



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

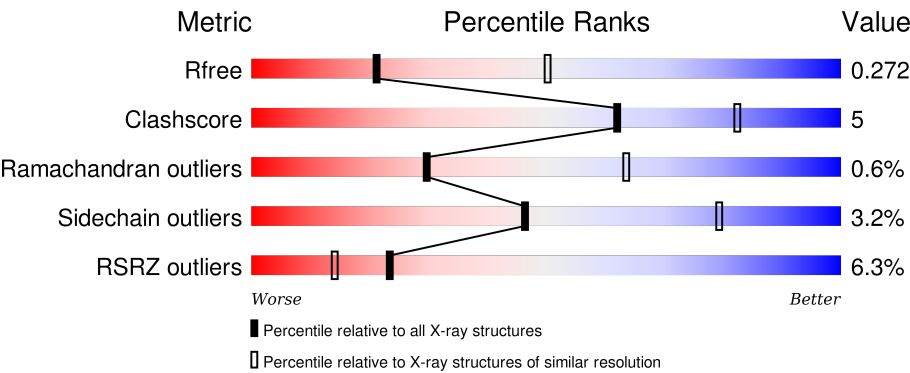
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (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 >=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 <=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></div><div>86%12% .</div></div>
1	B	450	<div><div>4%</div><div>86%11% ..</div></div>
1	C	450	<div><div>%</div><div>85%13% ..</div></div>
1	D	450	<div><div>3%</div><div>85%12% ..</div></div>
1	E	450	<div><div>%</div><div>84%14% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	450	<div><div></div><div>30%</div><div></div><div>84%</div><div></div><div>13%</div><div></div><div>..</div></div>
1	G	450	<div><div></div><div>88%</div><div></div><div>11%</div><div></div><div>.</div></div>
1	H	450	<div><div></div><div>3%</div><div></div><div>84%</div><div></div><div>14%</div><div></div><div>.</div></div>
1	I	450	<div><div></div><div>%</div><div></div><div>85%</div><div></div><div>13%</div><div></div><div>..</div></div>
1	J	450	<div><div></div><div>28%</div><div></div><div>82%</div><div></div><div>14%</div><div></div><div>..</div></div>
1	K	450	<div><div></div><div>%</div><div></div><div>83%</div><div></div><div>15%</div><div></div><div>..</div></div>
1	L	450	<div><div></div><div>2%</div><div></div><div>87%</div><div></div><div>12%</div><div></div><div>.</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

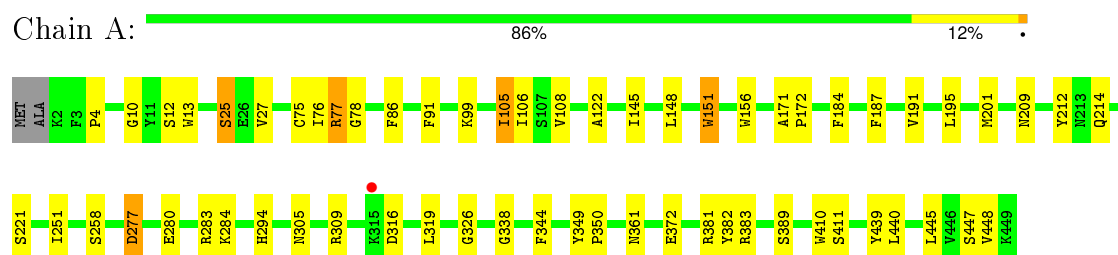
- Molecule 2 is water.

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

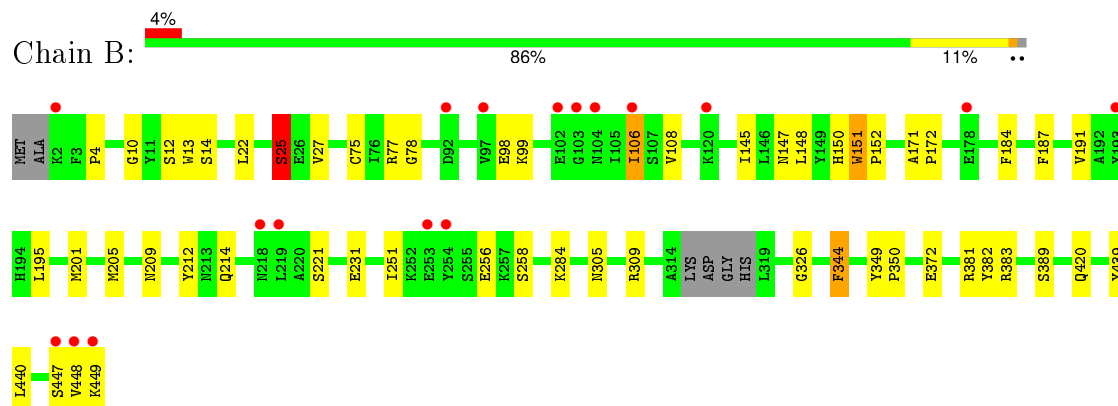
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

