



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:47 am GMT

PDB ID : 3WQ8  
Title : Monomer structure of hyperthermophilic beta-glucosidase mutant forming a dodecameric structure in the crystal form  
Authors : Nakabayashi, M.; Kataoka, M.; Watanabe, M.; Ishikawa, K.  
Deposited on : 2014-01-23  
Resolution : 2.81 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

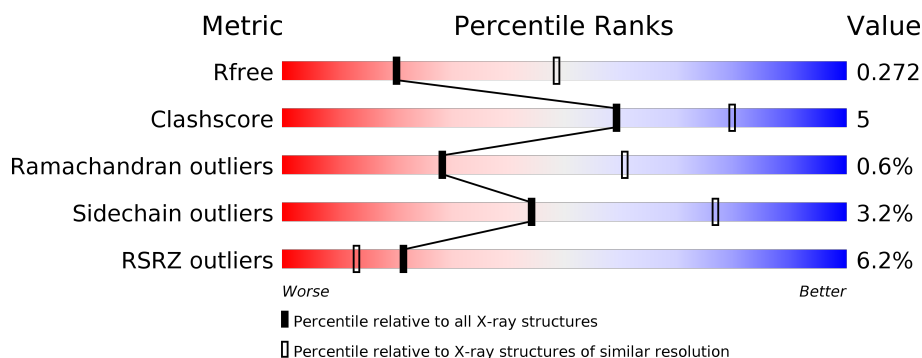
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	450	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	B	450	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	C	450	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>••</div> </div>
1	D	450	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>
1	E	450	<div> <div>%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
1	F	450	<div> <div>30%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div></div><div>88%11%.</div></div>
1	H	450	<div><div>3%</div><div></div><div>84%14%.</div></div>
1	I	450	<div><div>%</div><div></div><div>85%13%..</div></div>
1	J	450	<div><div>27%</div><div></div><div>82%14%..</div></div>
1	K	450	<div><div>%</div><div></div><div>83%15%..</div></div>
1	L	450	<div><div>2%</div><div></div><div>87%12%.</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43762 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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	B	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	C	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	D	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	E	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	F	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	G	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	H	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			
1	I	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	J	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	K	444	Total	C	N	O	S	0	0	0
			3626	2365	589	659	13			
1	L	448	Total	C	N	O	S	0	0	0
			3657	2383	596	665	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q51723
A	1	ALA	-	EXPRESSION TAG	UNP Q51723
A	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
A	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
A	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
A	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
A	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
A	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
B	0	MET	-	EXPRESSION TAG	UNP Q51723
B	1	ALA	-	EXPRESSION TAG	UNP Q51723
B	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
B	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
B	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
B	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
B	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
B	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
C	0	MET	-	EXPRESSION TAG	UNP Q51723
C	1	ALA	-	EXPRESSION TAG	UNP Q51723
C	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
C	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
C	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
C	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
C	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
C	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
D	0	MET	-	EXPRESSION TAG	UNP Q51723
D	1	ALA	-	EXPRESSION TAG	UNP Q51723
D	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
D	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
D	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
D	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
D	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
D	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
E	0	MET	-	EXPRESSION TAG	UNP Q51723
E	1	ALA	-	EXPRESSION TAG	UNP Q51723
E	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
E	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
E	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
E	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
E	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
E	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
F	0	MET	-	EXPRESSION TAG	UNP Q51723
F	1	ALA	-	EXPRESSION TAG	UNP Q51723
F	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
F	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
F	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
F	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
F	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
F	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
G	0	MET	-	EXPRESSION TAG	UNP Q51723
G	1	ALA	-	EXPRESSION TAG	UNP Q51723
G	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
G	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
G	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
G	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
G	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
G	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
H	0	MET	-	EXPRESSION TAG	UNP Q51723
H	1	ALA	-	EXPRESSION TAG	UNP Q51723
H	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
H	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
H	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
H	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
H	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
H	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
I	0	MET	-	EXPRESSION TAG	UNP Q51723
I	1	ALA	-	EXPRESSION TAG	UNP Q51723
I	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
I	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
I	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
I	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
I	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
I	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
J	0	MET	-	EXPRESSION TAG	UNP Q51723
J	1	ALA	-	EXPRESSION TAG	UNP Q51723
J	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
J	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
J	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
J	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
J	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
J	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
K	0	MET	-	EXPRESSION TAG	UNP Q51723
K	1	ALA	-	EXPRESSION TAG	UNP Q51723
K	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
K	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
K	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
K	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
K	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
K	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723
L	0	MET	-	EXPRESSION TAG	UNP Q51723

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ALA	-	EXPRESSION TAG	UNP Q51723
L	170	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
L	220	ALA	ARG	ENGINEERED MUTATION	UNP Q51723
L	227	PHE	TYR	ENGINEERED MUTATION	UNP Q51723
L	447	SER	PHE	ENGINEERED MUTATION	UNP Q51723
L	448	VAL	ARG	ENGINEERED MUTATION	UNP Q51723
L	449	LYS	GLU	ENGINEERED MUTATION	UNP Q51723

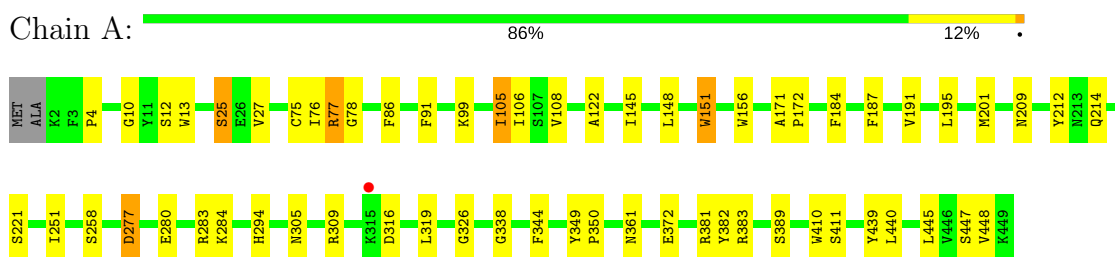
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	10	Total O 10 10	0	0
2	C	16	Total O 16 16	0	0
2	D	11	Total O 11 11	0	0
2	E	20	Total O 20 20	0	0
2	F	3	Total O 3 3	0	0
2	G	11	Total O 11 11	0	0
2	H	5	Total O 5 5	0	0
2	I	16	Total O 16 16	0	0
2	J	2	Total O 2 2	0	0
2	K	9	Total O 9 9	0	0
2	L	9	Total O 9 9	0	0

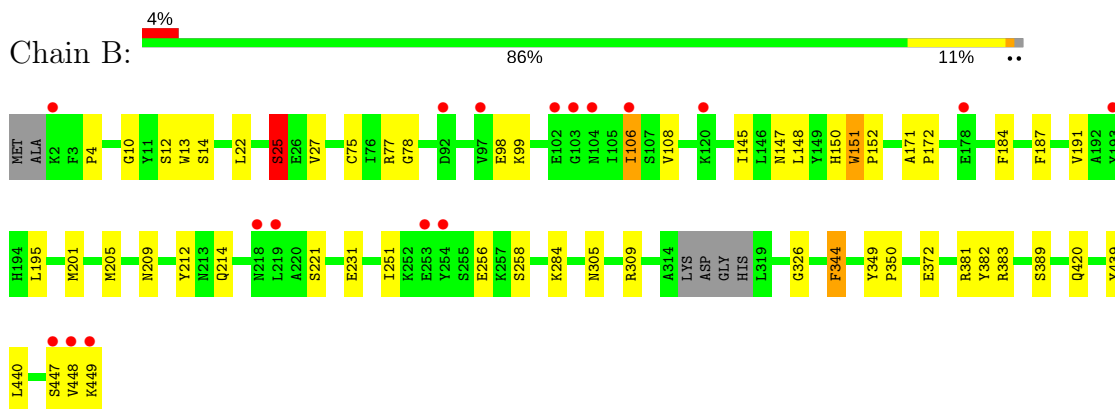
### 3 Residue-property plots [i](#)

