



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 PM UTC

PDB ID : 1BHG / pdb_00001bhg
Title : HUMAN BETA-GLUCURONIDASE AT 2.6 Å RESOLUTION
Authors : Jain, S.; Drendel, W.B.
Deposited on : 1996-03-04
Resolution : 2.53 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

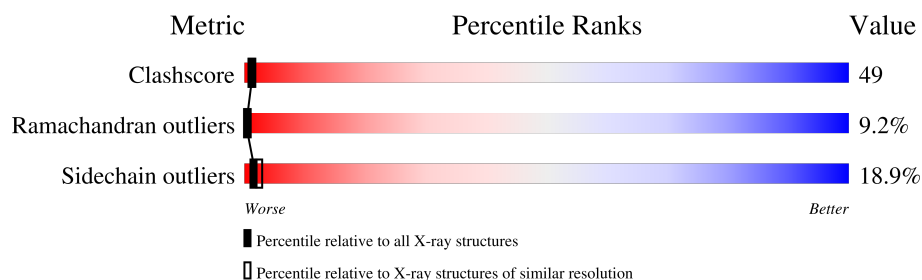
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	613	28% 47% 19% 5%
1	B	613	25% 48% 23% .
2	C	9	33% 56% 11%
2	D	9	22% 44% 33%

2 Entry composition [i](#)

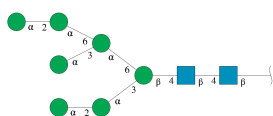
There are 2 unique types of molecules in this entry. The entry contains 10190 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			
1	B	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



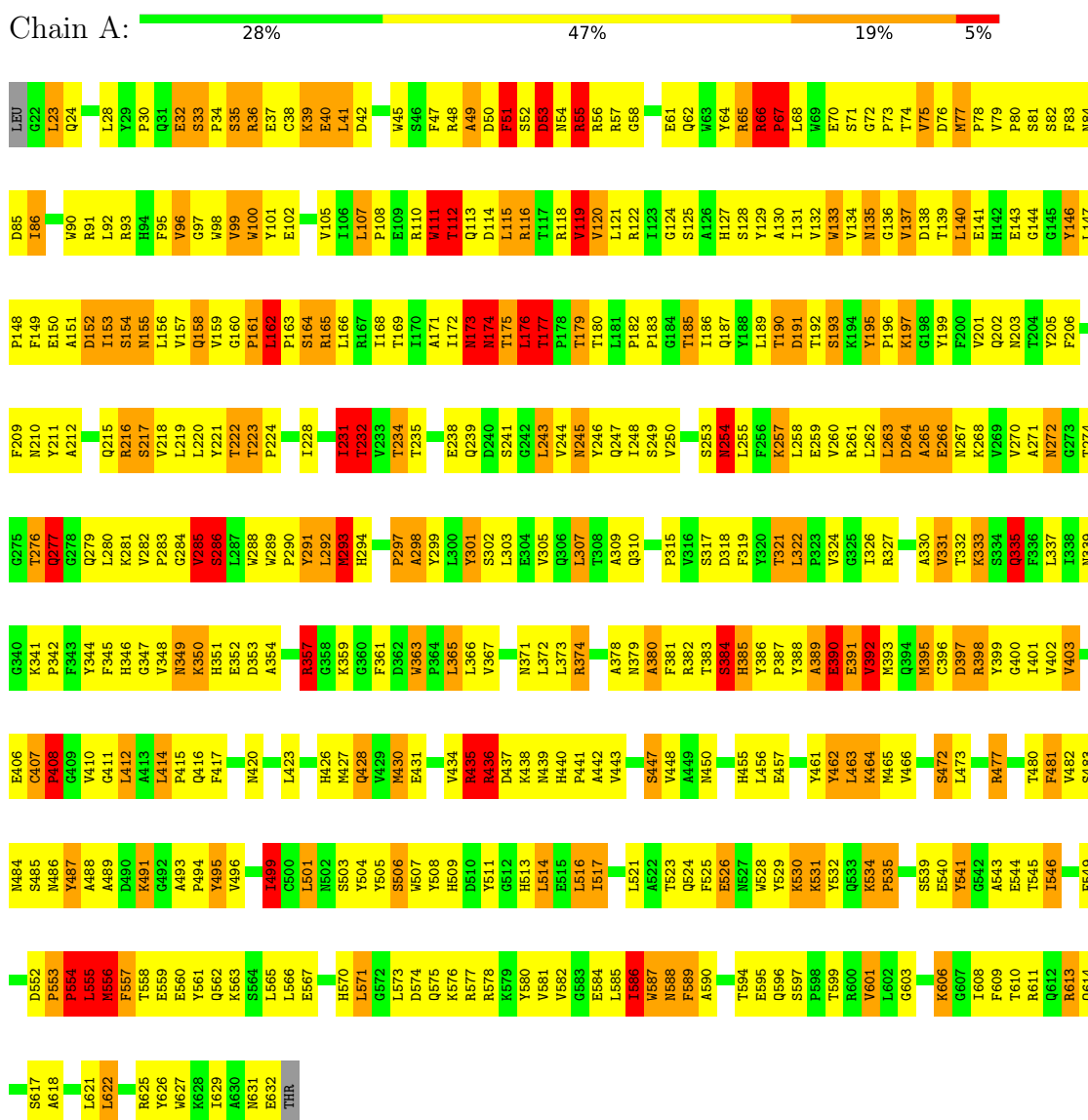
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	D	9	Total	C	N	O	0	0	0
			105	58	2	45			

3 Residue-property plots

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. 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. 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.

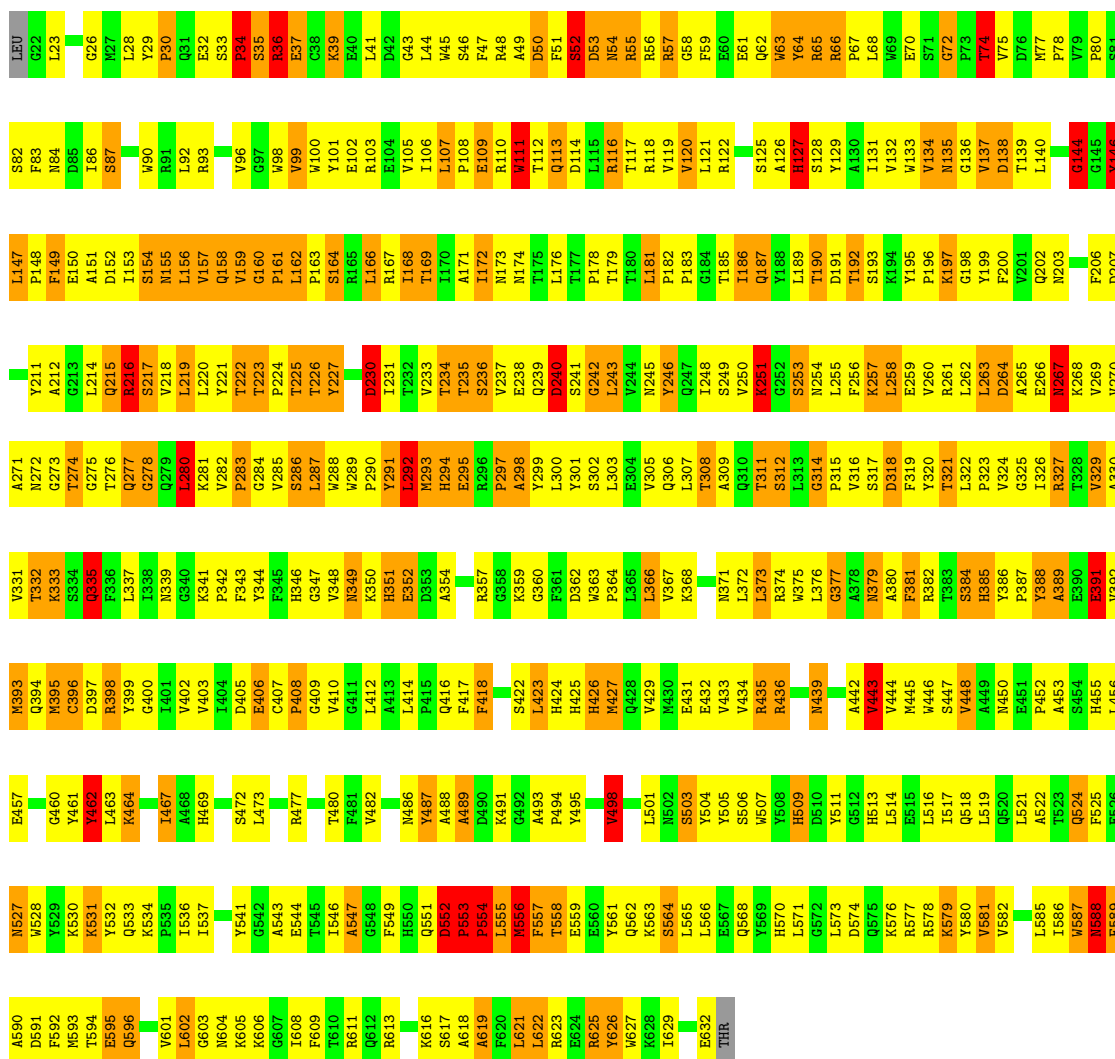
Note EDS was not executed.

• Molecule 1: BETA-GLUCURONIDASE



• Molecule 1: BETA-GLUCURONIDASE





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 56% 11%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 22% 44% 33%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.10Å 124.40Å 134.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.53	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.53)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.231 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10190	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.90	4/5139 (0.1%)	1.34	79/7000 (1.1%)
1	B	0.91	3/5139 (0.1%)	1.36	79/7000 (1.1%)
All	All	0.91	7/10278 (0.1%)	1.35	158/14000 (1.1%)

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	A	0	5
1	B	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	MET	SD-CE	7.86	1.99	1.79
1	B	556	MET	SD-CE	7.11	1.97	1.79
1	A	430	MET	SD-CE	-6.70	1.62	1.79
1	B	393	MET	SD-CE	5.58	1.93	1.79
1	A	177	THR	N-CA	5.38	1.50	1.46
1	A	392	VAL	CA-CB	5.16	1.60	1.54
1	A	77	MET	SD-CE	-5.12	1.66	1.79

