Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 06:00 am GMT

PDB ID	:	1QOX
Title	:	Beta-glucosidase from Bacillus circulans sp. alkalophilus
Authors	:	Hakulinen, N.; Rouvinen, J.
Deposited on	:	1999-11-24
Resolution	:	2.70 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:

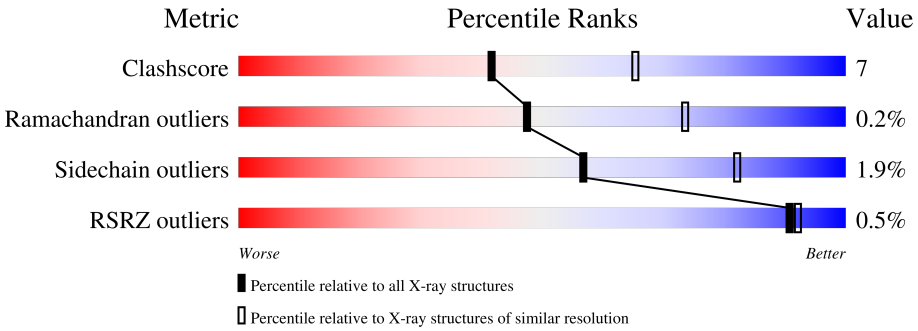
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.70 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.



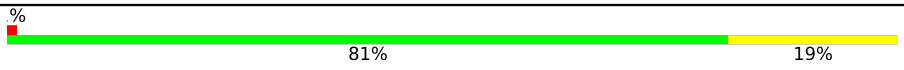
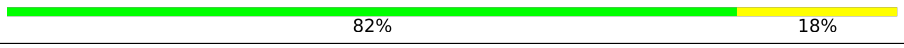
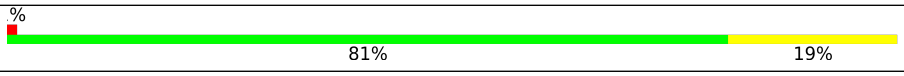
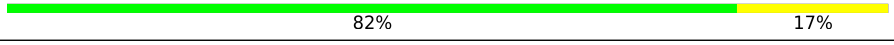
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	449	81% 19%
1	B	449	81% 19%
1	C	449	80% 20%
1	D	449	82% 18%
1	E	449	82% 18%
1	F	449	81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	449	
1	H	449	
1	I	449	
1	J	449	
1	K	449	
1	L	449	
1	M	449	
1	N	449	
1	O	449	
1	P	449	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 60304 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	B	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	C	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	D	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	E	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	F	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	G	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	H	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	I	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	J	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	K	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	L	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	M	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	N	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	O	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			
1	P	449	Total	C	N	O	S	0	0	0
			3616	2323	602	672	19			

- Molecule 2 is water.

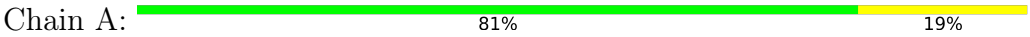
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	156	Total O 156 156	0	0
2	B	151	Total O 151 151	0	0
2	C	155	Total O 155 155	0	0
2	D	153	Total O 153 153	0	0
2	E	153	Total O 153 153	0	0
2	F	153	Total O 153 153	0	0
2	G	156	Total O 156 156	0	0
2	H	153	Total O 153 153	0	0
2	I	150	Total O 150 150	0	0
2	J	153	Total O 153 153	0	0
2	K	150	Total O 150 150	0	0
2	L	152	Total O 152 152	0	0
2	M	152	Total O 152 152	0	0
2	N	154	Total O 154 154	0	0
2	O	153	Total O 153 153	0	0
2	P	154	Total O 154 154	0	0

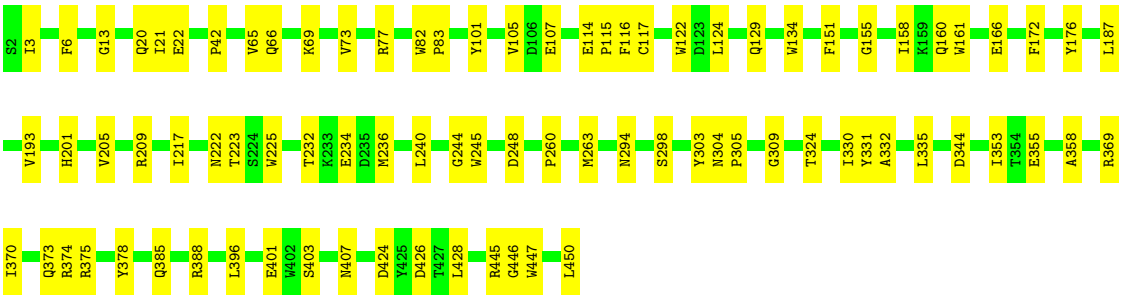
3 Residue-property plots (i)

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

• Molecule 1: BETA-GLUCOSIDASE

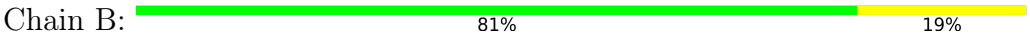
Chain A:

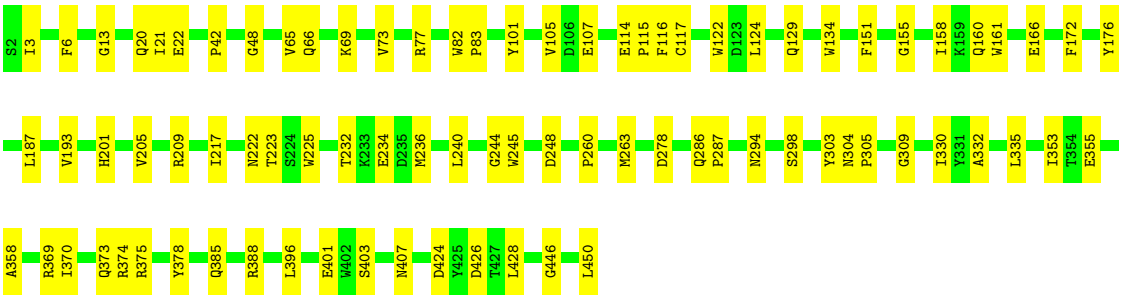




• Molecule 1: BETA-GLUCOSIDASE

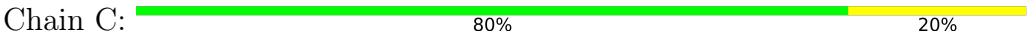
Chain B:

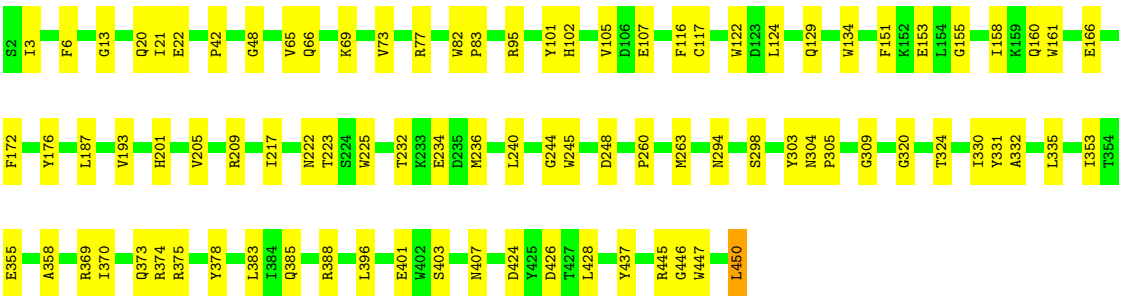




• Molecule 1: BETA-GLUCOSIDASE

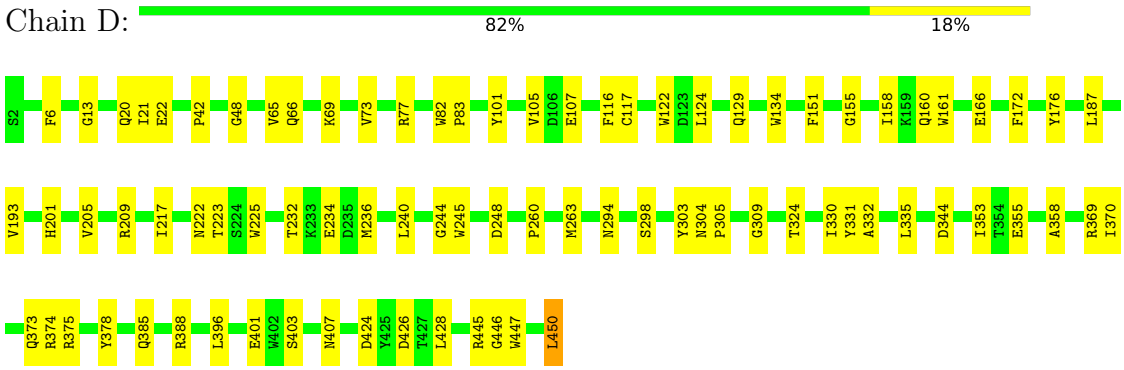
Chain C:





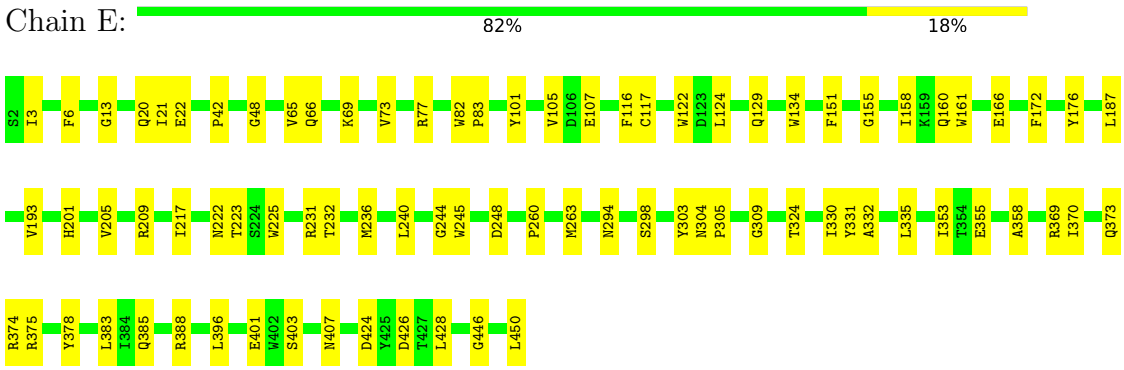
• Molecule 1: BETA-GLUCOSIDASE

Chain D:



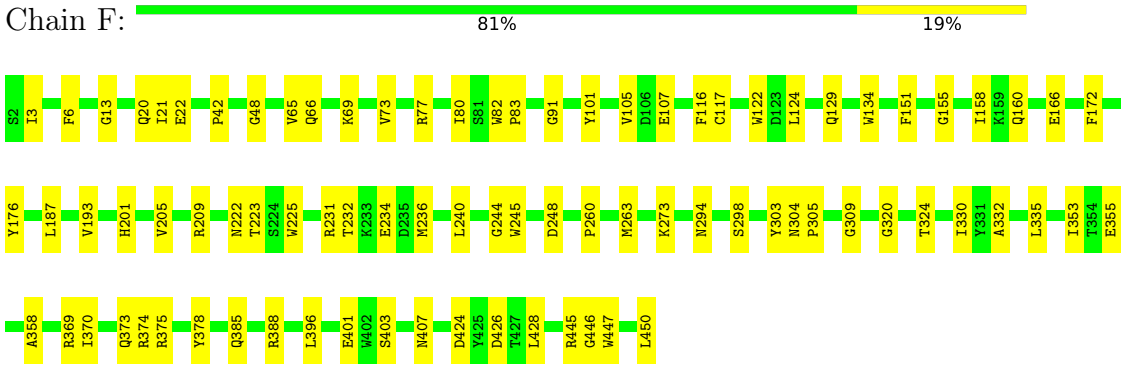
• Molecule 1: BETA-GLUCOSIDASE

Chain E:



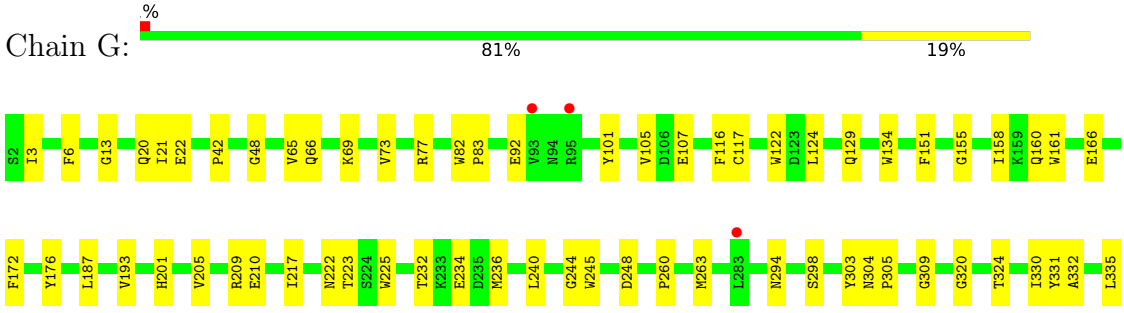
• Molecule 1: BETA-GLUCOSIDASE

Chain F:



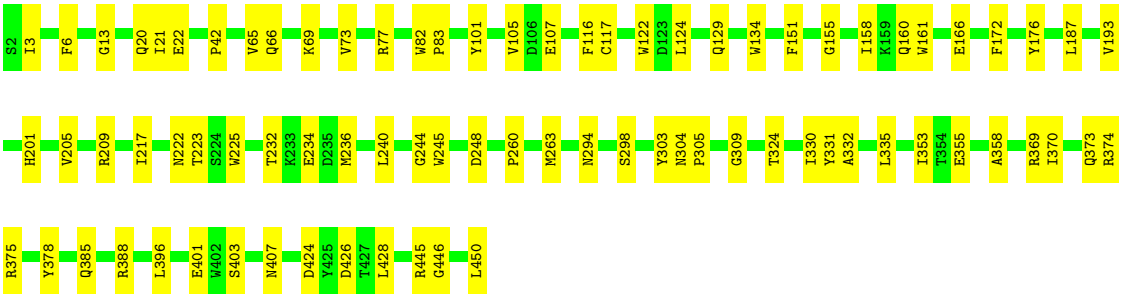
• Molecule 1: BETA-GLUCOSIDASE

Chain G:



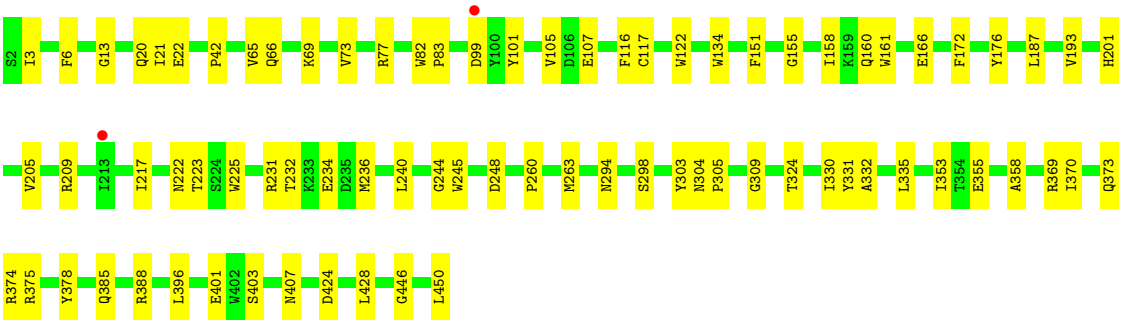
• Molecule 1: BETA-GLUCOSIDASE

Chain H:



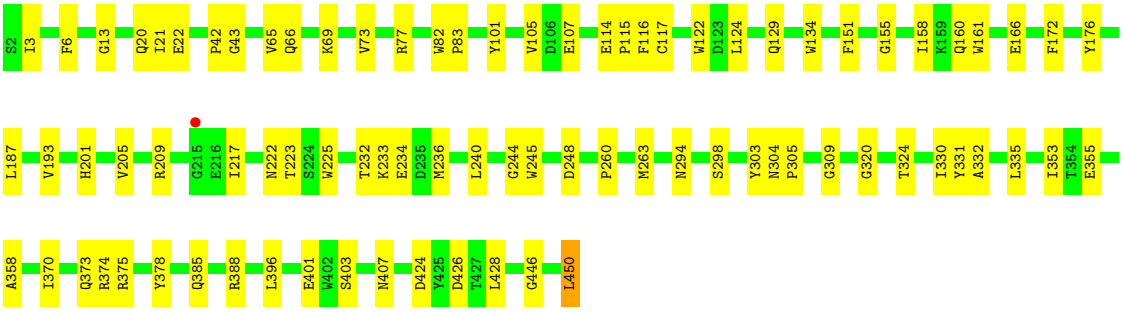
• Molecule 1: BETA-GLUCOSIDASE

Chain I:



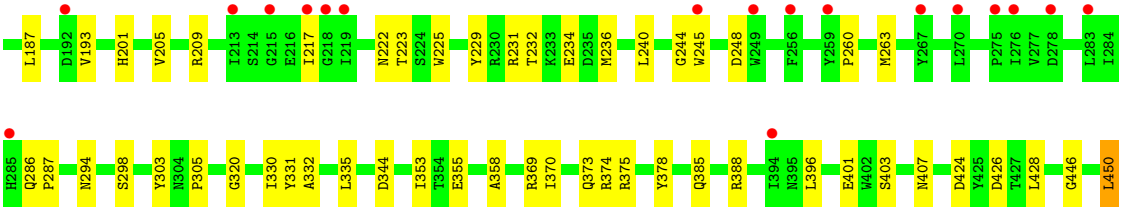
• Molecule 1: BETA-GLUCOSIDASE

Chain J:



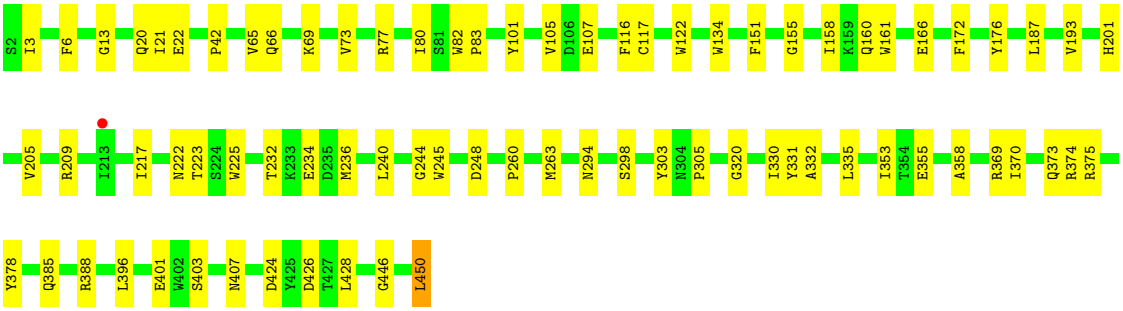
• Molecule 1: BETA-GLUCOSIDASE

Chain K:



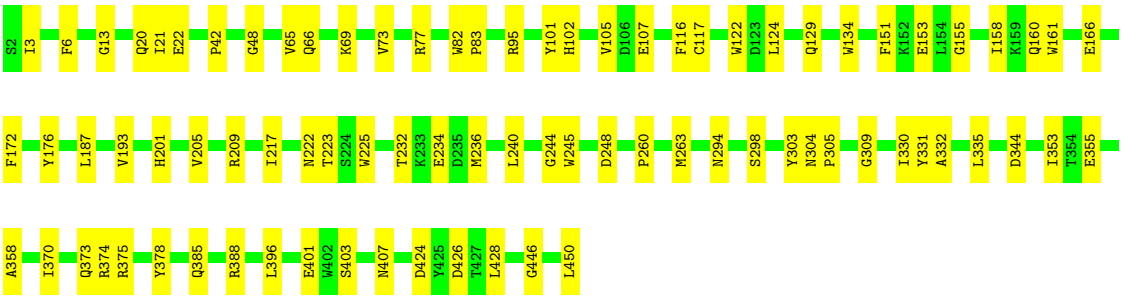
• Molecule 1: BETA-GLUCOSIDASE

Chain L:



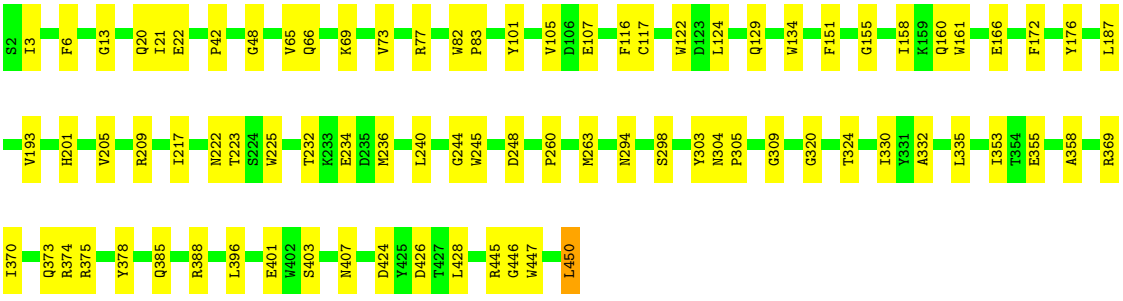
• Molecule 1: BETA-GLUCOSIDASE

Chain M:



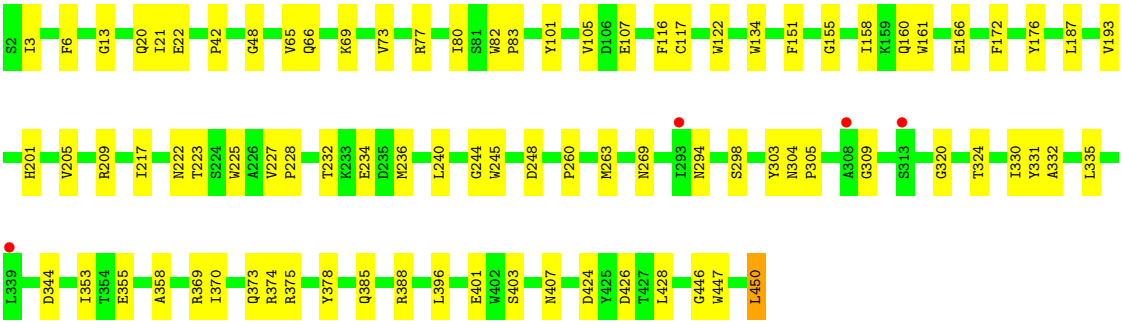
• Molecule 1: BETA-GLUCOSIDASE

Chain N:



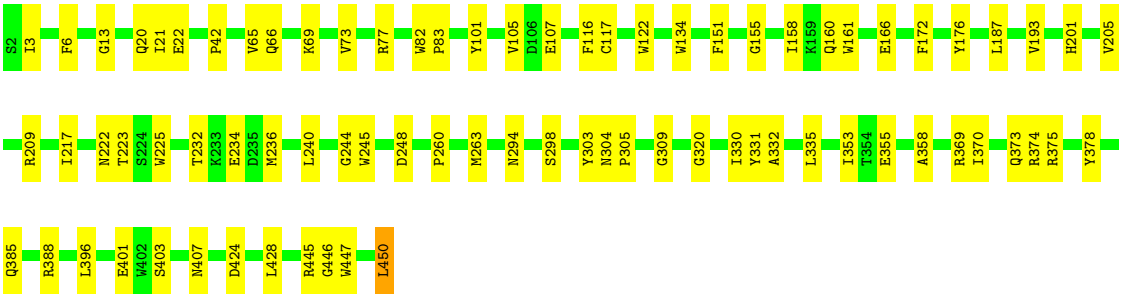
• Molecule 1: BETA-GLUCOSIDASE

Chain O:



• Molecule 1: BETA-GLUCOSIDASE

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	116.40Å 122.30Å 163.20Å 89.30° 74.30° 68.00°	Depositor
Resolution (Å)	10.00 – 2.70 97.14 – 2.69	Depositor EDS
% Data completeness (in resolution range)	84.0 (10.00-2.70) 77.5 (97.14-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , (Not available) 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	60304	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/3725	0.52	0/5061
1	B	0.26	0/3725	0.52	0/5061
1	C	0.26	0/3725	0.52	0/5061
1	D	0.26	0/3725	0.52	0/5061
1	E	0.26	0/3725	0.52	0/5061
1	F	0.26	0/3725	0.52	0/5061
1	G	0.26	0/3725	0.52	0/5061
1	H	0.26	0/3725	0.52	0/5061
1	I	0.26	0/3725	0.52	0/5061
1	J	0.26	0/3725	0.52	0/5061
1	K	0.26	0/3725	0.52	0/5061
1	L	0.26	0/3725	0.52	0/5061
1	M	0.26	0/3725	0.52	0/5061
1	N	0.26	0/3725	0.52	0/5061
1	O	0.26	0/3725	0.52	0/5061
1	P	0.26	0/3725	0.52	0/5061
All	All	0.26	0/59600	0.52	0/80976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3616	0	3424	56	0
1	B	3616	0	3424	57	1
1	C	3616	0	3424	68	0
1	D	3616	0	3424	58	0
1	E	3616	0	3424	55	0
1	F	3616	0	3424	56	6
1	G	3616	0	3424	58	1
1	H	3616	0	3424	53	0
1	I	3616	0	3424	48	1
1	J	3616	0	3424	55	1
1	K	3616	0	3424	59	6
1	L	3616	0	3424	51	0
1	M	3616	0	3424	59	0
1	N	3616	0	3424	58	0
1	O	3616	0	3424	61	0
1	P	3616	0	3424	51	0
2	A	156	0	0	2	0
2	B	151	0	0	2	0
2	C	155	0	0	2	0
2	D	153	0	0	2	0
2	E	153	0	0	2	0
2	F	153	0	0	2	0
2	G	156	0	0	3	0
2	H	153	0	0	2	0
2	I	150	0	0	2	0
2	J	153	0	0	2	0
2	K	150	0	0	2	0
2	L	152	0	0	2	0
2	M	152	0	0	2	0
2	N	154	0	0	3	0
2	O	153	0	0	3	0
2	P	154	0	0	2	0
All	All	60304	0	54784	787	8

