



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:18 AM UTC

PDB ID : 3WQ8 / pdb_00003wq8
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

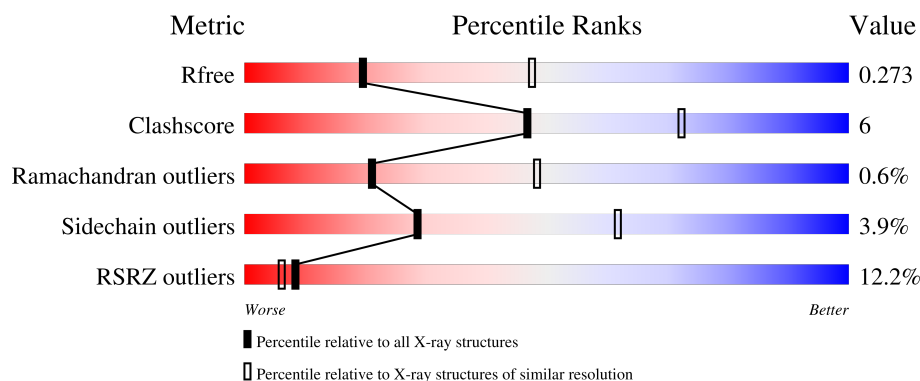
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 85% 14% .
1	B	450	7% 86% 12% ..
1	C	450	2% 84% 13% ..
1	D	450	7% 84% 13% ..
1	E	450	4% 82% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	450	53% 83% 14% ..
1	G	450	2% 86% 12% .
1	H	450	5% 82% 15% .
1	I	450	3% 84% 13% ..
1	J	450	52% 80% 16% ...
1	K	450	3% 82% 14% ..
1	L	450	5% 85% 14% .

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

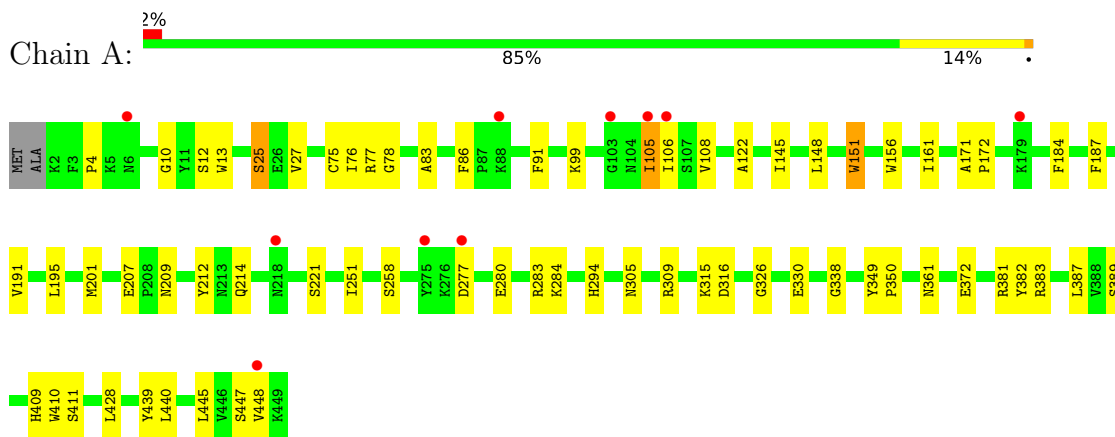
- Molecule 2 is water.

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

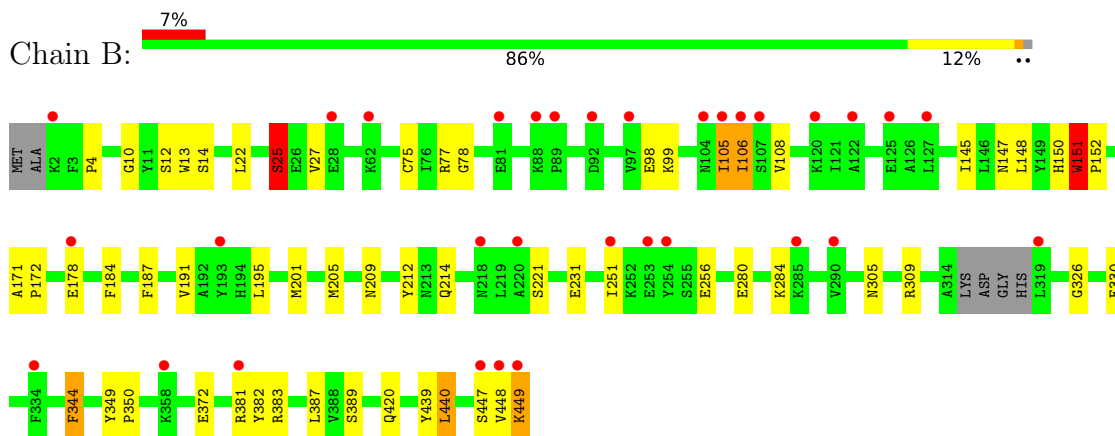
3 Residue-property plots [i](#)

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

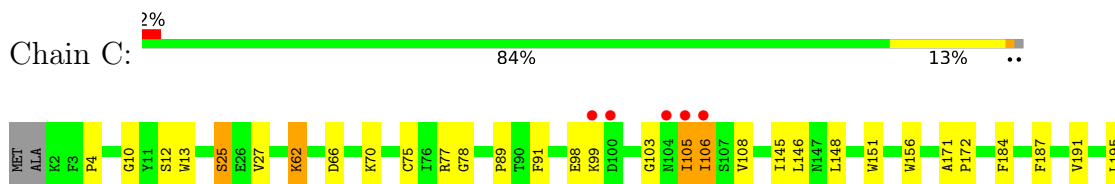
- Molecule 1: Beta-glucosidase

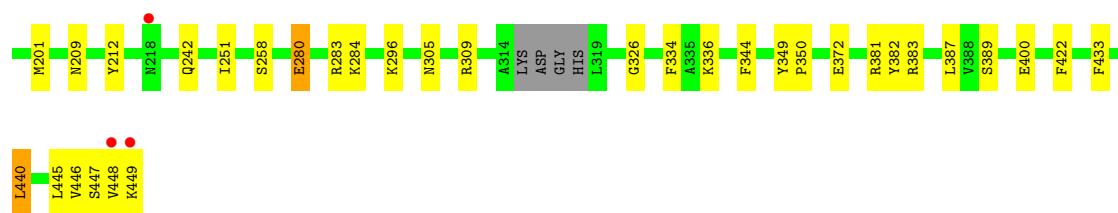


- Molecule 1: Beta-glucosidase

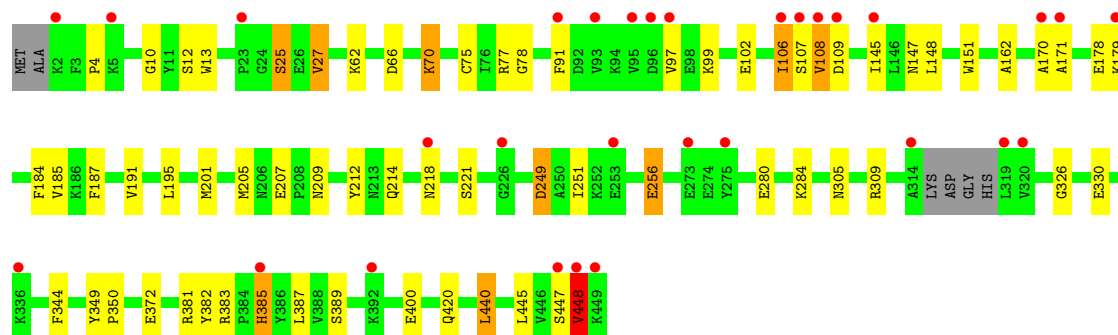
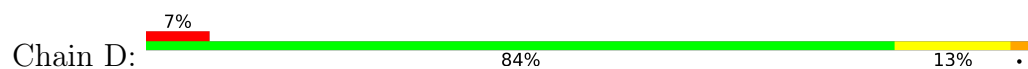


- Molecule 1: Beta-glucosidase

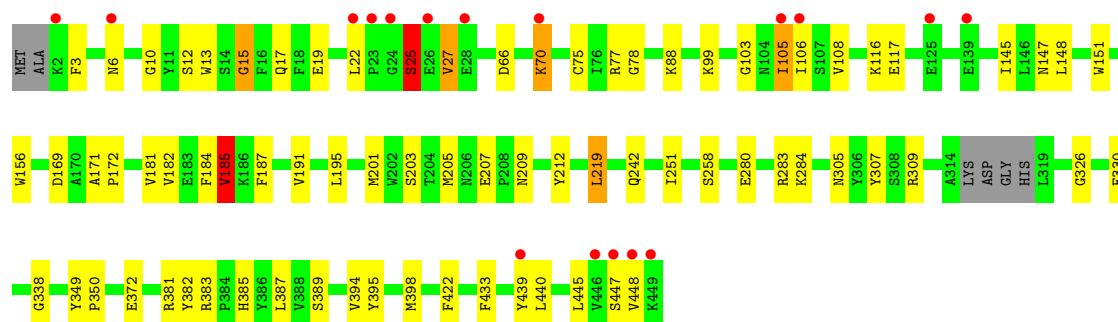
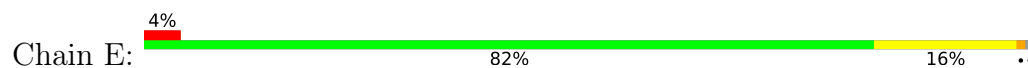




