



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:09 PM UTC

PDB ID : 8FAA / pdb_00008faa
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 : 4-5-2 with Phenix2.0
Xtrriage (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

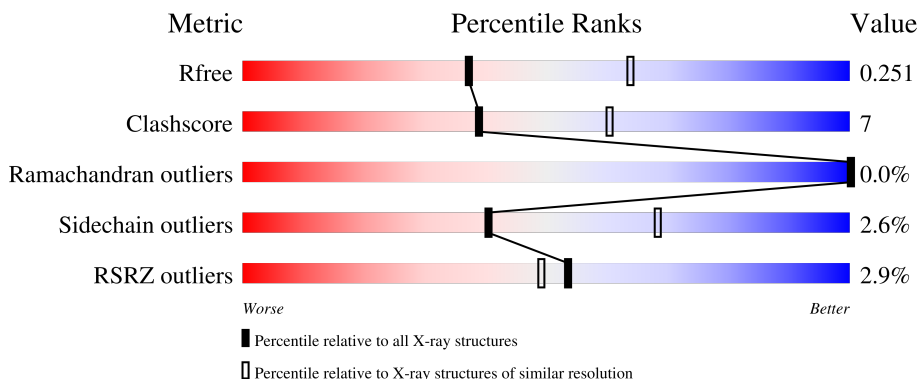
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	 85% 14% .
1	B	511	 2% 86% 13% .
1	C	511	 2% 86% 14% .
1	D	511	 4% 86% 12% .
1	E	511	 % 86% 13% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	511	 % 85% 13%
1	G	511	 3% 85% 15%
1	H	511	 % 87% 13%
1	I	511	 4% 86% 13%
1	J	511	 3% 87% 12%
1	K	511	 4% 85% 15%
1	L	511	 5% 86% 12%
1	M	511	 3% 87% 13%
1	N	511	 5% 84% 15%
1	O	511	 7% 81% 17%
1	P	511	 2% 86% 13%

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

Continued on next page...

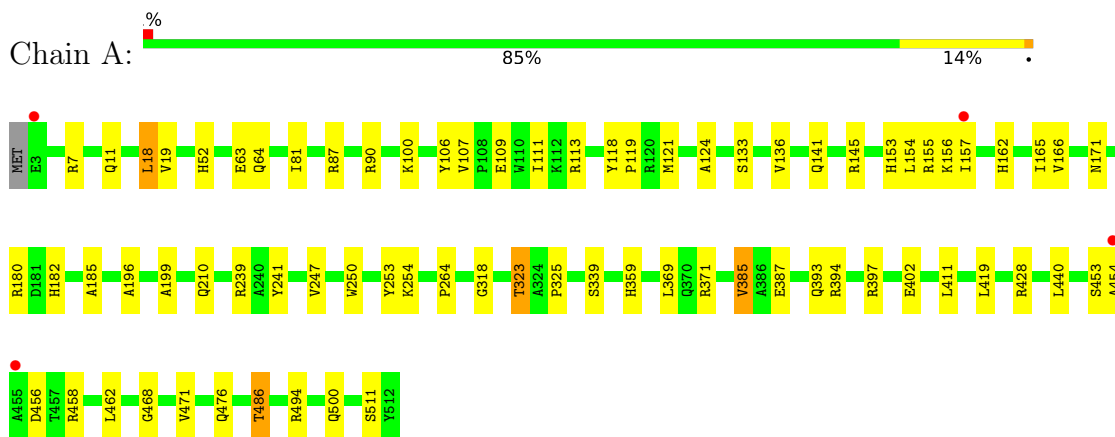
Continued from previous page...

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

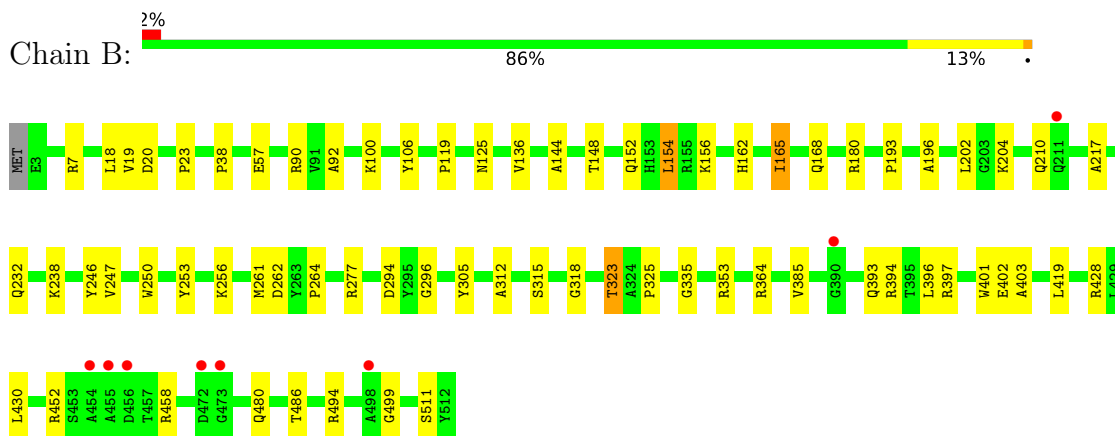
3 Residue-property plots [i](#)

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.