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 (787) 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:K:42:PRO:CB	1:L:3:ILE:HD13	1.71	1.18
1:I:42:PRO:HB3	1:J:3:ILE:HD13	1.23	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:PRO:HB3	1:L:3:ILE:CD1	1.92	0.99
1:G:210:GLU:O	2:G:2067:HOH:O	1.80	0.97
1:M:3:ILE:HD13	1:P:42:PRO:HB3	1.44	0.97
1:M:426:ASP:HB2	1:N:369:ARG:NH2	1.79	0.97
1:K:42:PRO:HB3	1:L:3:ILE:HD13	0.96	0.94
1:I:42:PRO:CB	1:J:3:ILE:HD13	1.98	0.92
1:M:426:ASP:HB2	1:N:369:ARG:HH22	1.31	0.92
1:J:42:PRO:HB3	1:K:3:ILE:HD13	1.56	0.87
1:N:42:PRO:HB3	1:O:3:ILE:HD13	1.55	0.87
1:I:3:ILE:HD13	1:L:42:PRO:HB3	1.57	0.87
1:J:42:PRO:CB	1:K:3:ILE:HD13	2.06	0.85
1:K:42:PRO:CB	1:L:3:ILE:CD1	2.52	0.84
1:M:426:ASP:CB	1:N:369:ARG:HH22	1.90	0.84
1:E:3:ILE:HD13	1:H:42:PRO:HB3	1.60	0.83
1:O:426:ASP:HB2	1:P:369:ARG:NH2	1.92	0.83
1:A:426:ASP:HB2	1:B:369:ARG:NH2	1.94	0.83
1:O:426:ASP:HB2	1:P:369:ARG:HH22	1.44	0.82
1:A:426:ASP:HB2	1:B:369:ARG:HH22	1.49	0.78
1:F:426:ASP:HB2	1:G:369:ARG:HH22	1.48	0.77
1:M:3:ILE:HD13	1:P:42:PRO:CB	2.15	0.77
1:O:269:ASN:ND2	2:O:2081:HOH:O	2.20	0.74
1:F:426:ASP:HB2	1:G:369:ARG:NH2	2.03	0.74
1:C:426:ASP:HB2	1:D:369:ARG:NH2	2.02	0.73
1:M:42:PRO:CB	1:N:3:ILE:HD13	2.18	0.73
1:F:42:PRO:CB	1:G:3:ILE:HD13	2.21	0.70
1:O:426:ASP:CB	1:P:369:ARG:HH22	2.04	0.70
1:F:42:PRO:HB3	1:G:3:ILE:HD13	1.72	0.70
1:A:426:ASP:CB	1:B:369:ARG:HH22	2.05	0.68
1:B:385:GLN:HE22	1:B:388:ARG:HH11	1.41	0.68
1:F:385:GLN:HE22	1:F:388:ARG:HH11	1.41	0.68
1:D:385:GLN:HE22	1:D:388:ARG:HH11	1.41	0.68
1:J:385:GLN:HE22	1:J:388:ARG:HH11	1.41	0.68
1:M:42:PRO:HB3	1:N:3:ILE:HD13	1.76	0.68
1:E:369:ARG:HH22	1:H:426:ASP:HB2	1.57	0.68
1:K:385:GLN:HE22	1:K:388:ARG:HH11	1.41	0.68
1:P:385:GLN:HE22	1:P:388:ARG:HH11	1.41	0.68
1:M:385:GLN:HE22	1:M:388:ARG:HH11	1.41	0.68
1:E:3:ILE:HD13	1:H:42:PRO:CB	2.23	0.68
1:A:385:GLN:HE22	1:A:388:ARG:HH11	1.41	0.68
1:L:385:GLN:HE22	1:L:388:ARG:HH11	1.41	0.68
1:N:42:PRO:CB	1:O:3:ILE:HD13	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:385:GLN:HE22	1:N:388:ARG:HH11	1.41	0.67
1:E:42:PRO:CB	1:F:3:ILE:HD13	2.25	0.67
1:E:385:GLN:HE22	1:E:388:ARG:HH11	1.41	0.67
1:C:385:GLN:HE22	1:C:388:ARG:HH11	1.41	0.67
1:H:385:GLN:HE22	1:H:388:ARG:HH11	1.41	0.67
1:A:42:PRO:HB3	1:B:3:ILE:HD13	1.76	0.67
1:C:426:ASP:HB2	1:D:369:ARG:HH22	1.59	0.67
1:G:385:GLN:HE22	1:G:388:ARG:HH11	1.41	0.66
1:O:385:GLN:HE22	1:O:388:ARG:HH11	1.41	0.66
1:C:48:GLY:HA3	1:D:445:ARG:HD3	1.76	0.66
1:G:426:ASP:HB2	1:H:369:ARG:NH2	2.10	0.66
1:I:385:GLN:HE22	1:I:388:ARG:HH11	1.41	0.66
1:I:3:ILE:HD13	1:L:42:PRO:CB	2.25	0.66
1:J:426:ASP:HB2	1:K:369:ARG:NH2	2.11	0.65
1:F:225:TRP:HB3	1:F:298:SER:HB3	1.79	0.65
1:E:225:TRP:HB3	1:E:298:SER:HB3	1.79	0.64
1:E:369:ARG:NH2	1:H:426:ASP:HB2	2.11	0.64
1:G:225:TRP:HB3	1:G:298:SER:HB3	1.79	0.64
1:G:426:ASP:HB2	1:H:369:ARG:HH22	1.62	0.64
1:J:225:TRP:HB3	1:J:298:SER:HB3	1.79	0.64
1:N:225:TRP:HB3	1:N:298:SER:HB3	1.79	0.64
1:B:225:TRP:HB3	1:B:298:SER:HB3	1.79	0.64
1:K:225:TRP:HB3	1:K:298:SER:HB3	1.79	0.64
1:L:225:TRP:HB3	1:L:298:SER:HB3	1.79	0.64
1:O:225:TRP:HB3	1:O:298:SER:HB3	1.79	0.64
1:O:42:PRO:CB	1:P:3:ILE:HD13	2.28	0.64
1:P:225:TRP:HB3	1:P:298:SER:HB3	1.79	0.64
1:I:225:TRP:HB3	1:I:298:SER:HB3	1.79	0.64
1:J:426:ASP:HB2	1:K:369:ARG:HH22	1.61	0.63
1:H:225:TRP:HB3	1:H:298:SER:HB3	1.79	0.63
1:A:225:TRP:HB3	1:A:298:SER:HB3	1.79	0.63
1:D:225:TRP:HB3	1:D:298:SER:HB3	1.79	0.63
1:E:42:PRO:HB3	1:F:3:ILE:HD13	1.79	0.63
1:M:117:CYS:HB2	1:M:158:ILE:HD13	1.82	0.62
1:M:225:TRP:HB3	1:M:298:SER:HB3	1.79	0.62
1:B:117:CYS:HB2	1:B:158:ILE:HD13	1.82	0.62
1:C:225:TRP:HB3	1:C:298:SER:HB3	1.79	0.62
1:J:117:CYS:HB2	1:J:158:ILE:HD13	1.82	0.62
1:F:117:CYS:HB2	1:F:158:ILE:HD13	1.82	0.62
1:H:117:CYS:HB2	1:H:158:ILE:HD13	1.82	0.62
1:O:117:CYS:HB2	1:O:158:ILE:HD13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:CYS:HB2	1:L:158:ILE:HD13	1.82	0.62
1:C:117:CYS:HB2	1:C:158:ILE:HD13	1.82	0.61
1:C:426:ASP:CB	1:D:369:ARG:HH22	2.14	0.61
1:I:117:CYS:HB2	1:I:158:ILE:HD13	1.82	0.61
1:K:117:CYS:HB2	1:K:158:ILE:HD13	1.82	0.61
1:A:42:PRO:CB	1:B:3:ILE:HD13	2.30	0.61
1:B:48:GLY:HA3	1:C:445:ARG:HD3	1.81	0.60
1:D:117:CYS:HB2	1:D:158:ILE:HD13	1.82	0.60
1:P:117:CYS:HB2	1:P:158:ILE:HD13	1.82	0.60
1:E:117:CYS:HB2	1:E:158:ILE:HD13	1.82	0.60
1:E:426:ASP:HB2	1:F:369:ARG:NH2	2.16	0.60
1:F:426:ASP:CB	1:G:369:ARG:HH22	2.14	0.60
1:G:117:CYS:HB2	1:G:158:ILE:HD13	1.82	0.60
1:A:117:CYS:HB2	1:A:158:ILE:HD13	1.82	0.60
1:N:117:CYS:HB2	1:N:158:ILE:HD13	1.82	0.60
1:O:42:PRO:HB3	1:P:3:ILE:HD13	1.82	0.60
1:K:426:ASP:HB2	1:L:369:ARG:HH22	1.66	0.59
1:D:13:GLY:HA2	1:D:73:VAL:HG22	1.85	0.59
1:B:13:GLY:HA2	1:B:73:VAL:HG22	1.85	0.59
1:J:13:GLY:HA2	1:J:73:VAL:HG22	1.85	0.59
1:B:426:ASP:HB2	1:C:369:ARG:HH22	1.65	0.59
1:H:13:GLY:HA2	1:H:73:VAL:HG22	1.85	0.59
1:F:13:GLY:HA2	1:F:73:VAL:HG22	1.85	0.59
1:L:13:GLY:HA2	1:L:73:VAL:HG22	1.85	0.59
1:O:13:GLY:HA2	1:O:73:VAL:HG22	1.85	0.59
1:N:13:GLY:HA2	1:N:73:VAL:HG22	1.85	0.58
1:K:231:ARG:NH2	1:O:344:ASP:OD2	2.36	0.58
1:B:42:PRO:HB3	1:C:3:ILE:HD13	1.86	0.58
1:M:13:GLY:HA2	1:M:73:VAL:HG22	1.85	0.58
1:P:13:GLY:HA2	1:P:73:VAL:HG22	1.85	0.58
1:I:244:GLY:HA2	1:I:248:ASP:HB2	1.86	0.58
1:C:244:GLY:HA2	1:C:248:ASP:HB2	1.86	0.58
1:E:244:GLY:HA2	1:E:248:ASP:HB2	1.86	0.58
1:E:13:GLY:HA2	1:E:73:VAL:HG22	1.85	0.58
1:G:13:GLY:HA2	1:G:73:VAL:HG22	1.85	0.58
1:I:13:GLY:HA2	1:I:73:VAL:HG22	1.85	0.58
1:A:13:GLY:HA2	1:A:73:VAL:HG22	1.85	0.58
1:J:244:GLY:HA2	1:J:248:ASP:HB2	1.86	0.58
1:K:13:GLY:HA2	1:K:73:VAL:HG22	1.85	0.58
1:P:244:GLY:HA2	1:P:248:ASP:HB2	1.86	0.57
1:N:244:GLY:HA2	1:N:248:ASP:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLY:HA2	1:C:73:VAL:HG22	1.85	0.57
1:O:244:GLY:HA2	1:O:248:ASP:HB2	1.86	0.57
1:L:244:GLY:HA2	1:L:248:ASP:HB2	1.86	0.57
1:B:244:GLY:HA2	1:B:248:ASP:HB2	1.86	0.57
1:D:244:GLY:HA2	1:D:248:ASP:HB2	1.86	0.57
1:K:244:GLY:HA2	1:K:248:ASP:HB2	1.86	0.57
1:A:244:GLY:HA2	1:A:248:ASP:HB2	1.86	0.56
1:G:244:GLY:HA2	1:G:248:ASP:HB2	1.86	0.56
1:F:244:GLY:HA2	1:F:248:ASP:HB2	1.86	0.56
1:H:244:GLY:HA2	1:H:248:ASP:HB2	1.86	0.56
1:B:260:PRO:HG2	1:B:263:MET:HB2	1.88	0.56
1:A:260:PRO:HG2	1:A:263:MET:HB2	1.88	0.56
1:B:42:PRO:CB	1:C:3:ILE:HD13	2.35	0.56
1:E:426:ASP:HB2	1:F:369:ARG:HH22	1.70	0.56
1:E:260:PRO:HG2	1:E:263:MET:HB2	1.88	0.56
1:J:260:PRO:HG2	1:J:263:MET:HB2	1.88	0.56
1:O:260:PRO:HG2	1:O:263:MET:HB2	1.88	0.56
1:A:353:ILE:HG13	1:A:396:LEU:HD11	1.88	0.56
1:B:353:ILE:HG13	1:B:396:LEU:HD11	1.88	0.56
1:M:260:PRO:HG2	1:M:263:MET:HB2	1.88	0.56
1:I:260:PRO:HG2	1:I:263:MET:HB2	1.88	0.55
1:I:353:ILE:HG13	1:I:396:LEU:HD11	1.88	0.55
1:K:260:PRO:HG2	1:K:263:MET:HB2	1.88	0.55
1:H:260:PRO:HG2	1:H:263:MET:HB2	1.88	0.55
1:M:244:GLY:HA2	1:M:248:ASP:HB2	1.86	0.55
1:C:260:PRO:HG2	1:C:263:MET:HB2	1.88	0.55
1:L:260:PRO:HG2	1:L:263:MET:HB2	1.88	0.55
1:F:260:PRO:HG2	1:F:263:MET:HB2	1.88	0.55
1:D:260:PRO:HG2	1:D:263:MET:HB2	1.88	0.55
1:E:353:ILE:HG13	1:E:396:LEU:HD11	1.88	0.55
1:G:260:PRO:HG2	1:G:263:MET:HB2	1.88	0.55
1:H:353:ILE:HG13	1:H:396:LEU:HD11	1.88	0.55
1:K:353:ILE:HG13	1:K:396:LEU:HD11	1.88	0.55
1:I:42:PRO:CB	1:J:3:ILE:CD1	2.79	0.55
1:J:353:ILE:HG13	1:J:396:LEU:HD11	1.88	0.55
1:C:320:GLY:HA2	1:G:450:LEU:HD12	1.89	0.54
1:D:353:ILE:HG13	1:D:396:LEU:HD11	1.88	0.54
1:P:260:PRO:HG2	1:P:263:MET:HB2	1.88	0.54
1:C:353:ILE:HG13	1:C:396:LEU:HD11	1.88	0.54
1:O:353:ILE:HG13	1:O:396:LEU:HD11	1.88	0.54
1:F:116:PHE:HA	1:F:160:GLN:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:PHE:HA	1:G:160:GLN:HB2	1.90	0.54
1:K:116:PHE:HA	1:K:160:GLN:HB2	1.90	0.54
1:E:116:PHE:HA	1:E:160:GLN:HB2	1.90	0.54
1:N:353:ILE:HG13	1:N:396:LEU:HD11	1.88	0.54
1:G:353:ILE:HG13	1:G:396:LEU:HD11	1.88	0.54
1:M:116:PHE:HA	1:M:160:GLN:HB2	1.90	0.54
1:N:260:PRO:HG2	1:N:263:MET:HB2	1.88	0.54
1:I:116:PHE:HA	1:I:160:GLN:HB2	1.90	0.54
1:P:353:ILE:HG13	1:P:396:LEU:HD11	1.88	0.54
1:L:116:PHE:HA	1:L:160:GLN:HB2	1.90	0.54
1:L:353:ILE:HG13	1:L:396:LEU:HD11	1.88	0.54
1:O:82:TRP:HB3	1:O:83:PRO:HD3	1.90	0.54
1:N:116:PHE:HA	1:N:160:GLN:HB2	1.90	0.54
1:C:82:TRP:HB3	1:C:83:PRO:HD3	1.90	0.54
1:M:353:ILE:HG13	1:M:396:LEU:HD11	1.88	0.54
1:P:116:PHE:HA	1:P:160:GLN:HB2	1.90	0.54
1:F:353:ILE:HG13	1:F:396:LEU:HD11	1.88	0.53
1:D:116:PHE:HA	1:D:160:GLN:HB2	1.90	0.53
1:A:82:TRP:HB3	1:A:83:PRO:HD3	1.90	0.53
1:M:42:PRO:HG3	1:N:447:TRP:CE2	2.43	0.53
1:P:82:TRP:HB3	1:P:83:PRO:HD3	1.90	0.53
1:B:116:PHE:HA	1:B:160:GLN:HB2	1.90	0.53
1:J:426:ASP:CB	1:K:369:ARG:HH22	2.20	0.53
1:M:294:ASN:OD1	1:M:355:GLU:HB2	2.09	0.53
1:N:82:TRP:HB3	1:N:83:PRO:HD3	1.90	0.53
1:C:294:ASN:OD1	1:C:355:GLU:HB2	2.09	0.53
1:E:82:TRP:HB3	1:E:83:PRO:HD3	1.90	0.53