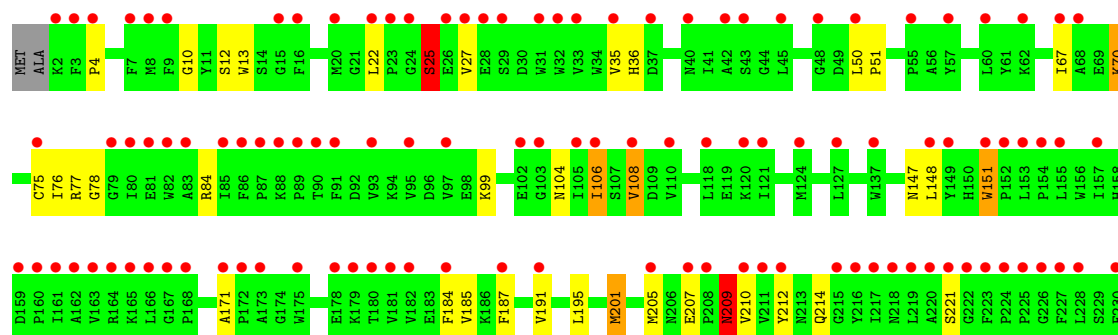
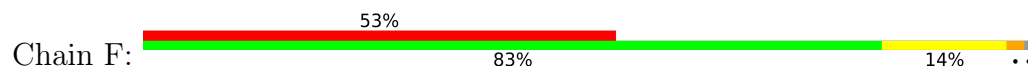
● Molecule 1: Beta-glucosidase

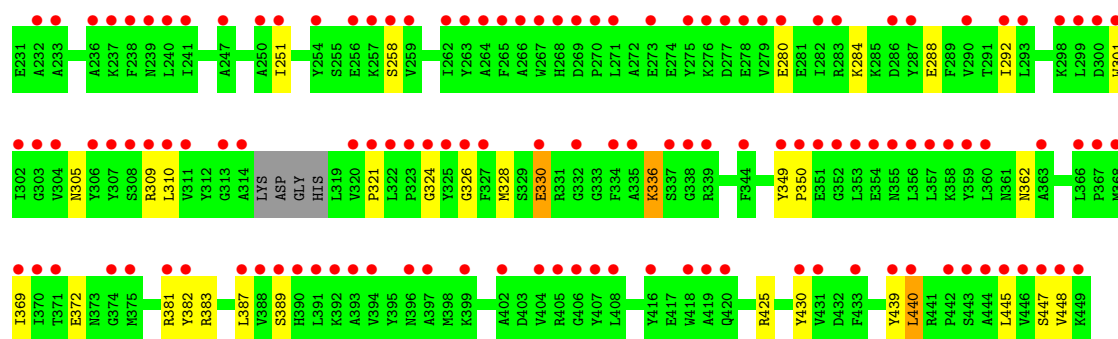


● Molecule 1: Beta-glucosidase

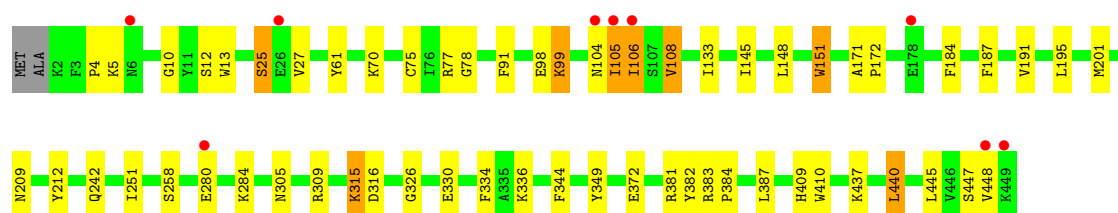
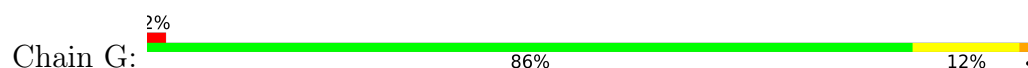


● Molecule 1: Beta-glucosidase

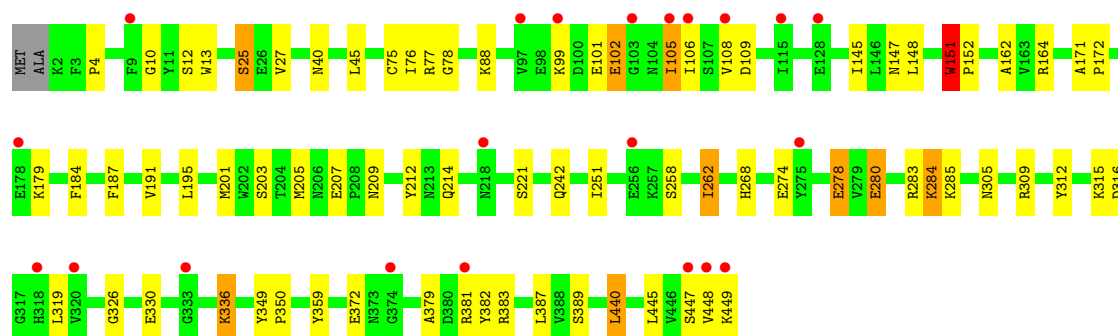
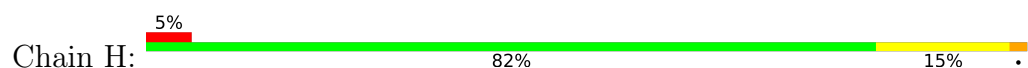




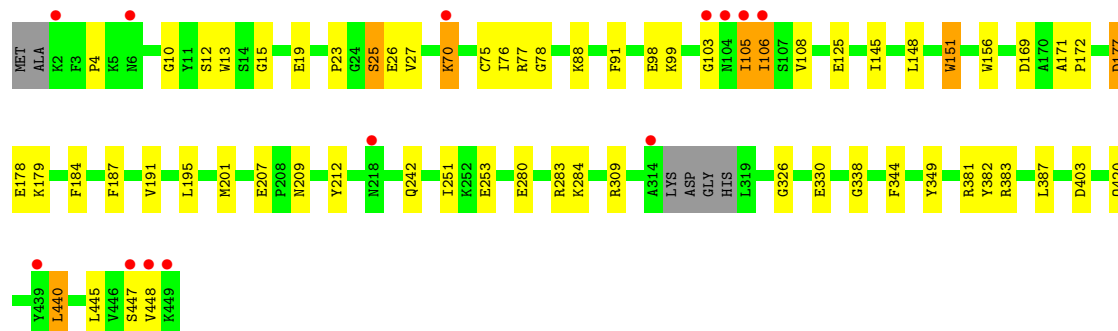
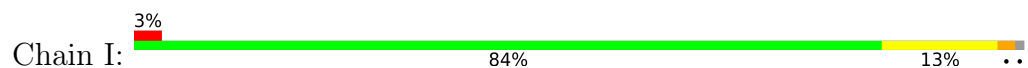
● Molecule 1: Beta-glucosidase



● Molecule 1: Beta-glucosidase



● Molecule 1: Beta-glucosidase



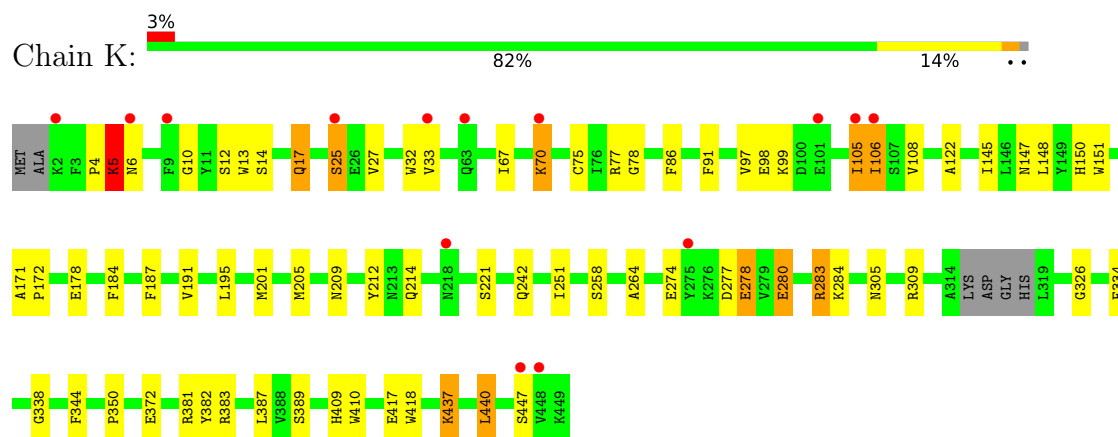
• Molecule 1: Beta-glucosidase

Chain J:



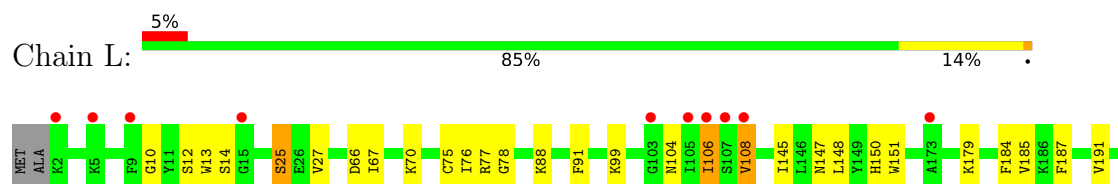
• Molecule 1: Beta-glucosidase

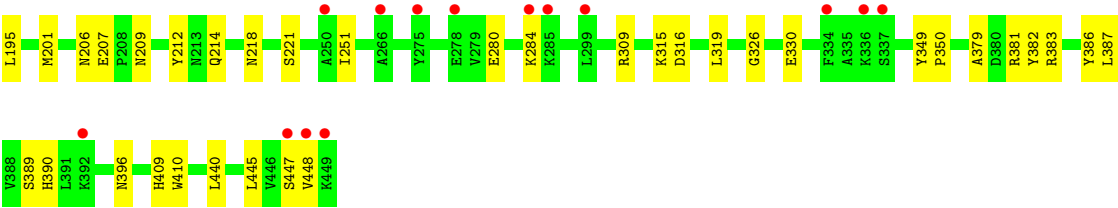
Chain K:



• Molecule 1: Beta-glucosidase

Chain L:





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) 96.7 (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 , 0.273	Depositor DCC
R_{free} test set	8299 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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 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, 0.333 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	0.99	4/3776 (0.1%)	1.02	3/5124 (0.1%)
1	B	0.77	0/3743	0.93	4/5079 (0.1%)
1	C	0.96	1/3743 (0.0%)	0.99	3/5079 (0.1%)
1	D	0.84	4/3743 (0.1%)	0.99	5/5079 (0.1%)
1	E	0.93	4/3743 (0.1%)	0.99	8/5079 (0.2%)
1	F	0.74	2/3743 (0.1%)	0.99	12/5079 (0.2%)
1	G	0.95	0/3776	0.97	3/5124 (0.1%)
1	H	0.83	1/3776 (0.0%)	0.99	9/5124 (0.2%)
1	I	0.92	1/3743 (0.0%)	0.98	5/5079 (0.1%)
1	J	0.75	5/3743 (0.1%)	1.02	15/5079 (0.3%)
1	K	0.93	0/3743	0.99	6/5079 (0.1%)
1	L	0.79	1/3776 (0.0%)	0.96	7/5124 (0.1%)
All	All	0.87	23/45048 (0.1%)	0.99	80/61128 (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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	207	GLU	CA-C	9.89	1.60	1.53
1	F	84	ARG	C-O	7.35	1.33	1.24
1	J	207	GLU	CA-C	6.76	1.58	1.53
1	D	448	VAL	CA-CB	6.58	1.62	1.54
1	D	207	GLU	CA-C	6.24	1.57	1.53
1	J	100	ASP	CA-CB	6.20	1.62	1.53
1	I	207	GLU	CA-C	6.06	1.60	1.52
1	J	41	ILE	CA-CB	6.00	1.61	1.54
1	D	109	ASP	N-CA	-5.96	1.39	1.46
1	J	100	ASP	CA-C	5.83	1.61	1.53
1	F	207	GLU	CA-C	5.82	1.57	1.53
1	E	207	GLU	CA-C	5.80	1.60	1.52
1	A	207	GLU	CA-C	5.65	1.59	1.52
1	C	146	LEU	CA-C	5.52	1.59	1.52
1	E	307	TYR	CA-C	5.48	1.60	1.52
1	A	361	ASN	CG-OD1	-5.37	1.13	1.23
1	E	203	SER	N-CA	-5.25	1.39	1.46
1	A	83	ALA	CA-C	5.19	1.59	1.52
1	L	207	GLU	CA-C	5.17	1.59	1.52
1	A	428	LEU	CA-C	5.16	1.59	1.52
1	E	17	GLN	CA-C	5.12	1.59	1.52
1	J	366	LEU	CA-C	5.11	1.60	1.53
1	D	256	GLU	CA-CB	5.08	1.60	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	161	ILE	N-CA-C	-15.27	99.55	111.62
1	D	249	ASP	CB-CA-C	-11.10	93.45	110.88
1	H	101	GLU	N-CA-C	-10.72	94.41	110.28
1	E	116	LYS	CG-CD-CE	10.26	134.89	111.30
1	F	84	ARG	CB-CA-C	-9.16	95.82	110.94
1	E	185	VAL	CB-CA-C	-9.09	100.14	112.04
1	J	160	PRO	CB-CA-C	-8.87	96.92	111.56
1	F	106	ILE	CB-CA-C	8.61	118.64	111.06
1	J	106	ILE	CB-CA-C	8.41	118.47	111.06
1	L	106	ILE	CB-CA-C	8.35	118.41	111.06
1	H	102	GLU	N-CA-CB	8.21	124.37	110.49
1	H	109	ASP	CB-CA-C	7.76	122.31	109.89
1	J	366	LEU	CB-CA-C	7.72	120.52	108.63
1	J	60	LEU	N-CA-C	-7.53	92.19	107.41
1	L	108	VAL	CB-CA-C	-7.52	98.96	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	5	LYS	N-CA-CB	-7.48	99.12	110.12
1	E	219	LEU	CA-CB-CG	7.32	141.91	116.30
1	B	105	ILE	N-CA-CB	7.13	119.56	111.21
1	J	361	ASN	CB-CG-ND2	7.05	126.97	116.40
1	F	201	MET	N-CA-CB	-6.98	98.64	110.99
1	A	361	ASN	CB-CG-ND2	6.98	126.86	116.40
1	F	108	VAL	CB-CA-C	-6.96	99.88	111.29
1	D	108	VAL	CB-CA-C	-6.75	100.23	111.29
1	G	5	LYS	CD-CE-NZ	6.66	133.21	111.90
1	K	278	GLU	CA-CB-CG	-6.49	101.11	114.10
1	F	425	ARG	CB-CG-CD	-6.46	96.43	111.30
1	D	106	ILE	N-CA-C	-6.28	105.61	111.45
1	H	278	GLU	CA-CB-CG	-6.25	101.61	114.10
1	C	62	LYS	CD-CE-NZ	6.19	131.70	111.90
1	F	201	MET	CB-CA-C	6.15	120.94	109.86
1	J	108	VAL	CB-CA-C	-6.10	101.29	111.29
1	L	108	VAL	CA-C-N	-5.93	114.82	123.00
1	L	108	VAL	C-N-CA	-5.93	114.82	123.00
1	K	283	ARG	CG-CD-NE	5.87	124.91	112.00
1	E	27	VAL	N-CA-C	5.85	116.29	108.27
1	F	209	ASN	CA-CB-CG	-5.84	106.76	112.60
1	E	15	GLY	N-CA-C	5.76	119.19	112.50
1	E	185	VAL	N-CA-CB	5.67	117.56	110.47
1	D	385	HIS	N-CA-CB	5.58	118.42	110.16
1	K	17	GLN	CB-CG-CD	5.57	122.07	112.60
1	G	151	TRP	CA-C-N	-5.48	114.28	119.76
1	G	151	TRP	C-N-CA	-5.48	114.28	119.76
1	K	437	LYS	CA-CB-CG	-5.43	103.23	114.10
1	J	151	TRP	CA-C-N	-5.42	114.34	119.76
1	J	151	TRP	C-N-CA	-5.42	114.34	119.76
1	J	361	ASN	CB-CG-OD1	-5.42	109.96	120.80
1	J	88	LYS	CA-C-N	5.42	125.36	119.78
1	J	88	LYS	C-N-CA	5.42	125.36	119.78
1	H	88	LYS	CA-C-N	5.41	125.35	119.78
1	H	88	LYS	C-N-CA	5.41	125.35	119.78
1	B	151	TRP	CA-C-N	-5.38	114.39	119.76
1	B	151	TRP	C-N-CA	-5.38	114.39	119.76
1	L	106	ILE	CA-CB-CG2	5.37	119.63	110.50
1	J	129	HIS	CA-CB-CG	5.37	119.17	113.80
1	I	177	ASP	CB-CA-C	-5.34	101.29	110.22
1	J	100	ASP	N-CA-CB	5.33	118.65	110.49
1	D	27	VAL	N-CA-C	5.29	115.52	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	151	TRP	CA-C-N	-5.29	114.51	119.85
1	I	151	TRP	C-N-CA	-5.29	114.51	119.85
1	C	296	LYS	CD-CE-NZ	5.23	128.64	111.90
1	H	151	TRP	CA-C-N	-5.23	114.57	119.85
1	H	151	TRP	C-N-CA	-5.23	114.57	119.85
1	J	106	ILE	CA-CB-CG2	5.23	119.38	110.50
1	F	106	ILE	CA-CB-CG2	5.22	119.37	110.50
1	C	280	GLU	CA-CB-CG	-5.20	103.70	114.10
1	E	88	LYS	CA-C-N	5.19	125.13	119.78
1	E	88	LYS	C-N-CA	5.19	125.13	119.78
1	F	108	VAL	CA-C-N	-5.19	115.83	123.00
1	F	108	VAL	C-N-CA	-5.19	115.83	123.00
1	K	280	GLU	CA-CB-CG	-5.18	103.75	114.10
1	I	88	LYS	CA-C-N	5.11	125.04	119.78
1	I	88	LYS	C-N-CA	5.11	125.04	119.78
1	H	101	GLU	CA-C-O	-5.09	115.46	121.16
1	L	88	LYS	CA-C-N	5.08	125.02	119.78
1	L	88	LYS	C-N-CA	5.08	125.02	119.78
1	A	361	ASN	CB-CG-OD1	-5.07	110.65	120.80
1	F	151	TRP	CA-C-N	-5.06	114.70	119.76
1	F	151	TRP	C-N-CA	-5.06	114.70	119.76
1	A	161	ILE	N-CA-C	-5.02	105.81	110.53
1	B	449	LYS	CB-CG-CD	5.01	122.82	111.30

