Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 09:16 PM EDT

PDB ID	:	6WIU
Title	:	Crystal structure of a beta-glucosidase from Exiguobacterium marinum
Authors	:	Zanphorlin, L.M.; Morais, M.A.B.; Murakami, M.T.
Deposited on	:	2020-04-10
Resolution	:	3.51 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 (i) 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 (1)) were used in the production of this report:

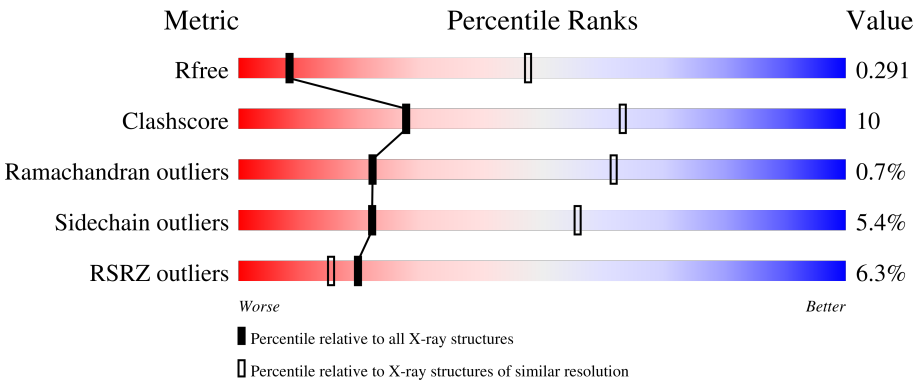
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	471	4% 78% 15% • 6%
1	B	471	4% 73% 19% • 6%
1	C	471	4% 77% 17% 5%
1	D	471	3% 75% 17% • 5%
1	E	471	3% 75% 19% • 5%

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Mol	Chain	Length	Quality of chain
1	F	471	6% 75% 19% 6%
1	G	471	4% 78% 17% 6%
1	H	471	6% 75% 18% 6%
1	I	471	8% 61% 25% 5% 7%
1	J	471	10% 65% 25% 6%
1	K	471	8% 53% 28% 7% 13%
1	L	471	10% 62% 28% 6%
1	M	471	8% 67% 24% 7%
1	N	471	5% 66% 24% 6%
1	O	471	6% 72% 20% 7%
1	P	471	5% 70% 22% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 57949 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.

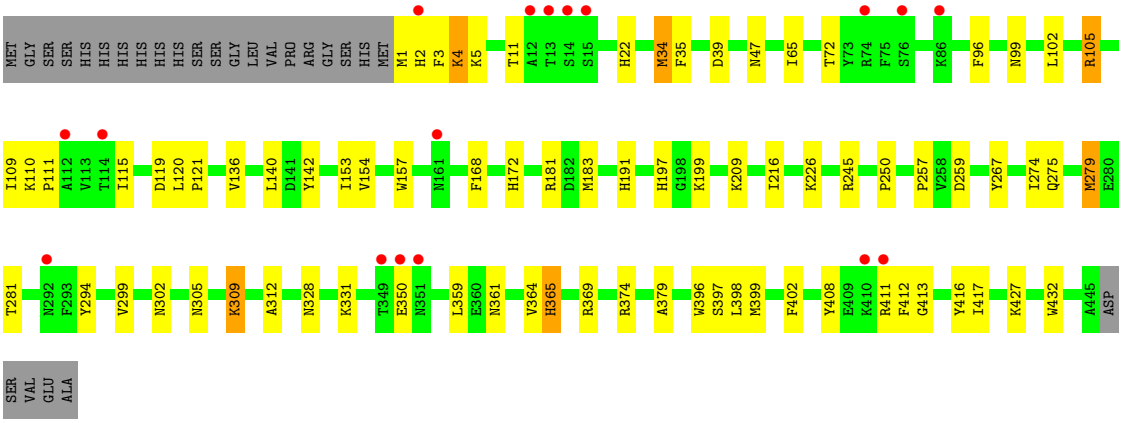
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3653	2337	615	681	20	0	0	0
1	B	444	3648	2334	614	680	20	0	0	0
1	C	446	3661	2342	616	682	21	0	0	0
1	D	446	3661	2342	616	682	21	0	0	0
1	E	447	3669	2346	617	685	21	0	0	0
1	F	445	3653	2337	615	681	20	0	0	0
1	G	444	3648	2334	614	680	20	0	0	0
1	H	445	3653	2337	615	681	20	0	0	0
1	I	438	3600	2304	604	672	20	0	0	0
1	J	444	3648	2334	614	680	20	0	0	0
1	K	412	3375	2160	570	627	18	0	0	0
1	L	443	3638	2328	611	679	20	0	0	0
1	M	438	3597	2301	605	671	20	0	0	0
1	N	441	3618	2313	608	677	20	0	0	0
1	O	438	3588	2293	603	673	19	0	0	0
1	P	443	3639	2329	613	677	20	0	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.

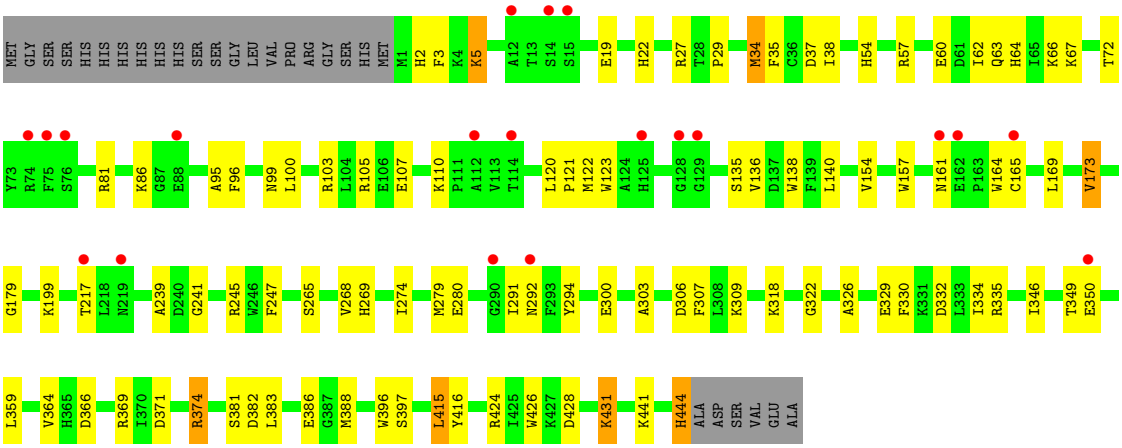
• Molecule 1: Beta-glucosidase

Chain A:



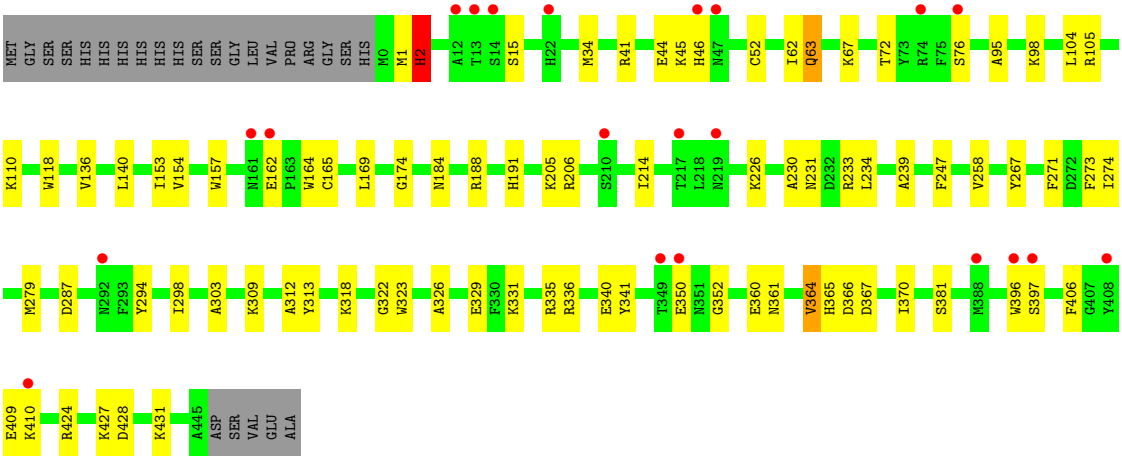
• Molecule 1: Beta-glucosidase

Chain B:



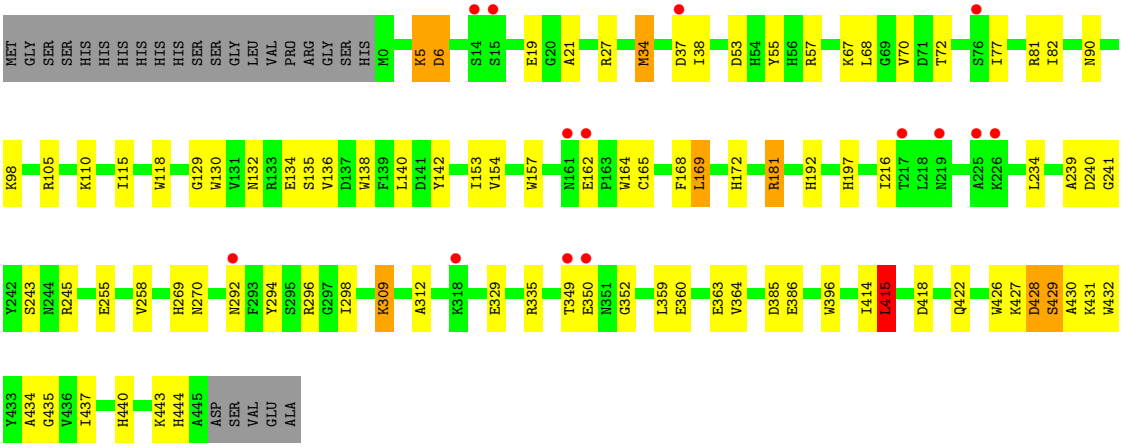
• Molecule 1: Beta-glucosidase

Chain C:



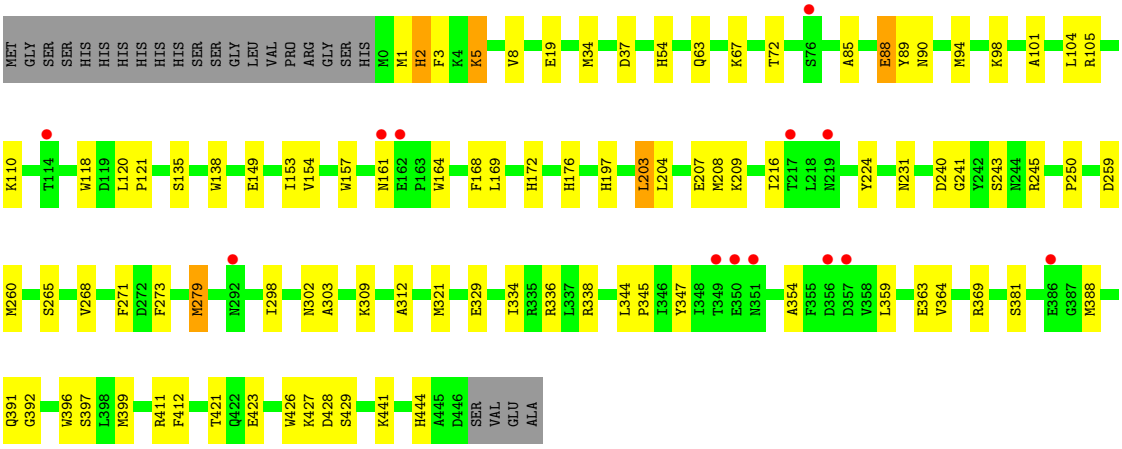
• Molecule 1: Beta-glucosidase

Chain D:



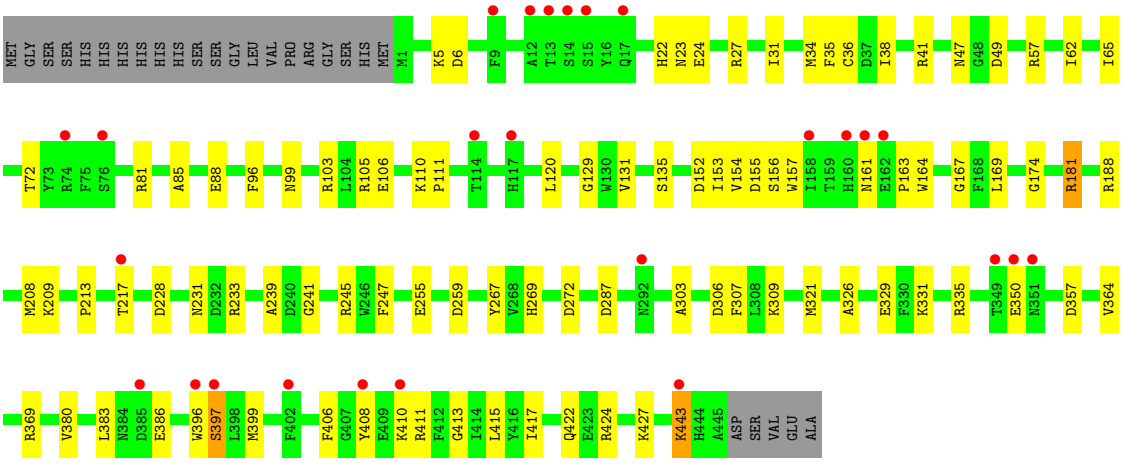
• Molecule 1: Beta-glucosidase

Chain E:



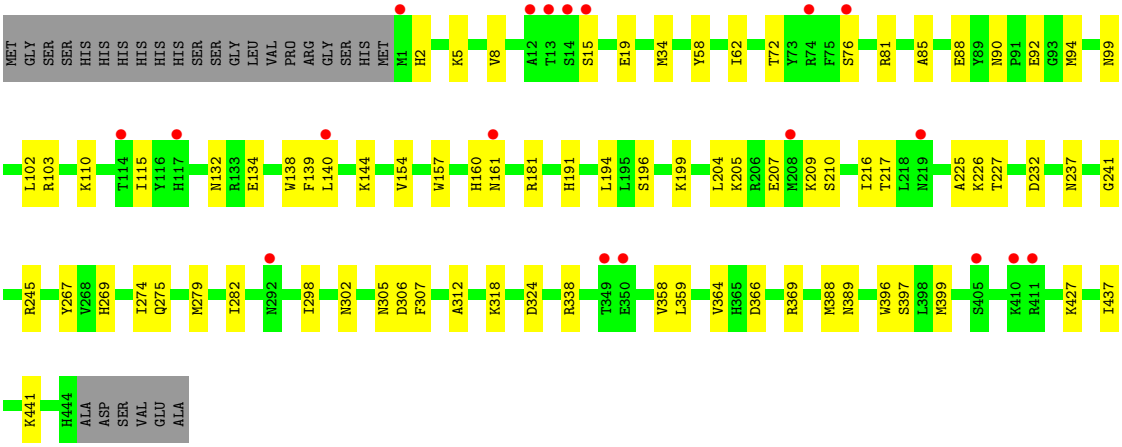
• Molecule 1: Beta-glucosidase

Chain F:



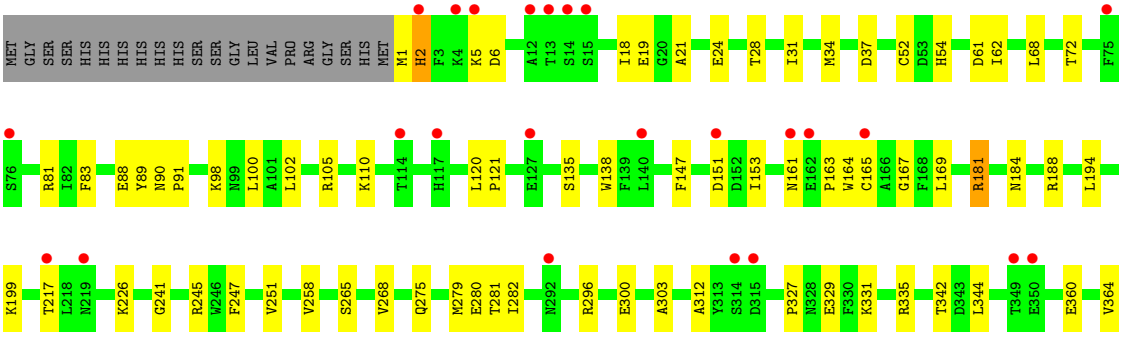
- Molecule 1: Beta-glucosidase

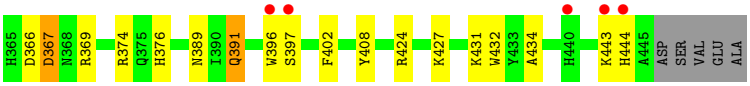
Chain G:



- Molecule 1: Beta-glucosidase

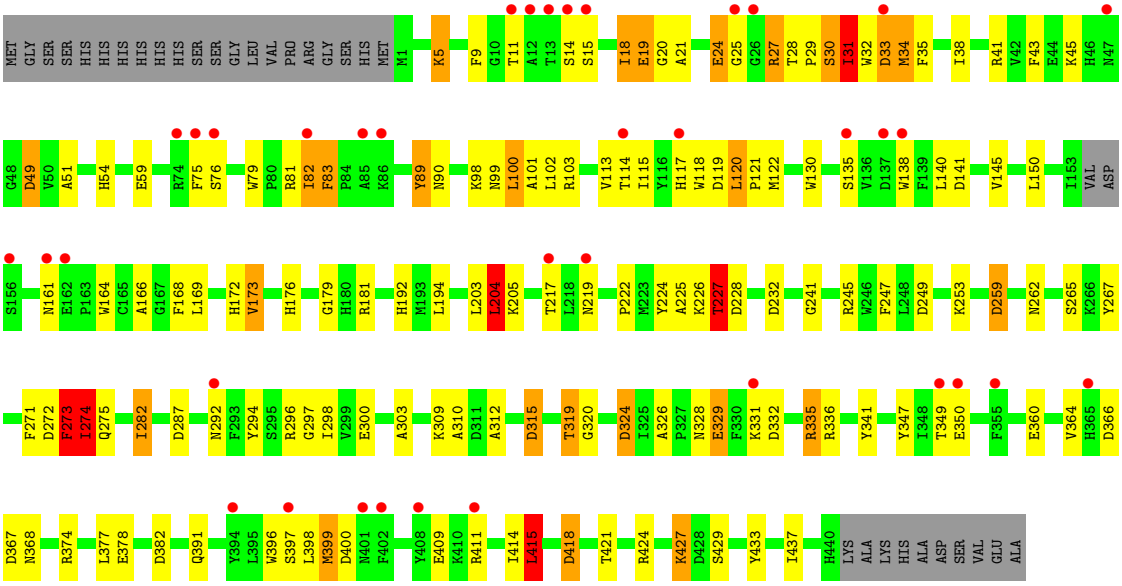
Chain H:





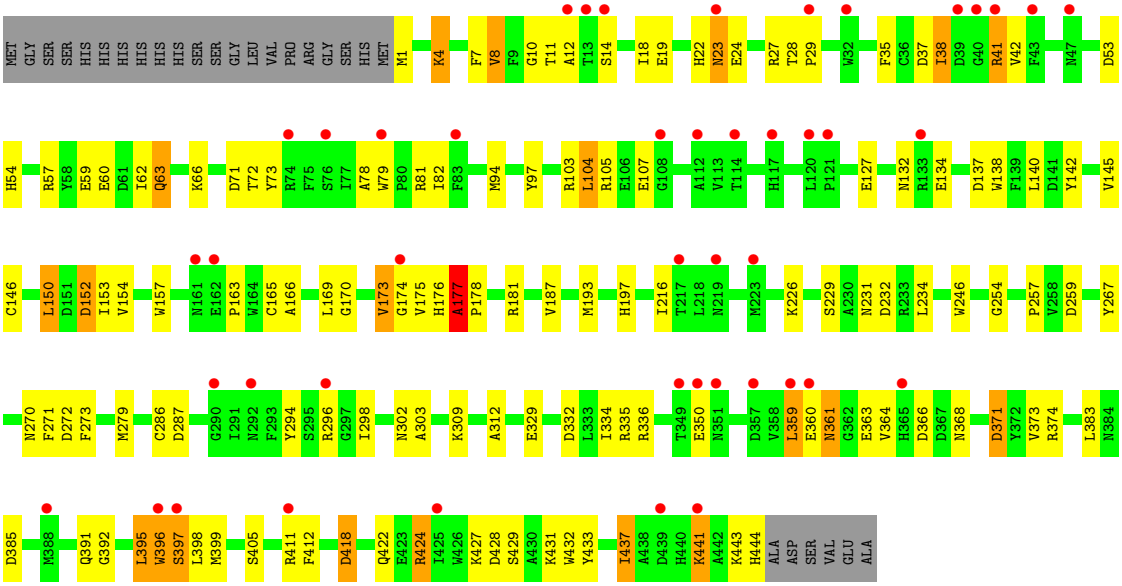
• Molecule 1: Beta-glucosidase

Chain I:



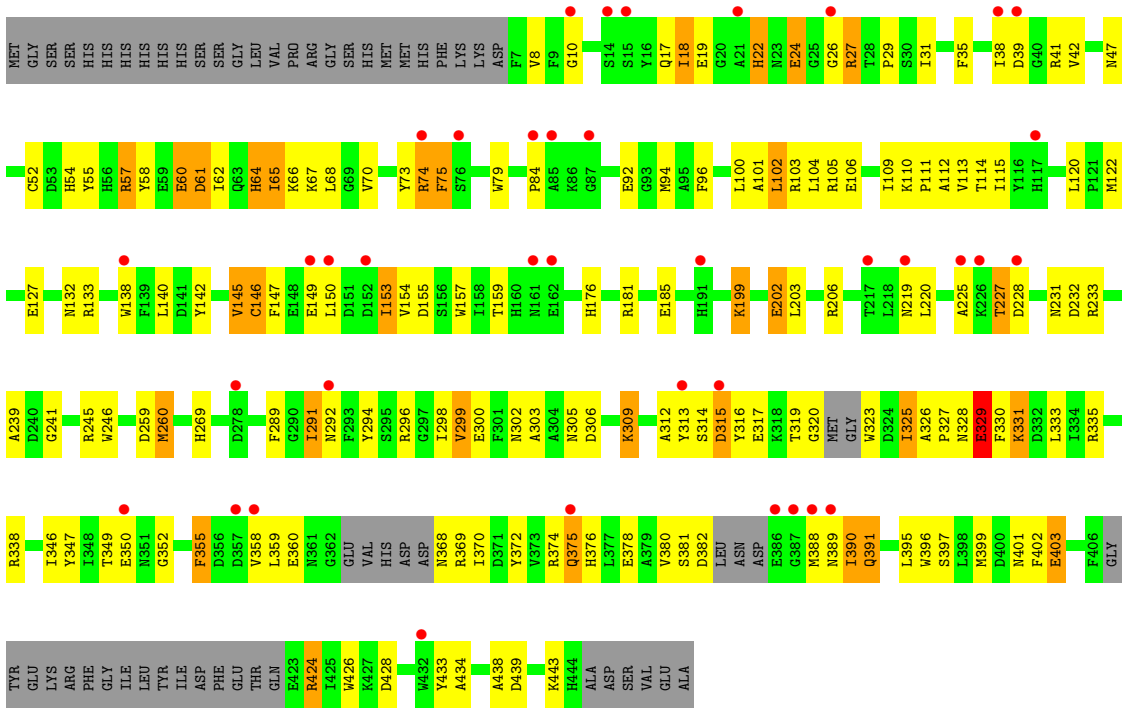
• Molecule 1: Beta-glucosidase

Chain J:



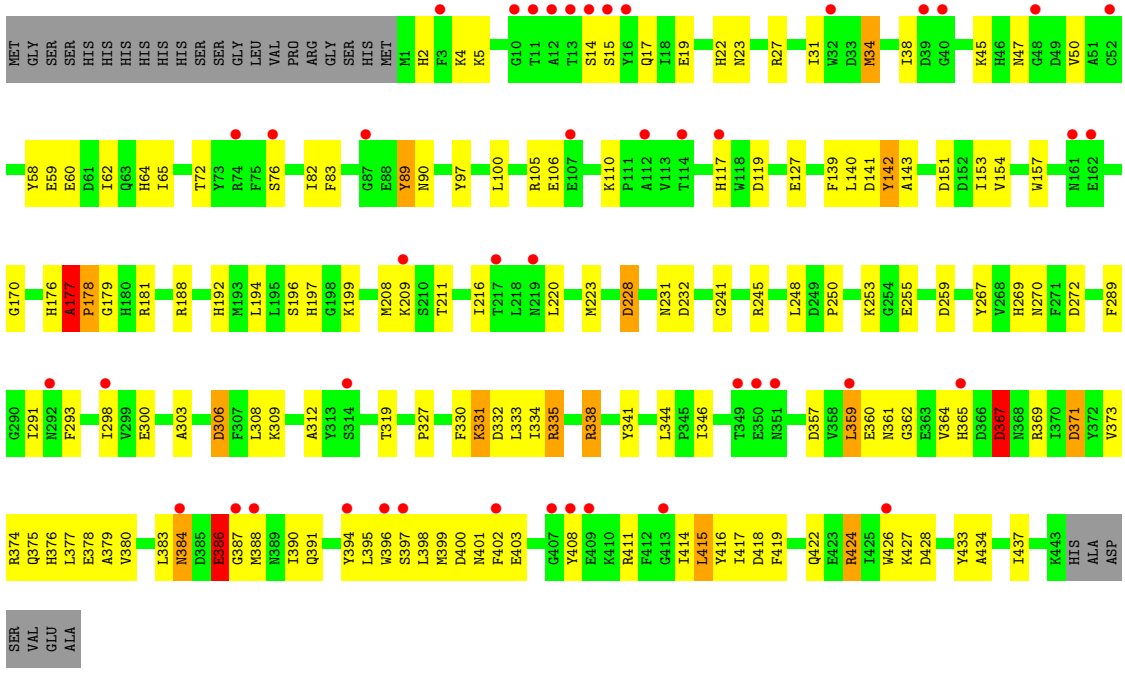
• Molecule 1: Beta-glucosidase

Chain K:



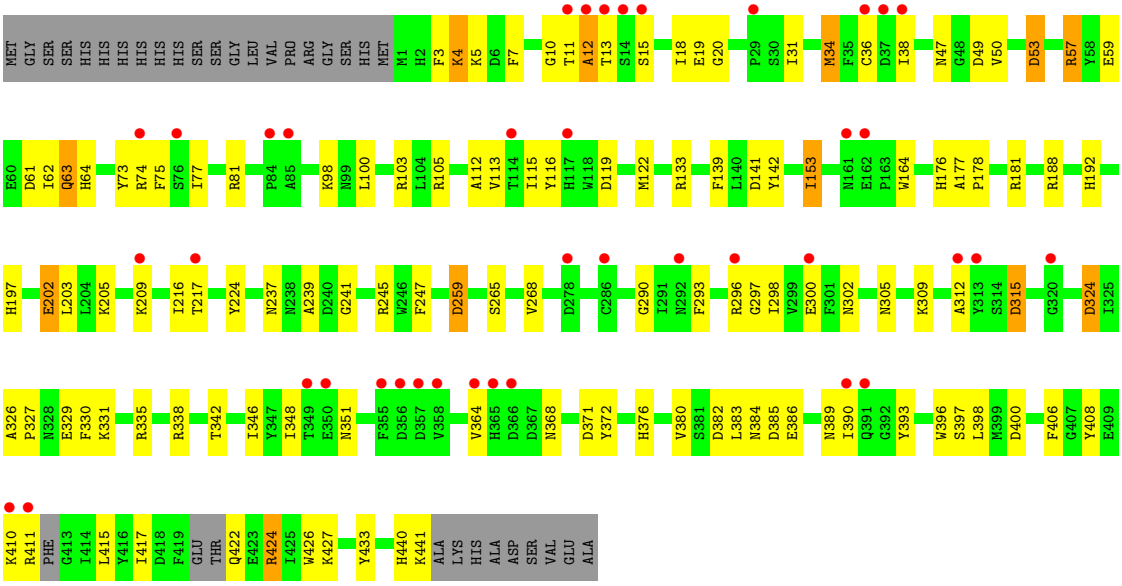
• Molecule 1: Beta-glucosidase

Chain L:



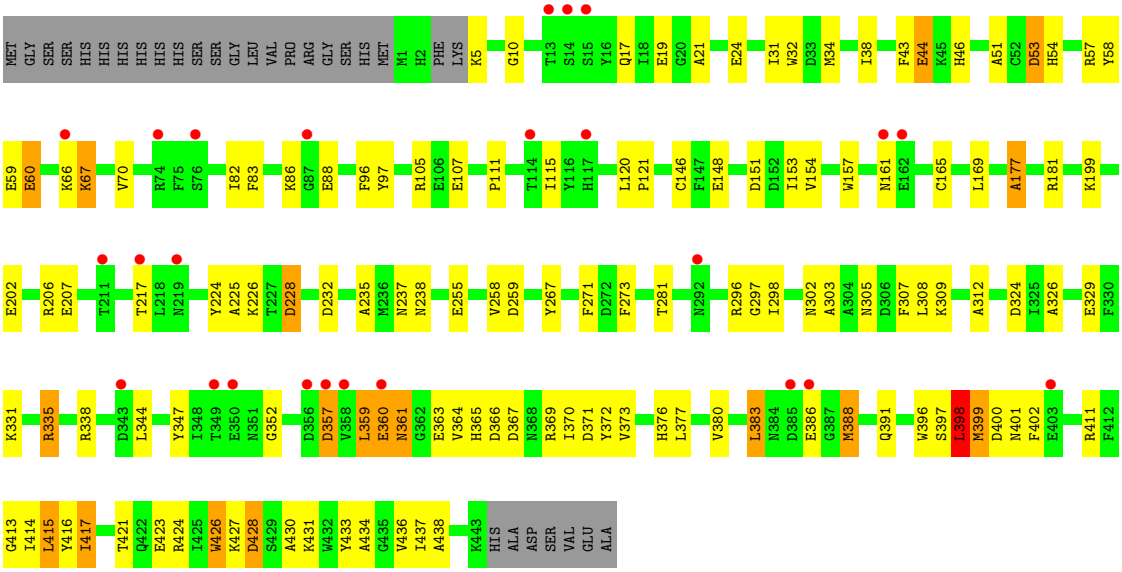
• Molecule 1: Beta-glucosidase

Chain M:



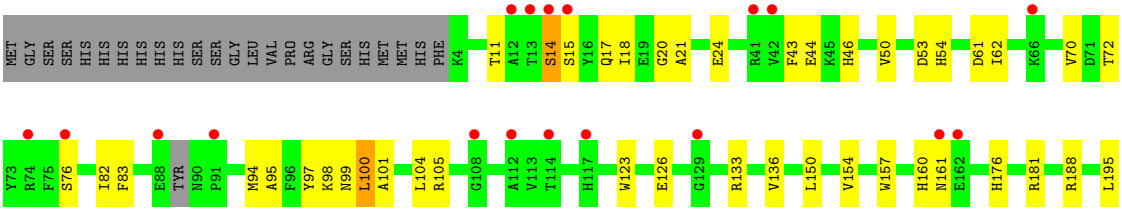
- Molecule 1: Beta-glucosidase

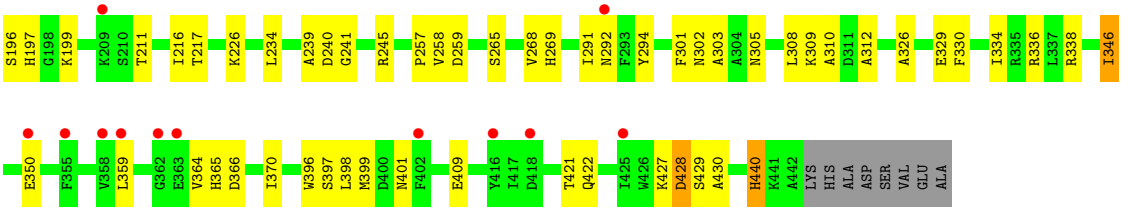
Chain N:



- Molecule 1: Beta-glucosidase

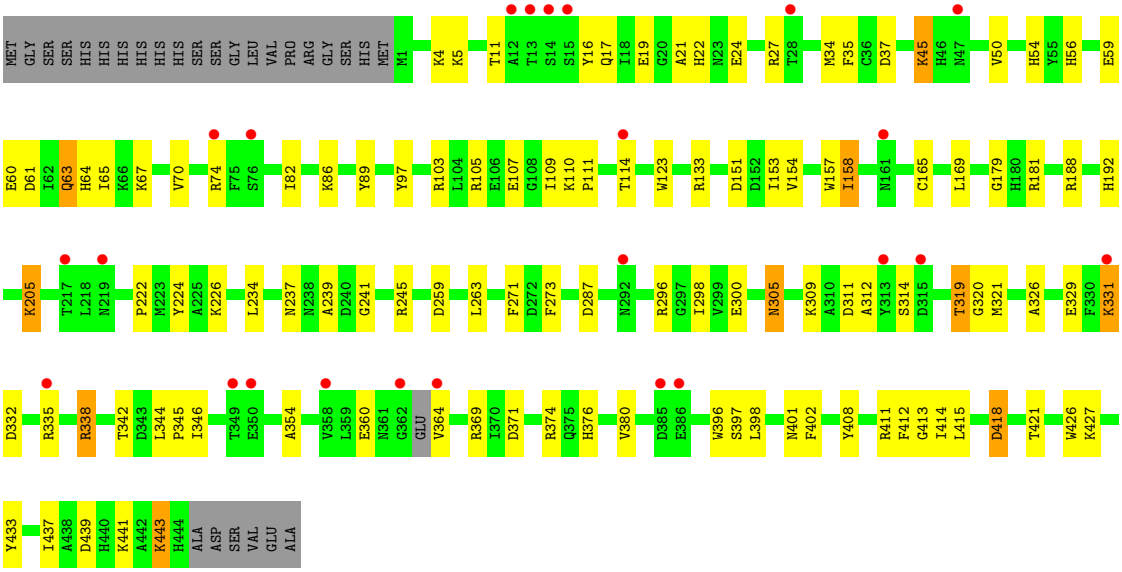
Chain O:





- Molecule 1: Beta-glucosidase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.16Å 171.90Å 213.52Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	32.71 – 3.51 34.15 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.71-3.51) 98.2 (34.15-3.51)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.8.3	Depositor
R, R_{free}	0.263 , 0.292 0.262 , 0.291	Depositor DCC
R_{free} test set	4497 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	94.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 4.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	57949	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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 (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	0.25	0/3765	0.49	0/5102
1	B	0.25	0/3760	0.51	0/5095
1	C	0.25	0/3773	0.50	0/5112
1	D	0.26	0/3773	0.52	2/5112 (0.0%)
1	E	0.24	0/3781	0.48	0/5123
1	F	0.25	0/3765	0.51	0/5102
1	G	0.24	0/3760	0.49	1/5095 (0.0%)
1	H	0.24	0/3765	0.48	0/5102
1	I	0.27	0/3710	0.63	4/5027 (0.1%)
1	J	0.30	0/3760	0.60	1/5095 (0.0%)
1	K	0.30	0/3476	0.70	2/4709 (0.0%)
1	L	0.29	0/3749	0.65	5/5080 (0.1%)
1	M	0.27	0/3705	0.55	2/5018 (0.0%)
1	N	0.28	0/3727	0.61	1/5050 (0.0%)
1	O	0.26	0/3695	0.55	2/5007 (0.0%)
1	P	0.25	0/3750	0.51	1/5080 (0.0%)
All	All	0.26	0/59714	0.55	21/80909 (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	L	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	177	ALA	C-N-CD	-9.41	99.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	387	GLY	N-CA-C	-8.10	92.85	113.10
1	L	386	GLU	N-CA-C	7.08	130.13	111.00
1	I	204	LEU	CA-CB-CG	6.85	131.06	115.30
1	I	415	LEU	CA-CB-CG	6.54	130.33	115.30
1	L	308	LEU	CA-CB-CG	6.52	130.29	115.30
1	I	100	LEU	CA-CB-CG	6.18	129.51	115.30
1	D	169	LEU	CA-CB-CG	6.16	129.46	115.30
1	J	177	ALA	C-N-CD	6.13	141.27	128.40
1	O	100	LEU	CA-CB-CG	5.99	129.08	115.30
1	K	65	ILE	CG1-CB-CG2	-5.92	98.39	111.40
1	L	359	LEU	CA-CB-CG	5.84	128.72	115.30
1	D	415	LEU	CA-CB-CG	5.71	128.42	115.30
1	I	259	ASP	CB-CG-OD2	5.65	123.38	118.30
1	O	188	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	P	82	ILE	CG1-CB-CG2	-5.54	99.22	111.40
1	K	102	LEU	CA-CB-CG	5.51	127.97	115.30
1	M	12	ALA	N-CA-C	5.44	125.68	111.00
1	M	15	SER	N-CA-C	5.15	124.90	111.00
1	N	398	LEU	CA-CB-CG	5.02	126.84	115.30
1	G	359	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	240	ASP	Sidechain
1	L	177	ALA	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	3653	0	3400	47	0
1	B	3648	0	3395	57	0
1	C	3661	0	3409	58	0
1	D	3661	0	3409	62	0
1	E	3669	0	3413	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3653	0	3400	64	0
1	G	3648	0	3395	45	0
1	H	3653	0	3400	47	0
1	I	3600	0	3343	100	0
1	J	3648	0	3395	93	2
1	K	3375	0	3138	119	0
1	L	3638	0	3388	109	0
1	M	3597	0	3346	78	2
1	N	3618	0	3365	103	0
1	O	3588	0	3337	57	0
1	P	3639	0	3388	68	0
All	All	57949	0	53921	1115	2

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 10.