1:H:116:PHE:HA	1:H:160:GLN:HB2	1.90	0.53
1:K:82:TRP:HB3	1:K:83:PRO:HD3	1.90	0.53
1:P:294:ASN:OD1	1:P:355:GLU:HB2	2.09	0.53
1:A:294:ASN:OD1	1:A:355:GLU:HB2	2.09	0.53
1:D:82:TRP:HB3	1:D:83:PRO:HD3	1.90	0.53
1:E:48:GLY:HA3	1:F:445:ARG:HD3	1.90	0.53
1:N:294:ASN:OD1	1:N:355:GLU:HB2	2.09	0.53
1:A:116:PHE:HA	1:A:160:GLN:HB2	1.90	0.53
1:B:294:ASN:OD1	1:B:355:GLU:HB2	2.09	0.53
1:E:294:ASN:OD1	1:E:355:GLU:HB2	2.09	0.53
1:C:95:ARG:CD	1:M:102:HIS:CE1	2.92	0.53
1:F:294:ASN:OD1	1:F:355:GLU:HB2	2.09	0.53
1:G:82:TRP:HB3	1:G:83:PRO:HD3	1.90	0.53
1:G:426:ASP:CB	1:H:369:ARG:HH22	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ARG:HH22	1:H:426:ASP:CB	2.22	0.53
1:B:426:ASP:HB2	1:C:369:ARG:NH2	2.24	0.52
1:C:116:PHE:HA	1:C:160:GLN:HB2	1.90	0.52
1:H:82:TRP:HB3	1:H:83:PRO:HD3	1.90	0.52
1:J:82:TRP:HB3	1:J:83:PRO:HD3	1.90	0.52
1:J:116:PHE:HA	1:J:160:GLN:HB2	1.90	0.52
1:O:116:PHE:HA	1:O:160:GLN:HB2	1.90	0.52
1:L:294:ASN:OD1	1:L:355:GLU:HB2	2.09	0.52
1:D:294:ASN:OD1	1:D:355:GLU:HB2	2.09	0.52
1:G:42:PRO:HB3	1:H:3:ILE:HD13	1.91	0.52
1:M:82:TRP:HB3	1:M:83:PRO:HD3	1.90	0.52
1:J:294:ASN:OD1	1:J:355:GLU:HB2	2.09	0.52
1:K:426:ASP:HB2	1:L:369:ARG:NH2	2.25	0.52
1:M:48:GLY:HA3	1:N:445:ARG:HD3	1.92	0.52
1:L:82:TRP:HB3	1:L:83:PRO:HD3	1.90	0.52
1:I:294:ASN:OD1	1:I:355:GLU:HB2	2.09	0.52
1:K:294:ASN:OD1	1:K:355:GLU:HB2	2.09	0.52
1:O:294:ASN:OD1	1:O:355:GLU:HB2	2.09	0.52
1:I:82:TRP:HB3	1:I:83:PRO:HD3	1.90	0.52
1:A:369:ARG:HH22	1:D:426:ASP:HB2	1.75	0.52
1:H:294:ASN:OD1	1:H:355:GLU:HB2	2.09	0.52
1:G:294:ASN:OD1	1:G:355:GLU:HB2	2.09	0.52
1:F:82:TRP:HB3	1:F:83:PRO:HD3	1.90	0.52
1:B:82:TRP:HB3	1:B:83:PRO:HD3	1.90	0.51
1:P:122:TRP:N	1:P:122:TRP:CD1	2.79	0.51
1:D:344:ASP:OD2	1:F:231:ARG:NH2	2.44	0.51
1:J:43:GLY:N	1:K:3:ILE:HD11	2.25	0.51
1:C:153:GLU:OE1	1:M:95:ARG:NH1	2.44	0.51
1:K:122:TRP:N	1:K:122:TRP:CD1	2.79	0.51
1:O:122:TRP:CD1	1:O:122:TRP:N	2.79	0.51
1:B:122:TRP:CD1	1:B:122:TRP:N	2.79	0.50
1:D:166:GLU:HG2	1:D:222:ASN:HB3	1.94	0.50
1:F:122:TRP:N	1:F:122:TRP:CD1	2.79	0.50
1:G:166:GLU:HG2	1:G:222:ASN:HB3	1.93	0.50
1:H:122:TRP:CD1	1:H:122:TRP:N	2.79	0.50
1:J:122:TRP:CD1	1:J:122:TRP:N	2.79	0.50
1:O:48:GLY:HA3	1:P:445:ARG:HD3	1.92	0.50
1:A:122:TRP:CD1	1:A:122:TRP:N	2.79	0.50
1:D:122:TRP:N	1:D:122:TRP:CD1	2.79	0.50
1:H:166:GLU:HG2	1:H:222:ASN:HB3	1.94	0.50
1:K:320:GLY:HA2	1:O:450:LEU:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG2	1:A:222:ASN:HB3	1.94	0.50
1:I:122:TRP:CD1	1:I:122:TRP:N	2.79	0.50
1:A:447:TRP:CH2	1:D:48:GLY:HA3	2.46	0.50
1:J:450:LEU:HD12	1:P:320:GLY:HA2	1.93	0.50
1:I:166:GLU:HG2	1:I:222:ASN:HB3	1.94	0.50
1:K:77:ARG:HH21	1:K:355:GLU:HG3	1.77	0.50
1:C:77:ARG:HH21	1:C:355:GLU:HG3	1.77	0.50
1:N:166:GLU:HG2	1:N:222:ASN:HB3	1.93	0.50
1:E:303:TYR:CZ	1:E:305:PRO:HG3	2.47	0.50
1:C:42:PRO:HG3	1:D:447:TRP:CE2	2.46	0.50
1:F:303:TYR:CZ	1:F:305:PRO:HG3	2.47	0.50
1:G:303:TYR:CZ	1:G:305:PRO:HG3	2.47	0.50
1:H:77:ARG:HH21	1:H:355:GLU:HG3	1.77	0.50
1:M:42:PRO:HA	1:N:447:TRP:CH2	2.47	0.50
1:P:166:GLU:HG2	1:P:222:ASN:HB3	1.94	0.50
1:P:303:TYR:CZ	1:P:305:PRO:HG3	2.47	0.50
1:B:303:TYR:CZ	1:B:305:PRO:HG3	2.47	0.49
1:N:77:ARG:HH21	1:N:355:GLU:HG3	1.77	0.49
1:N:122:TRP:N	1:N:122:TRP:CD1	2.79	0.49
1:P:77:ARG:HH21	1:P:355:GLU:HG3	1.77	0.49
1:B:77:ARG:HH21	1:B:355:GLU:HG3	1.77	0.49
1:C:95:ARG:HD2	1:M:102:HIS:CE1	2.47	0.49
1:D:77:ARG:HH21	1:D:355:GLU:HG3	1.77	0.49
1:E:166:GLU:HG2	1:E:222:ASN:HB3	1.94	0.49
1:O:77:ARG:HH21	1:O:355:GLU:HG3	1.77	0.49
1:E:122:TRP:N	1:E:122:TRP:CD1	2.79	0.49
1:I:77:ARG:HH21	1:I:355:GLU:HG3	1.77	0.49
1:J:77:ARG:HH21	1:J:355:GLU:HG3	1.77	0.49
1:L:320:GLY:HA2	1:N:450:LEU:HD12	1.94	0.49
1:M:166:GLU:HG2	1:M:222:ASN:HB3	1.93	0.49
1:N:303:TYR:CZ	1:N:305:PRO:HG3	2.47	0.49
1:B:166:GLU:HG2	1:B:222:ASN:HB3	1.93	0.49
1:C:166:GLU:HG2	1:C:222:ASN:HB3	1.93	0.49
1:L:450:LEU:HD12	1:N:320:GLY:HA2	1.95	0.49
1:E:77:ARG:HH21	1:E:355:GLU:HG3	1.77	0.49
1:F:48:GLY:HA3	1:G:445:ARG:HD3	1.94	0.49
1:I:303:TYR:CZ	1:I:305:PRO:HG3	2.47	0.49
1:L:166:GLU:HG2	1:L:222:ASN:HB3	1.94	0.49
1:A:77:ARG:HH21	1:A:355:GLU:HG3	1.77	0.49
1:C:450:LEU:HD12	1:G:320:GLY:HA2	1.94	0.49
1:H:303:TYR:CZ	1:H:305:PRO:HG3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:PHE:HB2	1:L:446:GLY:O	2.13	0.49
1:L:122:TRP:N	1:L:122:TRP:CD1	2.79	0.49
1:N:6:PHE:HB2	1:N:446:GLY:O	2.13	0.49
1:E:6:PHE:HB2	1:E:446:GLY:O	2.13	0.49
1:F:77:ARG:HH21	1:F:355:GLU:HG3	1.77	0.49
1:F:166:GLU:HG2	1:F:222:ASN:HB3	1.94	0.49
1:G:6:PHE:HB2	1:G:446:GLY:O	2.13	0.49
1:G:122:TRP:CD1	1:G:122:TRP:N	2.79	0.49
1:A:303:TYR:CZ	1:A:305:PRO:HG3	2.47	0.49
1:C:42:PRO:HA	1:D:447:TRP:CZ2	2.48	0.49
1:J:166:GLU:HG2	1:J:222:ASN:HB3	1.93	0.49
1:K:166:GLU:HG2	1:K:222:ASN:HB3	1.94	0.49
1:M:303:TYR:CZ	1:M:305:PRO:HG3	2.47	0.49
1:C:151:PHE:O	1:C:155:GLY:HA3	2.13	0.49
1:D:6:PHE:HB2	1:D:446:GLY:O	2.13	0.49
1:D:303:TYR:CZ	1:D:305:PRO:HG3	2.47	0.49
1:G:77:ARG:HH21	1:G:355:GLU:HG3	1.77	0.49
1:K:303:TYR:CZ	1:K:305:PRO:HG3	2.47	0.49
1:K:6:PHE:HB2	1:K:446:GLY:O	2.13	0.48
1:K:231:ARG:HH22	1:O:344:ASP:CG	2.16	0.48
1:M:122:TRP:N	1:M:122:TRP:CD1	2.79	0.48
1:L:77:ARG:HH21	1:L:355:GLU:HG3	1.77	0.48
1:B:6:PHE:HB2	1:B:446:GLY:O	2.13	0.48
1:D:151:PHE:O	1:D:155:GLY:HA3	2.14	0.48
1:H:6:PHE:HB2	1:H:446:GLY:O	2.13	0.48
1:I:6:PHE:HB2	1:I:446:GLY:O	2.13	0.48
1:J:151:PHE:O	1:J:155:GLY:HA3	2.13	0.48
1:J:303:TYR:CZ	1:J:305:PRO:HG3	2.47	0.48
1:J:320:GLY:HA2	1:P:450:LEU:HD12	1.96	0.48
1:L:151:PHE:O	1:L:155:GLY:HA3	2.14	0.48
1:L:303:TYR:CZ	1:L:305:PRO:HG3	2.47	0.48
1:M:6:PHE:HB2	1:M:446:GLY:O	2.13	0.48
1:M:151:PHE:O	1:M:155:GLY:HA3	2.13	0.48
1:B:151:PHE:O	1:B:155:GLY:HA3	2.13	0.48
1:C:303:TYR:CZ	1:C:305:PRO:HG3	2.47	0.48
1:F:6:PHE:HB2	1:F:446:GLY:O	2.13	0.48
1:G:151:PHE:O	1:G:155:GLY:HA3	2.14	0.48
1:A:6:PHE:HB2	1:A:446:GLY:O	2.13	0.48
1:A:151:PHE:O	1:A:155:GLY:HA3	2.14	0.48
1:C:6:PHE:HB2	1:C:446:GLY:O	2.13	0.48
1:K:151:PHE:O	1:K:155:GLY:HA3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:ARG:HH21	1:M:355:GLU:HG3	1.77	0.48
1:O:303:TYR:CZ	1:O:305:PRO:HG3	2.47	0.48
1:F:151:PHE:O	1:F:155:GLY:HA3	2.13	0.48
1:J:6:PHE:HB2	1:J:446:GLY:O	2.13	0.48
1:O:151:PHE:O	1:O:155:GLY:HA3	2.13	0.48
1:A:172:PHE:O	1:A:176:TYR:HB3	2.14	0.48
1:G:172:PHE:O	1:G:176:TYR:HB3	2.14	0.48
1:L:172:PHE:O	1:L:176:TYR:HB3	2.14	0.48
1:D:172:PHE:O	1:D:176:TYR:HB3	2.14	0.48
1:N:151:PHE:O	1:N:155:GLY:HA3	2.14	0.48
1:O:166:GLU:HG2	1:O:222:ASN:HB3	1.93	0.48
1:P:151:PHE:O	1:P:155:GLY:HA3	2.13	0.48
1:H:151:PHE:O	1:H:155:GLY:HA3	2.13	0.48
1:B:172:PHE:O	1:B:176:TYR:HB3	2.14	0.47
1:E:172:PHE:O	1:E:176:TYR:HB3	2.14	0.47
1:C:122:TRP:N	1:C:122:TRP:CD1	2.79	0.47
1:P:424:ASP:O	1:P:428:LEU:N	2.47	0.47
1:E:151:PHE:O	1:E:155:GLY:HA3	2.14	0.47
1:G:424:ASP:O	1:G:428:LEU:N	2.47	0.47
1:J:172:PHE:O	1:J:176:TYR:HB3	2.14	0.47
1:N:424:ASP:O	1:N:428:LEU:N	2.47	0.47
1:P:172:PHE:O	1:P:176:TYR:HB3	2.14	0.47
1:D:424:ASP:O	1:D:428:LEU:N	2.47	0.47
1:K:424:ASP:O	1:K:428:LEU:N	2.47	0.47
1:M:172:PHE:O	1:M:176:TYR:HB3	2.14	0.47
1:N:172:PHE:O	1:N:176:TYR:HB3	2.14	0.47
1:A:445:ARG:HD3	1:D:48:GLY:HA3	1.96	0.47
1:F:172:PHE:O	1:F:176:TYR:HB3	2.14	0.47
1:L:374:ARG:HD3	2:L:2114:HOH:O	2.15	0.47
1:H:172:PHE:O	1:H:176:TYR:HB3	2.14	0.47
1:M:374:ARG:HD3	2:M:2113:HOH:O	2.15	0.47
1:P:6:PHE:HB2	1:P:446:GLY:O	2.13	0.47
1:C:172:PHE:O	1:C:176:TYR:HB3	2.14	0.47
1:E:424:ASP:O	1:E:428:LEU:N	2.47	0.47
1:G:374:ARG:HD3	2:G:2117:HOH:O	2.15	0.47
1:I:172:PHE:O	1:I:176:TYR:HB3	2.14	0.47
1:O:172:PHE:O	1:O:176:TYR:HB3	2.14	0.47
1:B:424:ASP:O	1:B:428:LEU:N	2.47	0.47
1:C:95:ARG:NH1	1:M:153:GLU:OE1	2.47	0.47
1:H:374:ARG:HD3	2:H:2117:HOH:O	2.15	0.47
1:I:151:PHE:O	1:I:155:GLY:HA3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:PHE:O	1:K:176:TYR:HB3	2.14	0.47
1:L:424:ASP:O	1:L:428:LEU:N	2.47	0.47
1:O:6:PHE:HB2	1:O:446:GLY:O	2.13	0.47
1:A:374:ARG:HD3	2:A:2118:HOH:O	2.15	0.47
1:C:374:ARG:HD3	2:C:2115:HOH:O	2.15	0.47
1:E:374:ARG:HD3	2:E:2115:HOH:O	2.15	0.47
1:J:424:ASP:O	1:J:428:LEU:N	2.47	0.47
1:E:426:ASP:CB	1:F:369:ARG:HH22	2.28	0.47
1:O:424:ASP:O	1:O:428:LEU:N	2.47	0.47
1:I:42:PRO:HB3	1:J:3:ILE:CD1	2.16	0.46
1:N:445:ARG:HA	2:N:2153:HOH:O	2.14	0.46
1:P:374:ARG:HD3	2:P:2115:HOH:O	2.15	0.46
1:C:42:PRO:HG3	1:D:447:TRP:NE1	2.29	0.46
1:C:424:ASP:O	1:C:428:LEU:N	2.47	0.46
1:A:65:VAL:HG21	1:A:107:GLU:HB3	1.98	0.46
1:B:374:ARG:HD3	2:B:2113:HOH:O	2.15	0.46
1:J:65:VAL:HG21	1:J:107:GLU:HB3	1.98	0.46
1:K:374:ARG:HD3	2:K:2111:HOH:O	2.15	0.46
1:L:65:VAL:HG21	1:L:107:GLU:HB3	1.98	0.46
1:N:374:ARG:HD3	2:N:2116:HOH:O	2.15	0.46
1:O:65:VAL:HG21	1:O:107:GLU:HB3	1.98	0.46
1:C:370:ILE:HD12	1:C:370:ILE:N	2.31	0.46
1:D:374:ARG:HD3	2:D:2113:HOH:O	2.15	0.46
1:H:370:ILE:HD12	1:H:370:ILE:N	2.31	0.46