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	35	1
1	B	3626	0	3477	31	1
1	C	3626	0	3477	39	0
1	D	3626	0	3477	35	0
1	E	3626	0	3477	59	0
1	F	3626	0	3477	53	0
1	G	3657	0	3505	41	2
1	H	3657	0	3505	52	1
1	I	3626	0	3477	55	0
1	J	3626	0	3477	77	0
1	K	3626	0	3477	54	2
1	L	3657	0	3505	46	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	487	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (487) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:3:PHE:CE1	1:E:398:MET:HE1	1.91	1.04
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
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:E:3:PHE:HE1	1:E:398:MET:HE1	1.33	0.94
1:I:440:LEU:HD11	1:J:445:LEU:HD13	1.48	0.93
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: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:E:395:TYR:HA	1:E:398:MET:HE3	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:321:PRO:HB2	1:F:328:MET:HE1	1.69	0.72
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: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:E:3:PHE:HE1	1:E:398:MET:CE	2.06	0.68
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: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:C:336:LYS:HE2	1:E:169:ASP:C	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:VAL:HG11	1:L:185:VAL:HG11	1.80	0.63
1:C:440:LEU:HD11	1:D:445:LEU:HD11	1.79	0.63
1:G:336:LYS:HE2	1:I:169:ASP:C	2.24	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:C	1:E:185:VAL:HG23	2.23	0.61
1:E:182:VAL:HA	1:E:185:VAL:CG2	2.31	0.61
1:D:249:ASP:O	1:D:249:ASP:OD1	2.17	0.61
1:E:3:PHE:CD1	1:E:398:MET:HE1	2.36	0.61
1:F:36:HIS:ND1	1:F:50:LEU:HD22	2.15	0.61
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:105:ILE:HD11	1:G:108:VAL:HG23	1.84	0.58
1:C:336:LYS:CE	1:E:169:ASP:C	2.77	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:F:201:MET:HE1	1:F:369:ILE:HD12	1.86	0.57
1:J:300:ASP:C	1:J:366:LEU:HD21	2.29	0.57
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: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:C:77:ARG:C	1:C:77:ARG:HD2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:LEU:CD2	1:F:328:MET:HE2	2.36	0.55
1:H:305:ASN:CG	1:H:372:GLU:HB2	2.32	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:A:91:PHE:CE2	1:K:338:GLY:HA3	2.42	0.55
1:K:209:ASN:HA	1:K:212:TYR:CZ	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:HG23	1:A:105:ILE:O	2.07	0.54
1:G:105:ILE:HG23	1:G:105:ILE:O	2.08	0.54
1:I:448:VAL:HB	1:J:448:VAL:HG11	1.89	0.54
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:E:66:ASP:O	1:E:70:LYS:HG2	2.09	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:HG23	1:K:105:ILE:O	2.08	0.52
1:I:105:ILE:HG22	1:I:242:GLN:OE1	2.10	0.52
1:G:77:ARG:HD2	1:G:77:ARG:C	2.34	0.52
1:E:105:ILE:HG23	1:E:105:ILE:O	2.09	0.52
1:L:409:HIS:HD2	1:L:410:TRP:C	2.18	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:G:334:PHE:CD2	1:I:156:TRP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:LYS:HE2	1:I:103:GLY:C	2.35	0.51
1:F:310:LEU:HD23	1:F:328:MET:HE2	1.93	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: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
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:C:382:TYR:O	1:C:383:ARG:C	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:K:305:ASN:CG	1:K:372:GLU:HB2	2.38	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:A:294:HIS:ND1	1:A:294:HIS:C	2.69	0.49
1:G:437:LYS:HE3	1:H:379:ALA:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HD2	1:B:77:ARG:C	2.38	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:K:77:ARG:HD2	1:K:77:ARG:C	2.37	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:70:LYS:HZ1	1:L:445:LEU:HD13	1.77	0.49
1:K:214:GLN:HE21	1:K:221:SER:HB2	1.77	0.49
1:F:12:SER:HA	1:F:77:ARG:O	2.13	0.48
1:A:382:TYR:O	1:A:383:ARG:C	2.56	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:D:77:ARG:HD2	1:D:77:ARG:C	2.38	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:K:409:HIS:HD2	1:K:410:TRP:C	2.21	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
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:HA	1:H:179:LYS:HD3	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:A:77:ARG:HD2	1:A:77:ARG:C	2.39	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:F:77:ARG:HD2	1:F:77:ARG:C	2.39	0.48
1:G:409:HIS:HD2	1:G:410:TRP:C	2.22	0.48
1:I:382:TYR:O	1:I:383:ARG:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:107:SER:C	1:D:108:VAL:HG23	2.39	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:C:305:ASN:CG	1:C:372:GLU:HB2	2.39	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:C:445:LEU:HD11	1:D:440:LEU:HD11	1.97	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:E:171:ALA:HB1	1:E:172:PRO:HD2	1.97	0.47
1:H:77:ARG:C	1:H:77:ARG:HD2	2.40	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:B:305:ASN:CG	1:B:372:GLU:HB2	2.40	0.47
1:K:382:TYR:O	1:K:383:ARG:C	2.57	0.47
1:E:395:TYR:HA	1:E:398:MET:HE2	1.91	0.46
1:L:13:TRP:CE2	1:L:78:GLY:HA3	2.50	0.46
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:70:LYS:NZ	1:L:445:LEU:CD1	2.79	0.46
1:K:171:ALA:HB1	1:K:172:PRO:HD2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:77:ARG:C	1:E:77:ARG:HD2	2.40	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:382:TYR:O	1:B:383:ARG:C	2.59	0.46
1:B:448:VAL:O	1:B:449:LYS:HG3	2.14	0.46
1:D:382:TYR:O	1:D:383:ARG:C	2.58	0.46
1:E:394:VAL:HG12	1:E:398:MET:HE2	1.98	0.46
1:C:145:ILE:HG12	1:C:201:MET:HB2	1.98	0.46
1:E:305:ASN:CG	1:E:372:GLU:HB2	2.41	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:G:305:ASN:CG	1:G:372:GLU:HB2	2.41	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:I:77:ARG:HD2	1:I:77:ARG:C	2.41	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:F:305:ASN:CG	1:F:372:GLU:HB2	2.41	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:H:315:LYS:O	1:H:316:ASP:C	2.60	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
1:A:305:ASN:CG	1:A:372:GLU:HB2	2.42	0.45
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:C:445:LEU:HB3	1:D:70:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:HD11	1:D:251:ILE:HD11	1.98	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: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:J:305:ASN:CG	1:J:372:GLU:HB2	2.42	0.44
1:K:214:GLN:NE2	1:K:221:SER:CB	2.80	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: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: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:C:191:VAL:HG13	1:C:195:LEU:HD12	2.00	0.44
1:D:305:ASN:CG	1:D:372:GLU:HB2	2.43	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:F:201:MET:HE3	1:F:301:TRP:CE2	2.53	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
1:H:191:VAL:HG13	1:H:195:LEU:HD12	2.00	0.43
1:L:315:LYS:O	1:L:316:ASP:C	2.60	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:J:382:TYR:O	1:J:383:ARG:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:ASN:HD21	1:K:205:MET:C	2.26	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: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:G:70:LYS:HD3	1:H:445:LEU:O	2.18	0.43
1:D:309:ARG:HD3	1:D:349:TYR:CE2	2.54	0.43
1:I:171:ALA:HB1	1:I:172:PRO:HD2	1.99	0.43
1:G:315:LYS:O	1:G:316:ASP:C	2.61	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:G:336:LYS:CE	1:I:169:ASP:C	2.91	0.43
1:I:184:PHE:O	1:I:187:PHE:HB3	2.19	0.43
1:A:409:HIS:HD2	1:A:410:TRP:C	2.27	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:G:445:LEU:HD11	1:H:440:LEU:HD11	2.00	0.43
1:H:214:GLN:OE1	1:H:221:SER:HB3	2.19	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:E:382:TYR:O	1:E:383:ARG:C	2.58	0.42
1:F:382:TYR:O	1:F:383:ARG:C	2.62	0.42
1:I:98:GLU:HB2	1:I:106:ILE:HG22	2.01	0.42
1:J:77:ARG:C	1:J:77:ARG:HD2	2.43	0.42
1:K:70:LYS:HD2	1:L:445:LEU:HD22	2.02	0.42
1:J:160:PRO:O	1:J:160:PRO:HG2	2.19	0.42
1:L:147:ASN:HD21	1:L:206:ASN:HB2	1.85	0.42
1:H:382:TYR:O	1:H:383:ARG:C	2.61	0.42
1:J:214:GLN:OE1	1:J:221:SER:HB3	2.20	0.42
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:A:315:LYS:O	1:A:316:ASP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:448:VAL:HG12	1:J:448:VAL:HG12	2.01	0.42
1:L:77:ARG:HD2	1:L:77:ARG:C	2.45	0.42
1:D:249:ASP:OD1	1:D:249:ASP:C	2.62	0.42
1:H:171:ALA:HB1	1:H:172:PRO:HD2	2.02	0.42
1:A:151:TRP:CD1	1:A:151:TRP:N	2.85	0.42
1:B:344:PHE:CZ	1:B:420:GLN:HG3	2.55	0.42
1:D:107:SER:C	1:D:108:VAL:CG2	2.93	0.42
1:J:147:ASN:HD21	1:J:205:MET:CA	2.32	0.42
1:L:382:TYR:O	1:L:383:ARG:C	2.63	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:F:445:LEU:HA	1:F:448:VAL:HG23	2.02	0.41
1:L:396:ASN:HD22	1:L:396:ASN:HA	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:I:445:LEU:HD23	1:J:448:VAL:HG21	2.00	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:B:309:ARG:HD3	1:B:349:TYR:CE2	2.54	0.41
1:G:383:ARG:O	1:G:384:PRO:C	2.63	0.41
1:J:445:LEU:HA	1:J:448:VAL:HG23	2.02	0.41
1:K:14:SER:HB3	1:K:150:HIS:CE1	2.55	0.41
1:K:147:ASN:HD21	1:K:205:MET:CA	2.33	0.41
1:L:386:TYR:CZ	1:L:390:HIS:CE1	3.09	0.41
1:H:319:LEU:O	1:H:319:LEU:HD23	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:G:382:TYR:O	1:G:383:ARG:C	2.63	0.41
1:K:86:PHE:CE1	1:K:122:ALA:HB2	2.55	0.41
1:L:319:LEU:O	1:L:319:LEU:HD23	2.21	0.41
1:A:410:TRP:HA	1:A:411:SER:HA	1.84	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:E:22:LEU:O	1:E:25:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:86:PHE:CE1	1:A:122:ALA:HB2	2.56	0.41
1:H:319:LEU:HD23	1:H:319:LEU:C	2.46	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:J:22:LEU:O	1:J:25:SER:HB2	2.21	0.40
1:J:41:ILE:CG1	1:J:42:ALA:N	2.84	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:F:209:ASN:ND2	1:F:209:ASN:C	2.79	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:E:15:GLY:HA2	1:E:19:GLU:HG3	2.02	0.40
1:H:76:ILE:HG22	1:H:77:ARG:N	2.36	0.40
1:H:151:TRP:HB2	1:H:152:PRO:HD3	2.03	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
1:I:76:ILE:HG22	1:I:77:ARG:N	2.34	0.40
1:K:32:TRP:O	1:K:33:VAL:C	2.64	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	45
1	B	440/450 (98%)	424 (96%)	13 (3%)	3 (1%)	18	45
1	C	440/450 (98%)	422 (96%)	15 (3%)	3 (1%)	18	45
1	D	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	24	53
1	E	440/450 (98%)	422 (96%)	16 (4%)	2 (0%)	24	53
1	F	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	24	53
1	G	446/450 (99%)	427 (96%)	16 (4%)	3 (1%)	18	45
1	H	446/450 (99%)	428 (96%)	14 (3%)	4 (1%)	14	38
1	I	440/450 (98%)	423 (96%)	14 (3%)	3 (1%)	18	45
1	J	440/450 (98%)	423 (96%)	15 (3%)	2 (0%)	24	53
1	K	440/450 (98%)	426 (97%)	11 (2%)	3 (1%)	18	45
1	L	446/450 (99%)	428 (96%)	16 (4%)	2 (0%)	30	58
All	All	5304/5400 (98%)	5099 (96%)	173 (3%)	32 (1%)	21	48

