



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:31 AM UTC

PDB ID : 8P4L / pdb_00008p4l
Title : Beta-N-acetylgalactosaminidase from Niabella aurantiaca
Authors : Fjermedal, S.; Wilkens, C.
Deposited on : 2023-05-22
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

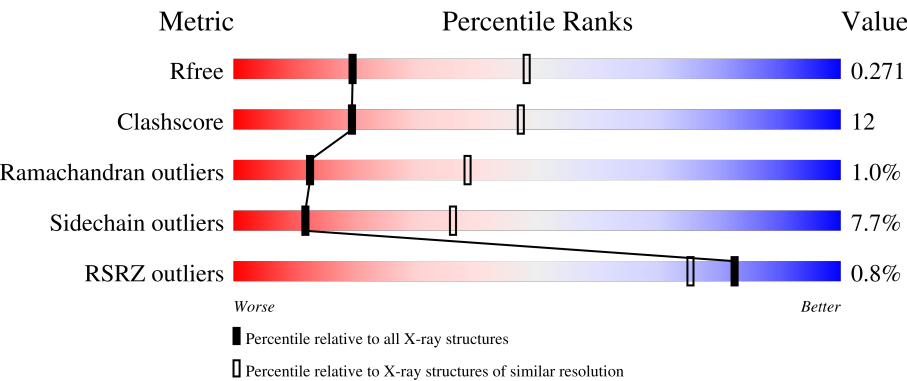
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	562	% 69% 24% • 5%
1	B	562	% 66% 27% • 5%
1	C	562	% 69% 25% • 5%
1	D	562	64% 28% • 5%
1	E	562	66% 25% • 5%

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Mol	Chain	Length	Quality of chain
1	F	562	% 67% 27% • 5%
1	G	562	% 66% 27% • 5%
1	H	562	% 66% 26% • 5%
1	I	562	% 69% 24% • 5%
1	J	562	% 63% 29% • 5%
1	K	562	% 65% 27% • 5%
1	L	562	2% 63% 28% • 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 53723 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-N-acetylgalactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	B	536	Total	C	N	O	S	0	1	0
			4466	2906	754	788	18			
1	C	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	D	536	Total	C	N	O	S	0	1	0
			4466	2906	754	788	18			
1	E	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	F	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	G	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	H	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	I	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	J	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	K	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			
1	L	536	Total	C	N	O	S	0	0	0
			4455	2896	753	788	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	18	Total	O	0	0
			18	18		

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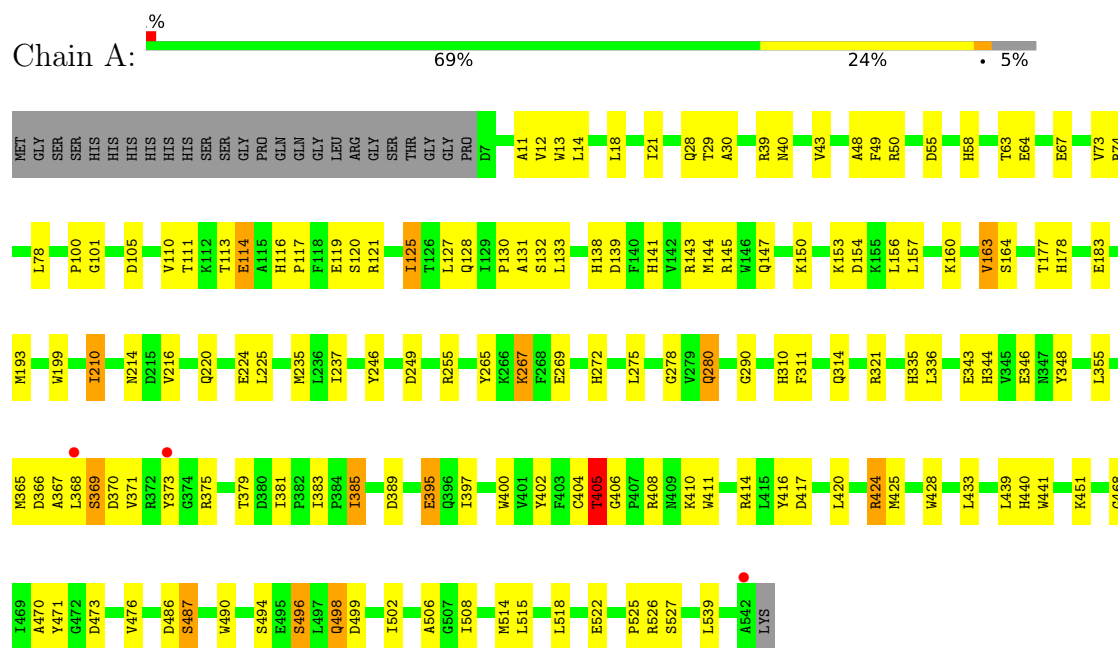
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	39	Total 39	O 39	0	0
2	D	28	Total 28	O 28	0	0
2	E	30	Total 30	O 30	0	0
2	F	26	Total 26	O 26	0	0
2	G	14	Total 14	O 14	0	0
2	H	14	Total 14	O 14	0	0
2	I	7	Total 7	O 7	0	0
2	J	13	Total 13	O 13	0	0
2	K	7	Total 7	O 7	0	0
2	L	5	Total 5	O 5	0	0

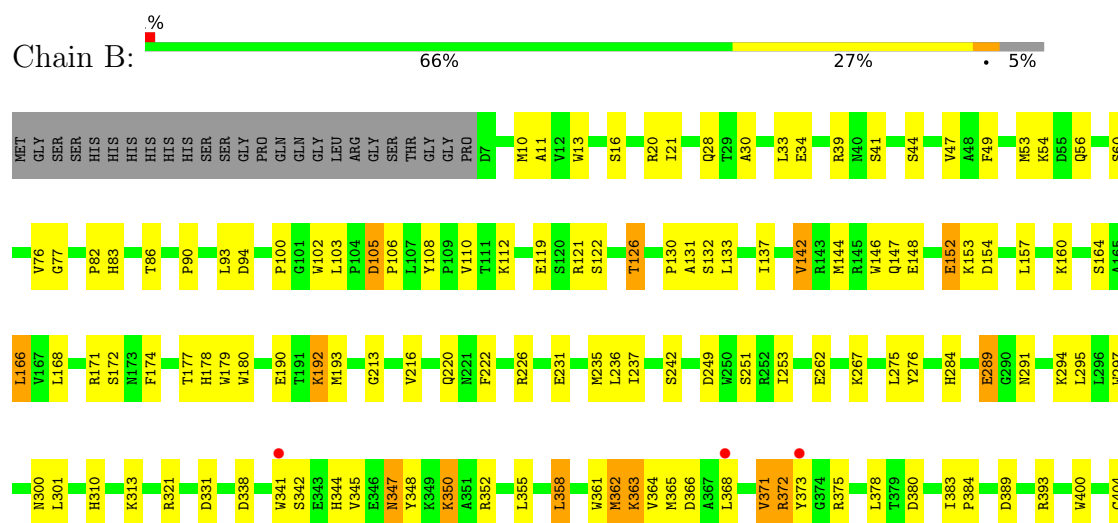
3 Residue-property plots [i](#)

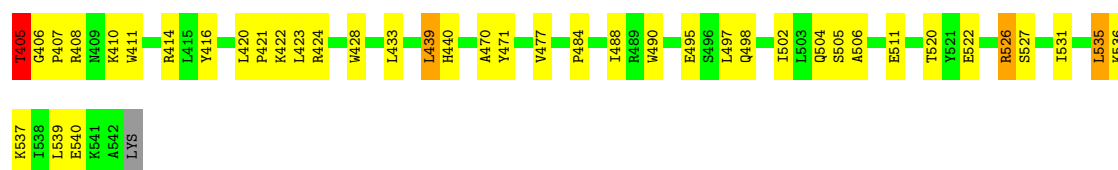
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-N-acetylgalactosaminidase

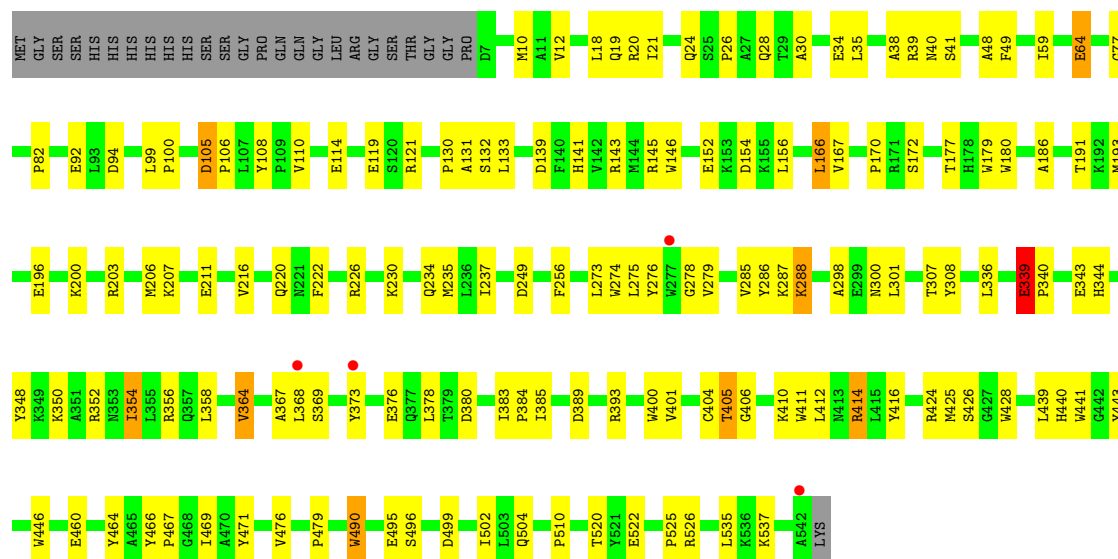


• Molecule 1: Beta-N-acetylgalactosaminidase

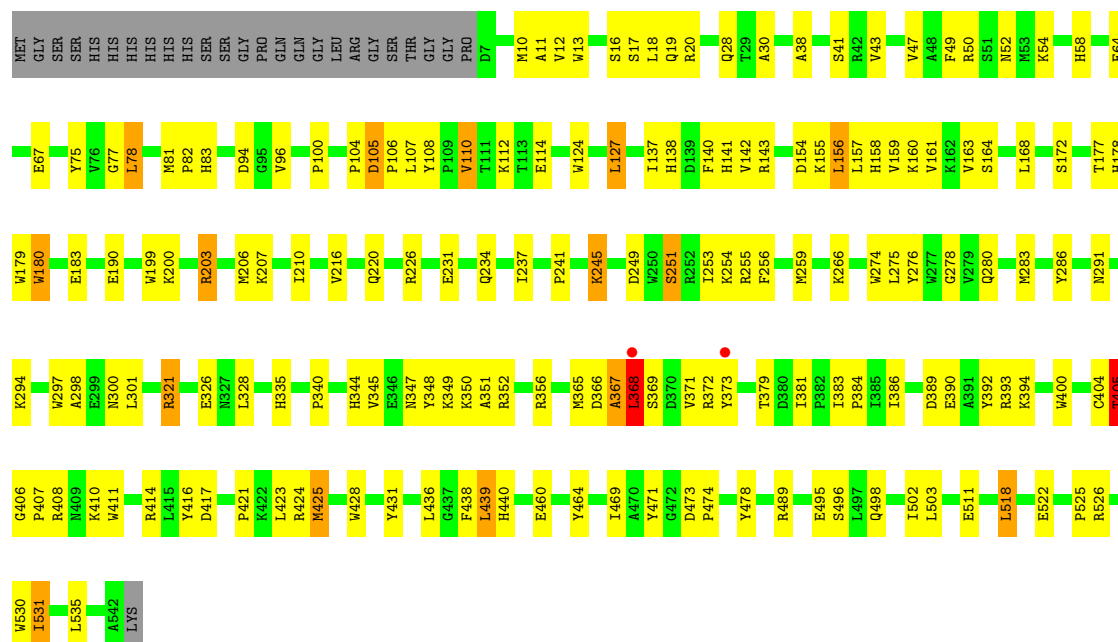




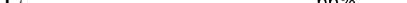
• Molecule 1: Beta-N-acetylgalactosaminidase

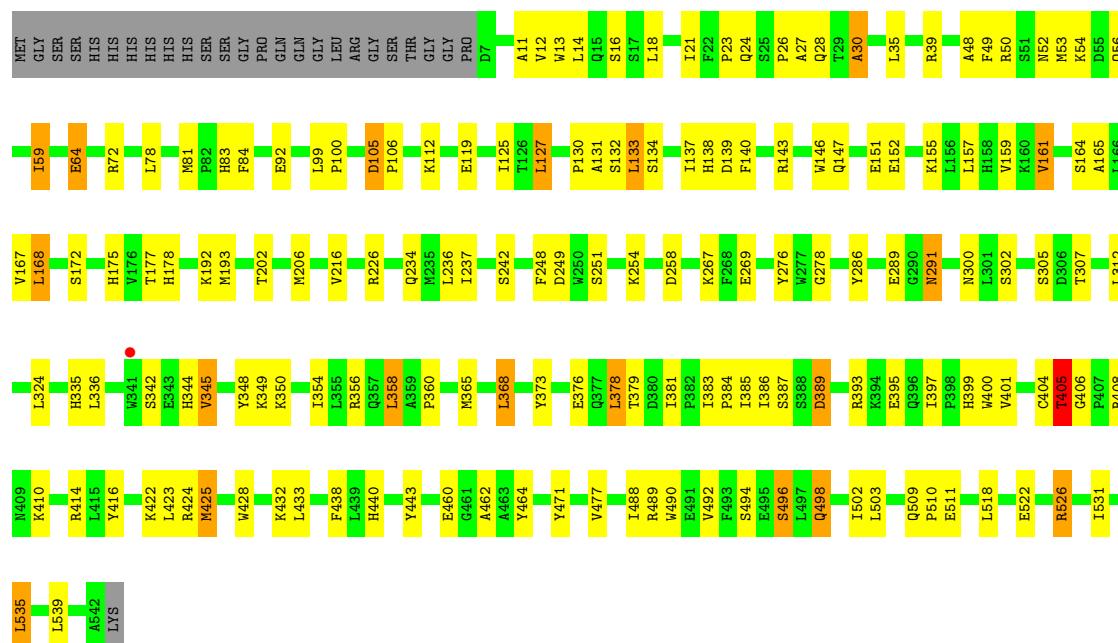


• Molecule 1: Beta-N-acetylgalactosaminidase

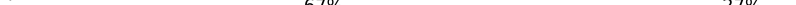


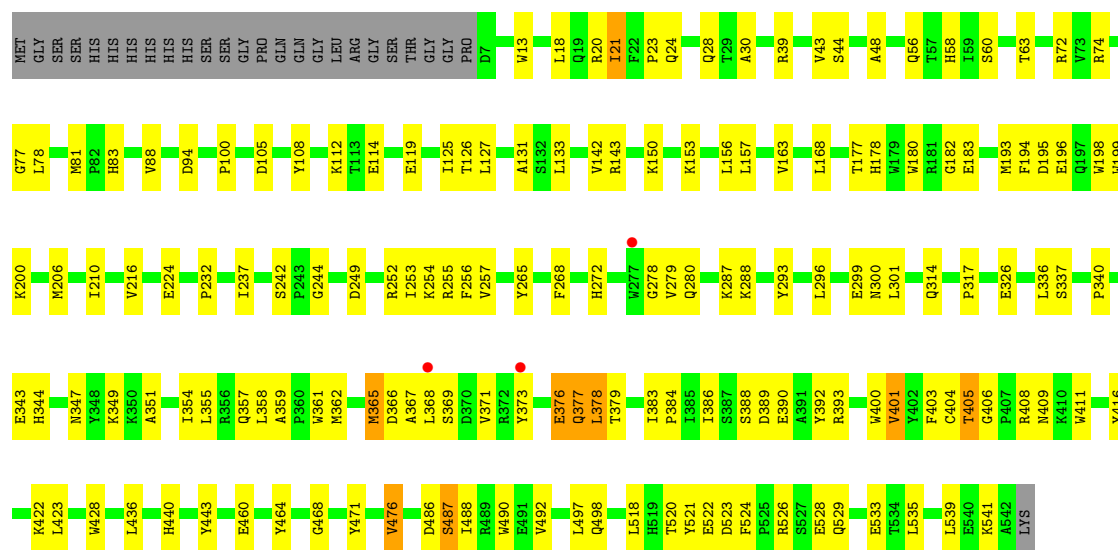
- Molecule 1: Beta-N-acetylgalactosaminidase

Chain E:  66% 25% • 5%

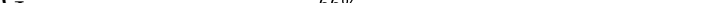


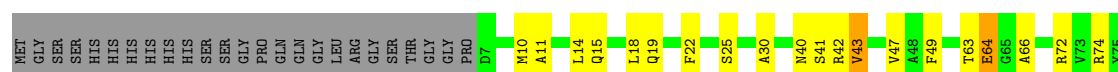
- Molecule 1: Beta-N-acetylgalactosaminidase