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

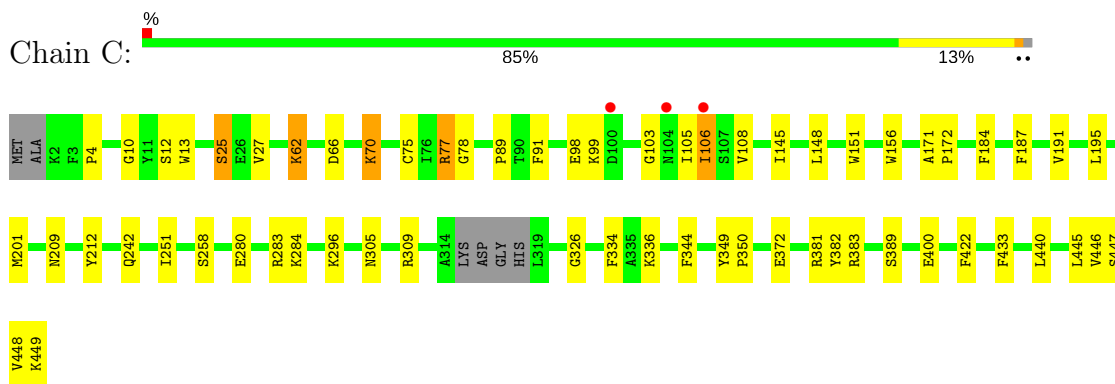
#### • Molecule 1: Beta-glucosidase



#### • Molecule 1: Beta-glucosidase

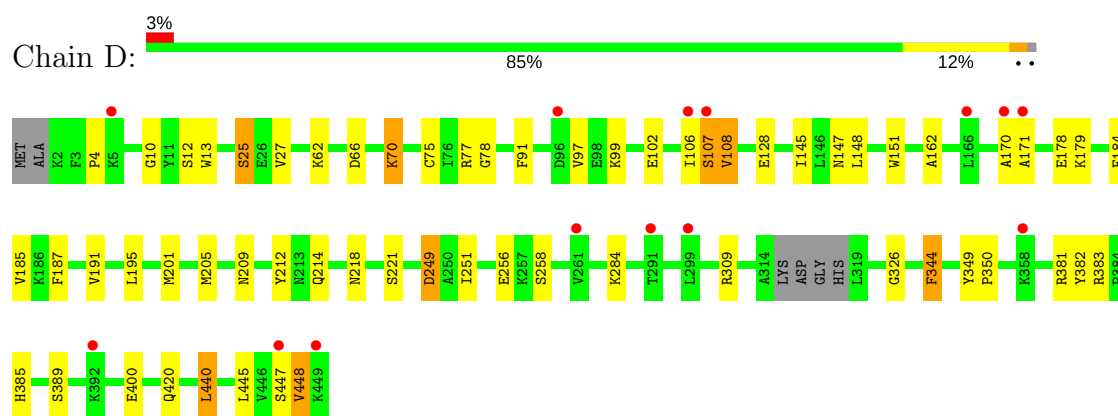


#### • Molecule 1: Beta-glucosidase

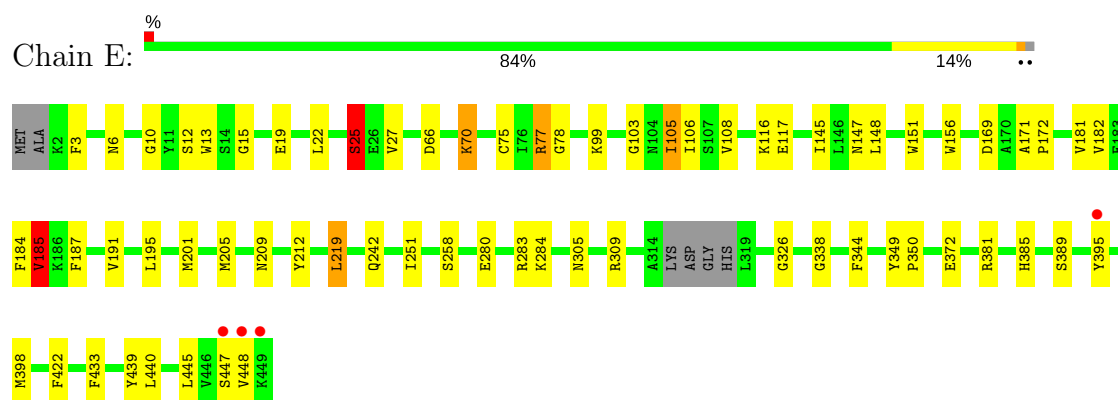


#### • Molecule 1: Beta-glucosidase

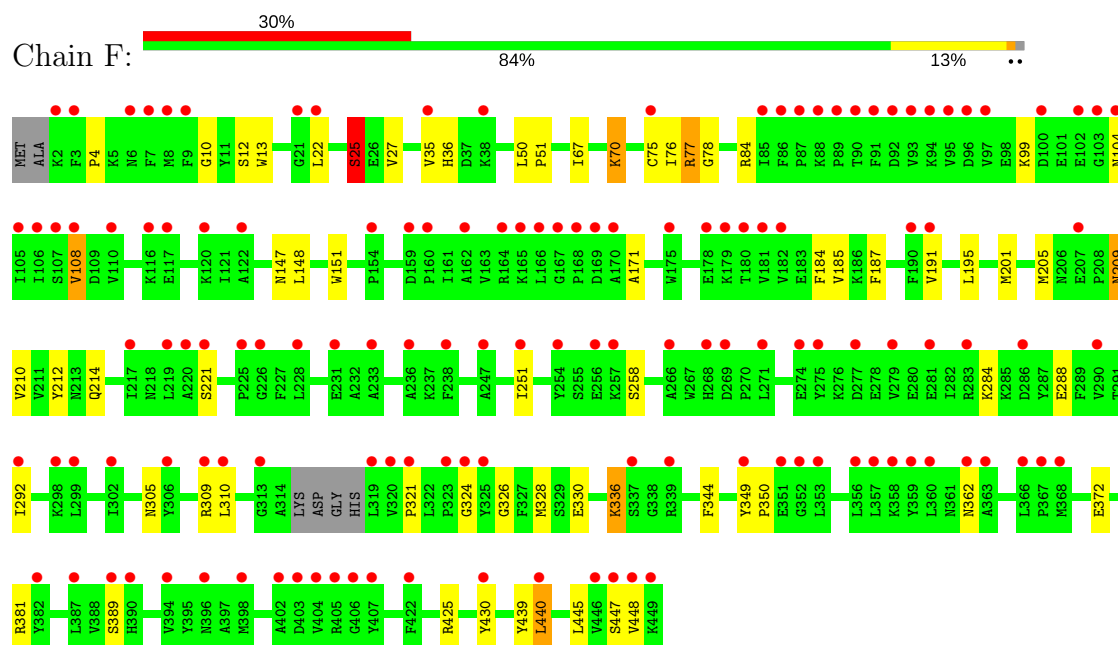




• Molecule 1: Beta-glucosidase



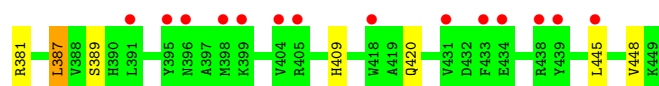
• Molecule 1: Beta-glucosidase



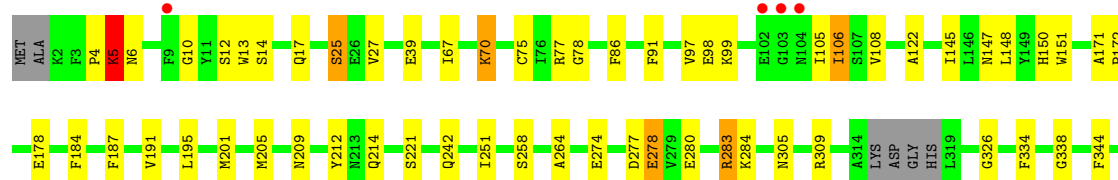
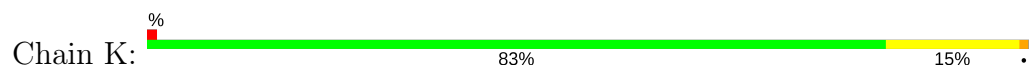
• Molecule 1: Beta-glucosidase



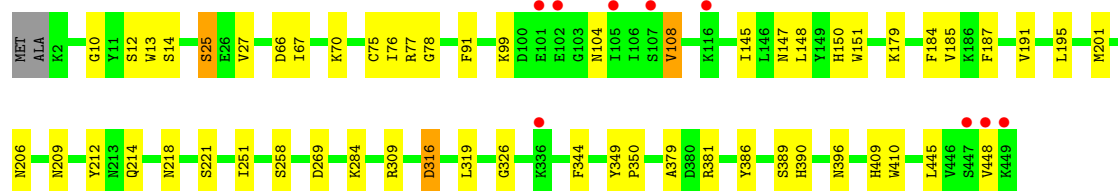
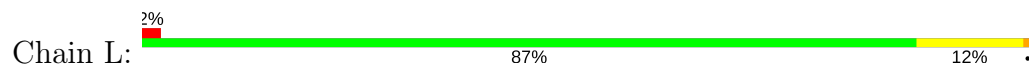




• Molecule 1: Beta-glucosidase



• Molecule 1: Beta-glucosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.36Å 148.87Å 148.56Å 120.08° 94.00° 99.70°	Depositor
Resolution (Å)	48.28 – 2.81 48.28 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.28-2.81) 78.5 (48.28-2.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.243 , 0.275 0.241 , 0.272	Depositor DCC
$R_{free}$ test set	8286 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	43762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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

### 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	0.77	0/3776	0.80	4/5124 (0.1%)
1	B	0.60	0/3743	0.71	0/5079
1	C	0.75	0/3743	0.77	2/5079 (0.0%)
1	D	0.63	2/3743 (0.1%)	0.75	2/5079 (0.0%)
1	E	0.72	0/3743	0.77	3/5079 (0.1%)
1	F	0.55	1/3743 (0.0%)	0.74	7/5079 (0.1%)
1	G	0.73	1/3776 (0.0%)	0.76	1/5124 (0.0%)
1	H	0.62	1/3776 (0.0%)	0.76	6/5124 (0.1%)
1	I	0.72	0/3743	0.77	5/5079 (0.1%)
1	J	0.54	0/3743	0.75	6/5079 (0.1%)
1	K	0.71	1/3743 (0.0%)	0.77	3/5079 (0.1%)
1	L	0.61	1/3776 (0.0%)	0.74	2/5124 (0.0%)
All	All	0.67	7/45048 (0.0%)	0.76	41/61128 (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	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	14