1:J:374:ARG:HD3	2:J:2114:HOH:O	2.15	0.46
1:M:65:VAL:HG21	1:M:107:GLU:HB3	1.98	0.46
1:M:424:ASP:O	1:M:428:LEU:N	2.48	0.46
1:B:48:GLY:HA2	1:C:447:TRP:HH2	1.81	0.46
1:B:370:ILE:N	1:B:370:ILE:HD12	2.31	0.46
1:E:65:VAL:HG21	1:E:107:GLU:HB3	1.98	0.46
1:L:370:ILE:N	1:L:370:ILE:HD12	2.31	0.46
1:M:370:ILE:HD12	1:M:370:ILE:N	2.31	0.46
1:N:370:ILE:N	1:N:370:ILE:HD12	2.31	0.46
1:A:424:ASP:O	1:A:428:LEU:N	2.47	0.46
1:L:205:VAL:O	1:L:209:ARG:HG2	2.16	0.46
1:N:65:VAL:HG21	1:N:107:GLU:HB3	1.98	0.46
1:A:370:ILE:HD12	1:A:370:ILE:N	2.31	0.46
1:F:424:ASP:O	1:F:428:LEU:N	2.47	0.46
1:I:65:VAL:HG21	1:I:107:GLU:HB3	1.98	0.46
1:F:374:ARG:HD3	2:F:2114:HOH:O	2.15	0.46
1:O:374:ARG:HD3	2:O:2116:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:205:VAL:O	1:P:209:ARG:HG2	2.16	0.46
1:A:205:VAL:O	1:A:209:ARG:HG2	2.16	0.46
1:F:205:VAL:O	1:F:209:ARG:HG2	2.16	0.46
1:I:231:ARG:NH2	1:M:344:ASP:OD2	2.49	0.46
1:I:370:ILE:N	1:I:370:ILE:HD12	2.31	0.46
1:I:374:ARG:HD3	2:I:2113:HOH:O	2.15	0.46
1:K:370:ILE:N	1:K:370:ILE:HD12	2.31	0.46
1:O:370:ILE:HD12	1:O:370:ILE:N	2.31	0.46
1:E:370:ILE:HD12	1:E:370:ILE:N	2.31	0.45
1:C:205:VAL:O	1:C:209:ARG:HG2	2.16	0.45
1:D:65:VAL:HG21	1:D:107:GLU:HB3	1.98	0.45
1:G:370:ILE:N	1:G:370:ILE:HD12	2.31	0.45
1:H:205:VAL:O	1:H:209:ARG:HG2	2.16	0.45
1:P:65:VAL:HG21	1:P:107:GLU:HB3	1.98	0.45
1:B:65:VAL:HG21	1:B:107:GLU:HB3	1.98	0.45
1:M:205:VAL:O	1:M:209:ARG:HG2	2.16	0.45
1:C:65:VAL:HG21	1:C:107:GLU:HB3	1.98	0.45
1:N:205:VAL:O	1:N:209:ARG:HG2	2.16	0.45
1:H:65:VAL:HG21	1:H:107:GLU:HB3	1.98	0.45
1:J:370:ILE:HD12	1:J:370:ILE:N	2.31	0.45
1:K:205:VAL:O	1:K:209:ARG:HG2	2.16	0.45
1:P:370:ILE:N	1:P:370:ILE:HD12	2.31	0.45
1:B:205:VAL:O	1:B:209:ARG:HG2	2.16	0.45
1:I:205:VAL:O	1:I:209:ARG:HG2	2.16	0.45
1:O:205:VAL:O	1:O:209:ARG:HG2	2.16	0.45
1:I:424:ASP:O	1:I:428:LEU:N	2.47	0.45
1:K:65:VAL:HG21	1:K:107:GLU:HB3	1.98	0.45
1:D:370:ILE:N	1:D:370:ILE:HD12	2.31	0.45
1:G:205:VAL:O	1:G:209:ARG:HG2	2.16	0.45
1:K:201:HIS:O	1:K:205:VAL:HG23	2.17	0.45
1:O:232:THR:O	1:O:236:MET:HG3	2.17	0.45
1:D:232:THR:O	1:D:236:MET:HG3	2.17	0.45
1:I:201:HIS:O	1:I:205:VAL:HG23	2.17	0.45
1:K:232:THR:O	1:K:236:MET:HG3	2.17	0.45
1:M:42:PRO:HB2	1:N:3:ILE:HD13	1.97	0.45
1:O:201:HIS:O	1:O:205:VAL:HG23	2.17	0.45
1:D:201:HIS:O	1:D:205:VAL:HG23	2.17	0.44
1:E:21:ILE:HG13	1:E:22:GLU:N	2.33	0.44
1:J:201:HIS:O	1:J:205:VAL:HG23	2.17	0.44
1:N:426:ASP:HB2	1:O:369:ARG:HH22	1.81	0.44
1:A:201:HIS:O	1:A:205:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:HIS:O	1:F:205:VAL:HG23	2.17	0.44
1:G:65:VAL:HG21	1:G:107:GLU:HB3	1.98	0.44
1:I:21:ILE:HG13	1:I:22:GLU:N	2.33	0.44
1:O:20:GLN:O	1:O:407:ASN:HB2	2.18	0.44
1:D:20:GLN:O	1:D:407:ASN:HB2	2.18	0.44
1:F:20:GLN:O	1:F:407:ASN:HB2	2.18	0.44
1:F:232:THR:O	1:F:236:MET:HG3	2.17	0.44
1:J:205:VAL:O	1:J:209:ARG:HG2	2.16	0.44
1:L:134:TRP:HB3	1:L:193:VAL:HG13	2.00	0.44
1:L:201:HIS:O	1:L:205:VAL:HG23	2.17	0.44
1:M:65:VAL:O	1:M:69:LYS:HG2	2.18	0.44
1:P:65:VAL:O	1:P:69:LYS:HG2	2.18	0.44
1:C:20:GLN:O	1:C:407:ASN:HB2	2.18	0.44
1:C:201:HIS:O	1:C:205:VAL:HG23	2.17	0.44
1:D:205:VAL:O	1:D:209:ARG:HG2	2.16	0.44
1:E:205:VAL:O	1:E:209:ARG:HG2	2.16	0.44
1:F:65:VAL:HG21	1:F:107:GLU:HB3	1.98	0.44
1:E:201:HIS:O	1:E:205:VAL:HG23	2.17	0.44
1:J:20:GLN:O	1:J:407:ASN:HB2	2.18	0.44
1:J:232:THR:O	1:J:236:MET:HG3	2.17	0.44
1:P:232:THR:O	1:P:236:MET:HG3	2.17	0.44
1:B:65:VAL:O	1:B:69:LYS:HG2	2.18	0.44
1:F:21:ILE:HG13	1:F:22:GLU:N	2.33	0.44
1:G:20:GLN:O	1:G:407:ASN:HB2	2.18	0.44
1:H:65:VAL:O	1:H:69:LYS:HG2	2.18	0.44
1:H:330:ILE:HD12	1:H:378:TYR:HD2	1.83	0.44
1:H:424:ASP:O	1:H:428:LEU:N	2.47	0.44
1:L:20:GLN:O	1:L:407:ASN:HB2	2.18	0.44
1:L:232:THR:O	1:L:236:MET:HG3	2.17	0.44
1:M:20:GLN:O	1:M:407:ASN:HB2	2.18	0.44
1:M:201:HIS:O	1:M:205:VAL:HG23	2.17	0.44
1:N:65:VAL:O	1:N:69:LYS:HG2	2.18	0.44
1:O:134:TRP:HB3	1:O:193:VAL:HG13	2.00	0.44
1:P:21:ILE:HG13	1:P:22:GLU:N	2.33	0.44
1:A:447:TRP:CH2	1:D:48:GLY:CA	3.01	0.44
1:B:134:TRP:HB3	1:B:193:VAL:HG13	2.00	0.44
1:D:21:ILE:HG13	1:D:22:GLU:N	2.33	0.44
1:F:370:ILE:N	1:F:370:ILE:HD12	2.31	0.44
1:G:232:THR:O	1:G:236:MET:HG3	2.17	0.44
1:M:134:TRP:HB3	1:M:193:VAL:HG13	2.00	0.44
1:N:201:HIS:O	1:N:205:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:VAL:O	1:O:69:LYS:HG2	2.18	0.44
1:A:21:ILE:HG13	1:A:22:GLU:N	2.33	0.44
1:B:201:HIS:O	1:B:205:VAL:HG23	2.17	0.44
1:E:330:ILE:HD12	1:E:378:TYR:HD2	1.83	0.44
1:F:65:VAL:O	1:F:69:LYS:HG2	2.18	0.44
1:H:134:TRP:HB3	1:H:193:VAL:HG13	2.00	0.44
1:P:201:HIS:O	1:P:205:VAL:HG23	2.17	0.44
1:B:232:THR:O	1:B:236:MET:HG3	2.17	0.43
1:C:42:PRO:HA	1:D:447:TRP:CH2	2.53	0.43
1:E:20:GLN:O	1:E:407:ASN:HB2	2.18	0.43
1:H:201:HIS:O	1:H:205:VAL:HG23	2.17	0.43
1:I:232:THR:O	1:I:236:MET:HG3	2.17	0.43
1:K:20:GLN:O	1:K:407:ASN:HB2	2.18	0.43
1:K:65:VAL:O	1:K:69:LYS:HG2	2.18	0.43
1:M:21:ILE:HG13	1:M:22:GLU:N	2.33	0.43
1:M:232:THR:O	1:M:236:MET:HG3	2.17	0.43
1:P:20:GLN:O	1:P:407:ASN:HB2	2.18	0.43
1:A:232:THR:O	1:A:236:MET:HG3	2.17	0.43
1:B:20:GLN:O	1:B:407:ASN:HB2	2.18	0.43
1:D:330:ILE:HD12	1:D:378:TYR:HD2	1.83	0.43
1:G:21:ILE:HG13	1:G:22:GLU:N	2.33	0.43
1:L:65:VAL:O	1:L:69:LYS:HG2	2.18	0.43
1:P:330:ILE:HD12	1:P:378:TYR:HD2	1.83	0.43
1:E:65:VAL:O	1:E:69:LYS:HG2	2.18	0.43
1:J:21:ILE:HG13	1:J:22:GLU:N	2.33	0.43
1:J:330:ILE:HD12	1:J:378:TYR:HD2	1.83	0.43
1:A:3:ILE:HD13	1:D:42:PRO:HB3	2.00	0.43
1:F:330:ILE:HD12	1:F:378:TYR:HD2	1.83	0.43
1:G:201:HIS:O	1:G:205:VAL:HG23	2.17	0.43
1:G:330:ILE:HD12	1:G:378:TYR:HD2	1.83	0.43
1:H:232:THR:O	1:H:236:MET:HG3	2.17	0.43
1:K:21:ILE:HG13	1:K:22:GLU:N	2.33	0.43
1:I:65:VAL:O	1:I:69:LYS:HG2	2.18	0.43
1:I:330:ILE:HD12	1:I:378:TYR:HD2	1.83	0.43
1:K:330:ILE:HD12	1:K:378:TYR:HD2	1.83	0.43
1:N:330:ILE:HD12	1:N:378:TYR:HD2	1.83	0.43
1:O:42:PRO:HG3	1:P:447:TRP:CE2	2.53	0.43
1:A:20:GLN:O	1:A:407:ASN:HB2	2.18	0.43
1:A:330:ILE:HD12	1:A:378:TYR:HD2	1.83	0.43
1:C:232:THR:O	1:C:236:MET:HG3	2.17	0.43
1:E:232:THR:O	1:E:236:MET:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:GLN:OE1	1:F:69:LYS:HE3	2.19	0.43
1:G:42:PRO:CB	1:H:3:ILE:HD13	2.48	0.43
1:H:66:GLN:OE1	1:H:69:LYS:HE3	2.19	0.43
1:I:66:GLN:OE1	1:I:69:LYS:HE3	2.19	0.43
1:N:21:ILE:HG13	1:N:22:GLU:N	2.33	0.43
1:C:21:ILE:HG13	1:C:22:GLU:N	2.33	0.43
1:I:134:TRP:HB3	1:I:193:VAL:HG13	2.00	0.43
1:J:65:VAL:O	1:J:69:LYS:HG2	2.18	0.43
1:K:114:GLU:HA	1:K:115:PRO:HD3	1.91	0.43
1:N:426:ASP:HB2	1:O:369:ARG:NH2	2.34	0.43
1:C:66:GLN:OE1	1:C:69:LYS:HE3	2.19	0.43
1:D:66:GLN:OE1	1:D:69:LYS:HE3	2.19	0.43
1:G:48:GLY:HA3	1:H:445:ARG:HD3	2.01	0.43
1:M:66:GLN:OE1	1:M:69:LYS:HE3	2.19	0.43
1:M:330:ILE:HD12	1:M:378:TYR:HD2	1.83	0.43
1:N:134:TRP:HB3	1:N:193:VAL:HG13	2.00	0.43
1:N:232:THR:O	1:N:236:MET:HG3	2.17	0.43
1:N:373:GLN:HG2	2:N:2148:HOH:O	2.19	0.43
1:P:66:GLN:OE1	1:P:69:LYS:HE3	2.19	0.43
1:A:65:VAL:O	1:A:69:LYS:HG2	2.18	0.43
1:C:65:VAL:O	1:C:69:LYS:HG2	2.18	0.43
1:C:134:TRP:HB3	1:C:193:VAL:HG13	2.00	0.43
1:G:65:VAL:O	1:G:69:LYS:HG2	2.18	0.43
1:H:21:ILE:HG13	1:H:22:GLU:N	2.33	0.43
1:L:66:GLN:OE1	1:L:69:LYS:HE3	2.19	0.43
1:O:66:GLN:OE1	1:O:69:LYS:HE3	2.19	0.43
1:O:225:TRP:HB3	1:O:298:SER:CB	2.49	0.43
1:O:330:ILE:HD12	1:O:378:TYR:HD2	1.83	0.43
1:A:134:TRP:HB3	1:A:193:VAL:HG13	2.00	0.43
1:A:369:ARG:NH2	1:D:426:ASP:HB2	2.33	0.43
1:B:21:ILE:HG13	1:B:22:GLU:N	2.33	0.43
1:D:134:TRP:HB3	1:D:193:VAL:HG13	2.00	0.43
1:G:66:GLN:OE1	1:G:69:LYS:HE3	2.19	0.43
1:J:66:GLN:OE1	1:J:69:LYS:HE3	2.19	0.43
1:J:134:TRP:HB3	1:J:193:VAL:HG13	2.00	0.43
1:K:373:GLN:HG2	2:K:2144:HOH:O	2.19	0.43
1:N:20:GLN:O	1:N:407:ASN:HB2	2.18	0.43
1:O:21:ILE:HG13	1:O:22:GLU:N	2.33	0.43
1:G:373:GLN:HG2	2:G:2151:HOH:O	2.19	0.42
1:H:20:GLN:O	1:H:407:ASN:HB2	2.18	0.42
1:I:20:GLN:O	1:I:407:ASN:HB2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ILE:HG13	1:L:22:GLU:N	2.33	0.42
1:B:66:GLN:OE1	1:B:69:LYS:HE3	2.19	0.42
1:B:358:ALA:O	1:B:375:ARG:NH1	2.52	0.42
1:G:134:TRP:HB3	1:G:193:VAL:HG13	2.00	0.42
1:I:373:GLN:HG2	2:I:2146:HOH:O	2.19	0.42
1:K:134:TRP:HB3	1:K:193:VAL:HG13	2.00	0.42
1:O:101:TYR:O	1:O:105:VAL:HG23	2.20	0.42
1:A:66:GLN:OE1	1:A:69:LYS:HE3	2.19	0.42
1:B:101:TYR:O	1:B:105:VAL:HG23	2.20	0.42
1:B:114:GLU:HA	1:B:115:PRO:HD3	1.91	0.42
1:C:101:TYR:O	1:C:105:VAL:HG23	2.20	0.42
1:C:330:ILE:HD12	1:C:378:TYR:HD2	1.83	0.42
1:E:101:TYR:O	1:E:105:VAL:HG23	2.20	0.42
1:E:134:TRP:HB3	1:E:193:VAL:HG13	2.00	0.42
1:E:358:ALA:O	1:E:375:ARG:NH1	2.53	0.42
1:F:358:ALA:O	1:F:375:ARG:NH1	2.53	0.42
1:I:358:ALA:O	1:I:375:ARG:NH1	2.53	0.42
1:K:66:GLN:OE1	1:K:69:LYS:HE3	2.19	0.42
1:N:358:ALA:O	1:N:375:ARG:NH1	2.53	0.42
1:B:225:TRP:HB3	1:B:298:SER:CB	2.49	0.42
1:D:65:VAL:O	1:D:69:LYS:HG2	2.18	0.42
1:P:358:ALA:O	1:P:375:ARG:NH1	2.53	0.42
1:A:101:TYR:O	1:A:105:VAL:HG23	2.20	0.42