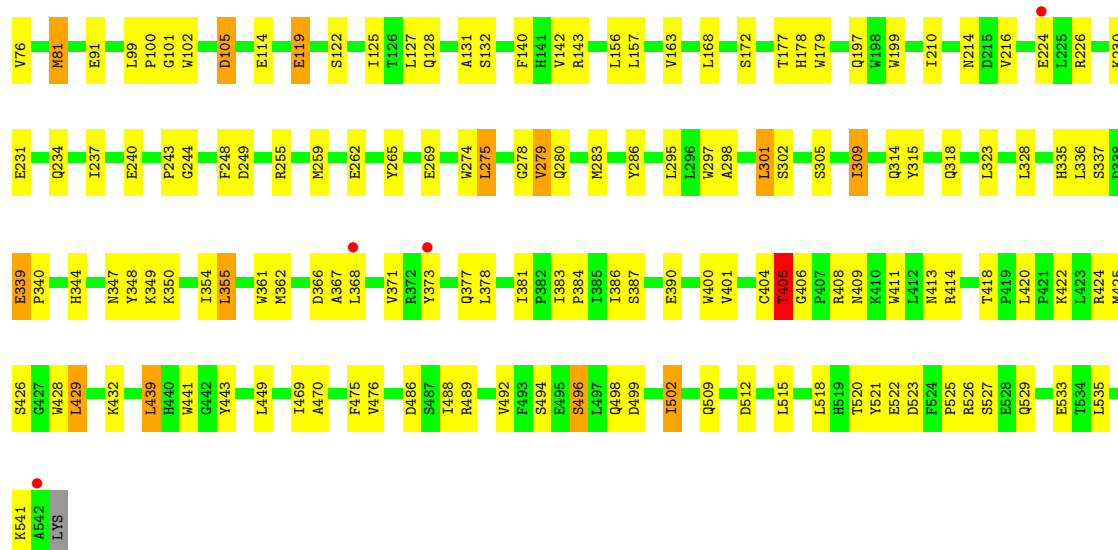
Chain F:  67% 27% 5%



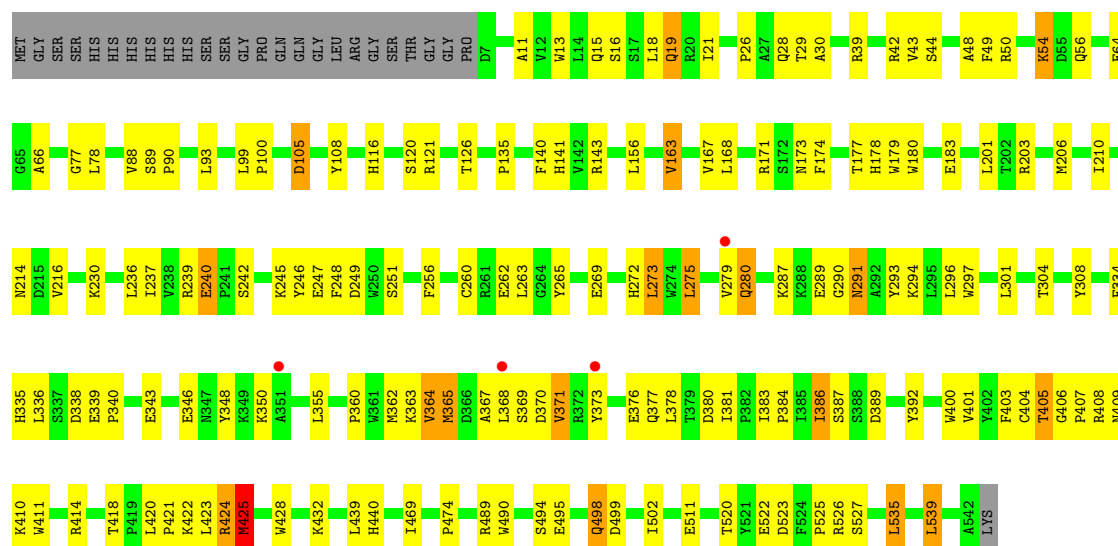
- Molecule 1: Beta-N-acetylgalactosaminidase

Chain G:  66% 27% 5%

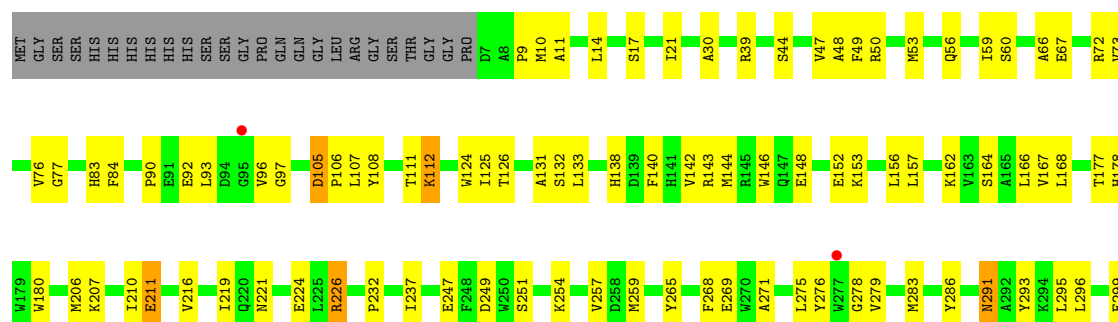


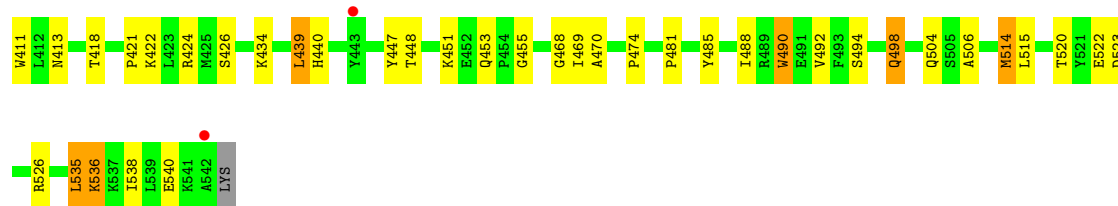


• Molecule 1: Beta-N-acetylgalactosaminidase

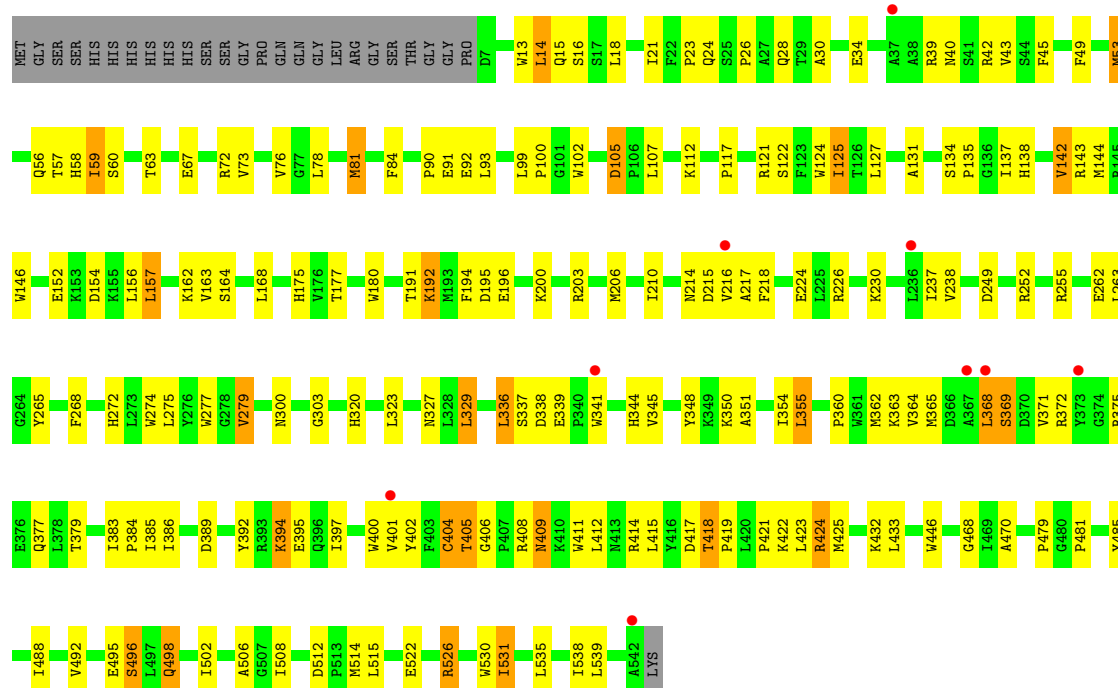


• Molecule 1: Beta-N-acetylgalactosaminidase





● Molecule 1: Beta-N-acetylgalactosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.46Å 117.62Å 282.44Å 90.00° 97.74° 90.00°	Depositor
Resolution (Å)	47.02 – 2.79 47.02 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.02-2.79) 98.6 (47.02-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.259 0.208 , 0.271	Depositor DCC
R_{free} test set	2263 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53723	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.41	0/4608	0.58	0/6269
1	B	0.38	0/4624	0.56	0/6292
1	C	0.44	0/4608	0.63	0/6269
1	D	0.41	0/4624	0.61	1/6292 (0.0%)
1	E	0.41	0/4608	0.59	0/6269
1	F	0.39	0/4608	0.58	0/6269
1	G	0.34	0/4608	0.53	0/6269
1	H	0.38	1/4608 (0.0%)	0.56	0/6269
1	I	0.33	0/4608	0.55	2/6269 (0.0%)
1	J	0.33	0/4608	0.55	1/6269 (0.0%)
1	K	0.32	0/4608	0.55	3/6269 (0.0%)
1	L	0.31	0/4608	0.52	1/6269 (0.0%)
All	All	0.37	1/55328 (0.0%)	0.57	8/75274 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	425	MET	CA-C	8.37	1.64	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	409	ASN	CB-CA-C	-8.45	106.82	116.54
1	L	409	ASN	CB-CA-C	-7.92	107.45	116.63
1	I	409	ASN	CB-CA-C	-7.79	107.59	116.63
1	J	409	ASN	CB-CA-C	-7.77	107.61	116.63
1	K	7	ASP	CA-C-N	7.23	134.67	120.94
1	K	7	ASP	C-N-CA	7.23	134.67	120.94
1	I	411	TRP	N-CA-C	5.16	116.94	110.24
1	D	368	LEU	CA-CB-CG	5.05	133.97	116.30

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	4455	0	4312	94	0
1	B	4466	0	4322	90	0
1	C	4455	0	4312	102	0
1	D	4466	0	4322	111	0
1	E	4455	0	4312	102	0
1	F	4455	0	4312	94	0
1	G	4455	0	4312	101	0
1	H	4455	0	4312	105	0
1	I	4455	0	4312	80	0
1	J	4455	0	4312	121	0
1	K	4455	0	4312	107	0
1	L	4455	0	4312	127	0
2	A	40	0	0	2	0
2	B	18	0	0	0	0
2	C	39	0	0	5	0
2	D	28	0	0	0	0
2	E	30	0	0	0	0
2	F	26	0	0	2	0
2	G	14	0	0	4	0
2	H	14	0	0	2	0
2	I	7	0	0	0	0
2	J	13	0	0	1	0
2	K	7	0	0	0	0
2	L	5	0	0	0	0
All	All	53723	0	51764	1217	0

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 12.