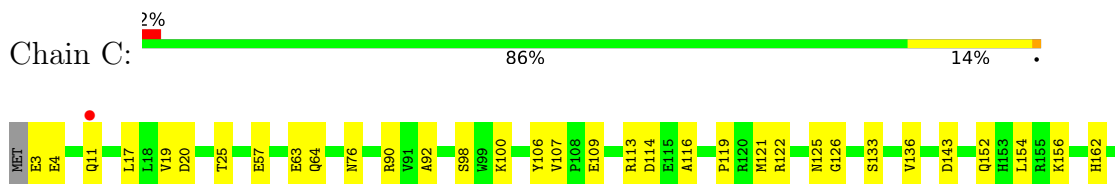
- Molecule 1: Beta-galactosidase

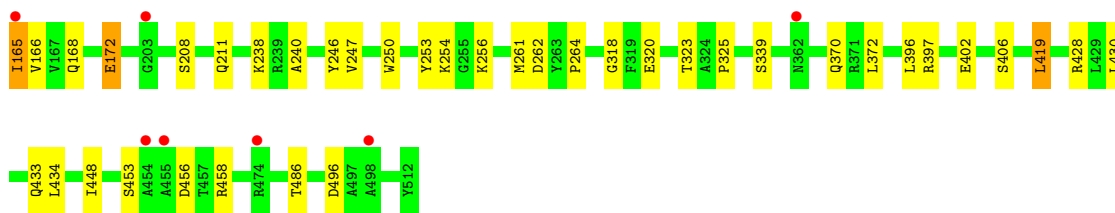


- Molecule 1: Beta-galactosidase

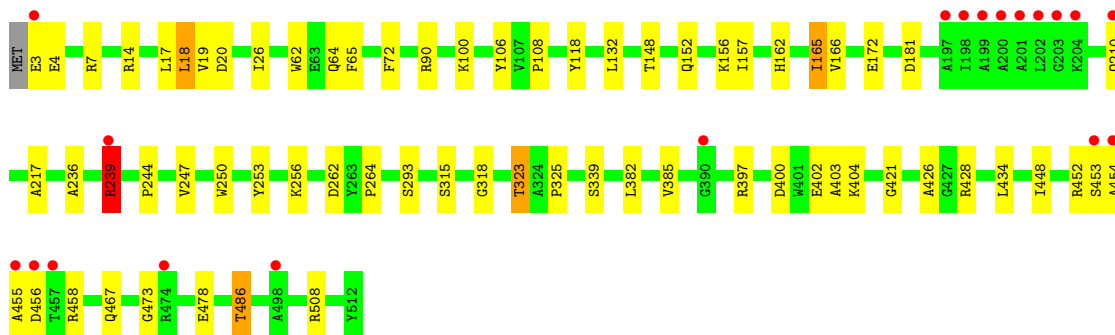
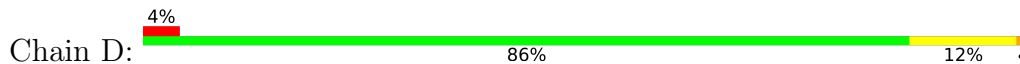


- Molecule 1: Beta-galactosidase

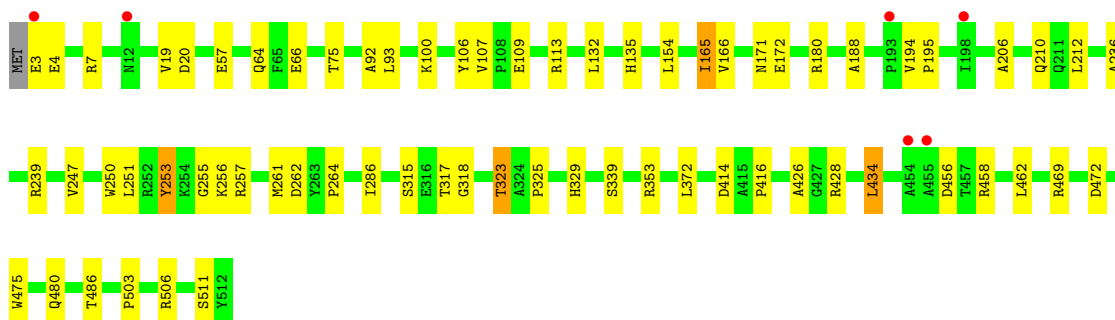
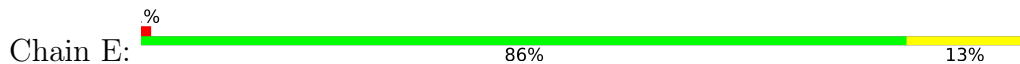




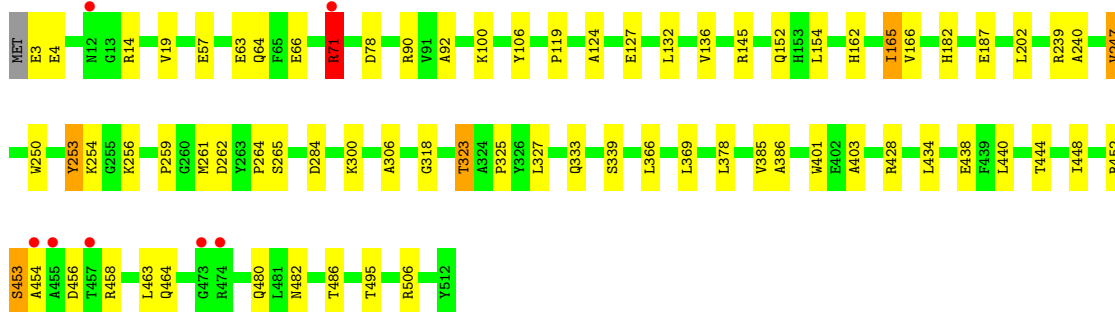
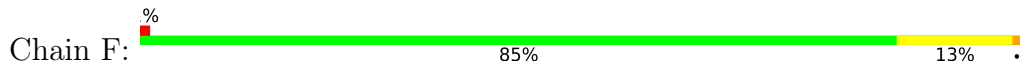
• Molecule 1: Beta-galactosidase