1:B:330:ILE:HD12	1:B:378:TYR:HD2	1.83	0.42
1:I:369:ARG:NH2	1:L:426:ASP:HB2	2.34	0.42
1:L:330:ILE:HD12	1:L:378:TYR:HD2	1.83	0.42
1:L:358:ALA:O	1:L:375:ARG:NH1	2.53	0.42
1:P:373:GLN:HG2	2:P:2148:HOH:O	2.19	0.42
1:D:101:TYR:O	1:D:105:VAL:HG23	2.20	0.42
1:F:134:TRP:HB3	1:F:193:VAL:HG13	2.00	0.42
1:G:225:TRP:HB3	1:G:298:SER:CB	2.49	0.42
1:G:330:ILE:HD12	1:G:378:TYR:CD2	2.55	0.42
1:G:358:ALA:O	1:G:375:ARG:NH1	2.53	0.42
1:L:101:TYR:O	1:L:105:VAL:HG23	2.20	0.42
1:M:225:TRP:HB3	1:M:298:SER:CB	2.49	0.42
1:A:358:ALA:O	1:A:375:ARG:NH1	2.53	0.42
1:C:358:ALA:O	1:C:375:ARG:NH1	2.53	0.42
1:G:101:TYR:O	1:G:105:VAL:HG23	2.20	0.42
1:H:101:TYR:O	1:H:105:VAL:HG23	2.20	0.42
1:H:358:ALA:O	1:H:375:ARG:NH1	2.53	0.42
1:J:330:ILE:HD12	1:J:378:TYR:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:66:GLN:OE1	1:N:69:LYS:HE3	2.19	0.42
1:O:330:ILE:HD12	1:O:378:TYR:CD2	2.55	0.42
1:P:134:TRP:HB3	1:P:193:VAL:HG13	2.00	0.42
1:A:114:GLU:HA	1:A:115:PRO:HD3	1.91	0.42
1:A:330:ILE:HD12	1:A:378:TYR:CD2	2.55	0.42
1:A:373:GLN:HG2	2:A:2150:HOH:O	2.19	0.42
1:D:373:GLN:HG2	2:D:2147:HOH:O	2.19	0.42
1:E:330:ILE:HD12	1:E:378:TYR:CD2	2.55	0.42
1:K:330:ILE:HD12	1:K:378:TYR:CD2	2.55	0.42
1:N:330:ILE:HD12	1:N:378:TYR:CD2	2.55	0.42
1:O:358:ALA:O	1:O:375:ARG:NH1	2.53	0.42
1:B:48:GLY:CA	1:C:447:TRP:CH2	3.03	0.42
1:B:330:ILE:HD12	1:B:378:TYR:CD2	2.55	0.42
1:B:373:GLN:HG2	2:B:2148:HOH:O	2.19	0.42
1:E:332:ALA:O	1:E:385:GLN:HG3	2.20	0.42
1:E:373:GLN:HG2	2:E:2148:HOH:O	2.19	0.42
1:K:358:ALA:O	1:K:375:ARG:NH1	2.53	0.42
1:P:101:TYR:O	1:P:105:VAL:HG23	2.20	0.42
1:A:332:ALA:O	1:A:385:GLN:HG3	2.20	0.42
1:C:225:TRP:HB3	1:C:298:SER:CB	2.49	0.42
1:C:373:GLN:HG2	2:C:2149:HOH:O	2.19	0.42
1:H:332:ALA:O	1:H:385:GLN:HG3	2.20	0.42
1:D:330:ILE:HD12	1:D:378:TYR:CD2	2.55	0.41
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.96	0.41
1:F:225:TRP:HB3	1:F:298:SER:CB	2.49	0.41
1:G:161:TRP:O	1:G:217:ILE:HA	2.20	0.41
1:J:358:ALA:O	1:J:375:ARG:NH1	2.53	0.41
1:L:225:TRP:HB3	1:L:298:SER:CB	2.49	0.41
1:M:101:TYR:O	1:M:105:VAL:HG23	2.20	0.41
1:M:332:ALA:O	1:M:385:GLN:HG3	2.20	0.41
1:M:358:ALA:O	1:M:375:ARG:NH1	2.53	0.41
1:C:332:ALA:O	1:C:385:GLN:HG3	2.20	0.41
1:F:101:TYR:O	1:F:105:VAL:HG23	2.20	0.41
1:H:161:TRP:O	1:H:217:ILE:HA	2.20	0.41
1:I:101:TYR:O	1:I:105:VAL:HG23	2.20	0.41
1:J:101:TYR:O	1:J:105:VAL:HG23	2.20	0.41
1:J:332:ALA:O	1:J:385:GLN:HG3	2.20	0.41
1:N:332:ALA:O	1:N:385:GLN:HG3	2.20	0.41
1:O:373:GLN:HG2	2:O:2148:HOH:O	2.19	0.41
1:P:161:TRP:O	1:P:217:ILE:HA	2.20	0.41
1:P:332:ALA:O	1:P:385:GLN:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLN:HA	1:B:287:PRO:HD3	1.95	0.41
1:C:330:ILE:HD12	1:C:378:TYR:CD2	2.55	0.41
1:D:161:TRP:O	1:D:217:ILE:HA	2.21	0.41
1:E:66:GLN:OE1	1:E:69:LYS:HE3	2.19	0.41
1:F:330:ILE:HD12	1:F:378:TYR:CD2	2.55	0.41
1:J:161:TRP:O	1:J:217:ILE:HA	2.21	0.41
1:M:373:GLN:HG2	2:M:2147:HOH:O	2.19	0.41
1:N:101:TYR:O	1:N:105:VAL:HG23	2.20	0.41
1:B:332:ALA:O	1:B:385:GLN:HG3	2.20	0.41
1:D:358:ALA:O	1:D:375:ARG:NH1	2.53	0.41
1:G:232:THR:CG2	1:G:234:GLU:HG2	2.51	0.41
1:G:304:ASN:O	1:G:309:GLY:HA3	2.21	0.41
1:H:330:ILE:HD12	1:H:378:TYR:CD2	2.55	0.41
1:H:373:GLN:HG2	2:H:2150:HOH:O	2.19	0.41
1:I:232:THR:CG2	1:I:234:GLU:HG2	2.51	0.41
1:K:450:LEU:HD12	1:O:320:GLY:HA2	2.03	0.41
1:L:332:ALA:O	1:L:385:GLN:HG3	2.20	0.41
1:M:161:TRP:O	1:M:217:ILE:HA	2.21	0.41
1:B:232:THR:CG2	1:B:234:GLU:HG2	2.51	0.41
1:C:102:HIS:CE1	1:M:95:ARG:CD	3.03	0.41
1:C:304:ASN:O	1:C:309:GLY:HA3	2.21	0.41
1:I:332:ALA:O	1:I:385:GLN:HG3	2.20	0.41
1:J:232:THR:CG2	1:J:234:GLU:HG2	2.51	0.41
1:K:101:TYR:O	1:K:105:VAL:HG23	2.20	0.41
1:K:161:TRP:O	1:K:217:ILE:HA	2.21	0.41
1:K:332:ALA:O	1:K:385:GLN:HG3	2.20	0.41
1:M:232:THR:CG2	1:M:234:GLU:HG2	2.51	0.41
1:M:330:ILE:HD12	1:M:378:TYR:CD2	2.55	0.41
1:O:161:TRP:O	1:O:217:ILE:HA	2.21	0.41
1:O:227:VAL:HA	1:O:228:PRO:HD3	1.95	0.41
1:A:344:ASP:OD2	1:E:231:ARG:NH2	2.53	0.41
1:C:232:THR:CG2	1:C:234:GLU:HG2	2.51	0.41
1:C:383:LEU:HD23	1:C:383:LEU:HA	1.96	0.41
1:E:161:TRP:O	1:E:217:ILE:HA	2.21	0.41
1:E:304:ASN:O	1:E:309:GLY:HA3	2.21	0.41
1:I:298:SER:OG	1:I:331:TYR:CD2	2.74	0.41
1:J:304:ASN:O	1:J:309:GLY:HA3	2.21	0.41
1:M:298:SER:OG	1:M:331:TYR:CD2	2.74	0.41
1:P:330:ILE:HD12	1:P:378:TYR:CD2	2.55	0.41
1:A:304:ASN:O	1:A:309:GLY:HA3	2.21	0.41
1:C:298:SER:OG	1:C:331:TYR:CD2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:THR:CG2	1:D:234:GLU:HG2	2.51	0.41
1:E:42:PRO:HG3	1:F:447:TRP:CE2	2.55	0.41
1:J:373:GLN:HG2	2:J:2147:HOH:O	2.19	0.41
1:L:298:SER:OG	1:L:331:TYR:CD2	2.74	0.41
1:O:298:SER:OG	1:O:331:TYR:CD2	2.74	0.41
1:A:124:LEU:HD23	1:A:129:GLN:HE21	1.86	0.41
1:A:447:TRP:HH2	1:D:48:GLY:HA2	1.86	0.41
1:C:161:TRP:O	1:C:217:ILE:HA	2.21	0.41
1:C:324:THR:HG23	1:C:330:ILE:HD11	2.03	0.41
1:E:324:THR:HG23	1:E:330:ILE:HD11	2.03	0.41
1:F:332:ALA:O	1:F:385:GLN:HG3	2.20	0.41
1:G:124:LEU:HD23	1:G:129:GLN:HE21	1.86	0.41
1:G:332:ALA:O	1:G:385:GLN:HG3	2.20	0.41
1:H:232:THR:CG2	1:H:234:GLU:HG2	2.51	0.41
1:O:332:ALA:O	1:O:385:GLN:HG3	2.20	0.41
1:A:77:ARG:NH2	1:A:355:GLU:HG3	2.36	0.41
1:B:304:ASN:O	1:B:309:GLY:HA3	2.21	0.41
1:C:124:LEU:HD23	1:C:129:GLN:HE21	1.86	0.41
1:D:298:SER:OG	1:D:331:TYR:CD2	2.74	0.41
1:D:304:ASN:O	1:D:309:GLY:HA3	2.21	0.41
1:D:332:ALA:O	1:D:385:GLN:HG3	2.20	0.41
1:E:124:LEU:HD23	1:E:129:GLN:HE21	1.86	0.41
1:F:373:GLN:HG2	2:F:2147:HOH:O	2.19	0.41
1:G:298:SER:OG	1:G:331:TYR:CD2	2.74	0.41
1:H:324:THR:HG23	1:H:330:ILE:HD11	2.03	0.41
1:I:161:TRP:O	1:I:217:ILE:HA	2.20	0.41
1:I:324:THR:HG23	1:I:330:ILE:HD11	2.03	0.41
1:I:330:ILE:HD12	1:I:378:TYR:CD2	2.55	0.41
1:K:286:GLN:HA	1:K:287:PRO:HD3	1.95	0.41
1:L:161:TRP:O	1:L:217:ILE:HA	2.20	0.41
1:L:232:THR:CG2	1:L:234:GLU:HG2	2.51	0.41
1:N:225:TRP:HB3	1:N:298:SER:CB	2.49	0.41
1:N:232:THR:CG2	1:N:234:GLU:HG2	2.51	0.41
1:O:232:THR:CG2	1:O:234:GLU:HG2	2.51	0.41
1:O:324:THR:HG23	1:O:330:ILE:HD11	2.03	0.41
1:B:161:TRP:O	1:B:217:ILE:HA	2.20	0.41
1:D:324:THR:HG23	1:D:330:ILE:HD11	2.03	0.41
1:F:304:ASN:O	1:F:309:GLY:HA3	2.21	0.41
1:G:77:ARG:NH2	1:G:355:GLU:HG3	2.36	0.41
1:I:304:ASN:O	1:I:309:GLY:HA3	2.21	0.41
1:J:324:THR:HG23	1:J:330:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:THR:CG2	1:K:234:GLU:HG2	2.51	0.41
1:L:330:ILE:HD12	1:L:378:TYR:CD2	2.55	0.41
1:L:373:GLN:HG2	2:L:2146:HOH:O	2.19	0.41
1:M:304:ASN:O	1:M:309:GLY:HA3	2.21	0.41
1:N:324:THR:HG23	1:N:330:ILE:HD11	2.03	0.41
1:O:304:ASN:O	1:O:309:GLY:HA3	2.21	0.41
1:P:304:ASN:O	1:P:309:GLY:HA3	2.21	0.41
1:A:324:THR:HG23	1:A:330:ILE:HD11	2.03	0.40
1:B:48:GLY:HA3	1:C:447:TRP:CH2	2.56	0.40
1:C:77:ARG:NH2	1:C:355:GLU:HG3	2.36	0.40
1:D:124:LEU:HD23	1:D:129:GLN:HE21	1.86	0.40
1:E:298:SER:OG	1:E:331:TYR:CD2	2.74	0.40
1:H:225:TRP:HB3	1:H:298:SER:CB	2.49	0.40
1:H:304:ASN:O	1:H:309:GLY:HA3	2.21	0.40
1:K:229:TYR:CD1	1:O:388:ARG:HG3	2.55	0.40
1:M:124:LEU:HD23	1:M:129:GLN:HE21	1.86	0.40
1:N:48:GLY:HA3	1:O:447:TRP:CH2	2.56	0.40
1:N:124:LEU:HD23	1:N:129:GLN:HE21	1.86	0.40
1:B:77:ARG:NH2	1:B:355:GLU:HG3	2.36	0.40
1:B:426:ASP:HB3	1:C:437:TYR:CE1	2.56	0.40
1:E:77:ARG:NH2	1:E:355:GLU:HG3	2.36	0.40
1:F:124:LEU:HD23	1:F:129:GLN:HE21	1.86	0.40
1:H:124:LEU:HD23	1:H:129:GLN:HE21	1.86	0.40
1:H:298:SER:OG	1:H:331:TYR:CD2	2.74	0.40
1:K:225:TRP:HB3	1:K:298:SER:CB	2.49	0.40
1:A:161:TRP:O	1:A:217:ILE:HA	2.21	0.40
1:A:232:THR:CG2	1:A:234:GLU:HG2	2.51	0.40
1:B:124:LEU:HD23	1:B:129:GLN:HE21	1.86	0.40
1:F:324:THR:HG23	1:F:330:ILE:HD11	2.03	0.40
1:J:42:PRO:HB3	1:K:3:ILE:HG21	2.04	0.40
1:J:298:SER:OG	1:J:331:TYR:CD2	2.74	0.40
1:M:77:ARG:NH2	1:M:355:GLU:HG3	2.36	0.40
1:N:161:TRP:O	1:N:217:ILE:HA	2.20	0.40
1:P:225:TRP:HB3	1:P:298:SER:CB	2.49	0.40
1:A:298:SER:OG	1:A:331:TYR:CD2	2.74	0.40
1:G:324:THR:HG23	1:G:330:ILE:HD11	2.03	0.40
1:J:114:GLU:HA	1:J:115:PRO:HD3	1.91	0.40
1:L:80:ILE:HG12	1:L:117:CYS:SG	2.62	0.40
1:O:80:ILE:HG12	1:O:117:CYS:SG	2.62	0.40
1:P:232:THR:CG2	1:P:234:GLU:HG2	2.51	0.40
1:D:450:LEU:HD12	1:F:320:GLY:HA2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:ILE:HG12	1:F:117:CYS:SG	2.62	0.40
1:F:232:THR:CG2	1:F:234:GLU:HG2	2.51	0.40
1:J:124:LEU:HD23	1:J:129:GLN:HE21	1.86	0.40
1:K:298:SER:OG	1:K:331:TYR:CD2	2.74	0.40
1:N:304:ASN:O	1:N:309:GLY:HA3	2.21	0.40
1:P:298:SER:OG	1:P:331:TYR:CD2	2.74	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:LYS:NZ	1:K:344:ASP:O[1_654]	0.89	1.31
1:F:273:LYS:NZ	1:K:344:ASP:C[1_654]	1.19	1.01
1:F:273:LYS:CE	1:K:344:ASP:O[1_654]	1.21	0.99
1:F:273:LYS:NZ	1:K:344:ASP:CA[1_654]	1.80	0.40
1:G:92:GLU:OE1	1:K:94:ASN:OD1[1_644]	1.85	0.35
1:B:278:ASP:OD2	1:J:233:LYS:N[1_645]	1.92	0.28
1:F:273:LYS:CD	1:K:344:ASP:O[1_654]	1.98	0.22
1:F:91:GLY:CA	1:I:99:ASP:OD2[1_644]	2.04	0.16

