



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BHG
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

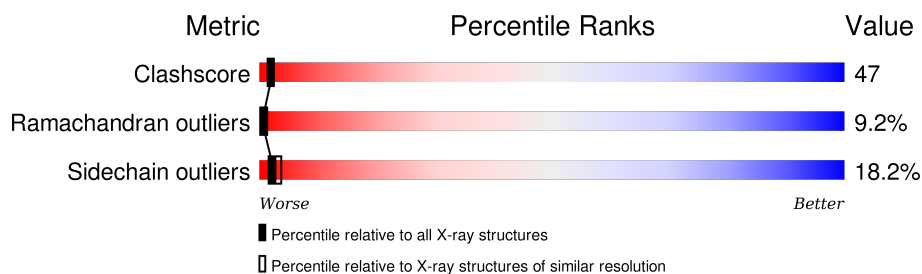
1 Overall quality at a glance

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	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	613	
1	B	613	

2 Entry composition

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 a polymer of unknown type called SUGAR (9-MER).

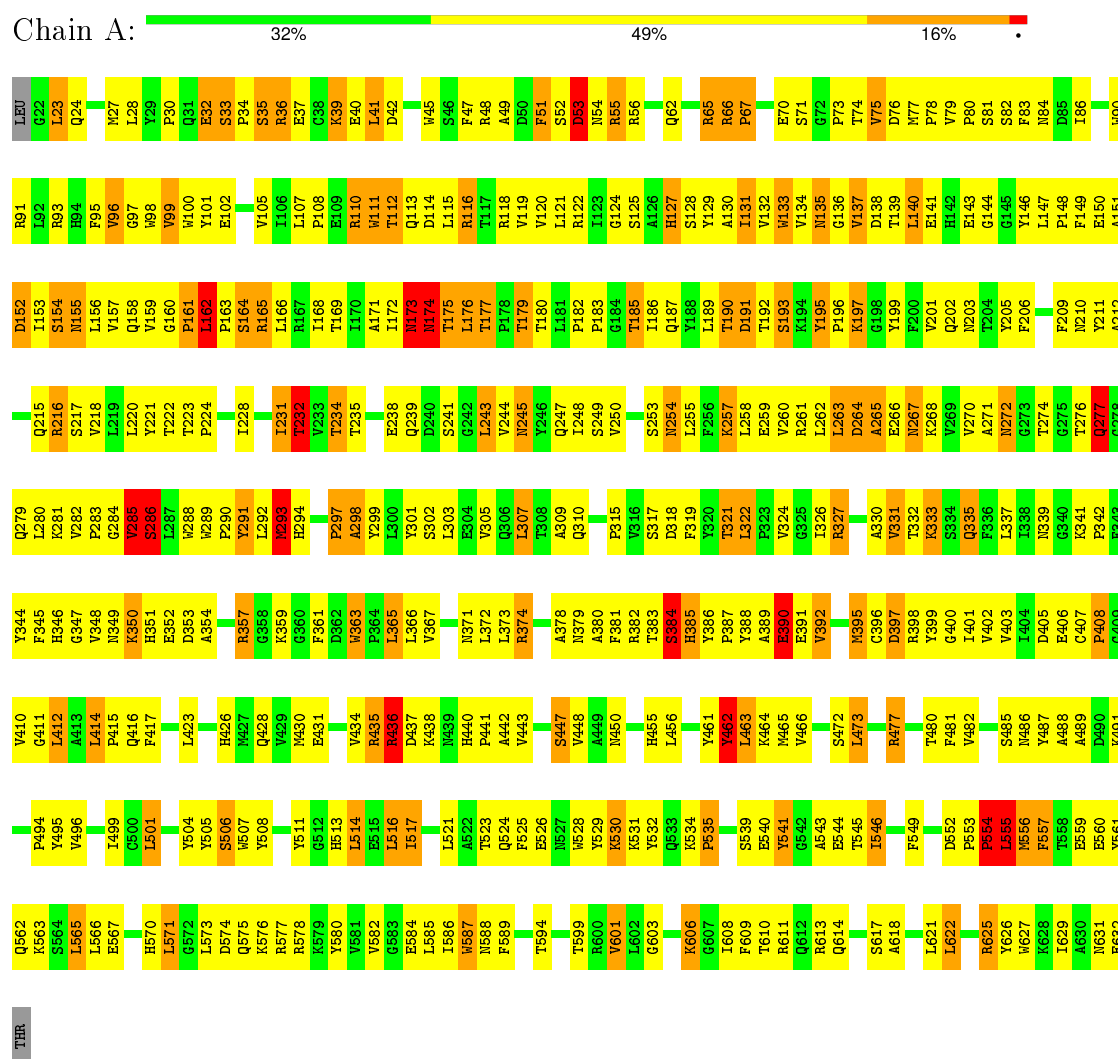
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			105	58	2	45		
2	B	9	Total	C	N	O	0	0
			105	58	2	45		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: BETA-GLUCURONIDASE



• Molecule 1: BETA-GLUCURONIDASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.10 Å 124.40 Å 134.50 Å 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	0.72	0/5139	0.97	13/7000 (0.2%)
1	B	0.74	0/5139	0.97	4/7000 (0.1%)
All	All	0.73	0/10278	0.97	17/14000 (0.1%)

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

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	140	LEU	CA-CB-CG	8.29	134.36	115.30
1	A	216	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	B	144	GLY	N-CA-C	6.86	130.26	113.10
1	B	23	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	293	MET	N-CA-C	6.06	127.36	111.00
1	A	405	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	216	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	36	ARG	N-CA-C	5.60	126.13	111.00
1	A	565	LEU	CA-CB-CG	5.51	127.99	115.30
1	A	447	SER	N-CA-C	-5.42	96.37	111.00
1	B	553	PRO	C-N-CD	-5.34	108.86	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	473	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	176	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	173	ASN	N-CA-C	5.12	124.84	111.00
1	A	131	ILE	CG1-CB-CG2	-5.08	100.22	111.40

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	424	0
1	B	4990	0	4845	518	0
2	A	105	0	88	4	0
2	B	105	0	88	7	0
All	All	10190	0	9867	945	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 47.