All (1217) 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:C:237:ILE:HB	1:C:249:ASP:HB3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:237:ILE:HB	1:I:249:ASP:HB3	1.50	0.92
1:F:232:PRO:HD2	1:F:293:TYR:HD2	1.33	0.91
1:A:143:ARG:HH21	1:A:156:LEU:HD21	1.35	0.90
1:H:237:ILE:HB	1:H:249:ASP:HB3	1.55	0.89
1:B:237:ILE:HB	1:B:249:ASP:HB3	1.55	0.87
1:G:237:ILE:HB	1:G:249:ASP:HB3	1.58	0.85
1:J:237:ILE:HB	1:J:249:ASP:HB3	1.60	0.83
1:K:313:LYS:HD3	1:K:358:LEU:HD11	1.61	0.82
1:L:59:ILE:HD12	1:L:146:TRP:HB3	1.61	0.81
1:E:404:CYS:O	1:E:406:GLY:N	2.14	0.81
1:C:404:CYS:O	1:C:406:GLY:N	2.11	0.80
1:F:404:CYS:O	1:F:406:GLY:N	2.14	0.80
1:D:237:ILE:HB	1:D:249:ASP:HB3	1.62	0.80
1:J:404:CYS:O	1:J:406:GLY:N	2.14	0.79
1:K:404:CYS:O	1:K:406:GLY:N	2.14	0.79
1:A:178:HIS:HD2	1:A:440:HIS:HB3	1.47	0.79
1:L:404:CYS:O	1:L:406:GLY:N	2.15	0.79
1:D:340:PRO:HD2	1:D:368:LEU:HB3	1.66	0.78
1:G:404:CYS:O	1:G:406:GLY:N	2.16	0.78
1:E:269:GLU:OE2	1:E:335:HIS:NE2	2.15	0.77
1:E:425:MET:HE3	1:E:531:ILE:HG12	1.67	0.77
1:C:520:THR:HG22	1:C:522:GLU:H	1.49	0.76
1:J:372:ARG:HD2	1:J:375:ARG:HH12	1.50	0.76
1:K:514:MET:HE1	1:K:538:ILE:HD11	1.68	0.76
1:J:520:THR:HG23	1:J:522:GLU:H	1.51	0.76
1:G:520:THR:HG23	1:G:522:GLU:H	1.50	0.76
1:K:237:ILE:HB	1:K:249:ASP:HB3	1.67	0.76
1:K:10:MET:HE3	1:K:59:ILE:HD12	1.68	0.75
1:F:74:ARG:HH22	1:F:486:ASP:HB2	1.50	0.75
1:K:405:THR:HG22	1:K:408:ARG:HH21	1.52	0.74
1:A:237:ILE:HB	1:A:249:ASP:HB3	1.70	0.74
1:C:288:LYS:NZ	2:C:601:HOH:O	2.18	0.74
1:I:404:CYS:O	1:I:406:GLY:N	2.19	0.74
1:K:284:HIS:HB3	1:K:286:TYR:HE1	1.52	0.74
1:E:130:PRO:HD2	1:E:133:LEU:HD13	1.70	0.73
1:A:267:LYS:NZ	2:A:601:HOH:O	2.19	0.73
1:C:234:GLN:HE22	1:C:285:VAL:HA	1.52	0.72
1:F:237:ILE:HB	1:F:249:ASP:HB3	1.71	0.72
1:L:168:LEU:HD21	1:L:502:ILE:HD13	1.71	0.72
1:D:404:CYS:O	1:D:406:GLY:N	2.22	0.72
1:J:284:HIS:HB3	1:J:286:TYR:HE1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:THR:HG23	1:B:522:GLU:H	1.55	0.72
1:A:395:GLU:HB3	1:A:397:ILE:HG13	1.73	0.71
1:K:232:PRO:HG3	1:K:286:TYR:HD2	1.56	0.71
1:B:171:ARG:NH2	1:B:213:GLY:O	2.24	0.71
1:J:206:MET:HE2	1:J:256:PHE:HZ	1.56	0.71
1:L:345:VAL:HG21	1:L:372:ARG:HH12	1.55	0.71
1:A:404:CYS:O	1:A:406:GLY:N	2.25	0.70
1:E:237:ILE:HB	1:E:249:ASP:HB3	1.73	0.70
1:F:74:ARG:NH2	1:F:486:ASP:HB2	2.07	0.70
1:I:59:ILE:HD12	1:I:146:TRP:HB3	1.73	0.70
1:I:143:ARG:HH21	1:I:156:LEU:HD21	1.57	0.70
1:G:522:GLU:O	1:G:526:ARG:NH2	2.24	0.70
1:K:302:SER:HB3	1:K:305:SER:HB2	1.74	0.70
1:K:269:GLU:OE2	1:K:335:HIS:NE2	2.25	0.69
1:L:203:ARG:NH2	1:L:262:GLU:OE2	2.25	0.69
1:C:59:ILE:HD12	1:C:146:TRP:HB3	1.74	0.69
1:E:349:LYS:HE2	1:E:378:LEU:HD21	1.74	0.69
1:B:20:ARG:HG3	1:B:420:LEU:HD11	1.75	0.69
1:I:389:ASP:OD2	1:I:393:ARG:NH1	2.21	0.69
1:L:423:LEU:HD23	1:L:492:VAL:HB	1.74	0.69
1:J:232:PRO:HG3	1:J:286:TYR:CD2	2.27	0.69
1:D:410:LYS:O	1:D:526:ARG:NH2	2.26	0.69
1:A:410:LYS:O	1:A:526:ARG:NH2	2.24	0.69
1:K:186:ALA:HA	1:K:191:THR:HG22	1.75	0.69
1:A:178:HIS:CD2	1:A:440:HIS:HB3	2.27	0.68
1:J:226:ARG:NH2	1:J:276:TYR:O	2.26	0.68
1:J:368:LEU:HD13	1:J:373:TYR:HB3	1.74	0.68
1:H:364:VAL:N	1:H:380:ASP:OD2	2.25	0.68
1:I:168:LEU:HD21	1:I:502:ILE:HG12	1.74	0.68
1:J:398:PRO:HB2	1:J:436:LEU:HD11	1.74	0.68
1:L:26:PRO:O	1:L:28:GLN:NE2	2.26	0.68
1:B:405:THR:HG22	1:B:408:ARG:HH21	1.59	0.68
1:L:368:LEU:HD13	1:L:369:SER:H	1.58	0.68
1:G:10:MET:HE2	1:G:49:PHE:HB2	1.75	0.68
1:B:226:ARG:HG3	1:B:276:TYR:CZ	2.30	0.67
1:F:18:LEU:HD12	1:F:528:GLU:HG3	1.76	0.67
1:K:232:PRO:HG3	1:K:286:TYR:CD2	2.29	0.67
1:B:371:VAL:O	1:B:373:TYR:N	2.26	0.67
1:J:414:ARG:HD2	2:J:605:HOH:O	1.93	0.67
1:B:172:SER:H	1:B:504:GLN:HE22	1.43	0.67
1:L:40:ASN:HB2	1:L:131:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:HIS:CD2	1:H:440:HIS:HB3	2.30	0.66
1:D:340:PRO:HB2	1:D:373:TYR:OH	1.95	0.66
1:G:262:GLU:OE1	2:G:601:HOH:O	2.13	0.66
1:K:422:LYS:HE2	1:K:526:ARG:HH11	1.60	0.66
1:D:10:MET:HE2	1:D:49:PHE:HB2	1.76	0.66
1:K:520:THR:HG23	1:K:522:GLU:H	1.60	0.66
1:B:166:LEU:HD11	1:B:506:ALA:HB2	1.76	0.66
1:B:404:CYS:O	1:B:406:GLY:N	2.29	0.66
1:K:448:THR:HG22	1:K:453:GLN:O	1.95	0.65
1:D:424:ARG:NH1	1:D:495:GLU:HB3	2.11	0.65
1:A:405:THR:HG22	1:A:408:ARG:HH21	1.62	0.65
1:E:383:ILE:HG12	1:E:400:TRP:HB2	1.76	0.65
1:C:404:CYS:C	1:C:406:GLY:H	2.03	0.65
1:F:383:ILE:HG12	1:F:400:TRP:HB2	1.79	0.65
1:F:520:THR:HG23	1:F:522:GLU:H	1.61	0.65
1:H:535:LEU:HD23	1:H:539:LEU:HD21	1.79	0.65
1:I:232:PRO:HD2	1:I:293:TYR:HD2	1.62	0.65
1:L:371:VAL:HA	1:L:392:TYR:CE1	2.31	0.65
1:B:424:ARG:HG2	1:B:531:ILE:HD13	1.78	0.65
1:K:316:LEU:HD13	1:K:358:LEU:HB3	1.79	0.64
1:C:77:GLY:HA3	1:C:108:TYR:CE2	2.33	0.64
1:L:142:VAL:HG13	1:L:157:LEU:HB2	1.79	0.64
1:F:340:PRO:HB2	1:F:373:TYR:OH	1.97	0.64
1:J:57:THR:HG23	1:J:115:ALA:HB3	1.78	0.64
1:C:234:GLN:NE2	1:C:285:VAL:HA	2.12	0.64
1:C:368:LEU:HD13	1:C:373:TYR:HB3	1.79	0.64
1:B:371:VAL:C	1:B:373:TYR:H	2.07	0.64
1:C:336:LEU:HD23	1:C:348:TYR:CZ	2.33	0.64
1:H:206:MET:HE3	1:H:256:PHE:HZ	1.63	0.64
1:H:520:THR:HG23	1:H:522:GLU:H	1.62	0.63
1:J:203:ARG:NH1	1:J:262:GLU:OE2	2.31	0.63
1:A:177:THR:HB	1:A:216:VAL:HB	1.79	0.63
1:A:100:PRO:HG2	1:B:119:GLU:HG3	1.81	0.63
1:G:408:ARG:HH21	1:G:470:ALA:HB2	1.64	0.63
1:G:234:GLN:HE22	1:G:286:TYR:H	1.45	0.63
1:I:14:LEU:HD11	1:I:157:LEU:HB3	1.80	0.63
1:I:207:LYS:O	1:I:211:GLU:HG2	1.98	0.63
1:E:137:ILE:HA	1:E:161:VAL:O	1.99	0.63
1:H:206:MET:HE3	1:H:256:PHE:CZ	2.34	0.63
1:I:77:GLY:HA3	1:I:108:TYR:HE2	1.64	0.63
1:K:447:TYR:HA	1:K:455:GLY:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HB3	1:B:131:ALA:HA	1.79	0.62
1:L:498:GLN:O	1:L:502:ILE:HG12	1.99	0.62
1:B:361:TRP:CZ3	1:B:362:MET:HG3	2.34	0.62
1:A:67:GLU:OE1	1:A:67:GLU:N	2.22	0.62
1:H:183:GLU:N	1:H:183:GLU:OE1	2.32	0.62
1:I:524:PHE:O	1:I:526:ARG:NH1	2.32	0.62
1:I:10:MET:HE2	1:I:49:PHE:HB2	1.81	0.62
1:G:349:LYS:HG3	1:G:378:LEU:HD21	1.80	0.62
1:E:425:MET:HE2	1:E:425:MET:HA	1.81	0.62
1:F:232:PRO:HD2	1:F:293:TYR:CD2	2.24	0.62
1:G:387:SER:HA	1:G:411:TRP:CH2	2.35	0.62
1:E:305:SER:HA	1:H:64:GLU:HG2	1.81	0.61
1:H:26:PRO:O	1:H:28:GLN:NE2	2.31	0.61
1:J:42:ARG:H	1:J:498:GLN:HE22	1.48	0.61
1:J:405:THR:HG22	1:J:408:ARG:HH21	1.63	0.61
1:J:78:LEU:HG	1:J:102:TRP:HB3	1.82	0.61
1:A:499:ASP:HA	1:A:502:ILE:HD12	1.82	0.61
1:K:240:GLU:H	1:K:287:LYS:NZ	1.97	0.61
1:E:26:PRO:O	1:E:28:GLN:NE2	2.33	0.61
1:E:226:ARG:HG3	1:E:276:TYR:CZ	2.36	0.61
1:H:77:GLY:HA3	1:H:108:TYR:HE2	1.66	0.61
1:C:460:GLU:HG2	1:C:464:TYR:CD1	2.35	0.61
1:F:366:ASP:HB3	1:F:368:LEU:HD21	1.83	0.61
1:G:76:VAL:HG12	1:G:122:SER:O	2.01	0.61
1:A:11:ALA:O	1:A:49:PHE:HA	2.01	0.61
1:F:520:THR:HG22	1:F:523:ASP:HB3	1.81	0.61
1:H:180:TRP:CD1	1:H:206:MET:HE1	2.35	0.61
1:I:361:TRP:CZ3	1:I:362:MET:HG3	2.35	0.61
1:H:171:ARG:HD3	1:H:174:PHE:HD2	1.65	0.61
1:H:203:ARG:NH2	1:H:262:GLU:OE2	2.34	0.61
1:H:90:PRO:HA	1:H:93:LEU:HD12	1.81	0.60
1:B:13:TRP:CG	1:B:28:GLN:HB2	2.35	0.60
1:H:355:LEU:HD13	1:H:362:MET:HE1	1.83	0.60
1:K:166:LEU:HD11	1:K:506:ALA:HB2	1.83	0.60
1:K:520:THR:HG22	1:K:523:ASP:HB3	1.83	0.60
1:J:206:MET:HE2	1:J:256:PHE:CZ	2.36	0.60
1:A:278:GLY:HA2	1:A:344:HIS:CG	2.36	0.60
1:B:536:LYS:HG2	1:B:540:GLU:CD	2.26	0.60
1:D:75:TYR:HB3	1:D:110:VAL:HG23	1.82	0.60
1:H:410:LYS:O	1:H:526:ARG:NH2	2.34	0.60
1:D:425:MET:HE1	1:D:530:TRP:CE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:424:ARG:HH11	1:L:495:GLU:HB3	1.66	0.60
1:E:59:ILE:HD12	1:E:146:TRP:HB3	1.84	0.60
1:G:14:LEU:HG	1:G:157:LEU:HD23	1.83	0.60
1:C:234:GLN:HE22	1:C:286:TYR:H	1.48	0.60
1:F:88:VAL:HG22	1:F:408:ARG:HB3	1.84	0.60
1:K:334:PHE:HB3	1:K:362:MET:HE3	1.83	0.60
1:L:73:VAL:HG22	1:L:125:ILE:HD13	1.83	0.60
1:D:424:ARG:O	1:D:496:SER:OG	2.12	0.60
1:A:383:ILE:HG12	1:A:400:TRP:HB2	1.84	0.59
1:F:416:TYR:CD2	1:F:471:TYR:HB3	2.36	0.59
1:C:226:ARG:HG3	1:C:276:TYR:CZ	2.37	0.59
1:K:18:LEU:HD21	1:K:424:ARG:NH1	2.18	0.59
1:L:164:SER:HB3	1:L:539:LEU:HD12	1.83	0.59
1:L:350:LYS:O	1:L:354:ILE:HG12	2.03	0.59
1:D:10:MET:HE3	1:D:11:ALA:H	1.68	0.59
1:D:460:GLU:HG2	1:D:464:TYR:CD1	2.37	0.59
1:D:460:GLU:HG2	1:D:464:TYR:CE1	2.37	0.59
1:G:297:TRP:HB2	1:G:301:LEU:HD13	1.85	0.59
1:L:226:ARG:HD3	1:L:275:LEU:HD13	1.84	0.59
1:D:365:MET:HB3	1:D:381:ILE:HB	1.84	0.59
1:E:405:THR:HG22	1:E:408:ARG:HH21	1.68	0.59
1:H:377:GLN:HG2	1:L:360:PRO:O	2.02	0.59
1:B:389:ASP:OD2	1:B:393:ARG:NH1	2.27	0.58
1:E:424:ARG:O	1:E:496:SER:OG	2.15	0.58
1:K:39:ARG:HB3	1:K:131:ALA:HA	1.84	0.58
1:K:234:GLN:NE2	1:K:286:TYR:O	2.36	0.58
1:L:67:GLU:H	1:L:67:GLU:CD	2.10	0.58
1:L:365:MET:HG3	1:L:383:ILE:HD11	1.84	0.58
1:G:323:LEU:HD23	1:G:328:LEU:HB2	1.86	0.58
1:I:226:ARG:HG3	1:I:276:TYR:CZ	2.39	0.58
1:K:448:THR:HG23	1:K:451:LYS:HB2	1.85	0.58
1:L:446:TRP:CE2	1:L:479:PRO:HD3	2.39	0.58
1:A:366:ASP:HB3	1:A:368:LEU:HD21	1.86	0.58
1:B:348:TYR:OH	1:B:366:ASP:OD2	2.20	0.58
1:E:354:ILE:HG23	1:E:358:LEU:HD23	1.84	0.58
1:L:237:ILE:HB	1:L:249:ASP:HB3	1.85	0.58
1:C:38:ALA:O	1:C:41:SER:OG	2.16	0.58
1:F:416:TYR:HD2	1:F:471:TYR:HB3	1.69	0.58
1:H:168:LEU:HD21	1:H:502:ILE:HG12	1.85	0.58
1:A:269:GLU:OE2	1:A:335:HIS:NE2	2.34	0.58
1:J:520:THR:HG22	1:J:523:ASP:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HA	1:A:383:ILE:HB	1.86	0.57
1:B:284:HIS:HB3	1:B:295:LEU:HD21	1.86	0.57
1:K:240:GLU:H	1:K:287:LYS:HZ2	1.52	0.57
1:L:339:GLU:HA	1:L:368:LEU:HB2	1.84	0.57
1:G:424:ARG:O	1:G:496:SER:HB2	2.03	0.57
1:C:278:GLY:HA2	1:C:344:HIS:CG	2.40	0.57
1:L:514:MET:HG3	1:L:515:LEU:HD13	1.87	0.57
1:F:180:TRP:CD1	1:F:206:MET:HE1	2.40	0.57
1:G:14:LEU:HD11	1:G:157:LEU:HB3	1.85	0.57
1:J:481:PRO:HD2	1:J:485:TYR:HE1	1.69	0.57
1:D:180[B]:TRP:CD1	1:D:206:MET:HE1	2.40	0.57
1:G:377:GLN:HG3	1:J:360:PRO:O	2.04	0.57
1:A:43:VAL:HG12	1:A:127:LEU:HB2	1.86	0.57
1:L:15:GLN:CD	1:L:21:ILE:HD11	2.30	0.57
1:L:60:SER:HB2	1:L:112:LYS:HG2	1.85	0.57
1:L:175:HIS:ND1	1:L:215:ASP:OD2	2.36	0.57
1:A:143:ARG:NH2	1:A:156:LEU:HD21	2.15	0.57
1:F:405:THR:HG22	1:F:408:ARG:HH21	1.69	0.57
1:E:345:VAL:HG11	1:E:373:TYR:CZ	2.38	0.57
1:F:20:ARG:HD2	1:F:94:ASP:OD2	2.04	0.57
1:G:269:GLU:OE2	1:G:335:HIS:NE2	2.30	0.57
1:E:39:ARG:HH21	1:E:165:ALA:HA	1.70	0.57
1:J:345:VAL:HG13	1:J:378:LEU:HD21	1.87	0.57
1:F:180:TRP:NE1	1:F:206:MET:HE1	2.20	0.57
1:A:73:VAL:HG22	1:A:125:ILE:HD13	1.86	0.56
1:G:529:GLN:NE2	1:G:533:GLU:OE2	2.33	0.56
1:H:383:ILE:HG12	1:H:400:TRP:HB2	1.86	0.56
1:D:518:LEU:HD22	1:D:525:PRO:HD2	1.87	0.56
1:F:206:MET:HE3	1:F:256:PHE:CZ	2.39	0.56
1:I:21:ILE:HD13	1:I:48:ALA:HB2	1.87	0.56
1:B:344:HIS:HB3	1:B:347:ASN:HB2	1.87	0.56
1:C:460:GLU:HG2	1:C:464:TYR:CE1	2.40	0.56
1:E:395:GLU:HB2	1:E:397:ILE:HG13	1.87	0.56
1:G:278:GLY:HA2	1:G:344:HIS:CG	2.40	0.56
1:J:18:LEU:HD21	1:J:424:ARG:HH11	1.70	0.56
1:J:142:VAL:HG13	1:J:157:LEU:HB2	1.86	0.56
1:K:305:SER:OG	1:K:306:ASP:N	2.38	0.56
1:L:425:MET:HE2	1:L:425:MET:HA	1.86	0.56
1:C:405:THR:N	2:C:607:HOH:O	2.37	0.56
1:D:297:TRP:CG	1:D:301:LEU:HD22	2.40	0.56
1:E:92:GLU:OE1	1:E:422:LYS:NZ	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:ILE:HB	1:G:265:TYR:CZ	2.40	0.56
1:H:66:ALA:HB2	1:H:140:PHE:CG	2.41	0.56
1:D:168:LEU:HD21	1:D:502:ILE:HG12	1.86	0.56
1:B:13:TRP:CD1	1:B:28:GLN:HB2	2.41	0.56
1:C:139:ASP:OD1	1:C:139:ASP:N	2.39	0.56
1:G:66:ALA:HB2	1:G:140:PHE:CG	2.41	0.56
1:L:23:PRO:HG2	1:L:102:TRP:HB2	1.88	0.56
1:L:336:LEU:HD11	1:L:355:LEU:HD23	1.87	0.56
1:G:367:ALA:HA	1:G:383:ILE:HB	1.88	0.56
1:L:76:VAL:HG12	1:L:122:SER:O	2.05	0.56
1:C:100:PRO:HG2	1:F:119:GLU:HG3	1.86	0.56
1:H:242:SER:HB2	1:H:245:LYS:HB2	1.87	0.56
1:F:244:GLY:O	1:F:314:GLN:NE2	2.38	0.55
1:I:180:TRP:NE1	1:I:206:MET:HE1	2.21	0.55
1:J:59:ILE:HG12	1:J:144:MET:HE3	1.89	0.55
1:L:14:LEU:HD21	1:L:157:LEU:HB3	1.89	0.55
1:L:386:ILE:HG22	1:L:401:VAL:HG22	1.88	0.55
1:D:406:GLY:HA2	1:D:407:PRO:C	2.31	0.55
1:E:422:LYS:HD2	1:E:526:ARG:HE	1.70	0.55
1:H:11:ALA:O	1:H:49:PHE:HA	2.07	0.55
1:K:361:TRP:CZ3	1:K:362:MET:HG3	2.41	0.55
1:F:476:VAL:O	1:F:487:SER:HB3	2.06	0.55
1:L:24:GLN:O	1:L:24:GLN:NE2	2.39	0.55
1:L:224:GLU:OE2	1:L:272:HIS:ND1	2.40	0.55
1:H:373:TYR:HA	1:H:378:LEU:HD13	1.89	0.55
1:K:143:ARG:CZ	1:K:156:LEU:HD21	2.37	0.55
1:K:356:ARG:O	1:K:360:PRO:HB3	2.07	0.55
1:L:371:VAL:HA	1:L:392:TYR:HE1	1.70	0.55
1:B:10:MET:HE2	1:B:49:PHE:HB2	1.89	0.55
1:L:226:ARG:HH21	1:L:277:TRP:HB2	1.72	0.55
1:H:143:ARG:HH21	1:H:156:LEU:HD11	1.73	0.54
1:J:481:PRO:HD2	1:J:485:TYR:CE1	2.41	0.54
1:I:77:GLY:HA3	1:I:108:TYR:CE2	2.42	0.54
1:E:509:GLN:C	1:E:511:GLU:H	2.14	0.54
1:L:177:THR:HB	1:L:216:VAL:HB	1.88	0.54
1:A:405:THR:HG21	1:A:468:GLY:O	2.08	0.54
1:B:90:PRO:HA	1:B:93:LEU:HD12	1.89	0.54
1:B:313:LYS:HG2	1:B:358:LEU:HD11	1.88	0.54
1:C:301:LEU:HD21	1:C:308:TYR:HB2	1.89	0.54
1:L:90:PRO:HA	1:L:93:LEU:HD12	1.88	0.54
1:C:180:TRP:CD1	1:C:206:MET:HE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:368:LEU:HG	1:I:373:TYR:CG	2.42	0.54
1:J:171:ARG:HD2	1:J:174:PHE:HD2	1.73	0.54
1:J:177:THR:HB	1:J:216:VAL:HB	1.88	0.54
1:G:422:LYS:HD2	1:G:526:ARG:NH1	2.23	0.54
1:L:323:LEU:HD13	1:L:329:LEU:HD23	1.89	0.54
1:D:511:GLU:H	1:D:511:GLU:CD	2.15	0.54
1:F:460:GLU:HG2	1:F:464:TYR:CE1	2.42	0.54
1:H:368:LEU:O	1:H:384:PRO:HA	2.08	0.54
1:I:152:GLU:O	1:I:153:LYS:HD2	2.08	0.54
1:L:384:PRO:HD2	1:L:400:TRP:O	2.08	0.54
1:A:199:TRP:CZ2	1:A:255:ARG:HD3	2.43	0.54
1:E:368:LEU:HD12	1:E:379:THR:HG22	1.90	0.54
1:G:143:ARG:NH1	1:G:156:LEU:HD21	2.23	0.54
1:E:138:HIS:O	1:E:161:VAL:HG23	2.08	0.54
1:I:269:GLU:OE2	1:I:335:HIS:NE2	2.26	0.54
1:I:376:GLU:HB3	1:I:378:LEU:HD13	1.89	0.54
1:A:144:MET:O	1:A:154:ASP:HA	2.08	0.53
1:B:172:SER:O	1:B:504:GLN:NE2	2.40	0.53
1:D:254:LYS:HE2	1:D:326:GLU:OE1	2.08	0.53
1:A:119:GLU:HG3	1:B:100:PRO:HG2	1.90	0.53
1:G:11:ALA:O	1:G:49:PHE:HA	2.08	0.53
1:G:348:TYR:OH	1:G:366:ASP:OD2	2.25	0.53
1:I:291:ASN:OD1	1:I:291:ASN:N	2.40	0.53
1:A:476:VAL:O	1:A:487:SER:HB3	2.08	0.53
1:C:376:GLU:HA	1:E:360:PRO:HB2	1.90	0.53
1:D:38:ALA:O	1:D:41:SER:OG	2.18	0.53
1:L:345:VAL:HG21	1:L:372:ARG:NH1	2.22	0.53
1:L:368:LEU:HD13	1:L:369:SER:N	2.24	0.53
1:B:177:THR:HB	1:B:216:VAL:HB	1.90	0.53
1:C:234:GLN:HE22	1:C:286:TYR:N	2.06	0.53
1:E:175:HIS:CE1	1:E:267:LYS:HD2	2.43	0.53
1:H:520:THR:HG23	1:H:523:ASP:H	1.73	0.53
1:J:466:TYR:CD1	1:J:467:PRO:HA	2.43	0.53
1:C:499:ASP:HA	1:C:502:ILE:HD12	1.90	0.53
1:D:226:ARG:HG3	1:D:276:TYR:CZ	2.44	0.53
1:G:429:LEU:HB3	1:G:521:TYR:CE1	2.43	0.53
1:J:11:ALA:O	1:J:49:PHE:HA	2.08	0.53
1:K:22:PHE:O	1:K:25:SER:HB2	2.08	0.53
1:C:40:ASN:HB2	1:C:131:ALA:HB2	1.91	0.53
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.74	0.53
1:J:434:LYS:HE2	1:J:510:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:MET:HE1	1:C:256:PHE:HB2	1.91	0.53
1:D:404:CYS:O	1:D:404:CYS:SG	2.66	0.53
1:F:206:MET:HE3	1:F:256:PHE:HZ	1.74	0.53
1:F:355:LEU:HD13	1:F:362:MET:HE3	1.90	0.53
1:H:77:GLY:HA3	1:H:108:TYR:CE2	2.43	0.53
1:K:209:LEU:HD23	1:K:490:TRP:HZ2	1.74	0.53
1:F:23:PRO:HD2	1:F:24:GLN:OE1	2.09	0.53
1:H:340:PRO:HD2	1:H:368:LEU:HD23	1.90	0.53
1:I:460:GLU:OE1	1:I:464:TYR:N	2.42	0.53
1:J:279:VAL:HG22	1:J:337:SER:HB3	1.91	0.52
1:K:514:MET:CE	1:K:538:ILE:HD11	2.38	0.52
1:G:366:ASP:O	1:G:368:LEU:HG	2.09	0.52
1:H:336:LEU:HD13	1:H:348:TYR:CZ	2.44	0.52
1:I:164:SER:HB3	1:I:539:LEU:HD12	1.91	0.52
1:A:441:TRP:HE1	1:A:473:ASP:CG	2.18	0.52
1:D:203:ARG:HG3	1:D:259:MET:HG3	1.91	0.52
1:G:367:ALA:O	1:G:368:LEU:HD23	2.10	0.52
1:F:389:ASP:OD1	1:F:393:ARG:HD3	2.09	0.52
1:F:524:PHE:O	1:F:526:ARG:NH1	2.43	0.52
1:J:210:ILE:HA	1:J:214:ASN:O	2.09	0.52
1:K:41:SER:HB2	1:K:498:GLN:OE1	2.10	0.52
1:B:365:MET:HG2	1:B:383:ILE:HD11	1.92	0.52
1:F:369:SER:O	1:F:388:SER:OG	2.27	0.52
1:G:275:LEU:HD22	1:G:283:MET:HA	1.92	0.52
1:I:72:ARG:O	1:I:125:ILE:HA	2.10	0.52
1:K:340:PRO:HB2	1:K:373:TYR:OH	2.09	0.52
1:A:272:HIS:HD1	1:A:272:HIS:H	1.57	0.52
1:K:488:ILE:O	1:K:492:VAL:HG23	2.10	0.52
1:D:141:HIS:HB3	1:D:156:LEU:HD12	1.90	0.52
1:J:352:ARG:NH2	1:J:380:ASP:OD2	2.43	0.52
1:B:405:THR:HG23	1:B:470:ALA:H	1.75	0.52
1:F:182:GLY:O	1:F:193:MET:HE1	2.10	0.52
1:H:44:SER:OG	1:H:126:THR:HG22	2.09	0.52
1:H:428:TRP:H	1:H:428:TRP:CD1	2.27	0.52
1:K:277:TRP:HZ3	1:K:339:GLU:HB2	1.74	0.52
1:I:39:ARG:HB2	1:I:167:VAL:HG22	1.92	0.52
1:A:21:ILE:HD13	1:A:48:ALA:HB2	1.92	0.51
1:A:369:SER:HB3	1:A:385:ILE:HG22	1.92	0.51
1:D:405:THR:HG22	1:D:408:ARG:HH21	1.75	0.51
1:F:386:ILE:HG22	1:F:401:VAL:HG22	1.91	0.51
1:K:387:SER:HA	1:K:411:TRP:CH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:405:THR:HG23	1:K:470:ALA:H	1.75	0.51
1:A:370:ASP:OD1	1:A:371:VAL:N	2.43	0.51
1:C:416:TYR:CD2	1:C:471:TYR:HB3	2.45	0.51
1:K:351:ALA:O	1:K:354:ILE:HB	2.09	0.51
1:A:164:SER:HB2	1:A:539:LEU:HB3	1.92	0.51
1:E:23:PRO:HG3	1:E:78:LEU:HD21	1.92	0.51
1:L:180:TRP:CD1	1:L:218:PHE:HB3	2.46	0.51
1:D:368:LEU:HG	1:D:373:TYR:CG	2.46	0.51
1:H:141:HIS:HB3	1:H:156:LEU:HD22	1.92	0.51
1:L:135:PRO:HA	1:L:163:VAL:HG13	1.93	0.51
1:H:56:GLN:HB2	2:H:605:HOH:O	2.09	0.51
1:H:180:TRP:NE1	1:H:206:MET:HE1	2.26	0.51
1:A:18:LEU:O	1:A:420:LEU:HB2	2.11	0.51
1:A:141:HIS:HB3	1:A:156:LEU:HD12	1.93	0.51
1:A:405:THR:HG23	1:A:470:ALA:H	1.76	0.51
1:C:49:PHE:CZ	1:C:121:ARG:HB2	2.46	0.51
1:E:460:GLU:HG2	1:E:464:TYR:CE1	2.46	0.51
1:E:522:GLU:O	1:E:526:ARG:NH2	2.41	0.51
1:F:142:VAL:HG13	1:F:157:LEU:HB2	1.91	0.51
1:J:39:ARG:HB3	1:J:131:ALA:HA	1.92	0.51
1:H:469:ILE:HG21	1:H:474:PRO:HG3	1.91	0.51
1:I:60:SER:HB3	1:I:112:LYS:HB3	1.93	0.51
1:L:339:GLU:HB3	1:L:368:LEU:HD23	1.92	0.51
1:B:477:VAL:HB	1:B:484:PRO:HB3	1.92	0.51
1:E:389:ASP:OD1	1:E:393:ARG:HD3	2.10	0.51
1:H:367:ALA:HA	1:H:383:ILE:HB	1.92	0.51
1:J:285:VAL:C	1:J:286:TYR:HD1	2.19	0.51
1:J:301:LEU:HD21	1:J:307:THR:HB	1.92	0.51
1:C:82:PRO:O	1:C:100:PRO:HB3	2.11	0.51
1:C:179:TRP:CZ2	1:C:439:LEU:HD11	2.46	0.51
1:D:384:PRO:HD2	1:D:400:TRP:O	2.11	0.51
1:I:226:ARG:HA	1:I:275:LEU:HD21	1.92	0.51
1:J:76:VAL:HG12	1:J:122:SER:O	2.10	0.51
1:C:206:MET:HE3	1:C:256:PHE:CZ	2.46	0.51