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	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73
1	B	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73
1	C	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73
1	D	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73
1	E	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73
1	F	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47 73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	H	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	I	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	J	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	K	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	L	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	M	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	N	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	O	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
1	P	447/449 (100%)	424 (95%)	22 (5%)	1 (0%)	47	73
All	All	7152/7184 (100%)	6784 (95%)	352 (5%)	16 (0%)	47	73

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	THR
1	D	223	THR
1	E	223	THR
1	F	223	THR
1	H	223	THR
1	J	223	THR
1	K	223	THR
1	L	223	THR
1	A	223	THR
1	B	223	THR
1	G	223	THR
1	I	223	THR
1	M	223	THR
1	N	223	THR
1	O	223	THR
1	P	223	THR

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	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	B	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	C	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	D	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	E	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	F	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	G	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	H	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	I	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	J	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	K	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	L	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	M	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	N	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	O	373/373 (100%)	366 (98%)	7 (2%)	57 82
1	P	373/373 (100%)	366 (98%)	7 (2%)	57 82
All	All	5968/5968 (100%)	5856 (98%)	112 (2%)	57 82

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LEU
1	A	240	LEU
1	A	245	TRP
1	A	335	LEU
1	A	401	GLU
1	A	403	SER
1	A	450	LEU
1	B	187	LEU
1	B	240	LEU
1	B	245	TRP
1	B	335	LEU
1	B	401	GLU
1	B	403	SER
1	B	450	LEU
1	C	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	240	LEU
1	C	245	TRP
1	C	335	LEU
1	C	401	GLU
1	C	403	SER
1	C	450	LEU
1	D	187	LEU
1	D	240	LEU
1	D	245	TRP
1	D	335	LEU
1	D	401	GLU
1	D	403	SER
1	D	450	LEU
1	E	187	LEU
1	E	240	LEU
1	E	245	TRP
1	E	335	LEU
1	E	401	GLU
1	E	403	SER
1	E	450	LEU
1	F	187	LEU
1	F	240	LEU
1	F	245	TRP
1	F	335	LEU
1	F	401	GLU
1	F	403	SER
1	F	450	LEU
1	G	187	LEU
1	G	240	LEU
1	G	245	TRP
1	G	335	LEU
1	G	401	GLU
1	G	403	SER
1	G	450	LEU
1	H	187	LEU
1	H	240	LEU
1	H	245	TRP
1	H	335	LEU
1	H	401	GLU
1	H	403	SER
1	H	450	LEU
1	I	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	240	LEU
1	I	245	TRP
1	I	335	LEU
1	I	401	GLU
1	I	403	SER
1	I	450	LEU
1	J	187	LEU
1	J	240	LEU
1	J	245	TRP
1	J	335	LEU
1	J	401	GLU
1	J	403	SER
1	J	450	LEU
1	K	187	LEU
1	K	240	LEU
1	K	245	TRP
1	K	335	LEU
1	K	401	GLU
1	K	403	SER
1	K	450	LEU
1	L	187	LEU
1	L	240	LEU
1	L	245	TRP
1	L	335	LEU
1	L	401	GLU
1	L	403	SER
1	L	450	LEU
1	M	187	LEU
1	M	240	LEU
1	M	245	TRP
1	M	335	LEU
1	M	401	GLU
1	M	403	SER
1	M	450	LEU
1	N	187	LEU
1	N	240	LEU
1	N	245	TRP
1	N	335	LEU
1	N	401	GLU
1	N	403	SER
1	N	450	LEU
1	O	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	240	LEU
1	O	245	TRP
1	O	335	LEU
1	O	401	GLU
1	O	403	SER
1	O	450	LEU
1	P	187	LEU
1	P	240	LEU
1	P	245	TRP
1	P	335	LEU
1	P	401	GLU
1	P	403	SER
1	P	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	129	GLN
1	A	165	ASN
1	A	356	ASN
1	A	385	GLN
1	B	126	GLN
1	B	129	GLN
1	B	165	ASN
1	B	356	ASN
1	B	385	GLN
1	C	126	GLN
1	C	129	GLN
1	C	165	ASN
1	C	356	ASN
1	C	385	GLN
1	D	126	GLN
1	D	129	GLN
1	D	165	ASN
1	D	356	ASN
1	D	385	GLN
1	E	126	GLN
1	E	129	GLN
1	E	165	ASN
1	E	356	ASN
1	E	385	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	126	GLN
1	F	129	GLN
1	F	165	ASN
1	F	356	ASN
1	F	385	GLN
1	G	126	GLN
1	G	129	GLN
1	G	165	ASN
1	G	356	ASN
1	G	385	GLN
1	H	126	GLN
1	H	129	GLN
1	H	165	ASN
1	H	356	ASN
1	H	385	GLN
1	I	126	GLN
1	I	129	GLN
1	I	165	ASN
1	I	356	ASN
1	I	385	GLN
1	J	126	GLN
1	J	129	GLN
1	J	165	ASN
1	J	356	ASN
1	J	385	GLN
1	K	126	GLN
1	K	129	GLN
1	K	165	ASN
1	K	356	ASN
1	K	385	GLN
1	L	126	GLN
1	L	129	GLN
1	L	165	ASN
1	L	356	ASN
1	L	385	GLN
1	M	126	GLN
1	M	129	GLN
1	M	165	ASN
1	M	356	ASN
1	M	385	GLN
1	N	126	GLN
1	N	129	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	165	ASN
1	N	356	ASN
1	N	385	GLN
1	O	126	GLN
1	O	129	GLN
1	O	165	ASN
1	O	356	ASN
1	O	385	GLN
1	P	126	GLN
1	P	129	GLN
1	P	165	ASN
1	P	356	ASN
1	P	385	GLN

