47	0.50
1:D:423:ASN:HA	1:D:426:ILE:HD12	1.93	0.50
1:E:285:GLY:HA3	1:E:326:TYR:HB2	1.93	0.50
1:A:377:ILE:HB	1:A:411:PHE:HA	1.94	0.50
1:D:99:VAL:CG1	1:D:106:LEU:HD12	2.42	0.49
1:E:413:VAL:HG21	1:E:418:ILE:HD13	1.93	0.49
1:A:362:LEU:HD23	1:A:456:VAL:HG12	1.93	0.49
1:E:531:ILE:O	1:E:532:LYS:CG	2.61	0.49
1:B:161:GLN:O	1:B:165:LYS:HG2	2.13	0.49
1:D:368:GLY:HA2	1:D:370:TYR:CZ	2.47	0.49
1:D:47:GLY:O	1:D:50:MET:HB2	2.12	0.49
1:C:241:LYS:HA	1:C:302:ASP:OD1	2.13	0.49
1:D:355:ARG:HH11	1:D:488:THR:HG22	1.78	0.49
1:D:483:VAL:HG12	1:D:485:PRO:HD3	1.93	0.49
1:B:47:GLY:O	1:B:50:MET:HB2	2.12	0.49
1:B:298:PRO:HG3	1:B:310:PRO:HG2	1.94	0.49
1:B:368:GLY:HA2	1:B:370:TYR:CE1	2.47	0.49
1:B:376:MET:HG2	1:B:412:SER:HB2	1.95	0.49
1:D:141:LEU:HB3	1:D:174:GLY:HA2	1.95	0.49
1:A:483:VAL:HG12	1:A:485:PRO:HD3	1.95	0.49
1:C:484:ALA:HB1	1:C:493:ARG:HE	1.76	0.49
1:A:79:GLY:HA2	1:A:114:THR:O	2.13	0.48
1:E:47:GLY:O	1:E:50:MET:HB2	2.13	0.48
1:E:162:TYR:CD1	1:E:176:PHE:CZ	3.00	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TRP:HZ2	1:A:252:TRP:HZ2	1.60	0.48
1:D:224:ASP:OD2	1:E:222:SER:HA	2.14	0.48
1:D:256:SER:OG	1:E:224:ASP:HB3	2.13	0.48
1:E:161:GLN:O	1:E:165:LYS:HG2	2.13	0.48
1:C:79:GLY:HA2	1:C:114:THR:O	2.13	0.48
1:C:292:ASP:HB2	1:C:295:TYR:CD2	2.49	0.48
1:A:132:GLN:NE2	1:C:490:GLY:HA2	2.29	0.48
1:B:203:THR:HG21	1:B:282:GLY:C	2.38	0.48
1:B:191:PHE:CZ	1:B:215:LEU:HD11	2.49	0.48
1:A:161:GLN:HE21	1:A:165:LYS:CE	2.25	0.48
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.96	0.48
1:D:358:ILE:HB	1:D:359:PRO:HD3	1.94	0.48
1:E:292:ASP:OD1	1:E:330:ARG:NH1	2.39	0.48
1:B:377:ILE:HG13	1:B:403:HIS:CE1	2.49	0.47
1:E:63:ARG:HE	1:E:298:PRO:HG2	1.79	0.47
1:C:47:GLY:O	1:C:50:MET:HB2	2.14	0.47
1:D:361:MET:SD	1:D:374:PRO:HB3	2.54	0.47
1:E:29:THR:HG23	1:E:99:VAL:HB	1.95	0.47
1:C:59:GLN:O	1:C:89:ARG:HA	2.13	0.47
1:D:79:GLY:HA2	1:D:118:ALA:HB2	1.96	0.47
1:E:59:GLN:O	1:E:89:ARG:HA	2.15	0.47
1:D:218:ALA:HA	1:D:317:TRP:CZ2	2.49	0.47
1:A:390:GLU:OE2	1:E:275:ARG:CD	2.62	0.47
1:E:358:ILE:HB	1:E:359:PRO:CD	2.44	0.47
1:A:203:THR:HG21	1:A:282:GLY:C	2.40	0.47
1:A:285:GLY:HA3	1:A:326:TYR:HB2	1.97	0.47
1:B:38:ARG:HG3	1:B:469:THR:HG21	1.97	0.47
1:D:29:THR:HG22	1:D:99:VAL:HB	1.94	0.47
1:C:344:LEU:HB2	1:C:375:ASP:HB2	1.97	0.47
1:D:38:ARG:HH11	1:D:38:ARG:HG3	1.80	0.47
1:D:79:GLY:HA2	1:D:114:THR:O	2.14	0.47