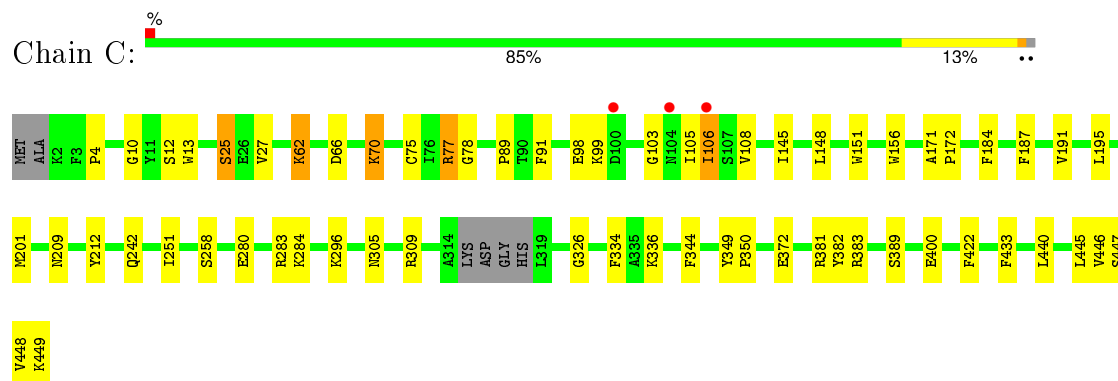
• Molecule 1: Beta-glucosidase



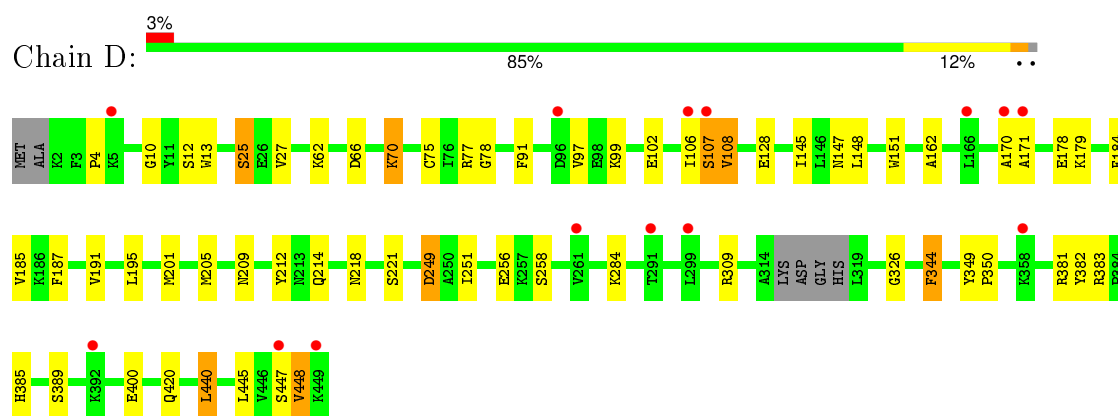
• Molecule 1: Beta-glucosidase



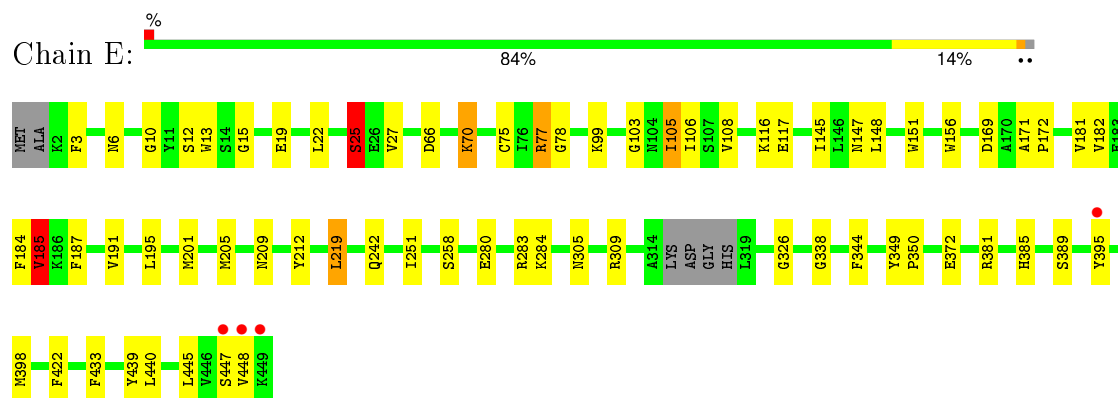
• Molecule 1: Beta-glucosidase



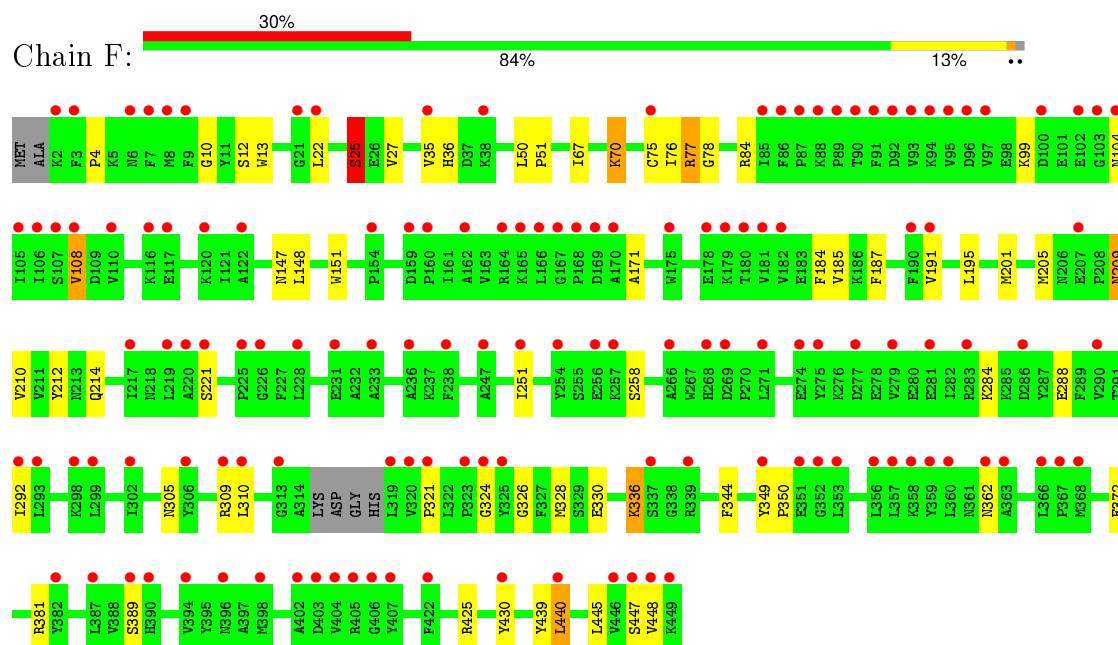
• Molecule 1: Beta-glucosidase



• Molecule 1: Beta-glucosidase

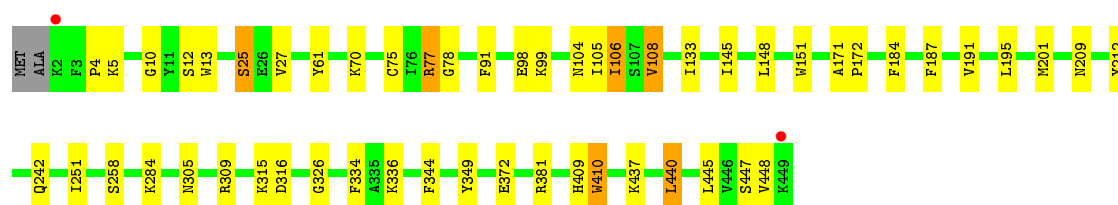


• Molecule 1: Beta-glucosidase

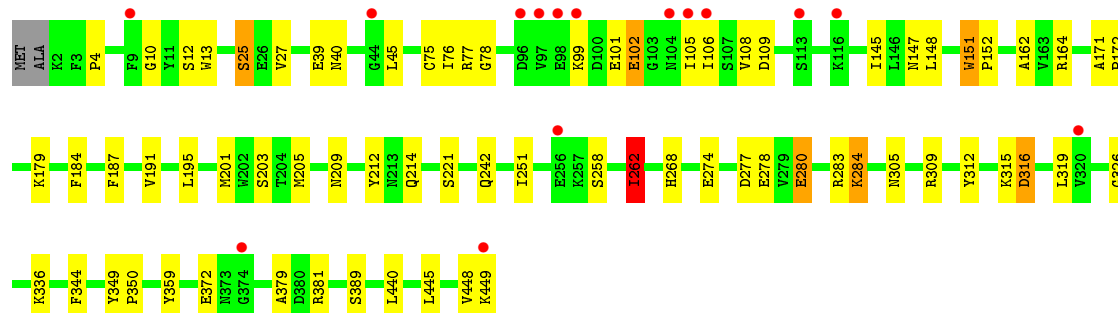