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	MET	N-CA-C	11.04	127.36	112.68
1	A	36	ARG	N-CA-C	10.80	126.13	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASN	N-CA-C	10.00	124.84	110.14
1	B	37	GLU	N-CA-C	9.81	122.99	110.33
1	A	472	SER	N-CA-C	-8.93	97.64	110.59
1	B	462	TYR	N-CA-C	-8.74	101.44	110.97
1	B	242	GLY	N-CA-C	8.66	123.01	110.80
1	A	40	GLU	N-CA-C	-8.62	102.32	112.92
1	B	613	ARG	N-CA-C	8.53	123.36	113.38
1	B	314	GLY	CA-C-N	8.45	130.40	119.84
1	B	314	GLY	C-N-CA	8.45	130.40	119.84
1	B	240	ASP	N-CA-C	8.43	119.70	108.07
1	A	534	LYS	N-CA-C	8.26	115.65	108.22
1	A	588	ASN	N-CA-C	8.25	123.30	109.76
1	B	36	ARG	N-CA-C	8.25	121.44	109.14
1	A	589	PHE	N-CA-C	-8.25	102.24	111.07
1	B	616	LYS	N-CA-C	-8.07	98.06	109.69
1	B	391	GLU	N-CA-C	-7.90	102.27	112.23
1	B	100	TRP	N-CA-C	7.79	124.31	107.49
1	A	112	THR	N-CA-C	7.67	121.52	112.93
1	A	392	VAL	N-CA-C	-7.67	102.64	113.07
1	B	595	GLU	N-CA-C	-7.65	100.70	110.19
1	A	553	PRO	N-CA-C	-7.61	101.42	110.70
1	A	534	LYS	CA-C-N	7.59	128.05	119.93
1	A	534	LYS	C-N-CA	7.59	128.05	119.93
1	A	72	GLY	CA-C-N	7.47	129.18	119.84
1	A	72	GLY	C-N-CA	7.47	129.18	119.84
1	B	547	ALA	N-CA-C	7.27	123.29	111.37
1	A	66	ARG	CA-C-N	7.24	128.89	119.84
1	A	66	ARG	C-N-CA	7.24	128.89	119.84
1	A	55	ARG	N-CA-C	-7.22	102.51	111.75
1	B	144	GLY	N-CA-C	7.21	130.26	113.18
1	A	335	GLN	N-CA-C	7.19	121.11	109.40
1	A	246	TYR	N-CA-C	7.12	121.18	110.14
1	B	396	CYS	N-CA-C	-7.07	103.50	111.14
1	B	406	GLU	N-CA-C	7.07	120.04	108.52
1	A	120	VAL	N-CA-C	7.03	118.99	108.23
1	A	389	ALA	N-CA-C	7.03	122.89	111.37
1	A	435	ARG	N-CA-C	-7.01	103.33	110.97
1	A	447	SER	N-CA-C	-6.96	96.37	108.69
1	B	74	THR	N-CA-C	6.88	119.60	109.69
1	A	586	ILE	N-CA-C	-6.87	102.45	110.21
1	A	484	ASN	N-CA-C	-6.81	103.27	112.26
1	B	147	LEU	CA-C-N	6.80	128.08	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LEU	C-N-CA	6.80	128.08	120.66
1	A	428	GLN	N-CA-C	-6.74	103.56	111.03
1	A	436	ARG	N-CA-C	6.74	119.48	111.33
1	B	426	HIS	N-CA-C	-6.65	103.95	111.07
1	A	111	TRP	N-CA-C	-6.60	103.78	110.97
1	A	349	ASN	N-CA-C	-6.58	98.18	108.90
1	B	72	GLY	CA-C-N	6.55	126.94	119.93
1	B	72	GLY	C-N-CA	6.55	126.94	119.93
1	B	553	PRO	CA-C-N	6.53	128.01	119.84
1	B	553	PRO	C-N-CA	6.53	128.01	119.84
1	B	377	GLY	N-CA-C	-6.52	105.87	115.72
1	B	448	VAL	N-CA-C	6.50	119.21	111.09
1	B	111	TRP	N-CA-C	-6.49	105.46	113.19
1	B	588	ASN	N-CA-C	6.48	120.47	110.42
1	A	85	ASP	N-CA-C	6.48	121.19	113.28
1	B	472	SER	N-CA-C	-6.48	105.33	112.72
1	A	493	ALA	CA-C-N	-6.46	113.15	119.87
1	A	493	ALA	C-N-CA	-6.46	113.15	119.87
1	B	26	GLY	N-CA-C	-6.43	102.74	112.89
1	B	349	ASN	N-CA-C	-6.43	98.42	108.90
1	B	556	MET	N-CA-C	6.42	124.47	110.80
1	B	335	GLN	N-CA-C	6.42	118.61	108.79
1	A	556	MET	N-CA-C	6.38	124.38	110.80
1	A	119	VAL	N-CA-C	6.37	116.57	106.88
1	A	407	CYS	N-CA-C	-6.35	100.39	110.10
1	A	176	LEU	N-CA-C	6.33	117.84	108.60
1	A	116	ARG	N-CA-C	-6.32	105.72	113.50
1	B	246	TYR	N-CA-C	6.31	118.70	108.41
1	B	46	SER	N-CA-C	-6.24	101.71	110.50
1	B	384	SER	N-CA-C	6.22	124.06	110.80
1	A	483	SER	N-CA-C	6.20	118.84	109.23
1	A	420	ASN	N-CA-C	6.19	118.83	111.71
1	B	439	ASN	N-CA-C	6.15	119.98	112.23
1	B	316	VAL	N-CA-C	6.11	116.67	107.80
1	A	254	ASN	N-CA-C	-6.10	97.82	110.80
1	B	489	ALA	N-CA-C	-6.03	105.65	114.39
1	A	158	GLN	N-CA-C	-6.02	104.84	111.82
1	B	467	ILE	N-CA-C	-5.99	104.51	110.62
1	B	619	ALA	N-CA-C	-5.99	104.09	111.75
1	A	153	ILE	N-CA-C	-5.98	107.10	112.12
1	A	597	SER	CA-C-N	5.95	127.28	119.84
1	A	597	SER	C-N-CA	5.95	127.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	THR	N-CA-C	-5.94	97.78	108.48
1	B	68	LEU	N-CA-C	5.91	117.72	111.28
1	A	100	TRP	N-CA-C	5.90	119.34	109.95
1	B	236	SER	N-CA-C	-5.89	102.22	110.35
1	A	120	VAL	CB-CA-C	-5.88	103.85	110.96
1	B	265	ALA	N-CA-C	5.86	119.96	112.34
1	A	301	TYR	N-CA-C	-5.85	100.75	110.17
1	B	168	ILE	N-CA-C	5.85	117.00	108.58
1	B	443	VAL	N-CA-C	5.85	121.50	109.34
1	A	499	ILE	N-CA-C	5.83	116.59	108.89
1	A	217	SER	N-CA-C	5.80	118.48	110.35
1	B	166	LEU	N-CA-C	5.80	118.90	108.17
1	A	38	CYS	N-CA-C	-5.76	102.24	110.59
1	B	581	VAL	N-CA-C	-5.74	100.32	108.58
1	A	487	TYR	N-CA-C	-5.70	102.60	110.35
1	B	626	TYR	N-CA-C	5.69	117.94	111.11
1	A	223	THR	CA-C-N	-5.67	114.91	120.98
1	A	223	THR	C-N-CA	-5.67	114.91	120.98
1	A	292	LEU	N-CA-C	5.63	117.89	111.02
1	A	357	ARG	N-CA-C	5.60	119.73	113.01
1	A	216	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A	596	GLN	N-CA-C	5.57	117.17	109.15
1	A	595	GLU	N-CA-C	-5.55	102.67	110.50
1	B	146	TYR	N-CA-C	-5.55	98.98	110.80
1	B	418	PHE	N-CA-C	5.55	119.36	112.59
1	B	602	LEU	N-CA-C	-5.52	101.28	109.83
1	B	611	ARG	N-CA-C	-5.51	104.66	111.33
1	B	273	GLY	N-CA-C	5.50	121.31	111.03
1	A	92	LEU	N-CA-C	-5.49	104.93	111.69
1	A	403	VAL	N-CA-C	5.48	116.56	108.45
1	B	591	ASP	N-CA-C	-5.45	103.33	110.53
1	A	49	ALA	N-CA-C	-5.45	101.29	109.95
1	A	495	TYR	N-CA-C	5.43	120.01	113.17
1	B	333	LYS	N-CA-C	-5.42	106.72	113.38
1	A	61	GLU	N-CA-C	-5.40	106.61	114.12
1	B	207	ASP	N-CA-C	5.40	116.78	109.11
1	B	217	SER	N-CA-C	5.40	118.19	108.48
1	B	192	THR	N-CA-C	-5.38	104.98	112.03
1	B	552	ASP	CA-C-N	-5.38	114.84	120.38
1	B	552	ASP	C-N-CA	-5.38	114.84	120.38
1	B	138	ASP	N-CA-C	-5.36	102.25	110.30
1	A	393	MET	N-CA-C	-5.36	106.25	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	PRO	N-CA-C	5.36	123.50	112.47
1	A	481	PHE	N-CA-C	-5.36	99.59	108.75
1	B	169	THR	N-CA-C	5.35	117.95	109.50
1	A	146	TYR	N-CA-C	-5.33	99.44	110.80
1	B	596	GLN	N-CA-C	5.33	118.30	109.46
1	A	581	VAL	N-CA-C	-5.33	100.08	108.23
1	B	49	ALA	N-CA-C	-5.31	98.92	108.48
1	B	513	HIS	N-CA-C	5.31	117.20	109.71
1	B	280	LEU	N-CA-C	5.30	118.02	108.48
1	B	589	PHE	N-CA-C	-5.29	105.19	111.69
1	A	276	THR	N-CA-C	-5.27	103.69	111.81
1	A	380	ALA	N-CA-C	5.26	117.08	108.76
1	B	127	HIS	N-CA-C	5.26	122.00	110.80
1	A	64	TYR	N-CA-C	5.25	117.75	111.71
1	B	389	ALA	N-CA-C	-5.22	101.93	109.29
1	A	115	LEU	N-CA-C	5.21	121.90	110.80
1	B	522	ALA	N-CA-C	-5.21	105.29	110.97
1	B	253	SER	N-CA-C	5.21	117.17	108.99
1	A	613	ARG	N-CA-C	5.21	118.77	111.90
1	B	186	ILE	N-CA-C	-5.20	100.96	108.87
1	A	219	LEU	N-CA-C	5.20	116.89	108.26
1	A	51	PHE	N-CA-C	5.18	116.40	108.42
1	A	222	THR	N-CA-C	5.17	117.24	109.23
1	B	148	PRO	N-CA-C	5.17	120.41	111.77
1	A	140	LEU	CA-CB-CG	5.16	134.36	116.30
1	B	109	GLU	N-CA-C	-5.13	105.69	111.28
1	B	498	VAL	N-CA-C	-5.13	101.58	108.35
1	B	293	MET	N-CA-C	5.07	117.00	108.73
1	A	590	ALA	N-CA-C	5.07	116.00	108.86
1	B	278	GLY	N-CA-C	5.04	117.40	110.69

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain
1	A	436	ARG	Sidechain
1	A	462	TYR	Sidechain
1	A	511	TYR	Sidechain
1	A	541	TYR	Sidechain
1	B	129	TYR	Sidechain
1	B	146	TYR	Sidechain

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	4990	0	4846	439	0
1	B	4990	0	4845	533	0
2	C	105	0	88	4	0
2	D	105	0	88	7	0
All	All	10190	0	9867	975	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 49.