1:A:363:ALA:O	1:A:364:ALA:C	2.57	0.46
1:A:191:PHE:CZ	1:A:215:LEU:HD11	2.50	0.46
1:B:79:GLY:HA2	1:B:114:THR:O	2.16	0.46
1:B:79:GLY:HA2	1:B:118:ALA:HB2	1.96	0.46
1:B:362:LEU:HD23	1:B:456:VAL:HG12	1.95	0.46
1:C:386:LEU:C	1:C:388:VAL:H	2.23	0.46
1:C:401:GLN:NE2	1:C:522:LEU:O	2.48	0.46
1:D:358:ILE:O	1:D:362:LEU:HG	2.16	0.46
1:E:377:ILE:HG13	1:E:403:HIS:CE1	2.50	0.46
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ALA:HA	1:A:317:TRP:CZ2	2.51	0.46
1:B:231:LEU:HD21	1:B:269:TYR:HE2	1.80	0.46
1:A:346:ASP:HA	1:A:375:ASP:OD1	2.16	0.46
1:E:79:GLY:HA2	1:E:114:THR:O	2.15	0.46
1:E:496:LYS:HG2	1:E:515:VAL:HG22	1.97	0.46
1:A:275:ARG:HD3	1:C:390:GLU:OE2	2.15	0.46
1:A:501:LYS:HB2	1:A:532:LYS:OXT	2.16	0.46
1:D:503:LYS:HB2	1:D:531:ILE:HD13	1.98	0.46
1:E:376:MET:SD	1:E:380:GLY:CA	3.02	0.46
1:B:270:LEU:HA	1:B:273:GLN:CG	2.46	0.46
1:A:141:LEU:HB3	1:A:174:GLY:HA2	1.98	0.46
1:D:401:GLN:NE2	1:D:522:LEU:O	2.49	0.45
1:B:395:LEU:HD23	1:B:395:LEU:O	2.17	0.45
1:C:152:TYR:HB3	1:C:181:ASN:HD22	1.81	0.45
1:C:231:LEU:HD21	1:C:269:TYR:HE2	1.81	0.45
1:A:38:ARG:HB3	1:A:51:PRO:HB2	1.98	0.45
1:A:100:TYR:CD1	1:A:100:TYR:N	2.83	0.45
1:B:482:LEU:HD23	1:B:483:VAL:N	2.31	0.45
1:A:183:GLN:HA	1:A:190:ASP:O	2.16	0.45
1:A:437:MET:HE1	1:A:481:TYR:CE2	2.52	0.45
1:B:267:MET:O	1:B:271:LYS:HG3	2.17	0.45
1:C:191:PHE:CZ	1:C:215:LEU:HD11	2.51	0.45
1:E:38:ARG:HD3	1:E:38:ARG:HA	1.90	0.45
1:B:264:PRO:CG	1:D:348:ASP:OD2	2.64	0.45
1:A:401:GLN:NE2	1:A:522:LEU:O	2.48	0.45
1:B:275:ARG:HH11	1:D:390:GLU:HB3	1.82	0.45
1:D:60:ASP:OD2	1:D:63:ARG:CZ	2.65	0.45
1:A:59:GLN:HE22	1:A:66:ARG:HH21	1.64	0.45
1:B:141:LEU:HD13	1:B:174:GLY:HA2	1.98	0.45
1:D:141:LEU:HD13	1:D:174:GLY:HA2	1.98	0.45
1:E:401:GLN:NE2	1:E:522:LEU:O	2.49	0.45
1:A:79:GLY:HA2	1:A:118:ALA:HB2	1.98	0.45
1:C:79:GLY:HA2	1:C:118:ALA:HB2	1.98	0.45
1:A:346:ASP:HB3	1:A:380:GLY:HA3	1.97	0.45
1:B:141:LEU:HB3	1:B:174:GLY:HA2	1.98	0.45
1:E:482:LEU:HD23	1:E:483:VAL:N	2.32	0.45
1:A:152:TYR:O	1:A:181:ASN:HB3	2.17	0.45
1:C:395:LEU:O	1:C:395:LEU:HD23	2.17	0.45
1:E:99:VAL:HG11	1:E:106:LEU:HD12	1.99	0.45
1:C:217:ILE:HD11	1:C:288:PHE:CD2	2.52	0.44
1:A:243:THR:C	1:A:245:GLN:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:O	1:A:395:LEU:HD23	2.17	0.44
1:D:270:LEU:HA	1:D:273:GLN:CG	2.48	0.44
1:E:398:ARG:HD2	1:E:486:MET:HB2	1.99	0.44
1:A:361:MET:HE2	1:A:361:MET:HB3	1.86	0.44
