



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:48 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

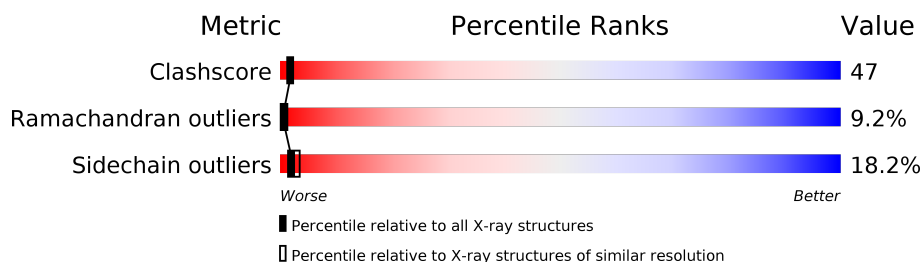
# 1 Overall quality at a glance

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	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (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  $\geq 3$ , 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: BETA-GLUCURONIDASE



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K606	G542	L467	L401	G340	L280	L219	S154	D85	LEU	
		A4543	V402	K341	K281	L220	N155	I86	G22	
		A469	A404	P342	V282	Y221	L156	S87	L23	
		L473	L405	F343	P283	T222	V157	L92	L28	
			A406	F344	G284	T223	Q168			
			E406	F345	V285	P224	V159			
		A618	A407	H346	S286	T225	G160	P96	P30	
			F349	P408	G347	L287	P161	G97	Q31	
			A619	G409	V348	V288	L162	W98	E32	
		F609	Q551	V410	N349	V289	P163	V99	S33	
Q612	G546	L477	G411	K350	P290	S164	Y100	P384		
			V482	H351	Y291	R165	Y101	S36		
			L412	L413	L292	L166	E102	R36		
				A414	M293	T232	R167	R103	E37	
				L415	A354	T234	L168	C38		
			Q416	D355	T235	T169	I106		K39	
			A417	T356	S236	T170	L107		E40	
			A628	A418	P357	P297	V237	A171	P108	L41
				K491	K357	A298	E238	E109	G42	
				L492	G358	A299	Q239	R110	G43	
E632	K663	A493	K359	V299	N173	W11	G43			
		P494	G360	L300	D240	N174	W11	L44		
		Y495	L423	F361	Y301	T175	T112	W45		
			A424	D362	S302	G242	L176	Q113	S46	
			H425	K363	L303	L243	D114	F47		
		V498	A426	K363	E304	V244	L115	R48		
			L427	L365	V305	N245	R116	A49		
			Q428	L366	G360	Y246	T117	D50		
		THR	G572	A502	L429	V367	L307	Q247	R181	G51
				S503	A430	V367	L308	T248	P182	S52
Y504	E431			K368	A309	S249	P183	D53		
L571	E432			N371	Q310	V250	G194	N54		
	S506			L433	T311	K251	T185	L121	R55	
	W507			L434	S312	G252	L186	R122	R56	
W508	R435			L373	S312	T186	S126	R57		
H509	R436			K374	L313	N254	A126	G58		
L575	L510			K375	G314	N254	Y188	A126	G58	
	K576			L511	L376	P315	L255	H127	F59	
	R577	V511	G377	V316	T256	E90	S128	E60		
R578	A442		S317	K257	T190	L131	Q62			
K579	D443		L258	T192	A130	W63				
L602	G580	L514	N379	F319	E259	V132	Y64			
		L517	A444	A380	V320	V260	W64	L132		
			M445	F381	V320	V260	W64			
			Q518	A446	T382	R261	W64			
		L521	A447	T383	L322	L262	K197	W64	L133	
			V448	S384	P323	L263	G198	V134		
			A449	H385	V324	D264	Y199	N135		P67
		L603	G588	F451	H385	G325	A265	F200	G136	R56
				E452	P387	L326	E266	W201	D138	S71
				A453	T388	R327	K267	Q202	T139	G72
L454	A389			A328	K268	M203	L140	T74		
W528	E390			V329	V269	F206	G144	W75		
K530	S391			A330	V270	D76	Y146	M77		
L531	L456			V392	V331	A271	L147	P78		
Y532	E457			T332	T332	N272	Y211	P78		
Q533	Q394			K393	K333	G273	A212	V79		
L604	G596			K534	K395	S394	G274	G213	P148	S81
		P535	C396	L314	T275	G215	F149	E150		
		L536	L462	D397	T276	Q215	S81	S82		
		Y537	L463	R398	Q277	R216	A151	S82		
		L537	L463	R398	L337	G278	D152	F83		
			K464	Y399	T338	G278	S217	D152	N94	
			W541	C400	N339	G279	V215	T152	N94	

## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: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:381:PHE:HE1	1:A:388:TYR:HE2	1.31	0.75
1:A:51:PHE:HB2	1:A:95:PHE:CE1	2.22	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:288:TRP:CE3	1:B:327:ARG:HD3	2.27	0.69
2:A:659:MAN:O2	2:A:659:MAN:H61	1.93	0.69
1:B:394:GLN:O	1:B:399:TYR:HD2	1.76	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: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: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

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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: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: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