All (1115) 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:D:364:VAL:HG22	1:D:427:LYS:HD2	1.52	0.92
1:J:66:LYS:HE2	1:J:107:GLU:HG3	1.50	0.90
1:K:241:GLY:HA2	1:K:245:ARG:HG2	1.52	0.90
1:N:105:ARG:NH1	1:N:153:ILE:O	2.05	0.89
1:M:11:THR:HG23	1:M:12:ALA:H	1.37	0.88
1:I:335:ARG:HH12	1:N:335:ARG:HG2	1.39	0.88
1:B:5:LYS:H	1:B:5:LYS:HD3	1.35	0.88
1:D:364:VAL:H	1:D:427:LYS:HD3	1.38	0.88
1:D:19:GLU:OE1	1:D:81:ARG:NH1	2.12	0.83
1:N:415:LEU:HD21	1:N:424:ARG:HG2	1.61	0.83
1:N:347:TYR:HE1	1:N:391:GLN:HB3	1.43	0.83
1:J:424:ARG:H	1:J:424:ARG:HE	1.23	0.82
1:N:235:ALA:HA	1:N:309:LYS:HD2	1.61	0.82
1:N:364:VAL:H	1:N:427:LYS:NZ	1.78	0.82
1:L:331:LYS:HZ3	1:L:379:ALA:HB1	1.44	0.81
1:C:406:PHE:HB3	1:C:410:LYS:HD3	1.63	0.81
1:L:374:ARG:NH1	1:L:378:GLU:OE2	2.15	0.79
1:I:30:SER:O	1:I:32:TRP:N	2.13	0.79
1:D:429:SER:O	1:D:431:LYS:N	2.14	0.79
1:P:369:ARG:NH1	1:P:413:GLY:O	2.16	0.79
1:N:331:LYS:HG2	1:N:383:LEU:HD11	1.64	0.78
1:N:360:GLU:O	1:N:361:ASN:ND2	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ASN:OD1	1:C:188:ARG:NH1	2.16	0.77
1:E:369:ARG:NH2	1:E:411:ARG:O	2.18	0.77
1:L:411:ARG:HH21	1:L:416:TYR:HA	1.49	0.77
1:P:305:ASN:HD21	1:P:309:LYS:H	1.30	0.77
1:K:320:GLY:HA3	1:K:355:PHE:HA	1.64	0.77
1:H:184:ASN:OD1	1:H:188:ARG:NH1	2.18	0.77
1:I:19:GLU:OE1	1:I:81:ARG:NH2	2.17	0.77
1:N:305:ASN:HD22	1:N:309:LYS:H	1.29	0.77
1:J:334:ILE:HD11	1:J:383:LEU:HD22	1.66	0.77
1:C:364:VAL:HB	1:C:427:LYS:HG3	1.67	0.76
1:L:364:VAL:HG21	1:L:427:LYS:HD3	1.67	0.76
1:N:398:LEU:HD13	1:N:399:MET:HG2	1.66	0.75
1:G:226:LYS:HG3	1:G:227:THR:HG23	1.68	0.75
1:B:72:THR:HG22	1:B:110:LYS:HB2	1.67	0.75
1:N:371:ASP:OD1	1:N:372:TYR:N	2.20	0.74
1:I:300:GLU:HG3	1:I:312:ALA:HB2	1.70	0.74
1:M:371:ASP:OD1	1:M:372:TYR:N	2.21	0.74
1:A:72:THR:HG22	1:A:110:LYS:HB2	1.69	0.74
1:F:380:VAL:HA	1:F:383:LEU:HD12	1.70	0.74
1:H:366:ASP:OD2	1:H:369:ARG:NH1	2.21	0.74
1:I:418:ASP:OD1	1:I:421:THR:OG1	2.06	0.73
1:L:170:GLY:HA3	1:L:177:ALA:HB3	1.69	0.73
1:K:314:SER:O	1:K:316:TYR:N	2.22	0.72
1:N:428:ASP:OD1	1:N:428:ASP:N	2.17	0.72
1:J:127:GLU:O	1:J:132:ASN:ND2	2.23	0.72
1:J:296:ARG:HD3	1:J:329:GLU:HG2	1.72	0.72
1:N:338:ARG:NH2	1:N:388:MET:O	2.21	0.72
1:N:238:ASN:HB2	1:N:309:LYS:HE3	1.71	0.71
1:N:364:VAL:H	1:N:427:LYS:HZ3	1.37	0.71
1:B:5:LYS:H	1:B:5:LYS:CD	2.04	0.71
1:C:72:THR:HG22	1:C:110:LYS:HB2	1.72	0.71
1:K:62:ILE:HG22	1:K:66:LYS:HE2	1.73	0.71
1:D:241:GLY:HA2	1:D:245:ARG:HB2	1.72	0.71
1:A:302:ASN:HD21	1:A:305:ASN:HB2	1.55	0.71
1:K:231:ASN:ND2	1:L:272:ASP:OD1	2.24	0.71
1:D:165:CYS:HA	1:D:169:LEU:HG	1.73	0.70
1:I:324:ASP:OD1	1:I:324:ASP:N	2.19	0.70
1:I:224:TYR:HD2	1:I:296:ARG:HD3	1.56	0.70
1:H:19:GLU:OE1	1:H:81:ARG:NH2	2.25	0.70
1:J:60:GLU:OE2	1:J:424:ARG:NH2	2.23	0.69
1:J:8:VAL:HG22	1:J:392:GLY:HA3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:TYR:HE1	1:K:75:PHE:HB3	1.55	0.69
1:K:68:LEU:HD22	1:K:70:VAL:HG22	1.73	0.69
1:K:60:GLU:O	1:K:424:ARG:NH2	2.23	0.69
1:H:1:MET:O	1:H:443:LYS:NZ	2.26	0.69
1:K:292:ASN:HD22	1:K:350:GLU:HB2	1.57	0.69
1:M:61:ASP:HA	1:M:424:ARG:HH12	1.57	0.69
1:J:424:ARG:H	1:J:424:ARG:NE	1.89	0.68
1:M:31:ILE:HG12	1:M:177:ALA:HB1	1.75	0.68
1:H:296:ARG:HD3	1:H:329:GLU:HG2	1.75	0.68
1:K:68:LEU:HB3	1:K:70:VAL:HG23	1.74	0.68
1:L:177:ALA:O	1:L:179:GLY:N	2.20	0.68
1:A:411:ARG:NH2	1:A:417:ILE:O	2.27	0.68
1:L:306:ASP:OD1	1:L:306:ASP:N	2.25	0.68
1:N:44:GLU:N	1:N:44:GLU:OE1	2.26	0.68
1:N:417:ILE:HG13	1:N:424:ARG:HG3	1.76	0.68
1:P:59:GLU:OE1	1:P:103:ARG:NH1	2.27	0.68
1:J:27:ARG:HH21	1:J:81:ARG:HD3	1.56	0.68
1:K:338:ARG:NH1	1:K:389:ASN:OD1	2.27	0.68
1:C:318:LYS:HZ1	1:C:322:GLY:C	1.97	0.67
1:L:395:LEU:HD13	1:L:414:ILE:HD11	1.74	0.67
1:J:81:ARG:NH1	1:J:97:TYR:OH	2.28	0.67
1:D:72:THR:HG22	1:D:110:LYS:HB2	1.76	0.67
1:I:5:LYS:H	1:I:5:LYS:HD3	1.59	0.67
1:D:364:VAL:HG13	1:D:427:LYS:HZ3	1.60	0.67
1:O:427:LYS:NZ	1:O:428:ASP:OD1	2.27	0.67
1:I:364:VAL:HG21	1:I:427:LYS:HB2	1.76	0.67
1:M:181:ARG:O	1:O:303:ALA:HB3	1.95	0.66
1:L:331:LYS:NZ	1:L:379:ALA:HB1	2.10	0.66
1:P:300:GLU:HG3	1:P:312:ALA:HB2	1.76	0.66
1:J:134:GLU:HG2	1:J:138:TRP:NE1	2.10	0.66
1:L:105:ARG:NH2	1:L:153:ILE:O	2.29	0.66
1:K:26:GLY:O	1:K:84:PRO:HB3	1.96	0.66
1:M:13:THR:HG23	1:M:398:LEU:HB3	1.77	0.66
1:O:160:HIS:NE2	1:O:196:SER:OG	2.28	0.65
1:K:74:ARG:NH1	1:K:114:THR:OG1	2.29	0.65
1:M:47:ASN:ND2	1:M:49:ASP:OD1	2.28	0.65
1:P:338:ARG:HH22	1:P:346:ILE:HD12	1.60	0.65
1:A:365:HIS:N	1:A:427:LYS:HE3	2.12	0.65
1:J:169:LEU:HD12	1:J:173:VAL:HG21	1.79	0.65
1:G:58:TYR:OH	1:G:99:ASN:ND2	2.29	0.65
1:C:365:HIS:ND1	1:C:428:ASP:OD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:ILE:HG12	1:L:312:ALA:HB3	1.79	0.65
1:O:11:THR:HG21	1:O:398:LEU:HD13	1.79	0.64
1:E:427:LYS:O	1:E:429:SER:N	2.26	0.64
1:C:63:GLN:OE1	1:C:63:GLN:N	2.30	0.64
1:I:11:THR:HG21	1:I:398:LEU:HD13	1.80	0.64
1:P:296:ARG:NH2	1:P:314:SER:OG	2.30	0.64
1:J:359:LEU:HA	1:J:364:VAL:HG12	1.80	0.64
1:M:188:ARG:O	1:M:192:HIS:ND1	2.28	0.64
1:L:332:ASP:OD1	1:L:335:ARG:NH2	2.31	0.64
1:P:326:ALA:HB1	1:P:329:GLU:HB2	1.78	0.64
1:D:364:VAL:N	1:D:427:LYS:HD3	2.12	0.64
1:J:63:GLN:OE1	1:J:66:LYS:NZ	2.22	0.64
1:M:296:ARG:HG2	1:M:297:GLY:N	2.12	0.64
1:F:228:ASP:OD1	1:F:233:ARG:NH2	2.31	0.63
1:F:131:VAL:HG12	1:F:188:ARG:HH21	1.63	0.63
1:H:194:LEU:HB3	1:H:282:ILE:HD13	1.80	0.63
1:M:400:ASP:HB2	1:M:417:ILE:HB	1.80	0.63
1:I:241:GLY:HA2	1:I:245:ARG:HB2	1.79	0.63
1:E:241:GLY:HA2	1:E:245:ARG:HB2	1.80	0.63
1:M:181:ARG:HD2	1:O:302:ASN:HA	1.79	0.63
1:C:318:LYS:NZ	1:C:323:TRP:O	2.28	0.63
1:C:331:LYS:O	1:C:335:ARG:HG2	1.98	0.63
1:E:67:LYS:HG3	1:E:426:TRP:HZ2	1.64	0.63
1:K:328:ASN:O	1:K:331:LYS:N	2.32	0.63
1:E:2:HIS:N	1:E:381:SER:OG	2.32	0.63
1:F:129:GLY:O	1:F:135:SER:OG	2.17	0.63
1:I:35:PHE:O	1:I:38:ILE:HG12	1.99	0.63
1:J:286:CYS:SG	1:J:287:ASP:N	2.71	0.63
1:K:259:ASP:OD1	1:K:260:MET:N	2.32	0.63
1:N:51:ALA:HA	1:N:402:PHE:HE1	1.64	0.63
1:J:105:ARG:NH2	1:J:153:ILE:O	2.31	0.63
1:K:331:LYS:O	1:K:335:ARG:NH1	2.32	0.63
1:I:319:THR:OG1	1:I:320:GLY:N	2.31	0.63
1:L:400:ASP:OD2	1:L:417:ILE:N	2.31	0.63
1:N:267:TYR:HA	1:O:269:HIS:HE2	1.63	0.63
1:D:298:ILE:HG12	1:D:312:ALA:HB3	1.80	0.62
1:C:95:ALA:HA	1:C:98:LYS:HE2	1.79	0.62
1:D:81:ARG:O	1:D:90:ASN:ND2	2.32	0.62
1:N:308:LEU:HB2	1:N:309:LYS:HE2	1.82	0.62
1:K:313:TYR:CE2	1:K:315:ASP:HB3	2.35	0.62
1:O:17:GLN:HB3	1:O:401:ASN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:421:THR:OG1	1:N:423:GLU:OE1	2.17	0.62
1:A:359:LEU:HA	1:A:364:VAL:HG12	1.82	0.61
1:K:326:ALA:O	1:K:375:GLN:NE2	2.33	0.61
1:P:319:THR:OG1	1:P:320:GLY:N	2.33	0.61
1:G:140:LEU:HD11	1:G:199:LYS:HE3	1.80	0.61
1:K:374:ARG:O	1:K:378:GLU:HG3	2.01	0.61
1:A:11:THR:HG21	1:A:398:LEU:HD13	1.82	0.61
1:N:357:ASP:OD1	1:N:411:ARG:NH1	2.24	0.61
1:O:291:ILE:HD12	1:O:346:ILE:HD12	1.81	0.61
1:C:298:ILE:HG12	1:C:312:ALA:HB3	1.81	0.61
1:F:161:ASN:HA	1:F:217:THR:HG23	1.83	0.61
1:M:63:GLN:N	1:M:63:GLN:OE1	2.34	0.61
1:F:181:ARG:NH1	1:H:300:GLU:OE2	2.33	0.61
1:D:53:ASP:OD2	1:D:57:ARG:NH1	2.33	0.61
1:C:41:ARG:NH1	1:C:174:GLY:O	2.34	0.61
1:K:300:GLU:HG3	1:K:312:ALA:HB2	1.83	0.61
1:P:11:THR:HG21	1:P:398:LEU:HD13	1.82	0.60
1:A:302:ASN:ND2	1:A:305:ASN:HB2	2.17	0.60
1:K:31:ILE:HD11	1:K:120:LEU:HD23	1.84	0.60
1:K:65:ILE:HG23	1:K:70:VAL:HG21	1.82	0.60
1:L:371:ASP:HA	1:L:374:ARG:HG2	1.83	0.60
1:A:120:LEU:HD12	1:A:121:PRO:HD2	1.82	0.60
1:B:274:ILE:HD12	1:B:279:MET:HE1	1.83	0.60
1:E:105:ARG:NH1	1:E:153:ILE:O	2.34	0.60
1:L:110:LYS:NZ	1:L:394:TYR:OH	2.34	0.60
1:M:296:ARG:NH2	1:M:324:ASP:OD2	2.27	0.60
1:I:130:TRP:O	1:I:192:HIS:ND1	2.26	0.60
1:P:86:LYS:HG2	1:P:123:TRP:CE3	2.36	0.60
1:E:203:LEU:HD12	1:E:207:GLU:HB2	1.81	0.60
1:K:439:ASP:O	1:K:443:LYS:HE2	2.02	0.60
1:D:364:VAL:HG13	1:D:427:LYS:NZ	2.17	0.60
1:F:38:ILE:HB	1:F:41:ARG:HD2	1.83	0.60
1:N:305:ASN:ND2	1:N:309:LYS:O	2.35	0.60
1:C:226:LYS:HD3	1:C:298:ILE:HD11	1.83	0.60
1:C:231:ASN:ND2	1:D:270:ASN:OD1	2.34	0.60
1:M:141:ASP:OD1	1:M:142:TYR:N	2.35	0.60
1:J:18:ILE:HG22	1:J:54:HIS:HB2	1.83	0.59
1:B:27:ARG:HD2	1:B:81:ARG:HE	1.66	0.59
1:I:347:TYR:HE1	1:I:391:GLN:HB2	1.65	0.59
1:C:2:HIS:O	1:C:381:SER:OG	2.20	0.59
1:D:105:ARG:NH1	1:D:153:ILE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:GLY:O	1:J:176:HIS:N	2.36	0.59
1:N:359:LEU:HD23	1:N:416:TYR:HE2	1.68	0.59
1:F:155:ASP:OD1	1:F:156:SER:N	2.36	0.59
1:I:427:LYS:HG3	1:I:429:SER:H	1.68	0.59
1:K:347:TYR:CZ	1:K:391:GLN:HB3	2.38	0.58
1:N:120:LEU:HD12	1:N:121:PRO:HD2	1.84	0.58
1:F:96:PHE:HA	1:F:99:ASN:HD21	1.68	0.58
1:J:154:VAL:HG21	1:J:157:TRP:CE2	2.38	0.58
1:K:17:GLN:HB3	1:K:401:ASN:HB2	1.84	0.58
1:K:325:ILE:HG12	1:K:326:ALA:H	1.67	0.58
1:F:36:CYS:SG	1:F:47:ASN:HB3	2.42	0.58
1:L:365:HIS:HA	1:L:428:ASP:OD2	2.04	0.58
1:P:133:ARG:HG2	1:P:192:HIS:NE2	2.18	0.58
1:C:105:ARG:NH2	1:C:153:ILE:O	2.36	0.58
1:K:185:GLU:OE2	1:K:185:GLU:N	2.35	0.58
1:L:72:THR:HG23	1:L:110:LYS:HG2	1.85	0.58
1:M:417:ILE:HG12	1:M:424:ARG:HB3	1.84	0.58
1:P:205:LYS:NZ	1:P:287:ASP:OD2	2.36	0.58
1:C:326:ALA:HB1	1:C:329:GLU:HB2	1.86	0.58
1:C:234:LEU:HD12	1:D:258:VAL:HG23	1.86	0.58
1:N:357:ASP:OD1	1:N:357:ASP:N	2.31	0.58
1:F:47:ASN:O	1:F:408:TYR:OH	2.19	0.58
1:I:332:ASP:O	1:I:335:ARG:HG3	2.04	0.58
1:O:83:PHE:O	1:O:123:TRP:NE1	2.34	0.58
1:O:95:ALA:HA	1:O:98:LYS:HD3	1.86	0.58
1:P:103:ARG:NH2	1:P:107:GLU:OE2	2.36	0.58
1:I:82:ILE:HD11	1:I:145:VAL:HG11	1.86	0.58
1:L:289:PHE:CE2	1:L:291:ILE:HD11	2.39	0.58
1:P:298:ILE:HG12	1:P:312:ALA:HB3	1.86	0.58
1:C:274:ILE:HD12	1:C:279:MET:HE3	1.85	0.57
1:E:5:LYS:HE2	1:E:444:HIS:HB3	1.86	0.57
1:P:21:ALA:HB1	1:P:24:GLU:HB2	1.86	0.57
1:P:60:GLU:HG2	1:P:64:HIS:CE1	2.38	0.57
1:A:369:ARG:NH1	1:A:413:GLY:O	2.37	0.57
1:B:383:LEU:HD22	1:B:388:MET:HG3	1.87	0.57
1:L:22:HIS:HA	1:L:27:ARG:HD3	1.86	0.57
1:L:346:ILE:HB	1:L:390:ILE:HG12	1.86	0.57
1:P:60:GLU:HG2	1:P:64:HIS:HE1	1.68	0.57
1:I:194:LEU:HB3	1:I:282:ILE:HD11	1.86	0.57
1:K:434:ALA:O	1:K:438:ALA:N	2.31	0.57
1:O:226:LYS:HE3	1:O:312:ALA:HB1	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:O	1:B:99:ASN:ND2	2.38	0.57
1:F:72:THR:HG22	1:F:110:LYS:HB2	1.86	0.57
1:B:428:ASP:O	1:B:431:LYS:NZ	2.33	0.57
1:K:338:ARG:HH12	1:K:388:MET:C	2.08	0.57
1:B:300:GLU:OE1	1:D:181:ARG:NH2	2.38	0.57
1:L:300:GLU:HG3	1:L:312:ALA:HB2	1.86	0.57
1:D:27:ARG:HD2	1:D:81:ARG:NH2	2.20	0.57
1:D:335:ARG:NH2	1:D:386:GLU:OE1	2.37	0.57
1:I:275:GLN:OE1	1:I:275:GLN:N	2.38	0.57
1:I:27:ARG:HE	1:I:81:ARG:HG2	1.69	0.57
1:J:298:ILE:HG12	1:J:312:ALA:HB3	1.85	0.57
1:K:355:PHE:CE2	1:K:369:ARG:HD3	2.40	0.57
1:L:338:ARG:NH2	1:L:344:LEU:O	2.37	0.57
1:M:382:ASP:OD1	1:M:383:LEU:N	2.37	0.57
1:A:34:MET:HG3	1:A:35:PHE:N	2.20	0.57
1:B:96:PHE:HA	1:B:99:ASN:HD21	1.69	0.57
1:C:205:LYS:NZ	1:C:287:ASP:OD1	2.33	0.57
1:D:129:GLY:O	1:D:135:SER:OG	2.15	0.57
1:K:153:ILE:HD13	1:K:153:ILE:H	1.69	0.57
1:C:318:LYS:HZ2	1:C:318:LYS:HB3	1.68	0.57
1:J:23:ASN:O	1:J:23:ASN:ND2	2.28	0.57
1:K:74:ARG:NH2	1:K:350:GLU:OE2	2.38	0.57
1:M:10:GLY:O	1:M:433:TYR:OH	2.22	0.57
1:P:19:GLU:OE2	1:P:97:TYR:OH	2.17	0.57
1:C:44:GLU:HB2	1:C:46:HIS:CE1	2.40	0.56
1:I:315:ASP:OD1	1:I:315:ASP:N	2.28	0.56
1:J:152:ASP:OD1	1:J:152:ASP:N	2.38	0.56
1:N:298:ILE:HG23	1:N:312:ALA:HB3	1.87	0.56
1:P:54:HIS:ND1	1:P:61:ASP:OD2	2.35	0.56
1:D:434:ALA:O	1:D:437:ILE:HG13	2.05	0.56
1:I:335:ARG:HB2	1:N:386:GLU:HG2	1.87	0.56
1:E:67:LYS:HG3	1:E:426:TRP:CZ2	2.40	0.56
1:I:271:PHE:HB2	1:J:231:ASN:OD1	2.06	0.56
1:O:99:ASN:OD1	1:O:100:LEU:N	2.39	0.56
1:O:294:TYR:OH	1:O:350:GLU:OE2	2.22	0.56
1:P:17:GLN:NE2	1:P:401:ASN:OD1	2.38	0.56
1:N:32:TRP:NE1	1:N:177:ALA:HB2	2.21	0.56
1:N:267:TYR:HA	1:O:269:HIS:NE2	2.20	0.56
1:O:365:HIS:O	1:O:365:HIS:ND1	2.38	0.56
1:K:19:GLU:HA	1:K:54:HIS:HB3	1.88	0.56
1:J:428:ASP:HA	1:J:431:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:VAL:HG23	1:P:234:LEU:HD22	1.88	0.56
1:K:352:GLY:HA3	1:K:396:TRP:O	2.06	0.56
1:O:195:LEU:HG	1:O:199:LYS:HE3	1.88	0.56
1:C:230:ALA:HA	1:C:233:ARG:HD3	1.88	0.56
1:G:72:THR:HG22	1:G:110:LYS:HB2	1.88	0.56
1:K:202:GLU:HG2	1:K:206:ARG:HD3	1.87	0.56
1:N:60:GLU:OE2	1:N:424:ARG:NH2	2.38	0.56
1:G:237:ASN:HD22	1:H:258:VAL:HG21	1.71	0.56
1:J:181:ARG:O	1:L:303:ALA:HB3	2.06	0.56
1:M:19:GLU:HG2	1:M:81:ARG:HH11	1.71	0.56
1:N:228:ASP:OD1	1:N:228:ASP:N	2.38	0.56
1:B:86:LYS:HG2	1:B:123:TRP:CE3	2.40	0.55
1:D:5:LYS:HD2	1:D:444:HIS:CD2	2.41	0.55
1:P:237:ASN:O	1:P:245:ARG:NH1	2.39	0.55
1:C:318:LYS:HZ2	1:C:318:LYS:CB	2.20	0.55
1:F:103:ARG:NH1	1:F:106:GLU:OE1	2.39	0.55
1:K:105:ARG:NH2	1:K:153:ILE:O	2.39	0.55
1:M:331:LYS:O	1:M:335:ARG:NE	2.39	0.55
1:P:63:GLN:HG3	1:P:64:HIS:N	2.19	0.55
1:A:154:VAL:HG21	1:A:157:TRP:CE2	2.42	0.55
1:L:267:TYR:OH	1:L:306:ASP:OD2	2.24	0.55
1:L:434:ALA:O	1:L:437:ILE:HG13	2.06	0.55
1:F:241:GLY:HA2	1:F:245:ARG:HB2	1.87	0.55
1:I:347:TYR:CE1	1:I:391:GLN:HB2	2.42	0.55
1:L:241:GLY:HA2	1:L:245:ARG:HB2	1.88	0.55
1:H:389:ASN:OD1	1:H:391:GLN:NE2	2.29	0.55
1:I:59:GLU:CD	1:I:103:ARG:HH12	2.10	0.55
1:I:82:ILE:HD13	1:I:83:PHE:HB2	1.88	0.55
1:I:224:TYR:CD2	1:I:296:ARG:HD3	2.40	0.55
1:L:331:LYS:CE	1:L:383:LEU:HD11	2.37	0.55
1:E:154:VAL:HG21	1:E:157:TRP:CE2	2.42	0.55
1:I:14:SER:O	1:I:18:ILE:HG22	2.06	0.55
1:I:253:LYS:HE3	1:I:341:TYR:CE1	2.42	0.55
1:L:228:ASP:OD1	1:L:228:ASP:N	2.40	0.55
1:L:197:HIS:CE1	1:L:216:ILE:HB	2.42	0.55
1:N:31:ILE:HD12	1:N:177:ALA:HB1	1.88	0.55
1:P:414:ILE:HG23	1:P:415:LEU:HD12	1.89	0.55
1:F:399:MET:HB2	1:F:417:ILE:HD11	1.89	0.54
1:G:298:ILE:HG12	1:G:312:ALA:HB3	1.89	0.54
1:N:357:ASP:CG	1:N:411:ARG:HH12	2.08	0.54
1:A:226:LYS:HD3	1:A:312:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:LYS:O	1:D:435:GLY:N	2.37	0.54
1:F:62:ILE:HA	1:F:65:ILE:HD12	1.89	0.54
1:H:72:THR:HG22	1:H:110:LYS:HB2	1.89	0.54
1:L:15:SER:H	1:L:76:SER:HB3	1.72	0.54
1:D:294:TYR:OH	1:D:350:GLU:OE1	2.22	0.54
1:F:181:ARG:O	1:H:303:ALA:HB3	2.07	0.54
1:I:19:GLU:N	1:I:51:ALA:O	2.39	0.54
1:J:11:THR:HG21	1:J:398:LEU:HD13	1.88	0.54
1:J:397:SER:OG	1:J:412:PHE:O	2.25	0.54
1:B:371:ASP:O	1:B:374:ARG:HG3	2.07	0.54
1:I:100:LEU:HD12	1:I:101:ALA:N	2.22	0.54
1:I:225:ALA:HB1	1:I:232:ASP:HB3	1.89	0.54
1:L:379:ALA:O	1:L:383:LEU:HD12	2.08	0.54
1:D:364:VAL:H	1:D:427:LYS:CD	2.17	0.54
1:D:429:SER:HA	1:D:432:TRP:HB3	1.90	0.54
1:L:371:ASP:OD1	1:L:371:ASP:N	2.31	0.54
1:P:105:ARG:NH2	1:P:153:ILE:O	2.41	0.54
1:B:120:LEU:HD12	1:B:121:PRO:HD2	1.90	0.54
1:E:441:LYS:O	1:E:444:HIS:ND1	2.40	0.54
1:I:326:ALA:HB1	1:I:329:GLU:OE2	2.08	0.54
1:L:19:GLU:OE1	1:L:97:TYR:OH	2.22	0.54
1:L:327:PRO:O	1:L:331:LYS:HD2	2.07	0.54
1:A:299:VAL:HG11	1:A:309:LYS:HB2	1.88	0.54
1:F:239:ALA:HB2	1:F:309:LYS:HD2	1.90	0.54
1:M:11:THR:HG23	1:M:12:ALA:N	2.17	0.54
1:D:414:ILE:HG13	1:D:415:LEU:HD13	1.90	0.54
1:J:35:PHE:CZ	1:J:41:ARG:HG2	2.42	0.54
1:J:66:LYS:HE2	1:J:107:GLU:CG	2.30	0.54
1:P:226:LYS:HD3	1:P:298:ILE:HD11	1.89	0.54
1:B:63:GLN:OE1	1:B:66:LYS:NZ	2.35	0.54
1:D:21:ALA:HB3	1:D:55:TYR:HD2	1.72	0.53
1:J:59:GLU:OE1	1:J:63:GLN:NE2	2.42	0.53
1:J:154:VAL:HG21	1:J:157:TRP:CZ2	2.42	0.53
1:L:369:ARG:NH2	1:L:411:ARG:O	2.41	0.53
1:M:59:GLU:HA	1:M:103:ARG:HH22	1.72	0.53
1:J:166:ALA:HB3	1:J:193:MET:HE1	1.89	0.53
1:O:302:ASN:ND2	1:O:305:ASN:HB2	2.23	0.53
1:C:62:ILE:HD12	1:C:104:LEU:HD21	1.91	0.53
1:K:74:ARG:C	1:K:74:ARG:HD2	2.29	0.53
1:K:319:THR:HG21	1:K:323:TRP:HB2	1.90	0.53
1:O:292:ASN:ND2	1:O:350:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:ARG:HG3	1:N:207:GLU:N	2.23	0.53
1:O:97:TYR:HA	1:O:100:LEU:HG	1.90	0.53
1:A:136:VAL:O	1:A:140:LEU:HD13	2.08	0.53
1:H:327:PRO:HB3	1:H:376:HIS:HD2	1.73	0.53
1:C:191:HIS:CE1	1:C:274:ILE:HD13	2.44	0.53
1:F:5:LYS:HB3	1:F:443:LYS:HG2	1.90	0.53
1:I:31:ILE:HD12	1:I:120:LEU:O	2.09	0.53
1:J:42:VAL:HG12	1:J:405:SER:HA	1.90	0.53
1:K:153:ILE:HG12	1:K:154:VAL:N	2.24	0.53
1:A:331:LYS:HE3	1:A:379:ALA:HA	1.91	0.53
1:I:31:ILE:HD11	1:I:119:ASP:HA	1.91	0.53
1:I:89:TYR:HD1	1:I:90:ASN:N	2.07	0.53
1:K:220:LEU:HD12	1:K:291:ILE:HD11	1.91	0.53
1:L:335:ARG:HG2	1:L:388:MET:HE3	1.91	0.53
1:A:359:LEU:HD22	1:A:416:TYR:HE2	1.74	0.53
1:D:363:GLU:HA	1:D:427:LYS:HD3	1.91	0.53
1:E:364:VAL:HB	1:E:427:LYS:HB3	1.90	0.53
1:H:280:GLU:N	1:H:280:GLU:OE2	2.41	0.53
1:J:373:VAL:HG21	1:J:433:TYR:OH	2.09	0.53
1:L:64:HIS:CE1	1:L:426:TRP:HE1	2.27	0.53