1:E:14:LEU:HD11	1:E:157:LEU:HB3	1.93	0.51
1:H:135:PRO:HA	1:H:163:VAL:HG22	1.91	0.51
1:I:178:HIS:CD2	1:I:440:HIS:HB3	2.45	0.51
1:I:180:TRP:CD1	1:I:206:MET:HE1	2.46	0.51
1:J:105:ASP:OD2	1:J:489:ARG:NH1	2.44	0.51
1:J:141:HIS:HD2	1:J:158:HIS:HA	1.75	0.51
1:L:78:LEU:HD13	1:L:121:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:385:ILE:HD12	1:L:402:TYR:O	2.11	0.51
1:L:425:MET:HE3	1:L:531:ILE:HG12	1.93	0.51
1:D:183:GLU:OE1	1:D:183:GLU:N	2.39	0.50
1:G:210:ILE:HA	1:G:214:ASN:O	2.11	0.50
1:J:178:HIS:CD2	1:J:440:HIS:HB3	2.46	0.50
1:K:277:TRP:CZ3	1:K:339:GLU:HB2	2.46	0.50
1:L:535:LEU:O	1:L:539:LEU:HD23	2.10	0.50
1:C:206:MET:HE3	1:C:256:PHE:HZ	1.76	0.50
1:C:384:PRO:HD2	1:C:400:TRP:O	2.11	0.50
1:H:105:ASP:OD2	1:H:489:ARG:NH1	2.45	0.50
1:A:13:TRP:CG	1:A:28:GLN:HB2	2.47	0.50
1:B:47:VAL:HG21	1:B:142:VAL:HG21	1.94	0.50
1:B:168:LEU:HD21	1:B:502:ILE:HG12	1.92	0.50
1:G:302:SER:HB3	1:G:305:SER:HB3	1.93	0.50
1:J:416:TYR:CD2	1:J:471:TYR:HB3	2.46	0.50
1:L:422:LYS:HG3	1:L:526:ARG:HD2	1.93	0.50
1:C:64:GLU:OE1	1:C:143:ARG:NH1	2.44	0.50
1:E:336:LEU:HD13	1:E:348:TYR:CZ	2.46	0.50
1:I:66:ALA:HB2	1:I:140:PHE:CG	2.46	0.50
1:I:210:ILE:HB	1:I:265:TYR:CZ	2.47	0.50
1:K:179:TRP:CE2	1:K:439:LEU:HD11	2.47	0.50
1:C:172:SER:O	1:C:504:GLN:NE2	2.43	0.50
1:D:416:TYR:CD2	1:D:471:TYR:HB3	2.47	0.50
1:F:299:GLU:C	1:F:301:LEU:H	2.18	0.50
1:F:423:LEU:HD23	1:F:492:VAL:HB	1.93	0.50
1:G:178:HIS:HB3	1:G:443:TYR:HB2	1.92	0.50
1:G:428:TRP:CD1	1:G:428:TRP:H	2.29	0.50
1:J:75:TYR:CZ	1:J:113:THR:HG21	2.46	0.50
1:K:178:HIS:CD2	1:K:440:HIS:HB3	2.47	0.50
1:L:432:LYS:HG3	1:L:515:LEU:HB3	1.93	0.50
1:A:74:ARG:HH12	1:A:486:ASP:HB2	1.76	0.50
1:E:13:TRP:CG	1:E:28:GLN:HB2	2.47	0.50
1:E:385:ILE:O	1:E:387:SER:N	2.45	0.50
1:F:133:LEU:HD23	1:F:163:VAL:HG11	1.93	0.50
1:H:105:ASP:OD1	1:H:489:ARG:HD3	2.11	0.50
1:A:368:LEU:HB3	1:A:373:TYR:CD2	2.46	0.50
1:F:359:ALA:HB1	1:F:361:TRP:CE2	2.46	0.50
1:G:43:VAL:HG12	1:G:127:LEU:HB2	1.94	0.50
1:I:66:ALA:HB2	1:I:140:PHE:CD2	2.47	0.50
1:L:196:GLU:OE1	1:L:255:ARG:NH2	2.45	0.50
1:D:43:VAL:HG12	1:D:127:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:LYS:HE2	1:F:378:LEU:HD11	1.94	0.50
1:G:499:ASP:HA	1:G:502:ILE:HG13	1.94	0.50
1:L:409:ASN:O	1:L:422:LYS:NZ	2.45	0.50
1:F:177:THR:HB	1:F:216:VAL:HB	1.94	0.49
1:H:178:HIS:HD2	1:H:440:HIS:HB3	1.73	0.49
1:I:143:ARG:NH2	1:I:156:LEU:HD21	2.25	0.49
1:L:191:THR:HB	1:L:195:ASP:OD2	2.11	0.49
1:E:64:GLU:OE2	1:E:143:ARG:HD2	2.12	0.49
1:G:47:VAL:HG21	1:G:142:VAL:HG11	1.93	0.49
1:H:387:SER:HA	1:H:411:TRP:CH2	2.46	0.49
1:H:406:GLY:HA2	1:H:407:PRO:C	2.37	0.49
1:C:186:ALA:HA	1:C:191:THR:OG1	2.13	0.49
1:F:43:VAL:HG12	1:F:127:LEU:HB2	1.95	0.49
1:F:367:ALA:C	1:F:368:LEU:HD23	2.38	0.49
1:K:295:LEU:HD11	1:K:299:GLU:HG2	1.94	0.49
1:K:514:MET:HE3	1:K:515:LEU:HD13	1.94	0.49
1:B:142:VAL:HG13	1:B:157:LEU:HB2	1.93	0.49
1:D:367:ALA:O	1:D:368:LEU:HD22	2.11	0.49
1:E:410:LYS:HB3	1:E:522:GLU:HG2	1.95	0.49
1:F:368:LEU:HD11	1:F:379:THR:HB	1.93	0.49
1:L:49:PHE:CZ	1:L:121:ARG:HB2	2.47	0.49
1:L:192:LYS:HB2	1:L:195:ASP:HB3	1.95	0.49
1:L:348:TYR:OH	1:L:379:THR:HG22	2.13	0.49
1:C:354:ILE:HG23	1:C:358:LEU:HD12	1.94	0.49
1:D:64:GLU:OE2	1:D:143:ARG:NE	2.27	0.49
1:D:348:TYR:OH	1:D:366:ASP:OD2	2.28	0.49
1:I:143:ARG:HE	1:I:156:LEU:HD21	1.78	0.49
1:J:49:PHE:CZ	1:J:121:ARG:HB2	2.47	0.49
1:D:138:HIS:HB2	1:D:161:VAL:HG22	1.93	0.49
1:E:13:TRP:HB2	1:E:30:ALA:HB3	1.93	0.49
1:E:134:SER:HB3	1:J:306:ASP:OD2	2.13	0.49
1:I:11:ALA:O	1:I:49:PHE:HA	2.12	0.49
1:J:413:ASN:O	1:J:418:THR:HG21	2.12	0.49
1:L:137:ILE:HG22	1:L:162:LYS:HG2	1.94	0.49
1:D:179:TRP:CZ2	1:D:439:LEU:HD11	2.47	0.49
1:L:39:ARG:HB3	1:L:131:ALA:HA	1.94	0.49
1:L:279:VAL:HG22	1:L:337:SER:HB3	1.93	0.49
1:G:339:GLU:HA	1:G:367:ALA:O	2.13	0.49
1:J:274:TRP:HZ3	1:J:355:LEU:HD21	1.78	0.49
1:B:20:ARG:HD2	1:B:94:ASP:OD2	2.12	0.49
1:B:297:TRP:CG	1:B:301:LEU:HD22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:CD2	1:B:471:TYR:HB3	2.47	0.49
1:C:77:GLY:HA3	1:C:108:TYR:HE2	1.76	0.49
1:C:411:TRP:CE3	1:C:522:GLU:HB2	2.48	0.49
1:D:81:MET:HE2	1:D:83:HIS:O	2.12	0.49
1:I:275:LEU:HA	1:I:283:MET:HE2	1.95	0.49
1:J:357:GLN:HB2	1:J:358:LEU:HD22	1.95	0.49
1:J:411:TRP:O	1:J:422:LYS:NZ	2.40	0.49
1:L:180:TRP:CD1	1:L:206:MET:HE1	2.48	0.49
1:B:179:TRP:CZ2	1:B:439:LEU:HD11	2.48	0.49
1:D:67:GLU:OE1	1:D:67:GLU:N	2.39	0.49
1:D:411:TRP:CE3	1:D:522:GLU:HB2	2.48	0.49
1:H:297:TRP:CD1	1:H:301:LEU:HD22	2.48	0.49
1:I:90:PRO:HA	1:I:93:LEU:HD12	1.94	0.49
1:D:58:HIS:HB3	1:D:112:LYS:HE3	1.94	0.48
1:E:399:HIS:HD2	1:E:400:TRP:O	1.96	0.48
1:G:40:ASN:HB2	1:G:131:ALA:HB2	1.95	0.48
1:H:273:LEU:O	1:H:308:TYR:OH	2.24	0.48
1:H:297:TRP:CG	1:H:301:LEU:HD22	2.47	0.48
1:J:339:GLU:HA	1:J:367:ALA:O	2.13	0.48
1:K:234:GLN:HE22	1:K:286:TYR:H	1.60	0.48
1:L:411:TRP:CD2	1:L:522:GLU:HB2	2.48	0.48
1:J:309:ILE:HA	1:J:312:LEU:HD12	1.96	0.48
1:K:17:SER:HB2	1:K:124:TRP:CH2	2.48	0.48
1:D:177:THR:HB	1:D:216:VAL:HB	1.95	0.48
1:H:376:GLU:HB2	1:H:378:LEU:CD1	2.44	0.48
1:H:384:PRO:HD2	1:H:400:TRP:O	2.14	0.48
1:I:44:SER:OG	1:I:126:THR:HG22	2.13	0.48
1:J:428:TRP:NE1	1:J:499:ASP:OD2	2.43	0.48
1:K:284:HIS:HB3	1:K:286:TYR:CE1	2.40	0.48
1:A:368:LEU:HD11	1:A:379:THR:OG1	2.13	0.48
1:C:220:GLN:HG2	1:C:222:PHE:O	2.13	0.48
1:G:15:GLN:HG2	2:G:611:HOH:O	2.12	0.48
1:K:99:LEU:HA	1:K:100:PRO:C	2.37	0.48
1:L:164:SER:CB	1:L:539:LEU:HD12	2.43	0.48
1:B:389:ASP:OD2	1:B:393:ARG:HD3	2.13	0.48
1:C:389:ASP:OD2	1:C:393:ARG:NH1	2.38	0.48
1:E:202:THR:O	1:E:206:MET:HG2	2.13	0.48
1:J:405:THR:O	1:J:408:ARG:NE	2.39	0.48
1:L:143:ARG:NH2	1:L:156:LEU:HD21	2.29	0.48
1:B:77:GLY:HA3	1:B:108:TYR:CE2	2.48	0.48
1:C:410:LYS:O	1:C:526:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TRP:CD1	1:F:28:GLN:HB2	2.48	0.48
1:F:365:MET:HE1	1:F:400:TRP:CE2	2.49	0.48
1:H:88:VAL:HG12	1:H:93:LEU:HG	1.96	0.48
1:C:119:GLU:HG3	1:F:100:PRO:HG2	1.95	0.48
1:C:368:LEU:HD13	1:C:373:TYR:CB	2.44	0.48
1:F:299:GLU:O	1:F:301:LEU:N	2.47	0.48
1:K:209:LEU:HD23	1:K:490:TRP:CZ2	2.47	0.48
1:C:368:LEU:HD22	1:C:373:TYR:CD1	2.49	0.48
1:D:82:PRO:O	1:D:100:PRO:HB3	2.14	0.48
1:D:383:ILE:HG23	1:D:400:TRP:HB2	1.96	0.48
1:D:469:ILE:HG21	1:D:474:PRO:HG3	1.96	0.48
1:F:178:HIS:HB3	1:F:443:TYR:HB2	1.94	0.48
1:I:428:TRP:CD1	1:I:428:TRP:H	2.29	0.48
1:J:384:PRO:HD2	1:J:400:TRP:O	2.13	0.48
1:J:181:ARG:NH1	1:J:441:TRP:O	2.47	0.48
1:K:249:ASP:OD1	1:K:251:SER:OG	2.31	0.48
1:K:418:THR:HG23	1:K:422:LYS:HD2	1.96	0.48
1:D:137:ILE:HA	1:D:161:VAL:O	2.14	0.48
1:E:291:ASN:OD1	1:E:291:ASN:N	2.40	0.48
1:F:411:TRP:O	1:F:422:LYS:HE3	2.14	0.48
1:H:424:ARG:NH1	1:H:499:ASP:OD1	2.47	0.48
1:I:219:ILE:O	1:I:221:ASN:N	2.44	0.48
1:J:313:LYS:HG2	1:J:358:LEU:HD11	1.96	0.48
1:L:124:TRP:CZ3	1:L:488:ILE:HD12	2.48	0.48
1:L:274:TRP:HZ3	1:L:355:LEU:HD21	1.78	0.48
1:A:210:ILE:HD12	1:A:265:TYR:CD2	2.48	0.47
1:C:520:THR:HG22	1:C:522:GLU:N	2.23	0.47
1:D:234:GLN:NE2	1:D:286:TYR:O	2.46	0.47
1:D:404:CYS:C	1:D:406:GLY:N	2.70	0.47
1:E:21:ILE:HD13	1:E:48:ALA:HB2	1.96	0.47
1:E:373:TYR:HB3	1:E:378:LEU:HG	1.95	0.47
1:F:279:VAL:HG22	1:F:337:SER:HB3	1.96	0.47
1:G:10:MET:CE	1:G:49:PHE:HB2	2.44	0.47
1:L:180:TRP:CG	1:L:206:MET:HE1	2.49	0.47
1:A:365:MET:HB3	1:A:381:ILE:HB	1.95	0.47
1:B:220:GLN:O	1:B:235:MET:HG3	2.14	0.47
1:B:414:ARG:NH2	1:B:440:HIS:CG	2.83	0.47
1:D:13:TRP:CD1	1:D:28:GLN:HB2	2.48	0.47
1:D:431:TYR:CD2	1:D:503:LEU:HD13	2.49	0.47
1:D:438:PHE:CE2	1:D:440:HIS:HB2	2.49	0.47
1:E:35:LEU:O	1:E:161:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ARG:HB3	1:F:126:THR:OG1	2.14	0.47
1:H:240:GLU:HG3	1:H:246:TYR:CD1	2.49	0.47
1:I:124:TRP:CZ3	1:I:488:ILE:HG12	2.49	0.47
1:I:408:ARG:NH2	1:I:470:ALA:HB2	2.28	0.47
1:K:66:ALA:HB2	1:K:140:PHE:CD2	2.48	0.47
1:L:168:LEU:HD21	1:L:502:ILE:HA	1.96	0.47
1:A:74:ARG:NH1	1:A:486:ASP:HB2	2.29	0.47
1:B:422:LYS:HE3	1:B:526:ARG:NH1	2.29	0.47
1:G:278:GLY:HA3	1:G:280:GLN:OE1	2.15	0.47
1:H:334:PHE:HB2	1:H:363:LYS:O	2.15	0.47
1:L:230:LYS:HA	1:L:230:LYS:HD3	1.56	0.47
1:C:105:ASP:H	1:C:106:PRO:HD2	1.80	0.47
1:E:404:CYS:O	1:E:404:CYS:SG	2.73	0.47
1:G:405:THR:HG23	1:G:470:ALA:H	1.79	0.47
1:H:511:GLU:CD	1:H:511:GLU:H	2.22	0.47
1:J:372:ARG:HD2	1:J:375:ARG:NH1	2.26	0.47
1:K:13:TRP:NE1	1:K:48:ALA:HB3	2.30	0.47
1:L:144:MET:O	1:L:154:ASP:HA	2.14	0.47
1:E:23:PRO:HD2	1:E:24:GLN:OE1	2.15	0.47
1:G:248:PHE:CZ	1:G:315:TYR:HB2	2.50	0.47
1:H:368:LEU:HD13	1:H:373:TYR:HB3	1.96	0.47
1:J:466:TYR:CG	1:J:467:PRO:HA	2.50	0.47
1:K:223:PHE:CZ	1:K:225:LEU:HD23	2.48	0.47
1:D:241:PRO:HD2	1:D:245:LYS:O	2.14	0.47
1:E:178:HIS:HB3	1:E:443:TYR:HB2	1.95	0.47
1:K:76:VAL:HG12	1:K:122:SER:O	2.15	0.47
1:L:134:SER:O	1:L:138:HIS:NE2	2.40	0.47
1:L:424:ARG:O	1:L:496:SER:OG	2.31	0.47
1:A:441:TRP:NE1	1:A:473:ASP:OD2	2.45	0.47
1:B:152:GLU:O	1:B:153:LYS:HD2	2.15	0.47
1:D:340:PRO:HB2	1:D:373:TYR:CZ	2.49	0.47
1:F:39:ARG:HB3	1:F:131:ALA:HA	1.96	0.47
1:G:18:LEU:O	1:G:420:LEU:HB2	2.14	0.47
1:H:346:GLU:H	1:H:346:GLU:CD	2.22	0.47
1:J:179:TRP:CE2	1:J:439:LEU:HD11	2.49	0.47
1:K:34:GLU:HA	1:K:160:LYS:HG2	1.96	0.47
1:E:425:MET:HE3	1:E:531:ILE:CG1	2.41	0.47
1:F:460:GLU:HG2	1:F:464:TYR:CD1	2.50	0.47
1:H:360:PRO:O	1:L:377:GLN:HG3	2.15	0.47
1:I:421:PRO:HB2	1:I:526:ARG:O	2.15	0.47
1:A:210:ILE:HA	1:A:214:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:CG2	1:D:155:LYS:HD3	2.44	0.47
1:F:428:TRP:CZ2	1:F:535:LEU:HD13	2.50	0.47
1:G:99:LEU:HA	1:G:100:PRO:C	2.40	0.47
1:H:428:TRP:NE1	1:H:499:ASP:OD2	2.42	0.47
1:L:192:LYS:HB3	1:L:192:LYS:HE3	1.56	0.47
1:A:101:GLY:HA2	1:B:102:TRP:CD1	2.50	0.47
1:B:60:SER:HB3	1:B:112:LYS:HG3	1.96	0.47
1:F:194:PHE:HA	1:F:198:TRP:CE3	2.49	0.47
1:H:42:ARG:N	1:H:498:GLN:OE1	2.41	0.47
1:K:45:PHE:CE1	1:K:125:ILE:HB	2.49	0.47
1:B:384:PRO:HD2	1:B:400:TRP:O	2.14	0.46
1:C:367:ALA:HA	1:C:383:ILE:HB	1.97	0.46
1:E:460:GLU:HG2	1:E:464:TYR:CD1	2.51	0.46
1:F:405:THR:N	2:F:602:HOH:O	2.48	0.46
1:G:179:TRP:CE2	1:G:439:LEU:HD11	2.50	0.46
1:I:232:PRO:HG3	1:I:286:TYR:CD2	2.49	0.46
1:J:355:LEU:HD13	1:J:355:LEU:HA	1.81	0.46
1:E:416:TYR:CD2	1:E:471:TYR:HB3	2.51	0.46
1:I:133:LEU:HD11	1:I:138:HIS:CE1	2.51	0.46
1:K:535:LEU:HD12	1:K:535:LEU:HA	1.81	0.46
1:E:254:LYS:HD3	1:E:258:ASP:OD2	2.15	0.46
1:G:237:ILE:CB	1:G:249:ASP:HB3	2.39	0.46
1:H:291:ASN:N	1:H:291:ASN:OD1	2.46	0.46
1:J:429:LEU:HB3	1:J:521:TYR:CE1	2.50	0.46
1:K:405:THR:HG21	1:K:468:GLY:O	2.15	0.46
1:C:39:ARG:HB3	1:C:131:ALA:HA	1.97	0.46
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.68	0.46
1:D:407:PRO:HB2	1:D:411:TRP:CD1	2.51	0.46
1:F:272:HIS:HD1	1:F:272:HIS:H	1.63	0.46
1:I:47:VAL:HG12	1:I:144:MET:HE2	1.98	0.46
1:L:92:GLU:O	1:L:419:PRO:HD3	2.16	0.46
1:C:404:CYS:C	1:C:406:GLY:N	2.69	0.46
1:G:19:GLN:HB2	2:G:611:HOH:O	2.15	0.46
1:H:39:ARG:HB2	1:H:167:VAL:HG22	1.97	0.46
1:I:177:THR:HB	1:I:216:VAL:HB	1.97	0.46
1:K:12:VAL:HG11	1:K:144:MET:HG3	1.96	0.46
1:A:58:HIS:HB2	1:A:147:GLN:OE1	2.16	0.46
1:B:171:ARG:NH1	1:B:174:PHE:O	2.49	0.46
1:C:336:LEU:HD23	1:C:348:TYR:CE1	2.50	0.46
1:F:254:LYS:HE2	1:F:326:GLU:OE1	2.16	0.46
1:G:274:TRP:HZ3	1:G:355:LEU:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HD2	1:B:133:LEU:HD22	1.97	0.46
1:D:20:ARG:HD2	1:D:94:ASP:OD2	2.16	0.46
1:D:278:GLY:HA2	1:D:344:HIS:CD2	2.51	0.46
1:D:335:HIS:ND1	1:D:365:MET:O	2.49	0.46
1:E:234:GLN:HE22	1:E:286:TYR:H	1.63	0.46
1:G:274:TRP:HB2	1:G:337:SER:HB2	1.96	0.46
1:G:350:LYS:O	1:G:354:ILE:HD12	2.15	0.46
1:G:386:ILE:HG22	1:G:401:VAL:HB	1.98	0.46
1:H:272:HIS:CD2	1:H:335:HIS:HB3	2.51	0.46
1:J:99:LEU:HA	1:J:100:PRO:C	2.41	0.46
1:B:289:GLU:OE2	1:B:294:LYS:HD3	2.16	0.46
1:C:180:TRP:CE2	1:C:206:MET:CE	2.99	0.46
1:E:234:GLN:NE2	1:E:286:TYR:O	2.48	0.46
1:F:368:LEU:HD13	1:F:373:TYR:CD1	2.50	0.46
1:H:177:THR:HB	1:H:216:VAL:HB	1.97	0.46
1:J:108:TYR:HD1	1:J:485:TYR:CD2	2.34	0.46
1:K:49:PHE:CZ	1:K:121:ARG:HB2	2.51	0.46
1:K:348:TYR:OH	1:K:366:ASP:OD2	2.26	0.46
1:L:91:GLU:OE1	1:L:91:GLU:N	2.38	0.46
1:A:220:GLN:O	1:A:235:MET:HG3	2.15	0.46
1:C:466:TYR:CG	1:C:467:PRO:HA	2.51	0.46
1:D:347:ASN:HA	1:D:350:LYS:HD2	1.98	0.46
1:G:432:LYS:HG3	1:G:515:LEU:HB3	1.98	0.46
1:H:365:MET:HE1	1:H:400:TRP:CE2	2.50	0.46
1:J:41:SER:HA	1:J:498:GLN:HE22	1.81	0.46
1:L:338:ASP:OD1	1:L:339:GLU:HG3	2.16	0.46
1:C:443:TYR:N	2:C:608:HOH:O	2.38	0.46
1:D:367:ALA:HA	1:D:383:ILE:HB	1.97	0.46
1:H:21:ILE:HD13	1:H:48:ALA:HB2	1.98	0.46
1:J:350:LYS:O	1:J:354:ILE:HG12	2.15	0.46
1:A:156:LEU:O	1:A:157:LEU:HD23	2.16	0.45
1:F:183:GLU:OE1	1:F:183:GLU:N	2.43	0.45
1:H:171:ARG:HD3	1:H:174:PHE:CD2	2.47	0.45
1:H:339:GLU:N	1:H:340:PRO:HD3	2.31	0.45
1:H:340:PRO:HD2	1:H:368:LEU:CD2	2.46	0.45
1:H:370:ASP:OD1	1:H:371:VAL:N	2.48	0.45
1:H:535:LEU:HD23	1:H:539:LEU:CD2	2.44	0.45
1:J:274:TRP:CZ3	1:J:355:LEU:HD21	2.51	0.45
1:J:387:SER:HA	1:J:411:TRP:CH2	2.50	0.45
1:L:272:HIS:HB3	1:L:336:LEU:O	2.15	0.45
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LEU:HD12	1:D:104:PRO:HA	1.96	0.45
1:E:438:PHE:CE2	1:E:440:HIS:HB2	2.51	0.45
1:F:336:LEU:HD21	1:F:351:ALA:HB3	1.98	0.45
1:F:405:THR:HG21	1:F:468:GLY:O	2.17	0.45
1:G:105:ASP:OD2	1:G:489:ARG:NH1	2.50	0.45
1:H:338:ASP:C	1:H:340:PRO:HD3	2.42	0.45
1:J:14:LEU:HD23	1:J:47:VAL:HG22	1.98	0.45
1:J:275:LEU:HG	1:J:283:MET:HA	1.98	0.45
1:B:363:LYS:HA	1:B:380:ASP:OD2	2.17	0.45
1:D:11:ALA:O	1:D:49:PHE:HA	2.16	0.45
1:G:449:LEU:HD22	1:G:469:ILE:HG13	1.97	0.45
1:I:383:ILE:HG23	1:I:400:TRP:HB2	1.98	0.45
1:J:40:ASN:HB2	1:J:131:ALA:HB2	1.97	0.45
1:K:386:ILE:HG22	1:K:401:VAL:HB	1.98	0.45
1:B:424:ARG:NH1	1:B:495:GLU:HB3	2.31	0.45
1:D:105:ASP:OD2	1:D:489:ARG:NH1	2.49	0.45
1:F:278:GLY:HA2	1:F:344:HIS:CG	2.51	0.45
1:H:179:TRP:CZ2	1:H:439:LEU:HD11	2.51	0.45
1:J:166:LEU:HD22	1:J:167:VAL:N	2.32	0.45
1:J:177:THR:HG23	1:J:439:LEU:HD12	1.98	0.45
1:J:368:LEU:HD23	1:J:368:LEU:HA	1.77	0.45
1:A:424:ARG:O	1:A:496:SER:OG	2.30	0.45
1:B:411:TRP:O	1:B:422:LYS:HE2	2.17	0.45
1:D:298:ALA:HB1	1:D:300:ASN:OD1	2.15	0.45
1:F:44:SER:OG	1:F:126:THR:HG22	2.16	0.45
1:G:280:GLN:HG3	1:G:347:ASN:OD1	2.16	0.45
1:H:99:LEU:HA	1:H:100:PRO:C	2.41	0.45
1:H:280:GLN:H	1:H:280:GLN:HG3	1.56	0.45
1:K:177:THR:HG23	1:K:439:LEU:HD12	1.98	0.45
1:C:235:MET:HE2	1:C:235:MET:HB3	1.63	0.45
1:D:417:ASP:OD1	1:D:417:ASP:N	2.33	0.45
1:E:105:ASP:HB3	1:E:106:PRO:HD3	1.99	0.45
1:F:58:HIS:HB3	1:F:112:LYS:HE2	1.99	0.45
1:H:18:LEU:O	1:H:421:PRO:HD3	2.16	0.45
1:H:116:HIS:HD2	2:H:605:HOH:O	1.99	0.45
1:J:368:LEU:HD22	1:J:373:TYR:CD2	2.51	0.45
1:J:386:ILE:HG22	1:J:401:VAL:HG22	1.97	0.45
1:L:210:ILE:HA	1:L:214:ASN:O	2.16	0.45
1:L:217:ALA:HB3	1:L:268:PHE:CD2	2.52	0.45
1:E:193:MET:HE2	1:E:193:MET:HB2	1.79	0.45
1:E:236:LEU:HD21	1:E:248:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:GLY:HA3	1:F:108:TYR:CE2	2.52	0.45
1:F:376:GLU:HB3	1:F:378:LEU:HD13	1.99	0.45
1:G:74:ARG:HH12	1:G:486:ASP:HB2	1.81	0.45
1:J:178:HIS:HB3	1:J:443:TYR:HB2	1.99	0.45
1:J:405:THR:HG23	1:J:470:ALA:H	1.81	0.45
1:K:296:LEU:H	1:K:296:LEU:HG	1.55	0.45
1:B:535:LEU:HD12	1:B:535:LEU:HA	1.67	0.45
1:C:414:ARG:HD2	1:C:476:VAL:CG1	2.46	0.45
1:D:199:TRP:CE2	1:D:255:ARG:HD3	2.51	0.45
1:E:350:LYS:HE3	1:E:350:LYS:HB2	1.74	0.45
1:G:309:ILE:HD13	1:G:309:ILE:HA	1.86	0.45
1:J:105:ASP:CG	1:J:489:ARG:HH11	2.25	0.45
1:A:498:GLN:HE21	1:A:498:GLN:HB3	1.51	0.45
1:B:424:ARG:O	1:B:424:ARG:HG3	2.17	0.45
1:E:13:TRP:CD1	1:E:28:GLN:HB2	2.52	0.45
1:F:224:GLU:OE2	1:F:272:HIS:ND1	2.41	0.45
1:J:41:SER:CA	1:J:498:GLN:HE22	2.29	0.45
1:K:365:MET:HE3	1:K:383:ILE:HD11	1.99	0.45
1:B:144:MET:O	1:B:154:ASP:HA	2.17	0.45
1:B:407:PRO:HB2	1:B:411:TRP:CD1	2.52	0.45
1:C:414:ARG:NH1	2:C:605:HOH:O	2.32	0.45
1:D:143:ARG:NH1	1:D:154:ASP:OD2	2.50	0.45
1:F:343:GLU:O	1:F:343:GLU:HG2	2.17	0.45
1:F:488:ILE:O	1:F:492:VAL:HG23	2.17	0.45
1:J:259:MET:HE3	1:J:259:MET:HB2	1.59	0.45
1:K:13:TRP:CD2	1:K:28:GLN:HB2	2.51	0.45
1:K:334:PHE:CB	1:K:362:MET:HE3	2.47	0.45
1:K:469:ILE:HG21	1:K:474:PRO:HG3	1.98	0.45
1:L:355:LEU:HG	1:L:362:MET:CE	2.47	0.45
1:L:481:PRO:HD2	1:L:485:TYR:CZ	2.52	0.45
1:D:414:ARG:HG3	1:D:423:LEU:HD11	1.99	0.44
1:D:531:ILE:O	1:D:535:LEU:HB2	2.16	0.44
1:E:39:ARG:HB3	1:E:131:ALA:HA	1.99	0.44
1:H:293:TYR:C	1:H:294:LYS:HD2	2.41	0.44
1:J:286:TYR:CD1	1:J:286:TYR:N	2.85	0.44
1:L:395:GLU:HB2	1:L:397:ILE:HG13	2.00	0.44
1:C:130:PRO:HD2	1:C:133:LEU:HB2	2.00	0.44
1:E:503:LEU:HD23	1:E:503:LEU:HA	1.75	0.44
1:G:22:PHE:O	1:G:25:SER:HB3	2.17	0.44
1:G:119:GLU:OE2	1:K:83:HIS:ND1	2.41	0.44
1:G:177:THR:HB	1:G:216:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:84:PHE:CD1	1:I:93:LEU:HD22	2.52	0.44
1:B:222:PHE:HE1	1:B:236:LEU:HD23	1.83	0.44
1:D:278:GLY:HA2	1:D:344:HIS:CG	2.53	0.44
1:E:127:LEU:HD21	1:E:140:PHE:CE1	2.51	0.44
1:E:365:MET:HE1	1:E:400:TRP:CE2	2.52	0.44
1:E:498:GLN:HE21	1:E:498:GLN:HB3	1.59	0.44
1:K:181:ARG:HB3	1:K:183:GLU:CD	2.42	0.44
1:B:421:PRO:HB2	1:B:526:ARG:O	2.17	0.44
1:E:127:LEU:HD21	1:E:140:PHE:CZ	2.52	0.44
1:F:178:HIS:HA	1:F:440:HIS:O	2.18	0.44
1:H:404:CYS:O	1:H:406:GLY:N	2.50	0.44
1:I:148:GLU:HG3	1:I:153:LYS:HG2	1.98	0.44
1:I:355:LEU:HD12	1:I:355:LEU:HA	1.82	0.44
1:I:363:LYS:HA	1:I:380:ASP:OD2	2.17	0.44
1:K:536:LYS:HG2	1:K:540:GLU:OE2	2.17	0.44
1:L:424:ARG:NH1	1:L:495:GLU:HB3	2.30	0.44
1:A:411:TRP:CE3	1:A:522:GLU:HB2	2.52	0.44
1:C:166:LEU:HD23	1:C:167:VAL:H	1.82	0.44
1:D:274:TRP:CZ3	1:D:351:ALA:HB1	2.52	0.44
1:G:101:GLY:HA2	1:K:102:TRP:CD1	2.53	0.44
1:I:39:ARG:HB3	1:I:131:ALA:HA	1.98	0.44
1:L:18:LEU:HD11	1:L:424:ARG:HB2	2.00	0.44
1:L:18:LEU:HD21	1:L:424:ARG:HD3	2.00	0.44
1:B:267:LYS:HD3	1:B:331:ASP:HB3	1.98	0.44
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.77	0.44
1:C:301:LEU:HD11	1:C:307:THR:HB	2.00	0.44
1:C:404:CYS:O	1:C:404:CYS:SG	2.76	0.44
1:D:294:LYS:HD2	1:D:294:LYS:HA	1.55	0.44
1:E:289:GLU:O	1:E:289:GLU:HG3	2.18	0.44
1:K:407:PRO:HG2	1:K:411:TRP:CG	2.52	0.44
1:B:44:SER:HG	1:B:126:THR:HG23	1.83	0.44