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: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:179:THR:HA	1:B:422:SER:HG	1.59	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

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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: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:233:VAL:HG22	1:B:439:ASN:ND2	2.12	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:O	1:A:276:THR:HG23	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: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: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: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: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: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: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: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: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: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: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:A:491:LYS:O	1:A:494:PRO:HD2	2.01	0.60
1:B:101:TYR:CE2	1:B:214:LEU:HB3	2.36	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: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:231:ILE:HG22	1:B:231:ILE: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: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: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:382:ARG:HD2	1:B:406:GLU:OE1	2.02	0.60
1:B:206:PHE:HB3	1:B:410:VAL:HG13	1.82	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:443:VAL:O	1:A:443:VAL:HG13	2.03	0.59
1:A:47:PHE:CG	1:A:77:MET:HG3	2.37	0.59
1:B:155:ASN:ND2	1:B:155:ASN:O	2.34	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: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:183:PRO:HG3	1:A:412:LEU:CD1	2.34	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: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: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:124:GLY:O	1:A:125:SER:HB3	2.02	0.58
1:A:174:ASN:C	1:A:174:ASN:HD22	2.07	0.58
1:B:189:LEU:HD12	1:B:199:TYR:CE2	2.39	0.57
1:B:445:MET:HE1	1:B:498:VAL:HG21	1.85	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:238:GLU:HB2	1:A:243:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:77:MET:SD	1:A:86:ILE:HD11	2.45	0.57
1:B:98:TRP:HE1	2:B:651:NAG:C7	2.18	0.57
1:A:288:TRP:CE3	1:A:288:TRP:O	2.57	0.56
1:B:258:LEU:HD12	1:B:275:GLY:HA2	1.87	0.56
1:B:461:TYR:HD1	1:B:464:LYS:HZ3	1.49	0.56
1:B:590:ALA:HA	1:B:609:PHE:O	2.06	0.56
1:A:464:LYS:HD3	1:A:495:TYR:CE1	2.40	0.56
1:B:195:TYR:HB3	1:B:196:PRO:HD2	1.87	0.56
1:B:29:TYR:CD2	1:B:393:MET:SD	2.97	0.56
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:158:GLN:O	1:A:161:PRO:HD3	2.05	0.56
1:A:90:TRP:CE2	1:A:91:ARG:HG2	2.40	0.56
1:B:155:ASN:ND2	1:B:155:ASN:C	2.59	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: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
1:B:34:PRO:O	1:B:35:SER:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:271:ALA:HB1	1:A:280:LEU:HD22	1.89	0.54
1:A:228:ILE:HD13	1:A:305:VAL:CG1	2.38	0.54
1:A:450:ASN:HA	1:A:482:VAL:CG2	2.37	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: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:263:LEU:HB2	1:A:267:ASN:HA	1.89	0.54
1:A:357:ARG:NH1	1:A:357:ARG:HB3	2.23	0.54
1:A:39:LYS:HB2	1:A:41:LEU:CD2	2.37	0.54
1:A:487:TYR:O	1:A:488:ALA:HB3	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:83:PHE:O	1:B:86:ILE:HG12	2.07	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:109:GLU:HG3	1:B:110:ARG:N	2.23	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:187:GLN:HE21	1:B:189:LEU:HG	1.73	0.53