1:L:376:HIS:O	1:L:380:VAL:N	2.39	0.53
1:N:398:LEU:HD13	1:N:399:MET:CG	2.38	0.53
1:H:241:GLY:HA2	1:H:245:ARG:HB2	1.90	0.52
1:M:300:GLU:HG3	1:M:312:ALA:HB2	1.91	0.52
1:P:241:GLY:HA2	1:P:245:ARG:HB2	1.90	0.52
1:P:418:ASP:OD2	1:P:421:THR:OG1	2.27	0.52
1:B:57:ARG:HG2	1:B:60:GLU:HB3	1.91	0.52
1:B:318:LYS:HE3	1:B:322:GLY:O	2.09	0.52
1:E:197:HIS:CE1	1:E:216:ILE:HB	2.43	0.52
1:I:59:GLU:OE1	1:I:103:ARG:NH1	2.39	0.52
1:I:303:ALA:HB3	1:K:181:ARG:O	2.09	0.52
1:K:326:ALA:HA	1:K:329:GLU:HG2	1.92	0.52
1:L:373:VAL:HG21	1:L:395:LEU:HD11	1.91	0.52
1:M:338:ARG:HD3	1:M:342:THR:O	2.10	0.52
1:D:136:VAL:O	1:D:140:LEU:HD13	2.09	0.52
1:E:334:ILE:HG22	1:E:388:MET:HE2	1.92	0.52
1:F:321:MET:HG2	1:F:410:LYS:HE2	1.92	0.52
1:G:204:LEU:HG	1:G:210:SER:HB3	1.91	0.52
1:H:62:ILE:HD11	1:H:100:LEU:HD12	1.90	0.52
1:K:298:ILE:HG12	1:K:312:ALA:HB3	1.91	0.52
1:L:17:GLN:OE1	1:L:401:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:HIS:ND1	1:O:61:ASP:OD2	2.38	0.52
1:I:161:ASN:HA	1:I:217:THR:HG23	1.91	0.52
1:I:335:ARG:NH1	1:N:335:ARG:HG2	2.19	0.52
1:J:79:TRP:HA	1:J:142:TYR:CE1	2.45	0.52
1:M:11:THR:CG2	1:M:12:ALA:H	2.15	0.52
1:N:400:ASP:N	1:N:413:GLY:HA3	2.24	0.52
1:K:38:ILE:HD12	1:K:41:ARG:HG3	1.92	0.52
1:O:100:LEU:HD12	1:O:101:ALA:N	2.25	0.52
1:J:177:ALA:HB1	1:J:178:PRO:CD	2.40	0.52
1:D:197:HIS:CE1	1:D:216:ILE:HB	2.45	0.52
1:F:35:PHE:CE1	1:F:41:ARG:HD3	2.44	0.52
1:G:132:ASN:OD1	1:G:134:GLU:HG2	2.09	0.52
1:I:204:LEU:HD12	1:I:205:LYS:N	2.24	0.52
1:L:376:HIS:O	1:L:380:VAL:HG23	2.10	0.52
1:P:35:PHE:CE1	1:P:179:GLY:HA3	2.44	0.52
1:G:237:ASN:OD1	1:G:245:ARG:NH1	2.43	0.52
1:I:25:GLY:O	1:I:90:ASN:ND2	2.34	0.52
1:K:349:THR:O	1:K:350:GLU:HG3	2.10	0.52
1:L:331:LYS:HE3	1:L:331:LYS:HA	1.91	0.52
1:L:383:LEU:HB3	1:L:390:ILE:HD12	1.90	0.52
1:I:329:GLU:H	1:I:329:GLU:CD	2.12	0.52
1:L:139:PHE:HD2	1:L:196:SER:HB2	1.75	0.52
1:M:62:ILE:HD12	1:M:103:ARG:NH2	2.25	0.52
1:O:240:ASP:OD2	1:O:336:ARG:NH2	2.40	0.51
1:G:191:HIS:HE1	1:G:274:ILE:HA	1.74	0.51
1:L:359:LEU:HD21	1:L:416:TYR:CD1	2.45	0.51
1:M:53:ASP:OD1	1:M:57:ARG:HD3	2.10	0.51
1:J:38:ILE:HD11	1:J:41:ARG:HD3	1.92	0.51
1:J:63:GLN:HA	1:J:66:LYS:HD2	1.92	0.51
1:K:55:TYR:HA	1:K:96:PHE:CZ	2.45	0.51
1:N:296:ARG:HG2	1:N:297:GLY:N	2.25	0.51
1:A:199:LYS:HG2	1:A:281:THR:HG21	1.93	0.51
1:C:154:VAL:HG21	1:C:157:TRP:CE2	2.46	0.51
1:E:169:LEU:HD12	1:E:176:HIS:CG	2.46	0.51
1:F:154:VAL:HG21	1:F:157:TRP:CE2	2.45	0.51
1:I:292:ASN:OD1	1:I:349:THR:OG1	2.20	0.51
1:L:369:ARG:HH22	1:L:411:ARG:NH1	2.08	0.51
1:P:331:LYS:NZ	1:P:335:ARG:HH21	2.08	0.51
1:B:165:CYS:HA	1:B:169:LEU:HB3	1.92	0.51
1:F:27:ARG:HD2	1:F:81:ARG:CZ	2.41	0.51
1:J:10:GLY:HA2	1:J:72:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:LEU:HG	1:J:433:TYR:CE2	2.46	0.51
1:M:259:ASP:HA	1:N:259:ASP:HA	1.93	0.51
1:K:73:TYR:CE1	1:K:75:PHE:HB3	2.40	0.51
1:N:44:GLU:HB2	1:N:46:HIS:CE1	2.45	0.51
1:E:101:ALA:HA	1:E:104:LEU:HD12	1.92	0.51
1:F:335:ARG:NH1	1:F:386:GLU:OE1	2.44	0.51
1:K:74:ARG:HD2	1:K:75:PHE:N	2.26	0.51
1:L:58:TYR:CE2	1:L:59:GLU:HG2	2.46	0.51
1:N:376:HIS:O	1:N:380:VAL:HG23	2.10	0.51
1:B:19:GLU:HA	1:B:54:HIS:HB3	1.93	0.51
1:C:1:MET:O	1:C:381:SER:OG	2.28	0.51
1:H:364:VAL:HG22	1:H:366:ASP:HB2	1.92	0.51
1:I:21:ALA:HB1	1:I:24:GLU:HB2	1.93	0.51
1:M:324:ASP:OD1	1:M:324:ASP:N	2.41	0.51
1:J:363:GLU:OE1	1:J:431:LYS:NZ	2.36	0.51
1:N:105:ARG:HH11	1:N:111:PRO:CD	2.24	0.51
1:O:14:SER:O	1:O:18:ILE:HG12	2.11	0.51
1:H:161:ASN:HA	1:H:217:THR:HG23	1.92	0.50
1:N:161:ASN:HA	1:N:217:THR:HG23	1.93	0.50
1:P:154:VAL:HG21	1:P:157:TRP:CE2	2.46	0.50
1:C:239:ALA:HB2	1:C:309:LYS:HD3	1.92	0.50
1:N:154:VAL:HG21	1:N:157:TRP:CE2	2.45	0.50
1:O:161:ASN:HA	1:O:217:THR:HG23	1.91	0.50
1:P:433:TYR:CZ	1:P:437:ILE:HD11	2.46	0.50
1:D:82:ILE:HD12	1:D:142:TYR:HE1	1.77	0.50
1:J:165:CYS:O	1:J:169:LEU:HB3	2.11	0.50
1:K:65:ILE:HG23	1:K:70:VAL:CG2	2.42	0.50
1:N:43:PHE:O	1:N:46:HIS:ND1	2.28	0.50
1:N:67:LYS:HB3	1:N:426:TRP:CZ2	2.46	0.50
1:P:369:ARG:NH2	1:P:411:ARG:O	2.44	0.50
1:A:402:PHE:HB2	1:A:408:TYR:HE1	1.76	0.50
1:B:415:LEU:HD21	1:B:426:TRP:CD1	2.46	0.50
1:I:18:ILE:O	1:I:54:HIS:HB3	2.11	0.50
1:K:376:HIS:O	1:K:380:VAL:N	2.42	0.50
1:J:73:TYR:HD2	1:J:104:LEU:HD21	1.76	0.50
1:N:400:ASP:OD1	1:N:417:ILE:HG22	2.12	0.50
1:B:441:LYS:O	1:B:444:HIS:NE2	2.44	0.50
1:I:294:TYR:OH	1:I:350:GLU:OE1	2.22	0.50
1:M:385:ASP:OD1	1:M:386:GLU:N	2.45	0.50
1:N:151:ASP:HA	1:N:154:VAL:HG22	1.94	0.50
1:N:226:LYS:HD2	1:N:312:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ARG:O	1:C:340:GLU:HG2	2.11	0.50
1:L:231:ASN:OD1	1:L:232:ASP:N	2.45	0.50
1:M:298:ILE:HG22	1:M:312:ALA:HB3	1.94	0.50
1:A:115:ILE:HG22	1:A:142:TYR:CE2	2.47	0.50
1:G:191:HIS:CE1	1:G:274:ILE:HA	2.46	0.50
1:K:115:ILE:HD11	1:K:159:THR:HA	1.93	0.50
1:L:89:TYR:HD1	1:L:90:ASN:N	2.10	0.50
1:L:411:ARG:NH2	1:L:416:TYR:HA	2.21	0.50
1:M:217:THR:HG22	1:M:290:GLY:HA3	1.93	0.50
1:N:296:ARG:NH2	1:N:324:ASP:OD2	2.45	0.50
1:D:134:GLU:HG3	1:D:138:TRP:CZ2	2.46	0.50
1:I:15:SER:HB3	1:I:76:SER:O	2.12	0.50
1:J:271:PHE:HA	1:J:273:PHE:CE2	2.47	0.50
1:P:70:VAL:HG12	1:P:437:ILE:HD13	1.93	0.50
1:C:340:GLU:HG3	1:C:341:TYR:CD2	2.47	0.49
1:N:224:TYR:HE2	1:N:329:GLU:HG3	1.77	0.49
1:F:24:GLU:N	1:F:24:GLU:OE1	2.45	0.49
1:J:27:ARG:NH2	1:J:81:ARG:HD3	2.25	0.49
1:K:319:THR:CG2	1:K:323:TRP:HB2	2.42	0.49
1:O:239:ALA:HB2	1:O:309:LYS:HD2	1.94	0.49
1:J:360:GLU:O	1:J:361:ASN:ND2	2.46	0.49
1:N:17:GLN:HB3	1:N:401:ASN:HB2	1.94	0.49
1:B:326:ALA:HB1	1:B:329:GLU:HB2	1.93	0.49
1:D:168:PHE:O	1:D:172:HIS:HB3	2.12	0.49
1:G:225:ALA:HB1	1:G:232:ASP:HB3	1.94	0.49
1:I:27:ARG:HD3	1:I:28:THR:O	2.12	0.49
1:J:82:ILE:HG21	1:J:145:VAL:HG21	1.95	0.49
1:J:187:VAL:HG13	1:J:246:TRP:HZ2	1.76	0.49
1:K:335:ARG:HG2	1:K:388:MET:CE	2.42	0.49
1:L:335:ARG:HA	1:L:388:MET:HE1	1.95	0.49
1:M:241:GLY:HA2	1:M:245:ARG:HB2	1.95	0.49
1:P:65:ILE:HG22	1:P:109:ILE:HD13	1.94	0.49
1:I:169:LEU:HA	1:I:173:VAL:HG23	1.94	0.49
1:I:181:ARG:O	1:K:303:ALA:HB3	2.12	0.49
1:N:307:PHE:O	1:N:309:LYS:HG2	2.13	0.49
1:P:114:THR:HA	1:P:158:ILE:HG12	1.94	0.49
1:D:296:ARG:HD3	1:D:329:GLU:HG2	1.95	0.49
1:K:142:TYR:O	1:K:145:VAL:HG22	2.13	0.49
1:N:58:TYR:CE2	1:N:59:GLU:HG2	2.47	0.49
1:N:303:ALA:HB3	1:P:181:ARG:O	2.13	0.49
1:F:22:HIS:HD2	1:F:49:ASP:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ARG:NH1	1:F:174:GLY:O	2.46	0.49
1:B:164:TRP:HD1	1:B:247:PHE:HE2	1.60	0.49
1:C:136:VAL:O	1:C:140:LEU:HD13	2.13	0.49
1:G:194:LEU:HB3	1:G:282:ILE:HD13	1.95	0.49
1:I:249:ASP:OD1	1:I:341:TYR:OH	2.24	0.49
1:I:300:GLU:HG3	1:I:312:ALA:CB	2.42	0.49
1:K:127:GLU:OE1	1:K:132:ASN:ND2	2.45	0.49
1:P:305:ASN:ND2	1:P:309:LYS:O	2.45	0.49
1:B:294:TYR:OH	1:B:350:GLU:OE1	2.23	0.48
1:H:68:LEU:HD23	1:H:434:ALA:HB2	1.96	0.48
1:J:27:ARG:HE	1:J:81:ARG:HD3	1.78	0.48
1:L:194:LEU:HD21	1:L:250:PRO:HB2	1.95	0.48
1:B:169:LEU:HD12	1:B:173:VAL:HG21	1.96	0.48
1:J:254:GLY:O	1:J:279:MET:HE2	2.13	0.48
1:N:347:TYR:CE1	1:N:391:GLN:HB3	2.35	0.48
1:N:415:LEU:HD12	1:N:426:TRP:HA	1.94	0.48
1:H:21:ALA:HB1	1:H:24:GLU:HB2	1.96	0.48
1:K:380:VAL:O	1:K:390:ILE:HD13	2.13	0.48
1:L:31:ILE:HD11	1:L:178:PRO:HD3	1.95	0.48
1:M:326:ALA:HB1	1:M:329:GLU:HB2	1.94	0.48
1:B:161:ASN:HA	1:B:217:THR:HG23	1.96	0.48
1:C:52:CYS:O	1:C:424:ARG:NH1	2.39	0.48
1:I:296:ARG:HD2	1:I:297:GLY:N	2.28	0.48
1:J:433:TYR:O	1:J:437:ILE:HG12	2.14	0.48
1:M:57:ARG:HH11	1:M:422:GLN:HG3	1.78	0.48
1:E:338:ARG:NH2	1:E:344:LEU:O	2.44	0.48
1:I:267:TYR:HA	1:L:269:HIS:NE2	2.28	0.48
1:I:309:LYS:HG2	1:I:310:ALA:N	2.28	0.48
1:M:351:ASN:OD1	1:M:376:HIS:ND1	2.30	0.48
1:O:440:HIS:O	1:O:440:HIS:CG	2.66	0.48
1:E:421:THR:HG23	1:E:423:GLU:H	1.79	0.48
1:I:24:GLU:O	1:I:27:ARG:HB3	2.14	0.48
1:N:235:ALA:HA	1:N:309:LYS:CD	2.37	0.48
1:B:140:LEU:HD21	1:B:199:LYS:HB3	1.94	0.48
1:B:366:ASP:OD2	1:B:369:ARG:HD2	2.13	0.48
1:B:382:ASP:O	1:B:386:GLU:HG3	2.13	0.48
1:G:318:LYS:NZ	1:G:324:ASP:OD1	2.46	0.48
1:J:169:LEU:O	1:J:173:VAL:HG22	2.14	0.48
1:K:227:THR:O	1:K:227:THR:OG1	2.27	0.48
1:P:45:LYS:HA	1:P:45:LYS:HD3	1.59	0.48
1:A:364:VAL:H	1:A:427:LYS:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:GLY:O	1:K:433:TYR:OH	2.32	0.48
1:A:267:TYR:HA	1:D:269:HIS:NE2	2.29	0.48
1:L:419:PHE:O	1:L:422:GLN:NE2	2.47	0.48
1:M:77:ILE:HD11	1:M:115:ILE:HG23	1.95	0.48
1:N:400:ASP:OD2	1:N:417:ILE:N	2.47	0.48
1:D:352:GLY:HA3	1:D:396:TRP:O	2.14	0.48
1:M:396:TRP:HA	1:M:397:SER:HA	1.59	0.48
1:O:326:ALA:HB1	1:O:329:GLU:HB2	1.96	0.48
1:E:72:THR:HG22	1:E:110:LYS:HB2	1.96	0.47
1:E:271:PHE:HB2	1:F:231:ASN:OD1	2.14	0.47
1:K:31:ILE:HD11	1:K:120:LEU:HB3	1.96	0.47
1:K:149:GLU:HB2	1:K:150:LEU:HD22	1.95	0.47
1:B:154:VAL:HG21	1:B:157:TRP:CE2	2.49	0.47
1:C:396:TRP:HA	1:C:397:SER:HA	1.60	0.47
1:D:359:LEU:CD1	1:D:427:LYS:HZ1	2.28	0.47
1:I:222:PRO:HB3	1:I:336:ARG:HH22	1.79	0.47
1:I:226:LYS:HG3	1:I:300:GLU:HG2	1.97	0.47
1:K:75:PHE:HD1	1:K:75:PHE:H	1.62	0.47
1:K:220:LEU:CD1	1:K:291:ILE:HD11	2.44	0.47
1:N:54:HIS:CD2	1:N:96:PHE:HZ	2.32	0.47
1:N:338:ARG:NH1	1:N:344:LEU:O	2.30	0.47
1:O:302:ASN:ND2	1:O:310:ALA:HB2	2.29	0.47
1:A:39:ASP:HB3	1:C:313:TYR:CD2	2.49	0.47
1:F:163:PRO:O	1:F:167:GLY:N	2.47	0.47
1:G:396:TRP:HA	1:G:397:SER:HA	1.67	0.47
1:I:31:ILE:HG22	1:I:122:MET:SD	2.54	0.47
1:L:62:ILE:HA	1:L:65:ILE:HD12	1.96	0.47
1:N:296:ARG:HG2	1:N:297:GLY:H	1.80	0.47
1:N:357:ASP:HB3	1:N:364:VAL:HG11	1.96	0.47
1:O:94:MET:O	1:O:98:LYS:HG3	2.15	0.47
1:B:396:TRP:HA	1:B:397:SER:HA	1.60	0.47
1:G:154:VAL:HG21	1:G:157:TRP:CE2	2.50	0.47
1:L:253:LYS:NZ	1:L:341:TYR:HA	2.29	0.47
1:M:364:VAL:CG1	1:M:427:LYS:HG2	2.44	0.47
1:M:383:LEU:HD12	1:M:384:ASN:N	2.29	0.47
1:P:344:LEU:HG	1:P:345:PRO:HD2	1.97	0.47
1:C:164:TRP:HD1	1:C:247:PHE:CE2	2.33	0.47
1:H:135:SER:HA	1:H:138:TRP:CE3	2.50	0.47
1:K:231:ASN:HD21	1:L:270:ASN:ND2	2.13	0.47
1:E:94:MET:CE	1:E:149:GLU:HG3	2.44	0.47
1:E:98:LYS:HE3	1:E:149:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:ASP:OD1	1:F:272:ASP:N	2.47	0.47
1:F:331:LYS:HB3	1:F:335:ARG:HH21	1.79	0.47
1:I:15:SER:H	1:I:76:SER:HB3	1.80	0.47
1:I:43:PHE:CE2	1:I:409:GLU:HG3	2.49	0.47
1:I:298:ILE:HG23	1:I:312:ALA:HB3	1.96	0.47
1:I:396:TRP:HA	1:I:397:SER:HA	1.55	0.47
1:M:406:PHE:HB3	1:M:410:LYS:HG2	1.95	0.47
1:N:21:ALA:HB1	1:N:24:GLU:HB2	1.96	0.47
1:O:44:GLU:HG3	1:O:46:HIS:CE1	2.49	0.47
1:B:105:ARG:HA	1:B:105:ARG:HD2	1.72	0.47
1:B:135:SER:HA	1:B:138:TRP:CE3	2.50	0.47
1:G:205:LYS:O	1:G:209:LYS:HA	2.14	0.47
1:J:170:GLY:HA3	1:J:177:ALA:HB3	1.97	0.47
1:J:418:ASP:OD1	1:J:418:ASP:N	2.31	0.47
1:K:296:ARG:NE	1:K:316:TYR:OH	2.47	0.47
1:M:239:ALA:HB2	1:M:309:LYS:HD2	1.97	0.47
1:A:65:ILE:HG22	1:A:109:ILE:HD13	1.96	0.47
1:G:160:HIS:HB2	1:G:216:ILE:HD11	1.97	0.47
1:I:140:LEU:HD11	1:I:203:LEU:HD13	1.97	0.47
1:L:154:VAL:HG21	1:L:157:TRP:CE2	2.50	0.47
1:B:136:VAL:O	1:B:140:LEU:HD13	2.14	0.47
1:E:118:TRP:NE1	1:E:161:ASN:O	2.38	0.47
1:E:321:MET:HG2	1:E:354:ALA:HB3	1.97	0.47
1:F:105:ARG:NH2	1:F:152:ASP:O	2.48	0.47
1:C:366:ASP:CG	1:C:427:LYS:HG2	2.36	0.46
1:H:2:HIS:HA	1:H:443:LYS:NZ	2.31	0.46
1:I:5:LYS:HD3	1:I:5:LYS:N	2.28	0.46
1:J:396:TRP:O	1:J:397:SER:OG	2.28	0.46
1:N:308:LEU:O	1:N:309:LYS:HD3	2.15	0.46
1:C:95:ALA:HA	1:C:98:LYS:CE	2.46	0.46
1:E:240:ASP:OD2	1:E:336:ARG:NH2	2.39	0.46
1:G:139:PHE:CD2	1:G:196:SER:HB2	2.50	0.46
1:K:338:ARG:NH2	1:K:346:ILE:HD13	2.30	0.46
1:L:411:ARG:HH12	1:L:427:LYS:HZ1	1.63	0.46
1:M:224:TYR:HD2	1:M:296:ARG:HG3	1.80	0.46
1:E:259:ASP:HA	1:F:259:ASP:HA	1.97	0.46
1:E:359:LEU:HD13	1:E:427:LYS:HZ3	1.80	0.46
1:M:73:TYR:CE1	1:M:75:PHE:HB3	2.50	0.46
1:M:197:HIS:CE1	1:M:216:ILE:HB	2.51	0.46
1:P:64:HIS:HD2	1:P:426:TRP:HE1	1.63	0.46
1:D:132:ASN:OD1	1:D:134:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:GLU:OE1	1:G:81:ARG:NH2	2.48	0.46
1:G:134:GLU:HG3	1:G:138:TRP:CZ2	2.51	0.46
1:I:259:ASP:N	1:I:259:ASP:OD1	2.47	0.46
1:J:62:ILE:HG22	1:J:66:LYS:HE3	1.98	0.46
1:K:58:TYR:O	1:K:62:ILE:HD11	2.14	0.46
1:L:364:VAL:HG11	1:L:427:LYS:HD3	1.97	0.46
1:N:335:ARG:HG3	1:N:388:MET:HE1	1.97	0.46
1:F:306:ASP:OD1	1:F:307:PHE:N	2.48	0.46
1:H:2:HIS:HA	1:H:443:LYS:HZ3	1.81	0.46
1:L:411:ARG:NH2	1:L:416:TYR:HD1	2.13	0.46
1:O:427:LYS:O	1:O:430:ALA:N	2.47	0.46
1:P:396:TRP:HA	1:P:397:SER:HA	1.60	0.46
1:J:7:PHE:HA	1:J:391:GLN:O	2.16	0.46
1:J:366:ASP:OD1	1:J:427:LYS:HB3	2.15	0.46
1:L:364:VAL:HG21	1:L:427:LYS:CD	2.43	0.46
1:B:62:ILE:HD11	1:B:100:LEU:HD12	1.98	0.46
1:C:271:PHE:HA	1:C:273:PHE:CE1	2.51	0.46
1:D:67:LYS:HB3	1:D:426:TRP:CH2	2.51	0.46
1:E:19:GLU:HA	1:E:54:HIS:HB3	1.98	0.46
1:I:332:ASP:HA	1:I:335:ARG:HD2	1.97	0.46
1:J:303:ALA:HB3	1:L:181:ARG:O	2.16	0.46
1:K:62:ILE:O	1:K:65:ILE:HB	2.15	0.46
1:L:14:SER:HB2	1:L:117:HIS:CE1	2.51	0.46
1:B:60:GLU:O	1:B:64:HIS:HD2	1.97	0.46
1:D:118:TRP:HZ2	1:D:162:GLU:HB2	1.80	0.46
1:K:225:ALA:HB1	1:K:232:ASP:HB3	1.98	0.46
1:K:228:ASP:O	1:K:233:ARG:NH1	2.49	0.46
1:L:60:GLU:O	1:L:64:HIS:HD2	1.98	0.46
1:M:12:ALA:HB1	1:M:74:ARG:O	2.15	0.46
1:J:437:ILE:HG12	1:J:437:ILE:H	1.33	0.46
1:L:62:ILE:HD11	1:L:100:LEU:HD12	1.97	0.46
1:O:259:ASP:HA	1:P:259:ASP:HA	1.98	0.46
1:B:241:GLY:HA2	1:B:245:ARG:HB2	1.97	0.46
1:H:54:HIS:ND1	1:H:61:ASP:OD2	2.37	0.46
1:I:168:PHE:O	1:I:172:HIS:HB3	2.16	0.46
1:J:66:LYS:HZ1	1:J:103:ARG:HH22	1.64	0.46
1:J:332:ASP:O	1:J:336:ARG:HG3	2.16	0.46
1:K:31:ILE:CD1	1:K:120:LEU:HB3	2.46	0.46
1:K:61:ASP:O	1:K:65:ILE:HD13	2.16	0.46
1:L:45:LYS:HB2	1:L:45:LYS:HE3	1.71	0.46
1:L:330:PHE:CE1	1:L:334:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:ARG:HA	1:M:112:ALA:O	2.15	0.46
1:O:364:VAL:H	1:O:427:LYS:HG2	1.81	0.46
1:P:16:TYR:HD1	1:P:27:ARG:HH22	1.63	0.46
1:A:47:ASN:O	1:A:408:TYR:OH	2.27	0.45
1:B:154:VAL:HG21	1:B:157:TRP:CZ2	2.51	0.45
1:G:90:ASN:OD1	1:G:92:GLU:HG2	2.16	0.45
1:H:364:VAL:HG11	1:H:427:LYS:HG2	1.97	0.45
1:H:367:ASP:OD1	1:H:367:ASP:N	2.50	0.45
1:I:222:PRO:O	1:I:296:ARG:HG2	2.16	0.45
1:P:4:LYS:HB3	1:P:4:LYS:HE2	1.82	0.45
1:A:245:ARG:NH1	1:A:259:ASP:OD2	2.44	0.45
1:C:118:TRP:HZ2	1:C:162:GLU:HB2	1.81	0.45
1:E:67:LYS:HE3	1:E:426:TRP:CZ2	2.51	0.45
1:K:29:PRO:O	1:K:122:MET:HB2	2.16	0.45
1:K:110:LYS:HA	1:K:111:PRO:HD3	1.71	0.45
1:K:127:GLU:HB3	1:K:138:TRP:HH2	1.81	0.45
1:L:367:ASP:OD2	1:L:367:ASP:N	2.35	0.45
1:M:31:ILE:HD11	1:M:178:PRO:HB3	1.98	0.45
1:M:346:ILE:HB	1:M:390:ILE:HG12	1.98	0.45
1:G:99:ASN:O	1:G:102:LEU:HG	2.17	0.45
1:G:241:GLY:HA2	1:G:245:ARG:HB2	1.98	0.45
1:H:83:PHE:HE1	1:H:89:TYR:HB2	1.81	0.45
1:J:137:ASP:HA	1:J:140:LEU:HG	1.97	0.45
1:J:441:LYS:HD3	1:J:441:LYS:HA	1.47	0.45
1:K:259:ASP:HA	1:L:259:ASP:HA	1.98	0.45
1:L:338:ARG:NH2	1:L:388:MET:O	2.49	0.45
1:N:326:ALA:HB1	1:N:329:GLU:HB2	1.97	0.45
1:P:165:CYS:HA	1:P:169:LEU:HB2	1.98	0.45
1:D:132:ASN:O	1:D:135:SER:OG	2.33	0.45
1:E:154:VAL:HG21	1:E:157:TRP:CZ2	2.51	0.45
1:E:298:ILE:HG12	1:E:312:ALA:HB3	1.98	0.45
1:G:161:ASN:HA	1:G:217:THR:HG23	1.97	0.45
1:K:61:ASP:HB3	1:K:64:HIS:ND1	2.32	0.45
1:L:359:LEU:HD12	1:L:359:LEU:O	2.17	0.45
1:O:396:TRP:HA	1:O:397:SER:HA	1.59	0.45
1:A:181:ARG:O	1:C:303:ALA:HB3	2.17	0.45
1:B:444:HIS:O	1:B:444:HIS:ND1	2.48	0.45
1:E:85:ALA:HB3	1:E:88:GLU:HB2	1.98	0.45
1:F:110:LYS:HA	1:F:111:PRO:HD3	1.77	0.45
1:H:265:SER:HA	1:H:268:VAL:O	2.16	0.45
1:K:154:VAL:HG21	1:K:157:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:18:ILE:HG13	1:M:19:GLU:N	2.32	0.45
1:M:348:ILE:HB	1:M:393:TYR:HD1	1.82	0.45
1:N:66:LYS:HD3	1:N:107:GLU:HB3	1.98	0.45
1:B:332:ASP:O	1:B:335:ARG:HG3	2.16	0.45
1:D:292:ASN:OD1	1:D:349:THR:OG1	2.29	0.45
1:E:271:PHE:HA	1:E:273:PHE:CE1	2.52	0.45
1:G:19:GLU:CD	1:G:81:ARG:HH22	2.20	0.45
1:G:62:ILE:HD13	1:G:103:ARG:HD2	1.99	0.45
1:G:279:MET:HA	1:G:282:ILE:HG22	1.98	0.45
1:L:293:PHE:CE2	1:L:330:PHE:HB2	2.52	0.45
1:M:389:ASN:ND2	1:M:389:ASN:O	2.49	0.45
1:N:433:TYR:O	1:N:436:VAL:HG22	2.17	0.45
1:O:133:ARG:O	1:O:136:VAL:HG22	2.16	0.45
1:P:402:PHE:HB2	1:P:408:TYR:HE1	1.81	0.45
1:C:205:LYS:HE3	1:C:214:ILE:HG22	1.98	0.45
1:D:418:ASP:O	1:D:422:GLN:N	2.49	0.45
1:L:338:ARG:HE	1:L:346:ILE:HD11	1.81	0.45
1:M:4:LYS:HB3	1:M:7:PHE:HB2	1.97	0.45
1:N:154:VAL:HG21	1:N:157:TRP:CZ2	2.52	0.45
1:C:410:LYS:N	1:C:410:LYS:HD2	2.32	0.45
1:P:151:ASP:HA	1:P:154:VAL:HG22	1.99	0.45
1:A:191:HIS:CE1	1:A:274:ILE:HA	2.52	0.45
1:A:374:ARG:HH21	1:A:432:TRP:HE1	1.64	0.45