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	449/449 (100%)	-0.36	0 100 100	4, 18, 42, 65	0
1	B	449/449 (100%)	-0.35	0 100 100	4, 18, 42, 65	0
1	C	449/449 (100%)	-0.28	0 100 100	4, 18, 42, 65	0
1	D	449/449 (100%)	-0.30	0 100 100	4, 18, 42, 65	0
1	E	449/449 (100%)	-0.38	0 100 100	4, 18, 42, 65	0
1	F	449/449 (100%)	-0.29	0 100 100	4, 18, 42, 65	0
1	G	449/449 (100%)	-0.21	3 (0%) 87 89	4, 18, 42, 65	0
1	H	449/449 (100%)	-0.37	0 100 100	4, 18, 42, 65	0
1	I	449/449 (100%)	-0.30	2 (0%) 92 93	4, 18, 42, 65	0
1	J	449/449 (100%)	-0.24	1 (0%) 95 96	4, 18, 42, 65	0
1	K	449/449 (100%)	0.32	22 (4%) 29 28	4, 18, 42, 65	0
1	L	449/449 (100%)	-0.33	1 (0%) 95 96	4, 18, 42, 65	0
1	M	449/449 (100%)	-0.37	0 100 100	4, 18, 42, 65	0
1	N	449/449 (100%)	-0.38	0 100 100	4, 18, 42, 65	0
1	O	449/449 (100%)	-0.17	4 (0%) 84 85	4, 18, 42, 65	0
1	P	449/449 (100%)	-0.36	0 100 100	4, 18, 42, 65	0
All	All	7184/7184 (100%)	-0.27	33 (0%) 91 92	4, 18, 43, 65	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	259	TYR	3.6
1	G	283	LEU	3.4
1	K	276	ILE	3.3
1	G	95	ARG	2.9
1	I	99	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	275	PRO	2.7
1	K	218	GLY	2.7
1	K	217	ILE	2.7
1	K	164	PHE	2.6
1	O	308	ALA	2.6
1	K	116	PHE	2.6
1	K	215	GLY	2.6
1	K	256	PHE	2.6
1	K	278	ASP	2.5
1	K	245	TRP	2.5
1	K	192	ASP	2.4
1	K	285	HIS	2.4
1	I	213	ILE	2.3
1	K	394	ILE	2.3
1	K	249	TRP	2.3
1	K	219	ILE	2.3
1	L	213	ILE	2.3
1	K	270	LEU	2.2
1	O	293	ILE	2.2
1	K	119	LEU	2.2
1	K	283	LEU	2.2
1	O	339	LEU	2.2
1	J	215	GLY	2.1
1	G	93	VAL	2.1
1	K	267	TYR	2.1
1	K	213	ILE	2.1
1	O	313	SER	2.1
1	K	161	TRP	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.