1:B:35:SER:CB	1:B:224:PRO:HD3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:CD1	1:B:149:PHE:N	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:159:VAL:HG23	1:A:159:VAL:O	2.08	0.52
1:A:157:VAL:O	1:A:161:PRO:HG3	2.09	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: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: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: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:B:376:LEU:HA	1:B:623:ARG:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:651:NAG:HN2	2:B:651:NAG:H5	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: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: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:B:416:GLN:OE1	1:B:416:GLN:N	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: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:B:50:ASP:HB3	1:B:63:TRP:CH2	2.45	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: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: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:59:PHE:HZ	1:B:131:ILE:HD12	1.76	0.51
1:B:243:LEU:HD13	1:B:243:LEU:O	2.11	0.51
1:B:276:THR:HG22	1:B:276:THR:O	2.11	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:53:ASP:HB2	1:B:56:ARG:HH11	1.76	0.51
1:A:186:ILE:HG22	1:A:187:GLN:N	2.26	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:134:VAL:HG22	1:B:135:ASN:N	2.25	0.50
1:B:179:THR:O	1:B:425:HIS:CD2	2.63	0.50
1:B:53:ASP:HB2	1:B:56:ARG:HD3	1.93	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: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:262:LEU:HD23	1:A:282:VAL:CG1	2.40	0.50
1:A:98:TRP:HA	1:A:172:ILE:O	2.12	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: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:O	1:B:423:LEU:HD22	2.12	0.49
1:B:445:MET:HE2	1:B:498:VAL:HG21	1.93	0.49
1:A:235:THR:HG22	1:A:244:VAL:HG22	1.95	0.49
1:B:460:GLY:O	1:B:495:TYR:HE2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:O	1:B:65:ARG:HG2	2.12	0.49
1:B:231:ILE:O	1:B:233:VAL:HG13	2.12	0.49
1:B:37:GLU:HB3	1:B:221:TYR:CD1	2.47	0.49
1:B:457:GLU:HA	1:B:491:LYS:HG3	1.94	0.49
1:B:50:ASP:HB3	1:B:63:TRP:HH2	1.77	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:292:LEU:CD2	1:B:379:ASN:ND2	2.73	0.49
1:B:65:ARG:O	1:B:66:ARG:HB3	2.11	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: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:309:ALA:O	1:B:315:PRO:HA	2.13	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: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: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: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:290:PRO:C	1:A:292:LEU:N	2.66	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:O	1:A:601:VAL:HG22	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:242:GLY:HA2	1:B:326:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLN:O	1:B:64:TYR:N	2.47	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
1:B:83:PHE:CE1	1:B:212:ALA:HB3	2.43	0.48
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:A:40:GLU:C	1:A:42:ASP:H	2.17	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:B:47:PHE:CB	1:B:77:MET:HB2	2.43	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: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: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: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:576:LYS:HB3	1:B:581:VAL:HG23	1.96	0.48