1:D:440:HIS:NE2	1:D:444:HIS:HE1	2.15	0.45
1:F:406:PHE:CG	1:F:410:LYS:HE3	2.51	0.45
1:G:364:VAL:HG21	1:G:427:LYS:HG2	1.99	0.45
1:I:31:ILE:HG12	1:I:32:TRP:N	2.32	0.45
1:C:431:LYS:HD3	1:C:431:LYS:HA	1.78	0.45
1:D:98:LYS:HB3	1:D:98:LYS:HE2	1.72	0.45
1:F:397:SER:O	1:F:413:GLY:HA2	2.16	0.45
1:K:294:TYR:O	1:K:372:TYR:OH	2.35	0.45
1:K:374:ARG:NH1	1:K:378:GLU:OE2	2.50	0.45
1:I:35:PHE:HE1	1:I:179:GLY:HA3	1.81	0.44
1:I:326:ALA:HB1	1:I:329:GLU:CD	2.37	0.44
1:J:197:HIS:CE1	1:J:216:ILE:HB	2.53	0.44
1:K:74:ARG:HA	1:K:112:ALA:O	2.17	0.44
1:A:257:PRO:HB2	1:A:259:ASP:OD1	2.17	0.44
1:C:294:TYR:OH	1:C:350:GLU:OE1	2.30	0.44
1:K:68:LEU:O	1:K:68:LEU:HD23	2.18	0.44
1:K:390:ILE:H	1:K:390:ILE:HG13	1.23	0.44
1:M:64:HIS:HD2	1:M:426:TRP:HE1	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:64:HIS:CD2	1:M:426:TRP:HE1	2.36	0.44
1:N:399:MET:SD	1:N:415:LEU:HD22	2.58	0.44
1:O:370:ILE:HD11	1:O:428:ASP:HB3	1.98	0.44
1:K:313:TYR:CZ	1:K:315:ASP:HB3	2.53	0.44
1:K:319:THR:HG1	1:K:323:TRP:N	2.15	0.44
1:N:53:ASP:OD1	1:N:57:ARG:HG3	2.17	0.44
1:N:82:ILE:O	1:N:83:PHE:HD1	2.00	0.44
1:N:199:LYS:HG2	1:N:281:THR:HG21	1.99	0.44
1:P:222:PRO:HB2	1:P:224:TYR:CE2	2.51	0.44
1:C:367:ASP:HA	1:C:370:ILE:HD12	1.99	0.44
1:E:354:ALA:HB2	1:E:412:PHE:CE1	2.53	0.44
1:F:105:ARG:HD2	1:F:153:ILE:HG23	1.99	0.44
1:G:85:ALA:HB3	1:G:88:GLU:HB3	1.99	0.44
1:G:140:LEU:HD11	1:G:199:LYS:HB3	2.00	0.44
1:J:432:TRP:HE3	1:J:433:TYR:CD1	2.35	0.44
1:M:119:ASP:OD1	1:M:119:ASP:N	2.51	0.44
1:M:383:LEU:HD13	1:M:390:ILE:HD12	1.99	0.44
1:O:330:PHE:O	1:O:334:ILE:HG12	2.18	0.44
1:A:197:HIS:CE1	1:A:216:ILE:HB	2.53	0.44
1:A:364:VAL:H	1:A:427:LYS:CE	2.30	0.44
1:D:132:ASN:CG	1:D:134:GLU:HG2	2.38	0.44
1:I:169:LEU:HD22	1:I:176:HIS:CG	2.52	0.44
1:J:395:LEU:HG	1:J:433:TYR:HE2	1.83	0.44
1:K:110:LYS:HB3	1:K:155:ASP:HB2	1.99	0.44
1:L:373:VAL:HG12	1:L:377:LEU:HD12	2.00	0.44
1:O:15:SER:H	1:O:76:SER:HG	1.63	0.44
1:P:60:GLU:O	1:P:64:HIS:ND1	2.51	0.44
1:B:34:MET:O	1:B:38:ILE:HG13	2.18	0.44
1:H:102:LEU:HG	1:H:153:ILE:HD13	1.98	0.44
1:H:342:THR:OG1	1:H:344:LEU:HD13	2.18	0.44
1:I:30:SER:C	1:I:31:ILE:HD13	2.37	0.44
1:I:118:TRP:CD1	1:I:166:ALA:HB2	2.52	0.44
1:L:220:LEU:HD11	1:L:248:LEU:HD21	2.00	0.44
1:N:430:ALA:O	1:N:434:ALA:N	2.41	0.44
1:E:231:ASN:ND2	1:F:272:ASP:OD1	2.44	0.44
1:I:14:SER:HB2	1:I:117:HIS:CD2	2.52	0.44
1:I:41:ARG:HA	1:I:41:ARG:HD2	1.85	0.44
1:K:291:ILE:HD12	1:K:291:ILE:HA	1.63	0.44
1:L:384:ASN:O	1:L:384:ASN:ND2	2.49	0.44
1:M:164:TRP:HD1	1:M:247:PHE:CE1	2.36	0.44
1:P:110:LYS:HA	1:P:111:PRO:HD3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ASN:HA	1:H:91:PRO:HD2	1.83	0.44
1:I:20:GLY:HA2	1:I:49:ASP:O	2.17	0.44
1:J:134:GLU:HG2	1:J:138:TRP:HE1	1.79	0.44
1:J:229:SER:OG	1:J:232:ASP:OD2	2.35	0.44
1:K:64:HIS:HD2	1:K:426:TRP:CZ2	2.35	0.44
1:K:368:ASN:N	1:K:368:ASN:HD22	2.16	0.44
1:A:294:TYR:OH	1:A:350:GLU:OE1	2.26	0.44
1:E:204:LEU:HA	1:E:208:MET:HB2	2.00	0.44
1:F:357:ASP:OD2	1:F:427:LYS:NZ	2.51	0.44
1:H:226:LYS:HE2	1:H:312:ALA:HB1	2.00	0.44
1:I:21:ALA:HB3	1:I:81:ARG:NH1	2.33	0.44
1:J:294:TYR:OH	1:J:350:GLU:OE1	2.31	0.44
1:N:267:TYR:HA	1:O:269:HIS:CD2	2.53	0.44
1:N:364:VAL:HB	1:N:427:LYS:HE3	2.00	0.44
1:A:427:LYS:HD2	1:A:427:LYS:HA	1.35	0.43
1:G:437:ILE:O	1:G:441:LYS:HG3	2.18	0.43
1:I:79:TRP:CD2	1:I:121:PRO:HD3	2.53	0.43
1:I:399:MET:HB3	1:I:415:LEU:CD2	2.47	0.43
1:I:400:ASP:OD2	1:I:411:ARG:HD3	2.18	0.43
1:K:41:ARG:HA	1:K:41:ARG:HD3	1.79	0.43
1:N:396:TRP:HA	1:N:397:SER:HA	1.52	0.43
1:A:1:MET:HG2	1:A:3:PHE:CE2	2.53	0.43
1:G:306:ASP:OD1	1:G:307:PHE:N	2.50	0.43
1:I:414:ILE:HG13	1:I:415:LEU:HD13	2.00	0.43
1:L:64:HIS:NE2	1:L:424:ARG:HD2	2.33	0.43
1:M:265:SER:HA	1:M:268:VAL:O	2.18	0.43
1:M:380:VAL:O	1:M:383:LEU:HG	2.19	0.43
1:N:10:GLY:HA2	1:N:70:VAL:HB	1.99	0.43
1:N:34:MET:O	1:N:38:ILE:HG13	2.18	0.43
1:O:53:ASP:OD2	1:O:422:GLN:NE2	2.51	0.43
1:O:350:GLU:HG3	1:O:396:TRP:HB2	2.00	0.43
1:K:146:CYS:SG	1:K:147:PHE:N	2.91	0.43
1:K:302:ASN:HB3	1:K:305:ASN:HB2	2.01	0.43
1:L:4:LYS:HD2	1:L:4:LYS:HA	1.81	0.43
1:M:293:PHE:CE2	1:M:330:PHE:HB2	2.53	0.43
1:N:271:PHE:HA	1:N:273:PHE:CE1	2.53	0.43
1:P:63:GLN:O	1:P:67:LYS:HG2	2.19	0.43
1:I:9:PHE:HB2	1:I:437:ILE:HD13	2.00	0.43
1:I:18:ILE:O	1:I:19:GLU:HG3	2.18	0.43
1:I:273:PHE:HB2	1:I:274:ILE:H	1.42	0.43
1:J:19:GLU:OE1	1:J:81:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:ARG:NH2	1:K:388:MET:O	2.51	0.43
1:N:366:ASP:OD2	1:N:369:ARG:NH1	2.51	0.43
1:B:29:PRO:HB2	1:B:122:MET:HE2	2.00	0.43
1:I:29:PRO:HB3	1:I:33:ASP:HB2	2.00	0.43
1:J:27:ARG:HG2	1:J:81:ARG:HG2	1.99	0.43
1:K:355:PHE:HE2	1:K:369:ARG:HA	1.84	0.43
1:O:43:PHE:CD2	1:O:44:GLU:HG2	2.54	0.43
1:E:168:PHE:O	1:E:172:HIS:HB3	2.18	0.43
1:F:34:MET:O	1:F:38:ILE:HG12	2.19	0.43
1:H:251:VAL:HG22	1:H:282:ILE:HD11	2.00	0.43
1:J:28:THR:HB	1:J:29:PRO:HD2	2.00	0.43
1:K:289:PHE:CE2	1:K:291:ILE:HD13	2.54	0.43
1:M:13:THR:OG1	1:M:18:ILE:HD13	2.18	0.43
1:M:59:GLU:OE1	1:M:103:ARG:NH2	2.52	0.43
1:N:19:GLU:OE2	1:N:97:TYR:OH	2.25	0.43
1:O:257:PRO:HB2	1:O:259:ASP:OD1	2.19	0.43
1:H:331:LYS:HE2	1:H:335:ARG:NH2	2.33	0.43
1:J:368:ASN:OD1	1:J:368:ASN:N	2.52	0.43
1:N:237:ASN:ND2	1:N:238:ASN:OD1	2.52	0.43
1:A:105:ARG:NH1	1:A:153:ILE:O	2.51	0.43
1:B:330:PHE:O	1:B:334:ILE:HD12	2.18	0.43
1:C:409:GLU:C	1:C:410:LYS:HD2	2.39	0.43
1:D:34:MET:O	1:D:38:ILE:HG12	2.18	0.43
1:E:63:GLN:O	1:E:67:LYS:HG2	2.19	0.43
1:K:74:ARG:NH1	1:K:114:THR:HG1	2.17	0.43
1:L:140:LEU:HD11	1:L:199:LYS:HG2	2.01	0.43
1:L:402:PHE:HB2	1:L:408:TYR:HE1	1.83	0.43
1:P:74:ARG:HH21	1:P:158:ILE:HD11	1.84	0.43
1:P:418:ASP:OD1	1:P:418:ASP:N	2.30	0.43
1:C:45:LYS:HE2	1:C:45:LYS:HB2	1.90	0.43
1:D:429:SER:C	1:D:431:LYS:N	2.71	0.43
1:J:94:MET:SD	1:J:150:LEU:HD21	2.58	0.43
1:N:437:ILE:HG13	1:N:438:ALA:N	2.33	0.43
1:A:4:LYS:H	1:A:4:LYS:HG3	1.51	0.43
1:A:110:LYS:HA	1:A:111:PRO:HD3	1.89	0.43
1:A:374:ARG:NH2	1:A:432:TRP:HE1	2.17	0.43
1:B:64:HIS:CE1	1:B:424:ARG:HB3	2.53	0.43
1:D:68:LEU:HB3	1:D:70:VAL:HG13	2.01	0.43
1:F:267:TYR:HA	1:G:269:HIS:NE2	2.32	0.43
1:I:34:MET:HG2	1:I:122:MET:CE	2.49	0.43
1:J:163:PRO:HA	1:J:193:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HD3	1:B:5:LYS:N	2.17	0.42
1:B:292:ASN:OD1	1:B:349:THR:OG1	2.24	0.42
1:C:335:ARG:HG2	1:C:335:ARG:H	1.62	0.42
1:F:326:ALA:HB1	1:F:329:GLU:HB2	2.01	0.42
1:G:144:LYS:NZ	1:G:207:GLU:OE2	2.52	0.42
1:G:338:ARG:NH2	1:G:388:MET:O	2.44	0.42
1:N:225:ALA:HB1	1:N:232:ASP:HB3	2.01	0.42
1:P:222:PRO:HB2	1:P:224:TYR:HE2	1.84	0.42
1:A:250:PRO:HB3	1:A:279:MET:HE1	2.02	0.42
1:C:15:SER:N	1:C:76:SER:OG	2.42	0.42
1:E:347:TYR:HE1	1:E:391:GLN:HB3	1.84	0.42
1:J:395:LEU:HD22	1:J:395:LEU:HA	1.72	0.42
1:N:115:ILE:HD11	1:N:157:TRP:CZ3	2.54	0.42
1:D:82:ILE:HD12	1:D:142:TYR:CE1	2.55	0.42
1:E:396:TRP:HA	1:E:397:SER:HA	1.65	0.42
1:G:15:SER:N	1:G:76:SER:OG	2.44	0.42
1:G:338:ARG:NH2	1:G:389:ASN:HB3	2.35	0.42
1:H:402:PHE:HB2	1:H:408:TYR:HE1	1.84	0.42
1:I:433:TYR:O	1:I:437:ILE:HG22	2.19	0.42
1:J:371:ASP:HA	1:J:374:ARG:HG2	2.00	0.42
1:K:402:PHE:O	1:K:402:PHE:CG	2.72	0.42
1:L:151:ASP:HA	1:L:154:VAL:HG22	2.00	0.42
1:L:411:ARG:CZ	1:L:416:TYR:HD1	2.32	0.42
1:M:202:GLU:HG3	1:M:203:LEU:N	2.34	0.42
1:M:351:ASN:HB3	1:M:393:TYR:CE1	2.54	0.42
1:M:411:ARG:HG3	1:M:411:ARG:HH11	1.82	0.42
1:N:302:ASN:ND2	1:P:181:ARG:HD2	2.34	0.42
1:O:301:PHE:CE1	1:O:308:LEU:HB3	2.54	0.42
1:P:369:ARG:NH1	1:P:427:LYS:HZ3	2.18	0.42
1:P:376:HIS:O	1:P:380:VAL:HG23	2.19	0.42
1:B:306:ASP:OD1	1:B:307:PHE:N	2.52	0.42
1:B:359:LEU:HD22	1:B:416:TYR:HE2	1.84	0.42
1:D:154:VAL:HG21	1:D:157:TRP:CE2	2.55	0.42
1:I:169:LEU:HD23	1:I:169:LEU:O	2.20	0.42
1:L:220:LEU:HB2	1:L:333:LEU:HD21	2.00	0.42
1:O:366:ASP:OD2	1:O:429:SER:OG	2.38	0.42
1:C:352:GLY:HA3	1:C:396:TRP:O	2.20	0.42
1:F:321:MET:HG2	1:F:410:LYS:CE	2.49	0.42
1:G:302:ASN:HB3	1:G:305:ASN:HB2	2.02	0.42
1:H:164:TRP:HD1	1:H:247:PHE:CE1	2.37	0.42
1:H:199:LYS:HG2	1:H:281:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:35:PHE:CD1	1:K:38:ILE:HD11	2.55	0.42
1:K:140:LEU:HD12	1:K:199:LYS:HG2	2.00	0.42
1:L:383:LEU:O	1:L:386:GLU:HB3	2.18	0.42
1:N:331:LYS:O	1:N:335:ARG:HD3	2.20	0.42
1:P:169:LEU:HD23	1:P:169:LEU:HA	1.90	0.42
1:A:96:PHE:HA	1:A:99:ASN:HD21	1.83	0.42
1:D:239:ALA:HB2	1:D:309:LYS:HD3	2.01	0.42
1:E:1:MET:HB3	1:E:3:PHE:CE2	2.54	0.42
1:E:164:TRP:NE1	1:E:243:SER:HA	2.35	0.42
1:I:135:SER:HA	1:I:138:TRP:CE3	2.55	0.42
1:I:164:TRP:HD1	1:I:247:PHE:HE2	1.68	0.42
1:K:74:ARG:HH11	1:K:114:THR:HG1	1.65	0.42
1:K:246:TRP:CE3	1:K:260:MET:HB3	2.54	0.42
1:L:253:LYS:HZ1	1:L:341:TYR:HA	1.85	0.42
1:L:416:TYR:HB2	1:L:427:LYS:HE2	2.02	0.42
1:A:209:LYS:HA	1:A:209:LYS:HD2	1.73	0.42
1:F:335:ARG:HH12	1:F:386:GLU:CD	2.22	0.42
1:J:78:ALA:HB3	1:J:81:ARG:HG3	2.01	0.42
1:J:270:ASN:ND2	1:J:272:ASP:OD2	2.53	0.42
1:K:57:ARG:O	1:K:60:GLU:HB2	2.19	0.42
1:O:154:VAL:HG21	1:O:157:TRP:CZ2	2.55	0.42
1:P:371:ASP:OD1	1:P:374:ARG:NH1	2.53	0.42
1:A:119:ASP:OD1	1:A:119:ASP:N	2.51	0.42
1:B:291:ILE:HD12	1:B:346:ILE:HG21	2.01	0.42
1:C:165:CYS:HA	1:C:169:LEU:HB2	2.01	0.42
1:D:77:ILE:HD11	1:D:115:ILE:HA	2.02	0.42
1:D:130:TRP:O	1:D:192:HIS:ND1	2.32	0.42
1:F:105:ARG:CZ	1:F:153:ILE:HA	2.50	0.42
1:H:147:PHE:O	1:H:151:ASP:HB2	2.19	0.42
1:K:355:PHE:HE2	1:K:369:ARG:HD3	1.82	0.42
1:L:142:TYR:CG	1:L:142:TYR:O	2.72	0.42
1:L:330:PHE:O	1:L:334:ILE:HD12	2.19	0.42
1:M:133:ARG:HA	1:M:192:HIS:CD2	2.54	0.42
1:P:354:ALA:HB2	1:P:412:PHE:CE1	2.55	0.42
1:C:360:GLU:HG3	1:C:361:ASN:OD1	2.20	0.42
1:E:135:SER:HA	1:E:138:TRP:CE3	2.54	0.42
1:I:331:LYS:O	1:I:335:ARG:HG2	2.20	0.42
1:J:257:PRO:HB2	1:J:259:ASP:OD1	2.20	0.42
1:J:429:SER:O	1:J:433:TYR:CD1	2.73	0.42
1:K:220:LEU:HD13	1:K:333:LEU:HD21	2.02	0.42
1:N:202:GLU:O	1:N:206:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:399:MET:HE1	1:N:415:LEU:HD13	2.01	0.42
1:D:385:ASP:OD1	1:P:59:GLU:HG3	2.20	0.42
1:D:440:HIS:O	1:D:443:LYS:HG2	2.20	0.42
1:J:302:ASN:OD1	1:L:181:ARG:HB3	2.20	0.42
1:K:299:VAL:HG21	1:K:309:LYS:HB2	2.01	0.42
1:O:43:PHE:HD2	1:O:44:GLU:HG2	1.84	0.42
1:B:269:HIS:NE2	1:C:267:TYR:HA	2.35	0.41
1:F:155:ASP:O	1:F:213:PRO:HD2	2.20	0.41
1:J:81:ARG:HE	1:J:97:TYR:HE2	1.67	0.41
1:K:101:ALA:HA	1:K:104:LEU:HD12	2.01	0.41
1:K:219:ASN:HA	1:K:292:ASN:O	2.20	0.41
1:N:105:ARG:HH11	1:N:111:PRO:HD2	1.84	0.41
1:N:165:CYS:HA	1:N:169:LEU:HB2	2.02	0.41
1:N:352:GLY:HA3	1:N:396:TRP:O	2.19	0.41
1:B:103:ARG:NH2	1:B:107:GLU:OE2	2.43	0.41
1:C:366:ASP:OD1	1:C:427:LYS:HG2	2.20	0.41
1:E:344:LEU:HG	1:E:345:PRO:HD2	2.03	0.41
1:F:154:VAL:HG21	1:F:157:TRP:CZ2	2.55	0.41
1:K:79:TRP:O	1:K:79:TRP:HD1	2.03	0.41
1:K:239:ALA:HB2	1:K:309:LYS:HG3	2.01	0.41
1:L:119:ASP:OD1	1:L:119:ASP:N	2.50	0.41
1:L:188:ARG:HG2	1:L:192:HIS:CE1	2.55	0.41
1:O:70:VAL:HG12	1:O:72:THR:H	1.85	0.41
1:E:8:VAL:HG23	1:E:392:GLY:HA3	2.02	0.41
1:E:303:ALA:HB3	1:G:181:ARG:O	2.20	0.41
1:F:31:ILE:HD13	1:F:120:LEU:HB3	2.02	0.41
1:F:57:ARG:NE	1:F:422:GLN:OE1	2.45	0.41
1:G:366:ASP:OD2	1:G:369:ARG:NH1	2.49	0.41
1:H:31:ILE:O	1:H:34:MET:HG3	2.20	0.41
1:J:173:VAL:HG23	1:J:174:GLY:N	2.36	0.41
1:K:18:ILE:HG13	1:K:52:CYS:HB2	2.03	0.41
1:L:34:MET:O	1:L:38:ILE:HG13	2.20	0.41
1:M:20:GLY:HA3	1:M:50:VAL:O	2.20	0.41
1:M:47:ASN:O	1:M:408:TYR:OH	2.27	0.41
1:M:209:LYS:HA	1:M:209:LYS:HD2	1.74	0.41
1:N:305:ASN:HD22	1:N:309:LYS:N	2.08	0.41
1:A:396:TRP:HA	1:A:397:SER:HA	1.66	0.41
1:B:3:PHE:CE1	1:B:381:SER:HB2	2.55	0.41
1:D:6:ASP:OD1	1:D:6:ASP:N	2.53	0.41
1:F:164:TRP:HD1	1:F:247:PHE:CE1	2.38	0.41
1:F:357:ASP:HB2	1:F:411:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:VAL:CG2	1:G:427:LYS:HG2	2.51	0.41
1:J:59:GLU:CD	1:J:63:GLN:HE22	2.24	0.41
1:K:231:ASN:HD21	1:L:270:ASN:HD21	1.69	0.41
1:L:357:ASP:OD1	1:L:357:ASP:N	2.48	0.41
1:M:315:ASP:OD1	1:M:315:ASP:N	2.52	0.41
1:N:31:ILE:CD1	1:N:120:LEU:HB3	2.50	0.41
1:O:150:LEU:O	1:O:154:VAL:HG22	2.20	0.41
1:O:197:HIS:CE1	1:O:216:ILE:HB	2.55	0.41
1:P:305:ASN:ND2	1:P:309:LYS:H	2.07	0.41
1:P:338:ARG:HA	1:P:342:THR:O	2.21	0.41
1:B:239:ALA:HA	1:B:309:LYS:HE2	2.02	0.41
1:F:213:PRO:HA	1:F:287:ASP:OD2	2.21	0.41
1:F:350:GLU:HG2	1:F:396:TRP:CE3	2.56	0.41
1:I:262:ASN:O	1:I:265:SER:HB3	2.20	0.41
1:J:66:LYS:HZ1	1:J:103:ARG:NH2	2.17	0.41
1:K:376:HIS:O	1:K:380:VAL:HG23	2.21	0.41
1:L:64:HIS:CE1	1:L:415:LEU:HD21	2.56	0.41
1:L:82:ILE:HG13	1:L:83:PHE:N	2.35	0.41
1:M:327:PRO:HB3	1:M:376:HIS:HD2	1.84	0.41
1:N:31:ILE:HD13	1:N:120:LEU:HB3	2.02	0.41
1:O:265:SER:HA	1:O:268:VAL:O	2.20	0.41
1:E:89:TYR:HE1	1:E:94:MET:HE2	1.86	0.41
1:E:302:ASN:ND2	1:G:181:ARG:HD2	2.35	0.41
1:H:18:ILE:HG13	1:H:19:GLU:N	2.35	0.41
1:J:27:ARG:HE	1:J:81:ARG:HG2	1.85	0.41
1:K:370:ILE:O	1:K:374:ARG:HB3	2.20	0.41
1:L:398:LEU:O	1:L:415:LEU:N	2.52	0.41
1:M:34:MET:O	1:M:38:ILE:HG13	2.20	0.41
1:M:338:ARG:HD3	1:M:338:ARG:HA	1.76	0.41
1:O:154:VAL:HG21	1:O:157:TRP:CE2	2.55	0.41
1:O:427:LYS:HA	1:O:427:LYS:HD2	1.49	0.41
1:P:239:ALA:HB2	1:P:309:LYS:HD2	2.01	0.41
1:P:271:PHE:HA	1:P:273:PHE:CE1	2.56	0.41
1:B:22:HIS:HA	1:B:27:ARG:HD3	2.02	0.41
1:E:209:LYS:HA	1:E:209:LYS:HD2	1.87	0.41
1:F:85:ALA:HB3	1:F:88:GLU:HB3	2.02	0.41
1:F:369:ARG:NH2	1:F:411:ARG:O	2.54	0.41
1:H:327:PRO:HB3	1:H:376:HIS:CD2	2.55	0.41
1:N:373:VAL:HG12	1:N:377:LEU:HD12	2.02	0.41
1:N:427:LYS:HA	1:N:427:LYS:HD2	1.76	0.41
1:E:5:LYS:N	1:E:5:LYS:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:LYS:O	1:F:335:ARG:HG2	2.21	0.41
1:F:369:ARG:NH1	1:F:427:LYS:HZ1	2.19	0.41
1:K:27:ARG:HG3	1:K:27:ARG:HH11	1.84	0.41
1:L:327:PRO:O	1:L:330:PHE:HB3	2.20	0.41
1:L:338:ARG:HE	1:L:346:ILE:CD1	2.34	0.41
1:M:116:TYR:HB2	1:M:139:PHE:HE2	1.86	0.41
1:D:67:LYS:HB3	1:D:426:TRP:HH2	1.85	0.41
1:E:120:LEU:HD12	1:E:121:PRO:HD2	2.01	0.41
1:E:224:TYR:HE2	1:E:329:GLU:HB3	1.85	0.41
1:E:250:PRO:HB3	1:E:279:MET:CE	2.51	0.41
1:F:303:ALA:HB3	1:H:181:ARG:O	2.21	0.41
1:H:52:CYS:O	1:H:424:ARG:NH1	2.32	0.41
1:H:163:PRO:O	1:H:167:GLY:N	2.51	0.41
1:J:334:ILE:HG13	1:J:335:ARG:N	2.35	0.41
1:L:360:GLU:O	1:L:362:GLY:N	2.54	0.41
1:L:396:TRP:HA	1:L:397:SER:HA	1.72	0.41
1:L:411:ARG:NH1	1:L:411:ARG:HB3	2.36	0.41
1:O:62:ILE:HD12	1:O:104:LEU:HD21	2.03	0.41
1:O:82:ILE:HG22	1:O:83:PHE:CD1	2.56	0.41
1:A:191:HIS:HE1	1:A:274:ILE:HA	1.86	0.41
1:B:35:PHE:HE1	1:B:179:GLY:HA3	1.86	0.41
1:G:226:LYS:HG2	1:G:232:ASP:OD2	2.21	0.41
1:H:374:ARG:HH21	1:H:432:TRP:HE1	1.69	0.41
1:L:374:ARG:HG3	1:L:375:GLN:N	2.35	0.41
1:M:153:ILE:H	1:M:153:ILE:HG12	1.50	0.41
1:N:366:ASP:O	1:N:370:ILE:HD12	2.21	0.41
1:B:67:LYS:HA	1:B:67:LYS:HD3	1.76	0.40
1:B:303:ALA:HB3	1:D:181:ARG:O	2.20	0.40
1:E:265:SER:HA	1:E:268:VAL:O	2.21	0.40
1:F:422:GLN:O	1:F:424:ARG:NH2	2.54	0.40
1:H:396:TRP:HA	1:H:397:SER:HA	1.72	0.40
1:I:227:THR:HB	1:I:228:ASP:H	1.38	0.40
1:K:396:TRP:HA	1:K:397:SER:HA	1.44	0.40
1:L:411:ARG:HH22	1:L:427:LYS:HE3	1.86	0.40
1:P:321:MET:HG2	1:P:354:ALA:HB3	2.03	0.40
1:P:364:VAL:HG11	1:P:427:LYS:HG2	2.04	0.40
1:A:299:VAL:CG1	1:A:309:LYS:HB2	2.51	0.40
1:B:265:SER:HA	1:B:268:VAL:O	2.22	0.40
1:C:206:ARG:HD3	1:C:206:ARG:HA	1.89	0.40
1:C:258:VAL:HG23	1:D:234:LEU:HD12	2.01	0.40
1:H:165:CYS:HA	1:H:169:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:ASN:HA	1:I:292:ASN:O	2.22	0.40
1:J:267:TYR:HA	1:K:269:HIS:NE2	2.36	0.40
1:L:369:ARG:HH12	1:L:427:LYS:HZ1	1.68	0.40
1:M:237:ASN:CG	1:N:258:VAL:HG21	2.42	0.40
1:A:168:PHE:O	1:A:172:HIS:HB3	2.20	0.40
1:C:44:GLU:HB2	1:C:46:HIS:HE1	1.84	0.40
1:F:269:HIS:NE2	1:G:267:TYR:HA	2.36	0.40
1:I:374:ARG:NH1	1:I:378:GLU:OE2	2.54	0.40
1:J:432:TRP:HE3	1:J:433:TYR:HD1	1.69	0.40
1:K:8:VAL:HG22	1:K:391:GLN:O	2.20	0.40
1:L:411:ARG:NH1	1:L:427:LYS:HZ1	2.19	0.40
1:D:164:TRP:CD1	1:D:243:SER:HA	2.57	0.40
1:E:241:GLY:HA3	1:E:260:MET:SD	2.62	0.40
1:F:364:VAL:HG11	1:F:427:LYS:HE3	2.02	0.40
1:H:120:LEU:HA	1:H:121:PRO:HD3	1.97	0.40
1:I:75:PHE:CZ	1:I:113:VAL:HG22	2.57	0.40
1:J:14:SER:O	1:J:18:ILE:HG12	2.21	0.40
1:K:17:GLN:NE2	1:K:403:GLU:HA	2.37	0.40
1:K:439:ASP:N	1:K:439:ASP:OD1	2.54	0.40
1:M:302:ASN:HB3	1:M:305:ASN:HB2	2.04	0.40
1:M:368:ASN:OD1	1:M:368:ASN:N	2.54	0.40
1:O:241:GLY:HA2	1:O:245:ARG:HB2	2.02	0.40
1:A:396:TRP:HE1	1:A:412:PHE:HD2	1.69	0.40
1:F:22:HIS:CE1	1:F:23:ASN:HD21	2.40	0.40
1:F:169:LEU:HD23	1:F:169:LEU:HA	1.93	0.40
1:J:429:SER:O	1:J:433:TYR:N	2.44	0.40
1:N:169:LEU:HD23	1:N:169:LEU:HA	1.88	0.40