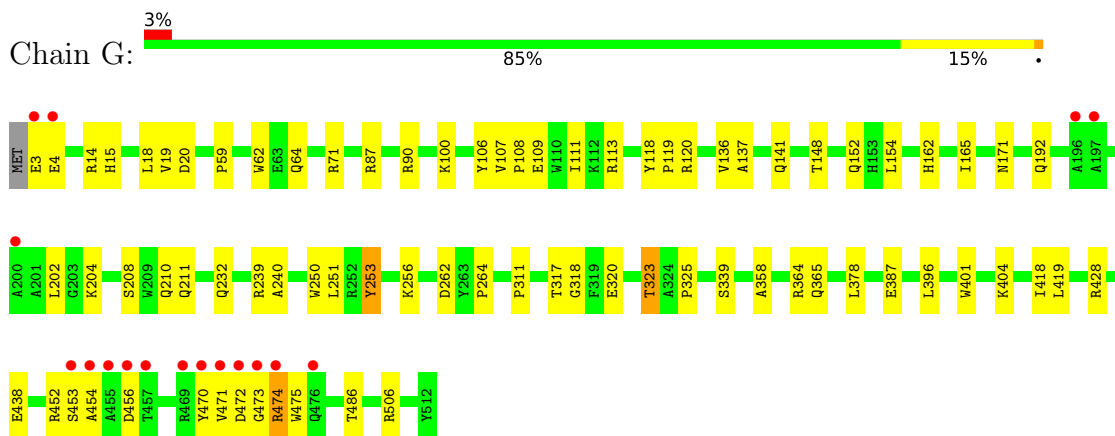
• Molecule 1: Beta-galactosidase



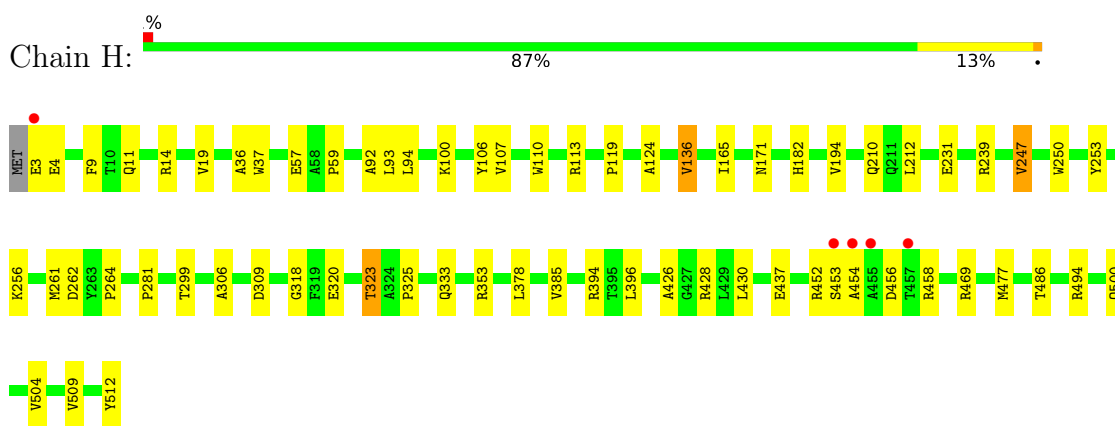
• Molecule 1: Beta-galactosidase



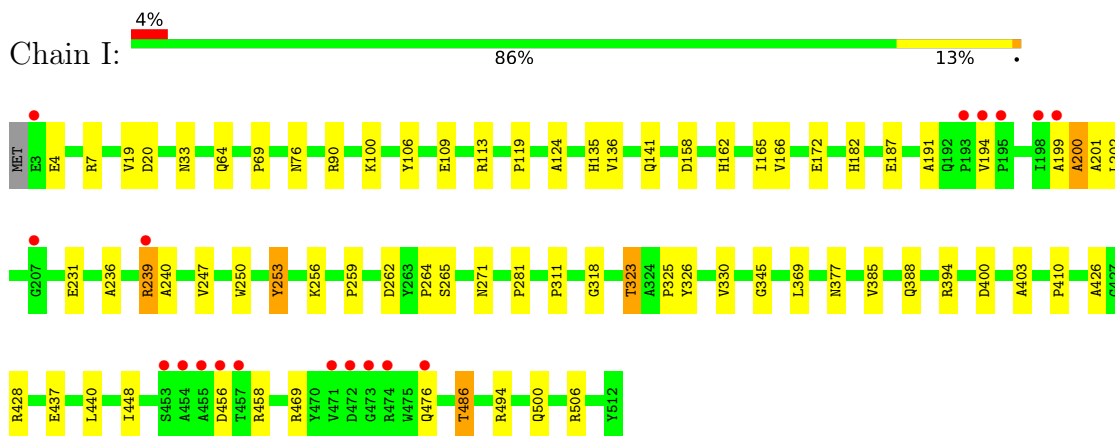
• Molecule 1: Beta-galactosidase



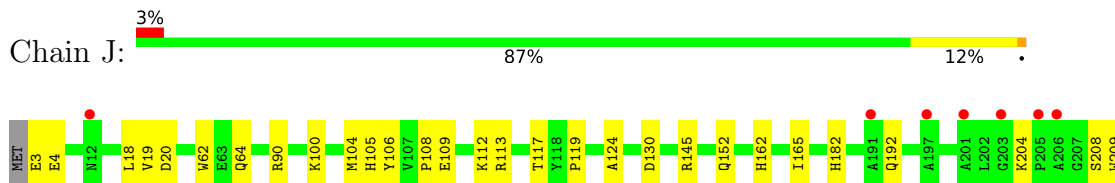
• Molecule 1: Beta-galactosidase

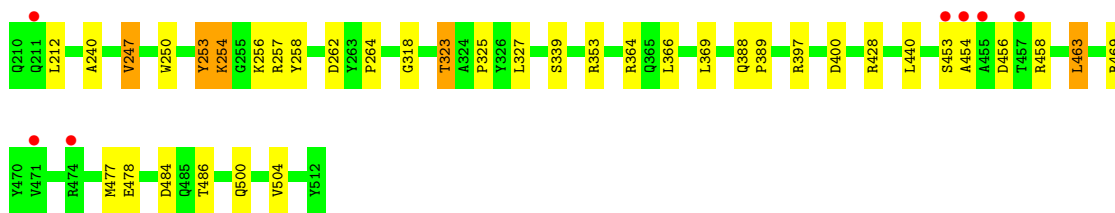


• Molecule 1: Beta-galactosidase

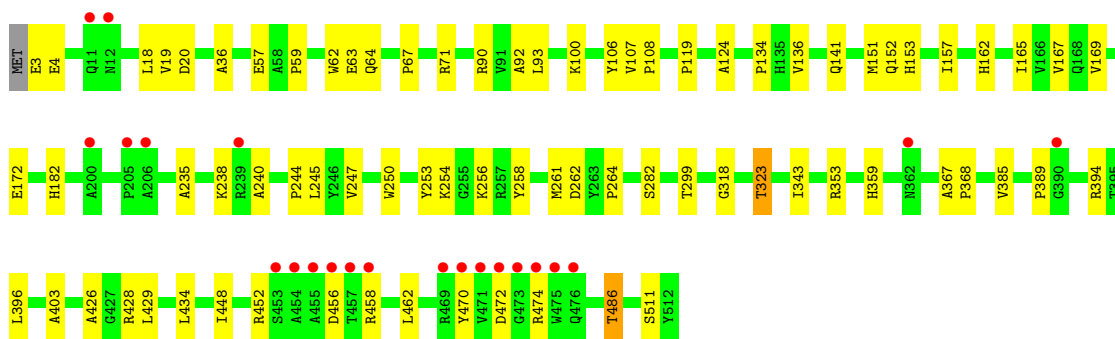
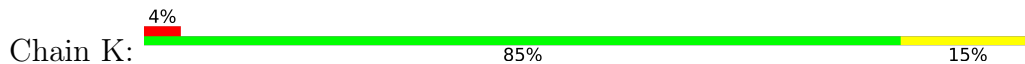