All (945) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:127:HIS:HD2	1:B:174:ASN:HA	1.44	0.81
1:B:107:LEU:HB3	1:B:111:TRP:CD1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:651: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:226:THR:HG21	1:B:309:ALA:CB	2.15	0.76
1:B:162:LEU:HB2	1:B:163:PRO:CD	2.16	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
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:B:125:SER:OG	1:B:216:ARG:HG3	1.89	0.72
1:A:382:ARG:HD3	1:A:406:GLU:OE2	1.89	0.72
1:A:120:VAL:HB	1:A:221:TYR:CE1	2.24	0.72
1:B:156:LEU:HD11	1:B:166:LEU:HD13	1.72	0.72
1:B:586:ILE:HG21	1:B:622:LEU:HD11	1.72	0.72
1:A:257:LYS:HD3	1:A:258:LEU:H	1.53	0.72
1:B:514:LEU:HD21	1:B:561:TYR:HE1	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD23	1:A:282:VAL:HG11	1.71	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: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:B:395:MET:HG2	1:B:403:VAL:CG2	2.21	0.70
1:A:137:VAL:HG22	1:A:138:ASP:H	1.55	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
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:A:659:MAN:O2	2:A:659:MAN:H61	1.93	0.69
1:A:175:THR:CG2	1:A:210:ASN:HB3	2.22	0.69
1:B:327:ARG:HH22	1:B:477:ARG:HH21	1.41	0.69
1:B:74:THR:HG22	1:B:75:VAL:H	1.57	0.69
1:A:23:LEU:H	1:A:23:LEU:HD23	1.56	0.69
1:B:227:TYR:HE1	1:B:251:LYS:HB3	1.57	0.69
1:A:352:GLU:O	1:A:359:LYS:HG2	1.92	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:447:SER:HA	1:A:480:THR:O	1.93	0.68
1:B:41:LEU:HD13	1:B:217:SER:HA	1.73	0.68
1:A:395:MET:HG2	1:A:403:VAL:CG2	2.23	0.68
1:A:531:LYS:HE2	1:A:532:TYR:CE2	2.28	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:B:135:ASN:HD22	1:B:136:GLY:N	1.90	0.68
1:A:499:ILE:HG22	1:A:501:LEU:HD22	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:32:GLU:CA	1:B:36:ARG:HD2	2.25	0.67
1:A:185:THR:HG23	2:A:655: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: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: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:349:ASN:ND2	1:A:585:LEU:HD23	2.10	0.67
1:B:395:MET:HG2	1:B:403:VAL:HG21	1.77	0.66
1:A:107:LEU:HD12	1:A:111:TRP:CD1	2.31	0.66
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:B:131:ILE:HG21	1:B:133:TRP:CZ2	2.31	0.66
1:A:415:PRO:HB3	1:A:456:LEU:HD21	1.78	0.66
1:B:178:PRO:HB3	1:B:417:PHE:CD1	2.31	0.66
1:B:146:TYR:HB2	1:B:387:PRO:HD2	1.77	0.66
1:A:397:ASP:O	1:A:399:TYR:N	2.29	0.66
1:A:288:TRP:HE3	1:A:288:TRP:O	1.79	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:B:455:HIS:HA	1:B:489:ALA:O	1.96	0.65
1:A:231:ILE:HG22	1:A:232:THR:H	1.62	0.65
1:B:179:THR:HA	1:B:422:SER:HG	1.59	0.65
1:B:216:ARG:HD3	1:B:389:ALA:HB2	1.77	0.65
1:B:107:LEU:HB3	1:B:111:TRP:HD1	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:TYR:CZ	1:B:374:ARG:HG3	2.32	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: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:406:GLU:HG2	1:A:447:SER:CB	2.26	0.64
1:A:276:THR:O	1:A:276:THR:HG23	1.97	0.64
1:B:407:CYS:SG	1:B:408:PRO:HD2	2.37	0.64
1:B:253:SER:HB3	1:B:311:THR:OG1	1.98	0.64
1:B:291:TYR:HB2	1:B:399:TYR:O	1.98	0.64
1:A:290:PRO:HG2	1:A:293:MET:SD	2.38	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:B:153:ILE:HG13	1:B:154:SER:N	2.12	0.64
1:A:107:LEU:HD23	1:A:164:SER:C	2.18	0.64
1:B:551:GLN:HG3	1:B:552:ASP:O	1.98	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
1:B:29:TYR:CE2	1:B:393:MET:SD	2.91	0.64
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:B:118:ARG:HA	1:B:154:SER:HB3	1.79	0.63
1:A:347:GLY:HA3	1:A:380:ALA:O	1.98	0.63
1:B:391:GLU:O	1:B:394:GLN:HB2	1.98	0.63
1:A:54:ASN:O	1:A:56:ARG:HG2	1.98	0.63
1:A:32:GLU:HB2	1:A:36:ARG:HG2	1.79	0.63
1:A:258:LEU:HG	1:A:307:LEU:HD12	1.81	0.63
1:A:183:PRO:HG3	1:A:412:LEU:HD12	1.80	0.63
1:B:119:VAL:N	1:B:154:SER:HB3	2.13	0.63
1:B:118:ARG:NH2	1:B:120:VAL:HB	2.14	0.63
1:A:352:GLU:O	1:A:359:LYS:NZ	2.29	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LYS:NZ	1:B:251:LYS:HB2	2.15	0.62
1:B:554:PRO:HB3	1:B:561:TYR:HA	1.82	0.62
1:A:381:PHE:HE1	1:A:388:TYR:CE2	2.15	0.62
1:A:348:VAL:HG23	1:A:586:ILE:CG2	2.30	0.62
1:A:298:ALA:HB1	1:A:396:CYS:O	2.00	0.62
1:A:39:LYS:HB2	1:A:41:LEU:HD23	1.82	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:H	1:A:557:PHE:HD1	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
1:B:120:VAL:HG13	1:B:221:TYR:HB3	1.82	0.61
1:A:430:MET:O	1:A:434:VAL:HG23	2.01	0.61
1:A:37:GLU:O	1:A:37:GLU:HG2	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: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: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: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: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:224:PRO:HD2	1:A:318:ASP:OD1	2.01	0.60
1:B:241:SER:O	1:B:326:ILE:HG21	2.01	0.60
1:A:415:PRO:HG2	1:A:416:GLN:HE21	1.64	0.60
1:A:410:VAL:HG23	1:A:411:GLY:N	2.14	0.60
1:B:231:ILE:HG22	1:B:231:ILE:O	2.01	0.60
1:A:349:ASN:HB2	1:A:587:TRP:O	2.01	0.60
1:B:178:PRO:HB3	1:B:417:PHE:HD1	1.66	0.60
1:A:554:PRO:HB3	1:A:561:TYR:HA	1.84	0.60
1:B:391:GLU:O	1:B:395:MET:SD	2.60	0.60
1:B:190:THR:HA	1:B:199:TYR:H	1.67	0.60
1:B:48:ARG:NH2	1:B:72:GLY:HA3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:TYR:CE2	1:B:374:ARG:HG3	2.37	0.59
1:B:163:PRO:O	1:B:164:SER:HB3	2.01	0.59
1:B:108:PRO:O	1:B:111:TRP:HB2	2.02	0.59
1:A:137:VAL:HG22	1:A:138:ASP:N	2.17	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:B:155:ASN:ND2	1:B:155:ASN:O	2.34	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: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:NH1	1:A:122:ARG:HG2	2.17	0.59
1:B:343:PHE:CE2	1:B:402:VAL:HG21	2.37	0.59
1:A:461:TYR:O	1:A:465:MET:HG2	2.03	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:B:426:HIS:O	1:B:429:VAL:HG22	2.03	0.58
1:A:183:PRO:HG3	1:A:412:LEU:CD1	2.34	0.58
1:B:233:VAL:H	1:B:439:ASN:HD21	1.50	0.58
1:A:543:ALA:HB2	1:A:565:LEU:HD13	1.85	0.58
1:B:120:VAL:CG2	1:B:150:GLU:HB2	2.34	0.58
1:B:386:TYR:CE1	1:B:388:TYR:CE1	2.91	0.58
1:B:335:GLN:HA	1:B:582:VAL:HG11	1.86	0.58
1:B:445:MET:SD	1:B:480:THR:HG22	2.44	0.58
1:A:174:ASN:C	1:A:174:ASN:HD22	2.07	0.58
1:A:124:GLY:O	1:A:125:SER:HB3	2.02	0.58
1:B:445:MET:HE1	1:B:498:VAL:HG21	1.85	0.57
1:B:189:LEU:HD12	1:B:199:TYR:CE2	2.39	0.57
1:A:231:ILE:HG23	1:A:248:ILE:HG12	1.85	0.57
1:A:67:PRO:HB2	1:A:70:GLU:HG3	1.86	0.57
1:A:48:ARG:NH1	1:A:71:SER:OG	2.37	0.57
1:A:160:GLY:N	1:A:161:PRO:HD3	2.19	0.57
1:A:531:LYS:HB3	1:A:531:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HD13	1:A:622:LEU:HD12	1.85	0.57
1:A:238:GLU:HB2	1:A:243:LEU:HD21	1.86	0.57
1:B:234:THR:O	1:B:245:ASN:HB2	2.03	0.57
1:B:263:LEU:HG	1:B:269:VAL:HG22	1.87	0.57
1:B:241:SER:HB2	1:B:285:VAL:N	2.18	0.57
1:B:552:ASP:CB	1:B:553:PRO:HD2	2.31	0.57
1:B:98:TRP:HE1	2:B:651:NAG:C7	2.18	0.57
1:A:77:MET:SD	1:A:86:ILE:HD11	2.45	0.57
1:B:258:LEU:HD12	1:B:275:GLY:HA2	1.87	0.56
1:A:288:TRP:CE3	1:A:288:TRP:O	2.57	0.56
1:B:29:TYR:CD2	1:B:393:MET:SD	2.97	0.56
1:B:590:ALA:HA	1:B:609:PHE:O	2.06	0.56
1:B:195:TYR:HB3	1:B:196:PRO:HD2	1.87	0.56
1:B:461:TYR:HD1	1:B:464:LYS:HZ3	1.49	0.56
1:A:464:LYS:HD3	1:A:495:TYR:CE1	2.40	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:383:THR:HG22	1:A:386:TYR:O	2.06	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:A:153:ILE:HG13	1:A:154:SER:N	2.21	0.56
1:B:445:MET:SD	1:B:480:THR:CG2	2.94	0.56
1:A:514:LEU:HD21	1:A:561:TYR:CE1	2.40	0.56
1:A:387:PRO:HD2	1:A:408:PRO:HD3	1.87	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:B:147:LEU:HD21	1:B:433:VAL:HG22	1.88	0.56
1:A:158:GLN:O	1:A:161:PRO:HD3	2.05	0.56
1:B:155:ASN:ND2	1:B:155:ASN:C	2.59	0.56
1:A:90:TRP:CE2	1:A:91:ARG:HG2	2.40	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:B:35:SER:HB3	1:B:223:THR:HA	1.88	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: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:B:34:PRO:O	1:B:35:SER:HB2	2.05	0.55