All (975) 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:B:118:ARG:HH21	1:B:153:ILE:HA	1.25	0.99
1:A:107:LEU:HG	1:A:156:LEU:HD21	1.42	0.99
1:A:156:LEU:HD11	1:A:166:LEU:HD13	1.43	0.99
1:B:146:TYR:HB3	1:B:216:ARG:HH22	1.30	0.97
1:B:162:LEU:HB2	1:B:163:PRO:HD3	1.48	0.94
1:A:162:LEU:HB3	1:A:163:PRO:HD3	1.47	0.94
1:B:258:LEU:HB3	1:B:307:LEU:HA	1.47	0.93
1:B:261:ARG:HB2	1:B:269:VAL:HG13	1.51	0.93
1:B:62:GLN:HB2	1:B:65:ARG:HD3	1.51	0.92
1:B:139:THR:HG22	1:B:151:ALA:HB1	1.49	0.92
1:B:543:ALA:HB2	1:B:565:LEU:HD13	1.50	0.90
1:B:77:MET:SD	1:B:86:ILE:HD13	2.13	0.89
1:B:179:THR:HA	1:B:422:SER:OG	1.72	0.89
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.56	0.88
1:A:410:VAL:HG23	1:A:411:GLY:H	1.38	0.88
1:A:344:TYR:CE2	1:A:577:ARG:HG3	2.09	0.87
1:B:32:GLU:HA	1:B:36:ARG:HD2	1.54	0.87
1:B:261:ARG:HH12	1:B:306:GLN:HE21	1.23	0.86
1:A:51:PHE:HB2	1:A:95:PHE:HE1	1.39	0.85
1:A:406:GLU:HG2	1:A:447:SER:HB3	1.59	0.84
1:A:175:THR:O	1:A:176:LEU:HD13	1.77	0.84
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.43	0.84
1:A:112:THR:HG23	1:A:156:LEU:HD23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HG22	1:B:226:THR:H	1.44	0.82
1:A:234:THR:HG23	1:A:245:ASN:HB2	1.61	0.82
1:B:233:VAL:HG22	1:B:439:ASN:HD22	1.44	0.82
1:B:119:VAL:H	1:B:154:SER:HB3	1.45	0.82
1:B:260:VAL:HG12	1:B:305:VAL:HG23	1.62	0.82
1:B:146:TYR:HB3	1:B:216:ARG:NH2	1.94	0.82
1:B:118:ARG:HH22	1:B:120:VAL:HB	1.45	0.81
1:B:107:LEU:HB3	1:B:111:TRP:CD1	2.16	0.81
1:B:127:HIS:HD2	1:B:174:ASN:HA	1.44	0.81
1:B:289:TRP:HZ3	1:B:293:MET:HE2	1.45	0.81
1:A:177:THR:HG23	1:A:179:THR:H	1.45	0.81
1:B:258:LEU:CB	1:B:307:LEU:HA	2.09	0.81
1:B:543:ALA:HB2	1:B:565:LEU:CD1	2.10	0.81
1:A:23:LEU:HD22	1:A:431:GLU:HB3	1.62	0.80
1:A:385:HIS:HB3	1:A:410:VAL:HG12	1.62	0.80
1:A:507:TRP:O	1:A:508:TYR:HB2	1.82	0.80
1:B:363:TRP:O	1:B:367:VAL:HG23	1.82	0.80
1:A:177:THR:HG22	1:A:180:THR:HG23	1.63	0.80
1:A:42:ASP:HA	1:A:79:VAL:O	1.82	0.79
1:B:349:ASN:HB2	1:B:587:TRP:O	1.82	0.79
1:B:118:ARG:NH2	1:B:153:ILE:HA	1.96	0.79
1:A:112:THR:CG2	1:A:156:LEU:HD23	2.12	0.78
1:A:361:PHE:CZ	1:A:366:LEU:HD12	2.19	0.78
1:B:463:LEU:O	1:B:467:ILE:HG12	1.81	0.78
1:B:341:LYS:HD2	1:B:342:PRO:HD2	1.64	0.78
1:B:287:LEU:HA	1:B:326:ILE:HB	1.65	0.78
1:B:137:VAL:HG13	1:B:138:ASP:H	1.50	0.77
1:A:136:GLY:O	1:A:137:VAL:HB	1.81	0.77
1:B:55:ARG:HG2	2:D:1:NAG:H83	1.67	0.77
1:B:577:ARG:HH12	1:B:629:ILE:HG12	1.48	0.77
1:B:487:TYR:CD2	1:B:527:ASN:HB3	2.20	0.76
1:B:394:GLN:OE1	1:B:399:TYR:HE2	1.67	0.76
1:B:140:LEU:HB2	1:B:151:ALA:HB2	1.68	0.76
1:A:118:ARG:HG3	1:A:153:ILE:O	1.84	0.76
1:B:41:LEU:HB3	1:B:218:VAL:H	1.48	0.76
1:B:162:LEU:HB2	1:B:163:PRO:CD	2.16	0.76
1:B:226:THR:HG21	1:B:309:ALA:CB	2.15	0.76
1:B:577:ARG:NH1	1:B:629:ILE:HG12	2.01	0.76
1:A:51:PHE:HB2	1:A:95:PHE:CE1	2.22	0.75
1:A:381:PHE:HE1	1:A:388:TYR:HE2	1.31	0.75
1:A:215:GLN:NE2	1:A:359:LYS:HB2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD12	1:A:111:TRP:HD1	1.52	0.74
1:B:544:GLU:HG3	1:B:605:LYS:HB2	1.67	0.74
1:A:241:SER:HA	1:A:285:VAL:HG23	1.69	0.74
1:A:371:ASN:O	1:A:374:ARG:HD3	1.86	0.74
1:A:327:ARG:HH22	1:A:477:ARG:HH21	1.33	0.74
1:A:108:PRO:HD2	1:A:111:TRP:CD1	2.23	0.74
1:B:352:GLU:O	1:B:359:LYS:HD3	1.87	0.74
1:A:303:LEU:O	1:A:321:THR:HA	1.88	0.73
1:B:271:ALA:HB1	1:B:280:LEU:HD13	1.71	0.73
1:A:450:ASN:HA	1:A:482:VAL:HG22	1.71	0.73
1:B:608:ILE:HD13	1:B:622:LEU:HD12	1.70	0.73
1:B:332:THR:OG1	1:B:335:GLN:HG2	1.89	0.73
1:A:552:ASP:HB3	1:A:553:PRO:HD3	1.70	0.73
1:A:120:VAL:HB	1:A:221:TYR:CE1	2.24	0.72
1:A:382:ARG:HD3	1:A:406:GLU:OE2	1.89	0.72
1:B:125:SER:OG	1:B:216:ARG:HG3	1.89	0.72
1:B:156:LEU:HD11	1:B:166:LEU:HD13	1.72	0.72
1:B:93:ARG:HH22	1:B:593:MET:HE3	1.54	0.72
1:A:257:LYS:HD3	1:A:258:LEU:H	1.53	0.72
1:B:586:ILE:HG21	1:B:622:LEU:HD11	1.72	0.72
1:A:262:LEU:HD23	1:A:282:VAL:HG11	1.71	0.72
1:B:514:LEU:HD21	1:B:561:TYR:HE1	1.55	0.72
1:B:457:GLU:HG3	1:B:491:LYS:HE2	1.71	0.71
1:B:118:ARG:O	1:B:222:THR:HA	1.89	0.71
1:B:176:LEU:HB2	1:B:202:GLN:OE1	1.90	0.71
1:A:563:LYS:O	1:A:567:GLU:HB2	1.90	0.71
1:B:397:ASP:O	1:B:399:TYR:N	2.24	0.71
1:B:289:TRP:CZ3	1:B:293:MET:HE2	2.25	0.71
1:B:555:LEU:O	1:B:561:TYR:HB2	1.91	0.71
1:B:514:LEU:HD21	1:B:561:TYR:CE1	2.25	0.71
1:A:156:LEU:HG	1:A:156:LEU:O	1.88	0.71
1:B:292:LEU:HD23	1:B:379:ASN:ND2	2.06	0.71
1:B:330:ALA:HB3	1:B:337:LEU:HB2	1.73	0.70
1:A:137:VAL:HG22	1:A:138:ASP:H	1.55	0.70
1:B:395:MET:HG2	1:B:403:VAL:CG2	2.21	0.70
1:B:261:ARG:HH12	1:B:306:GLN:NE2	1.90	0.70
1:A:257:LYS:HD3	1:A:258:LEU:N	2.05	0.70
1:A:395:MET:HG2	1:A:403:VAL:HG21	1.74	0.70
1:B:118:ARG:N	1:B:223:THR:O	2.25	0.70
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.57	0.70
1:B:158:GLN:O	1:B:161:PRO:HD3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TRP:CE3	1:B:327:ARG:HD3	2.27	0.69
1:B:394:GLN:O	1:B:399:TYR:HD2	1.76	0.69
2:C:6:MAN:O2	2:C:6:MAN:H61	1.93	0.69
1:A:175:THR:CG2	1:A:210:ASN:HB3	2.22	0.69
1:B:74:THR:HG22	1:B:75:VAL:H	1.57	0.69
1:B:327:ARG:HH22	1:B:477:ARG:HH21	1.41	0.69
1:A:23:LEU:HD23	1:A:23:LEU:H	1.56	0.69
1:A:352:GLU:O	1:A:359:LYS:HG2	1.92	0.69
1:B:227:TYR:HE1	1:B:251:LYS:HB3	1.57	0.69
1:A:156:LEU:O	1:A:157:VAL:HG12	1.93	0.69
1:B:66:ARG:HB2	1:B:67:PRO:HD2	1.75	0.69
1:A:361:PHE:CE1	1:A:366:LEU:HD12	2.27	0.68
1:A:395:MET:HG2	1:A:403:VAL:CG2	2.23	0.68
1:A:447:SER:HA	1:A:480:THR:O	1.93	0.68
1:A:531:LYS:HE2	1:A:532:TYR:CE2	2.28	0.68
1:B:41:LEU:HD13	1:B:217:SER:HA	1.73	0.68
1:A:107:LEU:HD23	1:A:164:SER:C	2.18	0.68
1:A:499:ILE:HG22	1:A:501:LEU:HD22	1.75	0.68
1:B:135:ASN:HD22	1:B:136:GLY:N	1.90	0.68
1:B:226:THR:HG21	1:B:309:ALA:HB2	1.76	0.68
1:B:558:THR:HG22	1:B:561:TYR:H	1.58	0.68
1:A:292:LEU:HB2	1:A:379:ASN:HD22	1.56	0.68
1:B:181:LEU:HD22	1:B:409:GLY:HA2	1.75	0.68
1:A:108:PRO:HD2	1:A:111:TRP:CG	2.28	0.68
1:B:403:VAL:O	1:B:444:VAL:HG22	1.93	0.68
1:B:227:TYR:CE1	1:B:251:LYS:HB3	2.30	0.67
1:B:303:LEU:O	1:B:321:THR:HA	1.94	0.67
1:A:162:LEU:HB3	1:A:163:PRO:CD	2.24	0.67
1:B:424:HIS:O	1:B:427:MET:HB3	1.94	0.67
1:A:185:THR:HG23	2:C:8:MAN:O4	1.94	0.67
1:A:192:THR:O	1:A:193:SER:HB2	1.94	0.67
1:A:372:LEU:HD22	1:A:609:PHE:CE1	2.29	0.67
1:B:32:GLU:CA	1:B:36:ARG:HD2	2.25	0.67
1:B:127:HIS:O	1:B:144:GLY:HA2	1.94	0.67
1:A:107:LEU:HB2	1:A:164:SER:HB3	1.75	0.67
1:A:107:LEU:HB2	1:A:164:SER:CB	2.24	0.67
1:A:349:ASN:ND2	1:A:585:LEU:HD23	2.10	0.67
1:B:162:LEU:CB	1:B:163:PRO:HD3	2.23	0.67
1:B:333:LYS:HE3	1:B:533:GLN:O	1.95	0.67
1:A:107:LEU:HD12	1:A:111:TRP:CD1	2.31	0.66
1:B:395:MET:HG2	1:B:403:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:N	1:B:107:LEU:HD22	2.10	0.66
1:B:134:VAL:HG22	1:B:135:ASN:H	1.60	0.66
1:B:83:PHE:HE1	1:B:212:ALA:HB3	1.60	0.66
1:A:415:PRO:HB3	1:A:456:LEU:HD21	1.78	0.66
1:B:131:ILE:HG21	1:B:133:TRP:CZ2	2.31	0.66
1:B:178:PRO:HB3	1:B:417:PHE:CD1	2.31	0.66
1:A:288:TRP:HE3	1:A:288:TRP:O	1.79	0.66
1:A:397:ASP:O	1:A:399:TYR:N	2.29	0.66
1:B:146:TYR:HB2	1:B:387:PRO:HD2	1.77	0.66
1:B:332:THR:HG1	1:B:335:GLN:HG2	1.58	0.66
1:A:309:ALA:O	1:A:315:PRO:HA	1.96	0.66
1:A:264:ASP:HB2	1:A:299:TYR:OH	1.95	0.66
1:A:47:PHE:CD2	1:A:77:MET:HG3	2.31	0.65
1:A:107:LEU:HG	1:A:156:LEU:CD2	2.22	0.65
1:A:231:ILE:HG22	1:A:232:THR:H	1.62	0.65
1:B:455:HIS:HA	1:B:489:ALA:O	1.96	0.65
1:B:107:LEU:HB3	1:B:111:TRP:HD1	1.61	0.65
1:B:216:ARG:HD3	1:B:389:ALA:HB2	1.77	0.65
1:B:521:LEU:HA	1:B:524:GLN:HG2	1.78	0.65
1:B:327:ARG:NH2	1:B:477:ARG:HH21	1.94	0.65
1:B:402:VAL:O	1:B:402:VAL:HG23	1.95	0.65
1:B:292:LEU:HD23	1:B:379:ASN:HD21	1.62	0.65
1:B:445:MET:CE	1:B:498:VAL:HG21	2.27	0.65
1:A:284:GLY:O	1:A:285:VAL:HG12	1.97	0.65
1:A:440:HIS:O	1:A:443:VAL:HG12	1.97	0.65
1:B:233:VAL:HG22	1:B:439:ASN:ND2	2.12	0.65
1:B:271:ALA:HB1	1:B:280:LEU:CD1	2.26	0.65
1:B:291:TYR:CZ	1:B:374:ARG:HG3	2.32	0.65
1:B:99:VAL:HG12	1:B:172:ILE:HD11	1.78	0.65
1:B:223:THR:HG21	1:B:227:TYR:HD2	1.62	0.64
1:A:627:TRP:O	1:A:631:ASN:ND2	2.30	0.64
1:A:276:THR:HG23	1:A:276:THR:O	1.97	0.64
1:A:406:GLU:HG2	1:A:447:SER:CB	2.26	0.64
1:B:253:SER:HB3	1:B:311:THR:OG1	1.98	0.64
1:B:407:CYS:SG	1:B:408:PRO:HD2	2.37	0.64
1:A:290:PRO:HG2	1:A:293:MET:SD	2.38	0.64
1:B:291:TYR:HB2	1:B:399:TYR:O	1.98	0.64
1:B:250:VAL:HG12	1:B:251:LYS:H	1.61	0.64
1:B:189:LEU:HD13	1:B:195:TYR:CZ	2.32	0.64
1:A:53:ASP:H	1:A:56:ARG:HD3	1.62	0.64
1:B:135:ASN:OD1	1:B:155:ASN:OD1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HG13	1:B:154:SER:N	2.12	0.64
1:B:551:GLN:HG3	1:B:552:ASP:O	1.98	0.64
1:B:29:TYR:CE2	1:B:393:MET:SD	2.91	0.64
1:A:555:LEU:HD13	1:A:556:MET:HE3	1.79	0.63
1:A:228:ILE:HD13	1:A:305:VAL:HG12	1.80	0.63
1:A:434:VAL:O	1:A:438:LYS:HB3	1.98	0.63
1:A:347:GLY:HA3	1:A:380:ALA:O	1.98	0.63
1:B:118:ARG:HA	1:B:154:SER:HB3	1.79	0.63
1:A:32:GLU:HB2	1:A:36:ARG:HG2	1.79	0.63
1:A:54:ASN:O	1:A:56:ARG:HG2	1.98	0.63
1:B:391:GLU:O	1:B:394:GLN:HB2	1.98	0.63
1:A:183:PRO:HG3	1:A:412:LEU:HD12	1.80	0.63
1:A:258:LEU:HG	1:A:307:LEU:HD12	1.81	0.63
1:B:119:VAL:N	1:B:154:SER:HB3	2.13	0.63
1:A:352:GLU:O	1:A:359:LYS:NZ	2.29	0.63
1:B:118:ARG:NH2	1:B:120:VAL:HB	2.14	0.63
1:A:174:ASN:HD22	1:A:174:ASN:C	2.07	0.62
1:A:175:THR:HG22	1:A:210:ASN:HB3	1.80	0.62
1:B:445:MET:HG2	1:B:446:TRP:N	2.12	0.62
1:A:570:HIS:HA	1:A:573:LEU:HD12	1.81	0.62
1:A:134:VAL:HG12	1:A:166:LEU:HD11	1.82	0.62
1:B:158:GLN:O	1:B:160:GLY:N	2.33	0.62
1:B:532:TYR:O	1:B:534:LYS:HG3	1.99	0.62
1:B:223:THR:OG1	1:B:227:TYR:HB3	1.98	0.62
1:B:251:LYS:HB2	1:B:251:LYS:NZ	2.15	0.62
1:A:298:ALA:HB1	1:A:396:CYS:O	2.00	0.62
1:A:348:VAL:HG23	1:A:586:ILE:CG2	2.30	0.62
1:A:381:PHE:HE1	1:A:388:TYR:CE2	2.15	0.62
1:B:445:MET:HE2	1:B:498:VAL:HG21	1.81	0.62
1:B:554:PRO:HB3	1:B:561:TYR:HA	1.82	0.62
1:A:39:LYS:HB2	1:A:41:LEU:HD23	1.82	0.62
1:A:531:LYS:HB3	1:A:531:LYS:HZ3	1.64	0.62
1:B:140:LEU:HD22	1:B:151:ALA:HB2	1.81	0.61
1:A:118:ARG:O	1:A:222:THR:HA	2.00	0.61
1:A:557:PHE:HD1	1:A:557:PHE:H	1.46	0.61
1:A:182:PRO:HB3	1:A:410:VAL:HG21	1.82	0.61
1:A:264:ASP:OD1	1:A:268:LYS:HB2	1.99	0.61
1:B:332:THR:HG23	1:B:337:LEU:HD11	1.82	0.61
1:B:134:VAL:HG13	1:B:135:ASN:N	2.15	0.61
1:B:594:THR:OG1	1:B:603:GLY:HA2	2.00	0.61
1:A:290:PRO:O	1:A:292:LEU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:HG13	1:B:221:TYR:HB3	1.82	0.61
1:A:37:GLU:O	1:A:37:GLU:HG2	2.01	0.61
1:A:430:MET:O	1:A:434:VAL:HG23	2.01	0.61
1:A:176:LEU:HD12	1:A:182:PRO:O	2.00	0.61
1:A:271:ALA:HB1	1:A:280:LEU:CD2	2.31	0.61
1:B:62:GLN:HB2	1:B:65:ARG:CD	2.29	0.60
1:B:155:ASN:C	1:B:155:ASN:ND2	2.59	0.60
1:A:491:LYS:O	1:A:494:PRO:HD2	2.01	0.60
1:B:52:SER:HB3	1:B:56:ARG:CZ	2.31	0.60
1:B:53:ASP:N	1:B:56:ARG:HD3	2.16	0.60
1:B:101:TYR:CE2	1:B:214:LEU:HB3	2.36	0.60
1:B:576:LYS:HE2	1:B:580:TYR:OH	2.00	0.60
1:B:372:LEU:HB2	1:B:589:PHE:HZ	1.66	0.60
1:A:327:ARG:NH2	1:A:477:ARG:HH21	1.96	0.60
1:A:224:PRO:HD2	1:A:318:ASP:OD1	2.01	0.60
1:A:291:TYR:HE2	1:A:374:ARG:HA	1.66	0.60
1:B:190:THR:HG22	1:B:198:GLY:HA2	1.84	0.60
1:A:415:PRO:HG2	1:A:416:GLN:HE21	1.64	0.60
1:B:241:SER:O	1:B:326:ILE:HG21	2.01	0.60
1:A:349:ASN:HB2	1:A:587:TRP:O	2.01	0.60
1:A:410:VAL:HG23	1:A:411:GLY:N	2.14	0.60
1:B:178:PRO:HB3	1:B:417:PHE:HD1	1.66	0.60
1:B:231:ILE:O	1:B:231:ILE:HG22	2.01	0.60
1:A:554:PRO:HB3	1:A:561:TYR:HA	1.84	0.60
1:B:48:ARG:NH2	1:B:72:GLY:HA3	2.16	0.60
1:B:190:THR:HA	1:B:199:TYR:H	1.67	0.60
1:B:391:GLU:O	1:B:395:MET:SD	2.60	0.60
1:A:108:PRO:O	1:A:111:TRP:HB2	2.02	0.60
1:B:206:PHE:HB3	1:B:410:VAL:HG13	1.82	0.60
1:B:382:ARG:HD2	1:B:406:GLU:OE1	2.02	0.60
1:B:139:THR:CG2	1:B:151:ALA:HB1	2.26	0.59
1:B:163:PRO:O	1:B:164:SER:HB3	2.01	0.59
1:B:291:TYR:CE2	1:B:374:ARG:HG3	2.37	0.59
1:A:137:VAL:HG22	1:A:138:ASP:N	2.17	0.59
1:B:108:PRO:O	1:B:111:TRP:HB2	2.02	0.59
1:A:116:ARG:O	1:A:224:PRO:HA	2.02	0.59
1:A:289:TRP:HB2	1:A:297:PRO:HA	1.85	0.59
1:B:261:ARG:HH22	1:B:306:GLN:NE2	2.00	0.59
1:A:47:PHE:CG	1:A:77:MET:HG3	2.37	0.59
1:A:443:VAL:O	1:A:443:VAL:HG13	2.03	0.59
1:B:155:ASN:ND2	1:B:155:ASN:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:CG1	1:B:172:ILE:HD11	2.33	0.59
1:B:66:ARG:HB2	1:B:67:PRO:CD	2.31	0.59
1:A:107:LEU:HD21	1:A:166:LEU:HB2	1.83	0.59
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.17	0.59
1:A:461:TYR:O	1:A:465:MET:HG2	2.03	0.59
1:B:343:PHE:CE2	1:B:402:VAL:HG21	2.37	0.59
1:B:238:GLU:HG2	1:B:239:GLN:HE22	1.66	0.59
1:A:504:TYR:O	1:A:507:TRP:O	2.21	0.58
1:B:190:THR:O	1:B:195:TYR:HB2	2.03	0.58
1:A:93:ARG:HG3	1:A:93:ARG:NH1	2.12	0.58
1:A:183:PRO:HG3	1:A:412:LEU:CD1	2.34	0.58
1:B:426:HIS:O	1:B:429:VAL:HG22	2.03	0.58
1:A:543:ALA:HB2	1:A:565:LEU:HD13	1.85	0.58
1:B:233:VAL:H	1:B:439:ASN:HD21	1.50	0.58
1:B:120:VAL:CG2	1:B:150:GLU:HB2	2.34	0.58
1:B:335:GLN:HA	1:B:582:VAL:HG11	1.86	0.58
1:B:386:TYR:CE1	1:B:388:TYR:CE1	2.91	0.58
1:B:445:MET:SD	1:B:480:THR:HG22	2.44	0.58
1:A:124:GLY:O	1:A:125:SER:HB3	2.02	0.58
1:B:552:ASP:O	1:B:553:PRO:C	2.46	0.58
1:B:189:LEU:HD12	1:B:199:TYR:CE2	2.39	0.57
1:A:48:ARG:NH1	1:A:71:SER:OG	2.37	0.57
1:A:67:PRO:HB2	1:A:70:GLU:HG3	1.86	0.57
1:A:231:ILE:HG23	1:A:248:ILE:HG12	1.85	0.57
1:A:160:GLY:N	1:A:161:PRO:HD3	2.19	0.57
1:A:238:GLU:HB2	1:A:243:LEU:HD21	1.86	0.57
1:A:531:LYS:HB3	1:A:531:LYS:NZ	2.19	0.57
1:A:608:ILE:HD13	1:A:622:LEU:HD12	1.85	0.57
1:B:234:THR:O	1:B:245:ASN:HB2	2.03	0.57
1:B:241:SER:HB2	1:B:285:VAL:N	2.18	0.57
1:B:263:LEU:HG	1:B:269:VAL:HG22	1.87	0.57
1:B:552:ASP:CB	1:B:553:PRO:HD2	2.31	0.57
1:A:77:MET:SD	1:A:86:ILE:HD11	2.45	0.57
1:A:390:GLU:C	1:A:392:VAL:H	2.13	0.57
1:B:98:TRP:HE1	2:D:1:NAG:C7	2.18	0.57
1:A:288:TRP:O	1:A:288:TRP:CE3	2.57	0.56
1:B:258:LEU:HD12	1:B:275:GLY:HA2	1.87	0.56
1:A:464:LYS:HD3	1:A:495:TYR:CE1	2.40	0.56
1:B:29:TYR:CD2	1:B:393:MET:SD	2.97	0.56
1:B:195:TYR:HB3	1:B:196:PRO:HD2	1.87	0.56
1:B:590:ALA:HA	1:B:609:PHE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:HG22	1:A:386:TYR:O	2.06	0.56
1:B:35:SER:OG	1:B:224:PRO:HD3	2.04	0.56
1:B:366:LEU:HD22	1:B:394:GLN:HE21	1.69	0.56
1:A:153:ILE:HG13	1:A:154:SER:N	2.21	0.56
1:A:387:PRO:HD2	1:A:408:PRO:HD3	1.87	0.56
1:A:514:LEU:HD21	1:A:561:TYR:CE1	2.40	0.56
1:B:32:GLU:HA	1:B:36:ARG:CD	2.31	0.56
1:B:348:VAL:HG22	1:B:349:ASN:N	2.20	0.56
1:B:445:MET:SD	1:B:480:THR:CG2	2.94	0.56
1:B:147:LEU:HD21	1:B:433:VAL:HG22	1.88	0.56
1:B:551:GLN:HG2	1:B:555:LEU:HB2	1.86	0.56