• Molecule 1: Beta-galactosidase

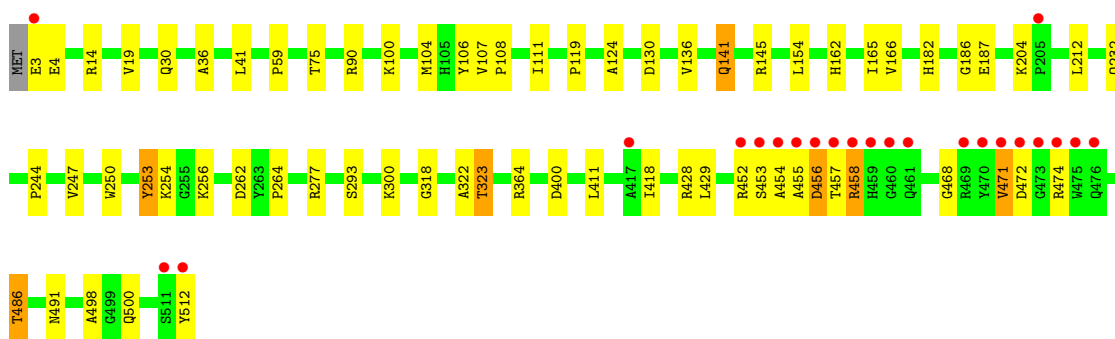
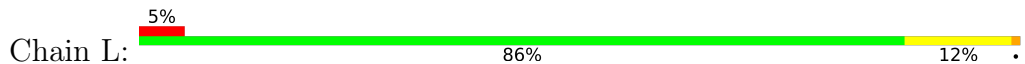




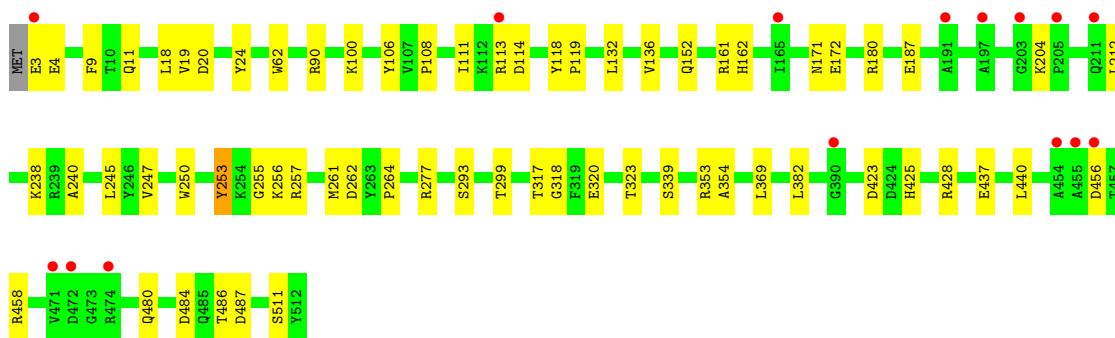
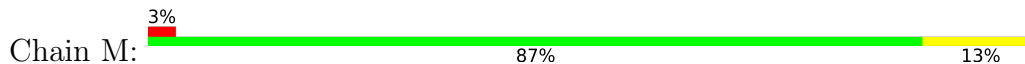
● Molecule 1: Beta-galactosidase