1:A:262:LEU:HD12	1:A:302:SER:O	2.05	0.55
1:A:32:GLU:HB3	1:A:37:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:HD3	1:A:373:LEU:HD21	1.88	0.55
1:A:257:LYS:NZ	1:A:274:THR:HG22	2.21	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:B:125:SER:O	1:B:214:LEU:HD13	2.06	0.55
1:A:387:PRO:CD	1:A:408:PRO:HD3	2.37	0.55
1:A:525:PHE:HD2	1:A:576:LYS:HE3	1.71	0.55
1:B:595:GLU:HG3	1:B:596:GLN:H	1.72	0.55
1:B:507:TRP:O	1:B:509:HIS:N	2.37	0.55
1:B:63:TRP:HA	1:B:65:ARG:HH21	1.73	0.54
1:A:259:GLU:HG2	1:A:272:ASN:HD21	1.72	0.54
1:B:557:PHE:HD1	1:B:557:PHE:H	1.55	0.54
1:B:450:ASN:HD22	1:B:482:VAL:HB	1.72	0.54
1:B:86:ILE:HG13	1:B:87:SER:N	2.22	0.54
1:A:545:THR:OG1	1:A:562:GLN:HB2	2.06	0.54
1:B:284:GLY:O	1:B:285:VAL:HG13	2.07	0.54
1:B:45:TRP:CH2	1:B:218:VAL:HG11	2.43	0.54
1:A:450:ASN:HA	1:A:482:VAL:CG2	2.37	0.54
1:A:228:ILE:HD13	1:A:305:VAL:CG1	2.38	0.54
1:A:271:ALA:HB1	1:A:280:LEU:HD22	1.89	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:B:156:LEU:CD1	1:B:166:LEU:HD13	2.38	0.54
1:A:584:GLU:O	1:A:585:LEU:HD12	2.07	0.54
1:B:256:PHE:HB2	1:B:308:THR:O	2.08	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:A:487:TYR:O	1:A:488:ALA:HB3	2.07	0.54
1:A:39:LYS:HB2	1:A:41:LEU:CD2	2.37	0.54
1:A:357:ARG:NH1	1:A:357:ARG:HB3	2.23	0.54
1:A:263:LEU:HB2	1:A:267:ASN:HA	1.89	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:109:GLU:HG3	1:B:110:ARG:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HG22	1:B:226:THR:N	2.19	0.53
1:A:112:THR:O	1:A:113:GLN:HG3	2.08	0.53
1:B:394:GLN:OE1	1:B:399:TYR:CE2	2.57	0.53
1:A:290:PRO:HD2	1:A:293:MET:SD	2.48	0.53
1:B:514:LEU:CD2	1:B:561:TYR:HE1	2.20	0.53
1:B:230:ASP:O	1:B:248:ILE:HA	2.08	0.53
1:B:552:ASP:O	1:B:553:PRO:C	2.46	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: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:557:PHE:N	1:B:557:PHE:CD1	2.77	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
1:B:149:PHE:CD1	1:B:149:PHE:N	2.77	0.52
1:A:385:HIS:O	1:A:386:TYR:HB3	2.09	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:157:VAL:O	1:A:161:PRO:HG3	2.09	0.52
1:A:96:VAL:HG12	1:A:175:THR:OG1	2.09	0.52
1:B:246:TYR:O	1:B:278:GLY:N	2.43	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:A:159:VAL:HG23	1:A:159:VAL:O	2.08	0.52
1:A:114:ASP:O	1:A:116:ARG:N	2.42	0.52
1:B:536:ILE:HG22	1:B:537:ILE:N	2.25	0.52
1:B:39:LYS:HA	1:B:219:LEU:CB	2.39	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: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:576:LYS:O	1:B:579:LYS:HB2	2.10	0.52
1:B:493:ALA:N	1:B:494:PRO:HD2	2.24	0.52
1:A:175:THR:HB	1:A:202:GLN:HG2	1.91	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:265:ALA:N	1:A:299:TYR:OH	2.39	0.52
1:B:263:LEU:N	1:B:263:LEU:HD12	2.24	0.52
1:A:291:TYR:CE2	1:A:374:ARG:HA	2.44	0.52
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.75	0.52
1:A:462:TYR:O	1:A:465:MET:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PHE:CZ	1:B:200:PHE:HZ	2.27	0.52
1:B:276:THR:O	1:B:277:GLN:HB3	2.10	0.52
1:B:329:VAL:O	1:B:329:VAL:HG22	2.10	0.52
1:A:49:ALA:HA	1:A:99:VAL:HG23	1.92	0.52
1:B:50:ASP:CB	1:B:63:TRP:HH2	2.22	0.52
2:B:651:NAG:HN2	2:B:651:NAG:H5	1.75	0.52
1:A:130:ALA:O	1:A:141:GLU:HA	2.10	0.52
1:B:257:LYS:HB3	1:B:257:LYS:NZ	2.25	0.52
1:B:307:LEU:HG	1:B:308:THR:H	1.75	0.52
1:A:156:LEU:CD1	1:A:166:LEU:HD13	2.30	0.52
1:B:172:ILE:H	1:B:172:ILE:HD13	1.74	0.52
1:B:189:LEU:HD13	1:B:195:TYR:CE2	2.45	0.52
1:A:562:GLN:O	1:A:566:LEU:HG	2.09	0.52
1:B:416:GLN:OE1	1:B:416:GLN:N	2.43	0.52
1:B:116:ARG:O	1:B:224:PRO:HA	2.11	0.51
1:B:50:ASP:HB3	1:B:63:TRP:CH2	2.45	0.51
1:A:385:HIS:HB3	1:A:410:VAL:CG1	2.36	0.51
1:B:592:PHE:CE2	1:B:604:ASN:ND2	2.78	0.51
1:A:129:TYR:O	1:A:172:ILE:HA	2.11	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:B:121:LEU:HD21	1:B:168:ILE:CD1	2.41	0.51
1:A:54:ASN:C	1:A:56:ARG:N	2.63	0.51
1:B:99:VAL:O	1:B:171:ALA:HA	2.09	0.51
1:B:368:LYS:O	1:B:371:ASN:HB2	2.10	0.51
1:B:59:PHE:HZ	1:B:131:ILE:HD12	1.76	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:433:VAL:HG12	1:B:446:TRP:HZ3	1.75	0.51
1:B:276:THR:HG22	1:B:276:THR:O	2.11	0.51
1:B:243:LEU:HD13	1:B:243:LEU:O	2.11	0.51
1:B:118:ARG:HH11	1:B:223:THR:HG23	1.75	0.51
1:B:107:LEU:HD21	1:B:166:LEU:HB2	1.93	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:B:224:PRO:HG2	1:B:318:ASP:OD2	2.11	0.51
1:A:359:LYS:NZ	1:A:386:TYR:OH	2.32	0.51
1:B:350:LYS:HG2	1:B:589:PHE:HB2	1.92	0.51
1:B:362:ASP:O	1:B:366:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:TYR:O	1:B:488:ALA:HB3	2.10	0.51
1:B:53:ASP:HB2	1:B:56:ARG:HH11	1.76	0.51
1:B:297:PRO:O	1:B:299:TYR:N	2.44	0.51
1:B:84:ASN:OD1	1:B:211:TYR:HD1	1.93	0.51
1:A:102:GLU:HG3	1:A:168:ILE:O	2.11	0.51
1:B:179:THR:O	1:B:425:HIS:CD2	2.63	0.50
1:B:134:VAL:HG22	1:B:135:ASN:N	2.25	0.50
1:A:390:GLU:C	1:A:392:VAL:H	2.13	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:A:186:ILE:HG22	1:A:187:GLN:N	2.26	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:B:140:LEU:HD13	1:B:150:GLU:O	2.10	0.50
1:B:134:VAL:O	1:B:137:VAL:N	2.45	0.50
1:B:385:HIS:O	1:B:408:PRO:HA	2.10	0.50
1:A:216:ARG:NH1	1:A:389:ALA:N	2.60	0.50
1:A:23:LEU:H	1:A:23:LEU:CD2	2.24	0.50
1:B:333:LYS:HE3	1:B:533:GLN:HB3	1.92	0.50
1:B:320:TYR:CD1	1:B:321:THR:O	2.65	0.50
1:B:29:TYR:CD1	1:B:30:PRO:HD2	2.47	0.50
1:B:250:VAL:HG12	1:B:251:LYS:N	2.26	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:A:136:GLY:O	1:A:137:VAL:CB	2.56	0.50
1:B:290:PRO:O	1:B:292:LEU:N	2.44	0.50
1:B:216:ARG:CZ	1:B:388:TYR:O	2.60	0.50
1:A:594:THR:OG1	1:A:603:GLY:HA2	2.12	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: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:A:98:TRP:HA	1:A:172:ILE:O	2.12	0.50
1:A:285:VAL:O	1:A:286:SER:HB2	2.11	0.50
1:B:445:MET:HE2	1:B:498:VAL:HG21	1.93	0.49
1:A:556:MET:HB3	1:A:557:PHE:HD1	1.76	0.49
1:A:514:LEU:HD21	1:A:561:TYR:CZ	2.46	0.49
1:A:333:LYS:H	1:A:333:LYS:HD3	1.77	0.49
1:B:423:LEU:O	1:B:423:LEU:HD22	2.12	0.49
1:B:65:ARG:O	1:B:65:ARG:HG2	2.12	0.49
1:A:235:THR:HG22	1:A:244:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:ARG:NH1	1:B:352:GLU:OE1	2.44	0.49
1:B:54:ASN:HB3	2:B:658:MAN:H61	1.95	0.49
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: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:B:274:THR:HG22	1:B:275:GLY:N	2.27	0.49
1:B:134:VAL:HG23	1:B:166:LEU:HD11	1.93	0.49
1:B:372:LEU:O	1:B:375:TRP:HB3	2.13	0.49
1:A:292:LEU:HD23	1:A:379:ASN:ND2	2.27	0.49
1:B:588:ASN:OD1	1:B:592:PHE:CE2	2.66	0.49
1:A:121:LEU:HD13	1:A:220:LEU:CD2	2.42	0.49
1:B:309:ALA:O	1:B:315:PRO:HA	2.13	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:A:472:SER:O	1:A:473:LEU:HB2	2.12	0.49
1:A:333:LYS:O	1:A:529:TYR:HE1	1.95	0.49
1:A:100:TRP:N	1:A:100:TRP:CD1	2.81	0.49
1:A:83:PHE:CE2	1:A:212:ALA:HB3	2.48	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:B:544:GLU:HG2	1:B:557:PHE:CD2	2.48	0.48
1:A:259:GLU:HA	1:A:274:THR:HA	1.94	0.48
1:A:357:ARG:CZ	1:A:357:ARG:HB3	2.43	0.48
1:A:286:SER:HB3	1:A:299:TYR:CD2	2.47	0.48
1:A:290:PRO:C	1:A:292:LEU:N	2.66	0.48
1:A:248:ILE:HG22	1:A:249:SER:N	2.28	0.48
1:B:531:LYS:HG3	1:B:532:TYR:CD2	2.48	0.48
1:A:423:LEU:HD23	1:A:423:LEU:O	2.12	0.48
1:B:32:GLU:HG2	1:B:36:ARG:CZ	2.44	0.48
1:A:110:ARG:O	1:A:110:ARG:NH1	2.47	0.48
1:A:601:VAL:O	1:A:601:VAL:HG22	2.12	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:A:39:LYS:HB2	1:A:41:LEU:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:SER:O	1:A:473:LEU:CB	2.61	0.48
1:B:261:ARG:NH1	1:B:306:GLN:HE21	2.02	0.48
1:B:83:PHE:CE1	1:B:212:ALA:HB3	2.43	0.48
1:B:623:ARG:O	1:B:627:TRP:HD1	1.95	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:A:40:GLU:C	1:A:42:ASP:H	2.17	0.48
1:A:262:LEU:HD11	1:A:301:TYR:HB3	1.96	0.48
1:B:447:SER:HA	1:B:480:THR:O	2.14	0.48
1:A:110:ARG:NH1	1:A:114:ASP:HB2	2.28	0.48