1:B:269:TYR:O	1:B:273:GLN:HG2	2.17	0.44
1:C:243:THR:C	1:C:245:GLN:N	2.72	0.44
1:B:38:ARG:HG3	1:B:38:ARG:HH11	1.83	0.44
1:D:48:HIS:CD2	1:D:49:GLN:HG3	2.52	0.44
1:D:482:LEU:HD23	1:D:483:VAL:N	2.33	0.44
1:A:224:ASP:OD2	1:B:186:TYR:HB2	2.16	0.44
1:A:470:ASP:O	1:A:472:LYS:HG3	2.18	0.44
1:B:180:ASP:O	1:B:181:ASN:HB2	2.17	0.44
1:B:217:ILE:HD11	1:B:288:PHE:CD2	2.53	0.44
1:C:38:ARG:HG3	1:C:469:THR:HG21	1.98	0.44
1:C:141:LEU:HD13	1:C:174:GLY:HA2	2.00	0.44
1:E:503:LYS:HB2	1:E:531:ILE:HD13	2.00	0.44
1:E:344:LEU:HB2	1:E:375:ASP:HB2	2.00	0.44
1:C:358:ILE:O	1:C:362:LEU:HG	2.17	0.44
1:C:456:VAL:HG13	1:C:475:TYR:CD2	2.52	0.44
1:C:486:MET:HE3	1:C:488:THR:O	2.17	0.44
1:E:217:ILE:HD11	1:E:288:PHE:CE2	2.53	0.44
1:B:27:PHE:HZ	1:D:94:ASN:HA	1.83	0.44
1:C:50:MET:HA	1:C:51:PRO:C	2.42	0.44
1:E:358:ILE:O	1:E:362:LEU:HG	2.18	0.44
1:A:50:MET:HA	1:A:51:PRO:C	2.42	0.44
1:E:347:LYS:HE2	1:E:356:MET:HE3	2.00	0.44
1:A:203:THR:HG21	1:A:282:GLY:O	2.18	0.43
1:B:292:ASP:HB2	1:B:295:TYR:CD2	2.53	0.43
1:B:401:GLN:NE2	1:B:522:LEU:O	2.51	0.43
1:C:26:VAL:O	1:C:27:PHE:C	2.61	0.43
1:C:218:ALA:HA	1:C:317:TRP:CZ2	2.53	0.43
1:E:218:ALA:HA	1:E:317:TRP:CZ2	2.53	0.43
1:E:395:LEU:HD23	1:E:395:LEU:O	2.18	0.43
1:A:252:TRP:HE3	1:A:295:TYR:OH	2.01	0.43
1:A:390:GLU:CD	1:E:275:ARG:HD3	2.43	0.43
1:C:482:LEU:HD23	1:C:483:VAL:N	2.33	0.43
1:D:285:GLY:HA3	1:D:326:TYR:HB2	1.99	0.43
1:D:89:ARG:HE	1:D:89:ARG:HB2	1.65	0.43
1:B:398:ARG:HD2	1:B:486:MET:HB2	2.01	0.43
1:D:346:ASP:HB3	1:D:380:GLY:HA3	2.00	0.43
1:C:74:MET:O	1:C:81:TYR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:MET:HA	1:D:51:PRO:C	2.43	0.43
1:D:185:TYR:CE1	1:D:188:ASN:HB2	2.53	0.43
1:D:203:THR:HG21	1:D:282:GLY:C	2.43	0.43
1:A:340:LEU:O	1:A:342:GLN:HG2	2.19	0.43
1:C:38:ARG:HG3	1:C:38:ARG:HH11	1.83	0.43
1:D:161:GLN:O	1:D:165:LYS:HG2	2.19	0.43
1:E:141:LEU:HB3	1:E:174:GLY:HA2	2.00	0.43
1:E:368:GLY:HA2	1:E:370:TYR:CE1	2.53	0.43
1:A:67:ASN:O	1:A:330:ARG:HD3	2.19	0.42
1:B:375:ASP:CG	1:B:376:MET:N	2.76	0.42
1:C:506:ARG:HH22	1:C:519:ASP:HB2	1.84	0.42
1:E:143:GLN:OE1	1:E:177:MET:HE3	2.19	0.42
1:E:217:ILE:HD11	1:E:288:PHE:CD2	2.54	0.42
1:A:123:ALA:HA	1:A:127:PHE:CD1	2.54	0.42
1:A:361:MET:O	1:A:362:LEU:C	2.62	0.42
1:B:59:GLN:O	1:B:89:ARG:HA	2.18	0.42
1:C:374:PRO:O	1:C:375:ASP:O	2.37	0.42
1:E:203:THR:HG21	1:E:282:GLY:C	2.45	0.42
1:C:225:SER:C	1:C:229:ARG:NH1	2.78	0.42
