



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:11 AM EST

PDB ID : 8FAA
Title : Crystal structure of Xanthomonas campestris GH35 beta-galactosidase
Authors : Godoy, A.S.; Polikarpov, I.
Deposited on : 2022-11-25
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

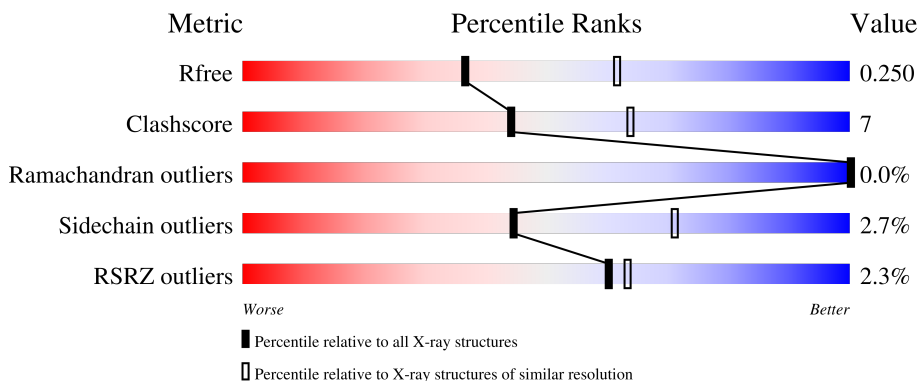
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	511	
1	B	511	
1	C	511	
1	D	511	
1	E	511	

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Mol	Chain	Length	Quality of chain
1	F	511	<p>2% 84% 15%</p>
1	G	511	<p>2% 85% 14%</p>
1	H	511	<p>1% 87% 12%</p>
1	I	511	<p>3% 86% 13%</p>
1	J	511	<p>2% 87% 12%</p>
1	K	511	<p>3% 86% 13%</p>
1	L	511	<p>5% 86% 12%</p>
1	M	511	<p>2% 87% 12%</p>
1	N	511	<p>4% 85% 14%</p>
1	O	511	<p>5% 82% 17%</p>
1	P	511	<p>1% 87% 12%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 65632 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	3921	2491	707	718	5	0	0	0
1	B	510	3921	2491	707	718	5	0	0	0
1	C	510	3921	2491	707	718	5	0	0	0
1	D	510	3921	2491	707	718	5	0	0	0
1	E	510	3921	2491	707	718	5	0	0	0
1	F	510	3921	2491	707	718	5	0	0	0
1	G	510	3921	2491	707	718	5	0	0	0
1	H	510	3921	2491	707	718	5	0	0	0
1	I	510	3921	2491	707	718	5	0	0	0
1	J	510	3921	2491	707	718	5	0	0	0
1	K	510	3921	2491	707	718	5	0	0	0
1	L	510	3921	2491	707	718	5	0	0	0
1	M	510	3921	2491	707	718	5	0	0	0
1	N	510	3921	2491	707	718	5	0	0	0
1	O	510	3921	2491	707	718	5	0	0	0
1	P	510	3921	2491	707	718	5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q8P844
B	2	MET	-	initiating methionine	UNP Q8P844
C	2	MET	-	initiating methionine	UNP Q8P844
D	2	MET	-	initiating methionine	UNP Q8P844
E	2	MET	-	initiating methionine	UNP Q8P844
F	2	MET	-	initiating methionine	UNP Q8P844
G	2	MET	-	initiating methionine	UNP Q8P844
H	2	MET	-	initiating methionine	UNP Q8P844
I	2	MET	-	initiating methionine	UNP Q8P844
J	2	MET	-	initiating methionine	UNP Q8P844
K	2	MET	-	initiating methionine	UNP Q8P844
L	2	MET	-	initiating methionine	UNP Q8P844
M	2	MET	-	initiating methionine	UNP Q8P844
N	2	MET	-	initiating methionine	UNP Q8P844
O	2	MET	-	initiating methionine	UNP Q8P844
P	2	MET	-	initiating methionine	UNP Q8P844

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	242	Total O 242 242	0	0
2	B	157	Total O 157 157	0	0
2	C	186	Total O 186 186	0	0
2	D	186	Total O 186 186	0	0
2	E	200	Total O 200 200	0	0
2	F	203	Total O 203 203	0	0
2	G	196	Total O 196 196	0	0
2	H	188	Total O 188 188	0	0
2	I	215	Total O 215 215	0	0
2	J	198	Total O 198 198	0	0
2	K	185	Total O 185 185	0	0

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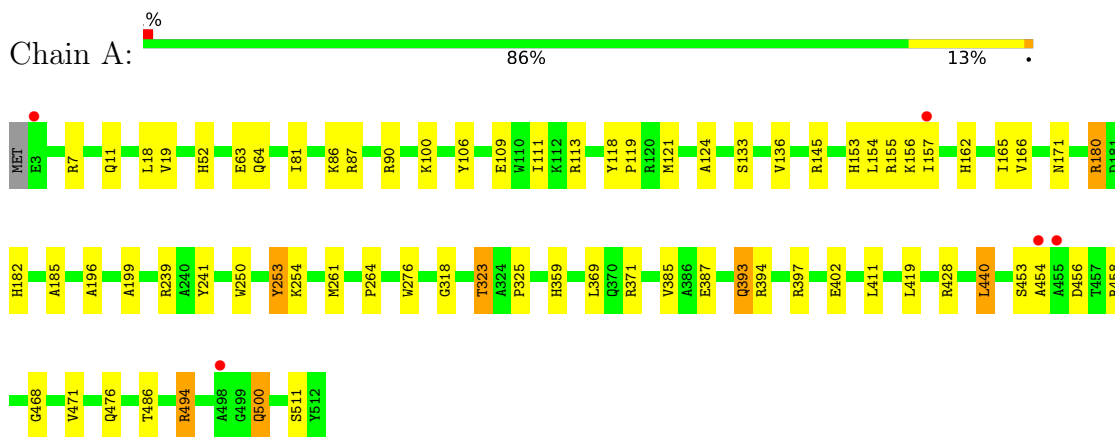
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	209	Total 209	O 209	0	0
2	M	129	Total 129	O 129	0	0
2	N	113	Total 113	O 113	0	0
2	O	94	Total 94	O 94	0	0
2	P	195	Total 195	O 195	0	0

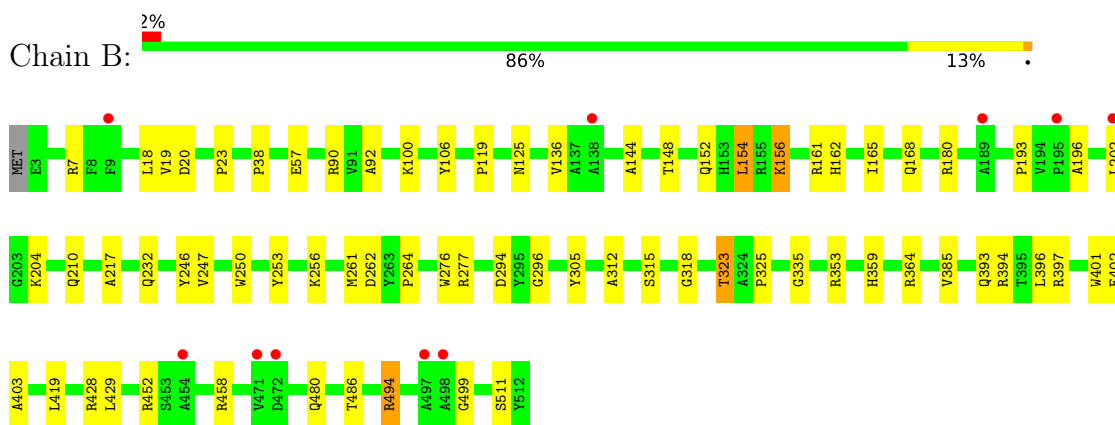
3 Residue-property plots [i](#)

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.

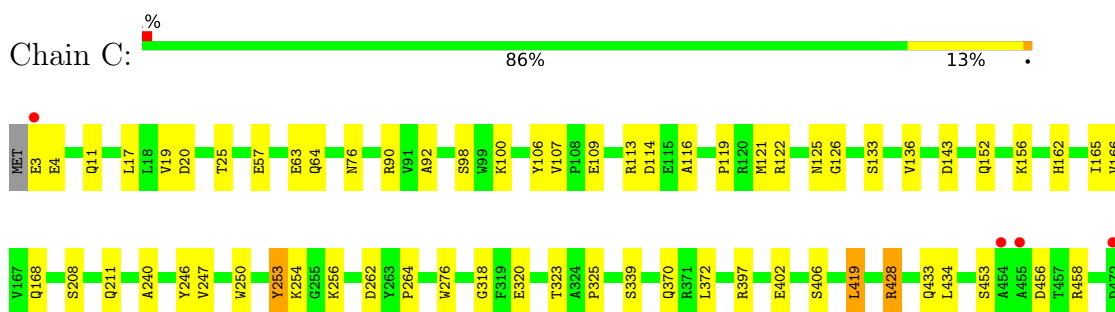
- Molecule 1: Beta-galactosidase



- Molecule 1: Beta-galactosidase

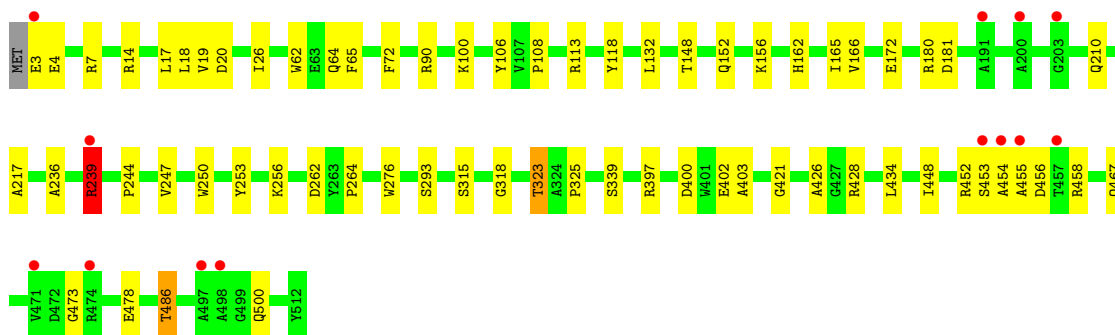
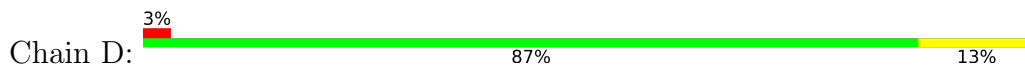


- Molecule 1: Beta-galactosidase

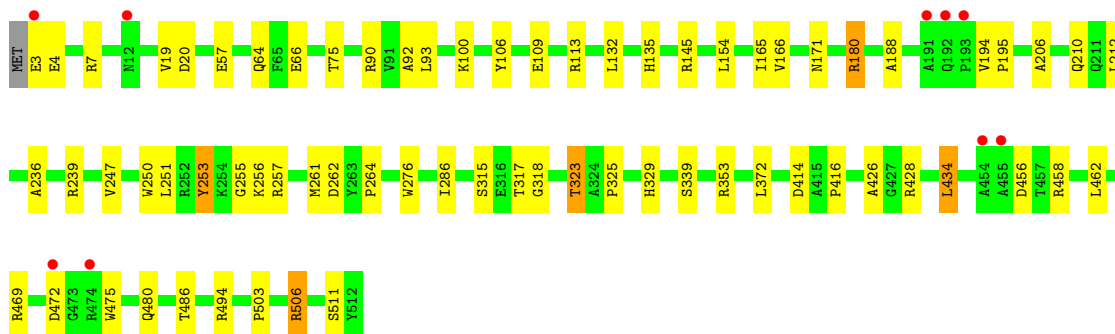
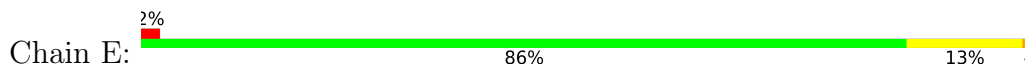




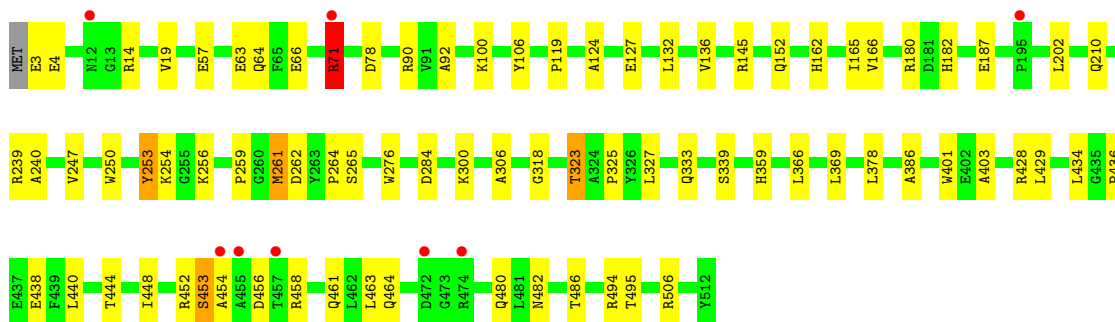
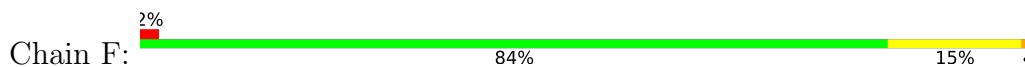
• Molecule 1: Beta-galactosidase