1:B:192:THR:O	1:B:192:THR:HG22	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: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:55:ARG:CG	2:B:651:NAG:H83	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: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: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:A:276:THR:O	1:A:277:GLN:HB2	2.13	0.47
1:B:343:PHE:CZ	1:B:402:VAL:HG21	2.49	0.47
1:B:64:TYR:CE2	1:B:133:TRP:CZ3	3.02	0.47
1:A:80:PRO:HB3	1:A:215:GLN:C	2.35	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:B:307:LEU:HG	1:B:308:THR:N	2.29	0.47
1:A:130:ALA:HA	1:A:171:ALA:O	2.15	0.47
1:A:78:PRO:HD2	1:A:86:ILE:HD13	1.96	0.47
1:A:32:GLU:HG2	1:A:32:GLU:O	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:HB3	1:A:110:ARG:NH1	2.29	0.47
1:A:505:TYR:CE2	1:A:521:LEU:HD12	2.48	0.47
1:A:555:LEU:HD13	1:A:556:MET:CE	2.45	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:283:PRO:C	1:A:285:VAL:H	2.17	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: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:B:651:NAG:H5	2:B:651:NAG:N2	2.30	0.46
1:A:410:VAL:CG2	1:A:411:GLY:H	2.21	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: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:35:SER:HB3	1:A:223:THR:HA	1.97	0.46
1:A:382:ARG:O	1:A:384:SER:N	2.47	0.46
1:B:268:LYS:HD3	1:B:268:LYS:HA	1.74	0.46
1:B:187:GLN:NE2	1:B:189:LEU:HG	2.31	0.46
1:B:450:ASN:C	1:B:452:PRO:HD3	2.36	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: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:A:430:MET:HE2	1:A:448:VAL:HG12	1.98	0.46
1:B:107:LEU:N	1:B:107:LEU:CD2	2.77	0.46
1:B:178:PRO:HA	1:B:183:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:LYS:HA	1:B:219:LEU:HB2	1.97	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:A:353:ASP:CG	1:A:611:ARG:HH21	2.19	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: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: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:423:LEU:HD11	1:A:465:MET:HG3	1.97	0.46
1:A:78:PRO:HG2	1:A:81:SER:OG	2.16	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: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: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:B:448:VAL:HG21	1:B:467:ILE:CD1	2.47	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:363:TRP:N	1:B:364:PRO:CD	2.80	0.45
1:B:110:ARG:C	1:B:112:THR:H	2.20	0.45
1:B:576:LYS:HD3	1:B:576:LYS:HA	1.70	0.45
1:A:156:LEU:O	1:A:156:LEU:CG	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	1:A:209:PHE:CE2	2.84	0.45
1:A:392:VAL:HA	1:A:395:MET:HE2	1.97	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:461:TYR:HD1	1:B:464:LYS:NZ	2.14	0.45
1:B:375:TRP:CZ2	1:B:623:ARG:HD3	2.52	0.45
1:A:335:GLN:HE21	1:A:335:GLN:N	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:333:LYS:HD3	1:A:333:LYS:N	2.32	0.45
1:A:54:ASN:HD22	1:A:55:ARG:HH11	1.65	0.45
1:B:140:LEU:HD11	1:B:149:PHE:HB2	1.97	0.45
1:B:102:GLU:OE2	1:B:167:ARG:HD2	2.17	0.45
1:B:573:LEU:O	1:B:577:ARG:HG3	2.17	0.45
1:A:438:LYS:HB2	1:A:438:LYS:HE3	1.68	0.45
1:B:146:TYR:C	1:B:216:ARG:HH21	2.20	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:HB3	1:A:350:LYS:NZ	2.32	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:B:77:MET:HA	1:B:78:PRO:HD2	1.89	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:410:VAL:HG23	1:B:450:ASN:HB3	1.99	0.45
1:B:375:TRP:HZ3	1:B:609:PHE:CZ	2.35	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
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:416:GLN:C	1:B:418:PHE:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:135:ASN:CG	1:B:155:ASN:OD1	2.56	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: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:A:507:TRP:CZ2	1:A:544:GLU:HB3	2.53	0.44