1:E:104:GLU:HG3	1:E:106:LEU:HD21	2.00	0.42
1:D:395:LEU:HD23	1:D:395:LEU:O	2.18	0.42
1:D:74:MET:O	1:D:81:TYR:HA	2.19	0.42
1:D:400:CYS:SG	1:D:409:MET:CE	3.08	0.42
1:E:521:PRO:HG2	1:E:524:ARG:HB2	2.02	0.42
1:C:86:ASN:ND2	1:C:103:SER:OG	2.53	0.42
1:C:291:ALA:HB1	1:C:314:MET:HA	2.02	0.42
1:E:25:ASN:O	1:E:27:PHE:N	2.52	0.42
1:B:72:PRO:HB2	1:B:84:ALA:HB3	2.02	0.42
1:C:89:ARG:NH2	1:C:102:ASP:OD1	2.52	0.42
1:C:488:THR:HB	1:C:489:PRO:CD	2.50	0.42
1:D:183:GLN:HA	1:D:190:ASP:O	2.20	0.42
1:C:398:ARG:HD2	1:C:486:MET:HB2	2.02	0.42
1:C:252:TRP:HE3	1:C:295:TYR:OH	2.03	0.42
1:D:43:VAL:HG11	1:D:66:ARG:HD2	2.02	0.42
1:E:501:LYS:CB	1:E:532:LYS:HB2	2.50	0.42
1:D:493:ARG:NH1	1:D:494:THR:O	2.53	0.41
1:A:375:ASP:CG	1:A:376:MET:H	2.27	0.41
1:C:386:LEU:C	1:C:388:VAL:N	2.77	0.41
1:D:217:ILE:HD11	1:D:288:PHE:CD2	2.55	0.41
1:D:290:GLY:C	1:D:292:ASP:H	2.28	0.41
1:D:358:ILE:N	1:D:359:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:HA	1:E:273:GLN:CG	2.51	0.41
1:C:218:ALA:HB1	1:C:219:PRO:HD2	2.02	0.41
1:D:191:PHE:CZ	1:D:215:LEU:HD11	2.56	0.41
1:E:100:TYR:CD1	1:E:100:TYR:N	2.88	0.41
1:E:299:GLY:C	1:E:301:TYR:H	2.28	0.41
1:C:521:PRO:HG2	1:C:524:ARG:HB2	2.02	0.41
1:D:38:ARG:HG3	1:D:469:THR:HG21	2.02	0.41
1:D:459:MET:HB2	1:D:468:PHE:HB3	2.02	0.41
1:E:50:MET:HA	1:E:51:PRO:C	2.46	0.41
1:E:79:GLY:HA2	1:E:118:ALA:HB2	2.01	0.41
1:C:203:THR:HG21	1:C:282:GLY:C	2.45	0.41
1:E:72:PRO:HB2	1:E:84:ALA:HB3	2.03	0.41
1:B:251:TRP:CH2	1:B:253:ASN:HB2	2.56	0.41
1:A:255:PHE:O	1:B:223:ALA:CB	2.68	0.41
1:A:482:LEU:HD23	1:A:483:VAL:N	2.36	0.41
1:B:468:PHE:HE1	1:B:496:LYS:HB3	1.86	0.41
1:D:382:TYR:CE2	1:D:386:LEU:HD11	2.55	0.41
1:E:74:MET:O	1:E:81:TYR:HA	2.20	0.41
1:A:217:ILE:HD11	1:A:288:PHE:CD2	2.55	0.41
1:B:413:VAL:CG2	1:B:418:ILE:HD13	2.51	0.41
1:D:223:ALA:HB3	1:E:255:PHE:O	2.21	0.41
1:D:241:LYS:HA	1:D:302:ASP:OD1	2.20	0.41
1:D:358:ILE:HB	1:D:359:PRO:CD	2.50	0.41
1:A:29:THR:HG23	1:A:99:VAL:HB	1.99	0.41
1:A:173:GLN:HB2	1:A:211:PHE:CD1	2.56	0.41
1:A:406:MET:HB3	1:A:407:PRO:CD	2.51	0.41
1:B:50:MET:HA	1:B:51:PRO:C	2.45	0.41
1:B:203:THR:HG21	1:B:282:GLY:O	2.21	0.41
1:B:385:PHE:CD2	1:B:391:PHE:HE2	2.39	0.41
1:B:406:MET:HB3	1:B:407:PRO:CD	2.51	0.41
1:C:358:ILE:N	1:C:359:PRO:HD2	2.35	0.41
1:E:471:CYS:SG	1:E:474:GLN:HG3	2.60	0.41
1:E:488:THR:HB	1:E:489:PRO:CD	2.51	0.41