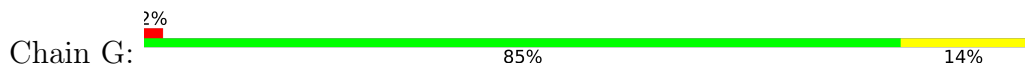
• Molecule 1: Beta-galactosidase

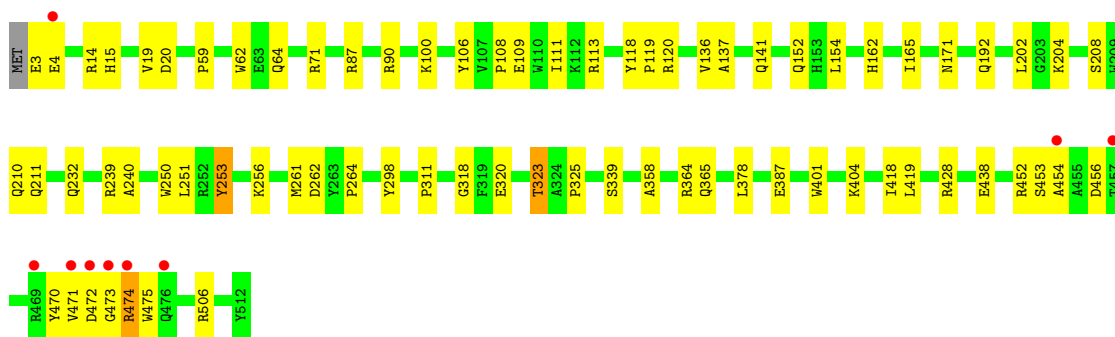


• Molecule 1: Beta-galactosidase

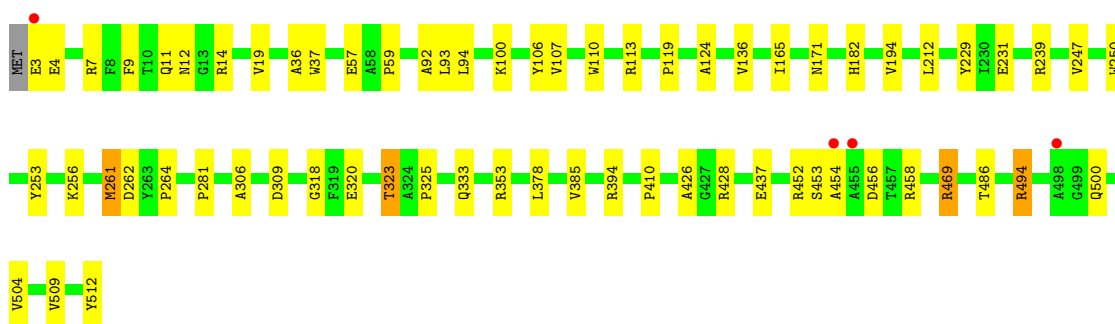
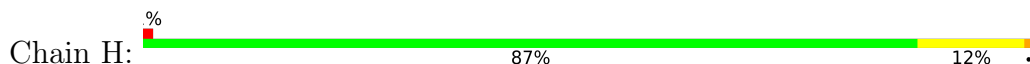


• Molecule 1: Beta-galactosidase

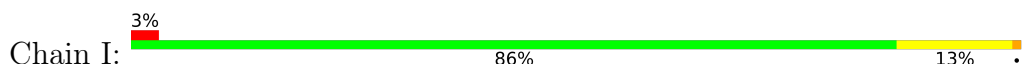




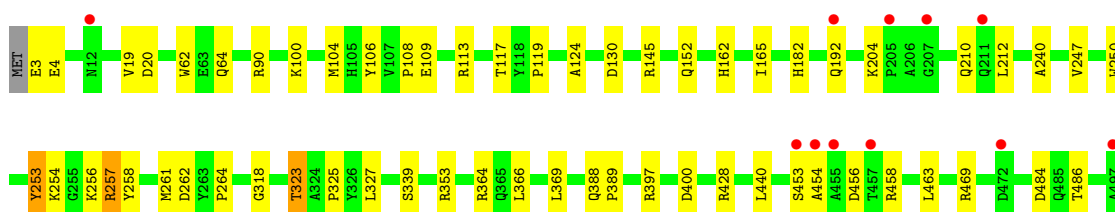
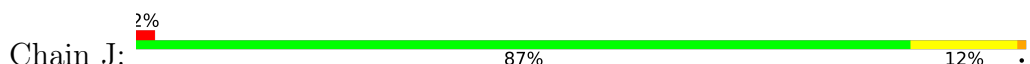
• Molecule 1: Beta-galactosidase

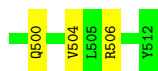


• Molecule 1: Beta-galactosidase

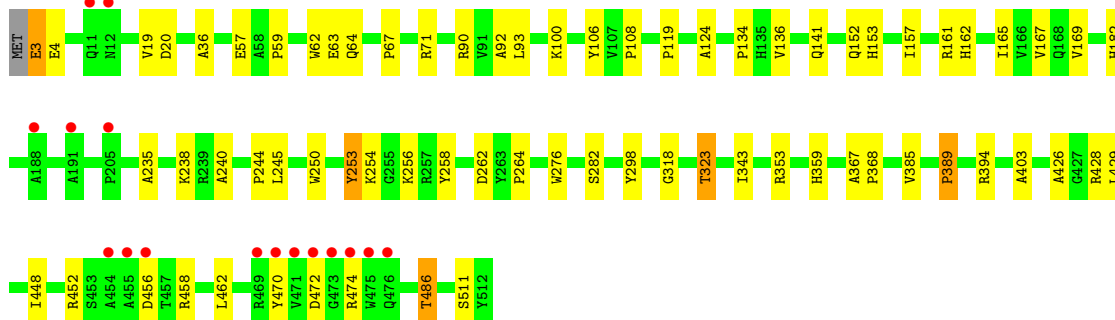
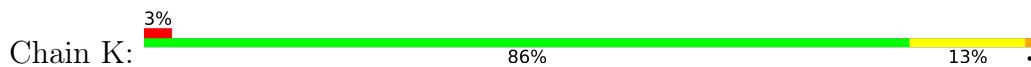


• Molecule 1: Beta-galactosidase

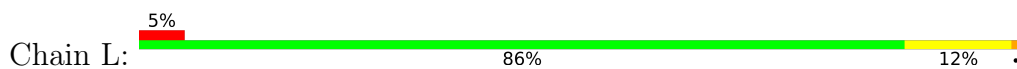




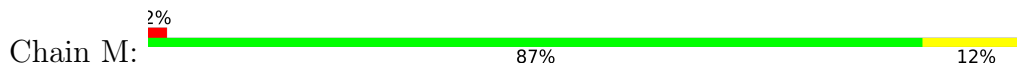
- Molecule 1: Beta-galactosidase



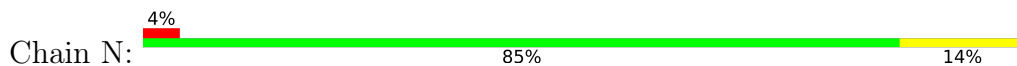
- Molecule 1: Beta-galactosidase

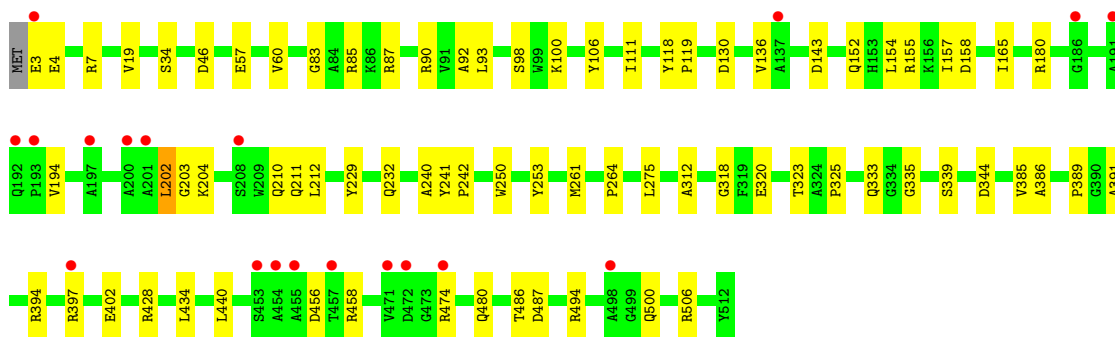


- Molecule 1: Beta-galactosidase

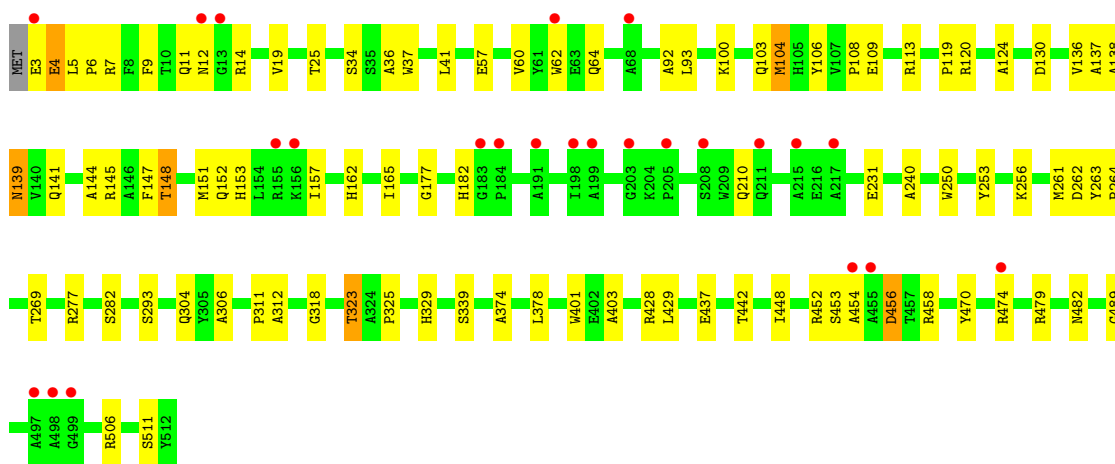
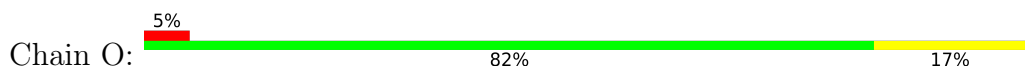


- Molecule 1: Beta-galactosidase

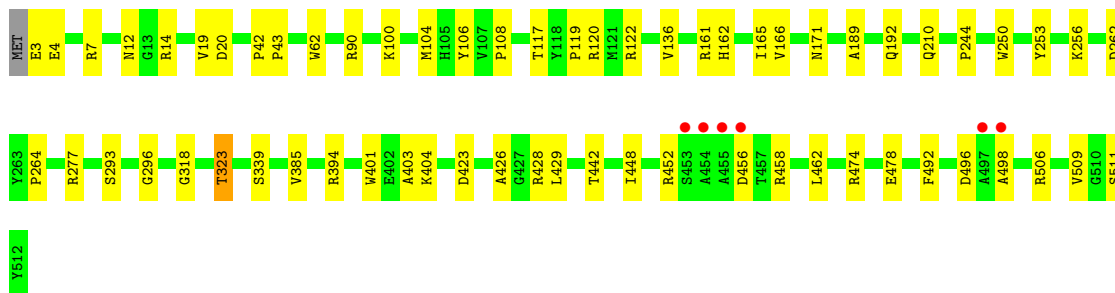
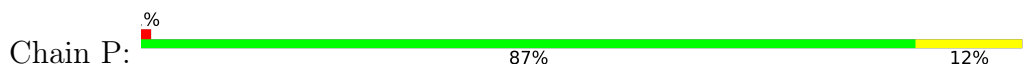




• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.27Å 162.99Å 235.48Å 90.00° 92.83° 90.00°	Depositor
Resolution (Å)	49.10 – 2.50 49.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.10-2.50) 99.1 (49.12-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.48Å)	Xtrriage
Refinement program	PHENIX v1	Depositor
R, R_{free}	0.211 , 0.251 0.211 , 0.250	Depositor DCC
R_{free} test set	16767 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	65632	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5908e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/4033	0.61	0/5508
1	B	0.34	0/4033	0.59	0/5508
1	C	0.34	0/4033	0.60	0/5508
1	D	0.37	1/4033 (0.0%)	0.63	2/5508 (0.0%)
1	E	0.36	0/4033	0.61	0/5508
1	F	0.37	0/4033	0.61	1/5508 (0.0%)
1	G	0.36	0/4033	0.62	1/5508 (0.0%)
1	H	0.35	0/4033	0.60	0/5508
1	I	0.39	0/4033	0.64	1/5508 (0.0%)
1	J	0.35	0/4033	0.59	0/5508
1	K	0.39	0/4033	0.61	1/5508 (0.0%)
1	L	0.42	4/4033 (0.1%)	0.69	7/5508 (0.1%)
1	M	0.32	0/4033	0.57	0/5508
1	N	0.33	0/4033	0.58	1/5508 (0.0%)
1	O	0.39	2/4033 (0.0%)	0.60	1/5508 (0.0%)
1	P	0.34	0/4033	0.59	0/5508
All	All	0.36	7/64528 (0.0%)	0.61	15/88128 (0.0%)

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	D	0	1
1	F	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	4	GLU	CB-CG	-9.03	1.34	1.52
1	L	456	ASP	CB-CG	6.26	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	458	ARG	CB-CG	5.91	1.68	1.52
1	L	458	ARG	CA-CB	5.80	1.66	1.53
1	D	239	ARG	CG-CD	-5.58	1.38	1.51
1	O	139	ASN	CB-CG	-5.42	1.38	1.51
1	L	472	ASP	CB-CG	5.11	1.62	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	458	ARG	CD-NE-CZ	9.30	136.62	123.60
1	L	458	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	D	239	ARG	CB-CG-CD	-8.85	88.58	111.60
1	L	472	ASP	CB-CG-OD2	8.73	126.15	118.30
1	L	472	ASP	CB-CG-OD1	-8.48	110.66	118.30
1	L	458	ARG	CA-CB-CG	7.83	130.62	113.40
1	D	239	ARG	CD-NE-CZ	-7.35	113.31	123.60
1	N	202	LEU	CA-CB-CG	6.73	130.78	115.30
1	F	71	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	L	456	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	K	389	PRO	C-N-CA	-5.52	110.72	122.30
1	O	4	GLU	OE1-CD-OE2	5.44	129.82	123.30
1	I	113	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	L	456	ASP	CB-CA-C	-5.23	99.94	110.40
1	G	474	ARG	CG-CD-NE	-5.11	101.06	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	239	ARG	Sidechain
1	F	71	ARG	Sidechain,Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3921	0	3780	55	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3921	0	3780	52	0
1	C	3921	0	3780	42	0
1	D	3921	0	3780	41	1
1	E	3921	0	3780	47	0
1	F	3921	0	3780	56	0
1	G	3921	0	3780	56	0
1	H	3921	0	3780	44	0
1	I	3921	0	3780	71	0
1	J	3921	0	3780	47	0
1	K	3921	0	3780	52	0
1	L	3921	0	3780	74	0
1	M	3921	0	3780	41	0
1	N	3921	0	3780	55	0
1	O	3921	0	3780	67	0
1	P	3921	0	3780	46	0
2	A	242	0	0	16	4
2	B	157	0	0	17	0
2	C	186	0	0	12	1
2	D	186	0	0	8	1
2	E	200	0	0	20	1
2	F	203	0	0	20	1
2	G	196	0	0	16	1
2	H	188	0	0	12	1
2	I	215	0	0	26	2
2	J	198	0	0	12	0
2	K	185	0	0	15	1
2	L	209	0	0	20	2
2	M	129	0	0	12	0
2	N	113	0	0	23	0
2	O	94	0	0	22	0
2	P	195	0	0	10	1
All	All	65632	0	60480	816	9

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 7.