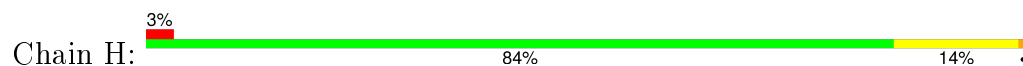


• Molecule 1: Beta-glucosidase

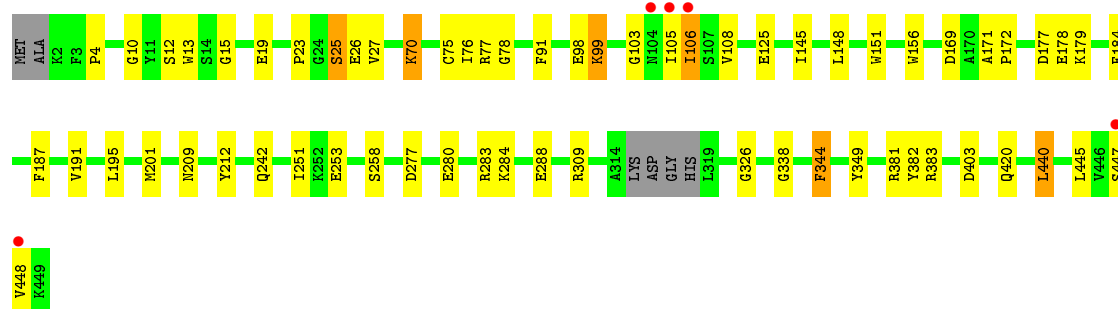
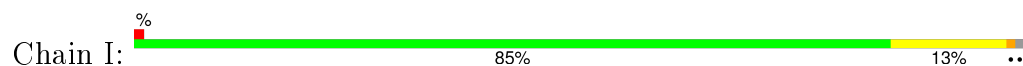




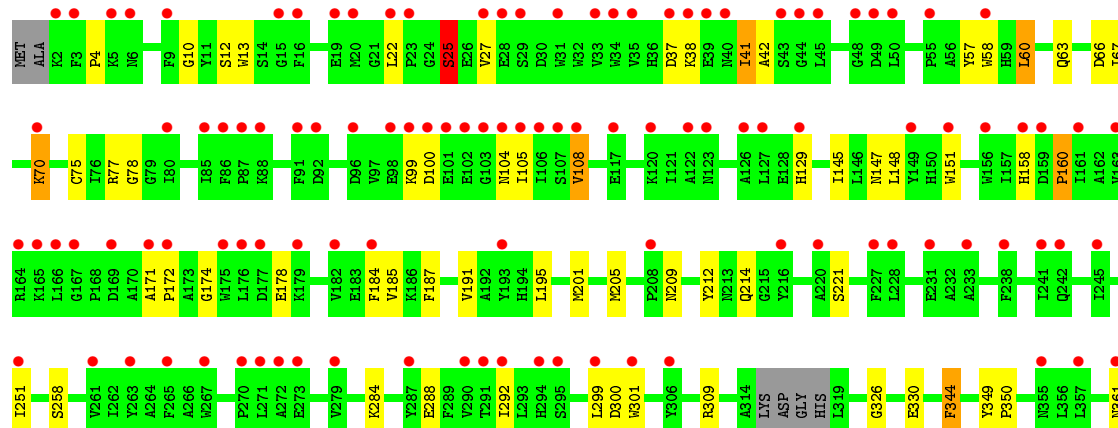
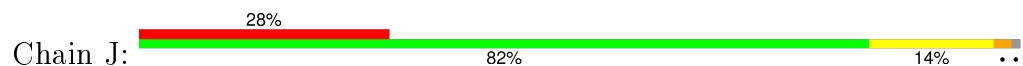
• Molecule 1: Beta-glucosidase

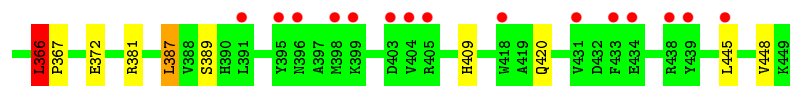


• Molecule 1: Beta-glucosidase

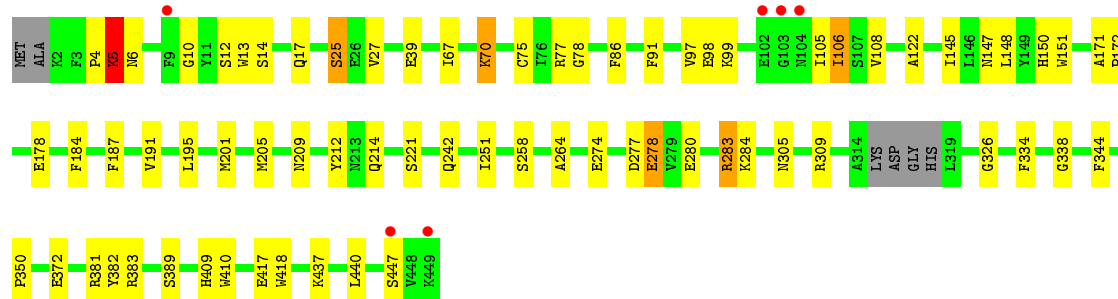
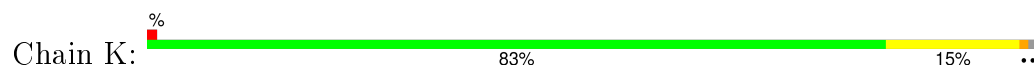