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

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Mol	Chain	Res	Type
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%)	366 (97%)	12 (3%)	34	68
1	B	375/379 (99%)	360 (96%)	15 (4%)	28	61
1	C	375/379 (99%)	362 (96%)	13 (4%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	375/379 (99%)	358 (96%)	17 (4%)	24	57
1	E	375/379 (99%)	360 (96%)	15 (4%)	28	61
1	F	375/379 (99%)	361 (96%)	14 (4%)	30	63
1	G	378/379 (100%)	363 (96%)	15 (4%)	28	61
1	H	378/379 (100%)	360 (95%)	18 (5%)	23	54
1	I	375/379 (99%)	361 (96%)	14 (4%)	30	63
1	J	375/379 (99%)	360 (96%)	15 (4%)	28	61
1	K	375/379 (99%)	359 (96%)	16 (4%)	26	58
1	L	378/379 (100%)	367 (97%)	11 (3%)	37	71
All	All	4512/4548 (99%)	4337 (96%)	175 (4%)	28	62

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	VAL
1	A	99	LYS
1	A	105	ILE
1	A	106	ILE
1	A	258	SER
1	A	284	LYS
1	A	330	GLU
1	A	381	ARG
1	A	387	LEU
1	A	440	LEU
1	A	447	SER
1	B	25	SER
1	B	27	VAL
1	B	99	LYS
1	B	105	ILE
1	B	106	ILE
1	B	178	GLU
1	B	256	GLU
1	B	280	GLU
1	B	284	LYS
1	B	330	GLU
1	B	344	PHE
1	B	381	ARG
1	B	387	LEU

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Mol	Chain	Res	Type
1	B	440	LEU
1	B	447	SER
1	C	25	SER
1	C	27	VAL
1	C	62	LYS
1	C	105	ILE
1	C	106	ILE
1	C	258	SER
1	C	284	LYS
1	C	344	PHE
1	C	381	ARG
1	C	387	LEU
1	C	400	GLU
1	C	440	LEU
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	218	ASN
1	D	256	GLU
1	D	280	GLU
1	D	284	LYS
1	D	330	GLU
1	D	381	ARG
1	D	385	HIS
1	D	387	LEU
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	105	ILE
1	E	106	ILE
1	E	117	GLU
1	E	185	VAL
1	E	219	LEU
1	E	258	SER
1	E	284	LYS

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Mol	Chain	Res	Type
1	E	330	GLU
1	E	381	ARG
1	E	387	LEU
1	E	440	LEU
1	E	447	SER
1	F	25	SER
1	F	27	VAL
1	F	70	LYS
1	F	106	ILE
1	F	258	SER
1	F	280	GLU
1	F	284	LYS
1	F	330	GLU
1	F	336	LYS
1	F	362	ASN
1	F	381	ARG
1	F	387	LEU
1	F	440	LEU
1	F	447	SER
1	G	25	SER
1	G	27	VAL
1	G	99	LYS
1	G	105	ILE
1	G	106	ILE
1	G	258	SER
1	G	280	GLU
1	G	284	LYS
1	G	315	LYS
1	G	330	GLU
1	G	344	PHE
1	G	381	ARG
1	G	387	LEU
1	G	440	LEU
1	G	447	SER
1	H	25	SER
1	H	27	VAL
1	H	99	LYS
1	H	105	ILE
1	H	106	ILE
1	H	258	SER
1	H	262	ILE
1	H	278	GLU