1:B:167:ARG:CG	1:B:167:ARG:O	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:HA	1:A:571:LEU:HD22	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:B:52:SER:C	1:B:56:ARG:HD3	2.38	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:159:VAL:HG13	1:B:160:GLY:H	1.83	0.44
1:B:51:PHE:HE2	1:B:96:VAL:O	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:197:LYS:HD3	1:B:197:LYS:C	2.38	0.43
1:B:258:LEU:HB2	1:B:307:LEU:HA	1.99	0.43
1:A:190:THR:O	1:A:191:ASP:C	2.57	0.43
1:A:346:HIS:O	1:A:378:ALA:HA	2.18	0.43
1:A:397:ASP:C	1:A:399:TYR:N	2.72	0.43
1:B:119:VAL:O	1:B:119:VAL:HG12	2.18	0.43
1:B:158:GLN:O	1:B:159:VAL:C	2.57	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:333:LYS:C	1:A:535:PRO:HD3	2.39	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:120:VAL:CG1	1:B:221:TYR:HB3	2.49	0.43
1:B:254:ASN:O	1:B:255:LEU:HB3	2.19	0.43
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: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: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: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:A:143:GLU:OE2	1:A:180:THR:HG22	2.19	0.42
1:A:28:LEU:HD11	1:A:231:ILE:HG13	2.00	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:A:65:ARG:O	1:A:66:ARG:HG3	2.20	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
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:HA	1:A:110:ARG:HD2	1.91	0.42
1:A:119:VAL:HG22	1:A:119:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:290:PRO:O	1:A:291:TYR:C	2.58	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:A:555:LEU:HD13	1:A:556:MET:HE2	2.01	0.42
1:B:37:GLU:HB3	1:B:221:TYR:HD1	1.82	0.42
1:A:332:THR:HB	1:A:333:LYS:HZ3	1.84	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:HB2	1:A:606:LYS:HE3	1.86	0.42
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.87	0.42
1:B:398:ARG:NH1	1:B:398:ARG:HG3	2.34	0.42
1:B:544:GLU:CG	1:B:605:LYS:HB2	2.44	0.42
1:B:67:PRO:HG2	1:B:70:GLU:HB2	2.00	0.42
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:A:97:GLY:O	1:A:173:ASN:HA	2.19	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:84:ASN:OD1	1:A:211:TYR:HA	2.20	0.41
1:A:54:ASN:HD22	1:A:55:ARG:HD2	1.84	0.41
1:B:118:ARG:HB3	1:B:118:ARG:CZ	2.50	0.41
1:B:156:LEU:O	1:B:157:VAL:C	2.58	0.41
1:B:263:LEU:HD23	1:B:267:ASN:CG	2.41	0.41
1:A:105:VAL:O	1:A:165:ARG:HA	2.20	0.41
1:A:353:ASP:OD1	1:A:611:ARG:NE	2.47	0.41
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: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:N	1:A:149:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:GLU:HB2	1:A:36:ARG:HA	2.03	0.41
1:A:383:THR:CG2	1:A:386:TYR:O	2.68	0.41
1:A:39:LYS:O	1:A:39:LYS:HG2	2.20	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:348:VAL:HG22	1:B:349:ASN:O	2.21	0.41
1:B:298:ALA:HB1	1:B:396:CYS:O	2.21	0.41
1:B:464:LYS:HB2	1:B:464:LYS:HZ2	1.85	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:A:513:HIS:HB3	1:A:516:LEU:HD22	2.03	0.41
1:B:507:TRP:C	1:B:509:HIS:H	2.21	0.41
1:A:140:LEU:HG	1:A:149:PHE:HD2	1.85	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: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:481:PHE:CD1	1:A:496:VAL:CG1	3.04	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:462:TYR:C	1:B:462:TYR:CD1	2.93	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: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: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:A:195:TYR:HA	1:A:196:PRO:HD3	1.88	0.41
1:A:535:PRO:HB3	1:A:582:VAL:HG21	2.02	0.41
1:A:197:LYS:HG3	2:A:659:MAN:H62	2.02	0.41
1:B:121:LEU:HD21	1:B:168:ILE:HD12	2.01	0.41