• Molecule 1: Beta-glucosidase

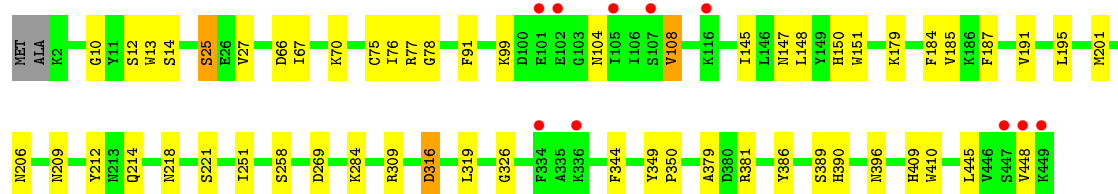
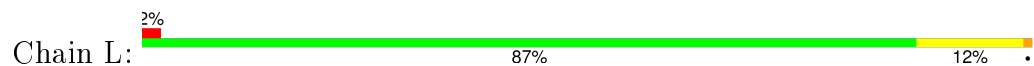




- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	49.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 165239 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	43762	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:J:60:LEU:HB3	1:J:63:GLN:OE1	1.51	1.11
1:E:182:VAL:O	1:E:185:VAL:HG23	1.50	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:K:70:LYS:HE3	1:L:445:LEU:HD13	1.63	0.79
1:J:99:LYS:NZ	1:J:178:GLU:OE2	2.16	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:OG	1:H:262:ILE:HD13	1.87	0.75
1:H:203:SER:CB	1:H:262:ILE:HD13	2.17	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:I:448:VAL:CG1	1:J:448:VAL:HG12	2.21	0.71
1:A:439:TYR:HB3	1:B:439:TYR:HB3	1.72	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:E:445:LEU:HD11	1:F:440:LEU:HD11	1.73	0.70
1:F:35:VAL:HG23	1:F:36:HIS:CE1	2.26	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:162:ALA:HB2	1:F:330:GLU:HG3	1.79	0.64
1:D:108:VAL:HG11	1:D:185:VAL:HG11	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:I:70:LYS:HE3	1:J:445:LEU:HD13	1.83	0.60
1:J:299:LEU:O	1:J:366:LEU:HD11	2.01	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:I:440:LEU:HD12	1:J:445:LEU:CD1	2.19	0.56
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: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:O	1:H:105:ILE:HG23	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:K:440:LEU:HD11	1:L:445:LEU:HD11	1.90	0.53
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: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:I:70:LYS:HE3	1:J:445:LEU:CB	2.39	0.53
1:J:300:ASP:C	1:J:366:LEU:HD21	2.29	0.53
1:E:66:ASP:O	1:E:70:LYS:HG2	2.09	0.53
1:H:162:ALA:HB2	1:J:330:GLU:CG	2.38	0.53
1:F:36:HIS:CE1	1:F:51:PRO:HD2	2.44	0.53
1:I:338:GLY:HA3	1:K:91:PHE:CE2	2.44	0.53
1:I:105:ILE:O	1:I:105:ILE:HG23	2.09	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:K:105:ILE:O	1:K:105:ILE:HG23	2.08	0.52
1:F:35:VAL:HG23	1:F:36:HIS:ND1	2.25	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:G:309:ARG:O	1:G:326:GLY:HA3	2.09	0.51
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:J:366:LEU:HD23	1:J:367:PRO:N	2.24	0.51
1:G:334:PHE:CD2	1:I:156:TRP:HB3	2.46	0.51
1:C:77:ARG:C	1:C:77:ARG:HD2	2.31	0.51
1:H:283:ARG:HD3	1:H:359:TYR:CE2	2.45	0.51
1:E:13:TRP:CE2	1:E:78:GLY:HA3	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:H:203:SER:HB2	1:H:262:ILE:CD1	2.40	0.50
1:D:10:GLY:HA3	1:D:75:CYS:O	2.11	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: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:A:309:ARG:O	1:A:326:GLY:HA3	2.12	0.50
1:H:280:GLU:HG2	1:H:283:ARG:HH21	1.75	0.50
1:L:145:ILE:HG12	1:L:201:MET:HB2	1.94	0.50
1:H:309:ARG:O	1:H:326:GLY:HA3	2.12	0.50
1:J:99:LYS:HE2	1:J:105:ILE:CG1	2.42	0.50
1:L:10:GLY:HA3	1:L:75:CYS:O	2.12	0.50
1:K:309:ARG:O	1:K:326:GLY:HA3	2.12	0.50
1:C:309:ARG:O	1:C:326:GLY:HA3	2.12	0.50
1:B:10:GLY:HA3	1:B:75:CYS:O	2.13	0.49
1:C:446:VAL:O	1:C:449:LYS:CG	2.56	0.49
1:B:309:ARG:O	1:B:326:GLY:HA3	2.12	0.49
1:K:437:LYS:HE3	1:L:379:ALA:CB	2.37	0.49
1:G:209:ASN:HA	1:G:212:TYR:CZ	2.48	0.49
1:I:10:GLY:HA3	1:I:75:CYS:O	2.12	0.49
1:L:67:ILE:HA	1:L:70:LYS:HE2	1.93	0.49
1:J:12:SER:HA	1:J:77:ARG:O	2.13	0.49
1:B:12:SER:HA	1:B:77:ARG:O	2.12	0.49
1:A:12:SER:HA	1:A:77:ARG:O	2.12	0.49
1:C:10:GLY:HA3	1:C:75:CYS:O	2.12	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:K:70:LYS:HZ1	1:L:445:LEU:HD13	1.77	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:C:209:ASN:HA	1:C:212:TYR:CZ	2.48	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:G:336:LYS:CE	1:I:169:ASP:O	2.61	0.48
1:C:12:SER:HA	1:C:77:ARG:O	2.13	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:K:70:LYS:HZ1	1:L:445:LEU:CD1	2.26	0.48
1:B:145:ILE:HG12	1:B:201:MET:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:CG2	1:C:242:GLN:OE1	2.54	0.48
1:B:13:TRP:CE2	1:B:78:GLY:HA3	2.49	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:G:10:GLY:HA3	1:G:75:CYS:O	2.14	0.48
1:J:309:ARG:O	1:J:326:GLY:HA3	2.14	0.48
1:I:148:LEU:HD11	1:I:251:ILE:HD11	1.96	0.48
1:E:12:SER:HA	1:E:77:ARG:O	2.14	0.48
1:D:12:SER:HA	1:D:77:ARG:O	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:I:70:LYS:CE	1:J:445:LEU:HB2	2.44	0.47