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Mol	Chain	Res	Type
1	H	280	GLU
1	H	284	LYS
1	H	285	LYS
1	H	330	GLU
1	H	336	LYS
1	H	381	ARG
1	H	387	LEU
1	H	440	LEU
1	H	447	SER
1	H	449	LYS
1	I	25	SER
1	I	27	VAL
1	I	70	LYS
1	I	105	ILE
1	I	106	ILE
1	I	125	GLU
1	I	177	ASP
1	I	253	GLU
1	I	284	LYS
1	I	330	GLU
1	I	381	ARG
1	I	387	LEU
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	106	ILE
1	J	155	LEU
1	J	258	SER
1	J	280	GLU
1	J	284	LYS
1	J	330	GLU
1	J	366	LEU
1	J	381	ARG
1	J	387	LEU
1	J	440	LEU
1	J	447	SER
1	K	5	LYS
1	K	25	SER
1	K	27	VAL

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Mol	Chain	Res	Type
1	K	70	LYS
1	K	99	LYS
1	K	105	ILE
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	387	LEU
1	K	440	LEU
1	K	447	SER
1	L	25	SER
1	L	27	VAL
1	L	106	ILE
1	L	218	ASN
1	L	280	GLU
1	L	284	LYS
1	L	330	GLU
1	L	381	ARG
1	L	387	LEU
1	L	440	LEU
1	L	447	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	59	HIS
1	A	150	HIS
1	A	373	ASN
1	A	409	HIS
1	B	17	GLN
1	B	59	HIS
1	B	147	ASN
1	B	150	HIS
1	B	206	ASN
1	B	214	GLN
1	B	373	ASN
1	C	17	GLN
1	C	53	ASN

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Mol	Chain	Res	Type
1	C	59	HIS
1	C	294	HIS
1	C	373	ASN
1	D	53	ASN
1	D	59	HIS
1	D	147	ASN
1	D	150	HIS
1	D	206	ASN
1	D	373	ASN
1	E	6	ASN
1	E	53	ASN
1	E	147	ASN
1	E	150	HIS
1	E	206	ASN
1	E	294	HIS
1	E	373	ASN
1	E	409	HIS
1	F	36	HIS
1	F	59	HIS
1	F	147	ASN
1	F	150	HIS
1	F	206	ASN
1	F	209	ASN
1	F	294	HIS
1	F	373	ASN
1	G	53	ASN
1	G	59	HIS
1	G	213	ASN
1	G	294	HIS
1	G	355	ASN
1	G	373	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	H	373	ASN
1	I	53	ASN
1	I	150	HIS

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Mol	Chain	Res	Type
1	I	373	ASN
1	J	17	GLN
1	J	53	ASN
1	J	59	HIS
1	J	147	ASN
1	J	150	HIS
1	J	242	GLN
1	J	373	ASN
1	K	59	HIS
1	K	147	ASN
1	K	214	GLN
1	K	355	ASN
1	K	373	ASN
1	K	409	HIS
1	L	59	HIS
1	L	294	HIS
1	L	355	ASN
1	L	373	ASN
1	L	396	ASN
1	L	409	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	0.11	10 (2%) 62 52	12, 38, 79, 120	0
1	B	444/450 (98%)	0.66	32 (7%) 21 15	33, 61, 106, 149	0
1	C	444/450 (98%)	0.15	8 (1%) 67 58	16, 40, 72, 160	0
1	D	444/450 (98%)	0.61	30 (6%) 23 17	26, 59, 94, 139	0
1	E	444/450 (98%)	0.25	17 (3%) 44 35	19, 42, 78, 159	0
1	F	444/450 (98%)	2.21	240 (54%) 0 0	43, 99, 142, 186	0
1	G	448/450 (99%)	0.15	9 (2%) 65 55	22, 41, 74, 134	0
1	H	448/450 (99%)	0.55	21 (4%) 36 28	31, 57, 97, 168	0
1	I	444/450 (98%)	0.19	13 (2%) 53 43	14, 42, 76, 146	0
1	J	444/450 (98%)	2.13	233 (52%) 0 0	54, 109, 165, 225	0
1	K	444/450 (98%)	0.31	14 (3%) 50 40	19, 45, 75, 147	0
1	L	448/450 (99%)	0.62	24 (5%) 31 23	24, 58, 98, 149	0
All	All	5344/5400 (98%)	0.66	651 (12%) 8 6	12, 52, 126, 225	0