1:B:622:LEU:O	1:B:625:ARG:HB3	2.06	0.56
1:A:90:TRP:CE2	1:A:91:ARG:HG2	2.40	0.56
1:A:158:GLN:O	1:A:161:PRO:HD3	2.05	0.56
1:A:128:SER:HA	1:A:144:GLY:HA2	1.86	0.56
1:A:363:TRP:O	1:A:367:VAL:HG23	2.06	0.56
1:A:120:VAL:HG13	1:A:151:ALA:O	2.06	0.56
1:A:349:ASN:HD21	1:A:585:LEU:HD23	1.68	0.56
1:B:35:SER:HB3	1:B:223:THR:HA	1.88	0.56
1:A:347:GLY:HA2	1:A:378:ALA:HB1	1.88	0.55
1:B:487:TYR:CE2	1:B:527:ASN:HB3	2.41	0.55
1:A:80:PRO:HB3	1:A:215:GLN:O	2.06	0.55
1:A:32:GLU:HB3	1:A:37:GLU:OE2	2.06	0.55
1:A:262:LEU:HD12	1:A:302:SER:O	2.05	0.55
1:B:34:PRO:O	1:B:35:SER:HB2	2.05	0.55
1:A:257:LYS:NZ	1:A:274:THR:HG22	2.21	0.55
1:A:350:LYS:HD3	1:A:373:LEU:HD21	1.88	0.55
1:B:191:ASP:HA	1:B:195:TYR:O	2.06	0.55
1:B:434:VAL:HA	1:B:446:TRP:CH2	2.42	0.55
1:A:387:PRO:CD	1:A:408:PRO:HD3	2.37	0.55
1:B:125:SER:O	1:B:214:LEU:HD13	2.06	0.55
1:A:525:PHE:HD2	1:A:576:LYS:HE3	1.71	0.55
1:B:507:TRP:O	1:B:509:HIS:N	2.37	0.55
1:B:595:GLU:HG3	1:B:596:GLN:H	1.72	0.55
1:A:259:GLU:HG2	1:A:272:ASN:HD21	1.72	0.54
1:B:63:TRP:HA	1:B:65:ARG:HH21	1.73	0.54
1:B:450:ASN:HD22	1:B:482:VAL:HB	1.72	0.54
1:B:557:PHE:HD1	1:B:557:PHE:H	1.55	0.54
1:A:545:THR:OG1	1:A:562:GLN:HB2	2.06	0.54
1:B:86:ILE:HG13	1:B:87:SER:N	2.22	0.54
1:A:228:ILE:HD13	1:A:305:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:HB1	1:A:280:LEU:HD22	1.89	0.54
1:A:450:ASN:HA	1:A:482:VAL:CG2	2.37	0.54
1:B:45:TRP:CH2	1:B:218:VAL:HG11	2.43	0.54
1:B:284:GLY:O	1:B:285:VAL:HG13	2.07	0.54
1:A:51:PHE:HA	1:A:56:ARG:HG3	1.88	0.54
1:B:595:GLU:HG3	1:B:596:GLN:N	2.21	0.54
1:A:584:GLU:O	1:A:585:LEU:HD12	2.07	0.54
1:B:156:LEU:CD1	1:B:166:LEU:HD13	2.38	0.54
1:A:39:LYS:HB2	1:A:41:LEU:CD2	2.37	0.54
1:A:263:LEU:HB2	1:A:267:ASN:HA	1.89	0.54
1:A:357:ARG:HB3	1:A:357:ARG:NH1	2.23	0.54
1:A:487:TYR:O	1:A:488:ALA:HB3	2.07	0.54
1:B:83:PHE:O	1:B:86:ILE:HG12	2.07	0.54
1:B:231:ILE:HG23	1:B:248:ILE:HG13	1.89	0.54
1:B:256:PHE:HB2	1:B:308:THR:O	2.08	0.54
1:B:237:VAL:HG22	1:B:326:ILE:HG22	1.89	0.54
1:B:629:ILE:O	1:B:632:GLU:HG2	2.08	0.54
1:A:107:LEU:CG	1:A:156:LEU:HD21	2.27	0.54
1:B:266:GLU:O	1:B:268:LYS:HG2	2.07	0.54
1:B:99:VAL:HG12	1:B:172:ILE:CD1	2.38	0.54
1:B:541:TYR:OH	1:B:570:HIS:HE1	1.91	0.54
1:B:248:ILE:HD12	1:B:248:ILE:N	2.23	0.53
1:B:35:SER:CB	1:B:224:PRO:HD3	2.37	0.53
1:B:187:GLN:HE21	1:B:189:LEU:HG	1.73	0.53
1:A:112:THR:O	1:A:113:GLN:HG3	2.08	0.53
1:B:225:THR:HG22	1:B:226:THR:N	2.19	0.53
1:A:290:PRO:C	1:A:292:LEU:N	2.66	0.53
1:A:290:PRO:HD2	1:A:293:MET:SD	2.48	0.53
1:B:394:GLN:OE1	1:B:399:TYR:CE2	2.57	0.53
1:B:230:ASP:O	1:B:248:ILE:HA	2.08	0.53
1:B:514:LEU:CD2	1:B:561:TYR:HE1	2.20	0.53
1:A:455:HIS:HA	1:A:489:ALA:O	2.09	0.53
1:B:541:TYR:OH	1:B:570:HIS:CE1	2.61	0.53
1:A:40:GLU:C	1:A:42:ASP:H	2.17	0.53
1:B:109:GLU:HG3	1:B:110:ARG:N	2.23	0.53
1:B:117:THR:HA	1:B:224:PRO:HA	1.90	0.53
1:B:233:VAL:H	1:B:439:ASN:ND2	2.07	0.53
1:B:552:ASP:C	1:B:554:PRO:N	2.67	0.53
1:B:577:ARG:C	1:B:579:LYS:H	2.17	0.53
1:A:488:ALA:H	1:A:531:LYS:HE3	1.74	0.53
1:A:557:PHE:CD1	1:A:557:PHE:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:PHE:N	1:B:557:PHE:CD1	2.77	0.53
1:A:385:HIS:O	1:A:386:TYR:HB3	2.09	0.52
1:B:149:PHE:N	1:B:149:PHE:CD1	2.77	0.52
1:B:281:LYS:HG3	1:B:282:VAL:N	2.24	0.52
1:B:266:GLU:O	1:B:268:LYS:N	2.42	0.52
1:A:96:VAL:HG12	1:A:175:THR:OG1	2.09	0.52
1:A:157:VAL:O	1:A:161:PRO:HG3	2.09	0.52
1:A:159:VAL:HG23	1:A:159:VAL:O	2.08	0.52
1:A:348:VAL:HG23	1:A:586:ILE:HG23	1.91	0.52
1:A:524:GLN:O	1:A:528:TRP:HD1	1.92	0.52
1:B:246:TYR:O	1:B:278:GLY:N	2.43	0.52
1:A:114:ASP:O	1:A:116:ARG:N	2.42	0.52
1:A:330:ALA:O	1:A:331:VAL:HG13	2.09	0.52
1:A:332:THR:HB	1:A:333:LYS:NZ	2.24	0.52
1:B:39:LYS:HA	1:B:219:LEU:CB	2.39	0.52
1:B:536:ILE:HG22	1:B:537:ILE:N	2.25	0.52
1:B:127:HIS:CD2	1:B:174:ASN:HA	2.34	0.52
1:B:376:LEU:HA	1:B:623:ARG:HB3	1.90	0.52
1:B:493:ALA:N	1:B:494:PRO:HD2	2.24	0.52
1:B:576:LYS:O	1:B:579:LYS:HB2	2.10	0.52
1:A:175:THR:HB	1:A:202:GLN:HG2	1.91	0.52
1:A:265:ALA:N	1:A:299:TYR:OH	2.39	0.52
1:A:504:TYR:HB3	1:A:507:TRP:HB3	1.90	0.52
1:B:348:VAL:HG22	1:B:349:ASN:H	1.74	0.52
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.75	0.52
1:A:291:TYR:CE2	1:A:374:ARG:HA	2.44	0.52
1:A:462:TYR:O	1:A:465:MET:HB2	2.10	0.52
1:B:51:PHE:CZ	1:B:200:PHE:HZ	2.27	0.52
1:B:263:LEU:N	1:B:263:LEU:HD12	2.24	0.52
1:A:49:ALA:HA	1:A:99:VAL:HG23	1.92	0.52
1:A:80:PRO:HB3	1:A:215:GLN:C	2.35	0.52
1:B:329:VAL:HG22	1:B:329:VAL:O	2.10	0.52
1:A:130:ALA:O	1:A:141:GLU:HA	2.10	0.52
1:B:50:ASP:CB	1:B:63:TRP:HH2	2.22	0.52
2:D:1:NAG:H5	2:D:1:NAG:HN2	1.75	0.52
1:A:156:LEU:CD1	1:A:166:LEU:HD13	2.30	0.52
1:A:562:GLN:O	1:A:566:LEU:HG	2.09	0.52
1:B:172:ILE:HD13	1:B:172:ILE:H	1.74	0.52
1:B:189:LEU:HD13	1:B:195:TYR:CE2	2.45	0.52
1:B:257:LYS:NZ	1:B:257:LYS:HB3	2.25	0.52
1:B:307:LEU:HG	1:B:308:THR:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:N	1:B:416:GLN:OE1	2.43	0.52
1:A:129:TYR:O	1:A:172:ILE:HA	2.11	0.51
1:A:385:HIS:HB3	1:A:410:VAL:CG1	2.36	0.51
1:B:50:ASP:HB3	1:B:63:TRP:CH2	2.45	0.51
1:B:116:ARG:O	1:B:224:PRO:HA	2.11	0.51
1:B:592:PHE:CE2	1:B:604:ASN:ND2	2.78	0.51
1:A:541:TYR:OH	1:A:570:HIS:HE1	1.92	0.51
1:A:53:ASP:N	1:A:56:ARG:HD3	2.24	0.51
1:A:283:PRO:C	1:A:285:VAL:H	2.17	0.51
1:B:121:LEU:HD21	1:B:168:ILE:CD1	2.41	0.51
1:B:99:VAL:O	1:B:171:ALA:HA	2.09	0.51
1:A:139:THR:HG22	1:A:151:ALA:HB1	1.93	0.51
1:A:395:MET:HG3	1:A:401:ILE:O	2.10	0.51
1:B:59:PHE:HZ	1:B:131:ILE:HD12	1.76	0.51
1:B:276:THR:O	1:B:277:GLN:HB3	2.10	0.51
1:B:368:LYS:O	1:B:371:ASN:HB2	2.10	0.51
1:B:433:VAL:HG12	1:B:446:TRP:HZ3	1.75	0.51
1:B:243:LEU:HD13	1:B:243:LEU:O	2.11	0.51
1:B:276:THR:O	1:B:276:THR:HG22	2.11	0.51
1:B:93:ARG:HH12	1:B:593:MET:HE3	1.76	0.51
1:B:107:LEU:HD21	1:B:166:LEU:HB2	1.93	0.51
1:B:118:ARG:HH11	1:B:223:THR:HG23	1.75	0.51
1:B:450:ASN:C	1:B:452:PRO:HD3	2.36	0.51
1:B:469:HIS:HE1	1:B:473:LEU:HD21	1.76	0.51
1:A:286:SER:HB3	1:A:299:TYR:CE2	2.46	0.51
1:A:631:ASN:N	1:A:631:ASN:HD22	2.09	0.51
1:B:189:LEU:HB2	1:B:199:TYR:HD2	1.75	0.51
1:A:353:ASP:CG	1:A:611:ARG:HH21	2.19	0.51
1:A:359:LYS:NZ	1:A:386:TYR:OH	2.32	0.51
1:B:224:PRO:HG2	1:B:318:ASP:OD2	2.11	0.51
1:B:350:LYS:HG2	1:B:589:PHE:HB2	1.92	0.51
1:A:102:GLU:HG3	1:A:168:ILE:O	2.11	0.51
1:B:53:ASP:HB2	1:B:56:ARG:HH11	1.76	0.51
1:B:84:ASN:OD1	1:B:211:TYR:HD1	1.93	0.51
1:B:297:PRO:O	1:B:299:TYR:N	2.44	0.51
1:B:362:ASP:O	1:B:366:LEU:HB2	2.10	0.51
1:B:487:TYR:O	1:B:488:ALA:HB3	2.10	0.51
1:A:186:ILE:HG22	1:A:187:GLN:N	2.26	0.50
1:A:570:HIS:O	1:A:574:ASP:OD2	2.28	0.50
1:B:53:ASP:HB2	1:B:56:ARG:HD3	1.93	0.50
1:B:134:VAL:HG22	1:B:135:ASN:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:O	1:B:425:HIS:CD2	2.63	0.50
1:A:107:LEU:HB2	1:A:164:SER:HB2	1.93	0.50
1:B:333:LYS:HG3	1:B:533:GLN:O	2.11	0.50
1:A:216:ARG:NH1	1:A:389:ALA:N	2.60	0.50
1:B:134:VAL:O	1:B:137:VAL:N	2.45	0.50
1:B:140:LEU:HD13	1:B:150:GLU:O	2.10	0.50
1:B:385:HIS:O	1:B:408:PRO:HA	2.10	0.50
1:A:23:LEU:H	1:A:23:LEU:CD2	2.24	0.50
1:B:320:TYR:CD1	1:B:321:THR:O	2.65	0.50
1:B:333:LYS:HE3	1:B:533:GLN:HB3	1.92	0.50
1:B:29:TYR:CD1	1:B:30:PRO:HD2	2.47	0.50
1:A:136:GLY:O	1:A:137:VAL:CB	2.56	0.50
1:A:182:PRO:HB3	1:A:410:VAL:CG2	2.41	0.50
1:B:107:LEU:HD22	1:B:107:LEU:H	1.77	0.50
1:B:110:ARG:C	1:B:112:THR:H	2.20	0.50
1:B:250:VAL:HG12	1:B:251:LYS:N	2.26	0.50
1:B:290:PRO:O	1:B:292:LEU:N	2.44	0.50
1:A:594:THR:OG1	1:A:603:GLY:HA2	2.12	0.50
1:B:216:ARG:CZ	1:B:388:TYR:O	2.60	0.50
1:A:54:ASN:C	1:A:56:ARG:N	2.63	0.50
1:A:98:TRP:HA	1:A:172:ILE:O	2.12	0.50
1:A:262:LEU:HD23	1:A:282:VAL:CG1	2.40	0.50
1:B:262:LEU:H	1:B:271:ALA:HB3	1.77	0.50
1:B:608:ILE:O	1:B:619:ALA:HB2	2.12	0.50
1:B:619:ALA:O	1:B:623:ARG:HG2	2.11	0.50
1:A:285:VAL:O	1:A:286:SER:HB2	2.11	0.50
1:B:461:TYR:HD1	1:B:464:LYS:HZ3	1.57	0.50
1:A:333:LYS:H	1:A:333:LYS:HD3	1.77	0.49
1:A:514:LEU:HD21	1:A:561:TYR:CZ	2.46	0.49
1:A:556:MET:HB3	1:A:557:PHE:HD1	1.76	0.49
1:B:423:LEU:HD22	1:B:423:LEU:O	2.12	0.49
1:A:235:THR:HG22	1:A:244:VAL:HG22	1.95	0.49
1:B:65:ARG:O	1:B:65:ARG:HG2	2.12	0.49
1:B:146:TYR:C	1:B:216:ARG:HH21	2.20	0.49
1:B:460:GLY:O	1:B:495:TYR:HE2	1.96	0.49
1:B:37:GLU:HB3	1:B:221:TYR:CD1	2.47	0.49
1:B:50:ASP:HB3	1:B:63:TRP:HH2	1.77	0.49
1:B:231:ILE:O	1:B:233:VAL:HG13	2.12	0.49
1:B:457:GLU:HA	1:B:491:LYS:HG3	1.94	0.49
1:B:54:ASN:HB3	2:D:5:MAN:H61	1.95	0.49
1:B:216:ARG:NH1	1:B:352:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:GLN:OE1	1:B:618:ALA:HB3	2.12	0.49
1:B:65:ARG:O	1:B:66:ARG:HB3	2.11	0.49
1:B:292:LEU:CD2	1:B:379:ASN:ND2	2.73	0.49
1:B:416:GLN:C	1:B:418:PHE:H	2.20	0.49
1:A:132:VAL:HG12	1:A:134:VAL:CG2	2.43	0.49
1:B:544:GLU:HG2	1:B:557:PHE:CE2	2.47	0.49
1:A:121:LEU:HD13	1:A:220:LEU:CD2	2.42	0.49
1:A:292:LEU:HD23	1:A:379:ASN:ND2	2.27	0.49
1:B:134:VAL:HG23	1:B:166:LEU:HD11	1.93	0.49
1:B:274:THR:HG22	1:B:275:GLY:N	2.27	0.49
1:B:372:LEU:O	1:B:375:TRP:HB3	2.13	0.49
1:B:507:TRP:C	1:B:509:HIS:H	2.21	0.49
1:B:588:ASN:OD1	1:B:592:PHE:CE2	2.66	0.49
1:A:472:SER:O	1:A:473:LEU:HB2	2.12	0.49
1:A:499:ILE:CG2	1:A:501:LEU:HD22	2.40	0.49
1:A:535:PRO:HA	1:A:580:TYR:O	2.12	0.49
1:B:135:ASN:CG	1:B:155:ASN:OD1	2.56	0.49
1:B:309:ALA:O	1:B:315:PRO:HA	2.13	0.49
1:A:83:PHE:CE2	1:A:212:ALA:HB3	2.48	0.49
1:A:100:TRP:N	1:A:100:TRP:CD1	2.81	0.49
1:A:333:LYS:O	1:A:529:TYR:HE1	1.95	0.49
1:B:186:ILE:HD13	1:B:202:GLN:HE21	1.77	0.49
1:B:385:HIS:ND1	1:B:385:HIS:N	2.61	0.49
1:A:259:GLU:HA	1:A:274:THR:HA	1.94	0.48
1:A:357:ARG:HB3	1:A:357:ARG:CZ	2.43	0.48
1:B:52:SER:C	1:B:56:ARG:HD3	2.38	0.48
1:B:544:GLU:HG2	1:B:557:PHE:CD2	2.48	0.48
1:A:248:ILE:HG22	1:A:249:SER:N	2.28	0.48
1:A:286:SER:HB3	1:A:299:TYR:CD2	2.47	0.48
1:A:423:LEU:HD23	1:A:423:LEU:O	2.12	0.48
1:B:531:LYS:HG3	1:B:532:TYR:CD2	2.48	0.48
1:A:110:ARG:O	1:A:110:ARG:NH1	2.47	0.48
1:A:601:VAL:HG22	1:A:601:VAL:O	2.12	0.48
1:B:32:GLU:HG2	1:B:36:ARG:CZ	2.44	0.48
1:A:39:LYS:HB2	1:A:41:LEU:CG	2.44	0.48
1:A:472:SER:O	1:A:473:LEU:CB	2.61	0.48
1:B:62:GLN:O	1:B:64:TYR:N	2.47	0.48
1:B:242:GLY:HA2	1:B:326:ILE:HG21	1.95	0.48
1:B:83:PHE:CE1	1:B:212:ALA:HB3	2.43	0.48
1:B:261:ARG:NH1	1:B:306:GLN:HE21	2.02	0.48
1:B:623:ARG:O	1:B:627:TRP:HD1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:A:114:ASP:HB2	2.28	0.48
1:A:133:TRP:CD1	1:A:133:TRP:N	2.81	0.48
1:A:262:LEU:HD11	1:A:301:TYR:HB3	1.96	0.48
1:B:47:PHE:CB	1:B:77:MET:HB2	2.43	0.48
1:B:128:SER:O	1:B:144:GLY:N	2.47	0.48
1:B:294:HIS:CG	1:B:295:GLU:N	2.81	0.48
1:B:447:SER:HA	1:B:480:THR:O	2.14	0.48
1:A:190:THR:O	1:A:192:THR:HG23	2.14	0.48
1:B:167:ARG:O	1:B:167:ARG:HG2	2.14	0.48
1:B:41:LEU:HD23	1:B:218:VAL:O	2.14	0.48
1:B:625:ARG:HG2	1:B:626:TYR:CD1	2.48	0.48
1:A:397:ASP:C	1:A:399:TYR:N	2.72	0.48
1:A:190:THR:O	1:A:191:ASP:C	2.57	0.48
1:A:396:CYS:SG	1:A:441:PRO:HD2	2.53	0.48
1:B:158:GLN:O	1:B:159:VAL:C	2.57	0.48
1:B:197:LYS:HD3	1:B:197:LYS:C	2.38	0.48
1:B:398:ARG:HG3	1:B:398:ARG:HH11	1.78	0.48
1:B:576:LYS:HB3	1:B:581:VAL:HG23	1.96	0.48
1:A:430:MET:HE2	1:A:448:VAL:HG12	1.96	0.47
1:B:48:ARG:HH22	1:B:72:GLY:HA3	1.78	0.47
1:B:55:ARG:CG	2:D:1:NAG:H83	2.41	0.47
1:B:192:THR:HG22	1:B:192:THR:O	2.13	0.47
1:B:223:THR:HG21	1:B:227:TYR:CD2	2.47	0.47
1:B:312:SER:O	1:B:314:GLY:N	2.46	0.47
1:B:547:ALA:O	1:B:559:GLU:OE2	2.32	0.47
1:A:271:ALA:CB	1:A:280:LEU:HD22	2.44	0.47
1:A:337:LEU:HD23	1:A:342:PRO:HA	1.95	0.47
1:B:608:ILE:CD1	1:B:622:LEU:HD12	2.41	0.47
1:A:147:LEU:HB3	1:A:148:PRO:HD2	1.96	0.47
1:A:206:PHE:HB3	1:A:410:VAL:HB	1.96	0.47
1:A:322:LEU:O	1:A:324:VAL:HG23	2.14	0.47
1:A:333:LYS:C	1:A:535:PRO:HD3	2.39	0.47
1:B:127:HIS:HB3	1:B:173:ASN:O	2.15	0.47
1:B:137:VAL:HG13	1:B:138:ASP:N	2.25	0.47
1:A:241:SER:CB	1:A:283:PRO:HA	2.44	0.47
1:B:344:TYR:CD1	1:B:344:TYR:C	2.92	0.47
1:B:461:TYR:HA	1:B:464:LYS:HZ3	1.79	0.47
1:A:276:THR:O	1:A:277:GLN:HB2	2.13	0.47
1:B:64:TYR:CE2	1:B:133:TRP:CZ3	3.02	0.47
1:B:343:PHE:CZ	1:B:402:VAL:HG21	2.49	0.47
1:A:78:PRO:HD2	1:A:86:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HA	1:A:171:ALA:O	2.15	0.47
1:A:496:VAL:O	1:A:534:LYS:NZ	2.44	0.47
1:B:146:TYR:CB	1:B:216:ARG:NH2	2.72	0.47
1:B:307:LEU:HG	1:B:308:THR:N	2.29	0.47
1:A:32:GLU:O	1:A:32:GLU:HG2	2.13	0.47
1:A:350:LYS:HD2	1:A:589:PHE:CG	2.49	0.47
1:A:435:ARG:HB3	1:A:435:ARG:HH11	1.79	0.47
1:A:586:ILE:O	1:A:587:TRP:O	2.32	0.47
1:B:276:THR:O	1:B:277:GLN:CB	2.62	0.47
1:A:110:ARG:NH1	1:A:110:ARG:HB3	2.29	0.47
1:A:505:TYR:CE2	1:A:521:LEU:HD12	2.48	0.47
1:B:51:PHE:CE2	1:B:96:VAL:O	2.67	0.47
1:A:156:LEU:O	1:A:157:VAL:CG1	2.62	0.47
1:A:260:VAL:O	1:A:272:ASN:ND2	2.48	0.47
1:A:486:ASN:HB3	1:A:489:ALA:HB3	1.96	0.47
1:B:215:GLN:HG2	1:B:216:ARG:HG2	1.97	0.47
1:B:504:TYR:CE2	1:B:606:LYS:HE2	2.50	0.47
1:A:152:ASP:OD1	1:A:153:ILE:N	2.48	0.46
1:A:290:PRO:O	1:A:291:TYR:C	2.58	0.46
1:A:293:MET:HG3	1:A:341:LYS:HE3	1.97	0.46
1:A:365:LEU:HD11	1:A:613:ARG:HD3	1.96	0.46
1:A:614:GLN:OE1	1:B:551:GLN:HA	2.15	0.46
2:D:1:NAG:H5	2:D:1:NAG:N2	2.30	0.46
1:A:410:VAL:CG2	1:A:411:GLY:H	2.21	0.46
1:B:93:ARG:NH2	1:B:593:MET:HE3	2.25	0.46
1:B:118:ARG:HB3	1:B:153:ILE:O	2.15	0.46
1:B:327:ARG:NH2	1:B:477:ARG:NH2	2.62	0.46
1:B:349:ASN:ND2	1:B:585:LEU:HB3	2.30	0.46
1:A:35:SER:HB3	1:A:223:THR:HA	1.97	0.46
1:A:261:ARG:HA	1:A:272:ASN:HA	1.97	0.46
1:A:298:ALA:HB2	1:A:400:GLY:CA	2.44	0.46
1:A:382:ARG:O	1:A:384:SER:N	2.47	0.46
1:B:156:LEU:O	1:B:157:VAL:C	2.58	0.46
1:B:268:LYS:HA	1:B:268:LYS:HD3	1.74	0.46
1:B:66:ARG:CB	1:B:67:PRO:CD	2.94	0.46
1:B:77:MET:SD	1:B:86:ILE:CD1	2.96	0.46
1:B:187:GLN:NE2	1:B:189:LEU:HG	2.31	0.46
1:B:426:HIS:HB2	1:B:462:TYR:OH	2.15	0.46
1:B:592:PHE:CZ	1:B:604:ASN:HB3	2.51	0.46
1:B:39:LYS:HA	1:B:219:LEU:HB2	1.97	0.46
1:B:107:LEU:N	1:B:107:LEU:CD2	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PRO:HA	1:B:183:PRO:HB3	1.98	0.46
1:B:246:TYR:HB2	1:B:248:ILE:HD11	1.98	0.46
1:B:261:ARG:NH1	1:B:306:GLN:NE2	2.59	0.46
1:B:462:TYR:CD1	1:B:462:TYR:C	2.93	0.46
1:B:588:ASN:OD1	1:B:592:PHE:CD2	2.68	0.46
1:A:175:THR:HG22	1:A:210:ASN:CB	2.44	0.46
1:B:64:TYR:CD2	1:B:133:TRP:CD2	3.04	0.46
1:B:227:TYR:O	1:B:227:TYR:CD1	2.69	0.46
1:B:376:LEU:HD11	1:B:608:ILE:HD11	1.97	0.46
1:A:185:THR:HG22	1:A:203:ASN:HD22	1.81	0.46
1:B:263:LEU:HD23	1:B:267:ASN:CG	2.41	0.46
1:B:455:HIS:CE1	1:B:456:LEU:HD21	2.51	0.46
1:B:511:TYR:CD1	1:B:511:TYR:N	2.79	0.46