1:K:105:ILE:CG2	1:K:242:GLN:OE1	2.52	0.47
1:K:17:GLN:OE1	1:K:418:TRP:CD1	2.67	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:A:184:PHE:O	1:A:187:PHE:HB3	2.14	0.47
1:J:145:ILE:HG12	1:J:201:MET:HB2	1.96	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:L:409:HIS:HD2	1:L:410:TRP:C	2.18	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:57:TYR:CA	1:J:60:LEU:O	2.53	0.47
1:J:38:LYS:HA	1:J:41:ILE:HD13	1.96	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:K:12:SER:HA	1:K:77:ARG:O	2.14	0.47
1:I:191:VAL:HG13	1:I:195:LEU:HD12	1.97	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:I:13:TRP:CE2	1:I:78:GLY:HA3	2.50	0.47
1:C:445:LEU:HD11	1:D:440:LEU:HD11	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:E:171:ALA:HB1	1:E:172:PRO:HD2	1.97	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:K:70:LYS:NZ	1:L:445:LEU:CD1	2.79	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: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: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: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:B:209:ASN:HA	1:B:212:TYR:CZ	2.51	0.46
1:I:145:ILE:HG12	1:I:201:MET:HB2	1.96	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:C:148:LEU:HD11	1:C:251:ILE:HD11	1.97	0.46
1:K:184:PHE:O	1:K:187:PHE:HB3	2.16	0.46
1:H:105:ILE:CG2	1:H:242:GLN:OE1	2.54	0.46
1:F:184:PHE:O	1:F:187:PHE:HB3	2.16	0.46
1:B:448:VAL:O	1:B:449:LYS:HG3	2.14	0.46
1:H:280:GLU:OE1	1:H:284:LYS:NZ	2.33	0.46
1:G:13:TRP:CE2	1:G:78:GLY:HA3	2.51	0.46
1:J:148:LEU:HD11	1:J:251:ILE:HD11	1.96	0.46
1:G:148:LEU:HD11	1:G:251:ILE:HD11	1.97	0.46
1:C:145:ILE:HG12	1:C:201:MET:HB2	1.98	0.46
1:J:184:PHE:O	1:J:187:PHE:HB3	2.16	0.45
1:E:184:PHE:O	1:E:187:PHE:HB3	2.16	0.45
1:F:310:LEU:HD22	1:F:328:MET:HE1	1.98	0.45
1:C:171:ALA:HB1	1:C:172:PRO:HD2	1.99	0.45
1:A:10:GLY:HA3	1:A:75:CYS:O	2.15	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: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:J:301:TRP:HA	1:J:366:LEU:CD2	2.45	0.45
1:F:99:LYS:HB3	1:F:104:ASN:O	2.16	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: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: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:B:191:VAL:HG13	1:B:195:LEU:HD12	1.99	0.45
1:C:445:LEU:HB3	1:D:70:LYS:HD3	1.99	0.45
1:D:148:LEU:HD11	1:D:251:ILE:HD11	1.98	0.45
1:B:214:GLN:NE2	1:B:221:SER:CB	2.79	0.45
1:A:309:ARG:HD3	1:A:349:TYR:CE2	2.52	0.45
1:H:309:ARG:HD3	1:H:349:TYR:CE2	2.52	0.45
1:B:148:LEU:HD11	1:B:251:ILE:HD11	1.98	0.45
1:G:334:PHE:CE2	1:I:156:TRP:HB3	2.51	0.45
1:C:382:TYR:O	1:C:383:ARG:C	2.56	0.45
1:K:214:GLN:NE2	1:K:221:SER:CB	2.80	0.44
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: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:L:309:ARG:HD3	1:L:349:TYR:CE2	2.52	0.44
1:D:66:ASP:O	1:D:70:LYS:HG2	2.17	0.44
1:B:184:PHE:O	1:B:187:PHE:HB3	2.17	0.44
1:E:191:VAL:HG13	1:E:195:LEU:HD12	2.00	0.44
1:C:336:LYS:HE3	1:E:169:ASP:HA	2.00	0.44
1:K:77:ARG:C	1:K:77:ARG:HD2	2.37	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:L:14:SER:HB3	1:L:150:HIS:CE1	2.52	0.44
1:D:191:VAL:HG13	1:D:195:LEU:HD12	1.98	0.44
1:L:66:ASP:O	1:L:70:LYS:HG2	2.18	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: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:L:409:HIS:CD2	1:L:410:TRP:N	2.85	0.44
1:E:209:ASN:HA	1:E:212:TYR:CZ	2.53	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:F:350:PRO:HG3	1:F:389:SER:HB2	2.00	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:305:ASN:CG	1:C:372:GLU:HB2	2.39	0.44
1:L:350:PRO:HB3	1:L:390:HIS:HD2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:VAL:HG11	1:D:448:VAL:HG21	2.00	0.43
1:H:191:VAL:HG13	1:H:195:LEU:HD12	2.00	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:I:70:LYS:HE3	1:J:445:LEU:CD1	2.47	0.43
1:E:350:PRO:HG3	1:E:389:SER:HB2	2.00	0.43
1:G:70:LYS:HD3	1:H:445:LEU:O	2.18	0.43
1:D:108:VAL:HG11	1:D:185:VAL:CG1	2.48	0.43
1:F:309:ARG:HD3	1:F:349:TYR:CE2	2.53	0.43
1:A:76:ILE:HG22	1:A:77:ARG:N	2.33	0.43
1:C:334:PHE:CD2	1:E:156:TRP:HB3	2.54	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:B:77:ARG:C	1:B:77:ARG:HD2	2.38	0.43
1:A:77:ARG:HD2	1:A:77:ARG:C	2.39	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: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:E:422:PHE:CD1	1:E:433:PHE:CE2	3.07	0.43