1:D:138:HIS:HB2	1:D:161:VAL:CG2	2.47	0.44
1:E:49:PHE:CE2	1:E:59:ILE:HG21	2.52	0.44
1:E:462:ALA:HB2	1:E:471:TYR:CD1	2.53	0.44
1:G:240:GLU:OE2	1:G:243:PRO:HA	2.18	0.44
1:G:408:ARG:NH2	1:G:470:ALA:HB2	2.33	0.44
1:H:210:ILE:HA	1:H:214:ASN:O	2.18	0.44
1:A:113:THR:OG1	1:A:114:GLU:N	2.50	0.44
1:B:82:PRO:HB2	1:B:83:HIS:CD2	2.52	0.44
1:B:178:HIS:CD2	1:B:440:HIS:HB3	2.53	0.44
1:D:142:VAL:CG1	1:D:157:LEU:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:MET:CE	1:E:531:ILE:HG12	2.43	0.44
1:G:81:MET:HE2	1:G:99:LEU:HD13	2.00	0.44
1:G:156:LEU:C	1:G:157:LEU:HD12	2.43	0.44
1:G:297:TRP:HB2	1:G:298:ALA:H	1.72	0.44
1:I:408:ARG:HH21	1:I:470:ALA:HB2	1.82	0.44
1:L:81:MET:HE3	1:L:99:LEU:HD13	2.00	0.44
1:C:34:GLU:O	1:C:35:LEU:HD23	2.18	0.44
1:C:92:GLU:OE1	1:C:526:ARG:NH1	2.51	0.44
1:D:416:TYR:HD2	1:D:471:TYR:HB3	1.83	0.44
1:K:295:LEU:HD23	1:K:295:LEU:H	1.83	0.44
1:A:405:THR:N	2:A:611:HOH:O	2.50	0.43
1:D:511:GLU:N	1:D:511:GLU:OE1	2.49	0.43
1:E:11:ALA:O	1:E:49:PHE:HA	2.17	0.43
1:E:300:ASN:OD1	1:E:300:ASN:N	2.47	0.43
1:E:358:LEU:HD13	1:E:358:LEU:HA	1.85	0.43
1:H:210:ILE:HB	1:H:265:TYR:CE1	2.53	0.43
1:H:346:GLU:O	1:H:350:LYS:HG2	2.18	0.43
1:H:405:THR:CG2	1:H:469:ILE:HA	2.48	0.43
1:I:164:SER:HB2	1:I:539:LEU:HB3	1.99	0.43
1:J:443:TYR:CZ	1:J:477:VAL:HG21	2.53	0.43
1:L:300:ASN:OD1	1:L:300:ASN:N	2.47	0.43
1:A:12:VAL:HA	1:A:48:ALA:O	2.18	0.43
1:B:53:MET:SD	1:B:148:GLU:HG2	2.58	0.43
1:D:178:HIS:CD2	1:D:440:HIS:HB3	2.52	0.43
1:D:206:MET:HE3	1:D:256:PHE:CZ	2.53	0.43
1:D:297:TRP:CD1	1:D:301:LEU:HD22	2.53	0.43
1:D:389:ASP:OD2	1:D:393:ARG:HD3	2.18	0.43
1:D:535:LEU:HD12	1:D:535:LEU:HA	1.86	0.43
1:H:177:THR:HG22	1:H:400:TRP:HZ3	1.82	0.43
1:H:287:LYS:HD3	1:H:296:LEU:HD21	1.99	0.43
1:H:376:GLU:HB2	1:H:378:LEU:HD12	2.00	0.43
1:I:73:VAL:HB	1:I:111:THR:HG22	2.00	0.43
1:J:34:GLU:C	1:J:35:LEU:HD12	2.43	0.43
1:K:223:PHE:CE2	1:K:225:LEU:HB2	2.52	0.43
1:A:514:MET:HG3	1:A:515:LEU:HD23	2.00	0.43
1:D:19:GLN:HA	1:D:19:GLN:OE1	2.18	0.43
1:J:146:TRP:CE2	1:J:153:LYS:HB2	2.54	0.43
1:J:390:GLU:HA	1:J:393:ARG:NH1	2.34	0.43
1:K:81:MET:HE2	1:K:83:HIS:O	2.18	0.43
1:K:366:ASP:O	1:K:368:LEU:HG	2.17	0.43
1:L:341:TRP:HB2	1:L:344:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HG23	1:A:439:LEU:HD13	2.00	0.43
1:A:183:GLU:OE1	1:A:183:GLU:N	2.43	0.43
1:B:105:ASP:H	1:B:106:PRO:HD2	1.83	0.43
1:B:383:ILE:HG12	1:B:400:TRP:HB2	2.01	0.43
1:B:536:LYS:O	1:B:537:LYS:C	2.61	0.43
1:D:275:LEU:HG	1:D:283:MET:HA	2.00	0.43
1:G:64:GLU:OE2	1:G:143:ARG:HD2	2.19	0.43
1:G:409:ASN:O	1:G:422:LYS:NZ	2.51	0.43
1:J:46:GLN:HA	1:J:123:PHE:O	2.19	0.43
1:L:341:TRP:HD1	1:L:344:HIS:CE1	2.36	0.43
1:F:404:CYS:O	1:F:404:CYS:SG	2.76	0.43
1:F:428:TRP:H	1:F:428:TRP:CD1	2.36	0.43
1:F:436:LEU:HA	1:F:436:LEU:HD23	1.80	0.43
1:G:72:ARG:HH21	1:G:74:ARG:NH1	2.16	0.43
1:I:410:LYS:HB3	1:I:410:LYS:HE2	1.72	0.43
1:K:50:ARG:HD2	1:K:120:SER:OG	2.19	0.43
1:K:383:ILE:HG12	1:K:400:TRP:HB2	2.01	0.43
1:L:99:LEU:HA	1:L:100:PRO:C	2.43	0.43
1:L:215:ASP:OD1	1:L:215:ASP:N	2.44	0.43
1:A:13:TRP:CD1	1:A:28:GLN:HB2	2.54	0.43
1:B:49:PHE:CZ	1:B:121:ARG:HB2	2.53	0.43
1:B:428:TRP:CD1	1:B:428:TRP:H	2.37	0.43
1:D:345:VAL:HG21	1:D:372:ARG:NH1	2.34	0.43
1:E:12:VAL:CG2	1:E:155:LYS:HD3	2.49	0.43
1:F:199:TRP:CZ2	1:F:255:ARG:HD3	2.53	0.43
1:G:425:MET:HE2	1:G:525:PRO:HG2	2.00	0.43
1:H:89:SER:HB3	1:H:409:ASN:OD1	2.18	0.43
1:I:10:MET:HE3	1:I:50:ARG:C	2.43	0.43
1:I:385:ILE:HD12	1:I:402:TYR:O	2.19	0.43
1:J:106:PRO:HB3	1:J:478:TYR:CD1	2.54	0.43
1:J:386:ILE:HG23	1:J:402:TYR:O	2.18	0.43
1:J:389:ASP:OD1	1:J:393:ARG:NH1	2.50	0.43
1:L:414:ARG:HA	1:L:423:LEU:HD13	2.00	0.43
1:A:78:LEU:HD13	1:A:121:ARG:NH2	2.34	0.43
1:A:416:TYR:CD2	1:A:471:TYR:HB3	2.54	0.43
1:B:404:CYS:O	1:B:404:CYS:SG	2.76	0.43
1:E:99:LEU:HA	1:E:100:PRO:C	2.44	0.43
1:E:105:ASP:OD2	1:E:489:ARG:NH1	2.52	0.43
1:F:408:ARG:HB3	1:F:409:ASN:H	1.66	0.43
1:F:521:TYR:O	1:F:524:PHE:HE2	2.02	0.43
1:J:105:ASP:OD1	1:J:489:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:383:ILE:HG12	1:J:400:TRP:HB2	2.00	0.43
1:L:42:ARG:HA	1:L:127:LEU:O	2.18	0.43
1:L:538:ILE:HG22	1:L:539:LEU:HD22	2.00	0.43
1:C:364:VAL:N	1:C:380:ASP:OD2	2.48	0.43
1:D:17:SER:HB2	1:D:124:TRP:CH2	2.53	0.43
1:E:84:PHE:CE1	1:E:99:LEU:HB2	2.54	0.43
1:E:278:GLY:HA2	1:E:344:HIS:CG	2.54	0.43
1:F:376:GLU:O	1:F:377:GLN:C	2.61	0.43
1:H:15:GLN:HE21	1:H:19:GLN:HB3	1.84	0.43
1:H:370:ASP:O	1:H:392:TYR:OH	2.31	0.43
1:J:18:LEU:HD11	1:J:424:ARG:HB2	2.00	0.43
1:K:23:PRO:HB3	1:K:119:GLU:HG3	2.01	0.43
1:A:224:GLU:OE2	1:A:272:HIS:ND1	2.50	0.43
1:B:420:LEU:HD12	1:B:420:LEU:H	1.84	0.43
1:C:350:LYS:HE3	1:C:350:LYS:HB2	1.50	0.43
1:D:47:VAL:HG21	1:D:142:VAL:HG21	2.01	0.43
1:D:352:ARG:HD2	1:D:352:ARG:HA	1.77	0.43
1:E:27:ALA:HB2	1:E:50:ARG:HD3	2.01	0.43
1:H:177:THR:OG1	1:H:269:GLU:OE1	2.34	0.43
1:J:14:LEU:HD11	1:J:157:LEU:HB3	2.00	0.43
1:J:368:LEU:HD22	1:J:373:TYR:CG	2.54	0.43
1:L:506:ALA:HB3	1:L:508:ILE:CD1	2.49	0.43
1:A:278:GLY:HA3	1:A:280:GLN:NE2	2.33	0.43
1:A:404:CYS:O	1:A:404:CYS:SG	2.77	0.43
1:C:237:ILE:CB	1:C:249:ASP:HB3	2.36	0.43
1:E:177:THR:HB	1:E:216:VAL:HB	2.00	0.43
1:F:257:VAL:HG13	1:F:268:PHE:CZ	2.53	0.43
1:F:384:PRO:HD2	1:F:400:TRP:O	2.19	0.43
1:H:405:THR:HG22	1:H:408:ARG:HH21	1.83	0.43
1:J:288:LYS:HE3	1:J:293:TYR:CE1	2.53	0.43
1:K:268:PHE:O	1:K:332:SER:HA	2.18	0.43
1:K:368:LEU:O	1:K:369:SER:OG	2.33	0.43
1:A:55:ASP:HA	1:B:86:THR:HG23	2.01	0.42
1:B:33:LEU:HD12	1:B:34:GLU:H	1.84	0.42
1:C:339:GLU:HA	1:C:367:ALA:O	2.18	0.42
1:E:423:LEU:HD23	1:E:492:VAL:HB	2.00	0.42
1:F:21:ILE:HD12	1:F:48:ALA:HB2	2.00	0.42
1:L:105:ASP:HA	1:L:488:ILE:HG12	2.01	0.42
1:A:130:PRO:HD2	1:A:133:LEU:HB2	2.00	0.42
1:A:310:HIS:O	1:A:314:GLN:HG3	2.19	0.42
1:A:336:LEU:HD22	1:A:348:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HD3	1:C:145:ARG:NH2	2.34	0.42
1:I:47:VAL:HG21	1:I:142:VAL:HG11	2.01	0.42
1:I:105:ASP:HB3	1:I:106:PRO:HD3	2.01	0.42
1:J:480:GLY:CA	1:J:485:TYR:HE1	2.32	0.42
1:A:39:ARG:HB3	1:A:131:ALA:HA	2.01	0.42
1:C:352:ARG:HD2	1:C:352:ARG:HA	1.86	0.42
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.87	0.42
1:F:81:MET:HE2	1:F:83:HIS:O	2.19	0.42
1:F:182:GLY:C	1:F:193:MET:HE1	2.43	0.42
1:G:428:TRP:CD1	1:G:428:TRP:N	2.87	0.42
1:H:343:GLU:CD	1:H:343:GLU:H	2.26	0.42
1:J:411:TRP:CD2	1:J:522:GLU:HB2	2.54	0.42
1:L:45:PHE:CE1	1:L:125:ILE:HB	2.54	0.42
1:L:351:ALA:O	1:L:355:LEU:HD22	2.19	0.42
1:C:99:LEU:HA	1:C:100:PRO:C	2.44	0.42
1:D:18:LEU:HD12	1:D:421:PRO:HA	2.01	0.42
1:D:207:LYS:O	1:D:210:ILE:HG22	2.19	0.42
1:D:404:CYS:C	1:D:406:GLY:H	2.27	0.42
1:G:230:LYS:HD3	1:G:230:LYS:HA	1.89	0.42
1:J:193:MET:HE2	1:J:193:MET:HB2	1.95	0.42
1:J:275:LEU:HD23	1:J:275:LEU:HA	1.81	0.42
1:J:366:ASP:C	1:J:383:ILE:HD12	2.44	0.42
1:K:341:TRP:CD1	1:K:341:TRP:N	2.86	0.42
1:L:320:HIS:HA	1:L:323:LEU:HD12	2.00	0.42
1:A:428:TRP:HB3	1:A:518:LEU:HD21	2.02	0.42
1:C:439:LEU:HD23	1:C:440:HIS:N	2.34	0.42
1:C:490:TRP:HA	1:C:490:TRP:CE3	2.55	0.42
1:D:371:VAL:HA	1:D:392:TYR:CE1	2.54	0.42
1:F:150:LYS:HA	1:F:150:LYS:HD3	1.83	0.42
1:F:371:VAL:HA	1:F:392:TYR:CE1	2.54	0.42
1:G:361:TRP:CD1	1:G:361:TRP:H	2.36	0.42
1:H:275:LEU:HA	1:H:275:LEU:HD13	1.78	0.42
1:H:414:ARG:HG3	1:H:423:LEU:HD11	2.01	0.42
1:L:57:THR:OG1	1:L:58:HIS:N	2.53	0.42
1:A:50:ARG:HD2	1:A:120:SER:OG	2.19	0.42
1:A:199:TRP:CE2	1:A:255:ARG:HD3	2.55	0.42
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.64	0.42
1:A:425:MET:HE2	1:A:525:PRO:O	2.20	0.42
1:B:321:ARG:HE	1:B:321:ARG:HB3	1.58	0.42
1:C:193:MET:HB2	1:C:193:MET:HE2	1.87	0.42
1:D:77:GLY:HA3	1:D:108:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:LYS:HD3	1:E:518:LEU:O	2.20	0.42
1:G:244:GLY:O	1:G:314:GLN:NE2	2.50	0.42
1:G:384:PRO:HD2	1:G:400:TRP:O	2.19	0.42
1:G:541:LYS:HA	1:G:541:LYS:HD2	1.95	0.42
1:H:362:MET:HE2	1:H:362:MET:HB3	1.87	0.42
1:K:405:THR:HG22	1:K:408:ARG:NH2	2.28	0.42
1:L:194:PHE:CG	1:L:252:ARG:HD3	2.54	0.42
1:A:138:HIS:HD2	1:A:163:VAL:CG1	2.32	0.42
1:B:11:ALA:O	1:B:49:PHE:HA	2.20	0.42
1:C:340:PRO:HG2	1:C:373:TYR:CZ	2.55	0.42
1:C:428:TRP:CD1	1:C:428:TRP:H	2.37	0.42
1:D:411:TRP:CD2	1:D:522:GLU:HB2	2.54	0.42
1:D:428:TRP:HZ2	1:D:535:LEU:HD13	1.85	0.42
1:E:164:SER:OG	1:E:539:LEU:O	2.26	0.42
1:E:428:TRP:CH2	1:E:535:LEU:HD13	2.54	0.42
1:H:340:PRO:HB2	1:H:373:TYR:OH	2.19	0.42
1:H:425:MET:HE2	1:H:525:PRO:O	2.20	0.42
1:I:339:GLU:HA	1:I:367:ALA:O	2.20	0.42
1:I:389:ASP:OD2	1:I:393:ARG:HD3	2.19	0.42
1:I:409:ASN:HB3	1:I:410:LYS:H	1.50	0.42
1:J:511:GLU:CD	1:J:511:GLU:H	2.28	0.42
1:L:84:PHE:CD1	1:L:93:LEU:HD22	2.55	0.42
1:L:415:LEU:O	1:L:418:THR:OG1	2.37	0.42
1:C:441:TRP:HD1	2:C:627:HOH:O	2.01	0.42
1:E:365:MET:HB3	1:E:381:ILE:HB	2.01	0.42
1:F:143:ARG:HH21	1:F:156:LEU:HD22	1.84	0.42
1:F:378:LEU:HD12	1:F:378:LEU:HA	1.83	0.42
1:G:199:TRP:CZ2	1:G:255:ARG:HD3	2.55	0.42
1:H:386:ILE:CD1	1:H:403:PHE:HB3	2.50	0.42
1:J:219:ILE:HG21	1:J:253:ILE:HG23	2.02	0.42
1:J:336:LEU:HD21	1:J:351:ALA:HB3	2.02	0.42
1:J:393:ARG:HG3	1:J:399:HIS:HE1	1.85	0.42
1:J:480:GLY:HA2	1:J:485:TYR:HE1	1.85	0.42
1:L:53:MET:O	1:L:117:PRO:HB3	2.19	0.42
1:L:404:CYS:O	1:L:404:CYS:SG	2.77	0.42
1:L:506:ALA:HB3	1:L:508:ILE:HD11	2.02	0.42
1:A:40:ASN:HB2	1:A:131:ALA:HB2	2.02	0.42
1:B:428:TRP:CH2	1:B:535:LEU:HD13	2.55	0.42
1:C:177:THR:HB	1:C:216:VAL:HB	2.02	0.42
1:D:180[B]:TRP:CE2	1:D:206:MET:CE	3.03	0.42
1:D:326:GLU:HB2	1:D:328:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ARG:O	1:E:125:ILE:HA	2.19	0.42
1:A:183:GLU:HA	1:A:193:MET:HE1	2.01	0.42
1:A:368:LEU:HD13	1:A:373:TYR:HB3	2.00	0.42
1:G:475:PHE:O	1:G:489:ARG:NH2	2.53	0.42
1:I:97:GLY:C	1:L:24:GLN:HG2	2.45	0.42
1:I:384:PRO:HD2	1:I:400:TRP:O	2.19	0.42
1:K:384:PRO:HD2	1:K:400:TRP:O	2.20	0.42
1:K:413:ASN:O	1:K:418:THR:HG21	2.19	0.42
1:L:13:TRP:CD1	1:L:28:GLN:HB2	2.55	0.42
1:B:164:SER:OG	1:B:539:LEU:O	2.29	0.41
1:C:274:TRP:CZ3	1:C:336:LEU:HD11	2.55	0.41
1:C:368:LEU:HA	1:C:368:LEU:HD23	1.44	0.41
1:D:348:TYR:OH	1:D:379:THR:HG22	2.19	0.41
1:D:436:LEU:HD23	1:D:436:LEU:HA	1.86	0.41
1:E:414:ARG:HA	1:E:423:LEU:HD13	2.00	0.41
1:I:166:LEU:HD11	1:I:506:ALA:HB2	2.02	0.41
1:L:180:TRP:CD2	1:L:206:MET:HE1	2.55	0.41
1:L:385:ILE:HD12	1:L:385:ILE:HA	1.90	0.41
1:A:143:ARG:HH11	1:A:145:ARG:HH21	1.67	0.41
1:B:10:MET:HG2	1:B:146:TRP:CE2	2.55	0.41
1:C:10:MET:HE3	1:C:59:ILE:HD13	2.03	0.41
1:C:156:LEU:HA	1:C:156:LEU:HD23	1.84	0.41
1:C:287:LYS:HE2	1:C:287:LYS:HB3	1.64	0.41
1:E:52:ASN:O	1:E:52:ASN:ND2	2.53	0.41
1:I:405:THR:HG22	1:I:408:ARG:HH21	1.85	0.41
1:J:200:LYS:HB3	1:J:200:LYS:HE2	1.70	0.41
1:J:411:TRP:CE3	1:J:522:GLU:HB2	2.55	0.41
1:K:47:VAL:HG21	1:K:142:VAL:HG11	2.02	0.41
1:K:368:LEU:HD13	1:K:373:TYR:CB	2.50	0.41
1:B:350:LYS:HD3	1:B:350:LYS:C	2.45	0.41
1:D:283:MET:HE3	1:D:283:MET:HB3	1.87	0.41
1:F:287:LYS:HG2	1:F:296:LEU:HD23	2.01	0.41
1:H:377:GLN:OE1	1:H:377:GLN:HA	2.20	0.41
1:I:257:VAL:HG22	1:I:268:PHE:CE2	2.55	0.41
1:L:355:LEU:HG	1:L:362:MET:HE1	2.02	0.41
1:L:394:LYS:HE2	1:L:394:LYS:HB3	1.86	0.41
1:A:153:LYS:HA	1:A:153:LYS:HD3	1.91	0.41
1:B:193:MET:HE2	1:B:193:MET:HB2	1.69	0.41
1:D:106:PRO:HB3	1:D:478:TYR:CD1	2.56	0.41
1:E:384:PRO:HD2	1:E:400:TRP:O	2.20	0.41
1:E:509:GLN:C	1:E:511:GLU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:LEU:HD22	1:G:348:TYR:CE2	2.55	0.41
1:K:538:ILE:HD13	1:K:538:ILE:HA	1.78	0.41
1:L:411:TRP:CE3	1:L:522:GLU:HB2	2.55	0.41
1:L:433:LEU:HD23	1:L:433:LEU:HA	1.83	0.41
1:B:41:SER:HB2	1:B:498:GLN:OE1	2.21	0.41
1:C:26:PRO:O	1:C:28:GLN:NE2	2.54	0.41
1:C:154:ASP:OD1	1:C:154:ASP:C	2.63	0.41
1:C:535:LEU:HA	1:C:535:LEU:HD23	1.82	0.41
1:E:302:SER:HB3	1:E:305:SER:HB3	2.02	0.41
1:F:336:LEU:HD21	1:F:351:ALA:CB	2.50	0.41
1:G:234:GLN:NE2	1:G:286:TYR:H	2.15	0.41
1:G:368:LEU:HD13	1:G:373:TYR:CG	2.55	0.41
1:I:278:GLY:HA2	1:I:344:HIS:CG	2.56	0.41
1:J:417:ASP:OD1	1:J:417:ASP:N	2.44	0.41
1:K:367:ALA:HA	1:K:383:ILE:O	2.19	0.41
1:A:138:HIS:HD2	1:A:163:VAL:HG11	1.85	0.41
1:A:143:ARG:NH1	1:A:145:ARG:HH21	2.18	0.41
1:C:234:GLN:HE22	1:C:285:VAL:CA	2.29	0.41
1:C:352:ARG:HG3	1:C:356:ARG:NH1	2.35	0.41
1:C:425:MET:HG3	1:C:525:PRO:O	2.21	0.41
1:D:158:HIS:CD2	1:D:160:LYS:HE2	2.55	0.41
1:D:249:ASP:OD1	1:D:251:SER:OG	2.35	0.41
1:E:81:MET:HE2	1:E:83:HIS:O	2.21	0.41
1:E:443:TYR:CZ	1:E:477:VAL:HG21	2.56	0.41
1:F:288:LYS:HD2	1:F:293:TYR:HE1	1.85	0.41
1:G:441:TRP:HD1	2:G:610:HOH:O	2.02	0.41
1:H:54:LYS:HE3	1:H:54:LYS:HB3	1.75	0.41
1:H:418:THR:HG23	1:H:422:LYS:HD3	2.03	0.41
1:I:366:ASP:HB2	1:I:379:THR:HG21	2.03	0.41
1:J:236:LEU:HD12	1:J:236:LEU:HA	1.77	0.41
1:J:286:TYR:HD1	1:J:286:TYR:N	2.18	0.41
1:J:313:LYS:HG2	1:J:358:LEU:CD1	2.50	0.41
1:J:439:LEU:HG	1:J:440:HIS:N	2.30	0.41
1:K:240:GLU:HG2	1:K:242:SER:O	2.20	0.41
1:K:275:LEU:HD23	1:K:275:LEU:HA	1.85	0.41
1:K:282:ALA:HB2	1:K:303:GLY:HA2	2.01	0.41
1:L:408:ARG:NH1	1:L:470:ALA:HB2	2.35	0.41
1:A:116:HIS:HA	1:A:117:PRO:HD3	1.89	0.41
1:A:506:ALA:HB3	1:A:508:ILE:HD12	2.03	0.41
1:C:412:LEU:HD11	1:C:426:SER:OG	2.20	0.41
1:D:75:TYR:CB	1:D:110:VAL:HG23	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:LEU:HA	1:E:324:LEU:HD23	1.80	0.41
1:G:413:ASN:O	1:G:418:THR:HG21	2.21	0.41
1:G:509:GLN:O	1:G:512:ASP:HB2	2.21	0.41
1:H:78:LEU:HG	1:H:121:ARG:CZ	2.50	0.41
1:J:128:GLN:O	1:J:130:PRO:HD3	2.20	0.41
1:J:404:CYS:O	1:J:404:CYS:SG	2.79	0.41
1:K:18:LEU:HD21	1:K:424:ARG:HH11	1.82	0.41
1:L:107:LEU:HD21	1:L:488:ILE:HD11	2.03	0.41
1:L:274:TRP:HE1	1:L:303:GLY:HA3	1.85	0.41
1:A:64:GLU:OE2	1:A:143:ARG:HD2	2.21	0.41
1:D:365:MET:HE1	1:D:400:TRP:CE2	2.56	0.41
1:E:312:LEU:HD23	1:E:312:LEU:HA	1.89	0.41
1:F:386:ILE:HD13	1:F:403:PHE:HD2	1.85	0.41
1:G:498:GLN:O	1:G:502:ILE:HG12	2.20	0.41
1:H:260:CYS:O	1:H:263:LEU:HB2	2.20	0.41
1:J:50:ARG:HD2	1:J:120:SER:OG	2.20	0.41
1:K:82:PRO:HB2	1:K:83:HIS:CD2	2.54	0.41
1:A:414:ARG:NH2	1:A:440:HIS:CE1	2.89	0.41
1:A:417:ASP:OD1	1:A:417:ASP:N	2.40	0.41
1:B:21:ILE:HD12	1:B:122:SER:HB3	2.02	0.41
1:B:352:ARG:HA	1:B:352:ARG:HD2	1.81	0.41
1:C:18:LEU:HD21	1:C:424:ARG:HD2	2.02	0.41
1:C:20:ARG:HD2	1:C:94:ASP:OD2	2.21	0.41
1:C:369:SER:HB3	1:C:385:ILE:HG22	2.03	0.41
1:C:446:TRP:CE2	1:C:479:PRO:HD3	2.56	0.41
1:D:127:LEU:HD21	1:D:140:PHE:HZ	1.86	0.41
1:D:473:ASP:N	1:D:474:PRO:HD3	2.36	0.41
1:E:139:ASP:HA	1:E:159:VAL:O	2.21	0.41
1:E:336:LEU:HD13	1:E:348:TYR:CE2	2.56	0.41
1:G:336:LEU:HD23	1:G:337:SER:HB3	2.02	0.41
1:G:488:ILE:O	1:G:492:VAL:HG23	2.20	0.41
1:H:236:LEU:HD21	1:H:248:PHE:CD1	2.55	0.41
1:I:9:PRO:HB2	1:I:53:MET:HE3	2.03	0.41
1:I:324:LEU:HA	1:I:324:LEU:HD23	1.74	0.41
1:I:416:TYR:CD2	1:I:471:TYR:HB3	2.55	0.41
1:K:481:PRO:HD2	1:K:485:TYR:CZ	2.55	0.41
1:L:143:ARG:HH21	1:L:156:LEU:HD21	1.86	0.41
1:L:405:THR:HG21	1:L:468:GLY:O	2.21	0.41
1:L:425:MET:HE1	1:L:530:TRP:CZ3	2.56	0.41
1:L:512:ASP:OD1	1:L:514:MET:HG2	2.20	0.41
1:A:139:ASP:HB3	1:A:160:LYS:HG2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HE2	1:B:192:LYS:HB2	1.73	0.41
1:C:207:LYS:O	1:C:211:GLU:HG3	2.20	0.41
1:C:298:ALA:HB1	1:C:300:ASN:OD1	2.20	0.41
1:E:168:LEU:HD11	1:E:502:ILE:HG12	2.01	0.41
1:F:529:GLN:O	1:F:533:GLU:HG3	2.20	0.41
1:G:119:GLU:HG3	1:K:100:PRO:HG2	2.02	0.41
1:G:520:THR:HG22	1:G:523:ASP:HB3	2.03	0.41
1:H:50:ARG:HD2	1:H:120:SER:OG	2.21	0.41
1:J:254:LYS:HE2	1:J:258:ASP:CG	2.46	0.41
1:L:210:ILE:HB	1:L:265:TYR:CZ	2.56	0.41
1:E:488:ILE:O	1:E:492:VAL:HG23	2.21	0.40
1:G:340:PRO:HD2	1:G:368:LEU:CD2	2.51	0.40
1:K:33:LEU:HA	1:K:33:LEU:HD12	1.79	0.40
1:K:421:PRO:HB2	1:K:526:ARG:O	2.21	0.40
1:L:13:TRP:HB2	1:L:30:ALA:HB3	2.02	0.40
1:L:18:LEU:HD12	1:L:421:PRO:HA	2.02	0.40
1:A:143:ARG:HD3	1:A:145:ARG:NE	2.36	0.40
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.84	0.40
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.95	0.40
1:B:404:CYS:O	1:B:406:GLY:O	2.39	0.40
1:E:236:LEU:HD21	1:E:248:PHE:HD2	1.85	0.40
1:F:74:ARG:HD3	2:F:605:HOH:O	2.20	0.40
1:G:361:TRP:CH2	1:G:362:MET:HE3	2.56	0.40
1:G:420:LEU:HD22	1:G:492:VAL:HG21	2.04	0.40
1:G:515:LEU:HA	1:G:518:LEU:HD13	2.04	0.40
1:I:498:GLN:O	1:I:502:ILE:HG13	2.21	0.40
1:J:367:ALA:HA	1:J:383:ILE:HB	2.03	0.40
1:K:367:ALA:HB1	1:K:402:TYR:CE1	2.56	0.40
1:A:14:LEU:HD11	1:A:157:LEU:HB3	2.02	0.40
1:A:402:TYR:HB2	1:A:439:LEU:O	2.22	0.40
1:B:76:VAL:HG11	1:B:488:ILE:HD11	2.03	0.40
1:C:141:HIS:HB3	1:C:156:LEU:HD22	2.04	0.40
1:C:424:ARG:O	1:C:496:SER:OG	2.32	0.40
1:D:414:ARG:HA	1:D:423:LEU:HD13	2.04	0.40
1:E:39:ARG:HB2	1:E:167:VAL:HG22	2.04	0.40
1:G:226:ARG:HG3	1:G:275:LEU:HG	2.04	0.40
1:G:424:ARG:C	1:G:426:SER:H	2.29	0.40
1:H:13:TRP:CE2	1:H:48:ALA:HB3	2.57	0.40
1:I:92:GLU:OE2	1:I:410:LYS:HG2	2.22	0.40
1:I:348:TYR:OH	1:I:379:THR:HG22	2.21	0.40
1:J:57:THR:OG1	1:J:58:HIS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:HD13	1:C:48:ALA:HB2	2.03	0.40
1:D:12:VAL:HG23	1:D:155:LYS:HD3	2.04	0.40
1:D:345:VAL:HG21	1:D:372:ARG:HH12	1.87	0.40
1:F:210:ILE:HB	1:F:265:TYR:CZ	2.56	0.40
1:F:314:GLN:O	1:F:317:PRO:HD2	2.21	0.40
1:G:91:GLU:H	1:G:91:GLU:CD	2.29	0.40
1:H:239:ARG:HB2	1:H:247:GLU:HB2	2.03	0.40
1:J:535:LEU:HD12	1:J:535:LEU:HA	1.83	0.40
1:K:183:GLU:OE1	1:K:183:GLU:N	2.43	0.40
1:K:309:ILE:O	1:K:313:LYS:HG2	2.21	0.40
1:K:447:TYR:HB2	1:K:453:GLN:O	2.22	0.40
1:A:138:HIS:CD2	1:A:163:VAL:HG11	2.57	0.40
1:A:246:TYR:CD2	1:A:311:PHE:HD1	2.39	0.40
1:B:414:ARG:HB3	1:B:423:LEU:CD1	2.51	0.40
1:C:424:ARG:C	1:C:426:SER:H	2.30	0.40
1:C:490:TRP:HA	1:C:490:TRP:HE3	1.87	0.40
1:D:321:ARG:HE	1:D:321:ARG:HB3	1.60	0.40
1:E:192:LYS:HD2	1:E:192:LYS:HA	1.82	0.40
1:G:72:ARG:HH21	1:G:74:ARG:CZ	2.35	0.40
1:G:102:TRP:CD1	1:K:101:GLY:HA2	2.56	0.40
1:I:224:GLU:OE1	1:I:271:ALA:HB1	2.21	0.40
1:I:309:ILE:HD13	1:I:309:ILE:HA	1.93	0.40
1:J:39:ARG:HD3	1:J:133:LEU:O	2.21	0.40
1:J:75:TYR:CE1	1:J:113:THR:HG21	2.57	0.40
1:J:428:TRP:HB3	1:J:518:LEU:HD21	2.03	0.40
1:K:409:ASN:HB3	1:K:410:LYS:H	1.42	0.40
1:L:341:TRP:HB2	1:L:344:HIS:HD1	1.86	0.40