All (816) 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:239:ARG:HD2	1:L:458:ARG:HB3	1.27	1.13
1:G:364:ARG:NH2	2:G:1301:HOH:O	1.81	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:GLN:NE2	2:I:603:HOH:O	1.89	1.02
1:P:428:ARG:NH2	2:P:602:HOH:O	1.93	1.01
1:B:428:ARG:NH2	2:B:601:HOH:O	1.95	0.98
1:G:387:GLU:O	2:G:1302:HOH:O	1.82	0.97
1:O:306:ALA:O	2:O:601:HOH:O	1.83	0.97
1:M:238:LYS:NZ	2:M:603:HOH:O	1.96	0.96
1:M:428:ARG:NH2	2:M:606:HOH:O	2.00	0.95
1:N:391:ALA:O	2:N:601:HOH:O	1.83	0.95
1:N:232:GLN:OE1	2:N:602:HOH:O	1.84	0.93
1:A:11:GLN:NE2	2:A:605:HOH:O	2.00	0.93
1:J:389:PRO:O	2:J:601:HOH:O	1.87	0.93
1:G:120:ARG:O	2:G:1303:HOH:O	1.87	0.92
1:I:69:PRO:O	2:I:601:HOH:O	1.85	0.92
1:N:500:GLN:OE1	2:N:603:HOH:O	1.85	0.92
1:C:428:ARG:NH2	2:C:605:HOH:O	2.03	0.91
1:E:353:ARG:NH2	2:E:604:HOH:O	2.00	0.91
1:L:130:ASP:OD1	2:L:601:HOH:O	1.86	0.91
1:K:428:ARG:NH2	2:K:603:HOH:O	2.04	0.91
1:I:200:ALA:O	1:I:202:LEU:N	2.04	0.90
1:C:98:SER:O	2:C:601:HOH:O	1.90	0.90
1:N:87:ARG:NH2	2:N:610:HOH:O	2.01	0.90
1:B:397:ARG:NH1	1:B:402:GLU:OE2	2.05	0.90
1:L:14:ARG:NH1	2:L:602:HOH:O	2.02	0.90
1:I:377:ASN:O	2:I:602:HOH:O	1.88	0.89
1:L:452:ARG:NH1	1:L:456:ASP:OD2	2.05	0.89
1:O:428:ARG:NH2	2:O:606:HOH:O	2.05	0.89
1:O:137:ALA:O	2:O:602:HOH:O	1.90	0.88
1:J:353:ARG:NH1	2:J:603:HOH:O	2.04	0.88
1:N:242:PRO:O	2:N:605:HOH:O	1.89	0.88
1:M:423:ASP:O	2:M:601:HOH:O	1.91	0.87
1:I:119:PRO:HD2	1:I:136:VAL:HG21	1.56	0.87
1:O:210:GLN:OE1	2:O:603:HOH:O	1.93	0.86
1:E:180:ARG:NH1	2:E:601:HOH:O	1.94	0.86
1:G:119:PRO:HD2	1:G:136:VAL:HG21	1.57	0.86
1:O:103:GLN:OE1	2:O:604:HOH:O	1.93	0.86
1:I:236:ALA:HA	1:L:458:ARG:HD3	1.57	0.85
1:K:119:PRO:HD2	1:K:136:VAL:HG21	1.59	0.85
1:A:185:ALA:O	2:A:601:HOH:O	1.94	0.85
1:C:90:ARG:NH1	1:C:162:HIS:O	2.09	0.85
1:J:428:ARG:NH2	2:J:604:HOH:O	2.09	0.84
1:N:344:ASP:OD2	2:N:606:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:OE1	2:A:604:HOH:O	1.95	0.84
1:K:235:ALA:O	2:K:601:HOH:O	1.94	0.84
1:N:333:GLN:O	2:N:607:HOH:O	1.96	0.84
1:F:66:GLU:OE2	2:F:602:HOH:O	1.96	0.84
1:C:433:GLN:OE1	2:C:602:HOH:O	1.94	0.84
1:M:354:ALA:O	2:M:602:HOH:O	1.95	0.84
1:E:428:ARG:NH2	2:E:611:HOH:O	2.11	0.83
1:D:236:ALA:O	1:D:239:ARG:HB2	1.77	0.83
1:A:387:GLU:O	2:A:603:HOH:O	1.95	0.83
1:A:468:GLY:O	2:A:602:HOH:O	1.95	0.83
1:A:180:ARG:NH1	2:A:606:HOH:O	2.10	0.83
1:B:296:GLY:O	2:B:602:HOH:O	1.96	0.83
1:G:473:GLY:N	2:G:1307:HOH:O	2.10	0.83
1:B:90:ARG:NH1	1:B:162:HIS:O	2.11	0.82
1:C:119:PRO:HD2	1:C:136:VAL:HG21	1.62	0.82
1:F:202:LEU:O	2:F:604:HOH:O	1.98	0.82
1:J:90:ARG:NH1	1:J:162:HIS:O	2.13	0.81
1:M:382:LEU:O	2:M:604:HOH:O	1.98	0.81
1:B:23:PRO:O	2:B:603:HOH:O	1.98	0.81
1:H:500:GLN:OE1	2:H:601:HOH:O	1.98	0.81
1:N:180:ARG:NH1	2:N:615:HOH:O	2.13	0.81
1:M:437:GLU:OE2	2:M:605:HOH:O	1.99	0.80
1:A:90:ARG:NH1	1:A:162:HIS:O	2.14	0.80
1:E:480:GLN:O	2:E:603:HOH:O	2.00	0.80
1:N:487:ASP:OD2	2:N:608:HOH:O	2.00	0.80
1:I:239:ARG:NH1	1:L:458:ARG:HD2	1.96	0.79
1:E:469:ARG:NH1	2:E:602:HOH:O	1.96	0.79
1:I:236:ALA:HA	1:L:458:ARG:CD	2.12	0.79
1:E:188:ALA:O	2:E:605:HOH:O	2.01	0.79
1:C:63:GLU:OE1	2:C:604:HOH:O	1.99	0.79
1:B:38:PRO:O	2:B:604:HOH:O	2.01	0.79
1:N:480:GLN:OE1	2:N:609:HOH:O	2.00	0.78
1:F:78:ASP:OD2	2:F:605:HOH:O	2.01	0.78
1:J:64:GLN:NE2	2:J:606:HOH:O	2.11	0.78
1:I:90:ARG:NH1	1:I:162:HIS:O	2.17	0.78
1:C:64:GLN:NE2	2:C:603:HOH:O	1.98	0.77
1:B:125:ASN:O	2:B:605:HOH:O	2.02	0.77
1:M:484:ASP:O	2:M:607:HOH:O	2.01	0.77
1:J:145:ARG:NH2	2:J:602:HOH:O	1.93	0.77
1:O:64:GLN:NE2	2:O:610:HOH:O	2.17	0.77
1:G:452:ARG:HH22	1:G:456:ASP:HB2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLN:NE2	2:D:604:HOH:O	2.09	0.76
1:C:114:ASP:OD2	2:C:606:HOH:O	2.03	0.76
1:F:428:ARG:NH2	2:F:614:HOH:O	2.15	0.76
1:E:64:GLN:NE2	2:E:607:HOH:O	2.03	0.76
1:C:11:GLN:NE2	2:C:609:HOH:O	2.10	0.76
1:E:416:PRO:O	2:E:606:HOH:O	2.02	0.76
1:L:232:GLN:OE1	2:L:604:HOH:O	2.03	0.76
1:O:6:PRO:O	2:O:605:HOH:O	2.03	0.76
1:B:196:ALA:HB1	1:L:471:VAL:HG12	1.66	0.76
1:G:404:LYS:NZ	2:G:1312:HOH:O	2.18	0.75
1:K:90:ARG:NH1	1:K:162:HIS:O	2.20	0.75
1:I:187:GLU:O	2:I:606:HOH:O	2.03	0.75
1:K:64:GLN:NE2	2:K:607:HOH:O	2.19	0.75
1:L:453:SER:OG	2:L:603:HOH:O	2.03	0.75
1:N:386:ALA:O	2:N:611:HOH:O	2.04	0.75
1:G:59:PRO:O	2:G:1304:HOH:O	2.05	0.75
1:A:458:ARG:NH1	1:A:511:SER:OG	2.20	0.74
1:F:187:GLU:O	2:F:606:HOH:O	2.05	0.74
1:N:203:GLY:O	2:N:612:HOH:O	2.05	0.74
1:K:3:GLU:N	2:K:609:HOH:O	2.21	0.74
1:L:452:ARG:NH1	2:L:606:HOH:O	2.08	0.74
1:N:60:VAL:HG23	1:N:93:LEU:HD11	1.68	0.74
1:K:3:GLU:HG3	1:K:4:GLU:H	1.52	0.74
1:F:63:GLU:OE2	2:F:608:HOH:O	2.07	0.73
1:L:90:ARG:NH1	1:L:162:HIS:O	2.22	0.73
1:H:119:PRO:HD2	1:H:136:VAL:HG21	1.69	0.73
1:O:12:ASN:N	2:O:612:HOH:O	2.20	0.73
1:G:473:GLY:O	2:G:1305:HOH:O	2.06	0.73
1:B:480:GLN:O	2:B:607:HOH:O	2.06	0.73
1:P:496:ASP:OD2	2:P:603:HOH:O	2.08	0.72
1:B:232:GLN:NE2	2:B:613:HOH:O	2.23	0.72
1:I:191:ALA:O	2:I:609:HOH:O	2.08	0.72
1:J:3:GLU:HG3	1:J:4:GLU:H	1.53	0.72
1:L:322:ALA:O	2:L:605:HOH:O	2.06	0.72
1:E:472:ASP:OD2	2:E:608:HOH:O	2.06	0.72
1:A:428:ARG:NH2	2:A:607:HOH:O	2.13	0.72
1:D:473:GLY:O	2:D:602:HOH:O	2.08	0.71
1:K:472:ASP:HB2	2:K:623:HOH:O	1.88	0.71
1:J:353:ARG:NH2	2:J:615:HOH:O	2.24	0.71
1:L:454:ALA:HB3	1:L:456:ASP:OD2	1.90	0.71
1:I:388:GLN:OE1	2:I:610:HOH:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:456:ASP:HB3	1:J:458:ARG:H	1.54	0.71
1:C:116:ALA:HB3	1:P:12:ASN:HD21	1.55	0.71
1:I:494:ARG:O	2:I:608:HOH:O	2.07	0.71
1:N:428:ARG:NH2	2:N:620:HOH:O	2.23	0.71
1:C:125:ASN:O	2:C:608:HOH:O	2.09	0.70
1:D:181:ASP:O	2:D:603:HOH:O	2.08	0.70
1:E:286:ILE:O	2:E:609:HOH:O	2.08	0.70
1:F:386:ALA:O	2:F:609:HOH:O	2.09	0.70
1:I:428:ARG:NH2	2:I:620:HOH:O	2.23	0.70
1:K:343:ILE:O	2:K:604:HOH:O	2.08	0.70
1:G:358:ALA:O	2:G:1306:HOH:O	2.09	0.70
1:I:239:ARG:CZ	1:L:458:ARG:HD2	2.21	0.70
1:L:498:ALA:O	2:L:608:HOH:O	2.10	0.70
1:E:469:ARG:HH12	1:E:503:PRO:HA	1.57	0.70
1:I:239:ARG:HH11	1:L:458:ARG:HB3	1.55	0.70
1:I:194:VAL:HB	1:I:199:ALA:HB2	1.74	0.70
1:L:454:ALA:CB	1:L:456:ASP:OD2	2.40	0.70
1:P:296:GLY:O	2:P:604:HOH:O	2.10	0.69
1:N:157:ILE:N	2:N:619:HOH:O	2.23	0.69
1:E:206:ALA:O	2:E:610:HOH:O	2.11	0.69
1:K:169:VAL:CG2	1:K:245:LEU:HD13	2.23	0.69
1:N:474:ARG:NH1	2:N:604:HOH:O	1.87	0.68
1:B:364:ARG:O	2:B:608:HOH:O	2.11	0.68
1:P:498:ALA:O	2:P:605:HOH:O	2.11	0.68
1:B:119:PRO:HD2	1:B:136:VAL:HG21	1.75	0.68
1:L:107:VAL:O	2:L:607:HOH:O	2.10	0.68
1:F:306:ALA:O	2:F:610:HOH:O	2.10	0.68
1:F:506:ARG:NH2	2:F:615:HOH:O	2.19	0.68
1:P:511:SER:OG	2:P:601:HOH:O	1.89	0.68
1:G:232:GLN:NE2	2:G:1315:HOH:O	2.25	0.68
1:I:458:ARG:O	2:I:612:HOH:O	2.12	0.67
1:J:484:ASP:OD1	2:J:605:HOH:O	2.11	0.67
1:D:90:ARG:NH1	1:D:162:HIS:O	2.27	0.67
1:I:437:GLU:OE2	2:I:613:HOH:O	2.12	0.67
1:L:108:PRO:HD2	1:L:111:ILE:HD12	1.75	0.67
1:A:456:ASP:HB3	1:A:458:ARG:H	1.60	0.67
1:H:494:ARG:NH1	2:H:607:HOH:O	2.24	0.67
1:B:458:ARG:NH1	1:B:511:SER:OG	2.27	0.67
1:K:169:VAL:HG21	1:K:245:LEU:HD13	1.77	0.66
1:N:4:GLU:OE1	1:N:7:ARG:NH1	2.29	0.66
1:K:141:GLN:NE2	2:K:615:HOH:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:GLY:O	2:O:607:HOH:O	2.14	0.66
1:D:456:ASP:HB3	1:D:458:ARG:H	1.61	0.66
1:F:90:ARG:NH1	1:F:162:HIS:O	2.29	0.66
1:G:418:ILE:O	2:G:1308:HOH:O	2.13	0.66
1:N:389:PRO:O	2:N:616:HOH:O	2.14	0.66
1:P:90:ARG:NH1	1:P:162:HIS:O	2.29	0.66
1:O:437:GLU:N	2:O:613:HOH:O	2.21	0.66
1:F:127:GLU:OE2	2:F:613:HOH:O	2.14	0.65
1:F:284:ASP:OD1	2:F:611:HOH:O	2.14	0.65
1:G:365:GLN:O	2:G:1309:HOH:O	2.13	0.65
1:F:333:GLN:O	2:F:612:HOH:O	2.14	0.65
1:K:63:GLU:OE2	2:K:605:HOH:O	2.15	0.65
1:A:494:ARG:NH1	2:A:610:HOH:O	2.24	0.65
1:I:239:ARG:HG2	1:L:512:TYR:C	2.17	0.65
1:O:489:GLY:O	2:O:608:HOH:O	2.15	0.64
1:J:262:ASP:OD1	2:J:608:HOH:O	2.15	0.64
1:K:167:VAL:HB	1:K:245:LEU:HD22	1.80	0.64
1:K:124:ALA:HA	1:K:182:HIS:ND1	2.12	0.64
1:B:294:ASP:OD1	2:B:609:HOH:O	2.15	0.64
1:E:132:LEU:N	2:E:613:HOH:O	2.18	0.64
1:G:87:ARG:NH2	2:G:1320:HOH:O	2.29	0.64
1:G:208:SER:H	1:G:211:GLN:NE2	1.95	0.64
1:M:180:ARG:NH2	1:M:187:GLU:OE2	2.29	0.64
1:O:458:ARG:NH1	1:O:511:SER:OG	2.30	0.63
1:C:402:GLU:OE2	2:C:610:HOH:O	2.14	0.63
1:G:90:ARG:NH1	1:G:162:HIS:O	2.31	0.63
1:H:309:ASP:OD2	2:H:602:HOH:O	2.16	0.63
1:F:3:GLU:HG2	1:F:4:GLU:H	1.63	0.63
1:O:162:HIS:ND1	2:O:623:HOH:O	2.30	0.63
1:B:256:LYS:HB3	1:B:262:ASP:HB3	1.80	0.63
1:A:124:ALA:HA	1:A:182:HIS:ND1	2.14	0.63
1:F:124:ALA:HA	1:F:182:HIS:ND1	2.14	0.63
1:N:98:SER:OG	1:N:143:ASP:OD2	2.14	0.63
1:G:19:VAL:HG13	1:G:165:ILE:HD11	1.80	0.62
1:I:109:GLU:O	1:I:113:ARG:HG2	1.99	0.62
1:C:325:PRO:HA	1:C:428:ARG:HD2	1.81	0.62
1:H:19:VAL:HG13	1:H:165:ILE:HD11	1.81	0.62
1:M:256:LYS:HB3	1:M:262:ASP:HB3	1.80	0.62
1:N:456:ASP:HB3	1:N:458:ARG:H	1.64	0.62
1:L:119:PRO:HD2	1:L:136:VAL:HG21	1.80	0.62
1:A:87:ARG:NH2	2:A:616:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:480:GLN:NE2	2:M:618:HOH:O	2.32	0.62
1:L:187:GLU:OE1	2:L:610:HOH:O	2.16	0.62
1:E:458:ARG:NH1	1:E:511:SER:OG	2.33	0.62
1:K:474:ARG:HB2	2:K:623:HOH:O	1.99	0.61
1:M:256:LYS:NZ	2:M:620:HOH:O	2.33	0.61
1:K:452:ARG:HH12	1:K:456:ASP:HB2	1.63	0.61
1:L:30:GLN:NE2	2:L:615:HOH:O	2.25	0.61
1:L:456:ASP:HB3	1:L:458:ARG:HG3	1.81	0.61
1:O:374:ALA:O	2:O:609:HOH:O	2.16	0.61
1:I:124:ALA:HA	1:I:182:HIS:ND1	2.15	0.61
1:O:456:ASP:HB3	1:O:458:ARG:H	1.65	0.61
1:C:318:GLY:O	1:C:323:THR:HG21	2.00	0.61
1:F:325:PRO:HA	1:F:428:ARG:HD2	1.83	0.61
1:E:135:HIS:HE1	2:E:645:HOH:O	1.84	0.61
1:M:119:PRO:HD2	1:M:136:VAL:HG11	1.81	0.61
1:P:4:GLU:HB2	2:P:720:HOH:O	2.00	0.61
1:F:100:LYS:HG2	1:F:106:TYR:CE2	2.36	0.61
1:M:20:ASP:OD2	1:M:90:ARG:NH2	2.33	0.60
1:B:499:GLY:O	2:B:610:HOH:O	2.16	0.60
1:I:247:VAL:HB	2:I:676:HOH:O	2.00	0.60
1:L:486:THR:HG22	2:L:632:HOH:O	2.00	0.60
1:L:124:ALA:HA	1:L:182:HIS:ND1	2.17	0.60
1:K:256:LYS:HB3	1:K:262:ASP:HB3	1.84	0.60
1:L:19:VAL:HG13	1:L:165:ILE:HD11	1.83	0.60
1:P:19:VAL:HG13	1:P:165:ILE:HD11	1.83	0.60
1:C:456:ASP:HB3	1:C:458:ARG:H	1.66	0.60
1:D:421:GLY:O	2:D:605:HOH:O	2.16	0.60
1:L:3:GLU:HG2	1:L:4:GLU:H	1.66	0.60
1:M:458:ARG:NH1	1:M:511:SER:OG	2.34	0.60
1:P:458:ARG:HG2	1:P:458:ARG:HH11	1.66	0.60
1:G:470:TYR:HA	1:G:474:ARG:O	2.02	0.60
1:P:20:ASP:OD2	1:P:90:ARG:NH2	2.35	0.60
1:P:119:PRO:HD2	1:P:136:VAL:HG21	1.84	0.60
1:E:20:ASP:OD1	2:E:612:HOH:O	2.16	0.60
1:N:19:VAL:HG13	1:N:165:ILE:HD11	1.84	0.60
1:I:239:ARG:HH11	1:L:458:ARG:CB	2.15	0.59
1:I:240:ALA:HA	1:L:457:THR:OG1	2.02	0.59
1:O:141:GLN:N	2:O:602:HOH:O	2.20	0.59
1:L:256:LYS:HB3	1:L:262:ASP:HB3	1.84	0.59
1:A:371:ARG:O	2:A:608:HOH:O	2.17	0.59
1:P:189:ALA:HA	1:P:192:GLN:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:ARG:NE	2:K:621:HOH:O	2.35	0.59
1:K:385:VAL:HG11	1:K:394:ARG:HG3	1.84	0.59
1:A:119:PRO:HG2	1:A:136:VAL:HG21	1.84	0.59
1:N:3:GLU:HG2	1:N:4:GLU:H	1.68	0.59
1:P:401:TRP:CZ2	1:P:452:ARG:HD2	2.37	0.59
1:D:256:LYS:HB3	1:D:262:ASP:HB3	1.85	0.58
1:E:469:ARG:NH1	1:E:503:PRO:HA	2.18	0.58
1:H:333:GLN:O	2:H:603:HOH:O	2.17	0.58
1:D:397:ARG:HG2	1:D:402:GLU:HG2	1.86	0.58
1:G:401:TRP:CE2	1:G:452:ARG:HG3	2.38	0.58
1:J:19:VAL:HG13	1:J:165:ILE:HD11	1.85	0.58
1:C:116:ALA:CB	1:P:12:ASN:HD21	2.16	0.58
1:E:325:PRO:HA	1:E:428:ARG:HD2	1.85	0.58
1:F:261:MET:HG3	1:F:262:ASP:N	2.17	0.58
1:J:250:TRP:HE1	1:J:256:LYS:HE2	1.68	0.58
1:H:353:ARG:NH2	2:H:616:HOH:O	2.36	0.58
1:J:100:LYS:HG2	1:J:106:TYR:CE2	2.39	0.58
1:N:119:PRO:HD2	1:N:136:VAL:HG21	1.85	0.58
1:N:194:VAL:HG21	1:N:212:LEU:HD12	1.86	0.58
1:D:100:LYS:HG2	1:D:106:TYR:CE2	2.39	0.58
1:M:113:ARG:HD2	1:M:114:ASP:HB2	1.86	0.57
1:N:152:GLN:HG3	1:N:240:ALA:HB1	1.85	0.57
1:P:14:ARG:HD2	2:P:713:HOH:O	2.03	0.57
1:K:20:ASP:OD2	1:K:90:ARG:NH2	2.37	0.57
1:I:4:GLU:OE1	1:I:7:ARG:NH2	2.37	0.57
1:E:329:HIS:HD2	2:E:689:HOH:O	1.86	0.57
1:I:100:LYS:HG2	1:I:106:TYR:CE2	2.39	0.57
1:J:400:ASP:OD1	2:J:610:HOH:O	2.17	0.57