All (651) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	266	ALA	7.1
1	J	16	PHE	6.8
1	F	366	LEU	6.1
1	J	175	TRP	6.1
1	J	439	TYR	5.8
1	F	9	PHE	5.5
1	J	265	PHE	5.5
1	J	33	VAL	5.4
1	J	81	GLU	5.3
1	F	360	LEU	5.3
1	F	217	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	L	2	LYS	5.2
1	J	86	PHE	5.2
1	F	3	PHE	5.2
1	F	293	LEU	5.2
1	F	367	PRO	5.2
1	D	106	ILE	5.1
1	F	310	LEU	5.1
1	F	247	ALA	5.1
1	F	389	SER	5.1
1	J	438	ARG	5.1
1	F	325	TYR	5.0
1	F	181	VAL	5.0
1	D	108	VAL	4.9
1	C	105	ILE	4.9
1	J	227	PHE	4.9
1	J	182	VAL	4.9
1	I	106	ILE	4.9
1	F	404	VAL	4.8
1	F	359	TYR	4.8
1	F	90	THR	4.7
1	H	105	ILE	4.7
1	D	447	SER	4.7
1	I	105	ILE	4.7
1	F	182	VAL	4.6
1	J	149	TYR	4.6
1	F	323	PRO	4.6
1	J	228	LEU	4.6
1	F	358	LYS	4.6
1	F	394	VAL	4.5
1	I	447	SER	4.5
1	F	22	LEU	4.5
1	J	31	TRP	4.5
1	F	357	LEU	4.5
1	J	105	ILE	4.4
1	F	219	LEU	4.4
1	F	275	TYR	4.4
1	J	28	GLU	4.4
1	J	84	ARG	4.4
1	F	233	ALA	4.4
1	J	160	PRO	4.4
1	F	207	GLU	4.4
1	J	121	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	88	LYS	4.3
1	E	105	ILE	4.3
1	F	108	VAL	4.3
1	F	279	VAL	4.3
1	F	407	TYR	4.3
1	F	283	ARG	4.3
1	F	308	SER	4.2
1	J	168	PRO	4.2
1	F	314	ALA	4.2
1	J	290	VAL	4.2
1	J	19	GLU	4.2
1	J	263	TYR	4.2
1	C	106	ILE	4.2
1	D	448	VAL	4.2
1	J	60	LEU	4.2
1	B	106	ILE	4.2
1	J	245	ILE	4.2
1	J	433	PHE	4.2
1	F	220	ALA	4.1
1	F	397	ALA	4.1
1	F	91	PHE	4.1
1	J	208	PRO	4.1
1	F	430	TYR	4.1
1	J	440	LEU	4.1
1	F	211	VAL	4.1
1	J	404	VAL	4.1
1	J	41	ILE	4.1
1	K	6	ASN	4.0
1	F	85	ILE	4.0
1	L	106	ILE	4.0
1	J	258	SER	4.0
1	F	225	PRO	4.0
1	F	106	ILE	4.0
1	F	16	PHE	4.0
1	F	45	LEU	4.0
1	J	156	TRP	4.0
1	F	306	TYR	3.9
1	J	233	ALA	3.9
1	F	356	LEU	3.9
1	F	160	PRO	3.9
1	J	291	THR	3.9
1	F	81	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	88	LYS	3.9
1	J	176	LEU	3.9
1	F	448	VAL	3.9
1	F	302	ILE	3.9
1	F	179	LYS	3.9
1	F	268	HIS	3.9
1	F	338	GLY	3.8
1	J	446	VAL	3.8
1	A	105	ILE	3.8
1	G	105	ILE	3.8
1	J	159	ASP	3.8
1	J	27	VAL	3.8
1	J	151	TRP	3.8
1	F	419	ALA	3.8
1	J	445	LEU	3.8
1	E	448	VAL	3.8
1	F	168	PRO	3.8
1	F	352	GLY	3.8
1	J	172	PRO	3.8
1	F	391	LEU	3.8
1	J	22	LEU	3.8
1	J	166	LEU	3.8
1	J	29	SER	3.7
1	F	159	ASP	3.7
1	J	48	GLY	3.7
1	J	164	ARG	3.7
1	F	97	VAL	3.7
1	F	237	LYS	3.7
1	G	449	LYS	3.7
1	F	309	ARG	3.7
1	L	448	VAL	3.7
1	J	89	PRO	3.7
1	H	374	GLY	3.7
1	G	106	ILE	3.7
1	J	241	ILE	3.7
1	J	87	PRO	3.7
1	J	58	TRP	3.7
1	F	339	ARG	3.7
1	J	80	ILE	3.7
1	J	279	VAL	3.7
1	F	4	PRO	3.6
1	J	91	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	216	TYR	3.6
1	J	431	VAL	3.6
1	F	353	LEU	3.6
1	F	154	PRO	3.6
1	J	55	PRO	3.6
1	J	106	ILE	3.6
1	F	390	HIS	3.6
1	B	447	SER	3.6
1	J	83	ALA	3.5
1	F	418	TRP	3.5
1	J	240	LEU	3.5
1	J	23	PRO	3.5
1	K	106	ILE	3.5
1	F	173	ALA	3.5
1	F	222	GLY	3.5
1	F	161	ILE	3.5
1	F	238	PHE	3.5
1	H	9	PHE	3.5
1	J	161	ILE	3.5
1	J	282	ILE	3.5
1	F	33	VAL	3.5
1	F	368	MET	3.5
1	F	155	LEU	3.5
1	F	23	PRO	3.5
1	F	363	ALA	3.5
1	H	449	LYS	3.4
1	F	350	PRO	3.4
1	F	180	THR	3.4
1	J	85	ILE	3.4
1	F	221	SER	3.4
1	J	49	ASP	3.4
1	J	355	ASN	3.4
1	F	299	LEU	3.4
1	J	447	SER	3.4
1	J	292	ILE	3.4
1	F	149	TYR	3.4
1	J	415	ASN	3.4
1	F	311	VAL	3.4
1	J	126	ALA	3.4
1	J	236	ALA	3.4
1	J	391	LEU	3.3
1	F	191	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	437	LYS	3.3
1	K	105	ILE	3.3
1	J	422	PHE	3.3
1	F	387	LEU	3.3
1	D	107	SER	3.3
1	F	304	VAL	3.3
1	J	107	SER	3.3
1	J	267	TRP	3.3
1	J	418	TRP	3.3
1	K	447	SER	3.3
1	D	170	ALA	3.3
1	F	75	CYS	3.3
1	F	127	LEU	3.3
1	F	263	TYR	3.3
1	J	70	LYS	3.3
1	L	105	ILE	3.3
1	J	397	ALA	3.3
1	J	163	VAL	3.3
1	J	122	ALA	3.2
1	J	35	VAL	3.2
1	J	15	GLY	3.2
1	B	2	LYS	3.2
1	F	28	GLU	3.2
1	J	148	LEU	3.2
1	J	230	PHE	3.2
1	F	89	PRO	3.2
1	J	251	ILE	3.2
1	F	240	LEU	3.2
1	K	9	PHE	3.2
1	F	449	LYS	3.2
1	F	324	GLY	3.2
1	F	337	SER	3.2
1	J	295	SER	3.2
1	J	6	ASN	3.2
1	F	35	VAL	3.2
1	L	284	LYS	3.2
1	F	20	MET	3.2
1	F	152	PRO	3.2
1	F	162	ALA	3.1
1	J	402	ALA	3.1
1	K	218	ASN	3.1
1	F	267	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	301	TRP	3.1
1	I	439	TYR	3.1
1	J	134	TYR	3.1
1	F	223	PHE	3.1
1	F	265	PHE	3.1
1	H	106	ILE	3.1
1	F	442	PRO	3.1
1	K	448	VAL	3.1
1	F	322	LEU	3.1
1	F	440	LEU	3.1
1	J	165	LYS	3.1
1	J	162	ALA	3.1
1	J	103	GLY	3.1
1	F	292	ILE	3.1
1	F	280	GLU	3.1
1	H	178	GLU	3.1
1	J	399	LYS	3.1
1	D	314	ALA	3.0
1	J	301	TRP	3.0
1	F	230	PHE	3.0
1	F	287	TYR	3.0
1	H	275	TYR	3.0
1	F	105	ILE	3.0
1	F	87	PRO	3.0
1	F	228	LEU	3.0
1	B	448	VAL	3.0
1	F	175	TRP	3.0
1	J	20	MET	3.0
1	F	307	TYR	3.0
1	D	449	LYS	3.0
1	E	449	LYS	3.0
1	F	370	ILE	3.0
1	F	408	LEU	3.0
1	F	178	GLU	3.0
1	F	224	PRO	3.0
1	H	256	GLU	3.0
1	J	154	PRO	3.0
1	J	124	MET	3.0
1	F	254	TYR	3.0
1	L	449	LYS	3.0
1	C	104	ASN	3.0
1	F	153	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	277	ASP	3.0
1	J	127	LEU	3.0
1	J	4	PRO	3.0
1	J	413	THR	3.0
1	F	103	GLY	3.0
1	J	299	LEU	3.0
1	B	253	GLU	3.0
1	F	86	PHE	3.0
1	F	290	VAL	3.0
1	B	449	LYS	2.9
1	F	416	TYR	2.9
1	J	357	LEU	2.9
1	B	218	ASN	2.9
1	L	447	SER	2.9
1	J	314	ALA	2.9
1	F	257	LYS	2.9
1	L	336	LYS	2.9
1	B	105	ILE	2.9
1	F	241	ILE	2.9
1	F	313	GLY	2.9
1	J	146	LEU	2.9
1	J	219	LEU	2.9
1	J	218	ASN	2.9
1	L	15	GLY	2.9
1	F	321	PRO	2.9
1	J	193	TYR	2.9
1	K	2	LYS	2.9
1	F	250	ALA	2.9
1	F	121	ILE	2.9
1	J	242	GLN	2.8
1	F	276	LYS	2.8
1	J	57	TYR	2.8
1	F	7	PHE	2.8
1	G	6	ASN	2.8
1	F	31	TRP	2.8
1	F	171	ALA	2.8
1	J	104	ASN	2.8
1	J	158	HIS	2.8
1	J	63	GLN	2.8
1	J	261	VAL	2.8
1	J	416	TYR	2.8
1	J	157	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	6	ASN	2.8
1	J	34	TRP	2.8
1	F	320	VAL	2.8
1	F	187	PHE	2.8
1	J	109	ASP	2.8
1	B	88	LYS	2.8
1	H	99	LYS	2.8
1	I	70	LYS	2.8
1	J	117	GLU	2.7
1	F	93	VAL	2.7
1	F	163	VAL	2.7
1	H	97	VAL	2.7
1	F	227	PHE	2.7
1	F	264	ALA	2.7
1	F	433	PHE	2.7
1	J	173	ALA	2.7
1	J	67	ILE	2.7
1	J	364	TYR	2.7
1	J	38	LYS	2.7
1	F	443	SER	2.7