1:B:189:LEU:HB3	1:B:195:TYR:CD2	2.55	0.41
1:B:80:PRO:HB3	1:B:215:GLN:HA	2.03	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:335:GLN:HG2	1:A:335:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:TYR:O	1:A:506:SER:HB2	2.21	0.41
1:A:75:VAL:HG13	1:A:76:ASP:N	2.36	0.41
1:B:161:PRO:HB2	1:B:164:SER:HA	2.02	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:39:LYS:HA	1:B:219:LEU:HB3	2.01	0.41
1:B:564:SER:O	1:B:568:GLN:HG2	2.21	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:270:VAL:HG22	1:A:270:VAL:O	2.21	0.40
1:A:264:ASP:HA	1:A:301:TYR:CD1	2.56	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:189:LEU:HD12	1:B:199:TYR:HE2	1.83	0.40
1:B:125:SER:CB	1:B:216:ARG:HG3	2.51	0.40
1:B:586:ILE:O	1:B:587:TRP:C	2.59	0.40
1:A:174:ASN:C	1:A:174:ASN:ND2	2.74	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:A:40:GLU:C	1:A:42:ASP:N	2.73	0.40
1:B:126:ALA:HB1	1:B:172:ILE:HG21	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:B:185:THR:HG23	2:B:655:MAN:H61	2.03	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:155:ASN:O	1:B:156:LEU:C	2.59	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:A:33:SER:CB	1:A:34:PRO:CD	2.99	0.40
1:A:350:LYS:HG3	1:A:381:PHE:CD1	2.57	0.40
1:A:463:LEU:HA	1:A:463:LEU:HD12	1.91	0.40
1:B:256:PHE:CD1	1:B:257:LYS:N	2.90	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:A:353:ASP:O	1:A:354:ALA:HB2	2.21	0.40
1:A:516:LEU:O	1:A:517:ILE:C	2.60	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:N	1:B:495:TYR:CD1	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ASN:O	1:B:528:TRP:C	2.58	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%)	0	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/542 (100%)	445 (82%)	95 (18%)	2	3
1	B	540/542 (100%)	438 (81%)	102 (19%)	2	2
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	0.84	1 (7%)	15,19,21	1.02	2 (13%)
2	NAG	A	652	2	14,14,15	0.57	0	15,19,21	0.68	0
2	BMA	A	653	2	11,11,12	0.40	0	13,15,17	1.19	2 (15%)
2	MAN	A	654	2	11,11,12	0.90	1 (9%)	13,15,17	0.74	0
2	MAN	A	655	2	11,11,12	0.59	0	13,15,17	0.64	0
2	MAN	A	656	2	11,11,12	0.65	0	13,15,17	1.73	2 (15%)
2	MAN	A	657	2	11,11,12	0.67	0	13,15,17	0.94	0
2	MAN	A	658	2	11,11,12	0.78	0	13,15,17	0.89	1 (7%)
2	MAN	A	659	2	11,11,12	0.51	0	13,15,17	1.02	1 (7%)
2	NAG	B	651	1,2	14,14,15	0.87	1 (7%)	15,19,21	0.48	0
2	NAG	B	652	2	14,14,15	0.58	0	15,19,21	0.75	0
2	BMA	B	653	2	11,11,12	0.70	0	13,15,17	0.88	0
2	MAN	B	654	2	11,11,12	0.55	0	13,15,17	1.33	2 (15%)
2	MAN	B	655	2	11,11,12	0.36	0	13,15,17	0.84	1 (7%)
2	MAN	B	656	2	11,11,12	0.50	0	13,15,17	1.07	1 (7%)
2	MAN	B	657	2	11,11,12	0.58	0	13,15,17	1.10	1 (7%)
2	MAN	B	658	2	11,11,12	0.65	0	13,15,17	0.93	1 (7%)
2	MAN	B	659	2	11,11,12	0.63	0	13,15,17	0.73	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	2.13	1.55	1.52
2	B	651	NAG	C1-C2	2.25	1.55	1.52
2	A	651	NAG	C1-C2	2.48	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	-2.69	106.24	109.65
2	A	653	BMA	O5-C1-C2	-2.40	107.03	110.79
2	A	651	NAG	C2-N2-C7	-2.13	119.83	122.94
2	B	654	MAN	C1-C2-C3	-2.10	106.99	109.65
2	A	658	MAN	C1-O5-C5	2.01	114.93	112.17
2	B	656	MAN	C1-O5-C5	2.15	115.13	112.17
2	B	659	MAN	C1-O5-C5	2.21	115.21	112.17
2	A	656	MAN	C2-C3-C4	2.22	114.75	110.88
2	A	651	NAG	C1-O5-C5	2.22	115.23	112.17
2	B	655	MAN	C1-O5-C5	2.27	115.29	112.17
2	B	658	MAN	C1-O5-C5	2.49	115.59	112.17
2	B	654	MAN	C1-O5-C5	2.77	115.98	112.17
2	B	657	MAN	C1-O5-C5	2.83	116.07	112.17
2	A	659	MAN	C1-O5-C5	2.91	116.17	112.17
2	A	656	MAN	C1-C2-C3	5.22	116.27	109.65

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

### 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.