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	39	GLU	CD-OE2	-6.01	1.19	1.25
1	K	39	GLU	CD-OE2	-5.65	1.19	1.25
1	D	128	GLU	CB-CG	5.43	1.62	1.52
1	L	316	ASP	CB-CG	5.39	1.63	1.51
1	D	128	GLU	CD-OE2	5.33	1.31	1.25
1	F	84	ARG	C-O	5.30	1.33	1.23
1	G	410	TRP	CB-CG	-5.06	1.41	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	219	LEU	CA-CB-CG	11.57	141.91	115.30
1	H	277	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	277	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	G	5	LYS	CD-CE-NZ	9.35	133.21	111.70
1	I	277	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	C	62	LYS	CD-CE-NZ	8.69	131.70	111.70
1	D	249	ASP	CB-CA-C	-8.47	93.45	110.40
1	L	316	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	277	ASP	CB-CG-OD1	8.05	125.55	118.30
1	E	116	LYS	CG-CD-CE	7.66	134.89	111.90
1	H	102	GLU	N-CA-CB	7.65	124.37	110.60
1	F	425	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	C	296	LYS	CD-CE-NZ	7.37	128.64	111.70
1	F	84	ARG	CB-CA-C	-7.29	95.82	110.40
1	J	60	LEU	N-CA-C	-6.96	92.19	111.00
1	I	277	ASP	CB-CG-OD1	6.90	124.51	118.30
1	F	201	MET	N-CA-CB	-6.64	98.64	110.60
1	L	108	VAL	CB-CA-C	-6.55	98.96	111.40
1	K	5	LYS	N-CA-CB	-6.38	99.12	110.60
1	K	283	ARG	CG-CD-NE	6.24	124.91	111.80
1	H	101	GLU	N-CA-C	-6.14	94.41	111.00
1	F	108	VAL	CB-CA-C	-6.07	99.88	111.40
1	I	99	LYS	CD-CE-NZ	6.05	125.62	111.70
1	J	160	PRO	CB-CA-C	-6.03	96.92	112.00
1	H	109	ASP	CB-CA-C	5.95	122.31	110.40
1	E	185	VAL	CB-CA-C	-5.93	100.14	111.40
1	D	108	VAL	CB-CA-C	-5.88	100.23	111.40
1	F	425	ARG	CB-CG-CD	-5.83	96.43	111.60
1	J	361	ASN	CB-CG-OD1	-5.82	109.96	121.60
1	K	278	GLU	CA-CB-CG	-5.58	101.11	113.40
1	F	201	MET	CA-CB-CG	5.53	122.70	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	288	GLU	CG-CD-OE1	5.48	129.27	118.30
1	A	361	ASN	CB-CG-OD1	-5.47	110.65	121.60
1	J	100	ASP	CB-CG-OD1	5.46	123.21	118.30
1	J	366	LEU	CB-CA-C	5.43	120.52	110.20
1	H	278	GLU	CA-CB-CG	-5.36	101.61	113.40
1	J	108	VAL	CB-CA-C	-5.32	101.29	111.40
1	F	201	MET	CB-CA-C	5.27	120.94	110.40
1	H	262	ILE	CG1-CB-CG2	-5.17	100.04	111.40
1	A	319	LEU	CB-CG-CD1	5.10	119.68	111.00
1	I	288	GLU	CG-CD-OE2	-5.09	108.11	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	SER	Peptide
1	A	448	VAL	Peptide
1	B	25	SER	Peptide
1	C	25	SER	Peptide
1	D	25	SER	Peptide
1	E	25	SER	Peptide
1	F	209	ASN	Sidechain
1	F	25	SER	Peptide
1	G	25	SER	Peptide
1	H	25	SER	Peptide
1	I	25	SER	Peptide
1	J	25	SER	Peptide
1	K	25	SER	Peptide
1	L	25	SER	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3657	0	3505	34	1
1	B	3626	0	3477	31	1
1	C	3626	0	3477	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3626	0	3477	32	0
1	E	3626	0	3477	58	0
1	F	3626	0	3477	48	0
1	G	3657	0	3505	38	2
1	H	3657	0	3505	50	1
1	I	3626	0	3477	55	0
1	J	3626	0	3477	74	0
1	K	3626	0	3477	52	2
1	L	3657	0	3505	43	2
2	A	14	0	0	0	0
2	B	10	0	0	0	0
2	C	16	0	0	0	0
2	D	11	0	0	1	0
2	E	20	0	0	2	0
2	F	3	0	0	0	0
2	G	11	0	0	0	0
2	H	5	0	0	0	1
2	I	16	0	0	1	0
2	J	2	0	0	1	0
2	K	9	0	0	2	0
2	L	9	0	0	1	0
All	All	43762	0	41836	464	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 5.