1	F	447	SER	2.7
1	J	25	SER	2.7
1	F	208	PRO	2.7
1	J	50	LEU	2.7
1	J	59	HIS	2.7
1	B	358	LYS	2.7
1	D	2	LYS	2.7
1	L	5	LYS	2.7
1	J	53	ASN	2.7
1	J	123	ASN	2.7
1	D	226	GLY	2.7
1	F	382	TYR	2.7
1	J	287	TYR	2.7
1	F	239	ASN	2.7
1	F	215	GLY	2.7
1	J	44	GLY	2.7
1	D	97	VAL	2.7
1	F	27	VAL	2.7
1	H	128	GLU	2.7
1	J	101	GLU	2.7
1	J	118	LEU	2.7
1	J	223	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	205	MET	2.7
1	F	355	ASN	2.7
1	J	226	GLY	2.7
1	G	448	VAL	2.7
1	J	231	GLU	2.7
1	D	5	LYS	2.6
1	E	106	ILE	2.6
1	F	80	ILE	2.6
1	F	393	ALA	2.6
1	J	430	TYR	2.6
1	J	381	ARG	2.6
1	F	226	GLY	2.6
1	F	148	LEU	2.6
1	F	269	ASP	2.6
1	J	394	VAL	2.6
1	F	327	PHE	2.6
1	J	268	HIS	2.6
1	F	55	PRO	2.6
1	J	406	GLY	2.6
1	D	392	LYS	2.6
1	J	271	LEU	2.6
1	E	139	GLU	2.6
1	F	278	GLU	2.6
1	A	277	ASP	2.6
1	F	68	ALA	2.6
1	F	216	TYR	2.6
1	F	392	LYS	2.6
1	J	358	LYS	2.6
1	K	70	LYS	2.6
1	J	2	LYS	2.6
1	F	369	ILE	2.6
1	H	320	VAL	2.6
1	J	320	VAL	2.6
1	F	42	ALA	2.6
1	F	396	ASN	2.6
1	K	25	SER	2.5
1	B	285	LYS	2.5
1	F	399	LYS	2.5
1	F	24	GLY	2.5
1	F	48	GLY	2.5
1	F	60	LEU	2.5
1	J	155	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	81	GLU	2.5
1	B	125	GLU	2.5
1	F	420	GLN	2.5
1	G	26	GLU	2.5
1	J	17	GLN	2.5
1	J	238	PHE	2.5
1	K	63	GLN	2.5
1	F	83	ALA	2.5
1	F	402	ALA	2.5
1	B	104	ASN	2.5
1	F	164	ARG	2.5
1	J	129	HIS	2.5
1	D	93	VAL	2.5
1	J	61	TYR	2.5
1	J	108	VAL	2.5
1	J	3	PHE	2.5
1	J	425	ARG	2.5
1	B	92	ASP	2.5
1	F	165	LYS	2.5
1	F	137	TRP	2.5
1	H	448	VAL	2.5
1	J	180	THR	2.5
1	J	62	LYS	2.5
1	J	66	ASP	2.5
1	F	326	GLY	2.5
1	F	210	VAL	2.5
1	J	95	VAL	2.5
1	J	311	VAL	2.5
1	L	392	LYS	2.5
1	A	6	ASN	2.5
1	I	218	ASN	2.5
1	C	100	ASP	2.4
1	F	8	MET	2.4
1	F	118	LEU	2.4
1	J	224	PRO	2.4
1	J	367	PRO	2.4
1	B	97	VAL	2.4
1	F	95	VAL	2.4
1	F	332	GLY	2.4
1	F	256	GLU	2.4
1	L	9	PHE	2.4
1	B	193	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	298	LYS	2.4
1	I	6	ASN	2.4
1	F	271	LEU	2.4
1	J	203	SER	2.4
1	C	99	LYS	2.4
1	J	434	GLU	2.4
1	L	334	PHE	2.4
1	D	171	ALA	2.4
1	F	371	THR	2.4
1	J	45	LEU	2.4
1	F	157	ILE	2.4
1	J	225	PRO	2.4
1	F	446	VAL	2.4
1	J	46	VAL	2.4
1	K	33	VAL	2.4
1	L	108	VAL	2.4
1	J	285	LYS	2.4
1	J	298	LYS	2.4
1	B	334	PHE	2.4
1	F	354	GLU	2.4
1	J	9	PHE	2.4
1	J	184	PHE	2.4
1	J	354	GLU	2.4
1	I	314	ALA	2.4
1	J	72	GLY	2.4
1	J	116	LYS	2.4
1	F	335	ALA	2.4
1	J	444	ALA	2.4
1	L	337	SER	2.4
1	J	435	THR	2.4
1	A	448	VAL	2.3
1	I	449	LYS	2.3
1	J	5	LYS	2.3
1	D	96	ASP	2.3
1	J	363	ALA	2.3
1	J	43	SER	2.3
1	D	319	LEU	2.3
1	J	395	TYR	2.3
1	F	251	ILE	2.3
1	B	381	ARG	2.3
1	F	381	ARG	2.3
1	J	304	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	218	ASN	2.3
1	B	127	LEU	2.3
1	J	293	LEU	2.3
1	J	82	TRP	2.3
1	J	254	TYR	2.3
1	K	275	TYR	2.3
1	J	179	LYS	2.3
1	J	51	PRO	2.3
1	I	448	VAL	2.3
1	J	429	VAL	2.3
1	J	448	VAL	2.3
1	F	303	GLY	2.3
1	C	218	ASN	2.3
1	I	104	ASN	2.3
1	F	236	ALA	2.3
1	L	173	ALA	2.3
1	F	124	MET	2.3
1	B	107	SER	2.3
1	E	2	LYS	2.3
1	H	447	SER	2.3
1	E	439	TYR	2.3
1	J	306	TYR	2.3
1	E	446	VAL	2.3
1	J	181	VAL	2.3
1	F	351	GLU	2.3
1	F	62	LYS	2.3
1	D	385	HIS	2.3
1	J	150	HIS	2.3
1	J	217	ILE	2.3
1	F	82	TRP	2.3
1	E	447	SER	2.3
1	F	258	SER	2.3
1	A	179	LYS	2.2
1	C	449	LYS	2.2
1	F	2	LYS	2.2
1	F	37	ASP	2.2
1	D	320	VAL	2.2
1	F	270	PRO	2.2
1	J	211	VAL	2.2
1	J	442	PRO	2.2
1	B	254	TYR	2.2
1	J	443	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	406	GLY	2.2
1	F	344	PHE	2.2
1	F	26	GLU	2.2
1	F	273	GLU	2.2
1	A	218	ASN	2.2
1	J	120	LYS	2.2
1	J	257	LYS	2.2
1	J	436	LYS	2.2
1	A	106	ILE	2.2
1	B	251	ILE	2.2
1	D	275	TYR	2.2
1	F	43	SER	2.2
1	F	349	TYR	2.2
1	F	15	GLY	2.2
1	F	334	PHE	2.2
1	B	220	ALA	2.2
1	J	26	GLU	2.2
1	J	393	ALA	2.2
1	F	282	ILE	2.2
1	J	194	HIS	2.2
1	J	92	ASP	2.2
1	J	270	PRO	2.2
1	F	439	TYR	2.2
1	J	359	TYR	2.2
1	L	103	GLY	2.2
1	F	300	ASP	2.2
1	A	103	GLY	2.2
1	F	374	GLY	2.2
1	H	103	GLY	2.2
1	J	137	TRP	2.2
1	J	167	GLY	2.2
1	F	57	TYR	2.2
1	J	130	TYR	2.2
1	B	319	LEU	2.2
1	L	107	SER	2.2
1	L	299	LEU	2.2
1	B	28	GLU	2.2
1	F	444	ALA	2.2
1	J	42	ALA	2.2
1	J	207	GLU	2.2
1	F	405	ARG	2.1
1	C	448	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	23	PRO	2.1
1	F	110	VAL	2.1
1	H	108	VAL	2.1
1	F	286	ASP	2.1
1	F	120	LYS	2.1
1	F	79	GLY	2.1
1	F	151	TRP	2.1
1	F	166	LEU	2.1
1	J	360	LEU	2.1
1	L	250	ALA	2.1
1	E	26	GLU	2.1
1	L	278	GLU	2.1
1	D	218	ASN	2.1
1	B	89	PRO	2.1
1	B	290	VAL	2.1
1	J	191	VAL	2.1
1	J	210	VAL	2.1
1	F	375	MET	2.1
1	B	62	LYS	2.1
1	J	237	LYS	2.1
1	L	285	LYS	2.1
1	J	334	PHE	2.1
1	J	32	TRP	2.1
1	B	122	ALA	2.1
1	L	266	ALA	2.1
1	H	115	ILE	2.1
1	F	388	VAL	2.1
1	E	23	PRO	2.1
1	F	172	PRO	2.1
1	I	2	LYS	2.1
1	J	235	LYS	2.1
1	J	396	ASN	2.1
1	F	50	LEU	2.1
1	J	153	LEU	2.1
1	J	366	LEU	2.1
1	F	184	PHE	2.1
1	H	381	ARG	2.1
1	A	275	TYR	2.1
1	B	178	GLU	2.1
1	F	102	GLU	2.1
1	F	212	TYR	2.1
1	G	280	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	29	SER	2.1
1	J	14	SER	2.1
1	B	120	LYS	2.1
1	D	95	VAL	2.1
1	F	259	VAL	2.1
1	F	431	VAL	2.1
1	F	218	ASN	2.1
1	E	22	LEU	2.1
1	J	174	GLY	2.1
1	J	286	ASP	2.1
1	J	432	ASP	2.1
1	D	145	ILE	2.1
1	J	220	ALA	2.1
1	J	379	ALA	2.1
1	D	253	GLU	2.1
1	F	330	GLU	2.1
1	G	178	GLU	2.1
1	L	275	TYR	2.1
1	J	132	LYS	2.0
1	J	205	MET	2.0
1	H	318	HIS	2.0
1	G	104	ASN	2.0
1	J	361	ASN	2.0
1	D	91	PHE	2.0
1	F	167	GLY	2.0
1	I	103	GLY	2.0
1	F	262	ILE	2.0
1	F	232	ALA	2.0
1	J	232	ALA	2.0
1	J	272	ALA	2.0
1	D	273	GLU	2.0
1	F	32	TRP	2.0
1	J	392	LYS	2.0
1	J	368	MET	2.0
1	J	97	VAL	2.0
1	F	445	LEU	2.0
1	F	40	ASN	2.0
1	E	24	GLY	2.0
1	H	333	GLY	2.0
1	J	222	GLY	2.0
1	F	67	ILE	2.0
1	J	266	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	109	ASP	2.0
1	A	88	LYS	2.0
1	D	179	LYS	2.0
1	D	336	LYS	2.0
1	E	28	GLU	2.0
1	E	70	LYS	2.0
1	E	125	GLU	2.0
1	J	94	LYS	2.0
1	K	101	GLU	2.0
1	J	212	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.