There are no symmetry-related clashes.

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	534/562 (95%)	507 (95%)	23 (4%)	4 (1%)	18	47
1	B	535/562 (95%)	504 (94%)	27 (5%)	4 (1%)	18	47
1	C	534/562 (95%)	505 (95%)	24 (4%)	5 (1%)	14	41
1	D	535/562 (95%)	509 (95%)	20 (4%)	6 (1%)	11	36
1	E	534/562 (95%)	502 (94%)	25 (5%)	7 (1%)	9	31
1	F	534/562 (95%)	506 (95%)	22 (4%)	6 (1%)	11	36
1	G	534/562 (95%)	507 (95%)	22 (4%)	5 (1%)	14	41
1	H	534/562 (95%)	509 (95%)	21 (4%)	4 (1%)	18	47
1	I	534/562 (95%)	505 (95%)	24 (4%)	5 (1%)	14	41
1	J	534/562 (95%)	507 (95%)	23 (4%)	4 (1%)	18	47
1	K	534/562 (95%)	494 (92%)	32 (6%)	8 (2%)	8	28
1	L	534/562 (95%)	500 (94%)	30 (6%)	4 (1%)	18	47
All	All	6410/6744 (95%)	6055 (94%)	293 (5%)	62 (1%)	12	38

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	ARG
1	C	339	GLU
1	C	405	THR
1	F	405	THR
1	H	30	ALA
1	I	30	ALA
1	A	405	THR
1	B	30	ALA
1	C	30	ALA
1	D	367	ALA
1	F	30	ALA
1	F	300	ASN
1	F	377	GLN
1	G	30	ALA
1	G	105	ASP
1	G	279	VAL
1	J	377	GLN
1	K	30	ALA
1	K	361	TRP
1	K	434	LYS
1	L	405	THR
1	A	30	ALA