All (464) 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:I:440:LEU:CD1	1:J:445:LEU:HD11	1.59	1.31
1:I:440:LEU:HD11	1:J:445:LEU:CD1	1.79	1.11
1:E:182:VAL:O	1:E:185:VAL:HG23	1.50	1.11
1:J:60:LEU:HB3	1:J:63:GLN:OE1	1.51	1.11
1:J:366:LEU:HD23	1:J:367:PRO:HD2	1.19	1.10
1:J:366:LEU:HD23	1:J:367:PRO:CD	1.82	1.09
1:I:440:LEU:CD1	1:J:445:LEU:CD1	2.32	1.07
1:I:99:LYS:NZ	1:I:178:GLU:OE2	1.87	1.07
1:I:440:LEU:HD12	1:J:445:LEU:HD11	1.37	1.04
1:J:37:ASP:O	1:J:41:ILE:HG23	1.62	0.99
1:K:70:LYS:HZ2	1:L:445:LEU:HB2	1.29	0.98
1:E:395:TYR:HA	1:E:398:MET:CE	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:ILE:HG22	1:K:242:GLN:OE1	1.66	0.95
1:E:439:TYR:HB3	1:F:439:TYR:CB	1.96	0.95
1:I:440:LEU:HD11	1:J:445:LEU:HD13	1.48	0.93
1:E:3:PHE:HE1	1:E:398:MET:HE1	1.34	0.92
1:E:105:ILE:HG22	1:E:242:GLN:OE1	1.69	0.92
1:J:57:TYR:HA	1:J:60:LEU:O	1.70	0.91
1:E:439:TYR:HB3	1:F:439:TYR:HB3	1.50	0.91
1:E:395:TYR:HA	1:E:398:MET:HE2	1.54	0.89
1:C:105:ILE:HG22	1:C:242:GLN:OE1	1.70	0.89
1:H:105:ILE:HG22	1:H:242:GLN:OE1	1.73	0.89
1:J:366:LEU:CD2	1:J:367:PRO:HD2	2.01	0.88
1:C:446:VAL:O	1:C:449:LYS:HG3	1.74	0.87
1:K:437:LYS:HE3	1:L:379:ALA:HB1	1.59	0.85
1:K:280:GLU:HG3	1:K:283:ARG:HH21	1.43	0.83
1:D:170:ALA:O	1:F:324:GLY:HA3	1.78	0.83
1:I:23:PRO:HA	1:I:26:GLU:OE2	1.80	0.82
1:C:280:GLU:HG3	1:C:283:ARG:HH21	1.46	0.80
1:I:280:GLU:HG3	1:I:283:ARG:HH21	1.46	0.80
1:A:280:GLU:HG3	1:A:283:ARG:HH21	1.47	0.79
1:I:448:VAL:HG11	1:J:448:VAL:CG1	2.12	0.79
1:J:99:LYS:NZ	1:J:178:GLU:OE2	2.16	0.79
1:K:70:LYS:HE3	1:L:445:LEU:HD13	1.63	0.79
1:K:280:GLU:HG3	1:K:283:ARG:NH2	1.99	0.77
1:K:417:GLU:OE2	2:K:505:HOH:O	2.01	0.77
1:G:105:ILE:HD11	1:G:108:VAL:CG2	2.15	0.77
1:C:280:GLU:HG3	1:C:283:ARG:NH2	2.00	0.76
1:K:17:GLN:OE1	1:K:418:TRP:NE1	2.17	0.76
1:L:99:LYS:O	2:L:504:HOH:O	2.03	0.76
1:H:162:ALA:HB2	1:J:330:GLU:HG3	1.68	0.76
1:D:99:LYS:NZ	1:D:178:GLU:OE2	2.19	0.76
1:F:67:ILE:HA	1:F:70:LYS:HE2	1.68	0.76
1:E:445:LEU:HD13	1:F:70:LYS:HE3	1.67	0.75
1:H:203:SER:CB	1:H:262:ILE:HD13	2.17	0.75
1:H:203:SER:OG	1:H:262:ILE:HD13	1.87	0.75
1:I:280:GLU:HG3	1:I:283:ARG:NH2	2.01	0.75
1:E:6:ASN:ND2	2:E:501:HOH:O	2.20	0.74
1:J:60:LEU:CB	1:J:63:GLN:OE1	2.33	0.73
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.02	0.73
1:G:440:LEU:HD11	1:H:445:LEU:HD11	1.69	0.72
1:L:91:PHE:CD1	1:L:179:LYS:HE2	2.24	0.72
1:K:70:LYS:CE	1:L:445:LEU:HD13	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:PHE:CE1	1:E:398:MET:HE1	2.23	0.71
1:A:439:TYR:HB3	1:B:439:TYR:HB3	1.72	0.71
1:I:448:VAL:CG1	1:J:448:VAL:HG12	2.21	0.71
1:K:70:LYS:HD3	1:L:445:LEU:HB3	1.71	0.71
1:H:40:ASN:HD21	1:H:164:ARG:HH12	1.37	0.70
1:F:35:VAL:HG23	1:F:36:HIS:CE1	2.26	0.70
1:E:445:LEU:HD11	1:F:440:LEU:HD11	1.73	0.70
1:L:350:PRO:HB3	1:L:390:HIS:CD2	2.28	0.69
1:I:440:LEU:CG	1:J:445:LEU:HD11	2.21	0.69
1:E:439:TYR:HB3	1:F:439:TYR:HB2	1.74	0.69
1:K:70:LYS:NZ	1:L:445:LEU:HB2	2.06	0.68
1:L:91:PHE:CE1	1:L:179:LYS:HE2	2.28	0.68
1:F:171:ALA:HA	1:H:336:LYS:HE2	1.76	0.67
1:E:3:PHE:HE1	1:E:398:MET:CE	2.06	0.67
1:I:448:VAL:CG1	1:J:448:VAL:CG1	2.71	0.67
1:J:37:ASP:O	1:J:41:ILE:CG2	2.41	0.67
1:I:445:LEU:CD2	1:J:448:VAL:HG21	2.25	0.66
1:I:70:LYS:HE3	1:J:445:LEU:HB2	1.78	0.66
1:F:108:VAL:HG11	1:F:185:VAL:HG11	1.78	0.66
1:A:338:GLY:HA3	1:C:91:PHE:CE2	2.31	0.65
1:H:280:GLU:HG2	1:H:283:ARG:NH2	2.11	0.65
1:K:67:ILE:HA	1:K:70:LYS:HE2	1.77	0.65
1:I:403:ASP:OD2	2:I:515:HOH:O	2.14	0.65
1:F:36:HIS:HE1	1:F:51:PRO:HD2	1.61	0.64
1:J:108:VAL:HG11	1:J:185:VAL:HG11	1.78	0.64
1:F:321:PRO:HB2	1:F:328:MET:HE1	1.79	0.64
1:H:203:SER:HB2	1:H:262:ILE:HD13	1.80	0.64
1:E:280:GLU:OE1	1:E:283:ARG:NH2	2.31	0.64
1:E:439:TYR:CB	1:F:439:TYR:HB3	2.27	0.64
1:D:108:VAL:HG11	1:D:185:VAL:HG11	1.79	0.64
1:D:162:ALA:HB2	1:F:330:GLU:HG3	1.79	0.64
1:L:108:VAL:HG11	1:L:185:VAL:HG11	1.80	0.63
1:E:3:PHE:CE1	1:E:398:MET:CE	2.80	0.63
1:C:440:LEU:HD11	1:D:445:LEU:HD11	1.79	0.63
1:H:268:HIS:HD2	1:H:312:TYR:OH	1.83	0.62
1:E:445:LEU:HD11	1:F:440:LEU:CD1	2.29	0.62
1:F:36:HIS:CE1	1:F:50:LEU:HD22	2.36	0.61
1:E:182:VAL:HA	1:E:185:VAL:CG2	2.31	0.61
1:D:249:ASP:OD1	1:D:249:ASP:O	2.17	0.61
1:C:336:LYS:HE2	1:E:169:ASP:C	2.21	0.61
1:F:36:HIS:ND1	1:F:50:LEU:HD22	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:299:LEU:O	1:J:366:LEU:HD11	2.01	0.60
1:I:70:LYS:HE3	1:J:445:LEU:HD13	1.83	0.60
1:H:40:ASN:ND2	1:H:45:LEU:HD23	2.16	0.60
1:F:209:ASN:HD21	1:F:210:VAL:HG23	1.65	0.60
1:J:301:TRP:HA	1:J:366:LEU:HD22	1.84	0.60
1:J:99:LYS:HE2	1:J:105:ILE:HG12	1.82	0.60
1:A:439:TYR:CB	1:B:439:TYR:HB3	2.32	0.60
1:J:300:ASP:O	1:J:366:LEU:HD21	2.02	0.59
1:E:439:TYR:CD1	1:F:430:TYR:CD2	2.90	0.59
1:J:38:LYS:O	1:J:41:ILE:HG12	2.03	0.59
1:I:448:VAL:HG11	1:J:448:VAL:HB	1.84	0.59
1:F:209:ASN:HA	1:F:212:TYR:CZ	2.38	0.59
1:C:66:ASP:O	1:C:70:LYS:HG2	2.03	0.59
1:G:99:LYS:HB3	1:G:104:ASN:O	2.02	0.58
1:G:437:LYS:HE3	1:H:379:ALA:HA	1.85	0.58
1:G:336:LYS:HE2	1:I:169:ASP:C	2.24	0.58
1:A:294:HIS:HD1	1:A:294:HIS:C	2.06	0.58
1:G:105:ILE:HD11	1:G:108:VAL:HG23	1.84	0.58
1:A:439:TYR:HB3	1:B:439:TYR:CB	2.32	0.58
1:B:214:GLN:HE21	1:B:221:SER:CB	2.17	0.58
1:I:448:VAL:HG11	1:J:448:VAL:CB	2.35	0.57
1:K:70:LYS:NZ	1:L:445:LEU:HD13	2.20	0.57
1:E:182:VAL:C	1:E:185:VAL:HG23	2.23	0.56
1:E:385:HIS:CE1	1:E:389:SER:HB3	2.40	0.56
1:I:440:LEU:HD12	1:J:445:LEU:CD1	2.19	0.56
1:B:214:GLN:NE2	1:B:221:SER:HB3	2.21	0.56
1:G:105:ILE:HG22	1:G:242:GLN:OE1	2.06	0.56
1:J:67:ILE:HA	1:J:70:LYS:HE2	1.87	0.55
1:A:445:LEU:HD11	1:B:440:LEU:HD11	1.88	0.55
1:E:439:TYR:CE1	1:F:430:TYR:CD2	2.95	0.55
1:H:105:ILE:HG23	1:H:105:ILE:O	2.07	0.55
1:K:209:ASN:HA	1:K:212:TYR:CZ	2.42	0.55
1:A:91:PHE:CE2	1:K:338:GLY:HA3	2.42	0.55
1:H:162:ALA:CB	1:J:330:GLU:HG3	2.34	0.55
1:K:70:LYS:CD	1:L:445:LEU:HB3	2.37	0.54
1:K:214:GLN:NE2	1:K:221:SER:HB3	2.23	0.54
1:E:338:GLY:HA3	1:G:91:PHE:CE2	2.42	0.54
1:A:156:TRP:HB3	1:K:334:PHE:CD2	2.42	0.54
1:A:105:ILE:O	1:A:105:ILE:HG23	2.07	0.54
1:G:105:ILE:O	1:G:105:ILE:HG23	2.08	0.54
1:I:448:VAL:HB	1:J:448:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:HD2	1:C:103:GLY:HA2	1.90	0.54
1:G:448:VAL:HG11	1:H:448:VAL:HG11	1.89	0.53
1:K:214:GLN:HE21	1:K:221:SER:CB	2.20	0.53
1:K:440:LEU:HD11	1:L:445:LEU:HD11	1.90	0.53
1:K:5:LYS:HG2	1:K:6:ASN:N	2.21	0.53
1:E:99:LYS:HD3	1:E:103:GLY:HA2	1.89	0.53
1:J:288:GLU:O	1:J:292:ILE:HG22	2.09	0.53
1:C:336:LYS:CE	1:E:169:ASP:C	2.77	0.53
1:E:66:ASP:O	1:E:70:LYS:HG2	2.09	0.53
1:J:300:ASP:C	1:J:366:LEU:HD21	2.29	0.53
1:I:70:LYS:HE3	1:J:445:LEU:CB	2.39	0.53
1:F:36:HIS:CE1	1:F:51:PRO:HD2	2.44	0.53
1:H:162:ALA:HB2	1:J:330:GLU:CG	2.38	0.53
1:I:105:ILE:O	1:I:105:ILE:HG23	2.09	0.53
1:I:338:GLY:HA3	1:K:91:PHE:CE2	2.44	0.53
1:C:105:ILE:HG23	1:C:105:ILE:O	2.10	0.53
1:J:372:GLU:OE1	2:J:502:HOH:O	2.19	0.52
1:F:35:VAL:HG23	1:F:36:HIS:ND1	2.25	0.52
1:K:105:ILE:O	1:K:105:ILE:HG23	2.08	0.52
1:I:105:ILE:HG22	1:I:242:GLN:OE1	2.10	0.52
1:E:105:ILE:O	1:E:105:ILE:HG23	2.09	0.52
1:H:40:ASN:ND2	1:H:45:LEU:CD2	2.73	0.52
1:I:209:ASN:HA	1:I:212:TYR:CZ	2.45	0.52
1:F:288:GLU:O	1:F:292:ILE:HG22	2.09	0.51
1:F:309:ARG:O	1:F:326:GLY:HA3	2.10	0.51
1:G:309:ARG:O	1:G:326:GLY:HA3	2.09	0.51
1:C:77:ARG:C	1:C:77:ARG:HD2	2.31	0.51
1:G:334:PHE:CD2	1:I:156:TRP:HB3	2.46	0.51
1:J:366:LEU:HD23	1:J:367:PRO:N	2.24	0.51
1:E:13:TRP:CE2	1:E:78:GLY:HA3	2.45	0.51
1:H:283:ARG:HD3	1:H:359:TYR:CE2	2.45	0.51
1:E:439:TYR:CB	1:F:439:TYR:CB	2.82	0.51
1:F:321:PRO:HB2	1:F:328:MET:CE	2.41	0.51
1:I:448:VAL:CB	1:J:448:VAL:HG11	2.41	0.51
1:E:309:ARG:O	1:E:326:GLY:HA3	2.11	0.51
1:E:6:ASN:HB2	2:E:502:HOH:O	2.10	0.50
1:H:305:ASN:CG	1:H:372:GLU:HB2	2.32	0.50
1:D:309:ARG:O	1:D:326:GLY:HA3	2.11	0.50
1:D:10:GLY:HA3	1:D:75:CYS:O	2.11	0.50
1:H:203:SER:HB2	1:H:262:ILE:CD1	2.40	0.50
1:L:309:ARG:O	1:L:326:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:O	1:A:326:GLY:HA3	2.12	0.50
1:B:214:GLN:HE21	1:B:221:SER:HB2	1.76	0.50
1:D:13:TRP:CE2	1:D:78:GLY:HA3	2.47	0.50
1:F:13:TRP:CE2	1:F:78:GLY:HA3	2.47	0.50
1:H:280:GLU:HG2	1:H:283:ARG:HH21	1.75	0.50
1:H:309:ARG:O	1:H:326:GLY:HA3	2.12	0.50
1:L:145:ILE:HG12	1:L:201:MET:HB2	1.94	0.50
1:C:309:ARG:O	1:C:326:GLY:HA3	2.12	0.50
1:J:99:LYS:HE2	1:J:105:ILE:CG1	2.42	0.50
1:K:309:ARG:O	1:K:326:GLY:HA3	2.12	0.50
1:L:10:GLY:HA3	1:L:75:CYS:O	2.12	0.50
1:B:10:GLY:HA3	1:B:75:CYS:O	2.13	0.49
1:B:309:ARG:O	1:B:326:GLY:HA3	2.12	0.49
1:C:446:VAL:O	1:C:449:LYS:CG	2.56	0.49
1:G:209:ASN:HA	1:G:212:TYR:CZ	2.48	0.49
1:K:437:LYS:HE3	1:L:379:ALA:CB	2.37	0.49
1:A:12:SER:HA	1:A:77:ARG:O	2.12	0.49
1:B:12:SER:HA	1:B:77:ARG:O	2.12	0.49
1:C:10:GLY:HA3	1:C:75:CYS:O	2.12	0.49
1:I:10:GLY:HA3	1:I:75:CYS:O	2.12	0.49
1:J:12:SER:HA	1:J:77:ARG:O	2.13	0.49
1:L:67:ILE:HA	1:L:70:LYS:HE2	1.93	0.49
1:A:209:ASN:HA	1:A:212:TYR:CZ	2.47	0.49
1:G:437:LYS:HE3	1:H:379:ALA:CA	2.43	0.49
1:E:439:TYR:CE1	1:F:430:TYR:CG	3.00	0.49
1:J:10:GLY:HA3	1:J:75:CYS:O	2.13	0.49
1:K:10:GLY:HA3	1:K:75:CYS:O	2.13	0.49
1:E:10:GLY:HA3	1:E:75:CYS:O	2.12	0.49
1:C:209:ASN:HA	1:C:212:TYR:CZ	2.48	0.49
1:F:209:ASN:ND2	1:F:210:VAL:N	2.61	0.49
1:K:214:GLN:HE21	1:K:221:SER:HB2	1.77	0.49
1:K:70:LYS:HZ1	1:L:445:LEU:HD13	1.77	0.49
1:F:12:SER:HA	1:F:77:ARG:O	2.13	0.48
1:E:148:LEU:HD11	1:E:251:ILE:HD11	1.95	0.48
1:C:12:SER:HA	1:C:77:ARG:O	2.13	0.48
1:G:336:LYS:CE	1:I:169:ASP:O	2.61	0.48
1:C:336:LYS:CE	1:E:169:ASP:O	2.62	0.48
1:I:12:SER:HA	1:I:77:ARG:O	2.14	0.48
1:L:209:ASN:HA	1:L:212:TYR:CZ	2.49	0.48
1:B:145:ILE:HG12	1:B:201:MET:HB2	1.96	0.48
1:K:70:LYS:HZ1	1:L:445:LEU:CD1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:CE2	1:B:78:GLY:HA3	2.49	0.48
1:C:105:ILE:CG2	1:C:242:GLN:OE1	2.54	0.48
1:H:179:LYS:HD3	1:H:179:LYS:HA	1.56	0.48
1:L:12:SER:HA	1:L:77:ARG:O	2.13	0.48
1:H:12:SER:HA	1:H:77:ARG:O	2.14	0.48
1:D:12:SER:HA	1:D:77:ARG:O	2.14	0.48
1:E:12:SER:HA	1:E:77:ARG:O	2.14	0.48
1:G:10:GLY:HA3	1:G:75:CYS:O	2.14	0.48
1:I:148:LEU:HD11	1:I:251:ILE:HD11	1.96	0.48
1:J:309:ARG:O	1:J:326:GLY:HA3	2.14	0.48
1:J:209:ASN:HA	1:J:212:TYR:CZ	2.49	0.48
1:K:145:ILE:HG12	1:K:201:MET:HB2	1.96	0.48
1:J:13:TRP:CE2	1:J:78:GLY:HA3	2.49	0.48
1:A:184:PHE:O	1:A:187:PHE:HB3	2.14	0.47
1:D:145:ILE:HG12	1:D:201:MET:HB2	1.96	0.47
1:H:10:GLY:HA3	1:H:75:CYS:O	2.13	0.47
1:I:70:LYS:CE	1:J:445:LEU:HB2	2.44	0.47
1:K:17:GLN:OE1	1:K:418:TRP:CD1	2.67	0.47