1:D:350:PRO:HG3	1:D:389:SER:HB2	2.01	0.43
1:H:214:GLN:OE1	1:H:221:SER:HB3	2.19	0.43
1:G:440:LEU:CD1	1:H:445:LEU:HD11	2.44	0.42
1:E:309:ARG:HD3	1:E:349:TYR:CE2	2.54	0.42
1:K:97:VAL:N	2:K:506:HOH:O	2.35	0.42
1:F:214:GLN:OE1	1:F:221:SER:HB3	2.19	0.42
1:D:184:PHE:O	1:D:187:PHE:HB3	2.19	0.42
1:K:70:LYS:HD2	1:L:445:LEU:HD22	2.02	0.42
1:I:98:GLU:HB2	1:I:106:ILE:HG22	2.01	0.42
1:D:171:ALA:N	1:F:336:LYS:HG3	2.34	0.42
1:L:147:ASN:HD21	1:L:206:ASN:HB2	1.85	0.42
1:J:160:PRO:HG2	1:J:160:PRO:O	2.19	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:J:66:ASP:O	1:J:70:LYS:HG2	2.19	0.42
1:C:13:TRP:CE2	1:C:78:GLY:HA3	2.55	0.42
1:I:448:VAL:HG12	1:J:448:VAL:HG12	2.01	0.42
1:H:77:ARG:HD2	1:H:77:ARG:C	2.40	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:K:382:TYR:O	1:K:383:ARG:C	2.57	0.42
1:H:171:ALA:HB1	1:H:172:PRO:HD2	2.02	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: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:G:445:LEU:HA	1:G:448:VAL:HG23	2.02	0.42
1:D:97:VAL:HG22	1:D:108:VAL:HG13	2.02	0.42
1:I:76:ILE:HG22	1:I:77:ARG:N	2.34	0.42
1:H:350:PRO:HG3	1:H:389:SER:HB2	2.01	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:I:445:LEU:HD23	1:J:448:VAL:HG21	2.00	0.41
1:J:41:ILE:CG1	1:J:42:ALA:N	2.84	0.41
1:J:387:LEU:HD21	1:J:409:HIS:NE2	2.34	0.41
1:B:14:SER:HB3	1:B:150:HIS:CE1	2.55	0.41
1:I:91:PHE:CD1	1:I:179:LYS:HE3	2.56	0.41
1:B:350:PRO:HG3	1:B:389:SER:HB2	2.02	0.41
1:J:350:PRO:HG3	1:J:389:SER:HB2	2.02	0.41
1:J:171:ALA:HB1	1:J:172:PRO:HD2	2.02	0.41
1:J:445:LEU:HA	1:J:448:VAL:HG23	2.02	0.41
1:L:386:TYR:CZ	1:L:390:HIS:CE1	3.09	0.41
1:B:309:ARG:HD3	1:B:349:TYR:CE2	2.54	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:214:GLN:OE1	1:L:221:SER:HB3	2.20	0.41
1:H:319:LEU:HD23	1:H:319:LEU:O	2.21	0.41
1:G:309:ARG:HD3	1:G:349:TYR:CE2	2.55	0.41
1:C:98:GLU:HB2	1:C:106:ILE:HG22	2.03	0.41
1:A:214:GLN:OE1	1:A:221:SER:HB3	2.21	0.41
1:E:77:ARG:C	1:E:77:ARG:HD2	2.40	0.41
1:C:445:LEU:HA	1:C:448:VAL:HG23	2.03	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:H:445:LEU:HA	1:H:448:VAL:HG23	2.02	0.41
1:E:305:ASN:CG	1:E:372:GLU:HB2	2.41	0.41
1:A:410:TRP:HA	1:A:411:SER:HA	1.84	0.41
1:G:336:LYS:HE2	1:I:169:ASP:O	2.21	0.41
1:I:77:ARG:HD2	1:I:77:ARG:C	2.41	0.41
1:D:62:LYS:NZ	2:D:501:HOH:O	2.53	0.41
1:B:171:ALA:HB1	1:B:172:PRO:HD2	2.03	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:I:344:PHE:CZ	1:I:420:GLN:HG3	2.55	0.41
1:E:22:LEU:O	1:E:25:SER:HB2	2.20	0.41
1:K:98:GLU:HB2	1:K:106:ILE:HG22	2.03	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:A:86:PHE:CE1	1:A:122:ALA:HB2	2.56	0.41
1:E:395:TYR:HA	1:E:398:MET:HE3	1.94	0.40
1:C:89:PRO:HA	1:C:156:TRP:CE2	2.56	0.40
1:B:151:TRP:HB2	1:B:152:PRO:HD3	2.03	0.40
1:D:214:GLN:OE1	1:D:221:SER:HB3	2.21	0.40
1:J:22:LEU:O	1:J:25:SER:HB2	2.21	0.40
1:E:147:ASN:HD21	1:E:205:MET:CA	2.34	0.40
1:H:315:LYS:O	1:H:316:ASP:C	2.60	0.40
1:E:445:LEU:HA	1:E:448:VAL:HG23	2.04	0.40
1:B:22:LEU:O	1:B:25:SER:HB2	2.21	0.40
1:L:350:PRO:HG3	1:L:389:SER:HB2	2.03	0.40
1:K:209:ASN:HD21	1:K:264:ALA:HB3	1.87	0.40
1:H:147:ASN:HD21	1:H:205:MET:CA	2.35	0.40
1:K:350:PRO:HG3	1:K:389:SER:HB2	2.03	0.40
1:H:76:ILE:HG22	1:H:77:ARG:N	2.36	0.40
1:I:309:ARG:HD3	1:I:349:TYR:CE2	2.55	0.40
1:H:151:TRP:HB2	1:H:152:PRO:HD3	2.03	0.40
1:A:305:ASN:CG	1:A:372:GLU:HB2	2.42	0.40
1:I:15:GLY:HA2	1:I:19:GLU:HG3	2.03	0.40
1:E:15:GLY:HA2	1:E:19:GLU:HG3	2.02	0.40
1:F:76:ILE:HG22	1:F:77:ARG:N	2.36	0.40
1:L:76:ILE:HG22	1:L:77:ARG:N	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:LEU:O	1:F:25:SER:HB2	2.21	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%)	26	60
1	B	440/450 (98%)	424 (96%)	13 (3%)	3 (1%)	26	60
1	C	440/450 (98%)	422 (96%)	15 (3%)	3 (1%)	26	60
1	D	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	E	440/450 (98%)	422 (96%)	16 (4%)	2 (0%)	34	68
1	F	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	G	446/450 (99%)	427 (96%)	16 (4%)	3 (1%)	26	60
1	H	446/450 (99%)	428 (96%)	14 (3%)	4 (1%)	21	53
1	I	440/450 (98%)	423 (96%)	14 (3%)	3 (1%)	26	60
1	J	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	34	68
1	K	440/450 (98%)	426 (97%)	11 (2%)	3 (1%)	26	60
1	L	446/450 (99%)	428 (96%)	16 (4%)	2 (0%)	39	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5304/5400 (98%)	5099 (96%)	173 (3%)	32 (1%)	30	63