1:A:43:VAL:HG11	1:A:66:ARG:HD2	2.02	0.41
1:A:185:TYR:CE1	1:A:188:ASN:HB2	2.56	0.41
1:A:453:GLU:OE2	1:A:457:ARG:NH1	2.54	0.41
1:C:406:MET:HB3	1:C:407:PRO:CD	2.51	0.41
1:D:38:ARG:HB3	1:D:51:PRO:HB2	2.03	0.41
1:D:413:VAL:CG2	1:D:418:ILE:HD13	2.49	0.41
1:E:292:ASP:HB2	1:E:295:TYR:CD2	2.56	0.41
1:A:292:ASP:HB2	1:A:295:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:HG2	1:A:524:ARG:HB2	2.04	0.40
1:E:362:LEU:HD23	1:E:456:VAL:HG12	2.02	0.40
1:B:80:ARG:HA	1:B:109:VAL:O	2.21	0.40
1:B:275:ARG:NH1	1:D:390:GLU:HB3	2.36	0.40
1:C:270:LEU:HA	1:C:273:GLN:CG	2.51	0.40
1:D:389:LYS:H	1:D:389:LYS:HG2	1.58	0.40
1:E:327:ASN:O	1:E:341:VAL:HB	2.21	0.40
1:A:72:PRO:HB2	1:A:84:ALA:HB3	2.02	0.40
1:A:217:ILE:HD11	1:A:288:PHE:CE2	2.56	0.40
1:A:496:LYS:HG2	1:A:515:VAL:HG22	2.03	0.40
1:D:99:VAL:HG12	1:D:106:LEU:HD12	2.03	0.40
1:A:151:MET:HG2	1:A:382:TYR:CD2	2.56	0.40
1:D:362:LEU:HD23	1:D:456:VAL:HG12	2.04	0.40
1:E:224:ASP:C	1:E:224:ASP:OD1	2.65	0.40
1:B:152:TYR:O	1:B:181:ASN:HB3	2.21	0.40
1:C:358:ILE:HB	1:C:359:PRO:HD3	2.03	0.40
1:C:496:LYS:HG2	1:C:515:VAL:HG22	2.03	0.40
1:D:180:ASP:OD2	1:D:253:ASN:ND2	2.55	0.40
1:D:291:ALA:HB1	1:D:314:MET:HA	2.04	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	505/532 (95%)	469 (93%)	34 (7%)	2 (0%)	30 62
1	B	499/532 (94%)	466 (93%)	32 (6%)	1 (0%)	43 74
1	C	506/532 (95%)	468 (92%)	34 (7%)	4 (1%)	16 49
1	D	508/532 (96%)	478 (94%)	29 (6%)	1 (0%)	43 74
1	E	507/532 (95%)	469 (92%)	34 (7%)	4 (1%)	16 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2525/2660 (95%)	2350 (93%)	163 (6%)	12 (0%)	24 57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	26	VAL
1	E	181	ASN
1	A	181	ASN
1	C	26	VAL
1	C	330	ARG
1	A	339	ALA
1	B	181	ASN
1	C	181	ASN
1	D	241	LYS
1	E	339	ALA
1	C	244	GLY
1	E	298	PRO

### 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	435/456 (95%)	424 (98%)	11 (2%)	42 63
1	B	431/456 (94%)	422 (98%)	9 (2%)	47 66
1	C	436/456 (96%)	420 (96%)	16 (4%)	30 56
1	D	438/456 (96%)	423 (97%)	15 (3%)	32 57
1	E	438/456 (96%)	420 (96%)	18 (4%)	27 53
All	All	2178/2280 (96%)	2109 (97%)	69 (3%)	34 59

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	151	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	222	SER
1	A	241	LYS
1	A	271	LYS
1	A	313	PHE
1	A	329	LEU
1	A	361	MET
1	A	367	LEU
1	A	371	TYR
1	A	377	ILE
1	B	29	THR
1	B	242	ASP
1	B	245	GLN
1	B	329	LEU