1:B:294:HIS:CG	1:B:295:GLU:N	2.81	0.48
1:A:133:TRP:CD1	1:A:133:TRP:N	2.81	0.48
1:B:552:ASP:C	1:B:554:PRO:N	2.67	0.48
1:B:577:ARG:C	1:B:579:LYS:H	2.17	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:625:ARG:HG2	1:B:626:TYR:CD1	2.48	0.48
1:B:41:LEU:HD23	1:B:218:VAL:O	2.14	0.48
1:B:576:LYS:HB3	1:B:581:VAL:HG23	1.96	0.48
1:A:396:CYS:SG	1:A:441:PRO:HD2	2.53	0.48
1:B:398:ARG:HG3	1:B:398:ARG:HH11	1.78	0.48
1:B:223:THR:HG21	1:B:227:TYR:CD2	2.47	0.47
1:B:55:ARG:CG	2:B:651:NAG:H83	2.41	0.47
1:B:312:SER:O	1:B:314:GLY:N	2.46	0.47
1:B:48:ARG:HH22	1:B:72:GLY:HA3	1.78	0.47
1:B:547:ALA:O	1:B:559:GLU:OE2	2.32	0.47
1:B:192:THR:O	1:B:192:THR:HG22	2.13	0.47
1:B:608:ILE:CD1	1:B:622:LEU:HD12	2.41	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: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:147:LEU:HB3	1:A:148:PRO:HD2	1.96	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: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:276:THR:O	1:A:277:GLN:HB2	2.13	0.47
1:B:307:LEU:HG	1:B:308:THR:N	2.29	0.47
1:B:146:TYR:CB	1:B:216:ARG:NH2	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HB3	1:A:215:GLN:C	2.35	0.47
1:A:78:PRO:HD2	1:A:86:ILE:HD13	1.96	0.47
1:A:130:ALA:HA	1:A:171:ALA:O	2.15	0.47
1:A:350:LYS:HD2	1:A:589:PHE:CG	2.49	0.47
1:A:586:ILE:O	1:A:587:TRP:O	2.32	0.47
1:A:32:GLU:HG2	1:A:32:GLU:O	2.13	0.47
1:B:276:THR:O	1:B:277:GLN:CB	2.62	0.47
1:A:435:ARG:HB3	1:A:435:ARG:HH11	1.79	0.47
1:A:555:LEU:HD13	1:A:556:MET:CE	2.45	0.47
1:A:110:ARG:HB3	1:A:110:ARG:NH1	2.29	0.47
1:B:51:PHE:CE2	1:B:96:VAL:O	2.67	0.47
1:A:505:TYR:CE2	1:A:521:LEU:HD12	2.48	0.47
1:A:156:LEU:O	1:A:157:VAL:CG1	2.62	0.47
1:B:215:GLN:HG2	1:B:216:ARG:HG2	1.97	0.47
1:A:283:PRO:C	1:A:285:VAL:H	2.17	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:504:TYR:CE2	1:B:606:LYS:HE2	2.50	0.47
1:A:614:GLN:OE1	1:B:551:GLN:HA	2.15	0.46
2:B:651:NAG:H5	2:B:651:NAG:N2	2.30	0.46
1:A:152:ASP:OD1	1:A:153:ILE:N	2.48	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:B:118:ARG:HB3	1:B:153:ILE:O	2.15	0.46
1:A:410:VAL:CG2	1:A:411:GLY:H	2.21	0.46
1:B:349:ASN:ND2	1:B:585:LEU:HB3	2.30	0.46
1:B:327:ARG:NH2	1:B:477:ARG:NH2	2.62	0.46
1:A:382:ARG:O	1:A:384:SER:N	2.47	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: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:426:HIS:HB2	1:B:462:TYR:OH	2.15	0.46
1:B:450:ASN:C	1:B:452:PRO:HD3	2.36	0.46
1:B:187:GLN:NE2	1:B:189:LEU:HG	2.31	0.46
1:B:592:PHE:CZ	1:B:604:ASN:HB3	2.51	0.46
1:B:261:ARG:NH1	1:B:306:GLN:NE2	2.59	0.46
1:B:246:TYR:HB2	1:B:248:ILE:HD11	1.98	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:A:430:MET:HE2	1:A:448:VAL:HG12	1.98	0.46
1:B:588:ASN:OD1	1:B:592:PHE:CD2	2.68	0.46
1:B:39:LYS:HA	1:B:219:LEU:HB2	1.97	0.46
1:B:227:TYR:O	1:B:227:TYR:CD1	2.69	0.46
1:B:64:TYR:CD2	1:B:133:TRP:CD2	3.04	0.46
1:A:175:THR:HG22	1:A:210:ASN:CB	2.44	0.46
1:B:376:LEU:HD11	1:B:608:ILE:HD11	1.97	0.46
1:A:353:ASP:CG	1:A:611:ARG:HH21	2.19	0.46
1:A:185:THR:HG22	1:A:203:ASN:HD22	1.81	0.46
1:B:455:HIS:CE1	1:B:456:LEU:HD21	2.51	0.46
1:B:511:TYR:N	1:B:511:TYR:CD1	2.79	0.46
1:B:240:ASP:HB3	1:B:284:GLY:O	2.16	0.46
1:B:460:GLY:HA3	1:B:491:LYS:HB3	1.98	0.46
1:A:186:ILE:HG22	1:A:187:GLN:H	1.80	0.46
1:B:264:ASP:HA	1:B:301:TYR:HD1	1.81	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: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:555:LEU:O	1:B:558:THR:HB	2.16	0.46
1:B:320:TYR:CE1	1:B:321:THR:O	2.69	0.46
1:A:45:TRP:HE3	1:A:102:GLU:H	1.63	0.46
1:A:107:LEU:HD22	1:A:107:LEU:N	2.31	0.45
1:A:135:ASN:O	1:A:137:VAL:HG12	2.16	0.45
1:A:118:ARG:N	1:A:223:THR:O	2.46	0.45
1:A:487:TYR:HB2	1:A:531:LYS:HZ1	1.81	0.45
1:B:453:ALA:O	1:B:456:LEU:HG	2.16	0.45
1:B:311:THR:OG1	1:B:312:SER:N	2.49	0.45
1:B:461:TYR:O	1:B:464:LYS:HB3	2.16	0.45
1:B:448:VAL:HG21	1:B:467:ILE:CD1	2.47	0.45
1:A:303:LEU:HB2	1:A:324:VAL:HG21	1.98	0.45
1:A:124:GLY:N	1:A:217:SER:O	2.48	0.45
1:A:102:GLU:HA	1:A:168:ILE:O	2.16	0.45
1:B:363:TRP:N	1:B:364:PRO:CD	2.80	0.45
2:A:659:MAN:O2	2:A:659:MAN:C6	2.64	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:576:LYS:HD3	1:B:576:LYS:HA	1.70	0.45
1:B:110:ARG:C	1:B:112:THR:H	2.20	0.45
1:B:140:LEU:CB	1:B:151:ALA:HB2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HB2	1:B:223:THR:HG23	1.98	0.45
1:A:156:LEU:O	1:A:156:LEU:CG	2.63	0.45
1:A:93:ARG:NH1	1:A:209:PHE:CE2	2.84	0.45
1:B:375:TRP:CZ2	1:B:623:ARG:HD3	2.52	0.45
1:B:287:LEU:N	1:B:287:LEU:HD12	2.32	0.45
1:A:392:VAL:HA	1:A:395:MET:HE2	1.97	0.45
1:B:461:TYR:HD1	1:B:464:LYS:NZ	2.14	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:335:GLN:N	1:A:335:GLN:HE21	2.14	0.45
1:B:140:LEU:HD11	1:B:149:PHE:HB2	1.97	0.45
1:A:54:ASN:HD22	1:A:55:ARG:HH11	1.65	0.45
1:B:573:LEU:O	1:B:577:ARG:HG3	2.17	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:122:ARG:HA	1:B:150:GLU:HA	1.97	0.45
1:B:146:TYR:C	1:B:216:ARG:HH21	2.20	0.45
1:A:438:LYS:HB2	1:A:438:LYS:HE3	1.68	0.45
1:B:77:MET:HA	1:B:78:PRO:HD2	1.89	0.45
1:B:551:GLN:HG2	1:B:555:LEU:CB	2.47	0.45
1:B:233:VAL:N	1:B:439:ASN:HD21	2.15	0.45
1:A:350:LYS:HB3	1:A:350:LYS:NZ	2.32	0.45
1:A:121:LEU:HD13	1:A:220:LEU:HD23	1.98	0.45
1:B:118:ARG:HH11	1:B:223:THR:CG2	2.31	0.45
1:B:375:TRP:HZ3	1:B:609:PHE:CZ	2.35	0.45
1:A:241:SER:HA	1:A:285:VAL:CG2	2.44	0.45
1:B:288:TRP:CH2	1:B:442:ALA:HA	2.52	0.45
1:A:372:LEU:HD22	1:A:609:PHE:CZ	2.52	0.45
1:B:410:VAL:HG23	1:B:450:ASN:HB3	1.99	0.45
1:A:524:GLN:O	1:A:528:TRP:CD1	2.70	0.45
1:A:426:HIS:CE1	1:A:466:VAL:HG11	2.52	0.45
1:A:526:GLU:O	1:A:530:LYS:HB3	2.16	0.45
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: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:257:LYS:HZ1	1:A:274:THR:HG22	1.82	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:416:GLN:C	1:B:418:PHE:H	2.20	0.44
1:A:172:ILE:HG22	1:A:173:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:HZ	1:A:366:LEU:HD12	1.76	0.44
1:A:120:VAL:CG1	1:A:150:GLU:HB2	2.47	0.44
1:B:196:PRO:HG2	1:B:199:TYR:HB2	2.00	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: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:135:ASN:CG	1:B:155:ASN:OD1	2.56	0.44
1:A:140:LEU:HD22	1:A:151:ALA:HB2	1.99	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:B:33:SER:O	1:B:35:SER:N	2.51	0.44
1:A:305:VAL:O	1:A:319:PHE:HA	2.17	0.44
1:A:127:HIS:O	1:A:144:GLY:HA2	2.17	0.44
1:A:507:TRP:CZ2	1:A:544:GLU:HB3	2.53	0.44
1:B:576:LYS:HB3	1:B:581:VAL:CG2	2.48	0.44
1:B:167:ARG:CG	1:B:167:ARG:O	2.66	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:A:39:LYS:HB2	1:A:41:LEU:HG	1.99	0.44
1:B:52:SER:C	1:B:56:ARG:HD3	2.38	0.44
1:A:575:GLN:HB3	1:A:576:LYS:HD3	1.99	0.44
1:B:354:ALA:HB3	1:B:357:ARG:CG	2.48	0.44
1:A:571:LEU:HA	1:A:571:LEU:HD22	1.80	0.44
1:B:159:VAL:HG13	1:B:160:GLY:H	1.83	0.44
1:A:385:HIS:ND1	1:A:385:HIS:N	2.66	0.44
1:A:192:THR:O	1:A:193:SER:CB	2.63	0.44
1:B:51:PHE:HE2	1:B:96:VAL:O	2.01	0.44
1:B:448:VAL:HG21	1:B:467:ILE:HD13	2.00	0.44
1:B:241:SER:O	1:B:326:ILE:HG13	2.18	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:299:TYR:O	1:B:300:LEU:HD23	2.17	0.44
1:A:488:ALA:N	1:A:531:LYS:HE3	2.33	0.43
1:B:181:LEU:HD11	1:B:426:HIS:ND1	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:A:485:SER:O	1:A:528:TRP:HZ2	2.01	0.43
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:B:153:ILE:O	1:B:154:SER:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:506:SER:HB3	1:B:561:TYR:OH	2.19	0.43
1:A:175:THR:HA	1:A:210:ASN:OD1	2.17	0.43
1:A:153:ILE:HG13	1:A:154:SER:H	1.83	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:B:172:ILE:HD13	1:B:172:ILE:N	2.33	0.43
1:A:279:GLN:O	1:A:280:LEU:HG	2.18	0.43
1:A:45:TRP:CE3	1:A:101:TYR:HB3	2.53	0.43
1:A:107:LEU:H	1:A:107:LEU:HD22	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:B:216:ARG:NH2	1:B:387:PRO:O	2.52	0.43
1:B:107:LEU:CD1	1:B:220:LEU:HD13	2.48	0.43