1:B:152:GLN:O	1:B:156:LYS:HG2	2.05	0.57
1:L:418:ILE:O	2:L:611:HOH:O	2.17	0.57
1:L:428:ARG:NH2	2:L:618:HOH:O	2.30	0.57
1:C:76:ASN:OD1	2:C:611:HOH:O	2.17	0.57
1:E:3:GLU:HG2	1:E:4:GLU:H	1.68	0.57
1:J:388:GLN:OE1	2:J:611:HOH:O	2.18	0.57
1:E:250:TRP:CD2	1:E:264:PRO:HD3	2.39	0.56
1:E:261:MET:HG3	1:E:262:ASP:N	2.19	0.56
1:P:100:LYS:HG2	1:P:106:TYR:CE2	2.39	0.56
1:H:456:ASP:HB3	1:H:458:ARG:H	1.71	0.56
1:B:210:GLN:OE1	1:B:210:GLN:N	2.35	0.56
1:H:14:ARG:HD3	1:H:378:LEU:O	2.05	0.56
1:J:124:ALA:HA	1:J:182:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:256:LYS:HB3	1:J:262:ASP:HB3	1.85	0.56
1:O:124:ALA:HA	1:O:182:HIS:ND1	2.20	0.56
1:D:3:GLU:HG2	1:D:4:GLU:H	1.70	0.56
1:D:20:ASP:OD2	1:D:90:ARG:NH2	2.38	0.56
1:F:165:ILE:HG23	1:F:166:VAL:HG13	1.87	0.56
1:I:239:ARG:HB2	1:L:458:ARG:CB	2.35	0.56
1:G:452:ARG:NH2	1:G:456:ASP:HB2	2.19	0.56
1:I:20:ASP:OD2	1:I:90:ARG:NH2	2.39	0.56
1:J:20:ASP:OD2	1:J:90:ARG:NH2	2.39	0.56
1:M:90:ARG:NH1	1:M:162:HIS:O	2.39	0.56
1:I:19:VAL:HG13	1:I:165:ILE:HD11	1.88	0.56
1:G:210:GLN:CD	1:G:210:GLN:H	2.09	0.55
1:H:458:ARG:HH11	1:H:458:ARG:HG2	1.71	0.55
1:I:64:GLN:NE2	2:I:623:HOH:O	2.28	0.55
1:M:318:GLY:O	1:M:323:THR:HG21	2.06	0.55
1:O:311:PRO:HA	2:O:618:HOH:O	2.05	0.55
1:K:253:TYR:CD1	1:K:254:LYS:HG3	2.42	0.55
1:N:85:ARG:NH1	2:N:625:HOH:O	2.30	0.55
1:G:137:ALA:HB1	1:G:141:GLN:NE2	2.22	0.55
1:I:239:ARG:CB	1:L:458:ARG:HA	2.37	0.55
1:B:20:ASP:OD2	1:B:90:ARG:NH2	2.39	0.55
1:C:250:TRP:CD2	1:C:264:PRO:HD3	2.42	0.55
1:H:124:ALA:HA	1:H:182:HIS:ND1	2.22	0.55
1:P:456:ASP:HB3	1:P:458:ARG:H	1.72	0.55
1:F:480:GLN:HB2	1:O:37:TRP:CZ2	2.42	0.55
1:J:257:ARG:HG3	1:J:258:TYR:CE2	2.41	0.55
1:A:325:PRO:HA	1:A:428:ARG:HD2	1.88	0.55
1:C:3:GLU:HG2	1:C:4:GLU:H	1.71	0.55
1:M:204:LYS:NZ	1:M:212:LEU:O	2.38	0.55
1:N:202:LEU:HD11	1:N:275:LEU:HD23	1.89	0.55
1:O:263:TYR:CE2	1:O:269:THR:HG21	2.42	0.55
1:B:57:GLU:HG2	1:B:92:ALA:HB3	1.89	0.54
1:D:325:PRO:HA	1:D:428:ARG:HD2	1.88	0.54
1:E:456:ASP:HB3	1:E:458:ARG:H	1.72	0.54
1:F:401:TRP:CZ2	1:F:452:ARG:HD2	2.42	0.54
1:I:486:THR:HG22	2:I:643:HOH:O	2.07	0.54
1:A:318:GLY:O	1:A:323:THR:HG21	2.07	0.54
1:I:158:ASP:OD2	2:I:614:HOH:O	2.18	0.54
1:D:318:GLY:O	1:D:323:THR:HG21	2.08	0.54
1:E:165:ILE:HG23	1:E:166:VAL:HG13	1.89	0.54
1:B:19:VAL:HG13	1:B:165:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:487:ASP:OD2	2:M:608:HOH:O	2.18	0.54
1:H:110:TRP:HA	1:H:113:ARG:HG2	1.88	0.54
1:H:452:ARG:HH12	1:H:456:ASP:HB2	1.72	0.54
1:I:311:PRO:O	2:I:615:HOH:O	2.19	0.54
1:A:250:TRP:CD2	1:A:264:PRO:HD3	2.43	0.54
1:D:148:THR:O	1:D:152:GLN:HG3	2.08	0.54
1:D:250:TRP:CD2	1:D:264:PRO:HD3	2.43	0.54
1:I:200:ALA:O	2:I:604:HOH:O	2.18	0.54
1:G:474:ARG:HG3	1:G:475:TRP:N	2.23	0.53
1:H:318:GLY:O	1:H:323:THR:HG21	2.07	0.53
1:O:104:MET:HE1	1:O:120:ARG:HG2	1.91	0.53
1:A:323:THR:HG22	1:A:359:HIS:HE2	1.73	0.53
1:C:165:ILE:HG23	1:C:166:VAL:HG13	1.90	0.53
1:D:19:VAL:HG13	1:D:165:ILE:HD11	1.89	0.53
1:I:33:ASN:ND2	2:I:622:HOH:O	2.26	0.53
1:A:486:THR:HG21	2:A:743:HOH:O	2.08	0.53
1:G:239:ARG:NH1	2:G:1332:HOH:O	2.41	0.53
1:N:34:SER:O	1:O:479:ARG:HD3	2.08	0.53
1:P:256:LYS:HB3	1:P:262:ASP:HB3	1.91	0.53
1:N:155:ARG:HG3	1:N:241:TYR:CD2	2.43	0.53
1:J:469:ARG:HH11	1:J:504:VAL:HG23	1.74	0.53
1:L:400:ASP:O	2:L:603:HOH:O	2.19	0.53
1:O:36:ALA:HA	1:O:41:LEU:HD21	1.91	0.53
1:K:167:VAL:HB	1:K:245:LEU:CD2	2.38	0.53
1:N:458:ARG:HG2	1:N:458:ARG:HH11	1.74	0.53
1:A:155:ARG:HB2	1:A:241:TYR:CG	2.44	0.52
1:C:256:LYS:HB3	1:C:262:ASP:HB3	1.90	0.52
1:G:3:GLU:HG2	1:G:4:GLU:H	1.73	0.52
1:G:64:GLN:NE2	2:G:1322:HOH:O	2.32	0.52
1:J:318:GLY:O	1:J:323:THR:HG21	2.09	0.52
1:K:19:VAL:HG13	1:K:165:ILE:HD11	1.91	0.52
1:N:250:TRP:CD2	1:N:264:PRO:HD3	2.44	0.52
1:J:247:VAL:HB	2:J:688:HOH:O	2.09	0.52
1:M:100:LYS:HG2	1:M:106:TYR:CE1	2.44	0.52
1:D:486:THR:HG21	2:D:662:HOH:O	2.08	0.52
1:J:469:ARG:NH1	1:J:504:VAL:HG23	2.24	0.52
1:K:36:ALA:HB2	1:K:59:PRO:HD2	1.92	0.52
1:K:389:PRO:O	2:K:606:HOH:O	2.18	0.52
1:A:154:LEU:HA	1:A:157:ILE:CG1	2.40	0.52
1:C:17:LEU:N	2:C:621:HOH:O	2.32	0.52
1:E:426:ALA:O	1:E:428:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:256:LYS:HB3	1:I:262:ASP:HB3	1.91	0.52
1:F:256:LYS:HB3	1:F:262:ASP:HB3	1.92	0.52
1:F:495:THR:OG1	2:F:603:HOH:O	1.96	0.52
1:P:478:GLU:OE1	2:P:606:HOH:O	2.18	0.52
1:C:57:GLU:HG2	1:C:92:ALA:HB3	1.92	0.52
1:H:239:ARG:NE	2:H:610:HOH:O	2.28	0.52
1:J:257:ARG:HG3	1:J:258:TYR:CD2	2.45	0.52
1:D:118:TYR:OH	2:D:606:HOH:O	2.19	0.52
1:O:144:ALA:O	1:O:148:THR:OG1	2.27	0.52
1:A:153:HIS:O	1:A:157:ILE:HG12	2.09	0.51
1:H:385:VAL:HG11	1:H:394:ARG:HG3	1.92	0.51
1:L:456:ASP:HB3	1:L:458:ARG:CB	2.39	0.51
1:B:401:TRP:CZ2	1:B:452:ARG:HD2	2.45	0.51
1:J:253:TYR:CZ	1:J:254:LYS:HD2	2.45	0.51
1:G:100:LYS:HG2	1:G:106:TYR:CE2	2.45	0.51
1:I:259:PRO:HB2	1:I:265:SER:HB2	1.93	0.51
1:I:494:ARG:HG3	2:I:753:HOH:O	2.11	0.51
1:B:217:ALA:HB3	2:B:643:HOH:O	2.09	0.51
1:B:396:LEU:HB2	1:B:403:ALA:HB3	1.91	0.51
1:E:109:GLU:O	1:E:113:ARG:HG2	2.11	0.51
1:I:165:ILE:HG23	1:I:166:VAL:HG13	1.91	0.51
1:K:403:ALA:HB1	1:K:448:ILE:HD11	1.93	0.51
1:M:456:ASP:HB3	1:M:458:ARG:H	1.76	0.51
1:I:236:ALA:CA	1:L:458:ARG:HD3	2.36	0.51
1:L:250:TRP:CD2	1:L:264:PRO:HD3	2.45	0.51
1:B:305:TYR:OH	2:B:606:HOH:O	2.03	0.51
1:E:372:LEU:HD21	1:E:434:LEU:HD11	1.93	0.51
1:O:256:LYS:HB3	1:O:262:ASP:HB3	1.93	0.51
1:J:250:TRP:CD2	1:J:264:PRO:HD3	2.46	0.51
1:A:109:GLU:O	1:A:113:ARG:HG3	2.11	0.51
1:H:458:ARG:HG2	1:H:458:ARG:NH1	2.25	0.51
1:K:4:GLU:O	2:K:608:HOH:O	2.19	0.51
1:P:3:GLU:HG2	2:P:720:HOH:O	2.11	0.51
1:G:251:LEU:HB2	1:G:253:TYR:CD2	2.46	0.50
1:O:139:ASN:N	1:O:139:ASN:ND2	2.57	0.50
1:B:250:TRP:CD2	1:B:264:PRO:HD3	2.46	0.50
1:D:152:GLN:O	1:D:156:LYS:HG2	2.11	0.50
1:D:325:PRO:HA	1:D:428:ARG:CD	2.41	0.50
1:J:204:LYS:HD2	1:J:212:LEU:HD13	1.93	0.50
1:M:3:GLU:HG2	1:M:4:GLU:H	1.76	0.50
1:O:250:TRP:CD2	1:O:264:PRO:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:TRP:CD2	1:I:264:PRO:HD3	2.47	0.50
1:D:210:GLN:H	1:D:210:GLN:CD	2.15	0.50
1:E:236:ALA:HA	1:E:239:ARG:NH1	2.27	0.50
1:P:166:VAL:HG12	1:P:244:PRO:HB2	1.94	0.50
2:E:610:HOH:O	1:P:474:ARG:NH2	2.23	0.50
1:G:109:GLU:O	1:G:113:ARG:HG2	2.11	0.50
1:F:250:TRP:CD2	1:F:264:PRO:HD3	2.46	0.50
1:F:444:THR:OG1	2:F:607:HOH:O	2.06	0.50
1:N:320:GLU:O	1:N:323:THR:HG22	2.12	0.50
1:H:325:PRO:HA	1:H:428:ARG:CD	2.41	0.50
1:L:100:LYS:HG2	1:L:106:TYR:CE2	2.46	0.50
1:O:304:GLN:OE1	2:O:611:HOH:O	2.18	0.50
1:P:104:MET:HE1	1:P:120:ARG:HG2	1.93	0.50
1:F:64:GLN:NE2	2:F:601:HOH:O	1.95	0.50
1:H:426:ALA:O	1:H:428:ARG:NH1	2.44	0.50
1:H:512:TYR:OXT	2:H:604:HOH:O	2.20	0.50
1:O:100:LYS:HG2	1:O:106:TYR:CE1	2.47	0.50
1:H:250:TRP:CD2	1:H:264:PRO:HD3	2.47	0.49
1:N:385:VAL:HG11	1:N:394:ARG:HG3	1.94	0.49
1:C:19:VAL:HG13	1:C:165:ILE:HD11	1.95	0.49
1:G:250:TRP:CD2	1:G:264:PRO:HD3	2.47	0.49
1:G:256:LYS:HB3	1:G:262:ASP:HB3	1.94	0.49
1:G:470:TYR:OH	2:G:1311:HOH:O	2.17	0.49
1:K:250:TRP:CD2	1:K:264:PRO:HD3	2.47	0.49
1:K:426:ALA:O	1:K:428:ARG:NH1	2.45	0.49
1:O:9:PHE:CZ	1:O:11:GLN:HB2	2.47	0.49
1:O:329:HIS:HD2	2:O:641:HOH:O	1.95	0.49
1:P:250:TRP:CD2	1:P:264:PRO:HD3	2.47	0.49
1:A:100:LYS:HG2	1:A:106:TYR:CE2	2.47	0.49
1:L:454:ALA:HB1	1:L:456:ASP:OD2	2.12	0.49
1:B:318:GLY:O	1:B:323:THR:HG21	2.11	0.49
1:A:64:GLN:NE2	2:A:617:HOH:O	2.33	0.49
1:E:325:PRO:HA	1:E:428:ARG:CD	2.42	0.49
1:F:453:SER:OG	1:F:454:ALA:N	2.43	0.49
1:G:318:GLY:O	1:G:323:THR:HG21	2.12	0.49
1:A:100:LYS:HD2	1:A:171:ASN:HD22	1.78	0.49
1:E:66:GLU:OE1	2:E:614:HOH:O	2.19	0.49
1:K:238:LYS:HE2	1:K:245:LEU:HG	1.94	0.49
1:B:385:VAL:HG11	1:B:394:ARG:HG3	1.93	0.49
1:O:231:GLU:OE2	1:O:282:SER:OG	2.30	0.49
1:I:239:ARG:HB3	1:L:458:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:HD12	1:A:157:ILE:HD12	1.94	0.49
1:M:108:PRO:HD2	1:M:111:ILE:HD12	1.95	0.49
1:D:17:LEU:HD22	1:D:26:ILE:HD11	1.94	0.48
1:G:152:GLN:HG3	1:G:240:ALA:HB1	1.95	0.48
1:C:152:GLN:HG3	1:C:240:ALA:HB1	1.95	0.48
1:E:251:LEU:HB2	1:E:253:TYR:CD2	2.47	0.48
1:F:253:TYR:CZ	1:F:254:LYS:HE2	2.47	0.48
1:N:204:LYS:NZ	1:N:212:LEU:O	2.37	0.48
1:O:19:VAL:HG13	1:O:165:ILE:HD11	1.95	0.48
1:O:119:PRO:HD2	1:O:136:VAL:HG21	1.94	0.48
1:C:496:ASP:OD2	2:C:612:HOH:O	2.20	0.48
1:D:14:ARG:HD2	2:D:720:HOH:O	2.12	0.48
1:E:100:LYS:HG2	1:E:106:TYR:CE2	2.48	0.48
1:A:63:GLU:HG3	1:A:106:TYR:O	2.13	0.48
1:B:353:ARG:NH2	2:B:630:HOH:O	2.46	0.48
1:C:253:TYR:CZ	1:C:254:LYS:HE2	2.48	0.48
1:E:255:GLY:O	1:E:257:ARG:HG3	2.13	0.48
1:F:19:VAL:HG13	1:F:165:ILE:HD11	1.94	0.48
1:K:323:THR:HG22	1:K:359:HIS:NE2	2.29	0.48
1:E:247:VAL:HB	2:E:666:HOH:O	2.13	0.48
1:M:9:PHE:HB2	1:M:18:LEU:HD11	1.96	0.48
1:J:453:SER:OG	1:J:454:ALA:N	2.46	0.48
1:K:100:LYS:HG2	1:K:106:TYR:CE2	2.49	0.48
1:G:471:VAL:HG12	1:G:472:ASP:OD2	2.14	0.48
1:I:135:HIS:HE1	2:I:708:HOH:O	1.97	0.48
1:I:410:PRO:O	2:I:616:HOH:O	2.20	0.48
1:M:320:GLU:O	1:M:323:THR:HG22	2.14	0.48
1:O:153:HIS:O	1:O:157:ILE:HG12	2.14	0.48
1:L:458:ARG:O	2:L:606:HOH:O	2.20	0.48
1:N:19:VAL:CG1	1:N:165:ILE:HD11	2.43	0.48
1:P:120:ARG:O	1:P:122:ARG:NH1	2.46	0.48
1:B:397:ARG:NH2	2:B:618:HOH:O	2.29	0.47
1:E:318:GLY:O	1:E:323:THR:HG21	2.14	0.47
1:F:63:GLU:OE1	2:F:617:HOH:O	2.20	0.47
1:H:36:ALA:HB2	1:H:59:PRO:HD2	1.95	0.47
1:L:456:ASP:HB3	1:L:458:ARG:CG	2.44	0.47
1:A:393:GLN:HG3	1:A:419:LEU:HD12	1.96	0.47
1:H:250:TRP:HA	2:H:731:HOH:O	2.13	0.47
1:K:486:THR:HG22	2:K:619:HOH:O	2.12	0.47
1:F:100:LYS:HG2	1:F:106:TYR:HE2	1.79	0.47
1:L:36:ALA:HB2	1:L:59:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:MET:HG2	1:L:130:ASP:O	2.14	0.47
1:M:261:MET:HG3	1:M:262:ASP:N	2.30	0.47
1:N:203:GLY:O	2:N:618:HOH:O	2.20	0.47
1:A:253:TYR:CZ	1:A:254:LYS:HE2	2.50	0.47
1:E:93:LEU:HD22	1:E:154:LEU:HD11	1.96	0.47
1:F:14:ARG:HD3	1:F:378:LEU:O	2.15	0.47
1:I:100:LYS:HG2	1:I:106:TYR:HE2	1.79	0.47
1:C:208:SER:H	1:C:211:GLN:NE2	2.12	0.47
1:F:463:LEU:HD12	1:O:109:GLU:HG3	1.96	0.47
1:H:3:GLU:HG2	1:H:4:GLU:H	1.80	0.47
1:I:456:ASP:HB3	1:I:458:ARG:H	1.79	0.47
1:J:3:GLU:HG3	1:J:4:GLU:N	2.24	0.47
1:P:42:PRO:HB2	1:P:43:PRO:HD3	1.97	0.47
1:P:458:ARG:HG2	1:P:458:ARG:NH1	2.30	0.47
1:F:259:PRO:HB2	1:F:265:SER:HB2	1.96	0.47
1:O:3:GLU:HG2	1:O:4:GLU:H	1.79	0.47
1:O:470:TYR:OH	1:O:506:ARG:NH1	2.47	0.47
1:E:210:GLN:H	1:E:210:GLN:CD	2.19	0.47
1:N:106:TYR:CE2	1:O:482:ASN:HB3	2.50	0.47
1:B:165:ILE:HA	1:B:165:ILE:HD12	1.76	0.47
1:H:231:GLU:CD	1:H:281:PRO:HD2	2.35	0.47
1:H:325:PRO:HA	1:H:428:ARG:HD3	1.97	0.47
1:L:19:VAL:CG1	1:L:165:ILE:HD11	2.45	0.47
1:O:14:ARG:HD3	1:O:378:LEU:O	2.15	0.47
1:I:318:GLY:O	1:I:323:THR:HG21	2.16	0.46
1:J:109:GLU:O	1:J:113:ARG:HG2	2.15	0.46
1:M:353:ARG:NE	2:M:628:HOH:O	2.48	0.46
1:B:247:VAL:HB	2:B:651:HOH:O	2.15	0.46
1:F:325:PRO:HA	1:F:428:ARG:CD	2.45	0.46
1:F:482:ASN:HB3	1:O:106:TYR:CZ	2.49	0.46
1:K:238:LYS:HE3	1:K:282:SER:O	2.15	0.46
1:N:154:LEU:C	2:N:619:HOH:O	2.53	0.46
1:I:400:ASP:OD2	2:I:617:HOH:O	2.21	0.46
1:L:452:ARG:NH1	1:L:454:ALA:HB3	2.30	0.46
1:B:168:GLN:HB2	1:B:246:TYR:CZ	2.51	0.46
1:M:100:LYS:HD2	1:M:171:ASN:HD22	1.81	0.46
1:B:325:PRO:HA	1:B:428:ARG:CD	2.46	0.46
1:E:19:VAL:HG13	1:E:165:ILE:HD11	1.98	0.46
1:E:247:VAL:HG22	1:E:286:ILE:HD12	1.96	0.46
1:F:403:ALA:HB1	1:F:448:ILE:HD11	1.96	0.46
1:I:239:ARG:HB2	1:L:458:ARG:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:GLU:HG2	1:F:92:ALA:HB3	1.98	0.46
1:G:452:ARG:HH22	1:G:456:ASP:CB	2.24	0.46
1:P:318:GLY:O	1:P:323:THR:HG21	2.15	0.46
1:B:210:GLN:H	1:B:210:GLN:CD	2.16	0.46
1:I:469:ARG:HD2	1:I:476:GLN:HB2	1.97	0.46
1:P:100:LYS:HD2	1:P:171:ASN:HD22	1.80	0.46
1:C:20:ASP:OD2	1:C:90:ARG:NH2	2.49	0.46
1:L:166:VAL:HG12	1:L:244:PRO:HB2	1.98	0.46
1:L:318:GLY:O	1:L:323:THR:HG21	2.16	0.46
1:L:411:LEU:HD13	1:L:491:ASN:HB3	1.97	0.46
1:O:138:ALA:C	2:O:602:HOH:O	2.54	0.46
1:G:428:ARG:NH2	2:G:1306:HOH:O	2.49	0.46