All (2) 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:J:385:ASP:O	1:M:331:LYS:NZ[2_455]	2.16	0.04
1:J:385:ASP:OD2	1:M:335:ARG:NH2[2_455]	2.19	0.01

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	443/471 (94%)	426 (96%)	16 (4%)	1 (0%)	47	80
1	B	442/471 (94%)	427 (97%)	14 (3%)	1 (0%)	47	80
1	C	444/471 (94%)	427 (96%)	16 (4%)	1 (0%)	47	80
1	D	444/471 (94%)	424 (96%)	17 (4%)	3 (1%)	22	62
1	E	445/471 (94%)	426 (96%)	18 (4%)	1 (0%)	47	80
1	F	443/471 (94%)	423 (96%)	19 (4%)	1 (0%)	47	80
1	G	442/471 (94%)	424 (96%)	18 (4%)	0	100	100
1	H	443/471 (94%)	426 (96%)	16 (4%)	1 (0%)	47	80
1	I	434/471 (92%)	400 (92%)	22 (5%)	12 (3%)	5	34
1	J	442/471 (94%)	412 (93%)	25 (6%)	5 (1%)	14	53
1	K	402/471 (85%)	360 (90%)	29 (7%)	13 (3%)	4	31
1	L	441/471 (94%)	413 (94%)	22 (5%)	6 (1%)	11	47
1	M	432/471 (92%)	414 (96%)	18 (4%)	0	100	100
1	N	437/471 (93%)	416 (95%)	20 (5%)	1 (0%)	47	80
1	O	434/471 (92%)	411 (95%)	19 (4%)	4 (1%)	17	57
1	P	439/471 (93%)	418 (95%)	19 (4%)	2 (0%)	29	67
All	All	7007/7536 (93%)	6647 (95%)	308 (4%)	52 (1%)	22	62