1	B	352	ASN
1	B	371	TYR
1	B	377	ILE
1	B	471	CYS
1	B	493	ARG
1	C	26	VAL
1	C	75	ILE
1	C	150	LEU
1	C	151	MET
1	C	240	LYS
1	C	241	LYS
1	C	242	ASP
1	C	243	THR
1	C	329	LEU
1	C	330	ARG
1	C	357	LEU
1	C	371	TYR
1	C	377	ILE
1	C	387	ASN
1	C	493	ARG
1	C	532	LYS
1	D	23	SER
1	D	24	GLN
1	D	25	ASN
1	D	89	ARG
1	D	229	ARG
1	D	240	LYS
1	D	241	LYS
1	D	242	ASP

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Mol	Chain	Res	Type
1	D	329	LEU
1	D	357	LEU
1	D	377	ILE
1	D	389	LYS
1	D	470	ASP
1	D	494	THR
1	D	518	THR
1	E	20	HIS
1	E	21	MET
1	E	24	GLN
1	E	25	ASN
1	E	26	VAL
1	E	29	THR
1	E	38	ARG
1	E	176	PHE
1	E	183	GLN
1	E	229	ARG
1	E	294	SER
1	E	323	SER
1	E	328	GLU
1	E	329	LEU
1	E	371	TYR
1	E	377	ILE
1	E	471	CYS
1	E	474	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	86	ASN
1	A	145	ASN
1	A	161	GLN
1	A	169	ASN
1	A	273	GLN
1	A	410	GLN
1	B	48	HIS
1	B	49	GLN
1	B	55	GLN
1	B	68	ASN
1	B	86	ASN
1	B	132	GLN

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Mol	Chain	Res	Type
1	B	145	ASN
1	B	169	ASN
1	B	273	GLN
1	B	403	HIS
1	B	429	HIS
1	B	474	GLN
1	C	48	HIS
1	C	49	GLN
1	C	68	ASN
1	C	69	GLN
1	C	86	ASN
1	C	145	ASN
1	C	207	HIS
1	C	342	GLN
1	C	410	GLN
1	D	48	HIS
1	D	49	GLN
1	D	55	GLN
1	D	68	ASN
1	D	86	ASN
1	D	94	ASN
1	D	273	GLN
1	D	410	GLN
1	D	429	HIS
1	D	474	GLN
1	E	24	GLN
1	E	48	HIS
1	E	49	GLN
1	E	68	ASN
1	E	86	ASN
1	E	145	ASN
1	E	169	ASN
1	E	273	GLN
1	E	338	GLN
1	E	410	GLN

### 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	507/532 (95%)	0.17	2 (0%) 88 72	24, 91, 126, 184	0
1	B	503/532 (94%)	0.23	6 (1%) 76 52	50, 103, 144, 178	0
1	C	508/532 (95%)	0.22	6 (1%) 76 52	40, 99, 137, 193	0
1	D	510/532 (95%)	0.26	5 (0%) 79 56	43, 109, 156, 212	0
1	E	511/532 (96%)	0.15	5 (0%) 79 56	48, 104, 141, 207	0
All	All	2539/2660 (95%)	0.21	24 (0%) 81 58	24, 101, 144, 212	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	378	GLY	3.6
1	E	331	ALA	3.1
1	D	411	PHE	3.0
1	E	366	LEU	2.8
1	B	378	GLY	2.7
1	D	349	TYR	2.6
1	B	346	ASP	2.5
1	B	418	ILE	2.3
1	D	405	LEU	2.3
1	C	456	VAL	2.3
1	A	290	GLY	2.2
1	B	407	PRO	2.2
1	B	357	LEU	2.2
1	C	386	LEU	2.2
1	C	41	GLY	2.1
1	D	458	SER	2.1
1	B	244	GLY	2.1
1	E	373	CYS	2.1
1	D	404	ALA	2.1
1	E	385	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	405	LEU	2.1
1	C	224	ASP	2.0
1	E	290	GLY	2.0
1	C	491	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.