1:I:426:ALA:O	1:I:428:ARG:NH1	2.48	0.46
1:M:425:HIS:O	2:M:609:HOH:O	2.21	0.46
1:N:506:ARG:NH1	2:N:633:HOH:O	2.48	0.46
1:C:100:LYS:HG2	1:C:106:TYR:CE2	2.51	0.46
1:P:426:ALA:O	1:P:428:ARG:NH1	2.48	0.46
1:A:196:ALA:HA	1:A:199:ALA:HB3	1.97	0.45
1:C:25:THR:HB	1:C:370:GLN:HB2	1.98	0.45
1:K:470:TYR:HA	1:K:474:ARG:O	2.16	0.45
1:N:397:ARG:NH1	1:N:402:GLU:OE2	2.48	0.45
1:G:14:ARG:HD2	1:G:378:LEU:O	2.16	0.45
1:I:19:VAL:CG1	1:I:165:ILE:HD11	2.47	0.45
1:I:236:ALA:O	1:L:458:ARG:HD3	2.16	0.45
1:L:186:GLY:N	2:L:609:HOH:O	2.13	0.45
1:A:471:VAL:HG23	1:A:476:GLN:HG3	1.99	0.45
1:F:132:LEU:HD23	1:F:132:LEU:HA	1.84	0.45
1:G:438:GLU:OE2	1:G:506:ARG:NH2	2.47	0.45
1:H:494:ARG:HG3	2:H:728:HOH:O	2.16	0.45
1:L:165:ILE:HG22	1:L:166:VAL:HG22	1.97	0.45
1:N:130:ASP:OD2	2:N:617:HOH:O	2.20	0.45
1:C:98:SER:OG	1:C:143:ASP:OD2	2.30	0.45
1:O:277:ARG:HD2	1:O:277:ARG:HA	1.84	0.45
1:P:452:ARG:HG2	1:P:452:ARG:HH11	1.81	0.45
1:A:19:VAL:HG22	1:A:165:ILE:HD12	1.98	0.45
1:D:100:LYS:HG2	1:D:106:TYR:HE2	1.80	0.45
1:E:3:GLU:HB3	2:E:612:HOH:O	2.15	0.45
1:N:434:LEU:HD21	1:N:440:LEU:HB2	1.98	0.45
1:B:393:GLN:HG3	1:B:419:LEU:HD12	1.99	0.45
1:M:152:GLN:HG3	1:M:240:ALA:HB1	1.98	0.45
1:N:458:ARG:HG2	1:N:458:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:LYS:HD2	1:M:171:ASN:ND2	2.30	0.45
1:N:90:ARG:HA	1:N:90:ARG:HD2	1.86	0.45
1:O:57:GLU:HG3	1:O:92:ALA:HB3	1.99	0.45
1:O:429:LEU:HD21	1:O:448:ILE:HD12	1.98	0.45
1:P:161:ARG:NH1	2:P:625:HOH:O	2.44	0.45
1:D:426:ALA:O	1:D:428:ARG:NH1	2.49	0.45
1:J:100:LYS:HG2	1:J:106:TYR:HE2	1.81	0.45
1:J:327:LEU:HD21	1:J:366:LEU:HD12	1.99	0.45
1:M:253:TYR:O	1:M:256:LYS:HG3	2.17	0.45
1:B:106:TYR:OH	2:B:611:HOH:O	2.20	0.45
1:M:255:GLY:O	1:M:257:ARG:HG3	2.17	0.45
1:P:104:MET:CE	1:P:120:ARG:HG2	2.47	0.45
1:F:152:GLN:HG3	1:F:240:ALA:HB1	1.98	0.44
1:G:202:LEU:HB2	1:G:204:LYS:HG3	1.99	0.44
1:N:100:LYS:HG3	1:N:106:TYR:CE1	2.51	0.44
1:O:318:GLY:O	1:O:323:THR:HG21	2.16	0.44
1:P:100:LYS:HG2	1:P:106:TYR:HE2	1.82	0.44
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.74	0.44
1:I:162:HIS:HA	2:I:614:HOH:O	2.18	0.44
1:M:62:TRP:CD2	1:M:108:PRO:HD3	2.52	0.44
1:D:172:GLU:CD	1:D:250:TRP:HB2	2.38	0.44
1:F:327:LEU:HD21	1:F:366:LEU:HD12	1.98	0.44
1:J:258:TYR:CE2	1:N:261:MET:HE1	2.52	0.44
1:L:75:THR:O	2:L:613:HOH:O	2.21	0.44
1:L:204:LYS:HE3	1:L:212:LEU:HD12	1.98	0.44
1:O:401:TRP:CZ2	1:O:452:ARG:HD2	2.51	0.44
1:A:111:ILE:HG23	1:A:118:TYR:CG	2.53	0.44
1:B:193:PRO:HG2	1:L:472:ASP:OD2	2.17	0.44
1:B:419:LEU:HD23	1:B:419:LEU:HA	1.81	0.44
1:B:480:GLN:HB2	1:H:37:TRP:CZ2	2.52	0.44
1:D:165:ILE:HA	1:D:165:ILE:HD12	1.82	0.44
1:D:453:SER:C	1:D:455:ALA:H	2.21	0.44
1:D:467:GLN:NE2	1:D:478:GLU:OE1	2.48	0.44
1:J:192:GLN:O	2:J:612:HOH:O	2.21	0.44
1:K:153:HIS:NE2	1:K:157:ILE:HD13	2.32	0.44
1:O:261:MET:HG3	1:O:262:ASP:N	2.32	0.44
1:B:7:ARG:O	1:B:18:LEU:HB2	2.18	0.44
1:J:204:LYS:HD3	1:J:212:LEU:HD22	2.00	0.44
1:K:452:ARG:NH2	1:K:456:ASP:OD2	2.28	0.44
1:K:458:ARG:NH1	1:K:511:SER:OG	2.51	0.44
1:N:93:LEU:HD23	1:N:154:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:TRP:CD2	1:O:108:PRO:HD3	2.52	0.44
1:A:7:ARG:O	1:A:18:LEU:HB2	2.18	0.44
1:C:168:GLN:HB2	1:C:246:TYR:CZ	2.51	0.44
1:D:62:TRP:CD2	1:D:108:PRO:HD3	2.53	0.44
1:J:325:PRO:HA	1:J:428:ARG:HD2	1.98	0.44
1:O:141:GLN:O	1:O:145:ARG:HB2	2.18	0.44
1:A:323:THR:HG22	1:A:359:HIS:NE2	2.32	0.44
1:G:474:ARG:CZ	1:G:474:ARG:HB2	2.46	0.44
1:H:256:LYS:HB3	1:H:262:ASP:HB3	1.99	0.44
1:F:300:LYS:HE2	2:F:704:HOH:O	2.18	0.44
1:H:57:GLU:HG2	1:H:92:ALA:HB3	1.98	0.44
1:H:320:GLU:OE1	2:H:605:HOH:O	2.21	0.44
1:H:437:GLU:HG2	1:H:509:VAL:HG23	2.00	0.44
1:M:238:LYS:HE2	1:M:245:LEU:HG	1.99	0.44
1:N:46:ASP:OD1	1:N:87:ARG:NH1	2.42	0.44
1:K:258:TYR:HD2	1:K:262:ASP:OD2	2.00	0.44
1:L:36:ALA:HA	1:L:41:LEU:HD21	2.00	0.44
1:F:239:ARG:NH2	2:F:636:HOH:O	2.49	0.43
1:M:9:PHE:CE2	1:M:11:GLN:HB2	2.53	0.43
1:C:397:ARG:HG3	1:C:397:ARG:HH11	1.83	0.43
1:D:65:PHE:O	1:D:72:PHE:HA	2.18	0.43
1:D:403:ALA:HB1	1:D:448:ILE:HD11	2.00	0.43
1:H:247:VAL:HB	2:H:611:HOH:O	2.18	0.43
1:O:25:THR:OG1	1:O:374:ALA:HB2	2.18	0.43
1:A:154:LEU:HA	1:A:157:ILE:HG12	2.00	0.43
1:L:364:ARG:HH21	1:L:500:GLN:NE2	2.17	0.43
1:B:323:THR:HG22	1:B:359:HIS:HE2	1.82	0.43
1:M:111:ILE:HG23	1:M:118:TYR:CG	2.53	0.43
1:A:121:MET:HG3	1:A:133:SER:HA	2.00	0.43
1:A:397:ARG:HG2	1:A:397:ARG:HH11	1.83	0.43
1:D:166:VAL:HG12	1:D:244:PRO:HB2	1.99	0.43
1:E:75:THR:O	2:E:615:HOH:O	2.21	0.43
1:K:244:PRO:O	1:K:245:LEU:HD23	2.19	0.43
1:E:475:TRP:CD2	1:E:506:ARG:HD2	2.53	0.43
1:G:100:LYS:HD2	1:G:171:ASN:HD22	1.83	0.43
1:G:475:TRP:CH2	1:G:506:ARG:HG3	2.54	0.43
1:H:59:PRO:HA	1:H:94:LEU:HB2	2.00	0.43
1:I:325:PRO:HA	1:I:428:ARG:HD2	1.99	0.43
1:O:5:LEU:HD12	1:O:6:PRO:HD2	2.01	0.43
1:E:256:LYS:HB3	1:E:262:ASP:HB3	2.00	0.43
1:F:323:THR:HG22	1:F:359:HIS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:PRO:HD2	1:K:71:ARG:O	2.19	0.43
1:L:468:GLY:O	2:L:612:HOH:O	2.21	0.43
1:N:158:ASP:N	2:N:619:HOH:O	2.50	0.43
1:A:154:LEU:HD12	1:A:157:ILE:HD11	2.00	0.43
1:D:400:ASP:OD2	1:D:454:ALA:HA	2.18	0.43
1:E:462:LEU:HD12	1:E:462:LEU:HA	1.82	0.43
1:H:261:MET:HG3	1:H:262:ASP:N	2.33	0.43
1:J:62:TRP:CD2	1:J:108:PRO:HD3	2.53	0.43
1:B:325:PRO:HA	1:B:428:ARG:HD2	2.01	0.43
1:D:239:ARG:HD3	1:D:239:ARG:HA	1.05	0.43
1:G:208:SER:H	1:G:211:GLN:HE21	1.64	0.43
1:G:320:GLU:O	1:G:323:THR:HG22	2.19	0.43
1:K:3:GLU:HG3	1:K:4:GLU:N	2.26	0.43
1:M:369:LEU:HD23	1:M:440:LEU:HD21	2.00	0.43
1:F:369:LEU:HD23	1:F:440:LEU:HD21	2.01	0.43
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.82	0.43
1:I:239:ARG:HD2	1:L:458:ARG:CB	2.20	0.43
1:M:250:TRP:CD2	1:M:264:PRO:HD3	2.54	0.43
1:O:312:ALA:N	2:O:618:HOH:O	2.25	0.43
1:P:404:LYS:HB2	1:P:404:LYS:HE3	1.64	0.43
1:B:494:ARG:NH1	2:B:627:HOH:O	2.40	0.42
1:C:406:SER:HB3	1:C:419:LEU:HD21	2.01	0.42
1:I:253:TYR:CE1	1:I:256:LYS:HE3	2.55	0.42
1:K:57:GLU:HG2	1:K:92:ALA:HB3	2.00	0.42
1:O:152:GLN:HG3	1:O:240:ALA:HB1	2.00	0.42
1:A:369:LEU:HD23	1:A:440:LEU:HD21	2.01	0.42
1:A:397:ARG:NH1	1:A:402:GLU:OE2	2.52	0.42
1:C:109:GLU:OE2	1:C:113:ARG:NH1	2.53	0.42
1:I:250:TRP:CG	1:I:264:PRO:HD3	2.55	0.42
1:I:369:LEU:HD23	1:I:440:LEU:HD21	2.01	0.42
1:K:238:LYS:HB2	2:K:601:HOH:O	2.20	0.42
1:P:403:ALA:HB1	1:P:448:ILE:HD11	2.00	0.42
1:A:154:LEU:HA	1:A:157:ILE:HG13	2.00	0.42
1:F:318:GLY:O	1:F:323:THR:HG21	2.20	0.42
1:H:453:SER:OG	1:H:454:ALA:N	2.52	0.42
1:I:403:ALA:HB1	1:I:448:ILE:HD11	2.02	0.42
1:O:277:ARG:O	2:O:614:HOH:O	2.22	0.42
1:D:210:GLN:HA	1:D:217:ALA:HB2	2.01	0.42
1:F:434:LEU:HD12	1:F:438:GLU:HG2	2.00	0.42
1:F:456:ASP:HB3	1:F:458:ARG:H	1.83	0.42
1:C:113:ARG:HA	1:C:113:ARG:HD2	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:PRO:HD2	2:I:665:HOH:O	2.20	0.42
1:J:256:LYS:HE3	1:J:262:ASP:O	2.20	0.42
1:K:62:TRP:CD2	1:K:108:PRO:HD3	2.55	0.42
1:N:318:GLY:O	1:N:323:THR:HG21	2.19	0.42
1:O:141:GLN:HB2	2:O:602:HOH:O	2.20	0.42
1:B:100:LYS:HD2	1:B:106:TYR:HE2	1.84	0.42
1:M:277:ARG:HA	1:M:277:ARG:HD2	1.90	0.42
1:P:385:VAL:HG11	1:P:394:ARG:HG3	2.01	0.42
1:A:145:ARG:HD2	2:A:788:HOH:O	2.19	0.42
1:A:453:SER:OG	1:A:454:ALA:N	2.51	0.42
1:E:100:LYS:HD2	1:E:171:ASN:HD22	1.85	0.42
1:G:62:TRP:CD2	1:G:108:PRO:HD3	2.54	0.42
1:I:345:GLY:O	2:I:618:HOH:O	2.22	0.42
1:K:318:GLY:O	1:K:323:THR:HG21	2.20	0.42
1:O:210:GLN:HB3	2:O:603:HOH:O	2.20	0.42
1:O:403:ALA:HB1	1:O:448:ILE:HD11	2.02	0.42
1:P:462:LEU:HD23	1:P:509:VAL:HG12	2.02	0.42
1:I:271:ASN:OD1	1:I:271:ASN:N	2.53	0.42
1:M:19:VAL:HB	1:M:24:TYR:HB2	2.01	0.42
1:A:165:ILE:HA	1:A:165:ILE:HD13	1.74	0.41
1:A:180:ARG:NH2	2:A:618:HOH:O	2.36	0.41
1:A:325:PRO:HA	1:A:428:ARG:CD	2.50	0.41
1:G:325:PRO:HA	1:G:428:ARG:CD	2.50	0.41
1:B:277:ARG:HA	1:B:277:ARG:HD2	1.77	0.41
1:C:165:ILE:HD12	1:C:165:ILE:HA	1.77	0.41
1:F:145:ARG:HE	1:F:145:ARG:HB2	1.64	0.41
1:L:300:LYS:NZ	2:L:640:HOH:O	2.53	0.41
1:N:312:ALA:O	1:N:335:GLY:HA2	2.20	0.41
1:O:453:SER:OG	1:O:454:ALA:N	2.52	0.41
1:A:52:HIS:HD2	2:A:781:HOH:O	2.02	0.41
1:G:20:ASP:OD2	1:G:90:ARG:NH2	2.53	0.41
1:H:93:LEU:HA	1:H:93:LEU:HD12	1.81	0.41
1:J:152:GLN:HG3	1:J:240:ALA:HB1	2.02	0.41
1:J:463:LEU:HD13	1:J:463:LEU:HA	1.94	0.41
1:O:325:PRO:HA	1:O:428:ARG:CD	2.50	0.41
1:O:452:ARG:HG2	1:O:452:ARG:HH11	1.85	0.41
1:B:312:ALA:HB3	1:B:335:GLY:HA2	2.02	0.41
1:C:121:MET:HG3	1:C:133:SER:HA	2.01	0.41
1:C:372:LEU:HD21	1:C:434:LEU:HD21	2.01	0.41
1:E:194:VAL:HG21	1:E:212:LEU:HD22	2.02	0.41
1:F:119:PRO:HG2	1:F:136:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:VAL:HG21	1:H:212:LEU:HD12	2.02	0.41
1:I:385:VAL:HG11	1:I:394:ARG:HG3	2.03	0.41
1:I:506:ARG:HD2	2:I:649:HOH:O	2.19	0.41
1:K:93:LEU:HD12	1:K:93:LEU:HA	1.80	0.41
1:O:37:TRP:O	1:O:41:LEU:HD23	2.20	0.41
1:P:19:VAL:CG1	1:P:165:ILE:HD11	2.49	0.41
1:A:165:ILE:HG22	1:A:166:VAL:HG13	2.02	0.41
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.89	0.41
1:B:261:MET:HG3	1:B:262:ASP:N	2.35	0.41
1:F:482:ASN:HB3	1:O:106:TYR:CE2	2.56	0.41
1:H:9:PHE:CE1	1:H:11:GLN:HB2	2.55	0.41
1:I:76:ASN:HB3	2:I:746:HOH:O	2.20	0.41
1:J:369:LEU:HD23	1:J:440:LEU:HD21	2.02	0.41
1:K:134:PRO:O	2:K:610:HOH:O	2.22	0.41
1:N:325:PRO:HA	1:N:428:ARG:HD2	2.02	0.41
1:O:104:MET:HE3	1:O:130:ASP:HA	2.01	0.41
1:P:442:THR:HA	1:P:492:PHE:CE2	2.55	0.41
1:D:452:ARG:HH12	1:D:456:ASP:HB2	1.84	0.41
1:D:486:THR:HG22	2:D:617:HOH:O	2.21	0.41
1:F:247:VAL:HB	2:F:674:HOH:O	2.20	0.41
1:F:464:GLN:NE2	1:F:480:GLN:OE1	2.50	0.41
1:G:192:GLN:HA	1:G:192:GLN:OE1	2.20	0.41
1:G:453:SER:OG	1:G:454:ALA:N	2.54	0.41
1:K:367:ALA:HB3	1:K:368:PRO:HD3	2.01	0.41
1:L:119:PRO:HG2	1:L:136:VAL:HG11	2.03	0.41
1:I:239:ARG:O	1:L:457:THR:OG1	2.38	0.41
1:J:253:TYR:O	1:J:256:LYS:HG3	2.21	0.41
1:L:253:TYR:CD1	1:L:254:LYS:HG3	2.56	0.41
1:P:62:TRP:CD2	1:P:108:PRO:HD3	2.56	0.41
1:A:239:ARG:NH1	2:A:629:HOH:O	2.53	0.41
1:B:90:ARG:NH1	1:B:165:ILE:HD13	2.36	0.41
1:G:19:VAL:CG1	1:G:165:ILE:HD11	2.47	0.41
1:H:469:ARG:NH1	1:H:504:VAL:HG23	2.36	0.41
1:J:117:THR:O	1:J:119:PRO:HD3	2.21	0.41
1:J:325:PRO:HA	1:J:428:ARG:CD	2.51	0.41
1:J:364:ARG:HH21	1:J:500:GLN:NE2	2.19	0.41
1:K:165:ILE:HA	1:K:165:ILE:HD12	1.87	0.41
1:L:204:LYS:CD	1:L:212:LEU:HD12	2.51	0.41
1:L:212:LEU:HD13	1:L:212:LEU:HA	1.87	0.41
1:N:111:ILE:HG23	1:N:118:TYR:CG	2.56	0.41
1:P:100:LYS:HD2	1:P:171:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:ARG:HA	1:P:277:ARG:HD2	1.90	0.41
1:A:100:LYS:HG2	1:A:106:TYR:HE2	1.85	0.41
1:B:144:ALA:O	1:B:148:THR:OG1	2.32	0.41
1:C:122:ARG:HD2	1:C:126:GLY:O	2.20	0.41
1:E:57:GLU:HG2	1:E:92:ALA:HB3	2.01	0.41
1:F:71:ARG:HG2	2:F:625:HOH:O	2.21	0.41
1:G:154:LEU:HD12	1:G:154:LEU:HA	1.87	0.41
1:L:141:GLN:O	1:L:145:ARG:HB2	2.21	0.41
1:N:57:GLU:HG2	1:N:92:ALA:HB3	2.03	0.41
1:A:385:VAL:HG11	1:A:394:ARG:HG3	2.02	0.40
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.93	0.40
1:G:15:HIS:HB2	1:G:311:PRO:HB3	2.04	0.40
1:H:100:LYS:HD2	1:H:106:TYR:HE2	1.86	0.40
1:O:60:VAL:CG2	1:O:93:LEU:HD21	2.50	0.40
1:B:202:LEU:HB2	1:B:204:LYS:HG3	2.03	0.40
1:D:7:ARG:O	1:D:18:LEU:HB2	2.21	0.40
1:G:419:LEU:HA	1:G:419:LEU:HD23	1.88	0.40
1:I:326:TYR:O	1:I:330:VAL:HG23	2.21	0.40
1:P:117:THR:O	1:P:119:PRO:HD3	2.21	0.40
1:F:480:GLN:O	1:O:34:SER:HB3	2.21	0.40
1:G:71:ARG:HG2	1:G:71:ARG:NH1	2.37	0.40
1:G:111:ILE:HG23	1:G:118:TYR:CG	2.57	0.40
1:J:104:MET:HG2	1:J:130:ASP:C	2.42	0.40
1:L:14:ARG:HH11	1:L:14:ARG:HG2	1.85	0.40
1:O:147:PHE:O	1:O:151:MET:HG2	2.22	0.40
1:P:165:ILE:HA	1:P:165:ILE:HD12	1.79	0.40
1:H:306:ALA:O	2:H:606:HOH:O	2.22	0.40
1:K:152:GLN:HG3	1:K:240:ALA:HB1	2.03	0.40
1:L:145:ARG:HG2	2:L:782:HOH:O	2.21	0.40
1:L:165:ILE:HG23	1:L:166:VAL:HG13	2.04	0.40
1:L:277:ARG:HD2	1:L:277:ARG:HA	1.84	0.40
1:C:320:GLU:O	1:C:323:THR:HG22	2.20	0.40
1:H:19:VAL:CG1	1:H:165:ILE:HD11	2.51	0.40
1:H:100:LYS:HG2	1:H:171:ASN:HB3	2.04	0.40
1:N:83:GLY:HA2	2:N:610:HOH:O	2.21	0.40