1:B:288:TRP:CE3	1:B:288:TRP:O	2.72	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:258:LEU:HB2	1:B:307:LEU:HA	1.99	0.43
1:A:544:GLU:N	1:A:606:LYS:HD3	2.33	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:B:197:LYS:HD3	1:B:197:LYS:C	2.38	0.43
1:B:119:VAL:HG12	1:B:119:VAL:O	2.18	0.43
1:B:225:THR:O	1:B:227:TYR:N	2.52	0.43
1:B:258:LEU:CD2	1:B:307:LEU:HD12	2.49	0.43
1:B:158:GLN:O	1:B:159:VAL:C	2.57	0.43
1:B:235:THR:OG1	1:B:326:ILE:HG23	2.18	0.43
1:B:556:MET:HB3	1:B:557:PHE:HD1	1.83	0.43
1:A:190:THR:O	1:A:191:ASP:C	2.57	0.43
1:A:397:ASP:C	1:A:399:TYR:N	2.72	0.43
1:A:346:HIS:O	1:A:378:ALA:HA	2.18	0.43
1:B:543:ALA:CB	1:B:565:LEU:HD13	2.35	0.43
1:B:135:ASN:ND2	1:B:136:GLY:N	2.63	0.43
1:A:395:MET:N	1:A:395:MET:SD	2.91	0.43
1:A:41:LEU:N	1:A:218:VAL:O	2.51	0.43
1:B:504:TYR:O	1:B:507:TRP:O	2.37	0.43
1:A:629:ILE:HA	1:A:632:GLU:OE1	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:B:327:ARG:HA	1:B:339:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLU:O	1:B:436:ARG:HB2	2.19	0.43
1:B:140:LEU:HB2	1:B:151:ALA:CB	2.44	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:A:244:VAL:HG21	1:A:324:VAL:HG11	2.01	0.43
1:A:333:LYS:C	1:A:535:PRO:HD3	2.39	0.43
1:A:131:ILE:HG12	1:A:141:GLU:HG2	2.01	0.43
1:B:254:ASN:O	1:B:255:LEU:HB3	2.19	0.43
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:395:MET:HB3	1:A:442:ALA:HB1	2.00	0.42
1:A:75:VAL:CG1	1:A:76:ASP:N	2.81	0.42
1:A:162:LEU:CB	1:A:163:PRO:HD3	2.31	0.42
1:B:182:PRO:HA	1:B:183:PRO:HD3	1.79	0.42
1:B:344:TYR:CD1	1:B:344:TYR:C	2.92	0.42
1:B:563:LYS:HG3	1:B:621:LEU:HD13	2.01	0.42
1:B:34:PRO:O	1:B:35:SER:CB	2.67	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:A:359:LYS:HG2	1:A:359:LYS:HZ3	1.57	0.42
1:A:143:GLU:OE2	1:A:180:THR:HG22	2.19	0.42
1:A:381:PHE:CE1	1:A:388:TYR:HE2	2.22	0.42
1:A:248:ILE:CG2	1:A:249:SER:N	2.81	0.42
1:A:28:LEU:HD11	1:A:231:ILE:HG13	2.00	0.42
1:A:545:THR:HG21	1:A:559:GLU:HA	2.00	0.42
1:B:257:LYS:O	1:B:258:LEU:HB3	2.20	0.42
1:B:594:THR:HG23	1:B:604:ASN:N	2.33	0.42
1:B:238:GLU:HB3	1:B:239:GLN:H	1.66	0.42
1:B:563:LYS:HG3	1:B:621:LEU:CD1	2.48	0.42
1:A:65:ARG:O	1:A:66:ARG:HG3	2.20	0.42
1:B:347:GLY:HA3	1:B:380:ALA:O	2.19	0.42
1:B:118:ARG:HA	1:B:154:SER:CB	2.49	0.42
1:B:460:GLY:HA3	1:B:491:LYS:CB	2.49	0.42
1:A:563:LYS:HD2	1:A:617:SER:HB2	2.01	0.42
1:B:99:VAL:O	1:B:172:ILE:HD13	2.20	0.42
1:A:247:GLN:HE22	1:A:277:GLN:NE2	2.18	0.42
1:A:110:ARG:HA	1:A:110:ARG:HD2	1.91	0.42
1:B:546:ILE:HD11	1:B:601:VAL:HG11	2.02	0.42
1:A:119:VAL:HG22	1:A:119:VAL:O	2.19	0.42
1:A:618:ALA:O	1:A:621:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:SER:OG	1:A:254:ASN:N	2.52	0.42
1:B:214:LEU:HD12	1:B:215:GLN:N	2.35	0.42
1:B:503:SER:HB3	1:B:524:GLN:NE2	2.35	0.42
1:B:402:VAL:O	1:B:402:VAL:CG2	2.64	0.42
1:B:37:GLU:HB3	1:B:221:TYR:HD1	1.82	0.42
1:A:290:PRO:O	1:A:291:TYR:C	2.58	0.42
1:A:395:MET:HB3	1:A:442:ALA:CB	2.50	0.42
1:A:555:LEU:HD13	1:A:556:MET:HE2	2.01	0.42
1:A:146:TYR:HB2	1:A:387:PRO:HG2	2.02	0.42
1:B:67:PRO:HG2	1:B:70:GLU:HB2	2.00	0.42
1:A:606:LYS:HB2	1:A:606:LYS:HE3	1.86	0.42
1:B:544:GLU:CG	1:B:605:LYS:HB2	2.44	0.42
1:A:563:LYS:HD2	1:A:617:SER:CB	2.50	0.42
1:A:332:THR:HB	1:A:333:LYS:HZ3	1.84	0.42
1:B:398:ARG:NH1	1:B:398:ARG:HG3	2.34	0.42
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.87	0.42
1:A:539:SER:O	1:A:540:GLU:HB2	2.20	0.42
1:B:248:ILE:HG22	1:B:249:SER:N	2.34	0.41
1:A:177:THR:CG2	1:A:180:THR:HG23	2.43	0.41
1:B:350:LYS:HB3	1:B:351:HIS:H	1.72	0.41
1:A:407:CYS:SG	1:A:448:VAL:HA	2.59	0.41
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:B:566:LEU:HD23	1:B:621:LEU:CD2	2.50	0.41
1:A:414:LEU:HD22	1:A:417:PHE:CZ	2.55	0.41
1:B:118:ARG:HB3	1:B:118:ARG:CZ	2.50	0.41
1:B:263:LEU:HD23	1:B:267:ASN:CG	2.41	0.41
1:A:54:ASN:HD22	1:A:55:ARG:HD2	1.84	0.41
1:B:156:LEU:O	1:B:157:VAL:C	2.58	0.41
1:A:84:ASN:OD1	1:A:211:TYR:HA	2.20	0.41
1:B:362:ASP:HB2	1:B:364:PRO:HD2	2.02	0.41
1:B:261:ARG:HB2	1:B:269:VAL:CG1	2.36	0.41
1:A:388:TYR:O	1:A:436:ARG:NH2	2.49	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:A:455:HIS:O	1:A:491:LYS:HG3	2.20	0.41
1:A:353:ASP:OD1	1:A:611:ARG:NE	2.47	0.41
1:A:105:VAL:O	1:A:165:ARG:HA	2.20	0.41
1:A:107:LEU:HD21	1:A:166:LEU:N	2.35	0.41
1:A:383:THR:CG2	1:A:386:TYR:O	2.68	0.41
1:B:348:VAL:HG22	1:B:349:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:THR:HG21	1:B:325:GLY:O	2.20	0.41
1:A:149:PHE:N	1:A:149:PHE:CD1	2.88	0.41
1:A:276:THR:O	1:A:276:THR:CG2	2.67	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:B:464:LYS:HB2	1:B:464:LYS:HZ2	1.85	0.41
1:A:146:TYR:CB	1:A:387:PRO:HG2	2.50	0.41
1:A:505:TYR:HE2	1:A:521:LEU:HD12	1.83	0.41
1:B:298:ALA:HB1	1:B:396:CYS:O	2.21	0.41
1:A:189:LEU:HD12	1:A:199:TYR:CD1	2.55	0.41
1:B:549:PHE:N	1:B:549:PHE:HD1	2.19	0.41
1:A:245:ASN:HD22	1:A:245:ASN:N	2.17	0.41
1:A:504:TYR:HE2	1:A:606:LYS:HZ3	1.68	0.41
1:A:507:TRP:O	1:A:508:TYR:CB	2.53	0.41
1:B:507:TRP:C	1:B:509:HIS:H	2.21	0.41
1:A:513:HIS:HB3	1:A:516:LEU:HD22	2.03	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:A:175:THR:C	1:A:176:LEU:HD22	2.41	0.41
1:A:327:ARG:O	1:A:327:ARG:NH1	2.49	0.41
1:A:140:LEU:HG	1:A:149:PHE:HD2	1.85	0.41
1:B:375:TRP:CZ3	1:B:609:PHE:CZ	3.08	0.41
1:B:462:TYR:C	1:B:462:TYR:CD1	2.93	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:A:481:PHE:CD1	1:A:496:VAL:CG1	3.04	0.41
1:B:47:PHE:CG	1:B:77:MET:HG3	2.56	0.41
1:A:614:GLN:OE1	1:A:614:GLN:HA	2.21	0.41
1:B:241:SER:OG	1:B:286:SER:N	2.54	0.41
1:B:56:ARG:O	1:B:57:ARG:O	2.39	0.41
1:B:51:PHE:CZ	1:B:200:PHE:CZ	3.07	0.41
1:B:431:GLU:O	1:B:435:ARG:HB2	2.20	0.41
1:B:251:LYS:HZ2	1:B:251:LYS:HB2	1.82	0.41
1:B:80:PRO:HB3	1:B:215:GLN:HA	2.03	0.41
1:B:161:PRO:HB2	1:B:164:SER:HA	2.02	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:197:LYS:HG3	2:A:659:MAN:H62	2.02	0.41
1:B:189:LEU:HB3	1:B:195:TYR:CD2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD21	1:B:168:ILE:HD12	2.01	0.41
1:A:505:TYR:O	1:A:506:SER:HB2	2.21	0.41
1:A:335:GLN:HG2	1:A:335:GLN:O	2.20	0.41
1:A:75:VAL:HG13	1:A:76:ASP:N	2.36	0.41
1:A:195:TYR:HA	1:A:196:PRO:HD3	1.88	0.41
1:B:564:SER:O	1:B:568:GLN:HG2	2.21	0.41
1:B:346:HIS:CE1	1:B:377:GLY:O	2.74	0.41
1:B:386:TYR:CE1	1:B:388:TYR:HE1	2.38	0.41
1:B:59:PHE:CZ	1:B:131:ILE:HD12	2.56	0.41
1:B:549:PHE:N	1:B:549:PHE:CD1	2.88	0.41
1:B:125:SER:CB	1:B:216:ARG:HG3	2.51	0.40
1:A:80:PRO:HB2	1:A:361:PHE:H	1.85	0.40
1:A:383:THR:HB	1:A:406:GLU:H	1.86	0.40
1:B:586:ILE:O	1:B:587:TRP:C	2.59	0.40
1:A:264:ASP:HA	1:A:301:TYR:CD1	2.56	0.40
1:B:189:LEU:HD12	1:B:199:TYR:HE2	1.83	0.40
1:A:270:VAL:HG22	1:A:270:VAL:O	2.21	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:40:GLU:C	1:A:42:ASP:N	2.73	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:A:174:ASN:C	1:A:174:ASN:ND2	2.74	0.40
1:B:185:THR:HG23	2:B:655:MAN:H61	2.03	0.40
1:B:80:PRO:HA	1:B:215:GLN:HA	2.04	0.40
1:B:47:PHE:HB3	1:B:77:MET:HB2	2.03	0.40
1:B:155:ASN:O	1:B:156:LEU:C	2.59	0.40
1:A:263:LEU:HD22	1:A:267:ASN:ND2	2.36	0.40
1:A:62:GLN:NE2	1:A:65:ARG:NH1	2.69	0.40
1:B:256:PHE:CD1	1:B:257:LYS:N	2.90	0.40
1:A:33:SER:CB	1:A:34:PRO:CD	2.99	0.40
1:B:41:LEU:HD22	1:B:218:VAL:N	2.37	0.40
1:A:350:LYS:HG3	1:A:381:PHE:CD1	2.57	0.40
1:B:53:ASP:HB3	1:B:54:ASN:H	1.48	0.40
1:A:463:LEU:HA	1:A:463:LEU:HD12	1.91	0.40
1:B:527:ASN:O	1:B:528:TRP:C	2.58	0.40
1:B:332:THR:HB	1:B:333:LYS:H	1.76	0.40
1:B:495:TYR:N	1:B:495:TYR:CD1	2.88	0.40
1:B:493:ALA:HB3	1:B:532:TYR:CZ	2.55	0.40
1:A:353:ASP:O	1:A:354:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:O	1:A:517:ILE:C	2.60	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	609/613 (99%)	462 (76%)	99 (16%)	48 (8%)	1	1
1	B	609/613 (99%)	442 (73%)	103 (17%)	64 (10%)	1	0
All	All	1218/1226 (99%)	904 (74%)	202 (17%)	112 (9%)	1	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	445 (82%)	95 (18%)	2	3
1	B	540/542 (100%)	438 (81%)	102 (19%)	2	3
All	All	1080/1084 (100%)	883 (82%)	197 (18%)	2	3