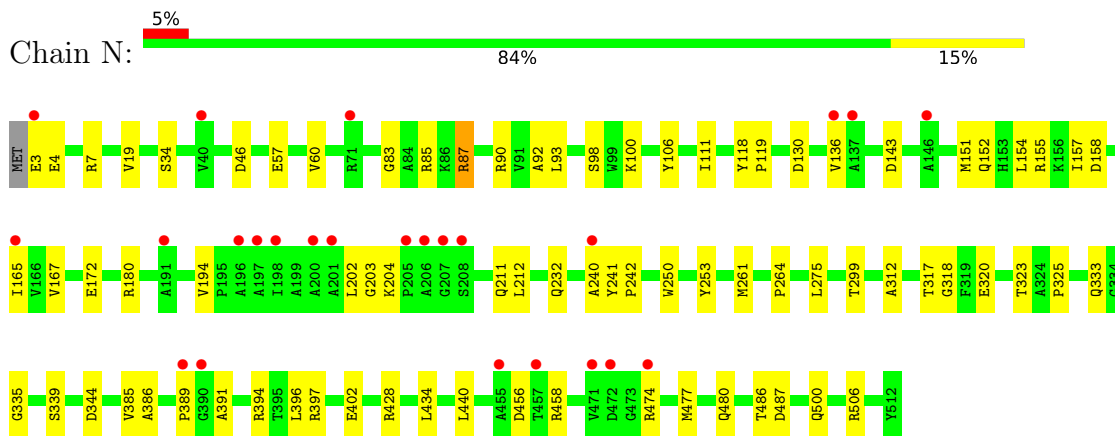
● Molecule 1: Beta-galactosidase



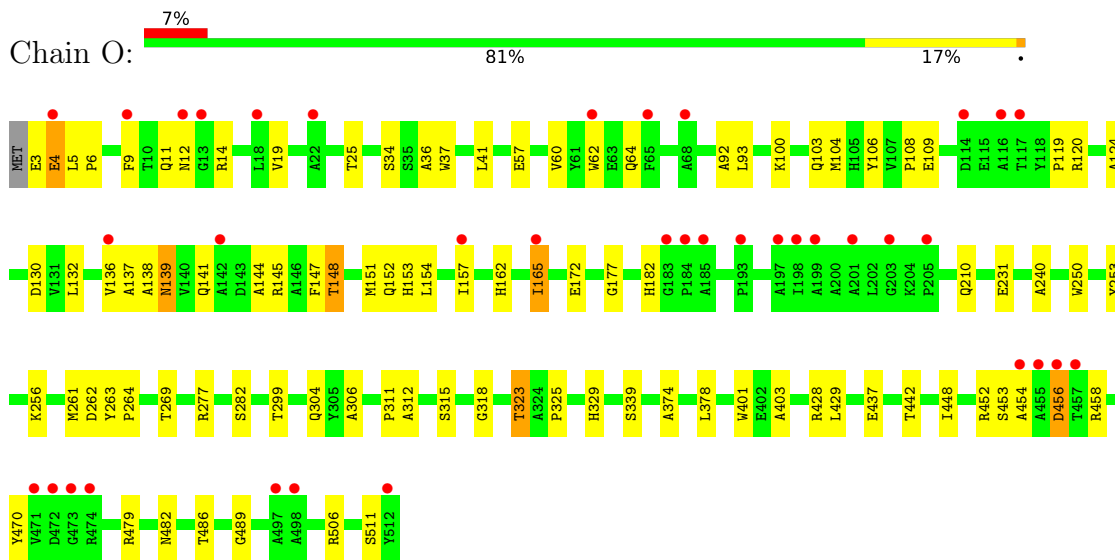
● Molecule 1: Beta-galactosidase



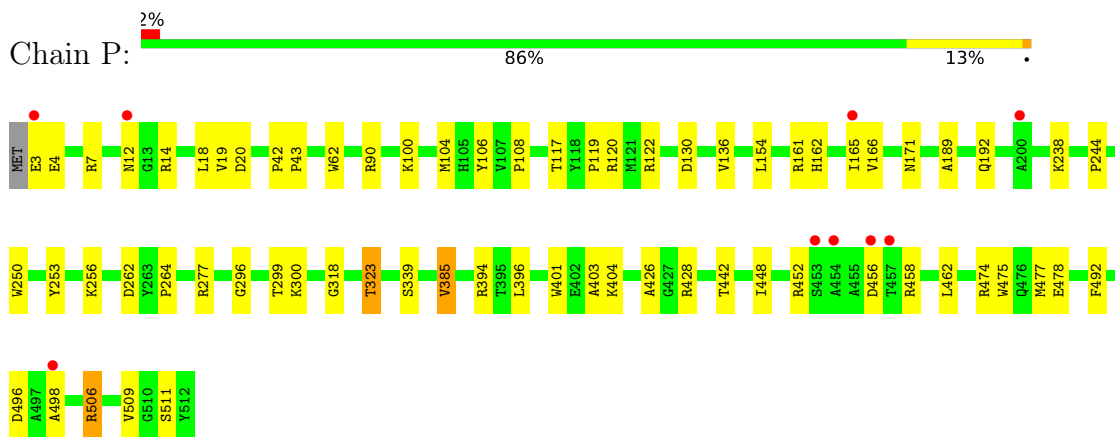
- Molecule 1: Beta-galactosidase



- 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 49.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.10-2.50) 99.4 (49.10-2.50)	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 , 0.251	Depositor DCC
R_{free} test set	16771 reflections (5.00%)	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)	0.32 , 35.3	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	0.30	0/4033	0.52	0/5508
1	B	0.25	0/4033	0.46	0/5508
1	C	0.29	1/4033 (0.0%)	0.47	0/5508
1	D	0.30	1/4033 (0.0%)	0.51	2/5508 (0.0%)
1	E	0.31	1/4033 (0.0%)	0.50	0/5508
1	F	0.29	0/4033	0.49	0/5508
1	G	0.27	0/4033	0.49	1/5508 (0.0%)
1	H	0.26	0/4033	0.47	0/5508
1	I	0.35	1/4033 (0.0%)	0.54	1/5508 (0.0%)
1	J	0.27	0/4033	0.47	0/5508
1	K	0.29	0/4033	0.49	0/5508
1	L	0.37	3/4033 (0.1%)	0.58	5/5508 (0.1%)
1	M	0.23	0/4033	0.43	0/5508
1	N	0.25	0/4033	0.45	0/5508
1	O	0.30	2/4033 (0.0%)	0.48	1/5508 (0.0%)
1	P	0.26	0/4033	0.45	0/5508
All	All	0.29	9/64528 (0.0%)	0.49	10/88128 (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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	172	GLU	C-O	8.57	1.28	1.23
1	C	172	GLU	C-O	8.40	1.27	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	172	GLU	C-O	7.94	1.27	1.23
1	L	458	ARG	CA-CB	7.54	1.66	1.53
1	O	4	GLU	CB-CG	-5.82	1.34	1.52
1	D	239	ARG	CD-NE	-5.76	1.38	1.46
1	O	139	ASN	CB-CG	-5.38	1.38	1.52
1	L	458	ARG	CB-CG	5.36	1.68	1.52
1	L	456	ASP	CB-CG	5.14	1.65	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	ARG	CB-CG-CD	-9.88	88.58	111.30
1	L	458	ARG	CD-NE-CZ	8.73	136.62	124.40
1	L	458	ARG	CA-CB-CG	8.26	130.62	114.10
1	D	239	ARG	CD-NE-CZ	-7.92	113.31	124.40
1	I	172	GLU	O-C-N	-6.39	118.59	121.53
1	L	455	ALA	CA-C-N	5.84	132.62	122.81
1	L	455	ALA	C-N-CA	5.84	132.62	122.81
1	O	4	GLU	CA-CB-CG	-5.63	102.83	114.10
1	G	474	ARG	CA-CB-CG	-5.11	103.89	114.10
1	L	456	ASP	CB-CA-C	-5.01	99.94	109.66

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
1	B	3921	0	3780	51	0
1	C	3921	0	3780	44	0
1	D	3921	0	3780	43	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3921	0	3780	47	0
1	F	3921	0	3780	55	0
1	G	3921	0	3780	56	0
1	H	3921	0	3780	46	0
1	I	3921	0	3780	72	0
1	J	3921	0	3780	51	0
1	K	3921	0	3780	55	0
1	L	3921	0	3780	75	0
1	M	3921	0	3780	42	0
1	N	3921	0	3780	58	0
1	O	3921	0	3780	69	0
1	P	3921	0	3780	49	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	9	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	11	1
All	All	65632	0	60480	836	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 (836) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:404:LYS:NZ	2:D:601:HOH:O	2.03	0.79
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
1:D:64:GLN:NE2	2:D:604:HOH:O	2.09	0.76
1:P:104:MET:HE1	1:P:120:ARG:HG2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:456:ASP:HB3	1:J:458:ARG:H	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:L:512:TYR:C	2.17	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

Continued on next page...

Continued from previous page...

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: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
1:M:480:GLN:NE2	2:M:618:HOH:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:210:GLN:CD	1:G:210:GLN:H	2.09	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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: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:D:210:GLN:CD	1:D:210:GLN:H	2.15	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

Continued on next page...

Continued from previous page...