All (9) 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)
2:E:696:HOH:O	2:K:729:HOH:O[2_655]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:794:HOH:O	2:G:1474:HOH:O[2_555]	1.96	0.24
2:H:716:HOH:O	2:L:604:HOH:O[1_655]	1.98	0.22
1:A:156:LYS:O	1:D:239:ARG:NH2[1_455]	2.03	0.17
2:A:606:HOH:O	2:P:692:HOH:O[1_565]	2.04	0.16
2:F:726:HOH:O	2:L:672:HOH:O[2_656]	2.04	0.16
2:A:779:HOH:O	2:I:636:HOH:O[1_565]	2.13	0.07
2:C:774:HOH:O	2:I:813:HOH:O[1_655]	2.13	0.07
2:A:812:HOH:O	2:D:770:HOH:O[1_455]	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	508/511 (99%)	491 (97%)	17 (3%)	0	100	100
1	B	508/511 (99%)	489 (96%)	19 (4%)	0	100	100
1	C	508/511 (99%)	489 (96%)	19 (4%)	0	100	100
1	D	508/511 (99%)	485 (96%)	22 (4%)	1 (0%)	47	68
1	E	508/511 (99%)	491 (97%)	16 (3%)	1 (0%)	47	68
1	F	508/511 (99%)	494 (97%)	14 (3%)	0	100	100
1	G	508/511 (99%)	490 (96%)	18 (4%)	0	100	100
1	H	508/511 (99%)	491 (97%)	17 (3%)	0	100	100
1	I	508/511 (99%)	490 (96%)	16 (3%)	2 (0%)	34	54
1	J	508/511 (99%)	493 (97%)	15 (3%)	0	100	100
1	K	508/511 (99%)	494 (97%)	14 (3%)	0	100	100
1	L	508/511 (99%)	491 (97%)	17 (3%)	0	100	100
1	M	508/511 (99%)	494 (97%)	14 (3%)	0	100	100
1	N	508/511 (99%)	491 (97%)	17 (3%)	0	100	100
1	O	508/511 (99%)	491 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	508/511 (99%)	493 (97%)	15 (3%)	0	100	100
All	All	8128/8176 (99%)	7857 (97%)	267 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	200	ALA
1	I	201	ALA
1	D	239	ARG
1	E	195	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/382 (100%)	371 (97%)	10 (3%)	46	72
1	B	381/382 (100%)	370 (97%)	11 (3%)	42	69
1	C	381/382 (100%)	369 (97%)	12 (3%)	40	67
1	D	381/382 (100%)	368 (97%)	13 (3%)	37	63
1	E	381/382 (100%)	366 (96%)	15 (4%)	32	57
1	F	381/382 (100%)	367 (96%)	14 (4%)	34	60
1	G	381/382 (100%)	376 (99%)	5 (1%)	69	87
1	H	381/382 (100%)	370 (97%)	11 (3%)	42	69
1	I	381/382 (100%)	372 (98%)	9 (2%)	49	74
1	J	381/382 (100%)	372 (98%)	9 (2%)	49	74
1	K	381/382 (100%)	372 (98%)	9 (2%)	49	74
1	L	381/382 (100%)	369 (97%)	12 (3%)	40	67
1	M	381/382 (100%)	371 (97%)	10 (3%)	46	72
1	N	381/382 (100%)	374 (98%)	7 (2%)	59	81
1	O	381/382 (100%)	370 (97%)	11 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	381/382 (100%)	372 (98%)	9 (2%)	49	74
All	All	6096/6112 (100%)	5929 (97%)	167 (3%)	44	71