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%)	44	77
1	B	375/379 (99%)	365 (97%)	10 (3%)	52	84
1	C	375/379 (99%)	363 (97%)	12 (3%)	46	79
1	D	375/379 (99%)	358 (96%)	17 (4%)	34	67
1	E	375/379 (99%)	360 (96%)	15 (4%)	38	72
1	F	375/379 (99%)	363 (97%)	12 (3%)	46	79
1	G	378/379 (100%)	367 (97%)	11 (3%)	50	82
1	H	378/379 (100%)	366 (97%)	12 (3%)	46	79
1	I	375/379 (99%)	362 (96%)	13 (4%)	43	76
1	J	375/379 (99%)	365 (97%)	10 (3%)	52	84
1	K	375/379 (99%)	362 (96%)	13 (4%)	43	76
1	L	378/379 (100%)	370 (98%)	8 (2%)	61	89
All	All	4512/4548 (99%)	4366 (97%)	146 (3%)	46	79

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/450 (99%)	-0.35	1 (0%) 95 94	12, 38, 79, 120	0
1	B	444/450 (98%)	0.09	17 (3%) 44 32	33, 61, 106, 149	0
1	C	444/450 (98%)	-0.34	3 (0%) 89 84	16, 40, 72, 160	0
1	D	444/450 (98%)	-0.02	14 (3%) 51 39	26, 59, 95, 139	0
1	E	444/450 (98%)	-0.23	4 (0%) 85 79	19, 42, 78, 159	0
1	F	444/450 (98%)	1.56	136 (30%) 1 0	43, 99, 143, 186	0
1	G	448/450 (99%)	-0.34	2 (0%) 93 90	22, 41, 74, 134	0
1	H	448/450 (99%)	-0.06	15 (3%) 50 38	31, 57, 97, 168	0
1	I	444/450 (98%)	-0.30	5 (1%) 82 75	14, 42, 76, 146	0
1	J	444/450 (98%)	1.37	126 (28%) 1 0	54, 109, 165, 225	0
1	K	444/450 (98%)	-0.22	6 (1%) 78 69	19, 45, 75, 147	0
1	L	448/450 (99%)	-0.01	10 (2%) 65 54	24, 58, 98, 149	0
All	All	5344/5400 (98%)	0.10	339 (6%) 23 14	12, 52, 126, 225	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	366	LEU	10.6
1	E	449	LYS	10.6
1	F	367	PRO	10.2
1	J	28	GLU	9.4
1	J	122	ALA	9.3
1	F	275	TYR	8.8
1	J	31	TRP	8.8
1	F	448	VAL	8.8
1	C	104	ASN	8.6
1	F	93	VAL	8.3
1	K	447	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	F	363	ALA	7.5
1	B	448	VAL	7.5
1	J	164	ARG	7.4
1	D	106	ILE	7.3
1	F	310	LEU	7.0
1	B	449	LYS	6.8
1	J	16	PHE	6.8
1	J	105	ILE	6.6
1	F	309	ARG	6.6
1	F	107	SER	6.5
1	K	449	LYS	6.3
1	F	97	VAL	6.3
1	F	108	VAL	6.3
1	F	106	ILE	6.2
1	J	434	GLU	6.2
1	F	105	ILE	6.1
1	F	228	LEU	6.1
1	J	104	ASN	6.0
1	F	110	VAL	5.9
1	F	360	LEU	5.9
1	F	181	VAL	5.9
1	J	117	GLU	5.9
1	F	390	HIS	5.8
1	J	159	ASP	5.8
1	J	182	VAL	5.7
1	F	353	LEU	5.6
1	F	220	ALA	5.5
1	F	3	PHE	5.5
1	J	172	PRO	5.5
1	J	279	VAL	5.4
1	F	277	ASP	5.4
1	H	106	ILE	5.3
1	F	90	THR	5.3
1	F	404	VAL	5.3
1	E	448	VAL	5.2
1	J	35	VAL	5.2
1	F	266	ALA	5.2
1	F	274	GLU	5.1
1	H	99	LYS	5.1
1	I	447	SER	5.0
1	D	447	SER	5.0
1	J	433	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	389	SER	5.0
1	J	91	PHE	4.9
1	F	313	GLY	4.8
1	J	45	LEU	4.8
1	F	162	ALA	4.8
1	H	105	ILE	4.7
1	I	104	ASN	4.7
1	F	102	GLU	4.7
1	J	49	ASP	4.7
1	B	102	GLU	4.6
1	F	302	ILE	4.6
1	F	219	LEU	4.6
1	F	368	MET	4.6
1	J	291	THR	4.6
1	J	272	ALA	4.5
1	J	404	VAL	4.5
1	J	301	TRP	4.4
1	F	449	LYS	4.4
1	F	430	TYR	4.4
1	B	254	TYR	4.3
1	F	247	ALA	4.3
1	J	165	LYS	4.3
1	F	254	TYR	4.3
1	F	394	VAL	4.3
1	F	85	ILE	4.3
1	C	106	ILE	4.2
1	F	325	TYR	4.2
1	J	273	GLU	4.2
1	F	92	ASP	4.2
1	J	44	GLY	4.2
1	J	43	SER	4.2
1	B	97	VAL	4.2
1	F	191	VAL	4.1
1	L	448	VAL	4.1
1	F	257	LYS	4.1
1	J	171	ALA	4.1
1	J	242	GLN	4.1
1	J	15	GLY	4.1
1	F	122	ALA	4.0
1	F	398	MET	4.0
1	J	265	PHE	4.0
1	F	362	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	166	LEU	4.0
1	J	5	LYS	4.0
1	J	193	TYR	3.9
1	F	226	GLY	3.9
1	F	178	GLU	3.9
1	J	167	GLY	3.9
1	J	6	ASN	3.9
1	J	295	SER	3.9
1	J	58	TRP	3.8
1	J	399	LYS	3.8
1	F	182	VAL	3.8
1	J	40	ASN	3.8
1	B	447	SER	3.8
1	F	279	VAL	3.8
1	J	3	PHE	3.8
1	J	123	ASN	3.8
1	F	159	ASP	3.8
1	L	447	SER	3.8
1	F	324	GLY	3.8
1	J	156	TRP	3.8
1	H	449	LYS	3.7
1	F	306	TYR	3.7
1	J	99	LYS	3.7
1	F	231	GLU	3.7
1	J	107	SER	3.7
1	F	396	ASN	3.6
1	J	48	GLY	3.6
1	J	299	LEU	3.6
1	J	438	ARG	3.6
1	B	103	GLY	3.6
1	I	106	ILE	3.6
1	J	85	ILE	3.6
1	J	290	VAL	3.6
1	J	271	LEU	3.5