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	27	MET
1	A	32	GLU
1	A	39	LYS
1	A	51	PHE
1	A	53	ASP
1	A	55	ARG
1	A	65	ARG
1	A	74	THR
1	A	75	VAL
1	A	96	VAL
1	A	99	VAL

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Mol	Chain	Res	Type
1	A	110	ARG
1	A	111	TRP
1	A	112	THR
1	A	116	ARG
1	A	127	HIS
1	A	133	TRP
1	A	155	ASN
1	A	162	LEU
1	A	165	ARG
1	A	173	ASN
1	A	174	ASN
1	A	175	THR
1	A	177	THR
1	A	179	THR
1	A	185	THR
1	A	190	THR
1	A	201	VAL
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	267	ASN
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
1	A	322	LEU
1	A	327	ARG
1	A	331	VAL
1	A	333	LYS
1	A	335	GLN
1	A	345	PHE
1	A	350	LYS
1	A	351	HIS

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Mol	Chain	Res	Type
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	436	ARG
1	A	437	ASP
1	A	462	TYR
1	A	463	LEU
1	A	477	ARG
1	A	501	LEU
1	A	514	LEU
1	A	516	LEU
1	A	523	THR
1	A	530	LYS
1	A	534	LYS
1	A	535	PRO
1	A	546	ILE
1	A	554	PRO
1	A	555	LEU
1	A	557	PHE
1	A	560	GLU
1	A	571	LEU
1	A	578	ARG
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	A	625	ARG
1	B	23	LEU