1:A:175:THR:C	1:A:176:LEU:HD22	2.41	0.46
1:A:186:ILE:HG22	1:A:187:GLN:H	1.80	0.46
1:B:240:ASP:HB3	1:B:284:GLY:O	2.16	0.46
1:B:264:ASP:HA	1:B:301:TYR:HD1	1.81	0.46
1:B:460:GLY:HA3	1:B:491:LYS:HB3	1.98	0.46
1:A:78:PRO:HG2	1:A:81:SER:OG	2.16	0.46
1:A:423:LEU:HD11	1:A:465:MET:HG3	1.97	0.46
1:B:30:PRO:HA	1:B:221:TYR:CZ	2.50	0.46
1:B:375:TRP:CZ2	1:B:623:ARG:CD	2.98	0.46
1:A:45:TRP:HE3	1:A:102:GLU:H	1.63	0.46
1:B:320:TYR:CE1	1:B:321:THR:O	2.69	0.46
1:B:555:LEU:O	1:B:558:THR:HB	2.16	0.46
1:A:107:LEU:N	1:A:107:LEU:HD22	2.31	0.45
1:A:118:ARG:N	1:A:223:THR:O	2.46	0.45
1:A:135:ASN:O	1:A:137:VAL:HG12	2.16	0.45
1:A:391:GLU:HG3	1:A:395:MET:HE1	1.97	0.45
1:B:311:THR:OG1	1:B:312:SER:N	2.49	0.45
1:B:453:ALA:O	1:B:456:LEU:HG	2.16	0.45
1:B:461:TYR:O	1:B:464:LYS:HB3	2.16	0.45
1:A:102:GLU:HA	1:A:168:ILE:O	2.16	0.45
1:A:124:GLY:N	1:A:217:SER:O	2.48	0.45
1:A:303:LEU:HB2	1:A:324:VAL:HG21	1.98	0.45
1:A:555:LEU:HD13	1:A:556:MET:CE	2.45	0.45
1:B:448:VAL:HG21	1:B:467:ILE:CD1	2.47	0.45
1:A:332:THR:HB	1:A:333:LYS:HZ3	1.81	0.45
1:B:185:THR:HB	1:B:203:ASN:HB2	1.98	0.45
1:B:322:LEU:HA	1:B:323:PRO:HD3	1.84	0.45
1:B:363:TRP:N	1:B:364:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:MAN:O2	2:C:6:MAN:C6	2.64	0.45
1:B:576:LYS:HD3	1:B:576:LYS:HA	1.70	0.45
1:B:586:ILE:O	1:B:587:TRP:C	2.59	0.45
1:A:40:GLU:C	1:A:42:ASP:N	2.73	0.45
1:A:93:ARG:NH1	1:A:209:PHE:CE2	2.84	0.45
1:A:156:LEU:O	1:A:156:LEU:CG	2.63	0.45
1:B:118:ARG:HB2	1:B:223:THR:HG23	1.98	0.45
1:B:140:LEU:CB	1:B:151:ALA:HB2	2.43	0.45
1:B:287:LEU:N	1:B:287:LEU:HD12	2.32	0.45
1:B:375:TRP:CZ2	1:B:623:ARG:HD3	2.52	0.45
1:B:461:TYR:HD1	1:B:464:LYS:NZ	2.14	0.45
1:A:335:GLN:HE21	1:A:335:GLN:N	2.14	0.45
1:B:155:ASN:O	1:B:156:LEU:C	2.59	0.45
1:B:183:PRO:HG2	1:B:412:LEU:HD23	1.98	0.45
1:B:343:PHE:CG	1:B:344:TYR:N	2.84	0.45
1:A:54:ASN:HD22	1:A:55:ARG:HH11	1.65	0.45
1:A:333:LYS:HD3	1:A:333:LYS:N	2.32	0.45
1:B:102:GLU:OE2	1:B:167:ARG:HD2	2.17	0.45
1:B:140:LEU:HD11	1:B:149:PHE:HB2	1.97	0.45
1:B:527:ASN:O	1:B:528:TRP:C	2.58	0.45
1:B:573:LEU:O	1:B:577:ARG:HG3	2.17	0.45
1:A:438:LYS:HE3	1:A:438:LYS:HB2	1.68	0.45
1:A:516:LEU:O	1:A:517:ILE:C	2.60	0.45
1:B:122:ARG:HA	1:B:150:GLU:HA	1.97	0.45
1:A:121:LEU:HD13	1:A:220:LEU:HD23	1.98	0.45
1:A:350:LYS:NZ	1:A:350:LYS:HB3	2.32	0.45
1:B:77:MET:HA	1:B:78:PRO:HD2	1.89	0.45
1:B:233:VAL:N	1:B:439:ASN:HD21	2.15	0.45
1:B:551:GLN:HG2	1:B:555:LEU:CB	2.47	0.45
1:A:62:GLN:CD	1:A:65:ARG:NH1	2.75	0.45
1:A:241:SER:HA	1:A:285:VAL:CG2	2.44	0.45
1:A:372:LEU:HD22	1:A:609:PHE:CZ	2.52	0.45
1:A:426:HIS:CE1	1:A:466:VAL:HG11	2.52	0.45
1:A:524:GLN:O	1:A:528:TRP:CD1	2.70	0.45
1:A:526:GLU:O	1:A:530:LYS:HB3	2.16	0.45
1:B:118:ARG:HH11	1:B:223:THR:CG2	2.31	0.45
1:B:288:TRP:CH2	1:B:442:ALA:HA	2.52	0.45
1:B:375:TRP:HZ3	1:B:609:PHE:CZ	2.35	0.45
1:B:410:VAL:HG23	1:B:450:ASN:HB3	1.99	0.45
1:A:172:ILE:HG22	1:A:173:ASN:N	2.32	0.44
1:A:257:LYS:HZ1	1:A:274:THR:HG22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:TYR:CZ	1:B:374:ARG:CG	3.00	0.44
1:B:291:TYR:N	1:B:400:GLY:O	2.50	0.44
1:B:391:GLU:C	1:B:395:MET:SD	3.00	0.44
1:B:461:TYR:CD1	1:B:464:LYS:NZ	2.81	0.44
1:B:501:LEU:HD12	1:B:536:ILE:HG21	1.99	0.44
1:B:525:PHE:HE2	1:B:573:LEU:HD23	1.82	0.44
1:B:577:ARG:O	1:B:578:ARG:HB3	2.17	0.44
1:A:120:VAL:CG1	1:A:150:GLU:HB2	2.47	0.44
1:A:361:PHE:HZ	1:A:366:LEU:HD12	1.76	0.44
1:B:196:PRO:HG2	1:B:199:TYR:HB2	2.00	0.44
1:B:240:ASP:CG	1:B:283:PRO:HA	2.42	0.44
1:A:289:TRP:CG	1:A:294:HIS:HB2	2.52	0.44
1:A:546:ILE:HD11	1:A:549:PHE:CE1	2.53	0.44
1:B:132:VAL:HG21	1:B:140:LEU:HD23	1.99	0.44
1:B:307:LEU:O	1:B:317:SER:HA	2.17	0.44
1:A:140:LEU:HD22	1:A:151:ALA:HB2	1.99	0.44
1:A:427:MET:HE3	1:A:465:MET:HB3	2.00	0.44
1:B:281:LYS:CG	1:B:282:VAL:N	2.81	0.44
1:B:354:ALA:HB3	1:B:357:ARG:HG3	2.00	0.44
1:A:112:THR:C	1:A:113:GLN:HG3	2.41	0.44
1:A:127:HIS:O	1:A:144:GLY:HA2	2.17	0.44
1:A:305:VAL:O	1:A:319:PHE:HA	2.17	0.44
1:B:33:SER:O	1:B:35:SER:N	2.51	0.44
1:B:90:TRP:CD1	1:B:90:TRP:H	2.35	0.44
1:A:507:TRP:CZ2	1:A:544:GLU:HB3	2.53	0.44
1:B:167:ARG:O	1:B:167:ARG:CG	2.66	0.44
1:B:576:LYS:HB3	1:B:581:VAL:CG2	2.48	0.44
1:A:39:LYS:HB2	1:A:41:LEU:HG	1.99	0.44
1:A:571:LEU:HD22	1:A:571:LEU:HA	1.80	0.44
1:A:575:GLN:HB3	1:A:576:LYS:HD3	1.99	0.44
1:B:241:SER:HB2	1:B:285:VAL:CA	2.48	0.44
1:B:333:LYS:HD2	1:B:333:LYS:HA	1.84	0.44
1:B:354:ALA:HB3	1:B:357:ARG:CG	2.48	0.44
1:A:192:THR:O	1:A:193:SER:CB	2.63	0.44
1:A:385:HIS:ND1	1:A:385:HIS:N	2.66	0.44
1:B:51:PHE:HE2	1:B:96:VAL:O	2.01	0.44
1:B:159:VAL:HG13	1:B:160:GLY:H	1.83	0.44
1:A:266:GLU:N	1:A:266:GLU:CD	2.75	0.44
1:A:327:ARG:HB2	1:A:339:ASN:OD1	2.18	0.44
1:A:524:GLN:HG3	1:A:525:PHE:N	2.33	0.44
1:B:241:SER:O	1:B:326:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:TYR:O	1:B:300:LEU:HD23	2.17	0.44
1:B:448:VAL:HG21	1:B:467:ILE:HD13	2.00	0.44
1:A:82:SER:HA	1:A:212:ALA:O	2.18	0.43
1:A:335:GLN:HE21	1:A:335:GLN:H	1.65	0.43
1:A:485:SER:O	1:A:528:TRP:HZ2	2.01	0.43
1:A:488:ALA:N	1:A:531:LYS:HE3	2.33	0.43
1:A:541:TYR:OH	1:A:570:HIS:CE1	2.71	0.43
1:A:555:LEU:O	1:A:561:TYR:CD1	2.71	0.43
1:B:181:LEU:HD11	1:B:426:HIS:ND1	2.33	0.43
1:A:137:VAL:CG2	1:A:138:ASP:H	2.27	0.43
1:A:535:PRO:HB3	1:A:582:VAL:CG2	2.47	0.43
1:B:153:ILE:O	1:B:154:SER:CB	2.66	0.43
1:A:33:SER:HB2	1:A:34:PRO:CD	2.48	0.43
1:A:33:SER:O	1:A:35:SER:N	2.51	0.43
1:A:45:TRP:CE3	1:A:101:TYR:HB3	2.53	0.43
1:A:153:ILE:HG13	1:A:154:SER:H	1.83	0.43
1:A:175:THR:HA	1:A:210:ASN:OD1	2.17	0.43
1:A:279:GLN:O	1:A:280:LEU:HG	2.18	0.43
1:A:392:VAL:HA	1:A:395:MET:HE2	2.00	0.43
1:B:172:ILE:HD13	1:B:172:ILE:N	2.33	0.43
1:B:506:SER:HB3	1:B:561:TYR:OH	2.19	0.43
1:A:107:LEU:HD22	1:A:107:LEU:H	1.83	0.43
1:B:162:LEU:CB	1:B:163:PRO:CD	2.91	0.43
1:B:405:ASP:OD2	1:B:443:VAL:HG11	2.18	0.43
1:A:397:ASP:HB3	1:A:399:TYR:HD1	1.83	0.43
1:A:505:TYR:O	1:A:506:SER:CB	2.66	0.43
1:B:107:LEU:CD1	1:B:220:LEU:HD13	2.48	0.43
1:B:216:ARG:NH2	1:B:387:PRO:O	2.52	0.43
1:B:288:TRP:CE3	1:B:288:TRP:O	2.72	0.43
1:A:259:GLU:CG	1:A:272:ASN:HD21	2.31	0.43
1:A:281:LYS:O	1:A:281:LYS:HD3	2.19	0.43
1:A:544:GLU:N	1:A:606:LYS:HD3	2.33	0.43
1:B:258:LEU:HB2	1:B:307:LEU:HA	1.99	0.43
1:A:346:HIS:O	1:A:378:ALA:HA	2.18	0.43
1:B:119:VAL:O	1:B:119:VAL:HG12	2.18	0.43
1:B:225:THR:O	1:B:227:TYR:N	2.52	0.43
1:B:235:THR:OG1	1:B:326:ILE:HG23	2.18	0.43
1:B:258:LEU:CD2	1:B:307:LEU:HD12	2.49	0.43
1:B:556:MET:HB3	1:B:557:PHE:HD1	1.83	0.43
1:A:41:LEU:N	1:A:218:VAL:O	2.51	0.43
1:A:395:MET:SD	1:A:395:MET:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ILE:HA	1:A:632:GLU:OE1	2.19	0.43
1:B:135:ASN:ND2	1:B:136:GLY:N	2.63	0.43
1:B:504:TYR:O	1:B:507:TRP:O	2.37	0.43
1:B:543:ALA:CB	1:B:565:LEU:HD13	2.35	0.43
1:B:327:ARG:HA	1:B:339:ASN:OD1	2.19	0.43
1:B:432:GLU:O	1:B:436:ARG:HB2	2.19	0.43
1:B:552:ASP:CB	1:B:553:PRO:CD	2.96	0.43
1:B:586:ILE:O	1:B:587:TRP:O	2.36	0.43
1:A:131:ILE:HG12	1:A:141:GLU:HG2	2.01	0.43
1:A:244:VAL:HG21	1:A:324:VAL:HG11	2.01	0.43
1:B:120:VAL:CG1	1:B:221:TYR:HB3	2.49	0.43
1:B:134:VAL:HG13	1:B:135:ASN:H	1.82	0.43
1:B:140:LEU:HB2	1:B:151:ALA:CB	2.44	0.43
1:B:254:ASN:O	1:B:255:LEU:HB3	2.19	0.43
1:A:75:VAL:CG1	1:A:76:ASP:N	2.81	0.42
1:A:395:MET:HB3	1:A:442:ALA:HB1	2.00	0.42
1:B:256:PHE:HA	1:B:309:ALA:HA	2.01	0.42
1:B:393:MET:O	1:B:397:ASP:HB2	2.19	0.42
1:A:162:LEU:CB	1:A:163:PRO:HD3	2.31	0.42
1:A:507:TRP:C	1:A:509:HIS:H	2.27	0.42
1:B:110:ARG:C	1:B:112:THR:N	2.76	0.42
1:B:182:PRO:HA	1:B:183:PRO:HD3	1.79	0.42
1:B:563:LYS:HG3	1:B:621:LEU:HD13	2.01	0.42
1:A:57:ARG:O	1:A:58:GLY:C	2.63	0.42
1:A:175:THR:O	1:A:176:LEU:HD22	2.19	0.42
1:A:250:VAL:HG21	1:A:307:LEU:HD13	2.01	0.42
1:A:625:ARG:HG3	1:A:626:TYR:N	2.34	0.42
1:B:34:PRO:O	1:B:35:SER:CB	2.67	0.42
1:B:225:THR:O	1:B:226:THR:C	2.62	0.42
1:A:28:LEU:HD11	1:A:231:ILE:HG13	2.00	0.42
1:A:143:GLU:OE2	1:A:180:THR:HG22	2.19	0.42
1:A:248:ILE:CG2	1:A:249:SER:N	2.81	0.42
1:A:359:LYS:HG2	1:A:359:LYS:HZ3	1.57	0.42
1:A:381:PHE:CE1	1:A:388:TYR:HE2	2.22	0.42
1:A:545:THR:HG21	1:A:559:GLU:HA	2.00	0.42
1:B:445:MET:HE1	1:B:498:VAL:HG21	1.98	0.42
1:A:65:ARG:O	1:A:66:ARG:HG3	2.20	0.42
1:A:290:PRO:C	1:A:292:LEU:H	2.27	0.42
1:B:238:GLU:HB3	1:B:239:GLN:H	1.66	0.42
1:B:257:LYS:O	1:B:258:LEU:HB3	2.20	0.42
1:B:347:GLY:HA3	1:B:380:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:LYS:HG3	1:B:621:LEU:CD1	2.48	0.42
1:B:594:THR:HG23	1:B:604:ASN:N	2.33	0.42
1:B:118:ARG:HA	1:B:154:SER:CB	2.49	0.42
1:A:110:ARG:HD2	1:A:110:ARG:HA	1.91	0.42
1:A:119:VAL:O	1:A:119:VAL:HG22	2.19	0.42
1:A:247:GLN:HE22	1:A:277:GLN:NE2	2.18	0.42
1:A:253:SER:OG	1:A:254:ASN:N	2.52	0.42
1:A:563:LYS:HD2	1:A:617:SER:HB2	2.01	0.42
1:A:618:ALA:O	1:A:621:LEU:HB3	2.20	0.42
1:B:99:VAL:O	1:B:172:ILE:HD13	2.20	0.42
1:B:460:GLY:HA3	1:B:491:LYS:CB	2.49	0.42
1:B:546:ILE:HD11	1:B:601:VAL:HG11	2.02	0.42
1:B:214:LEU:HD12	1:B:215:GLN:N	2.35	0.42
1:B:402:VAL:O	1:B:402:VAL:CG2	2.64	0.42
1:B:503:SER:HB3	1:B:524:GLN:NE2	2.35	0.42
1:A:146:TYR:HB2	1:A:387:PRO:HG2	2.02	0.42
1:A:395:MET:HB3	1:A:442:ALA:CB	2.50	0.42
1:B:37:GLU:HB3	1:B:221:TYR:HD1	1.82	0.42
1:B:381:PHE:CE2	1:B:395:MET:HE3	2.55	0.42
1:A:382:ARG:HD3	1:A:406:GLU:CD	2.44	0.42
1:A:539:SER:O	1:A:540:GLU:HB2	2.20	0.42
1:A:563:LYS:HD2	1:A:617:SER:CB	2.50	0.42
1:A:606:LYS:HE3	1:A:606:LYS:HB2	1.86	0.42
1:B:67:PRO:HG2	1:B:70:GLU:HB2	2.00	0.42
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.87	0.42
1:B:398:ARG:HG3	1:B:398:ARG:NH1	2.34	0.42
1:B:544:GLU:CG	1:B:605:LYS:HB2	2.44	0.42
1:A:97:GLY:O	1:A:173:ASN:HA	2.19	0.41
1:A:133:TRP:CD1	1:A:169:THR:HB	2.55	0.41
1:A:177:THR:CG2	1:A:180:THR:HG23	2.43	0.41
1:A:407:CYS:SG	1:A:448:VAL:HA	2.59	0.41
1:A:414:LEU:HD22	1:A:417:PHE:CZ	2.55	0.41
1:B:248:ILE:HG22	1:B:249:SER:N	2.34	0.41
1:B:350:LYS:HB3	1:B:351:HIS:H	1.72	0.41
1:B:566:LEU:HD23	1:B:621:LEU:CD2	2.50	0.41
1:A:54:ASN:HD22	1:A:55:ARG:HD2	1.84	0.41
1:A:84:ASN:OD1	1:A:211:TYR:HA	2.20	0.41
1:B:118:ARG:HB3	1:B:118:ARG:CZ	2.50	0.41
1:A:105:VAL:O	1:A:165:ARG:HA	2.20	0.41
1:A:155:ASN:C	1:A:155:ASN:HD22	2.28	0.41
1:A:353:ASP:OD1	1:A:611:ARG:NE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TYR:O	1:A:436:ARG:NH2	2.49	0.41
1:A:455:HIS:O	1:A:491:LYS:HG3	2.20	0.41
1:B:182:PRO:HG3	1:B:410:VAL:HG12	2.00	0.41
1:B:189:LEU:HA	1:B:189:LEU:HD23	1.81	0.41
1:B:261:ARG:HB2	1:B:269:VAL:CG1	2.36	0.41
1:B:362:ASP:HB2	1:B:364:PRO:HD2	2.02	0.41
1:A:32:GLU:HB2	1:A:36:ARG:HA	2.03	0.41
1:A:39:LYS:O	1:A:39:LYS:HG2	2.20	0.41
1:A:107:LEU:HD21	1:A:166:LEU:N	2.35	0.41
1:A:146:TYR:CB	1:A:387:PRO:HG2	2.50	0.41
1:A:149:PHE:CD1	1:A:149:PHE:N	2.88	0.41
1:A:189:LEU:HD12	1:A:199:TYR:CD1	2.55	0.41
1:A:276:THR:O	1:A:276:THR:CG2	2.67	0.41
1:A:383:THR:CG2	1:A:386:TYR:O	2.68	0.41
1:A:505:TYR:HE2	1:A:521:LEU:HD12	1.83	0.41
1:B:235:THR:HG21	1:B:325:GLY:O	2.20	0.41
1:B:298:ALA:HB1	1:B:396:CYS:O	2.21	0.41
1:B:348:VAL:HG22	1:B:349:ASN:O	2.21	0.41
1:B:505:TYR:C	1:B:507:TRP:H	2.28	0.41
1:B:549:PHE:N	1:B:549:PHE:HD1	2.19	0.41
1:A:245:ASN:N	1:A:245:ASN:HD22	2.17	0.41
1:A:507:TRP:O	1:A:508:TYR:CB	2.53	0.41
1:A:513:HIS:HB3	1:A:516:LEU:HD22	2.03	0.41
1:A:54:ASN:C	1:A:56:ARG:H	2.28	0.41
1:A:140:LEU:HG	1:A:149:PHE:HD2	1.85	0.41
1:A:327:ARG:O	1:A:327:ARG:NH1	2.49	0.41
1:B:258:LEU:HD22	1:B:307:LEU:HD12	2.01	0.41
1:B:367:VAL:HG12	1:B:371:ASN:ND2	2.35	0.41
1:B:427:MET:HE2	1:B:469:HIS:HB2	2.01	0.41
1:A:481:PHE:CD1	1:A:496:VAL:CG1	3.04	0.41
1:B:62:GLN:O	1:B:63:TRP:C	2.64	0.41
1:B:109:GLU:O	1:B:112:THR:N	2.49	0.41
1:B:121:LEU:CD2	1:B:168:ILE:HD12	2.50	0.41
1:B:375:TRP:CZ3	1:B:609:PHE:CZ	3.08	0.41
1:A:614:GLN:OE1	1:A:614:GLN:HA	2.21	0.41
1:B:47:PHE:CG	1:B:77:MET:HG3	2.56	0.41
1:B:51:PHE:CZ	1:B:200:PHE:CZ	3.07	0.41
1:B:56:ARG:O	1:B:57:ARG:O	2.39	0.41
1:B:241:SER:OG	1:B:286:SER:N	2.54	0.41
1:B:431:GLU:O	1:B:435:ARG:HB2	2.20	0.41
1:A:50:ASP:CG	1:A:56:ARG:HB2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG13	1:A:76:ASP:N	2.36	0.41
1:A:118:ARG:HA	1:A:153:ILE:O	2.21	0.41
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.27	0.41
1:A:195:TYR:HA	1:A:196:PRO:HD3	1.88	0.41
1:A:197:LYS:HG3	2:C:6:MAN:H62	2.02	0.41
1:A:335:GLN:O	1:A:335:GLN:HG2	2.20	0.41
1:A:505:TYR:O	1:A:506:SER:HB2	2.21	0.41
1:A:535:PRO:HB3	1:A:582:VAL:HG21	2.02	0.41
1:B:39:LYS:HA	1:B:219:LEU:HB3	2.01	0.41
1:B:80:PRO:HB3	1:B:215:GLN:HA	2.03	0.41
1:B:121:LEU:HD21	1:B:168:ILE:HD12	2.01	0.41
1:B:161:PRO:HB2	1:B:164:SER:HA	2.02	0.41
1:B:189:LEU:HB3	1:B:195:TYR:CD2	2.55	0.41
1:B:251:LYS:HB2	1:B:251:LYS:HZ2	1.82	0.41
1:B:346:HIS:CE1	1:B:377:GLY:O	2.74	0.41
1:B:564:SER:O	1:B:568:GLN:HG2	2.21	0.41
1:A:390:GLU:C	1:A:392:VAL:N	2.78	0.41
1:A:397:ASP:O	1:A:398:ARG:C	2.63	0.41
1:B:59:PHE:CZ	1:B:131:ILE:HD12	2.56	0.41
1:B:386:TYR:CE1	1:B:388:TYR:HE1	2.38	0.41
1:B:549:PHE:N	1:B:549:PHE:CD1	2.88	0.41
1:A:80:PRO:HB2	1:A:361:PHE:H	1.85	0.40
1:A:264:ASP:HA	1:A:301:TYR:CD1	2.56	0.40
1:A:270:VAL:O	1:A:270:VAL:HG22	2.21	0.40
1:A:383:THR:HB	1:A:406:GLU:H	1.86	0.40
1:B:29:TYR:O	1:B:30:PRO:C	2.63	0.40
1:B:125:SER:CB	1:B:216:ARG:HG3	2.51	0.40
1:B:189:LEU:HD12	1:B:199:TYR:HE2	1.83	0.40
1:A:67:PRO:O	1:A:68:LEU:C	2.63	0.40
1:A:241:SER:OG	1:A:283:PRO:HA	2.21	0.40
1:A:244:VAL:HG23	1:A:326:ILE:HD11	2.03	0.40
1:B:126:ALA:HB1	1:B:172:ILE:HG21	2.03	0.40
1:B:185:THR:HG23	2:D:8:MAN:H61	2.03	0.40
1:B:261:ARG:NH2	1:B:306:GLN:NE2	2.67	0.40
1:B:305:VAL:O	1:B:319:PHE:HA	2.21	0.40
1:A:62:GLN:NE2	1:A:65:ARG:NH1	2.69	0.40
1:A:263:LEU:HD22	1:A:267:ASN:ND2	2.36	0.40
1:A:487:TYR:C	1:A:489:ALA:H	2.28	0.40
1:B:47:PHE:HB3	1:B:77:MET:HB2	2.03	0.40
1:B:80:PRO:HA	1:B:215:GLN:HA	2.04	0.40
1:A:33:SER:CB	1:A:34:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:HG3	1:A:381:PHE:CD1	2.57	0.40
1:A:463:LEU:HD12	1:A:463:LEU:HA	1.91	0.40
1:B:41:LEU:HD22	1:B:218:VAL:N	2.37	0.40
1:B:53:ASP:HB3	1:B:54:ASN:H	1.48	0.40
1:B:256:PHE:CD1	1:B:257:LYS:N	2.90	0.40
1:A:353:ASP:O	1:A:354:ALA:HB2	2.21	0.40
1:B:332:THR:HB	1:B:333:LYS:H	1.76	0.40
1:B:493:ALA:HB3	1:B:532:TYR:CZ	2.55	0.40
1:B:495:TYR:CD1	1:B:495:TYR:N	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	609/613 (99%)	462 (76%)	99 (16%)	48 (8%)	1	0
1	B	609/613 (99%)	442 (73%)	103 (17%)	64 (10%)	0	0
All	All	1218/1226 (99%)	904 (74%)	202 (17%)	112 (9%)	0	0