1:K:105:ILE:CG2	1:K:242:GLN:OE1	2.52	0.47
1:F:10:GLY:HA3	1:F:75:CYS:O	2.13	0.47
1:G:145:ILE:HG12	1:G:201:MET:HB2	1.96	0.47
1:H:209:ASN:HA	1:H:212:TYR:CZ	2.49	0.47
1:I:309:ARG:O	1:I:326:GLY:HA3	2.14	0.47
1:J:145:ILE:HG12	1:J:201:MET:HB2	1.96	0.47
1:L:409:HIS:HD2	1:L:410:TRP:C	2.18	0.47
1:J:38:LYS:HA	1:J:41:ILE:HD13	1.96	0.47
1:J:57:TYR:CA	1:J:60:LEU:O	2.53	0.47
1:F:148:LEU:HD11	1:F:251:ILE:HD11	1.97	0.47
1:G:77:ARG:C	1:G:77:ARG:HD2	2.34	0.47
1:I:191:VAL:HG13	1:I:195:LEU:HD12	1.97	0.47
1:K:12:SER:HA	1:K:77:ARG:O	2.14	0.47
1:A:148:LEU:HD11	1:A:251:ILE:HD11	1.96	0.47
1:L:148:LEU:HD11	1:L:251:ILE:HD11	1.96	0.47
1:D:209:ASN:HA	1:D:212:TYR:CZ	2.49	0.47
1:C:445:LEU:HD11	1:D:440:LEU:HD11	1.97	0.47
1:I:13:TRP:CE2	1:I:78:GLY:HA3	2.50	0.47
1:E:171:ALA:HB1	1:E:172:PRO:HD2	1.97	0.47
1:E:395:TYR:CA	1:E:398:MET:HE2	2.37	0.47
1:H:145:ILE:HG12	1:H:201:MET:HB2	1.95	0.47
1:H:184:PHE:O	1:H:187:PHE:HB3	2.15	0.47
1:L:13:TRP:CE2	1:L:78:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:CE2	1:A:78:GLY:HA3	2.50	0.46
1:E:181:VAL:O	1:E:185:VAL:HG22	2.14	0.46
1:J:58:TRP:NE1	1:J:129:HIS:CE1	2.83	0.46
1:K:171:ALA:HB1	1:K:172:PRO:HD2	1.97	0.46
1:K:70:LYS:NZ	1:L:445:LEU:CD1	2.79	0.46
1:I:99:LYS:HE2	1:I:103:GLY:C	2.35	0.46
1:K:191:VAL:HG13	1:K:195:LEU:HD12	1.97	0.46
1:H:283:ARG:CD	1:H:359:TYR:CE2	2.98	0.46
1:B:209:ASN:HA	1:B:212:TYR:CZ	2.51	0.46
1:G:12:SER:HA	1:G:77:ARG:O	2.15	0.46
1:G:184:PHE:O	1:G:187:PHE:HB3	2.15	0.46
1:I:145:ILE:HG12	1:I:201:MET:HB2	1.96	0.46
1:J:99:LYS:HB3	1:J:104:ASN:O	2.16	0.46
1:L:99:LYS:HB3	1:L:104:ASN:O	2.16	0.46
1:C:148:LEU:HD11	1:C:251:ILE:HD11	1.97	0.46
1:G:437:LYS:HE3	1:H:379:ALA:CB	2.46	0.46
1:H:148:LEU:HD11	1:H:251:ILE:HD11	1.97	0.46
1:K:184:PHE:O	1:K:187:PHE:HB3	2.16	0.46
1:F:184:PHE:O	1:F:187:PHE:HB3	2.16	0.46
1:H:105:ILE:CG2	1:H:242:GLN:OE1	2.54	0.46
1:B:448:VAL:O	1:B:449:LYS:HG3	2.14	0.46
1:C:145:ILE:HG12	1:C:201:MET:HB2	1.98	0.46
1:G:13:TRP:CE2	1:G:78:GLY:HA3	2.51	0.46
1:G:148:LEU:HD11	1:G:251:ILE:HD11	1.97	0.46
1:H:280:GLU:OE1	1:H:284:LYS:NZ	2.33	0.46
1:J:148:LEU:HD11	1:J:251:ILE:HD11	1.96	0.46
1:E:184:PHE:O	1:E:187:PHE:HB3	2.16	0.45
1:J:184:PHE:O	1:J:187:PHE:HB3	2.16	0.45
1:A:10:GLY:HA3	1:A:75:CYS:O	2.15	0.45
1:C:171:ALA:HB1	1:C:172:PRO:HD2	1.99	0.45
1:F:310:LEU:HD22	1:F:328:MET:HE1	1.98	0.45
1:A:145:ILE:HG12	1:A:201:MET:HB2	1.97	0.45
1:C:184:PHE:O	1:C:187:PHE:HB3	2.17	0.45
1:I:448:VAL:HG11	1:J:448:VAL:HG12	1.84	0.45
1:K:148:LEU:HD11	1:K:251:ILE:HD11	1.99	0.45
1:A:171:ALA:HB1	1:A:172:PRO:HD2	1.98	0.45
1:E:145:ILE:HG12	1:E:201:MET:HB2	1.98	0.45
1:F:99:LYS:HB3	1:F:104:ASN:O	2.16	0.45
1:J:301:TRP:HA	1:J:366:LEU:CD2	2.45	0.45
1:A:338:GLY:HA3	1:C:91:PHE:CD2	2.52	0.45
1:K:13:TRP:CE2	1:K:78:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:VAL:HG13	1:B:195:LEU:HD12	1.99	0.45
1:E:448:VAL:HG11	1:F:448:VAL:HG11	1.98	0.45
1:L:184:PHE:O	1:L:187:PHE:HB3	2.17	0.45
1:D:148:LEU:HD11	1:D:251:ILE:HD11	1.98	0.45
1:C:445:LEU:HB3	1:D:70:LYS:HD3	1.99	0.45
1:A:309:ARG:HD3	1:A:349:TYR:CE2	2.52	0.45
1:B:148:LEU:HD11	1:B:251:ILE:HD11	1.98	0.45
1:B:214:GLN:NE2	1:B:221:SER:CB	2.79	0.45
1:H:309:ARG:HD3	1:H:349:TYR:CE2	2.52	0.45
1:C:382:TYR:O	1:C:383:ARG:C	2.56	0.45
1:G:334:PHE:CE2	1:I:156:TRP:HB3	2.51	0.45
1:E:338:GLY:HA3	1:G:91:PHE:CD2	2.52	0.44
1:H:13:TRP:CE2	1:H:78:GLY:HA3	2.52	0.44
1:K:214:GLN:NE2	1:K:221:SER:CB	2.80	0.44
1:K:305:ASN:CG	1:K:372:GLU:HB2	2.38	0.44
1:A:445:LEU:HD11	1:B:440:LEU:CD1	2.47	0.44
1:B:184:PHE:O	1:B:187:PHE:HB3	2.17	0.44
1:D:66:ASP:O	1:D:70:LYS:HG2	2.17	0.44
1:E:191:VAL:HG13	1:E:195:LEU:HD12	2.00	0.44
1:L:309:ARG:HD3	1:L:349:TYR:CE2	2.52	0.44
1:C:336:LYS:HE3	1:E:169:ASP:HA	2.00	0.44
1:G:171:ALA:HB1	1:G:172:PRO:HD2	1.99	0.44
1:J:191:VAL:HG13	1:J:195:LEU:HD12	1.99	0.44
1:K:77:ARG:C	1:K:77:ARG:HD2	2.37	0.44
1:D:191:VAL:HG13	1:D:195:LEU:HD12	1.98	0.44
1:L:14:SER:HB3	1:L:150:HIS:CE1	2.52	0.44
1:A:191:VAL:HG13	1:A:195:LEU:HD12	1.99	0.44
1:K:409:HIS:HD2	1:K:410:TRP:C	2.21	0.44
1:L:66:ASP:O	1:L:70:LYS:HG2	2.18	0.44
1:B:147:ASN:HD21	1:B:205:MET:CA	2.31	0.44
1:A:294:HIS:C	1:A:294:HIS:ND1	2.69	0.44
1:C:191:VAL:HG13	1:C:195:LEU:HD12	2.00	0.44
1:A:382:TYR:O	1:A:383:ARG:C	2.56	0.44
1:C:350:PRO:HG3	1:C:389:SER:HB2	2.00	0.44
1:E:209:ASN:HA	1:E:212:TYR:CZ	2.53	0.44
1:F:350:PRO:HG3	1:F:389:SER:HB2	2.00	0.44
1:L:409:HIS:CD2	1:L:410:TRP:N	2.85	0.44
1:C:305:ASN:CG	1:C:372:GLU:HB2	2.39	0.44
1:D:77:ARG:C	1:D:77:ARG:HD2	2.38	0.44
1:G:191:VAL:HG13	1:G:195:LEU:HD12	2.00	0.44
1:C:448:VAL:HG11	1:D:448:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:VAL:HG13	1:H:195:LEU:HD12	2.00	0.43
1:L:350:PRO:HB3	1:L:390:HIS:HD2	1.78	0.43
1:A:350:PRO:HG3	1:A:389:SER:HB2	2.00	0.43
1:F:191:VAL:HG13	1:F:195:LEU:HD12	1.99	0.43
1:G:409:HIS:CD2	1:G:410:TRP:N	2.86	0.43
1:E:350:PRO:HG3	1:E:389:SER:HB2	2.00	0.43
1:I:70:LYS:HE3	1:J:445:LEU:CD1	2.47	0.43
1:A:76:ILE:HG22	1:A:77:ARG:N	2.33	0.43
1:D:108:VAL:HG11	1:D:185:VAL:CG1	2.48	0.43
1:C:334:PHE:CD2	1:E:156:TRP:HB3	2.54	0.43
1:F:309:ARG:HD3	1:F:349:TYR:CE2	2.53	0.43
1:G:70:LYS:HD3	1:H:445:LEU:O	2.18	0.43
1:A:77:ARG:HD2	1:A:77:ARG:C	2.39	0.43
1:B:77:ARG:C	1:B:77:ARG:HD2	2.38	0.43
1:D:107:SER:C	1:D:108:VAL:HG23	2.39	0.43
1:D:309:ARG:HD3	1:D:349:TYR:CE2	2.54	0.43
1:G:409:HIS:HD2	1:G:410:TRP:C	2.22	0.43
1:F:77:ARG:HD2	1:F:77:ARG:C	2.39	0.43
1:I:171:ALA:HB1	1:I:172:PRO:HD2	1.99	0.43
1:I:382:TYR:O	1:I:383:ARG:C	2.56	0.43
1:J:344:PHE:CZ	1:J:420:GLN:HG3	2.54	0.43
1:C:309:ARG:HD3	1:C:349:TYR:CE2	2.54	0.43
1:D:344:PHE:CZ	1:D:420:GLN:HG3	2.54	0.43
1:I:184:PHE:O	1:I:187:PHE:HB3	2.19	0.43
1:D:350:PRO:HG3	1:D:389:SER:HB2	2.01	0.43
1:E:422:PHE:CD1	1:E:433:PHE:CE2	3.07	0.43
1:H:214:GLN:OE1	1:H:221:SER:HB3	2.19	0.43
1:G:445:LEU:HD11	1:H:440:LEU:HD11	2.00	0.43
1:J:309:ARG:HD3	1:J:349:TYR:CE2	2.54	0.43
1:L:191:VAL:HG13	1:L:195:LEU:HD12	2.01	0.43
1:D:184:PHE:O	1:D:187:PHE:HB3	2.19	0.42
1:E:309:ARG:HD3	1:E:349:TYR:CE2	2.54	0.42
1:F:214:GLN:OE1	1:F:221:SER:HB3	2.19	0.42
1:G:440:LEU:CD1	1:H:445:LEU:HD11	2.44	0.42
1:K:97:VAL:N	2:K:506:HOH:O	2.35	0.42
1:D:171:ALA:N	1:F:336:LYS:HG3	2.34	0.42
1:I:98:GLU:HB2	1:I:106:ILE:HG22	2.01	0.42
1:K:70:LYS:HD2	1:L:445:LEU:HD22	2.02	0.42
1:J:160:PRO:HG2	1:J:160:PRO:O	2.19	0.42
1:L:147:ASN:HD21	1:L:206:ASN:HB2	1.85	0.42
1:J:214:GLN:OE1	1:J:221:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:TRP:CE2	1:C:78:GLY:HA3	2.55	0.42
1:J:66:ASP:O	1:J:70:LYS:HG2	2.19	0.42
1:D:147:ASN:HD21	1:D:205:MET:CA	2.33	0.42
1:G:98:GLU:HB2	1:G:106:ILE:HG22	2.02	0.42
1:H:77:ARG:C	1:H:77:ARG:HD2	2.40	0.42
1:I:448:VAL:HG12	1:J:448:VAL:HG12	2.01	0.42
1:H:171:ALA:HB1	1:H:172:PRO:HD2	2.02	0.42
1:K:382:TYR:O	1:K:383:ARG:C	2.57	0.42
1:A:151:TRP:CD1	1:A:151:TRP:N	2.85	0.42
1:B:305:ASN:CG	1:B:372:GLU:HB2	2.40	0.42
1:B:344:PHE:CZ	1:B:420:GLN:HG3	2.55	0.42
1:G:305:ASN:CG	1:G:372:GLU:HB2	2.41	0.42
1:J:147:ASN:HD21	1:J:205:MET:CA	2.32	0.42
1:D:97:VAL:HG22	1:D:108:VAL:HG13	2.02	0.42
1:G:445:LEU:HA	1:G:448:VAL:HG23	2.02	0.42
1:H:350:PRO:HG3	1:H:389:SER:HB2	2.01	0.42
1:I:76:ILE:HG22	1:I:77:ARG:N	2.34	0.42
1:F:445:LEU:HA	1:F:448:VAL:HG23	2.02	0.41
1:L:396:ASN:HA	1:L:396:ASN:HD22	1.64	0.41
1:B:14:SER:HB3	1:B:150:HIS:CE1	2.55	0.41
1:B:350:PRO:HG3	1:B:389:SER:HB2	2.02	0.41
1:I:91:PHE:CD1	1:I:179:LYS:HE3	2.56	0.41
1:J:171:ALA:HB1	1:J:172:PRO:HD2	2.02	0.41
1:J:350:PRO:HG3	1:J:389:SER:HB2	2.02	0.41
1:J:387:LEU:HD21	1:J:409:HIS:NE2	2.34	0.41
1:J:41:ILE:CG1	1:J:42:ALA:N	2.84	0.41
1:I:445:LEU:HD23	1:J:448:VAL:HG21	2.00	0.41
1:B:309:ARG:HD3	1:B:349:TYR:CE2	2.54	0.41
1:J:445:LEU:HA	1:J:448:VAL:HG23	2.02	0.41
1:K:147:ASN:HD21	1:K:205:MET:CA	2.33	0.41
1:K:14:SER:HB3	1:K:150:HIS:CE1	2.55	0.41
1:L:386:TYR:CZ	1:L:390:HIS:CE1	3.09	0.41
1:H:319:LEU:HD23	1:H:319:LEU:O	2.21	0.41
1:L:214:GLN:OE1	1:L:221:SER:HB3	2.20	0.41
1:A:214:GLN:OE1	1:A:221:SER:HB3	2.21	0.41
1:C:98:GLU:HB2	1:C:106:ILE:HG22	2.03	0.41
1:G:309:ARG:HD3	1:G:349:TYR:CE2	2.55	0.41
1:C:445:LEU:HA	1:C:448:VAL:HG23	2.03	0.41
1:E:77:ARG:HD2	1:E:77:ARG:C	2.40	0.41
1:K:86:PHE:CE1	1:K:122:ALA:HB2	2.55	0.41
1:L:319:LEU:HD23	1:L:319:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TYR:O	1:B:383:ARG:C	2.59	0.41
1:D:382:TYR:O	1:D:383:ARG:C	2.58	0.41
1:A:410:TRP:HA	1:A:411:SER:HA	1.84	0.41
1:E:305:ASN:CG	1:E:372:GLU:HB2	2.41	0.41
1:H:445:LEU:HA	1:H:448:VAL:HG23	2.02	0.41
1:B:171:ALA:HB1	1:B:172:PRO:HD2	2.03	0.41
1:D:62:LYS:NZ	2:D:501:HOH:O	2.53	0.41
1:F:147:ASN:HD21	1:F:205:MET:CA	2.33	0.41
1:G:61:TYR:CD2	1:G:133:ILE:HG12	2.56	0.41
1:E:22:LEU:O	1:E:25:SER:HB2	2.20	0.41
1:G:336:LYS:HE2	1:I:169:ASP:O	2.21	0.41
1:I:344:PHE:CZ	1:I:420:GLN:HG3	2.55	0.41
1:I:77:ARG:HD2	1:I:77:ARG:C	2.41	0.41
1:A:86:PHE:CE1	1:A:122:ALA:HB2	2.56	0.41
1:F:305:ASN:CG	1:F:372:GLU:HB2	2.41	0.41
1:J:158:HIS:ND1	1:J:174:GLY:HA3	2.35	0.41
1:K:98:GLU:HB2	1:K:106:ILE:HG22	2.03	0.41
1:B:151:TRP:HB2	1:B:152:PRO:HD3	2.03	0.40
1:C:89:PRO:HA	1:C:156:TRP:CE2	2.56	0.40
1:D:214:GLN:OE1	1:D:221:SER:HB3	2.21	0.40
1:E:147:ASN:HD21	1:E:205:MET:CA	2.34	0.40
1:E:395:TYR:HA	1:E:398:MET:HE3	1.94	0.40
1:H:315:LYS:O	1:H:316:ASP:C	2.60	0.40
1:J:22:LEU:O	1:J:25:SER:HB2	2.21	0.40
1:B:22:LEU:O	1:B:25:SER:HB2	2.21	0.40
1:E:445:LEU:HA	1:E:448:VAL:HG23	2.04	0.40
1:H:147:ASN:HD21	1:H:205:MET:CA	2.35	0.40
1:K:209:ASN:HD21	1:K:264:ALA:HB3	1.87	0.40
1:K:350:PRO:HG3	1:K:389:SER:HB2	2.03	0.40
1:L:350:PRO:HG3	1:L:389:SER:HB2	2.03	0.40
1:A:305:ASN:CG	1:A:372:GLU:HB2	2.42	0.40
1:E:15:GLY:HA2	1:E:19:GLU:HG3	2.02	0.40
1:H:151:TRP:HB2	1:H:152:PRO:HD3	2.03	0.40
1:H:76:ILE:HG22	1:H:77:ARG:N	2.36	0.40
1:I:15:GLY:HA2	1:I:19:GLU:HG3	2.03	0.40
1:I:309:ARG:HD3	1:I:349:TYR:CE2	2.55	0.40
1:B:98:GLU:HB2	1:B:106:ILE:HG22	2.04	0.40
1:C:422:PHE:CD1	1:C:433:PHE:CE2	3.09	0.40
1:D:91:PHE:CD1	1:D:179:LYS:HE3	2.56	0.40
1:F:22:LEU:O	1:F:25:SER:HB2	2.21	0.40
1:F:76:ILE:HG22	1:F:77:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:ILE:HG22	1:L:77:ARG:N	2.37	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)
1:K:274:GLU:O	1:L:316:ASP:OD2[1_655]	1.81	0.39
1:G:316:ASP:OD2	1:H:274:GLU:O[1_655]	1.92	0.28
1:G:316:ASP:OD2	2:H:504:HOH:O[1_655]	2.03	0.17
1:K:277:ASP:OD2	1:L:316:ASP:N[1_655]	2.09	0.11
1:A:277:ASP:OD2	1:B:231:GLU:OE1[1_655]	2.18	0.02