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:F:444:THR:OG1	2:F:607:HOH:O	2.06	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: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
1:I:256:LYS:HB3	1:I:262:ASP:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:231:GLU:CD	1:H:281:PRO:HD2	2.35	0.52
1:O:144:ALA:O	1:O:148:THR:OG1	2.27	0.52
1:P:300:LYS:NZ	2:P:623:HOH:O	2.43	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:O:104:MET:HE1	1:O:120:ARG:HG2	1.93	0.51
1:B:401:TRP:CZ2	1:B:452:ARG:HD2	2.45	0.51
1:E:210:GLN:CD	1:E:210:GLN:H	2.19	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:N:154:LEU:C	2:N:619:HOH:O	2.53	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: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:B:210:GLN:H	1:B:210:GLN:CD	2.16	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:B:305:TYR:OH	2:B:606:HOH:O	2.03	0.50
1:G:251:LEU:HB2	1:G:253:TYR:CD2	2.46	0.50
1:O:138:ALA:C	2:O:602:HOH:O	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:250:TRP:CD2	1:I:264:PRO:HD3	2.47	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: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: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:K:151:MET:HE1	1:K:167:VAL:HG21	1.94	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:D:453:SER:C	1:D:455:ALA:H	2.21	0.49
1:E:66:GLU:OE1	2:E:614:HOH:O	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:239:ARG:HB3	1:L:458:ARG:HA	1.95	0.49
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:O:231:GLU:OE2	1:O:282:SER:OG	2.30	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:D:172:GLU:CD	1:D:250:TRP:HB2	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:P:477:MET:HE3	1:P:477:MET:HB3	1.85	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:H:477:MET:HE3	1:H:477:MET:HB3	1.87	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:118:TYR:OH	2:D:606:HOH:O	2.19	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:J:104:MET:HG2	1:J:130:ASP:C	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:508:ARG:HH22	1:J:109:GLU:CD	2.25	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:F:327:LEU:HD21	1:F:366:LEU:HD12	1.98	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: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:A:323:THR:HG22	1:A:359:HIS:NE2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:477:MET:HE3	1:J:478:GLU:C	2.43	0.44
1:N:151:MET:HE1	1:N:167:VAL:HG21	1.99	0.44
1:O:141:GLN:O	1:O:145:ARG:HB2	2.18	0.44
1:O:172:GLU:CD	1:O:250:TRP:HB2	2.42	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: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:A:210:GLN:H	1:A:210:GLN:CD	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:325:PRO:HA	1:I:428:ARG:HD2	1.99	0.43
1:J:105:HIS:O	1:J:112:LYS:NZ	2.47	0.43
1:O:5:LEU:HD12	1:O:6:PRO:HD2	2.01	0.43
1:O:261:MET:HE3	1:O:261:MET:HB2	1.85	0.43
1:E:256:LYS:HB3	1:E:262:ASP:HB3	2.00	0.43
1:K:67:PRO:HD2	1:K:71:ARG:O	2.19	0.43
1:K:172:GLU:CD	1:K:250:TRP:HB2	2.44	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:O:104:MET:HE3	1:O:130:ASP:HA	1.99	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:231:GLU:CD	1:I:281:PRO:HD2	2.44	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:P:475:TRP:CG	1:P:506:ARG:HH21	2.37	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:H:210:GLN:H	1:H:210:GLN:CD	2.27	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:P:104:MET:HG2	1:P:130:ASP:C	2.44	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:SER:O	1:J:209:TRP:C	2.62	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:C:261:MET:SD	1:K:261:MET:HE1	2.59	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
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:C:172:GLU:CD	1:C:250:TRP:HB2	2.45	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:J:258:TYR:CZ	1:N:261:MET:HE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:P:442:THR:HA	1:P:492:PHE:CE2	2.55	0.41
1:M:172:GLU:CD	1:M:250:TRP:HB2	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:512:TYR:C	1:L:512:TYR:CD1	2.99	0.41
1:N:111:ILE:HG23	1:N:118:TYR:CG	2.56	0.41
1:N:477:MET:HE3	1:N:477:MET:HB3	1.78	0.41
1:P:100:LYS:HD2	1:P:171:ASN:ND2	2.36	0.41
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:N:172:GLU:CD	1:N:250:TRP:HB2	2.46	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:L:14:ARG:HH11	1:L:14:ARG:HG2	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	63
1	E	508/511 (99%)	491 (97%)	16 (3%)	1 (0%)	43	63
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%)	30	49
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
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%)	372 (98%)	9 (2%)	43	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	381/382 (100%)	372 (98%)	9 (2%)	43	70
1	C	381/382 (100%)	368 (97%)	13 (3%)	32	60
1	D	381/382 (100%)	367 (96%)	14 (4%)	30	57
1	E	381/382 (100%)	370 (97%)	11 (3%)	37	65
1	F	381/382 (100%)	371 (97%)	10 (3%)	40	68
1	G	381/382 (100%)	372 (98%)	9 (2%)	43	70
1	H	381/382 (100%)	372 (98%)	9 (2%)	43	70
1	I	381/382 (100%)	376 (99%)	5 (1%)	61	82
1	J	381/382 (100%)	372 (98%)	9 (2%)	43	70
1	K	381/382 (100%)	371 (97%)	10 (3%)	40	68
1	L	381/382 (100%)	371 (97%)	10 (3%)	40	68
1	M	381/382 (100%)	372 (98%)	9 (2%)	43	70
1	N	381/382 (100%)	373 (98%)	8 (2%)	47	74
1	O	381/382 (100%)	369 (97%)	12 (3%)	35	62
1	P	381/382 (100%)	370 (97%)	11 (3%)	37	65
All	All	6096/6112 (100%)	5938 (97%)	158 (3%)	40	68