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Mol	Chain	Res	Type
1	B	28	LEU
1	B	30	PRO
1	B	34	PRO
1	B	36	ARG
1	B	39	LYS
1	B	41	LEU
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	66	ARG
1	B	74	THR
1	B	76	ASP
1	B	82	SER
1	B	87	SER
1	B	92	LEU
1	B	103	ARG
1	B	106	ILE
1	B	107	LEU
1	B	111	TRP
1	B	113	GLN
1	B	127	HIS
1	B	135	ASN
1	B	149	PHE
1	B	155	ASN
1	B	158	GLN
1	B	161	PRO
1	B	169	THR
1	B	172	ILE
1	B	187	GLN
1	B	215	GLN
1	B	216	ARG
1	B	219	LEU
1	B	221	TYR
1	B	222	THR
1	B	223	THR
1	B	227	TYR
1	B	230	ASP
1	B	235	THR
1	B	236	SER

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Mol	Chain	Res	Type
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	327	ARG
1	B	329	VAL
1	B	332	THR
1	B	335	GLN
1	B	344	TYR
1	B	351	HIS
1	B	355	ASP
1	B	379	ASN
1	B	381	PHE
1	B	385	HIS
1	B	391	GLU
1	B	392	VAL
1	B	414	LEU
1	B	423	LEU
1	B	425	HIS
1	B	427	MET
1	B	435	ARG
1	B	436	ARG
1	B	462	TYR
1	B	477	ARG
1	B	481	PHE
1	B	486	ASN
1	B	487	TYR
1	B	498	VAL
1	B	503	SER
1	B	509	HIS
1	B	511	TYR
1	B	524	GLN