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	429	SER
1	E	428	ASP
1	I	30	SER
1	I	31	ILE
1	I	49	ASP
1	I	273	PHE

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Mol	Chain	Res	Type
1	I	274	ILE
1	J	4	LYS
1	J	12	ALA
1	J	175	VAL
1	J	397	SER
1	K	60	GLU
1	K	315	ASP
1	L	178	PRO
1	L	386	GLU
1	N	177	ALA
1	O	21	ALA
1	A	365	HIS
1	D	428	ASP
1	D	430	ALA
1	F	397	SER
1	I	19	GLU
1	I	34	MET
1	I	227	THR
1	J	177	ALA
1	K	24	GLU
1	K	327	PRO
1	K	329	GLU
1	K	403	GLU
1	O	428	ASP
1	O	440	HIS
1	P	441	LYS
1	P	443	LYS
1	I	33	ASP
1	I	367	ASP
1	I	382	ASP
1	K	103	ARG
1	K	381	SER
1	B	431	LYS
1	H	444	HIS
1	K	22	HIS
1	K	317	GLU
1	K	331	LYS
1	L	361	ASN
1	L	142	TYR
1	L	367	ASP
1	C	2	HIS
1	I	272	ASP

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Mol	Chain	Res	Type
1	K	145	VAL
1	L	143	ALA
1	O	20	GLY
1	K	325	ILE

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	379/401 (94%)	365 (96%)	14 (4%)	34	65
1	B	379/401 (94%)	369 (97%)	10 (3%)	46	74
1	C	380/401 (95%)	375 (99%)	5 (1%)	69	86
1	D	380/401 (95%)	370 (97%)	10 (3%)	46	74
1	E	381/401 (95%)	370 (97%)	11 (3%)	42	71
1	F	379/401 (94%)	372 (98%)	7 (2%)	59	81
1	G	379/401 (94%)	370 (98%)	9 (2%)	49	76
1	H	379/401 (94%)	364 (96%)	15 (4%)	31	64
1	I	374/401 (93%)	335 (90%)	39 (10%)	7	32
1	J	379/401 (94%)	344 (91%)	35 (9%)	9	37
1	K	350/401 (87%)	303 (87%)	47 (13%)	4	22
1	L	378/401 (94%)	345 (91%)	33 (9%)	10	39
1	M	374/401 (93%)	350 (94%)	24 (6%)	17	51
1	N	376/401 (94%)	346 (92%)	30 (8%)	12	42
1	O	373/401 (93%)	358 (96%)	15 (4%)	31	64
1	P	378/401 (94%)	355 (94%)	23 (6%)	18	52
All	All	6018/6416 (94%)	5691 (95%)	327 (5%)	22	56

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	4	LYS
1	A	5	LYS
1	A	22	HIS
1	A	34	MET
1	A	102	LEU
1	A	105	ARG
1	A	183	MET
1	A	275	GLN
1	A	279	MET
1	A	309	LYS
1	A	328	ASN
1	A	361	ASN
1	A	399	MET
1	B	2	HIS
1	B	5	LYS
1	B	34	MET
1	B	37	ASP
1	B	173	VAL
1	B	280	GLU
1	B	364	VAL
1	B	374	ARG
1	B	415	LEU
1	B	444	HIS
1	C	2	HIS
1	C	34	MET
1	C	63	GLN
1	C	67	LYS
1	C	364	VAL
1	D	5	LYS
1	D	6	ASP
1	D	34	MET
1	D	37	ASP
1	D	181	ARG
1	D	255	GLU
1	D	309	LYS
1	D	360	GLU
1	D	415	LEU
1	D	428	ASP
1	E	2	HIS
1	E	5	LYS
1	E	34	MET
1	E	37	ASP

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Mol	Chain	Res	Type
1	E	88	GLU
1	E	90	ASN
1	E	203	LEU
1	E	279	MET
1	E	309	LYS
1	E	363	GLU
1	E	399	MET
1	F	6	ASP
1	F	181	ARG
1	F	208	MET
1	F	209	LYS
1	F	255	GLU
1	F	415	LEU
1	F	443	LYS
1	G	2	HIS
1	G	5	LYS
1	G	8	VAL
1	G	34	MET
1	G	94	MET
1	G	115	ILE
1	G	275	GLN
1	G	358	VAL
1	G	399	MET
1	H	2	HIS
1	H	5	LYS
1	H	6	ASP
1	H	28	THR
1	H	37	ASP
1	H	88	GLU
1	H	98	LYS
1	H	105	ARG
1	H	181	ARG
1	H	275	GLN
1	H	279	MET
1	H	360	GLU
1	H	367	ASP
1	H	391	GLN
1	H	431	LYS
1	I	5	LYS
1	I	18	ILE
1	I	24	GLU
1	I	27	ARG

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Mol	Chain	Res	Type
1	I	31	ILE
1	I	45	LYS
1	I	82	ILE
1	I	83	PHE
1	I	89	TYR
1	I	98	LYS
1	I	99	ASN
1	I	102	LEU
1	I	114	THR
1	I	115	ILE
1	I	120	LEU
1	I	141	ASP
1	I	150	LEU
1	I	173	VAL
1	I	204	LEU
1	I	227	THR
1	I	273	PHE
1	I	274	ILE
1	I	282	ILE
1	I	287	ASP
1	I	315	ASP
1	I	319	THR
1	I	324	ASP
1	I	328	ASN
1	I	329	GLU
1	I	335	ARG
1	I	360	GLU
1	I	366	ASP
1	I	368	ASN
1	I	377	LEU
1	I	399	MET
1	I	415	LEU
1	I	418	ASP
1	I	424	ARG
1	I	427	LYS
1	J	1	MET
1	J	4	LYS
1	J	8	VAL
1	J	22	HIS
1	J	23	ASN
1	J	24	GLU
1	J	37	ASP

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Mol	Chain	Res	Type
1	J	38	ILE
1	J	41	ARG
1	J	53	ASP
1	J	57	ARG
1	J	63	GLN
1	J	71	ASP
1	J	104	LEU
1	J	146	CYS
1	J	150	LEU
1	J	152	ASP
1	J	173	VAL
1	J	226	LYS
1	J	234	LEU
1	J	309	LYS
1	J	359	LEU
1	J	361	ASN
1	J	371	ASP
1	J	395	LEU
1	J	396	TRP
1	J	399	MET
1	J	411	ARG
1	J	418	ASP
1	J	422	GLN
1	J	424	ARG
1	J	437	ILE
1	J	441	LYS
1	J	443	LYS
1	J	444	HIS
1	K	18	ILE
1	K	22	HIS
1	K	24	GLU
1	K	27	ARG
1	K	39	ASP
1	K	42	VAL
1	K	47	ASN
1	K	57	ARG
1	K	61	ASP
1	K	64	HIS
1	K	67	LYS
1	K	74	ARG
1	K	75	PHE
1	K	92	GLU