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	107	VAL
1	A	141	GLN
1	A	247	VAL
1	A	323	THR
1	A	339	SER
1	A	385	VAL
1	A	462	LEU
1	A	486	THR
1	B	154	LEU
1	B	165	ILE
1	B	180	ARG
1	B	238	LYS
1	B	253	TYR
1	B	315	SER
1	B	323	THR
1	B	430	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	486	THR
1	C	107	VAL
1	C	154	LEU
1	C	156	LYS
1	C	165	ILE
1	C	238	LYS
1	C	247	VAL
1	C	339	SER
1	C	396	LEU
1	C	419	LEU
1	C	430	LEU
1	C	448	ILE
1	C	453	SER
1	C	486	THR
1	D	18	LEU
1	D	157	ILE
1	D	165	ILE
1	D	239	ARG
1	D	247	VAL
1	D	253	TYR
1	D	293	SER
1	D	315	SER
1	D	323	THR
1	D	339	SER
1	D	382	LEU
1	D	385	VAL
1	D	434	LEU
1	D	486	THR
1	E	7	ARG
1	E	107	VAL
1	E	165	ILE
1	E	253	TYR
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	F	71	ARG
1	F	154	LEU
1	F	165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	247	VAL
1	F	253	TYR
1	F	323	THR
1	F	339	SER
1	F	385	VAL
1	F	453	SER
1	F	486	THR
1	G	18	LEU
1	G	107	VAL
1	G	148	THR
1	G	253	TYR
1	G	317	THR
1	G	323	THR
1	G	339	SER
1	G	396	LEU
1	G	486	THR
1	H	107	VAL
1	H	136	VAL
1	H	247	VAL
1	H	253	TYR
1	H	299	THR
1	H	323	THR
1	H	396	LEU
1	H	430	LEU
1	H	486	THR
1	I	239	ARG
1	I	253	TYR
1	I	323	THR
1	I	486	THR
1	I	500	GLN
1	J	18	LEU
1	J	247	VAL
1	J	253	TYR
1	J	254	LYS
1	J	323	THR
1	J	339	SER
1	J	397	ARG
1	J	463	LEU
1	J	486	THR
1	K	18	LEU
1	K	107	VAL
1	K	247	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	299	THR
1	K	323	THR
1	K	396	LEU
1	K	429	LEU
1	K	434	LEU
1	K	462	LEU
1	K	486	THR
1	L	141	GLN
1	L	154	LEU
1	L	247	VAL
1	L	253	TYR
1	L	293	SER
1	L	323	THR
1	L	429	LEU
1	L	471	VAL
1	L	474	ARG
1	L	486	THR
1	M	132	LEU
1	M	161	ARG
1	M	247	VAL
1	M	253	TYR
1	M	293	SER
1	M	299	THR
1	M	317	THR
1	M	339	SER
1	M	486	THR
1	N	87	ARG
1	N	211	GLN
1	N	253	TYR
1	N	299	THR
1	N	317	THR
1	N	339	SER
1	N	396	LEU
1	N	486	THR
1	O	132	LEU
1	O	148	THR
1	O	154	LEU
1	O	165	ILE
1	O	253	TYR
1	O	299	THR
1	O	315	SER
1	O	323	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	339	SER
1	O	442	THR
1	O	456	ASP
1	O	486	THR
1	P	7	ARG
1	P	18	LEU
1	P	154	LEU
1	P	238	LYS
1	P	253	TYR
1	P	299	THR
1	P	323	THR
1	P	339	SER
1	P	385	VAL
1	P	396	LEU
1	P	506	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	103	GLN
1	A	141	GLN
1	A	222	ASN
1	A	333	GLN
1	A	383	GLN
1	A	467	GLN
1	B	467	GLN
1	C	52	HIS
1	C	76	ASN
1	C	103	GLN
1	C	168	GLN
1	C	171	ASN
1	C	182	HIS
1	C	211	GLN
1	C	222	ASN
1	C	346	ASN
1	C	352	ASN
1	C	383	GLN
1	C	464	GLN
1	D	171	ASN
1	D	467	GLN
1	E	52	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	135	HIS
1	E	168	GLN
1	E	222	ASN
1	E	329	HIS
1	E	346	ASN
1	E	393	GLN
1	E	467	GLN
1	F	52	HIS
1	F	346	ASN
1	F	393	GLN
1	F	459	HIS
1	F	461	GLN
1	F	467	GLN
1	G	141	GLN
1	G	211	GLN
1	G	222	ASN
1	G	346	ASN
1	G	461	GLN
1	G	467	GLN
1	G	485	GLN
1	G	500	GLN
1	H	103	GLN
1	H	346	ASN
1	H	433	GLN
1	H	467	GLN
1	I	101	ASN
1	I	135	HIS
1	I	168	GLN
1	I	224	HIS
1	I	329	HIS
1	I	352	ASN
1	I	388	GLN
1	J	168	GLN
1	J	210	GLN
1	J	346	ASN
1	J	393	GLN
1	K	135	HIS
1	K	168	GLN
1	K	171	ASN
1	K	192	GLN
1	K	333	GLN
1	K	346	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	464	GLN
1	K	480	GLN
1	L	52	HIS
1	L	222	ASN
1	L	224	HIS
1	L	232	GLN
1	L	333	GLN
1	L	346	ASN
1	L	461	GLN
1	L	464	GLN
1	L	500	GLN
1	M	383	GLN
1	M	467	GLN
1	N	11	GLN
1	N	103	GLN
1	N	125	ASN
1	N	182	HIS
1	N	210	GLN
1	N	211	GLN
1	N	375	GLN
1	N	476	GLN
1	N	500	GLN
1	O	12	ASN
1	O	103	GLN
1	O	139	ASN
1	O	304	GLN
1	O	329	HIS
1	O	333	GLN
1	O	346	ASN
1	P	12	ASN
1	P	103	GLN
1	P	141	GLN
1	P	333	GLN
1	P	346	ASN
1	P	393	GLN
1	P	467	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data 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%)	-0.20	4 (0%) 82 80	15, 25, 40, 66	0
1	B	510/511 (99%)	0.14	8 (1%) 70 67	21, 31, 48, 68	0
1	C	510/511 (99%)	-0.04	8 (1%) 70 67	19, 28, 43, 69	0
1	D	510/511 (99%)	0.04	19 (3%) 45 40	19, 27, 46, 71	0
1	E	510/511 (99%)	-0.16	6 (1%) 76 73	18, 25, 43, 64	0
1	F	510/511 (99%)	-0.01	7 (1%) 73 70	16, 27, 46, 70	0
1	G	510/511 (99%)	0.00	17 (3%) 49 45	17, 26, 45, 72	0
1	H	510/511 (99%)	0.03	5 (0%) 79 76	20, 29, 43, 68	0
1	I	510/511 (99%)	0.06	18 (3%) 47 42	17, 29, 47, 72	0
1	J	510/511 (99%)	0.06	14 (2%) 56 51	19, 29, 49, 69	0
1	K	510/511 (99%)	0.09	22 (4%) 40 35	19, 30, 45, 74	0
1	L	510/511 (99%)	0.15	23 (4%) 38 33	18, 28, 50, 78	0
1	M	510/511 (99%)	0.28	15 (2%) 53 49	25, 37, 55, 76	0
1	N	510/511 (99%)	0.65	25 (4%) 35 31	25, 42, 59, 84	0