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Mol	Chain	Res	Type
1	B	530	LYS
1	B	531	LYS
1	B	544	GLU
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	612	GLN
1	B	621	LEU
1	B	622	LEU
1	B	625	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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
1	A	215	GLN
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	469	HIS
1	A	551	GLN
1	A	570	HIS
1	A	631	ASN
1	B	127	HIS

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Mol	Chain	Res	Type
1	B	135	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	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	439	ASN
1	B	524	GLN
1	B	570	HIS
1	B	588	ASN
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 carbohydrates 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	A	651	1,2	14,14,15	0.83	1 (7%)	15,19,21	1.13	2 (13%)
2	NAG	A	652	2	14,14,15	0.56	0	15,19,21	0.63	0
2	BMA	A	653	2	11,11,12	0.39	0	14,15,17	1.16	2 (14%)
2	MAN	A	654	2	11,11,12	0.89	1 (9%)	14,15,17	0.74	0
2	MAN	A	655	2	11,11,12	0.58	0	14,15,17	0.59	0
2	MAN	A	656	2	11,11,12	0.64	0	14,15,17	1.77	2 (14%)
2	MAN	A	657	2	11,11,12	0.65	0	14,15,17	0.92	0
2	MAN	A	658	2	11,11,12	0.76	0	14,15,17	0.88	1 (7%)
2	MAN	A	659	2	11,11,12	0.49	0	14,15,17	1.03	1 (7%)
2	NAG	B	651	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.48	0
2	NAG	B	652	2	14,14,15	0.57	0	15,19,21	0.72	0
2	BMA	B	653	2	11,11,12	0.68	0	14,15,17	0.88	0
2	MAN	B	654	2	11,11,12	0.54	0	14,15,17	1.34	2 (14%)
2	MAN	B	655	2	11,11,12	0.36	0	14,15,17	0.85	1 (7%)
2	MAN	B	656	2	11,11,12	0.49	0	14,15,17	1.07	1 (7%)
2	MAN	B	657	2	11,11,12	0.56	0	14,15,17	1.11	1 (7%)
2	MAN	B	658	2	11,11,12	0.63	0	14,15,17	0.93	1 (7%)
2	MAN	B	659	2	11,11,12	0.61	0	14,15,17	0.74	1 (7%)

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	A	651	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	652	2	-	0/6/23/26	0/1/1/1
2	BMA	A	653	2	-	0/2/19/22	0/1/1/1
2	MAN	A	654	2	-	0/2/19/22	0/1/1/1
2	MAN	A	655	2	-	0/2/19/22	0/1/1/1
2	MAN	A	656	2	-	0/2/19/22	0/1/1/1
2	MAN	A	657	2	-	0/2/19/22	0/1/1/1
2	MAN	A	658	2	-	0/2/19/22	0/1/1/1
2	MAN	A	659	2	-	0/2/19/22	1/1/1/1
2	NAG	B	651	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	652	2	-	0/6/23/26	0/1/1/1
2	BMA	B	653	2	-	0/2/19/22	0/1/1/1
2	MAN	B	654	2	-	0/2/19/22	0/1/1/1
2	MAN	B	655	2	-	0/2/19/22	0/1/1/1
2	MAN	B	656	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	657	2	-	0/2/19/22	0/1/1/1
2	MAN	B	658	2	-	0/2/19/22	0/1/1/1
2	MAN	B	659	2	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	654	MAN	C2-C3	2.10	1.55	1.52
2	B	651	NAG	C1-C2	2.22	1.55	1.52
2	A	651	NAG	C1-C2	2.46	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	653	BMA	C1-C2-C3	-2.79	106.24	109.54
2	A	651	NAG	C2-N2-C7	-2.49	119.83	123.04
2	A	653	BMA	O5-C1-C2	-2.36	107.03	110.86
2	B	654	MAN	C1-C2-C3	-2.16	106.99	109.54
2	A	658	MAN	C1-O5-C5	2.11	114.93	112.25
2	A	656	MAN	C2-C3-C4	2.18	114.75	111.04
2	B	656	MAN	C1-O5-C5	2.27	115.13	112.25
2	B	659	MAN	C1-O5-C5	2.33	115.21	112.25
2	A	651	NAG	C1-O5-C5	2.35	115.23	112.25
2	B	655	MAN	C1-O5-C5	2.40	115.29	112.25
2	B	658	MAN	C1-O5-C5	2.64	115.59	112.25
2	B	654	MAN	C1-O5-C5	2.94	115.98	112.25
2	B	657	MAN	C1-O5-C5	3.01	116.07	112.25
2	A	659	MAN	C1-O5-C5	3.09	116.17	112.25
2	A	656	MAN	C1-C2-C3	5.69	116.27	109.54

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	659	MAN	C1-C2-C3-C4-C5-O5
2	A	659	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	655	MAN	1	0
2	A	659	MAN	3	0
2	B	651	NAG	5	0
2	B	655	MAN	1	0
2	B	658	MAN	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.