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Mol	Chain	Res	Type
1	K	94	MET
1	K	100	LEU
1	K	102	LEU
1	K	106	GLU
1	K	109	ILE
1	K	113	VAL
1	K	133	ARG
1	K	146	CYS
1	K	153	ILE
1	K	176	HIS
1	K	199	LYS
1	K	202	GLU
1	K	203	LEU
1	K	227	THR
1	K	260	MET
1	K	291	ILE
1	K	299	VAL
1	K	306	ASP
1	K	309	LYS
1	K	329	GLU
1	K	330	PHE
1	K	355	PHE
1	K	358	VAL
1	K	359	LEU
1	K	360	GLU
1	K	375	GLN
1	K	382	ASP
1	K	390	ILE
1	K	391	GLN
1	K	395	LEU
1	K	399	MET
1	K	424	ARG
1	K	428	ASP
1	L	2	HIS
1	L	5	LYS
1	L	23	ASN
1	L	34	MET
1	L	47	ASN
1	L	50	VAL
1	L	89	TYR
1	L	106	GLU
1	L	127	GLU

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Mol	Chain	Res	Type
1	L	141	ASP
1	L	176	HIS
1	L	208	MET
1	L	209	LYS
1	L	211	THR
1	L	223	MET
1	L	228	ASP
1	L	255	GLU
1	L	306	ASP
1	L	309	LYS
1	L	319	THR
1	L	331	LYS
1	L	335	ARG
1	L	338	ARG
1	L	367	ASP
1	L	371	ASP
1	L	384	ASN
1	L	391	GLN
1	L	399	MET
1	L	403	GLU
1	L	415	LEU
1	L	418	ASP
1	L	424	ARG
1	L	433	TYR
1	M	3	PHE
1	M	4	LYS
1	M	5	LYS
1	M	34	MET
1	M	36	CYS
1	M	53	ASP
1	M	57	ARG
1	M	63	GLN
1	M	98	LYS
1	M	100	LEU
1	M	105	ARG
1	M	113	VAL
1	M	122	MET
1	M	153	ILE
1	M	176	HIS
1	M	202	GLU
1	M	205	LYS
1	M	259	ASP

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Mol	Chain	Res	Type
1	M	315	ASP
1	M	324	ASP
1	M	415	LEU
1	M	424	ARG
1	M	440	HIS
1	M	441	LYS
1	N	5	LYS
1	N	44	GLU
1	N	53	ASP
1	N	60	GLU
1	N	67	LYS
1	N	86	LYS
1	N	88	GLU
1	N	146	CYS
1	N	148	GLU
1	N	181	ARG
1	N	228	ASP
1	N	255	GLU
1	N	335	ARG
1	N	357	ASP
1	N	359	LEU
1	N	360	GLU
1	N	361	ASN
1	N	363	GLU
1	N	365	HIS
1	N	367	ASP
1	N	383	LEU
1	N	388	MET
1	N	398	LEU
1	N	399	MET
1	N	414	ILE
1	N	415	LEU
1	N	417	ILE
1	N	426	TRP
1	N	428	ASP
1	N	431	LYS
1	O	14	SER
1	O	24	GLU
1	O	50	VAL
1	O	105	ARG
1	O	126	GLU
1	O	176	HIS

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Mol	Chain	Res	Type
1	O	181	ARG
1	O	211	THR
1	O	234	LEU
1	O	338	ARG
1	O	346	ILE
1	O	359	LEU
1	O	399	MET
1	O	409	GLU
1	O	421	THR
1	P	5	LYS
1	P	22	HIS
1	P	34	MET
1	P	37	ASP
1	P	45	LYS
1	P	50	VAL
1	P	56	HIS
1	P	63	GLN
1	P	89	TYR
1	P	158	ILE
1	P	188	ARG
1	P	205	LYS
1	P	263	LEU
1	P	305	ASN
1	P	311	ASP
1	P	319	THR
1	P	331	LYS
1	P	332	ASP
1	P	338	ARG
1	P	360	GLU
1	P	418	ASP
1	P	439	ASP
1	P	443	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	HIS
1	B	99	ASN
1	D	99	ASN
1	D	444	HIS
1	F	22	HIS
1	G	191	HIS

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Mol	Chain	Res	Type
1	J	269	HIS
1	K	351	ASN
1	L	270	ASN
1	N	269	HIS
1	N	305	ASN
1	O	270	ASN
1	P	17	GLN
1	P	231	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	445/471 (94%)	-0.09	17 (3%)	40	30	64, 78, 100, 196	0
1	B	444/471 (94%)	0.07	20 (4%)	33	24	65, 96, 125, 197	0
1	C	446/471 (94%)	-0.01	21 (4%)	31	23	66, 82, 99, 185	0
1	D	446/471 (94%)	0.04	14 (3%)	49	36	64, 88, 111, 166	0
1	E	447/471 (94%)	-0.17	13 (2%)	51	38	63, 82, 106, 147	0
1	F	445/471 (94%)	0.14	26 (5%)	23	17	65, 97, 124, 281	0
1	G	444/471 (94%)	-0.02	19 (4%)	35	26	63, 91, 115, 215	0
1	H	445/471 (94%)	0.13	29 (6%)	18	14	64, 90, 115, 159	0
1	I	438/471 (92%)	0.35	37 (8%)	11	9	80, 118, 170, 267	0
1	J	444/471 (94%)	0.36	45 (10%)	7	6	77, 111, 152, 460	0
1	K	412/471 (87%)	0.35	38 (9%)	9	7	90, 139, 204, 347	0
1	L	443/471 (94%)	0.34	45 (10%)	6	6	83, 111, 151, 205	0
1	M	438/471 (92%)	0.36	40 (9%)	9	7	76, 112, 143, 245	0
1	N	441/471 (93%)	0.12	25 (5%)	23	17	77, 106, 149, 430	0
1	O	438/471 (92%)	0.26	30 (6%)	17	14	81, 106, 154, 276	0
1	P	443/471 (94%)	0.12	24 (5%)	25	19	75, 98, 124, 185	0
All	All	7059/7536 (93%)	0.14	443 (6%)	20	15	63, 98, 149, 460	0

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	161	ASN	6.8
1	K	386	GLU	6.6
1	K	292	ASN	6.3
1	I	292	ASN	6.1
1	L	76	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	14	SER	5.5
1	L	161	ASN	5.5
1	M	161	ASN	5.5
1	F	14	SER	5.4
1	I	162	GLU	5.3
1	H	161	ASN	5.3
1	F	161	ASN	5.3
1	I	219	ASN	5.3
1	O	15	SER	5.2
1	O	14	SER	5.2
1	C	217	THR	5.2
1	F	76	SER	5.1
1	L	350	GLU	5.1
1	J	350	GLU	5.0
1	F	114	THR	5.0
1	B	114	THR	5.0
1	O	161	ASN	4.9
1	I	349	THR	4.9
1	H	292	ASN	4.9
1	B	76	SER	4.9
1	I	217	THR	4.9
1	K	387	GLY	4.8
1	M	358	VAL	4.8
1	L	292	ASN	4.8
1	L	349	THR	4.8
1	L	162	GLU	4.7
1	H	162	GLU	4.7
1	I	350	GLU	4.7
1	C	13	THR	4.7
1	C	161	ASN	4.6
1	I	14	SER	4.6
1	G	76	SER	4.6
1	K	226	LYS	4.5
1	L	408	TYR	4.5
1	C	292	ASN	4.5
1	K	161	ASN	4.5
1	I	13	THR	4.5
1	I	402	PHE	4.5
1	M	357	ASP	4.4
1	K	76	SER	4.4
1	A	76	SER	4.4
1	H	13	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	411	ARG	4.4
1	J	76	SER	4.4
1	K	39	ASP	4.4
1	H	350	GLU	4.3
1	H	76	SER	4.3
1	N	76	SER	4.3
1	E	292	ASN	4.3
1	O	76	SER	4.3
1	K	10	GLY	4.3
1	E	350	GLU	4.3
1	G	14	SER	4.3
1	K	87	GLY	4.3
1	I	12	ALA	4.3
1	N	161	ASN	4.3
1	I	74	ARG	4.2
1	P	350	GLU	4.2
1	J	292	ASN	4.2
1	M	350	GLU	4.2
1	J	40	GLY	4.2
1	M	356	ASP	4.1
1	F	13	THR	4.1
1	J	161	ASN	4.1
1	I	114	THR	4.1
1	N	357	ASP	4.1
1	G	292	ASN	4.0
1	I	86	LYS	4.0
1	M	292	ASN	4.0
1	H	15	SER	4.0
1	D	161	ASN	4.0
1	G	161	ASN	4.0
1	P	161	ASN	3.9
1	F	350	GLU	3.9
1	A	14	SER	3.9
1	M	162	GLU	3.9
1	P	292	ASN	3.8
1	P	386	GLU	3.8
1	N	114	THR	3.8
1	H	217	THR	3.8
1	K	162	GLU	3.8
1	L	219	ASN	3.8
1	L	117	HIS	3.8
1	L	40	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	12	ALA	3.8
1	J	13	THR	3.8
1	G	117	HIS	3.7
1	F	117	HIS	3.7
1	G	114	THR	3.7
1	L	365	HIS	3.7
1	M	278	ASP	3.7
1	C	408	TYR	3.7
1	F	15	SER	3.7
1	J	41	ARG	3.7
1	M	14	SER	3.7
1	O	350	GLU	3.7
1	O	425	ILE	3.7
1	E	114	THR	3.7
1	A	350	GLU	3.7
1	G	350	GLU	3.7
1	O	117	HIS	3.7
1	K	350	GLU	3.6
1	K	14	SER	3.6
1	H	315	ASP	3.6
1	D	14	SER	3.6
1	E	219	ASN	3.6
1	C	76	SER	3.6
1	M	114	THR	3.6
1	K	219	ASN	3.6
1	K	389	ASN	3.6
1	O	162	GLU	3.6
1	J	349	THR	3.6
1	I	117	HIS	3.6
1	K	15	SER	3.6
1	D	76	SER	3.5
1	C	350	GLU	3.5
1	F	162	GLU	3.5
1	P	349	THR	3.5
1	F	292	ASN	3.5
1	G	15	SER	3.5
1	B	217	THR	3.5
1	K	228	ASP	3.5
1	C	14	SER	3.5
1	L	209	LYS	3.5
1	E	217	THR	3.5
1	D	292	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	O	42	VAL	3.5
1	M	296	ARG	3.5
1	G	12	ALA	3.5
1	A	114	THR	3.5
1	J	397	SER	3.5
1	J	23	ASN	3.4
1	I	401	ASN	3.4
1	C	12	ALA	3.4
1	M	390	ILE	3.4
1	L	396	TRP	3.4
1	N	350	GLU	3.4
1	P	217	THR	3.4
1	I	138	TRP	3.4
1	M	29	PRO	3.4
1	N	360	GLU	3.4
1	H	219	ASN	3.4
1	K	217	THR	3.4
1	O	114	THR	3.4
1	O	292	ASN	3.4
1	P	364	VAL	3.4
1	A	161	ASN	3.3
1	J	162	GLU	3.3
1	B	219	ASN	3.3
1	H	397	SER	3.3
1	A	112	ALA	3.3
1	H	12	ALA	3.3
1	N	349	THR	3.2
1	A	292	ASN	3.2
1	O	74	ARG	3.2
1	M	76	SER	3.2
1	P	15	SER	3.2
1	L	3	PHE	3.2
1	O	12	ALA	3.2
1	P	76	SER	3.2
1	P	14	SER	3.2
1	M	365	HIS	3.2
1	L	39	ASP	3.2
1	K	84	PRO	3.2
1	M	117	HIS	3.2
1	P	13	THR	3.2
1	P	28	THR	3.2
1	E	161	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	386	GLU	3.2
1	M	300	GLU	3.2
1	L	114	THR	3.1
1	N	292	ASN	3.1
1	H	443	LYS	3.1
1	D	219	ASN	3.1
1	K	375	GLN	3.1
1	M	312	ALA	3.1
1	D	162	GLU	3.1
1	D	349	THR	3.1
1	M	366	ASP	3.1
1	K	225	ALA	3.1
1	O	362	GLY	3.1
1	A	13	THR	3.1
1	J	396	TRP	3.1
1	O	91	PRO	3.1
1	L	14	SER	3.1
1	L	351	ASN	3.1
1	I	76	SER	3.1
1	N	117	HIS	3.1
1	H	396	TRP	3.1
1	F	385	ASP	3.1
1	I	33	ASP	3.1
1	J	114	THR	3.0
1	N	386	GLU	3.0
1	J	411	ARG	3.0
1	A	2	HIS	3.0
1	H	2	HIS	3.0
1	C	349	THR	3.0
1	E	162	GLU	3.0
1	B	14	SER	3.0
1	K	388	MET	3.0
1	L	359	LEU	3.0
1	N	358	VAL	3.0
1	F	12	ALA	3.0
1	F	74	ARG	3.0
1	N	217	THR	3.0
1	O	41	ARG	3.0
1	D	217	THR	3.0
1	P	219	ASN	3.0
1	K	138	TRP	2.9
1	L	397	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	74	ARG	2.9
1	E	356	ASP	2.9
1	P	12	ALA	2.9
1	L	388	MET	2.9
1	H	4	LYS	2.9
1	P	385	ASP	2.9
1	G	13	THR	2.9
1	L	107	GLU	2.9
1	G	410	LYS	2.9
1	M	217	THR	2.9
1	C	397	SER	2.9
1	L	52	CYS	2.9
1	J	12	ALA	2.9
1	L	13	THR	2.9
1	N	74	ARG	2.9
1	K	117	HIS	2.9
1	J	441	LYS	2.8
1	L	387	GLY	2.8
1	I	156	SER	2.8
1	M	15	SER	2.8
1	M	74	ARG	2.8
1	A	15	SER	2.8
1	H	444	HIS	2.8
1	K	357	ASP	2.8
1	B	129	GLY	2.8
1	I	26	GLY	2.8
1	J	108	GLY	2.8
1	O	13	THR	2.8
1	A	86	LYS	2.8
1	N	219	ASN	2.8
1	I	355	PHE	2.8
1	E	76	SER	2.8
1	L	32	TRP	2.8
1	P	313	TYR	2.8
1	C	162	GLU	2.8
1	L	48	GLY	2.8
1	H	117	HIS	2.7
1	F	217	THR	2.7
1	K	85	ALA	2.7
1	L	217	THR	2.7
1	P	74	ARG	2.7
1	M	411	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	38	ILE	2.7
1	D	350	GLU	2.7
1	K	149	GLU	2.7
1	I	408	TYR	2.7
1	A	74	ARG	2.7
1	F	443	LYS	2.7
1	H	114	THR	2.7
1	L	12	ALA	2.7
1	K	150	LEU	2.7
1	N	162	GLU	2.7
1	O	416	TYR	2.7
1	N	15	SER	2.6
1	H	127	GLU	2.6
1	K	315	ASP	2.6
1	N	87	GLY	2.6
1	J	43	PHE	2.6
1	B	161	ASN	2.6
1	I	137	ASP	2.6
1	B	74	ARG	2.6
1	L	15	SER	2.6
1	A	411	ARG	2.6
1	P	114	THR	2.6
1	F	17	GLN	2.6
1	G	349	THR	2.6
1	C	388	MET	2.6
1	K	74	ARG	2.6
1	C	46	HIS	2.6
1	I	365	HIS	2.6
1	C	219	ASN	2.6
1	N	211	THR	2.6
1	F	408	TYR	2.6
1	C	210	SER	2.6
1	D	226	LYS	2.6
1	H	440	HIS	2.6
1	J	219	ASN	2.6
1	L	10	GLY	2.6
1	N	13	THR	2.6
1	I	397	SER	2.6
1	L	394	TYR	2.5
1	G	74	ARG	2.5
1	J	14	SER	2.5
1	I	85	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	385	ASP	2.5
1	L	11	THR	2.5
1	G	208	MET	2.5
1	J	74	ARG	2.5
1	A	351	ASN	2.5
1	F	9	PHE	2.5
1	J	365	HIS	2.5
1	G	140	LEU	2.5
1	J	217	THR	2.5
1	G	405	SER	2.5
1	L	407	GLY	2.5
1	M	410	LYS	2.5
1	C	396	TRP	2.5
1	K	21	ALA	2.5
1	M	85	ALA	2.5
1	J	79	TRP	2.5
1	B	162	GLU	2.5
1	D	318	LYS	2.5
1	K	26	GLY	2.5
1	M	36	CYS	2.5
1	N	356	ASP	2.5
1	E	349	THR	2.5
1	M	349	THR	2.5
1	P	331	LYS	2.5
1	G	1	MET	2.5
1	C	47	ASN	2.5
1	J	29	PRO	2.5
1	A	410	LYS	2.4
1	B	88	GLU	2.4
1	I	47	ASN	2.4
1	K	432	TRP	2.4
1	J	296	ARG	2.4
1	L	112	ALA	2.4
1	L	402	PHE	2.4
1	C	410	LYS	2.4
1	J	439	ASP	2.4
1	E	357	ASP	2.4
1	M	13	THR	2.4
1	G	219	ASN	2.4
1	M	84	PRO	2.4
1	M	37	ASP	2.4
1	B	350	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	360	GLU	2.4
1	N	14	SER	2.4
1	O	112	ALA	2.4
1	K	191	HIS	2.4
1	H	349	THR	2.4
1	J	357	ASP	2.4
1	B	128	GLY	2.3
1	D	225	ALA	2.3
1	J	290	GLY	2.3
1	G	411	ARG	2.3
1	M	355	PHE	2.3
1	J	425	ILE	2.3
1	O	363	GLU	2.3
1	I	25	GLY	2.3
1	D	15	SER	2.3
1	P	47	ASN	2.3
1	H	165	CYS	2.3
1	O	359	LEU	2.3
1	O	402	PHE	2.3
1	N	343	ASP	2.3
1	O	209	LYS	2.3
1	J	174	GLY	2.3
1	F	349	THR	2.3
1	J	223	MET	2.3
1	I	82	ILE	2.3
1	L	413	GLY	2.3
1	L	426	TRP	2.3
1	A	349	THR	2.3
1	B	290	GLY	2.2
1	E	351	ASN	2.2
1	H	75	PHE	2.2
1	M	38	ILE	2.2
1	B	125	HIS	2.2
1	F	160	HIS	2.2
1	B	292	ASN	2.2
1	O	355	PHE	2.2
1	D	37	ASP	2.2
1	H	151	ASP	2.2
1	L	384	ASN	2.2
1	F	351	ASN	2.2
1	F	410	LYS	2.2
1	M	364	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	298	ILE	2.2
1	J	351	ASN	2.2
1	I	15	SER	2.2
1	M	391	GLN	2.2
1	H	140	LEU	2.2
1	M	11	THR	2.2
1	P	335	ARG	2.2
1	M	313	TYR	2.2
1	J	39	ASP	2.2
1	J	120	LEU	2.2
1	F	397	SER	2.2
1	H	314	SER	2.2
1	J	83	PHE	2.2
1	O	108	GLY	2.2
1	J	121	PRO	2.2
1	I	75	PHE	2.2
1	J	133	ARG	2.2
1	B	75	PHE	2.1
1	B	112	ALA	2.1
1	O	88	GLU	2.1
1	I	331	LYS	2.1
1	J	112	ALA	2.1
1	P	358	VAL	2.1
1	L	409	GLU	2.1
1	F	402	PHE	2.1
1	K	152	ASP	2.1
1	P	362	GLY	2.1
1	I	11	THR	2.1
1	I	135	SER	2.1
1	F	396	TRP	2.1
1	A	12	ALA	2.1
1	B	15	SER	2.1
1	F	158	ILE	2.1
1	K	313	TYR	2.1
1	K	358	VAL	2.1
1	N	403	GLU	2.1
1	I	394	TYR	2.1
1	O	66	LYS	2.1
1	M	286	CYS	2.1
1	M	320	GLY	2.1
1	P	315	ASP	2.1
1	M	209	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	32	TRP	2.1
1	N	66	LYS	2.1
1	L	16	TYR	2.1
1	J	117	HIS	2.1
1	J	359	LEU	2.1
1	L	87	GLY	2.1
1	H	5	LYS	2.0
1	J	388	MET	2.0
1	B	165	CYS	2.0
1	O	358	VAL	2.0
1	L	314	SER	2.0
1	K	278	ASP	2.0
1	B	12	ALA	2.0
1	J	47	ASN	2.0
1	C	22	HIS	2.0
1	O	129	GLY	2.0
1	O	418	ASP	2.0
1	L	74	ARG	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.