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	180	ARG
1	A	253	TYR
1	A	261	MET
1	A	276	TRP
1	A	323	THR
1	A	393	GLN
1	A	440	LEU
1	A	494	ARG
1	A	500	GLN
1	B	154	LEU
1	B	156	LYS
1	B	161	ARG
1	B	180	ARG
1	B	253	TYR
1	B	276	TRP
1	B	315	SER
1	B	323	THR
1	B	429	LEU
1	B	486	THR
1	B	494	ARG
1	C	107	VAL
1	C	156	LYS
1	C	247	VAL
1	C	253	TYR
1	C	276	TRP
1	C	339	SER
1	C	419	LEU
1	C	428	ARG
1	C	453	SER
1	C	476	GLN
1	C	486	THR
1	C	494	ARG
1	D	113	ARG
1	D	180	ARG
1	D	239	ARG

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Mol	Chain	Res	Type
1	D	247	VAL
1	D	253	TYR
1	D	276	TRP
1	D	293	SER
1	D	315	SER
1	D	323	THR
1	D	339	SER
1	D	434	LEU
1	D	486	THR
1	D	500	GLN
1	E	7	ARG
1	E	90	ARG
1	E	145	ARG
1	E	180	ARG
1	E	253	TYR
1	E	276	TRP
1	E	315	SER
1	E	317	THR
1	E	323	THR
1	E	339	SER
1	E	414	ASP
1	E	434	LEU
1	E	486	THR
1	E	494	ARG
1	E	506	ARG
1	F	71	ARG
1	F	180	ARG
1	F	210	GLN
1	F	253	TYR
1	F	261	MET
1	F	276	TRP
1	F	323	THR
1	F	339	SER
1	F	429	LEU
1	F	436	PRO
1	F	453	SER
1	F	461	GLN
1	F	486	THR
1	F	494	ARG
1	G	253	TYR
1	G	261	MET
1	G	298	TYR