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	35	SER
1	A	52	SER
1	A	115	LEU
1	A	137	VAL
1	A	152	ASP
1	A	161	PRO
1	A	162	LEU
1	A	285	VAL

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Mol	Chain	Res	Type
1	A	286	SER
1	A	297	PRO
1	A	298	ALA
1	A	390	GLU
1	A	391	GLU
1	A	398	ARG
1	A	554	PRO
1	A	556	MET
1	A	587	TRP
1	B	34	PRO
1	B	35	SER
1	B	53	ASP
1	B	54	ASN
1	B	57	ARG
1	B	63	TRP
1	B	66	ARG
1	B	113	GLN
1	B	134	VAL
1	B	135	ASN
1	B	137	VAL
1	B	144	GLY
1	B	152	ASP
1	B	154	SER
1	B	159	VAL
1	B	162	LEU
1	B	267	ASN
1	B	274	THR
1	B	277	GLN
1	B	286	SER
1	B	287	LEU
1	B	291	TYR
1	B	292	LEU
1	B	295	GLU
1	B	298	ALA
1	B	311	THR
1	B	398	ARG
1	B	408	PRO
1	B	443	VAL
1	B	552	ASP
1	B	553	PRO
1	B	554	PRO
1	B	556	MET

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Mol	Chain	Res	Type
1	B	587	TRP
1	A	53	ASP
1	A	67	PRO
1	A	135	ASN
1	A	164	SER
1	A	174	ASN
1	A	191	ASP
1	A	232	THR
1	A	239	GLN
1	A	265	ALA
1	A	277	GLN
1	A	291	TYR
1	A	384	SER
1	B	114	ASP
1	B	116	ARG
1	B	156	LEU
1	B	157	VAL
1	B	226	THR
1	B	243	LEU
1	B	297	PRO
1	B	360	GLY
1	A	24	GLN
1	A	73	PRO
1	A	155	ASN
1	A	193	SER
1	A	254	ASN
1	A	321	THR
1	A	506	SER
1	B	164	SER
1	B	190	THR
1	B	264	ASP
1	B	272	ASN
1	B	384	SER
1	B	388	TYR
1	B	518	GLN
1	A	41	LEU
1	A	154	SER
1	A	195	TYR
1	A	197	LYS
1	A	264	ASP
1	A	555	LEU
1	B	52	SER