1	J	261	VAL	3.5
1	F	207	GLU	3.5
1	J	263	TYR	3.5
1	F	89	PRO	3.5
1	F	292	ILE	3.4
1	F	179	LYS	3.4
1	F	356	LEU	3.4
1	J	50	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	225	PRO	3.4
1	F	286	ASP	3.4
1	F	167	GLY	3.4
1	F	87	PRO	3.4
1	F	165	LYS	3.4
1	F	269	ASP	3.3
1	G	449	LYS	3.3
1	J	102	GLU	3.3
1	F	238	PHE	3.3
1	J	20	MET	3.3
1	F	407	TYR	3.3
1	J	86	PHE	3.3
1	F	403	ASP	3.3
1	F	6	ASN	3.3
1	J	106	ILE	3.3
1	F	299	LEU	3.2
1	F	91	PHE	3.2
1	F	339	ARG	3.2
1	D	449	LYS	3.2
1	H	104	ASN	3.2
1	F	268	HIS	3.2
1	F	104	ASN	3.2
1	J	177	ASP	3.2
1	J	23	PRO	3.2
1	F	120	LYS	3.1
1	J	101	GLU	3.1
1	F	406	GLY	3.1
1	J	231	GLU	3.1
1	J	267	TRP	3.1
1	F	86	PHE	3.1
1	H	97	VAL	3.1
1	F	236	ALA	3.1
1	F	154	PRO	3.1
1	L	336	LYS	3.1
1	J	100	ASP	3.0
1	L	105	ILE	3.0
1	F	180	THR	3.0
1	F	88	LYS	3.0
1	F	22	LEU	3.0
1	F	337	SER	3.0
1	D	170	ALA	3.0
1	F	35	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	126	ALA	3.0
1	J	398	MET	3.0
1	J	216	TYR	3.0
1	F	166	LEU	3.0
1	F	168	PRO	2.9
1	F	319	LEU	2.9
1	J	9	PHE	2.9
1	F	447	SER	2.9
1	J	431	VAL	2.9
1	J	241	ILE	2.9
1	F	271	LEU	2.9
1	J	405	ARG	2.9
1	B	104	ASN	2.9
1	F	357	LEU	2.9
1	J	55	PRO	2.9
1	J	87	PRO	2.9
1	F	164	ARG	2.9
1	J	439	TYR	2.9
1	J	33	VAL	2.9
1	J	306	TYR	2.9
1	J	292	ILE	2.9
1	F	7	PHE	2.9
1	D	96	ASP	2.9
1	J	120	LYS	2.9
1	F	117	GLU	2.9
1	J	80	ILE	2.9
1	J	37	ASP	2.8
1	F	9	PHE	2.8
1	F	446	VAL	2.8
1	B	92	ASP	2.8
1	B	253	GLU	2.8
1	J	233	ALA	2.8
1	J	27	VAL	2.8
1	J	19	GLU	2.8
1	F	94	LYS	2.8
1	F	251	ILE	2.8
1	D	358	LYS	2.8
1	F	387	LEU	2.8
1	J	227	PHE	2.8
1	J	103	GLY	2.8
1	A	315	LYS	2.7
1	D	392	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	217	ILE	2.7
1	D	261	VAL	2.7
1	B	219	LEU	2.7
1	F	402	ALA	2.7
1	F	233	ALA	2.7
1	F	440	LEU	2.7
1	J	163	VAL	2.7
1	F	283	ARG	2.6
1	F	321	PRO	2.6
1	F	2	LYS	2.6
1	H	374	GLY	2.6
1	J	92	ASP	2.6
1	F	175	TRP	2.6
1	D	299	LEU	2.6
1	F	382	TYR	2.6
1	J	287	TYR	2.6
1	J	108	VAL	2.6
1	F	221	SER	2.6
1	J	175	TRP	2.6
1	F	8	MET	2.6
1	H	320	VAL	2.6
1	L	116	LYS	2.6
1	K	104	ASN	2.6
1	F	281	GLU	2.5
1	E	395	TYR	2.5
1	F	320	VAL	2.5
1	F	103	GLY	2.5
1	F	352	GLY	2.5
1	F	75	CYS	2.5
1	J	88	LYS	2.5
1	J	238	PHE	2.5
1	B	120	LYS	2.5
1	F	96	ASP	2.5
1	F	358	LYS	2.5
1	J	445	LEU	2.5
1	F	256	GLU	2.5
1	J	396	ASN	2.4
1	K	102	GLU	2.4
1	J	391	LEU	2.4
1	J	151	TRP	2.4
1	J	38	LYS	2.4
1	J	228	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	179	LYS	2.4
1	J	395	TYR	2.4
1	D	107	SER	2.4
1	L	101	GLU	2.4
1	H	44	GLY	2.4
1	K	9	PHE	2.4
1	J	245	ILE	2.4
1	J	208	PRO	2.4
1	J	158	HIS	2.4
1	F	21	GLY	2.4
1	H	98	GLU	2.4
1	J	251	ILE	2.4
1	J	34	TRP	2.4
1	F	95	VAL	2.4
1	L	449	LYS	2.3
1	F	160	PRO	2.3
1	B	178	GLU	2.3
1	J	29	SER	2.3
1	H	113	SER	2.3
1	D	291	THR	2.3
1	F	190	PHE	2.3
1	F	349	TYR	2.3
1	B	106	ILE	2.3
1	D	166	LEU	2.3
1	F	298	LYS	2.3
1	J	220	ALA	2.3
1	I	105	ILE	2.3
1	B	2	LYS	2.3
1	F	38	LYS	2.3
1	F	100	ASP	2.2
1	J	357	LEU	2.3
1	D	5	LYS	2.2
1	J	22	LEU	2.2
1	J	70	LYS	2.2
1	E	447	SER	2.2
1	J	355	ASN	2.2
1	H	256	GLU	2.2
1	J	98	GLU	2.2
1	L	107	SER	2.2
1	B	193	TYR	2.2
1	J	418	TRP	2.2
1	F	116	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	2	LYS	2.2
1	J	161	ILE	2.2
1	C	100	ASP	2.2
1	J	361	ASN	2.2
1	F	323	PRO	2.1
1	I	448	VAL	2.1
1	F	351	GLU	2.1
1	J	176	LEU	2.1
1	H	96	ASP	2.1
1	H	116	LYS	2.1
1	B	218	ASN	2.1
1	J	270	PRO	2.1
1	J	39	GLU	2.1
1	J	129	HIS	2.1
1	F	169	ASP	2.1
1	F	405	ARG	2.1
1	D	171	ALA	2.1
1	F	359	TYR	2.1
1	J	184	PHE	2.1
1	L	102	GLU	2.1
1	K	103	GLY	2.1
1	J	149	TYR	2.1
1	F	422	PHE	2.0
1	G	2	LYS	2.0
1	J	96	ASP	2.0
1	F	290	VAL	2.0
1	J	169	ASP	2.0
1	J	403	ASP	2.0
1	F	170	ALA	2.0
1	H	9	PHE	2.0
1	L	334	PHE	2.0
1	J	294	HIS	2.0
1	F	293	LEU	2.0
1	J	127	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.