1	O	510/511 (99%)	0.75	37 (7%) 21 19	27, 39, 56, 78	0
1	P	510/511 (99%)	-0.01	9 (1%) 67 64	19, 29, 46, 69	0
All	All	8160/8176 (99%)	0.11	237 (2%) 53 49	15, 30, 50, 84	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	471	VAL	11.1
1	K	471	VAL	8.5
1	L	476	GLN	8.1
1	K	472	ASP	7.8
1	L	457	THR	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	512	TYR	7.5
1	L	472	ASP	7.4
1	L	473	GLY	7.0
1	L	474	ARG	6.5
1	D	454	ALA	5.9
1	L	475	TRP	5.8
1	G	473	GLY	5.8
1	K	474	ARG	5.6
1	D	203	GLY	5.3
1	K	473	GLY	5.3
1	D	455	ALA	5.3
1	L	469	ARG	5.2
1	G	474	ARG	5.2
1	L	511	SER	5.2
1	K	475	TRP	5.2
1	D	457	THR	5.2
1	K	469	ARG	5.2
1	L	470	TYR	5.2
1	F	455	ALA	5.1
1	L	458	ARG	4.9
1	I	472	ASP	4.9
1	I	476	GLN	4.9
1	L	453	SER	4.9
1	F	454	ALA	4.8
1	L	459	HIS	4.8
1	K	470	TYR	4.7
1	L	456	ASP	4.6
1	C	454	ALA	4.6
1	G	471	VAL	4.5
1	G	472	ASP	4.5
1	I	471	VAL	4.4
1	L	455	ALA	4.4
1	H	455	ALA	4.3
1	L	454	ALA	4.2
1	H	454	ALA	3.9
1	K	456	ASP	3.9
1	I	454	ALA	3.9
1	G	454	ALA	3.9
1	A	157	ILE	3.9
1	I	239	ARG	3.8
1	F	71	ARG	3.7
1	N	3	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	202	LEU	3.7
1	J	454	ALA	3.7
1	N	206	ALA	3.7
1	G	455	ALA	3.6
1	O	455	ALA	3.6
1	N	137	ALA	3.5
1	D	453	SER	3.5
1	N	201	ALA	3.5
1	D	201	ALA	3.5
1	I	193	PRO	3.5
1	K	476	GLN	3.4
1	I	453	SER	3.4
1	F	457	THR	3.4
1	D	204	LYS	3.3
1	G	457	THR	3.3
1	L	460	GLY	3.3
1	D	200	ALA	3.3
1	I	455	ALA	3.3
1	B	472	ASP	3.3
1	O	498	ALA	3.3
1	M	454	ALA	3.2
1	J	453	SER	3.2
1	D	239	ARG	3.2
1	N	455	ALA	3.1
1	I	456	ASP	3.1
1	O	457	THR	3.1
1	N	136	VAL	3.1
1	I	457	THR	3.1
1	J	457	THR	3.1
1	I	199	ALA	3.1
1	D	197	ALA	3.1
1	O	473	GLY	3.1
1	J	455	ALA	3.0
1	K	455	ALA	3.0
1	O	184	PRO	3.0
1	N	474	ARG	3.0
1	N	200	ALA	3.0
1	P	454	ALA	3.0
1	N	197	ALA	3.0
1	M	390	GLY	3.0
1	D	498	ALA	2.9
1	M	455	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	12	ASN	2.9
1	E	454	ALA	2.9
1	P	498	ALA	2.9
1	G	456	ASP	2.9
1	J	211	GLN	2.9
1	O	18	LEU	2.9
1	J	206	ALA	2.8
1	O	62	TRP	2.8
1	N	205	PRO	2.8
1	D	3	GLU	2.8
1	G	453	SER	2.8
1	K	453	SER	2.8
1	K	205	PRO	2.8
1	H	457	THR	2.8
1	O	198	ILE	2.7
1	H	453	SER	2.7
1	D	199	ALA	2.7
1	M	197	ALA	2.7
1	N	457	THR	2.7
1	O	203	GLY	2.7
1	O	197	ALA	2.7
1	N	390	GLY	2.7
1	O	13	GLY	2.7
1	M	472	ASP	2.7
1	G	3	GLU	2.7
1	J	201	ALA	2.7
1	P	3	GLU	2.7
1	G	476	GLN	2.7
1	O	454	ALA	2.6
1	N	471	VAL	2.6
1	K	206	ALA	2.6
1	K	457	THR	2.6
1	O	68	ALA	2.6
1	M	3	GLU	2.6
1	A	455	ALA	2.6
1	B	455	ALA	2.6
1	O	199	ALA	2.6
1	D	390	GLY	2.6
1	D	474	ARG	2.6
1	I	195	PRO	2.6
1	P	456	ASP	2.6
1	B	454	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	11	GLN	2.5
1	O	12	ASN	2.5
1	C	455	ALA	2.5
1	B	211	GLN	2.5
1	O	117	THR	2.5
1	C	498	ALA	2.5
1	E	455	ALA	2.5
1	O	201	ALA	2.5
1	E	193	PRO	2.5
1	I	194	VAL	2.5
1	C	474	ARG	2.5
1	K	454	ALA	2.5
1	M	205	PRO	2.4
1	O	4	GLU	2.4
1	M	471	VAL	2.4
1	P	453	SER	2.4
1	G	469	ARG	2.4
1	N	196	ALA	2.4
1	N	207	GLY	2.4
1	B	456	ASP	2.4
1	O	9	PHE	2.4
1	O	471	VAL	2.4
1	F	12	ASN	2.4
1	O	497	ALA	2.4
1	I	3	GLU	2.4
1	L	461	GLN	2.4
1	O	136	VAL	2.4
1	G	196	ALA	2.4
1	O	116	ALA	2.4
1	B	390	GLY	2.3
1	C	165	ILE	2.3
1	P	165	ILE	2.3
1	G	470	TYR	2.3
1	P	457	THR	2.3
1	N	208	SER	2.3
1	P	12	ASN	2.3
1	J	474	ARG	2.3
1	D	456	ASP	2.3
1	L	205	PRO	2.3
1	K	390	GLY	2.3
1	B	498	ALA	2.2
1	J	197	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	11	GLN	2.2
1	M	211	GLN	2.2
1	N	165	ILE	2.2
1	F	474	ARG	2.2
1	I	474	ARG	2.2
1	O	142	ALA	2.2
1	O	185	ALA	2.2
1	M	203	GLY	2.2
1	M	456	ASP	2.2
1	O	456	ASP	2.2
1	G	4	GLU	2.2
1	N	71	ARG	2.2
1	J	471	VAL	2.2
1	N	389	PRO	2.2
1	K	200	ALA	2.2
1	K	362	ASN	2.2
1	O	183	GLY	2.2
1	D	198	ILE	2.2
1	N	198	ILE	2.2
1	N	472	ASP	2.2
1	A	454	ALA	2.2
1	N	240	ALA	2.2
1	P	200	ALA	2.2
1	E	3	GLU	2.2
1	J	205	PRO	2.2
1	N	146	ALA	2.1
1	N	191	ALA	2.1
1	F	473	GLY	2.1
1	O	165	ILE	2.1
1	M	474	ARG	2.1
1	O	474	ARG	2.1
1	O	157	ILE	2.1
1	K	239	ARG	2.1
1	O	193	PRO	2.1
1	G	200	ALA	2.1
1	J	12	ASN	2.1
1	J	203	GLY	2.1
1	M	165	ILE	2.1
1	O	512	TYR	2.1
1	L	417	ALA	2.1
1	O	22	ALA	2.1
1	K	12	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	473	GLY	2.1
1	I	207	GLY	2.1
1	M	113	ARG	2.1
1	A	3	GLU	2.1
1	E	198	ILE	2.1
1	I	198	ILE	2.1
1	O	114	ASP	2.1
1	O	472	ASP	2.1
1	D	210	GLN	2.0
1	N	40	VAL	2.0
1	O	65	PHE	2.0
1	G	197	ALA	2.0
1	M	191	ALA	2.0
1	I	473	GLY	2.0
1	O	205	PRO	2.0
1	K	458	ARG	2.0
1	L	452	ARG	2.0
1	J	191	ALA	2.0
1	H	3	GLU	2.0
1	L	3	GLU	2.0
1	C	203	GLY	2.0
1	C	362	ASN	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.