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Mol	Chain	Res	Type
1	B	216	ARG
1	B	527	ASN
1	A	517	ILE
1	B	230	ASP
1	B	251	LYS
1	B	258	LEU
1	B	58	GLY
1	B	64	TYR
1	B	225	THR
1	A	408	PRO
1	B	160	GLY
1	B	270	VAL
1	A	66	ARG
1	B	43	GLY
1	B	331	VAL
1	A	30	PRO
1	A	231	ILE
1	B	283	PRO
1	B	517	ILE

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	540/542 (100%)	440 (82%)	100 (18%)	1	3
1	B	540/542 (100%)	436 (81%)	104 (19%)	1	2
All	All	1080/1084 (100%)	876 (81%)	204 (19%)	1	2

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	32	GLU
1	A	39	LYS
1	A	51	PHE

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Mol	Chain	Res	Type
1	A	53	ASP
1	A	55	ARG
1	A	65	ARG
1	A	67	PRO
1	A	74	THR
1	A	75	VAL
1	A	86	ILE
1	A	96	VAL
1	A	99	VAL
1	A	107	LEU
1	A	111	TRP
1	A	112	THR
1	A	119	VAL
1	A	133	TRP
1	A	162	LEU
1	A	165	ARG
1	A	173	ASN
1	A	174	ASN
1	A	175	THR
1	A	176	LEU
1	A	177	THR
1	A	179	THR
1	A	185	THR
1	A	190	THR
1	A	201	VAL
1	A	231	ILE
1	A	232	THR
1	A	234	THR
1	A	243	LEU
1	A	245	ASN
1	A	255	LEU
1	A	257	LYS
1	A	263	LEU
1	A	266	GLU
1	A	272	ASN
1	A	277	GLN
1	A	285	VAL
1	A	286	SER
1	A	293	MET
1	A	307	LEU
1	A	310	GLN
1	A	317	SER