## 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	446/450 (99%)	430 (96%)	13 (3%)	3 (1%)	25	57
1	B	440/450 (98%)	424 (96%)	13 (3%)	3 (1%)	25	57
1	C	440/450 (98%)	422 (96%)	15 (3%)	3 (1%)	25	57
1	D	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	32	65
1	E	440/450 (98%)	422 (96%)	16 (4%)	2 (0%)	32	65
1	F	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	32	65
1	G	446/450 (99%)	427 (96%)	16 (4%)	3 (1%)	25	57
1	H	446/450 (99%)	428 (96%)	14 (3%)	4 (1%)	20	50
1	I	440/450 (98%)	423 (96%)	14 (3%)	3 (1%)	25	57
1	J	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	32	65
1	K	440/450 (98%)	426 (97%)	11 (2%)	3 (1%)	25	57
1	L	446/450 (99%)	428 (96%)	16 (4%)	2 (0%)	38	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5304/5400 (98%)	5099 (96%)	173 (3%)	32 (1%)	28 61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	B	151	TRP
1	C	151	TRP
1	D	151	TRP
1	E	151	TRP
1	F	151	TRP
1	G	151	TRP
1	H	151	TRP
1	I	151	TRP
1	J	151	TRP
1	K	151	TRP
1	L	151	TRP
1	H	102	GLU
1	A	4	PRO
1	F	4	PRO
1	K	4	PRO
1	B	4	PRO
1	B	108	VAL
1	D	4	PRO
1	H	4	PRO
1	I	4	PRO
1	J	4	PRO
1	K	108	VAL
1	L	448	VAL
1	C	108	VAL
1	E	108	VAL
1	G	4	PRO
1	G	108	VAL
1	H	108	VAL
1	I	108	VAL
1	A	108	VAL
1	C	4	PRO