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Mol	Chain	Res	Type
1	A	105	ASP
1	B	105	ASP
1	C	105	ASP
1	D	30	ALA
1	D	105	ASP
1	D	405	THR
1	D	425	MET
1	E	30	ALA
1	E	105	ASP
1	E	386	ILE
1	E	405	THR
1	E	510	PRO
1	F	105	ASP
1	H	105	ASP
1	H	425	MET
1	I	105	ASP
1	I	405	THR
1	J	105	ASP
1	J	405	THR
1	K	105	ASP
1	K	405	THR
1	L	105	ASP
1	L	279	VAL
1	B	405	THR
1	G	405	THR
1	K	290	GLY
1	K	369	SER
1	A	290	GLY
1	D	369	SER
1	E	425	MET
1	F	518	LEU
1	L	404	CYS
1	E	376	GLU
1	J	279	VAL
1	C	170	PRO
1	G	339	GLU
1	I	454	PRO
1	I	279	VAL
1	H	290	GLY
1	K	279	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/494 (96%)	442 (93%)	32 (7%)	14	42
1	B	475/494 (96%)	423 (89%)	52 (11%)	6	21
1	C	474/494 (96%)	446 (94%)	28 (6%)	18	48
1	D	475/494 (96%)	435 (92%)	40 (8%)	10	32
1	E	474/494 (96%)	437 (92%)	37 (8%)	11	35
1	F	474/494 (96%)	442 (93%)	32 (7%)	14	42
1	G	474/494 (96%)	436 (92%)	38 (8%)	11	34
1	H	474/494 (96%)	437 (92%)	37 (8%)	11	35
1	I	474/494 (96%)	436 (92%)	38 (8%)	11	34
1	J	474/494 (96%)	439 (93%)	35 (7%)	13	37
1	K	474/494 (96%)	441 (93%)	33 (7%)	14	40
1	L	474/494 (96%)	437 (92%)	37 (8%)	11	35
All	All	5690/5928 (96%)	5251 (92%)	439 (8%)	12	36