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Mol	Chain	Res	Type
1	G	323	THR
1	G	339	SER
1	H	7	ARG
1	H	12	ASN
1	H	107	VAL
1	H	229	TYR
1	H	253	TYR
1	H	261	MET
1	H	323	THR
1	H	410	PRO
1	H	469	ARG
1	H	486	THR
1	H	494	ARG
1	I	122	ARG
1	I	239	ARG
1	I	253	TYR
1	I	276	TRP
1	I	323	THR
1	I	404	LYS
1	I	429	LEU
1	I	469	ARG
1	I	486	THR
1	J	210	GLN
1	J	253	TYR
1	J	257	ARG
1	J	261	MET
1	J	323	THR
1	J	339	SER
1	J	397	ARG
1	J	486	THR
1	J	506	ARG
1	K	3	GLU
1	K	161	ARG
1	K	253	TYR
1	K	276	TRP
1	K	298	TYR
1	K	323	THR
1	K	429	LEU
1	K	462	LEU
1	K	486	THR
1	L	141	GLN
1	L	180	ARG

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Mol	Chain	Res	Type
1	L	192	GLN
1	L	247	VAL
1	L	253	TYR
1	L	276	TRP
1	L	293	SER
1	L	323	THR
1	L	429	LEU
1	L	474	ARG
1	L	486	THR
1	L	494	ARG
1	M	14	ARG
1	M	132	LEU
1	M	161	ARG
1	M	253	TYR
1	M	276	TRP
1	M	293	SER
1	M	339	SER
1	M	429	LEU
1	M	456	ASP
1	M	486	THR
1	N	210	GLN
1	N	211	GLN
1	N	229	TYR
1	N	253	TYR
1	N	339	SER
1	N	486	THR
1	N	494	ARG
1	O	7	ARG
1	O	104	MET
1	O	113	ARG
1	O	148	THR
1	O	253	TYR
1	O	293	SER
1	O	323	THR
1	O	339	SER
1	O	442	THR
1	O	456	ASP
1	O	474	ARG
1	P	7	ARG
1	P	210	GLN
1	P	253	TYR
1	P	293	SER

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Mol	Chain	Res	Type
1	P	323	THR
1	P	339	SER
1	P	423	ASP
1	P	429	LEU
1	P	506	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	C	76	ASN
1	C	182	HIS
1	C	211	GLN
1	C	329	HIS
1	C	464	GLN
1	E	135	HIS
1	E	141	GLN
1	E	329	HIS
1	F	224	HIS
1	F	393	GLN
1	F	461	GLN
1	G	103	GLN
1	G	211	GLN
1	G	346	ASN
1	I	135	HIS
1	I	224	HIS
1	I	346	ASN
1	I	388	GLN
1	J	103	GLN
1	K	52	HIS
1	K	393	GLN
1	K	464	GLN
1	K	480	GLN
1	L	232	GLN
1	L	329	HIS
1	L	461	GLN
1	L	500	GLN
1	N	210	GLN
1	N	211	GLN
1	N	232	GLN
1	N	500	GLN
1	O	103	GLN

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Mol	Chain	Res	Type
1	O	139	ASN
1	O	304	GLN
1	O	329	HIS
1	P	12	ASN
1	P	141	GLN
1	P	352	ASN

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 monosaccharides 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 i

6.1 Protein, DNA and RNA chains i

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	510/511 (99%)	-0.25	5 (0%) 82 84	15, 25, 40, 66	0
1	B	510/511 (99%)	-0.05	10 (1%) 65 68	21, 31, 48, 68	0
1	C	510/511 (99%)	-0.18	7 (1%) 75 77	19, 28, 43, 69	0
1	D	510/511 (99%)	-0.17	13 (2%) 57 61	19, 27, 46, 71	0
1	E	510/511 (99%)	-0.28	9 (1%) 68 71	18, 25, 43, 64	0
1	F	510/511 (99%)	-0.19	8 (1%) 72 74	16, 27, 46, 70	0
1	G	510/511 (99%)	-0.19	9 (1%) 68 71	17, 26, 45, 72	0
1	H	510/511 (99%)	-0.22	4 (0%) 86 87	20, 29, 43, 68	0
1	I	510/511 (99%)	-0.09	13 (2%) 57 61	17, 29, 47, 72	0
1	J	510/511 (99%)	-0.11	11 (2%) 62 65	19, 29, 49, 69	0
1	K	510/511 (99%)	-0.11	16 (3%) 49 52	19, 30, 45, 74	0
1	L	510/511 (99%)	0.01	24 (4%) 31 33	18, 28, 50, 78	0
1	M	510/511 (99%)	0.00	12 (2%) 59 62	25, 37, 55, 76	0
1	N	510/511 (99%)	0.22	19 (3%) 41 45	25, 42, 59, 84	0
1	O	510/511 (99%)	0.30	24 (4%) 31 33	27, 39, 56, 78	0
1	P	510/511 (99%)	-0.17	6 (1%) 79 80	19, 29, 46, 69	0
All	All	8160/8176 (99%)	-0.09	190 (2%) 60 63	15, 30, 50, 84	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	471	VAL	10.8
1	L	472	ASP	10.7
1	K	472	ASP	8.7
1	L	457	THR	8.2
1	D	454	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
1	F	454	ALA	8.2
1	K	471	VAL	7.8
1	L	454	ALA	7.7
1	G	474	ARG	7.5
1	L	455	ALA	7.4
1	L	458	ARG	7.2
1	L	456	ASP	6.9
1	L	476	GLN	6.7
1	C	454	ALA	6.5
1	K	474	ARG	6.4
1	L	474	ARG	6.3
1	O	454	ALA	6.3
1	L	512	TYR	6.2
1	H	454	ALA	6.0
1	G	472	ASP	6.0
1	D	455	ALA	5.5
1	D	457	THR	5.5
1	L	473	GLY	5.3
1	O	497	ALA	5.2
1	G	471	VAL	5.0
1	I	472	ASP	4.9
1	F	455	ALA	4.9
1	G	473	GLY	4.7
1	M	454	ALA	4.7
1	J	454	ALA	4.7
1	L	459	HIS	4.6
1	I	454	ALA	4.6
1	K	455	ALA	4.5
1	K	469	ARG	4.3
1	I	457	THR	4.3
1	L	475	TRP	4.3
1	P	454	ALA	4.2
1	G	454	ALA	4.2
1	E	474	ARG	4.1
1	K	473	GLY	4.1
1	L	470	TYR	4.1
1	I	455	ALA	4.0
1	O	498	ALA	4.0
1	D	474	ARG	4.0
1	O	455	ALA	4.0
1	B	498	ALA	3.9
1	J	457	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	474	ARG	3.9
1	P	497	ALA	3.9
1	B	454	ALA	3.8
1	N	472	ASP	3.8
1	H	455	ALA	3.7
1	N	191	ALA	3.7
1	L	453	SER	3.7
1	O	12	ASN	3.6
1	K	475	TRP	3.6
1	C	498	ALA	3.5
1	N	455	ALA	3.5
1	K	191	ALA	3.5
1	L	469	ARG	3.4
1	L	511	SER	3.4
1	C	474	ARG	3.4
1	O	13	GLY	3.4
1	B	202	LEU	3.4
1	O	198	ILE	3.4
1	P	498	ALA	3.3
1	N	471	VAL	3.3
1	F	457	THR	3.3
1	A	3	GLU	3.3
1	I	239	ARG	3.2
1	D	3	GLU	3.2
1	M	205	PRO	3.2
1	F	472	ASP	3.1
1	L	192	GLN	3.1
1	C	497	ALA	3.1
1	A	498	ALA	3.1
1	M	472	ASP	3.1
1	M	455	ALA	3.1
1	K	470	TYR	3.1
1	O	199	ALA	3.1
1	H	3	GLU	3.1
1	O	68	ALA	3.0
1	N	498	ALA	3.0
1	E	454	ALA	3.0
1	N	137	ALA	3.0
1	N	200	ALA	2.9
1	B	472	ASP	2.9
1	J	12	ASN	2.9
1	L	191	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	217	ALA	2.8
1	K	12	ASN	2.8
1	E	472	ASP	2.7
1	I	476	GLN	2.7
1	A	455	ALA	2.7
1	N	3	GLU	2.7
1	K	205	PRO	2.7
1	L	207	GLY	2.7
1	N	197	ALA	2.7
1	J	192	GLN	2.7
1	A	454	ALA	2.7
1	N	397	ARG	2.6
1	I	456	ASP	2.6
1	E	455	ALA	2.6
1	F	71	ARG	2.6
1	M	202	LEU	2.6
1	I	193	PRO	2.6
1	O	155	ARG	2.6
1	B	497	ALA	2.5
1	B	9	PHE	2.5
1	C	472	ASP	2.5
1	E	192	GLN	2.5
1	K	454	ALA	2.5
1	O	474	ARG	2.5
1	D	203	GLY	2.5
1	K	11	GLN	2.5
1	D	191	ALA	2.5
1	K	476	GLN	2.5
1	O	211	GLN	2.5
1	D	200	ALA	2.5
1	J	211	GLN	2.4
1	J	472	ASP	2.4
1	J	455	ALA	2.4
1	G	476	GLN	2.4
1	N	201	ALA	2.4
1	J	207	GLY	2.4
1	E	191	ALA	2.4
1	L	417	ALA	2.4
1	J	497	ALA	2.3
1	C	3	GLU	2.3
1	I	199	ALA	2.3
1	E	3	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	156	LYS	2.3
1	D	471	VAL	2.3
1	B	189	ALA	2.3
1	O	215	ALA	2.3
1	G	457	THR	2.3
1	O	205	PRO	2.3
1	J	205	PRO	2.3
1	I	200	ALA	2.3
1	L	206	ALA	2.3
1	N	454	ALA	2.3
1	N	192	GLN	2.2
1	O	499	GLY	2.2
1	F	195	PRO	2.2
1	O	203	GLY	2.2
1	M	457	THR	2.2
1	D	239	ARG	2.2
1	P	455	ALA	2.2
1	O	3	GLU	2.2
1	M	207	GLY	2.2
1	M	471	VAL	2.2
1	A	157	ILE	2.2
1	F	12	ASN	2.2
1	M	12	ASN	2.2
1	N	474	ARG	2.2
1	M	198	ILE	2.2
1	I	195	PRO	2.2
1	B	138	ALA	2.2
1	D	497	ALA	2.2
1	P	456	ASP	2.2
1	L	460	GLY	2.2
1	O	184	PRO	2.2
1	N	457	THR	2.1
1	G	4	GLU	2.1
1	G	469	ARG	2.1
1	M	196	ALA	2.1
1	E	193	PRO	2.1
1	N	453	SER	2.1
1	P	453	SER	2.1
1	B	471	VAL	2.1
1	D	498	ALA	2.1
1	K	456	ASP	2.1
1	K	188	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	62	TRP	2.1
1	O	183	GLY	2.1
1	C	455	ALA	2.1
1	B	195	PRO	2.1
1	I	471	VAL	2.1
1	D	453	SER	2.1
1	M	3	GLU	2.1
1	H	498	ALA	2.1
1	E	12	ASN	2.0
1	I	453	SER	2.0
1	N	208	SER	2.0
1	O	208	SER	2.0
1	O	191	ALA	2.0
1	N	193	PRO	2.0
1	L	200	ALA	2.0
1	J	453	SER	2.0
1	N	186	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.