### 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	378/379 (100%)	365 (97%)	13 (3%)	42	75
1	B	375/379 (99%)	365 (97%)	10 (3%)	50	82
1	C	375/379 (99%)	363 (97%)	12 (3%)	44	77
1	D	375/379 (99%)	358 (96%)	17 (4%)	32	64
1	E	375/379 (99%)	360 (96%)	15 (4%)	36	69
1	F	375/379 (99%)	363 (97%)	12 (3%)	44	77
1	G	378/379 (100%)	367 (97%)	11 (3%)	48	79
1	H	378/379 (100%)	366 (97%)	12 (3%)	44	77
1	I	375/379 (99%)	362 (96%)	13 (4%)	41	74
1	J	375/379 (99%)	365 (97%)	10 (3%)	50	82
1	K	375/379 (99%)	362 (96%)	13 (4%)	41	74
1	L	378/379 (100%)	370 (98%)	8 (2%)	59	87
All	All	4512/4548 (99%)	4366 (97%)	146 (3%)	44	77

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	VAL
1	A	77	ARG
1	A	99	LYS
1	A	105	ILE
1	A	106	ILE
1	A	258	SER
1	A	284	LYS
1	A	316	ASP
1	A	344	PHE
1	A	381	ARG
1	A	440	LEU
1	A	447	SER
1	B	25	SER
1	B	27	VAL
1	B	99	LYS
1	B	106	ILE
1	B	256	GLU

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Mol	Chain	Res	Type
1	B	258	SER
1	B	284	LYS
1	B	344	PHE
1	B	381	ARG
1	B	447	SER
1	C	25	SER
1	C	27	VAL
1	C	62	LYS
1	C	70	LYS
1	C	77	ARG
1	C	106	ILE
1	C	258	SER
1	C	284	LYS
1	C	344	PHE
1	C	381	ARG
1	C	400	GLU
1	C	447	SER
1	D	25	SER
1	D	27	VAL
1	D	70	LYS
1	D	102	GLU
1	D	106	ILE
1	D	107	SER
1	D	218	ASN
1	D	256	GLU
1	D	258	SER
1	D	284	LYS
1	D	344	PHE
1	D	381	ARG
1	D	385	HIS
1	D	400	GLU
1	D	440	LEU
1	D	447	SER
1	D	448	VAL
1	E	25	SER
1	E	27	VAL
1	E	70	LYS
1	E	77	ARG
1	E	105	ILE
1	E	106	ILE
1	E	117	GLU
1	E	185	VAL

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Mol	Chain	Res	Type
1	E	219	LEU
1	E	258	SER
1	E	284	LYS
1	E	344	PHE
1	E	381	ARG
1	E	440	LEU
1	E	447	SER
1	F	25	SER
1	F	27	VAL
1	F	70	LYS
1	F	77	ARG
1	F	258	SER
1	F	284	LYS
1	F	336	LYS
1	F	344	PHE
1	F	362	ASN
1	F	381	ARG
1	F	440	LEU
1	F	447	SER
1	G	25	SER
1	G	27	VAL
1	G	77	ARG
1	G	106	ILE
1	G	258	SER
1	G	284	LYS
1	G	315	LYS
1	G	344	PHE
1	G	381	ARG
1	G	440	LEU
1	G	447	SER
1	H	25	SER
1	H	27	VAL
1	H	99	LYS
1	H	106	ILE
1	H	258	SER
1	H	262	ILE
1	H	280	GLU
1	H	284	LYS
1	H	316	ASP
1	H	344	PHE
1	H	381	ARG
1	H	449	LYS

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Mol	Chain	Res	Type
1	I	25	SER
1	I	27	VAL
1	I	70	LYS
1	I	106	ILE
1	I	125	GLU
1	I	177	ASP
1	I	253	GLU
1	I	258	SER
1	I	284	LYS
1	I	344	PHE
1	I	381	ARG
1	I	440	LEU
1	I	447	SER
1	J	25	SER
1	J	27	VAL
1	J	41	ILE
1	J	70	LYS
1	J	258	SER
1	J	284	LYS
1	J	344	PHE
1	J	366	LEU
1	J	381	ARG
1	J	387	LEU
1	K	5	LYS
1	K	25	SER
1	K	27	VAL
1	K	70	LYS
1	K	99	LYS
1	K	106	ILE
1	K	178	GLU
1	K	258	SER
1	K	278	GLU
1	K	284	LYS
1	K	344	PHE
1	K	381	ARG
1	K	447	SER
1	L	25	SER
1	L	27	VAL
1	L	218	ASN
1	L	258	SER
1	L	269	ASP
1	L	284	LYS

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Mol	Chain	Res	Type
1	L	344	PHE
1	L	381	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	409	HIS
1	B	59	HIS
1	B	147	ASN
1	B	150	HIS
1	B	206	ASN
1	B	214	GLN
1	C	150	HIS
1	D	147	ASN
1	D	150	HIS
1	D	206	ASN
1	E	147	ASN
1	E	150	HIS
1	E	206	ASN
1	F	147	ASN
1	F	150	HIS
1	F	206	ASN
1	F	209	ASN
1	G	213	ASN
1	G	218	ASN
1	G	355	ASN
1	G	409	HIS
1	H	40	ASN
1	H	59	HIS
1	H	147	ASN
1	H	150	HIS
1	H	206	ASN
1	H	268	HIS
1	H	355	ASN
1	I	150	HIS
1	J	147	ASN
1	J	150	HIS
1	K	147	ASN
1	K	150	HIS
1	K	214	GLN
1	K	355	ASN

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Mol	Chain	Res	Type
1	K	409	HIS
1	L	150	HIS
1	L	355	ASN
1	L	396	ASN
1	L	409	HIS

### 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 carbohydrates 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	448/450 (99%)	-0.36	1 (0%) 94 94	12, 38, 79, 120	0
1	B	444/450 (98%)	0.08	17 (3%) 41 30	33, 61, 106, 149	0
1	C	444/450 (98%)	-0.34	3 (0%) 87 84	16, 40, 72, 160	0
1	D	444/450 (98%)	-0.03	14 (3%) 48 37	26, 59, 95, 139	0
1	E	444/450 (98%)	-0.24	4 (0%) 84 79	19, 42, 78, 159	0
1	F	444/450 (98%)	1.53	135 (30%) 0 0	43, 99, 143, 186	0
1	G	448/450 (99%)	-0.34	1 (0%) 94 94	22, 41, 74, 134	0
1	H	448/450 (99%)	-0.07	14 (3%) 49 38	31, 57, 97, 168	0
1	I	444/450 (98%)	-0.30	5 (1%) 80 75	14, 42, 76, 146	0
1	J	444/450 (98%)	1.33	121 (27%) 1 0	54, 109, 165, 225	0
1	K	444/450 (98%)	-0.23	6 (1%) 75 69	19, 45, 75, 147	0
1	L	448/450 (99%)	-0.02	9 (2%) 65 56	24, 58, 98, 149	0
All	All	5344/5400 (98%)	0.08	330 (6%) 21 13	12, 52, 126, 225	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	366	LEU	10.4
1	E	449	LYS	10.4
1	F	367	PRO	9.9
1	J	122	ALA	9.3
1	J	28	GLU	9.2
1	F	448	VAL	8.7
1	F	275	TYR	8.6
1	J	31	TRP	8.5
1	C	104	ASN	8.3
1	F	93	VAL	8.2
1	J	164	ARG	7.7