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	331	VAL
1	A	333	LYS
1	A	335	GLN
1	A	345	PHE
1	A	350	LYS
1	A	351	HIS
1	A	357	ARG
1	A	363	TRP
1	A	365	LEU
1	A	374	ARG
1	A	384	SER
1	A	385	HIS
1	A	390	GLU
1	A	392	VAL
1	A	395	MET
1	A	397	ASP
1	A	402	VAL
1	A	412	LEU
1	A	414	LEU
1	A	428	GLN
1	A	435	ARG
1	A	437	ASP
1	A	439	ASN
1	A	457	GLU
1	A	463	LEU
1	A	464	LYS
1	A	477	ARG
1	A	491	LYS
1	A	499	ILE
1	A	501	LEU
1	A	503	SER
1	A	514	LEU
1	A	516	LEU
1	A	523	THR
1	A	526	GLU
1	A	530	LYS
1	A	531	LYS
1	A	535	PRO
1	A	546	ILE
1	A	554	PRO
1	A	555	LEU

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Mol	Chain	Res	Type
1	A	557	PHE
1	A	558	THR
1	A	560	GLU
1	A	571	LEU
1	A	578	ARG
1	A	586	ILE
1	A	588	ASN
1	A	599	THR
1	A	601	VAL
1	A	606	LYS
1	A	610	THR
1	A	622	LEU
1	B	23	LEU
1	B	28	LEU
1	B	30	PRO
1	B	34	PRO
1	B	36	ARG
1	B	39	LYS
1	B	44	LEU
1	B	50	ASP
1	B	52	SER
1	B	55	ARG
1	B	61	GLU
1	B	65	ARG
1	B	74	THR
1	B	82	SER
1	B	87	SER
1	B	92	LEU
1	B	99	VAL
1	B	103	ARG
1	B	105	VAL
1	B	106	ILE
1	B	107	LEU
1	B	111	TRP
1	B	113	GLN
1	B	120	VAL
1	B	127	HIS
1	B	149	PHE
1	B	155	ASN
1	B	158	GLN
1	B	161	PRO
1	B	169	THR

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Mol	Chain	Res	Type
1	B	172	ILE
1	B	181	LEU
1	B	187	GLN
1	B	193	SER
1	B	197	LYS
1	B	215	GLN
1	B	216	ARG
1	B	219	LEU
1	B	222	THR
1	B	223	THR
1	B	227	TYR
1	B	230	ASP
1	B	235	THR
1	B	236	SER
1	B	240	ASP
1	B	251	LYS
1	B	257	LYS
1	B	259	GLU
1	B	263	LEU
1	B	267	ASN
1	B	280	LEU
1	B	292	LEU
1	B	294	HIS
1	B	302	SER
1	B	308	THR
1	B	312	SER
1	B	318	ASP
1	B	321	THR
1	B	324	VAL
1	B	327	ARG
1	B	329	VAL
1	B	332	THR
1	B	335	GLN
1	B	351	HIS
1	B	352	GLU
1	B	366	LEU
1	B	373	LEU
1	B	379	ASN
1	B	381	PHE
1	B	385	HIS
1	B	391	GLU
1	B	392	VAL

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Mol	Chain	Res	Type
1	B	414	LEU
1	B	423	LEU
1	B	427	MET
1	B	435	ARG
1	B	436	ARG
1	B	462	TYR
1	B	464	LYS
1	B	486	ASN
1	B	487	TYR
1	B	498	VAL
1	B	503	SER
1	B	509	HIS
1	B	516	LEU
1	B	519	LEU
1	B	524	GLN
1	B	530	LYS
1	B	531	LYS
1	B	553	PRO
1	B	554	PRO
1	B	555	LEU
1	B	557	PHE
1	B	558	THR
1	B	564	SER
1	B	571	LEU
1	B	574	ASP
1	B	579	LYS
1	B	588	ASN
1	B	602	LEU
1	B	617	SER
1	B	621	LEU
1	B	622	LEU
1	B	625	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	142	HIS
1	A	155	ASN
1	A	174	ASN
1	A	202	GLN
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	267	ASN
1	A	272	ASN
1	A	277	GLN
1	A	335	GLN
1	A	416	GLN
1	A	420	ASN
1	A	425	HIS
1	A	439	ASN
1	A	455	HIS
1	A	469	HIS
1	A	518	GLN
1	A	538	GLN
1	A	551	GLN
1	A	568	GLN
1	A	570	HIS
1	A	631	ASN
1	B	158	GLN
1	B	187	GLN
1	B	202	GLN
1	B	203	ASN
1	B	215	GLN
1	B	239	GLN
1	B	279	GLN
1	B	306	GLN
1	B	335	GLN
1	B	351	HIS
1	B	371	ASN
1	B	379	ASN
1	B	385	HIS
1	B	394	GLN
1	B	424	HIS
1	B	439	ASN
1	B	440	HIS
1	B	486	ASN
1	B	524	GLN
1	B	570	HIS
1	B	612	GLN

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 ⓘ

18 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.87	1 (7%)	17,19,21	1.00	2 (11%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	0.67	0
2	BMA	C	3	2	11,11,12	0.38	0	15,15,17	0.94	1 (6%)
2	MAN	C	4	2	11,11,12	0.86	0	15,15,17	0.68	0
2	MAN	C	5	2	11,11,12	0.79	0	15,15,17	0.79	1 (6%)
2	MAN	C	6	2	11,11,12	0.50	0	15,15,17	0.93	1 (6%)
2	MAN	C	7	2	11,11,12	0.67	0	15,15,17	0.84	0
2	MAN	C	8	2	11,11,12	0.59	0	15,15,17	0.60	0
2	MAN	C	9	2	11,11,12	0.62	0	15,15,17	1.47	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.58	0	17,19,21	0.76	0
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	MAN	D	4	2	11,11,12	0.56	0	15,15,17	1.23	1 (6%)
2	MAN	D	5	2	11,11,12	0.65	0	15,15,17	0.85	1 (6%)
2	MAN	D	6	2	11,11,12	0.61	0	15,15,17	0.68	1 (6%)
2	MAN	D	7	2	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
2	MAN	D	8	2	11,11,12	0.36	0	15,15,17	0.78	1 (6%)
2	MAN	D	9	2	11,11,12	0.51	0	15,15,17	0.94	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '–' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	1/2/19/22	1/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
2	MAN	C	8	2	-	1/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	1/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
2	MAN	D	8	2	-	0/2/19/22	0/1/1/1
2	MAN	D	9	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.58	1.55	1.52
2	D	1	NAG	C1-C2	2.34	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	MAN	C1-C2-C3	4.55	116.27	109.64
2	C	6	MAN	C1-O5-C5	2.97	116.17	112.19
2	D	7	MAN	C1-O5-C5	2.90	116.07	112.19
2	D	4	MAN	C1-O5-C5	2.83	115.98	112.19
2	D	5	MAN	C1-O5-C5	2.54	115.59	112.19
2	C	3	BMA	C1-C2-C3	-2.34	106.24	109.64
2	D	8	MAN	C1-O5-C5	2.32	115.29	112.19
2	C	1	NAG	C2-N2-C7	-2.29	119.83	122.90
2	C	1	NAG	C1-O5-C5	2.27	115.23	112.19
2	D	6	MAN	C1-O5-C5	2.26	115.21	112.19
2	C	9	MAN	C2-C3-C4	2.21	114.75	110.86
2	D	9	MAN	C1-O5-C5	2.19	115.13	112.19
2	C	5	MAN	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	9	MAN	O5-C5-C6-O6
2	C	8	MAN	C4-C5-C6-O6

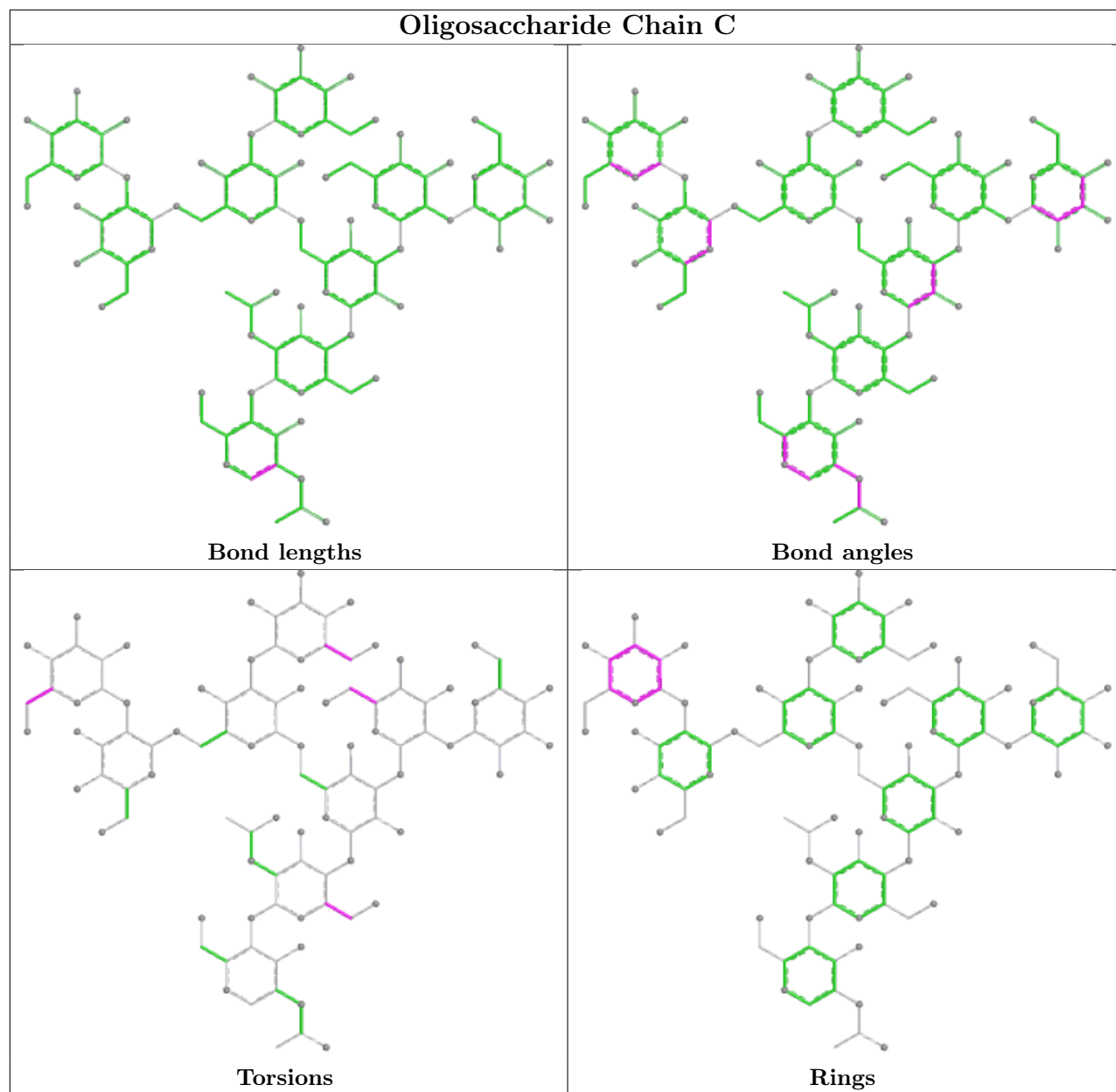
All (2) ring outliers are listed below:

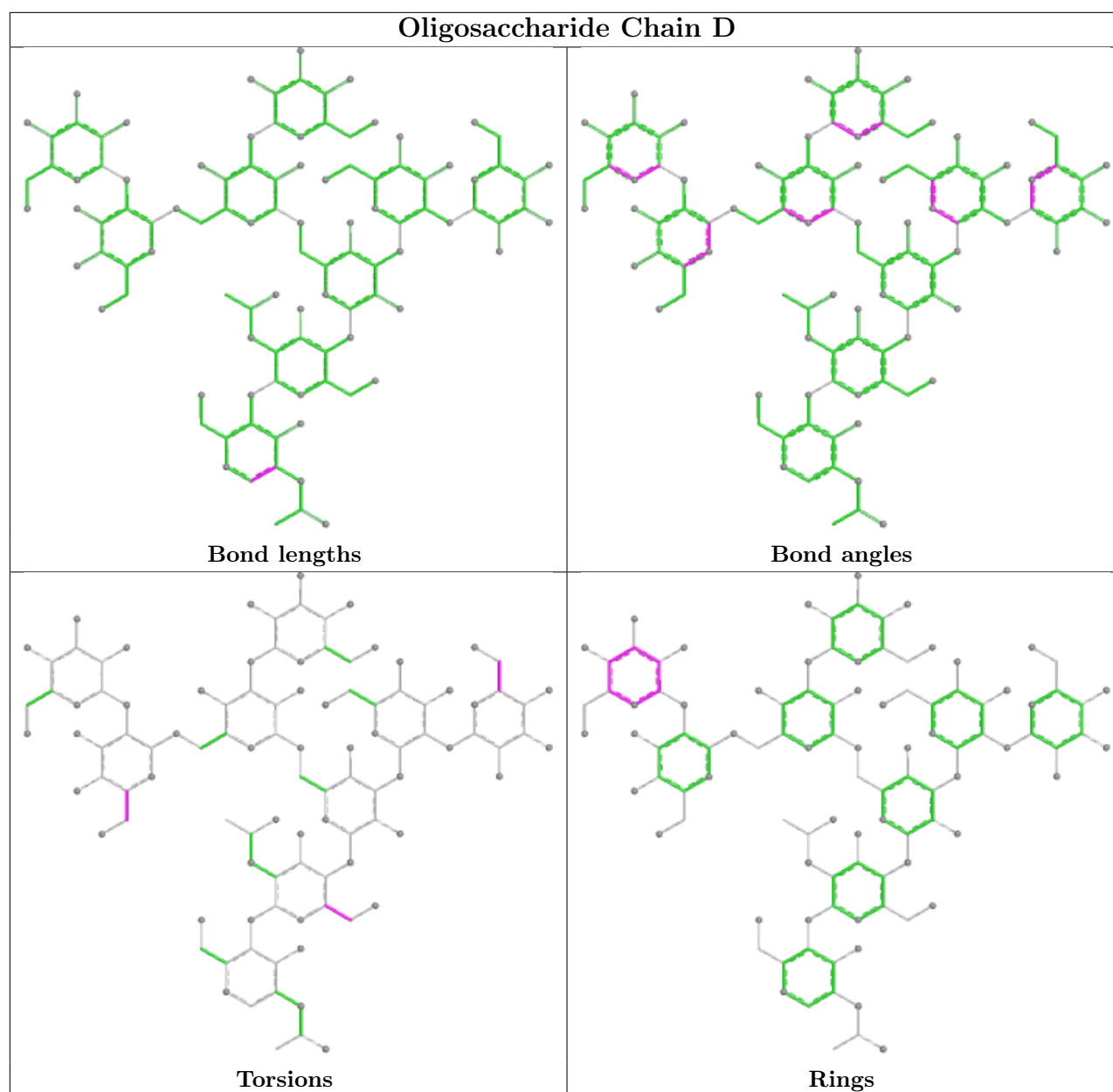
Mol	Chain	Res	Type	Atoms
2	D	6	MAN	C1-C2-C3-C4-C5-O5
2	C	6	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	5	0
2	D	5	MAN	1	0
2	D	8	MAN	1	0
2	C	6	MAN	3	0
2	C	8	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.