All (439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	63	THR
1	A	110	VAL
1	A	111	THR
1	A	114	GLU
1	A	125	ILE
1	A	128	GLN
1	A	132	SER
1	A	150	LYS
1	A	163	VAL
1	A	210	ILE
1	A	225	LEU
1	A	267	LYS
1	A	280	GLN

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Mol	Chain	Res	Type
1	A	321	ARG
1	A	343	GLU
1	A	346	GLU
1	A	355	LEU
1	A	369	SER
1	A	375	ARG
1	A	385	ILE
1	A	389	ASP
1	A	395	GLU
1	A	405	THR
1	A	424	ARG
1	A	451	LYS
1	A	487	SER
1	A	490	TRP
1	A	494	SER
1	A	496	SER
1	A	498	GLN
1	A	527	SER
1	B	16	SER
1	B	54	LYS
1	B	56	GLN
1	B	103	LEU
1	B	110	VAL
1	B	126	THR
1	B	132	SER
1	B	137	ILE
1	B	142	VAL
1	B	147	GLN
1	B	152	GLU
1	B	160	LYS
1	B	166	LEU
1	B	180[A]	TRP
1	B	180[B]	TRP
1	B	190	GLU
1	B	192	LYS
1	B	231	GLU
1	B	242	SER
1	B	251	SER
1	B	253	ILE
1	B	262	GLU
1	B	289	GLU
1	B	291	ASN

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Mol	Chain	Res	Type
1	B	300	ASN
1	B	310	HIS
1	B	338	ASP
1	B	341	TRP
1	B	342	SER
1	B	345	VAL
1	B	347	ASN
1	B	350	LYS
1	B	358	LEU
1	B	362	MET
1	B	363	LYS
1	B	364	VAL
1	B	368	LEU
1	B	371	VAL
1	B	372	ARG
1	B	375	ARG
1	B	378	LEU
1	B	405	THR
1	B	410	LYS
1	B	433	LEU
1	B	439	LEU
1	B	490	TRP
1	B	497	LEU
1	B	505	SER
1	B	511	GLU
1	B	526	ARG
1	B	527	SER
1	B	535	LEU
1	C	12	VAL
1	C	19	GLN
1	C	24	GLN
1	C	64	GLU
1	C	110	VAL
1	C	114	GLU
1	C	132	SER
1	C	152	GLU
1	C	166	LEU
1	C	196	GLU
1	C	200	LYS
1	C	203	ARG
1	C	230	LYS
1	C	273	LEU

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Mol	Chain	Res	Type
1	C	279	VAL
1	C	288	LYS
1	C	339	GLU
1	C	343	GLU
1	C	354	ILE
1	C	364	VAL
1	C	378	LEU
1	C	401	VAL
1	C	414	ARG
1	C	469	ILE
1	C	490	TRP
1	C	495	GLU
1	C	510	PRO
1	C	537	LYS
1	D	16	SER
1	D	50	ARG
1	D	52	ASN
1	D	54	LYS
1	D	78	LEU
1	D	96	VAL
1	D	107	LEU
1	D	110	VAL
1	D	114	GLU
1	D	127	LEU
1	D	156	LEU
1	D	159	VAL
1	D	163	VAL
1	D	164	SER
1	D	172	SER
1	D	180[A]	TRP
1	D	180[B]	TRP
1	D	190	GLU
1	D	200	LYS
1	D	203	ARG
1	D	220	GLN
1	D	231	GLU
1	D	245	LYS
1	D	251	SER
1	D	253	ILE
1	D	266	LYS
1	D	280	GLN
1	D	291	ASN

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Mol	Chain	Res	Type
1	D	321	ARG
1	D	349	LYS
1	D	356	ARG
1	D	368	LEU
1	D	386	ILE
1	D	390	GLU
1	D	394	LYS
1	D	405	THR
1	D	439	LEU
1	D	498	GLN
1	D	518	LEU
1	D	531	ILE
1	E	16	SER
1	E	18	LEU
1	E	53	MET
1	E	54	LYS
1	E	56	GLN
1	E	59	ILE
1	E	64	GLU
1	E	112	LYS
1	E	119	GLU
1	E	127	LEU
1	E	132	SER
1	E	133	LEU
1	E	147	GLN
1	E	151	GLU
1	E	152	GLU
1	E	161	VAL
1	E	168	LEU
1	E	172	SER
1	E	242	SER
1	E	251	SER
1	E	291	ASN
1	E	307	THR
1	E	342	SER
1	E	345	VAL
1	E	356	ARG
1	E	358	LEU
1	E	368	LEU
1	E	378	LEU
1	E	389	ASP
1	E	401	VAL

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Mol	Chain	Res	Type
1	E	405	THR
1	E	490	TRP
1	E	494	SER
1	E	496	SER
1	E	498	GLN
1	E	526	ARG
1	E	535	LEU
1	F	21	ILE
1	F	56	GLN
1	F	60	SER
1	F	63	THR
1	F	78	LEU
1	F	114	GLU
1	F	125	ILE
1	F	153	LYS
1	F	168	LEU
1	F	195	ASP
1	F	196	GLU
1	F	200	LYS
1	F	242	SER
1	F	252	ARG
1	F	253	ILE
1	F	280	GLN
1	F	347	ASN
1	F	354	ILE
1	F	357	GLN
1	F	358	LEU
1	F	365	MET
1	F	376	GLU
1	F	378	LEU
1	F	390	GLU
1	F	401	VAL
1	F	476	VAL
1	F	487	SER
1	F	490	TRP
1	F	497	LEU
1	F	498	GLN
1	F	539	LEU
1	F	541	LYS
1	G	41	SER
1	G	42	ARG
1	G	43	VAL

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Mol	Chain	Res	Type
1	G	63	THR
1	G	64	GLU
1	G	81	MET
1	G	114	GLU
1	G	119	GLU
1	G	125	ILE
1	G	128	GLN
1	G	132	SER
1	G	163	VAL
1	G	168	LEU
1	G	172	SER
1	G	197	GLN
1	G	224	GLU
1	G	231	GLU
1	G	259	MET
1	G	275	LEU
1	G	279	VAL
1	G	295	LEU
1	G	301	LEU
1	G	309	ILE
1	G	318	GLN
1	G	355	LEU
1	G	371	VAL
1	G	381	ILE
1	G	390	GLU
1	G	405	THR
1	G	414	ARG
1	G	429	LEU
1	G	439	LEU
1	G	476	VAL
1	G	494	SER
1	G	496	SER
1	G	502	ILE
1	G	527	SER
1	G	535	LEU
1	H	16	SER
1	H	19	GLN
1	H	29	THR
1	H	43	VAL
1	H	54	LYS
1	H	163	VAL
1	H	173	ASN

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Mol	Chain	Res	Type
1	H	201	LEU
1	H	230	LYS
1	H	240	GLU
1	H	251	SER
1	H	273	LEU
1	H	275	LEU
1	H	279	VAL
1	H	280	GLN
1	H	289	GLU
1	H	291	ASN
1	H	304	THR
1	H	364	VAL
1	H	365	MET
1	H	369	SER
1	H	371	VAL
1	H	381	ILE
1	H	386	ILE
1	H	389	ASP
1	H	401	VAL
1	H	405	THR
1	H	420	LEU
1	H	424	ARG
1	H	432	LYS
1	H	490	TRP
1	H	494	SER
1	H	495	GLU
1	H	498	GLN
1	H	527	SER
1	H	535	LEU
1	H	539	LEU
1	I	17	SER
1	I	56	GLN
1	I	67	GLU
1	I	76	VAL
1	I	83	HIS
1	I	96	VAL
1	I	107	LEU
1	I	112	LYS
1	I	132	SER
1	I	162	LYS
1	I	211	GLU
1	I	226	ARG

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Mol	Chain	Res	Type
1	I	247	GLU
1	I	251	SER
1	I	254	LYS
1	I	259	MET
1	I	291	ASN
1	I	295	LEU
1	I	296	LEU
1	I	299	GLU
1	I	304	THR
1	I	339	GLU
1	I	345	VAL
1	I	358	LEU
1	I	363	LYS
1	I	366	ASP
1	I	368	LEU
1	I	371	VAL
1	I	372	ARG
1	I	376	GLU
1	I	378	LEU
1	I	401	VAL
1	I	405	THR
1	I	417	ASP
1	I	439	LEU
1	I	460	GLU
1	I	487	SER
1	I	494	SER
1	J	12	VAL
1	J	16	SER
1	J	55	ASP
1	J	63	THR
1	J	78	LEU
1	J	107	LEU
1	J	114	GLU
1	J	142	VAL
1	J	152	GLU
1	J	155	LYS
1	J	156	LEU
1	J	166	LEU
1	J	190	GLU
1	J	191	THR
1	J	209	LEU
1	J	210	ILE

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Mol	Chain	Res	Type
1	J	228	VAL
1	J	234	GLN
1	J	253	ILE
1	J	259	MET
1	J	262	GLU
1	J	273	LEU
1	J	286	TYR
1	J	291	ASN
1	J	329	LEU
1	J	389	ASP
1	J	401	VAL
1	J	405	THR
1	J	439	LEU
1	J	449	LEU
1	J	476	VAL
1	J	477	VAL
1	J	502	ILE
1	J	526	ARG
1	J	535	LEU
1	K	25	SER
1	K	35	LEU
1	K	42	ARG
1	K	74	ARG
1	K	76	VAL
1	K	91	GLU
1	K	96	VAL
1	K	166	LEU
1	K	225	LEU
1	K	231	GLU
1	K	247	GLU
1	K	251	SER
1	K	252	ARG
1	K	259	MET
1	K	263	LEU
1	K	286	TYR
1	K	287	LYS
1	K	296	LEU
1	K	324	LEU
1	K	345	VAL
1	K	352	ARG
1	K	389	ASP
1	K	395	GLU

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Mol	Chain	Res	Type
1	K	405	THR
1	K	426	SER
1	K	439	LEU
1	K	490	TRP
1	K	494	SER
1	K	498	GLN
1	K	504	GLN
1	K	514	MET
1	K	535	LEU
1	K	536	LYS
1	L	14	LEU
1	L	16	SER
1	L	34	GLU
1	L	43	VAL
1	L	53	MET
1	L	56	GLN
1	L	59	ILE
1	L	63	THR
1	L	72	ARG
1	L	81	MET
1	L	125	ILE
1	L	142	VAL
1	L	152	GLU
1	L	157	LEU
1	L	192	LYS
1	L	200	LYS
1	L	238	VAL
1	L	263	LEU
1	L	327	ASN
1	L	329	LEU
1	L	336	LEU
1	L	355	LEU
1	L	363	LYS
1	L	364	VAL
1	L	368	LEU
1	L	369	SER
1	L	375	ARG
1	L	389	ASP
1	L	394	LYS
1	L	412	LEU
1	L	417	ASP
1	L	418	THR

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Mol	Chain	Res	Type
1	L	424	ARG
1	L	496	SER
1	L	498	GLN
1	L	526	ARG
1	L	531	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	58	HIS
1	A	83	HIS
1	A	178	HIS
1	A	280	GLN
1	B	36	GLN
1	B	504	GLN
1	B	509	GLN
1	C	56	GLN
1	C	116	HIS
1	C	234	GLN
1	C	409	ASN
1	D	15	GLN
1	D	83	HIS
1	D	220	GLN
1	D	347	ASN
1	D	532	ASN
1	E	320	HIS
1	F	58	HIS
1	F	173	ASN
1	F	347	ASN
1	F	409	ASN
1	G	141	HIS
1	G	188	GLN
1	G	532	ASN
1	H	318	GLN
1	H	347	ASN
1	I	28	GLN
1	I	70	HIS
1	I	141	HIS
1	J	58	HIS
1	J	498	GLN
1	K	15	GLN

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Mol	Chain	Res	Type
1	K	46	GLN
1	K	188	GLN
1	K	509	GLN
1	L	28	GLN
1	L	310	HIS
1	L	344	HIS
1	L	409	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	536/562 (95%)	-0.27	3 (0%) 85 80	42, 61, 89, 120	0
1	B	536/562 (95%)	-0.12	3 (0%) 85 80	41, 70, 100, 197	1 (0%)
1	C	536/562 (95%)	-0.30	4 (0%) 84 77	38, 56, 88, 133	0
1	D	536/562 (95%)	-0.21	2 (0%) 88 84	33, 61, 93, 114	1 (0%)
1	E	536/562 (95%)	-0.22	1 (0%) 91 88	44, 63, 93, 154	0
1	F	536/562 (95%)	-0.19	3 (0%) 85 80	48, 65, 93, 131	0
1	G	536/562 (95%)	-0.07	4 (0%) 84 77	53, 74, 112, 151	0
1	H	536/562 (95%)	0.00	4 (0%) 84 77	50, 74, 115, 147	0
1	I	536/562 (95%)	-0.04	5 (0%) 81 74	56, 77, 112, 170	0
1	J	536/562 (95%)	0.11	6 (1%) 78 70	58, 87, 119, 159	0
1	K	536/562 (95%)	0.13	8 (1%) 72 63	64, 93, 127, 166	0
1	L	536/562 (95%)	0.30	9 (1%) 69 60	72, 101, 132, 197	0
All	All	6432/6744 (95%)	-0.07	52 (0%) 82 75	33, 72, 115, 197	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	373	TYR	6.3
1	B	373	TYR	6.1
1	C	373	TYR	5.6
1	I	373	TYR	4.7
1	G	373	TYR	4.7
1	J	373	TYR	4.5
1	G	368	LEU	4.4
1	I	368	LEU	3.9
1	F	373	TYR	3.7
1	B	368	LEU	3.7
1	E	341	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	368	LEU	3.5
1	H	373	TYR	3.4
1	C	368	LEU	3.4
1	H	279	VAL	3.3
1	F	368	LEU	3.2
1	A	373	TYR	3.2
1	L	367	ALA	3.1
1	L	341	TRP	3.0
1	K	443	TYR	2.8
1	K	369	SER	2.7
1	K	542	ALA	2.7
1	L	542	ALA	2.6
1	A	368	LEU	2.6
1	L	216	VAL	2.6
1	I	277	TRP	2.5
1	L	236	LEU	2.5
1	D	373	TYR	2.5
1	I	345	VAL	2.5
1	A	542	ALA	2.5
1	K	27	ALA	2.5
1	J	341	TRP	2.5
1	D	368	LEU	2.5
1	H	368	LEU	2.5
1	G	542	ALA	2.5
1	I	95	GLY	2.4
1	K	373	TYR	2.4
1	H	351	ALA	2.4
1	L	37	ALA	2.4
1	K	205	CYS	2.3
1	L	368	LEU	2.3
1	C	277	TRP	2.3
1	J	277	TRP	2.3
1	J	236	LEU	2.3
1	F	277	TRP	2.2
1	C	542	ALA	2.1
1	J	367	ALA	2.1
1	K	277	TRP	2.1
1	G	224	GLU	2.1
1	L	401	VAL	2.0
1	B	341	TRP	2.0
1	K	368	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.