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Mol	Chain	Res	Type	RSRZ
1	F	363	ALA	7.6
1	K	447	SER	7.5
1	B	448	VAL	7.4
1	D	106	ILE	7.2
1	F	309	ARG	6.9
1	F	310	LEU	6.9
1	B	449	LYS	6.6
1	J	16	PHE	6.6
1	J	105	ILE	6.5
1	F	107	SER	6.4
1	F	97	VAL	6.3
1	K	449	LYS	6.2
1	F	108	VAL	6.2
1	F	106	ILE	6.1
1	J	434	GLU	6.1
1	F	105	ILE	6.0
1	F	228	LEU	6.0
1	F	110	VAL	5.9
1	F	181	VAL	5.9
1	F	360	LEU	5.8
1	J	104	ASN	5.8
1	J	117	GLU	5.8
1	F	390	HIS	5.8
1	J	182	VAL	5.6
1	J	159	ASP	5.6
1	F	220	ALA	5.5
1	F	353	LEU	5.5
1	F	3	PHE	5.4
1	J	279	VAL	5.3
1	J	172	PRO	5.3
1	H	106	ILE	5.2
1	F	266	ALA	5.2
1	F	404	VAL	5.2
1	E	448	VAL	5.2
1	F	277	ASP	5.2
1	F	90	THR	5.2
1	J	35	VAL	5.1
1	F	274	GLU	5.0
1	H	99	LYS	5.0
1	I	447	SER	4.9
1	J	433	PHE	4.9
1	D	447	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	389	SER	4.9
1	F	162	ALA	4.8
1	J	91	PHE	4.8
1	F	313	GLY	4.8
1	J	45	LEU	4.7
1	H	105	ILE	4.6
1	F	102	GLU	4.6
1	F	302	ILE	4.5
1	J	272	ALA	4.5
1	J	49	ASP	4.5
1	B	102	GLU	4.5
1	I	104	ASN	4.5
1	F	219	LEU	4.5
1	F	368	MET	4.5
1	J	291	THR	4.5
1	J	404	VAL	4.4
1	F	247	ALA	4.3
1	F	449	LYS	4.3
1	J	301	TRP	4.3
1	F	430	TYR	4.3
1	F	394	VAL	4.3
1	B	254	TYR	4.2
1	F	85	ILE	4.2
1	J	165	LYS	4.2
1	F	254	TYR	4.2
1	C	106	ILE	4.2
1	J	44	GLY	4.2
1	B	97	VAL	4.2
1	F	325	TYR	4.1
1	J	273	GLU	4.1
1	J	171	ALA	4.1
1	J	43	SER	4.1
1	F	92	ASP	4.1
1	F	191	VAL	4.1
1	L	448	VAL	4.1
1	F	122	ALA	4.0
1	J	15	GLY	4.0
1	F	257	LYS	4.0
1	J	242	GLN	3.9
1	F	398	MET	3.9
1	J	166	LEU	3.9
1	J	265	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	226	GLY	3.9
1	J	5	LYS	3.9
1	J	193	TYR	3.8
1	J	167	GLY	3.8
1	F	362	ASN	3.8
1	F	182	VAL	3.8
1	F	178	GLU	3.8
1	J	399	LYS	3.8
1	J	295	SER	3.8
1	J	438	ARG	3.8
1	F	279	VAL	3.7
1	J	6	ASN	3.7
1	B	447	SER	3.7
1	J	58	TRP	3.7
1	F	324	GLY	3.7
1	J	3	PHE	3.7
1	J	40	ASN	3.7
1	J	123	ASN	3.7
1	L	447	SER	3.7
1	H	449	LYS	3.7
1	J	156	TRP	3.7
1	F	306	TYR	3.7
1	F	159	ASP	3.6
1	J	99	LYS	3.6
1	J	48	GLY	3.6
1	F	231	GLU	3.6
1	J	107	SER	3.6
1	J	299	LEU	3.6
1	J	290	VAL	3.6
1	F	396	ASN	3.5
1	B	103	GLY	3.5
1	I	106	ILE	3.5
1	J	85	ILE	3.5
1	J	261	VAL	3.5
1	J	271	LEU	3.5
1	F	207	GLU	3.4
1	J	263	TYR	3.4
1	F	292	ILE	3.4
1	F	356	LEU	3.4
1	J	50	LEU	3.4
1	F	89	PRO	3.4
1	F	179	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	339	ARG	3.3
1	F	167	GLY	3.3
1	F	225	PRO	3.3
1	F	165	LYS	3.3
1	F	286	ASP	3.3
1	G	449	LYS	3.3
1	F	238	PHE	3.3
1	J	102	GLU	3.3
1	F	87	PRO	3.3
1	F	407	TYR	3.2
1	J	106	ILE	3.2
1	J	20	MET	3.2
1	F	269	ASP	3.2
1	J	86	PHE	3.2
1	F	299	LEU	3.2
1	F	6	ASN	3.2
1	F	403	ASP	3.2
1	F	91	PHE	3.2
1	F	268	HIS	3.2
1	D	449	LYS	3.2
1	F	236	ALA	3.1
1	H	104	ASN	3.1
1	F	120	LYS	3.1
1	F	406	GLY	3.1
1	F	104	ASN	3.1
1	H	97	VAL	3.1
1	J	177	ASP	3.1
1	J	101	GLU	3.1
1	F	86	PHE	3.1
1	J	23	PRO	3.1
1	J	405	ARG	3.0
1	J	231	GLU	3.0
1	D	170	ALA	3.0
1	J	126	ALA	3.0
1	F	164	ARG	3.0
1	J	267	TRP	3.0
1	L	336	LYS	3.0
1	L	105	ILE	3.0
1	F	154	PRO	3.0
1	F	35	VAL	3.0
1	F	22	LEU	2.9
1	F	180	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	100	ASP	2.9
1	F	88	LYS	2.9
1	F	166	LEU	2.9
1	F	337	SER	2.9
1	J	431	VAL	2.9
1	J	216	TYR	2.9
1	J	398	MET	2.9
1	F	319	LEU	2.9
1	J	241	ILE	2.9
1	J	9	PHE	2.9
1	F	271	LEU	2.9
1	J	33	VAL	2.9
1	F	357	LEU	2.9
1	F	447	SER	2.9
1	F	168	PRO	2.8
1	J	292	ILE	2.8
1	J	233	ALA	2.8
1	J	439	TYR	2.8
1	F	7	PHE	2.8
1	J	80	ILE	2.8
1	J	306	TYR	2.8
1	B	104	ASN	2.8
1	J	55	PRO	2.8
1	J	87	PRO	2.8
1	F	446	VAL	2.8
1	J	120	LYS	2.8
1	D	96	ASP	2.8
1	F	9	PHE	2.8
1	J	27	VAL	2.8
1	F	117	GLU	2.8
1	F	251	ILE	2.8
1	F	387	LEU	2.8
1	J	103	GLY	2.7
1	F	94	LYS	2.7
1	F	283	ARG	2.7
1	D	358	LYS	2.7
1	J	37	ASP	2.7
1	F	402	ALA	2.7
1	B	253	GLU	2.7
1	J	19	GLU	2.7
1	J	227	PHE	2.7
1	B	92	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	261	VAL	2.7
1	F	233	ALA	2.7
1	A	315	LYS	2.7
1	F	217	ILE	2.7
1	B	219	LEU	2.7
1	D	392	LYS	2.7
1	J	163	VAL	2.6
1	F	440	LEU	2.6
1	H	374	GLY	2.6
1	D	299	LEU	2.6
1	J	108	VAL	2.6
1	F	2	LYS	2.6
1	F	321	PRO	2.6
1	H	320	VAL	2.5
1	F	382	TYR	2.5
1	J	287	TYR	2.5
1	F	175	TRP	2.5
1	J	92	ASP	2.5
1	F	221	SER	2.5
1	F	8	MET	2.5
1	F	320	VAL	2.5
1	L	116	LYS	2.5
1	J	175	TRP	2.5
1	F	103	GLY	2.5
1	F	352	GLY	2.5
1	F	281	GLU	2.5
1	J	238	PHE	2.5
1	E	395	TYR	2.5
1	J	88	LYS	2.5
1	K	104	ASN	2.4
1	B	120	LYS	2.4
1	J	445	LEU	2.4
1	F	358	LYS	2.4
1	F	75	CYS	2.4
1	J	391	LEU	2.4
1	F	96	ASP	2.4
1	J	228	LEU	2.4
1	F	256	GLU	2.4
1	K	102	GLU	2.4
1	J	396	ASN	2.4
1	J	38	LYS	2.4
1	J	179	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	44	GLY	2.3
1	J	395	TYR	2.3
1	J	245	ILE	2.3
1	K	9	PHE	2.3
1	F	95	VAL	2.3
1	D	107	SER	2.3
1	J	151	TRP	2.3
1	J	251	ILE	2.3
1	F	21	GLY	2.3
1	J	158	HIS	2.3
1	L	101	GLU	2.3
1	J	208	PRO	2.3
1	J	220	ALA	2.3
1	H	98	GLU	2.3
1	J	34	TRP	2.3
1	L	449	LYS	2.3
1	B	106	ILE	2.3
1	F	190	PHE	2.3
1	J	29	SER	2.2
1	H	113	SER	2.2
1	D	166	LEU	2.2
1	F	160	PRO	2.2
1	I	105	ILE	2.2
1	B	178	GLU	2.2
1	D	291	THR	2.2
1	F	349	TYR	2.2
1	J	22	LEU	2.2
1	J	357	LEU	2.2
1	F	298	LYS	2.2
1	B	2	LYS	2.2
1	F	38	LYS	2.2
1	D	5	LYS	2.2
1	F	100	ASP	2.2
1	F	405	ARG	2.2
1	J	70	LYS	2.2
1	E	447	SER	2.2
1	J	161	ILE	2.1
1	J	98	GLU	2.1
1	I	448	VAL	2.1
1	B	193	TYR	2.1
1	H	256	GLU	2.1
1	J	355	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	107	SER	2.1
1	F	116	LYS	2.1
1	D	171	ALA	2.1
1	J	2	LYS	2.1
1	J	418	TRP	2.1
1	J	176	LEU	2.1
1	C	100	ASP	2.1
1	H	116	LYS	2.1
1	F	323	PRO	2.1
1	J	361	ASN	2.1
1	F	351	GLU	2.1
1	J	129	HIS	2.1
1	H	96	ASP	2.0
1	F	359	TYR	2.0
1	J	270	PRO	2.0
1	J	184	PHE	2.0
1	F	170	ALA	2.0
1	J	39	GLU	2.0
1	K	103	GLY	2.0
1	F	169	ASP	2.0
1	F	422	PHE	2.0
1	B	218	ASN	2.0
1	L	102	GLU	2.0
1	J	149	TYR	2.0
1	F	290	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 carbohydrates 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.