



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:19 AM GMT

PDB ID : 1VFU  
Title : Crystal structure of Thermoactinomyces vulgaris R-47 amylase 2/gamma-cyclodextrin complex  
Authors : Ohtaki, A.; Mizuno, M.; Tonozuka, T.; Sakano, Y.; Kamitori, S.  
Deposited on : 2004-04-19  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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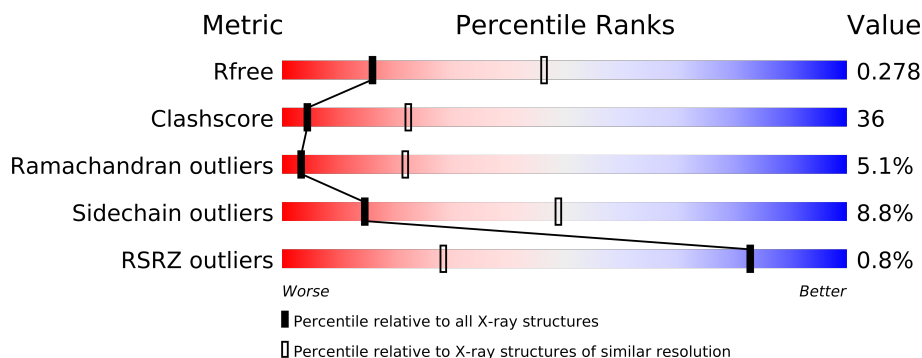
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9863 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Neopullulanase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	833	872	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	ENGINEERED	UNP Q08751
A	421	ASN	ASP	ENGINEERED	UNP Q08751
B	325	ASN	ASP	ENGINEERED	UNP Q08751
B	421	ASN	ASP	ENGINEERED	UNP Q08751

- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	8	Total	C	O	0	0
			88	48	40		
2	B	8	Total	C	O	0	0
			88	48	40		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	ENGINEERED	UNP Q08751
A	421	ASN	ASP	ENGINEERED	UNP Q08751
B	325	ASN	ASP	ENGINEERED	UNP Q08751
B	421	ASN	ASP	ENGINEERED	UNP Q08751

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

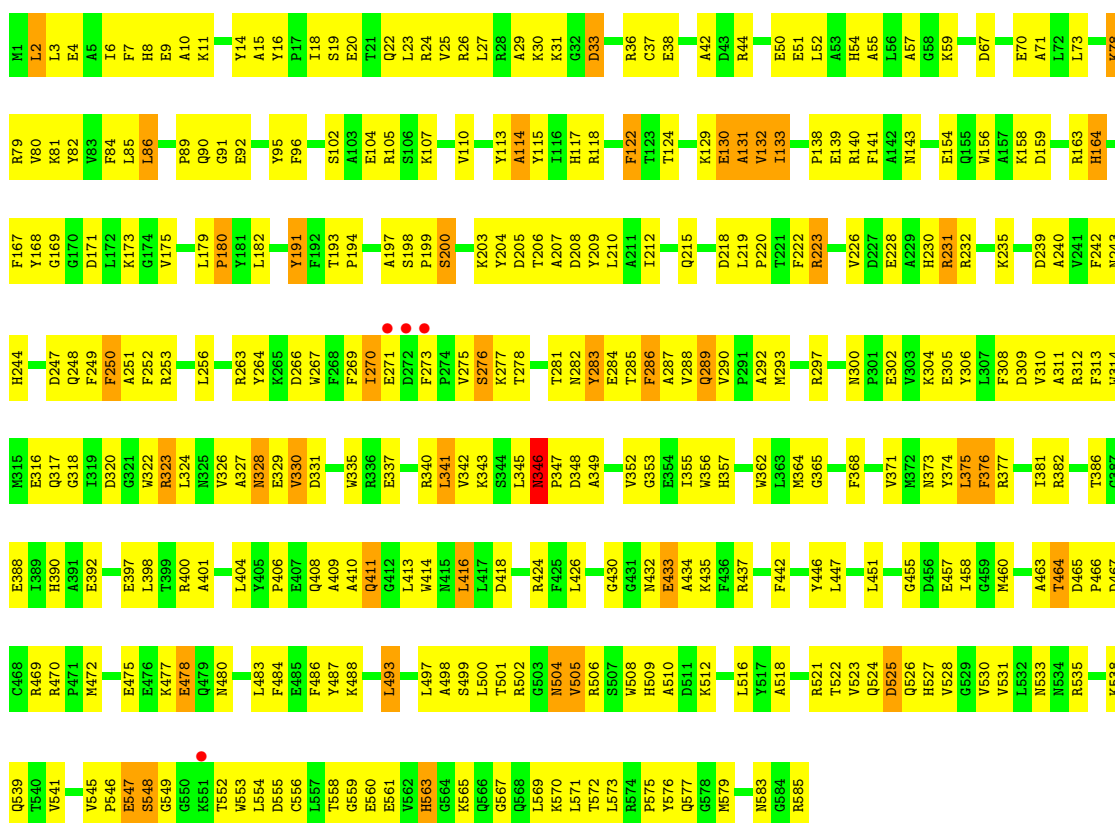
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total 60	O 60	0	0
4	B	73	Total 73	O 73	0	0

### 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.

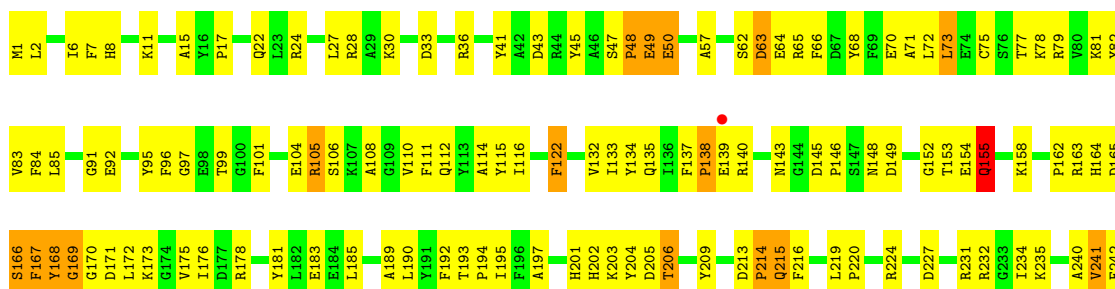
#### • Molecule 1: Neopullulanase 2

Chain A: 



#### • Molecule 1: Neopullulanase 2

Chain B: 



N243	L307	M372	G448	D525
H244	F308	N373	T449	L532
A245	D309	Y374	P450	N533
G246	V310	L375	L451	R534
		F376	Y454	R535
	F313	R377	G455	G536
F249	M314		D456	E537
F250	M315	V380	E457	K538
A251	E316	I381	I458	
F252		R382	G459	V541
R253	I319	F383	M460	L542
D254	D320	F384		L543
V255	G321	L385	A463	Q544
L256	M322	T386	T464	V545
Q257	R323	G387	D465	P546
K258	L324	E388	P466	E547
K259	N325	I389	D467	
E260	V326	H390	G468	K551
Q261	A327	A391	R469	T552
S262	R328	E392	R470	M553
R263	E329	R393	P471	L554
Y264	E330		M472	D555
K265	D331	A396	I473	C556
K266	H332	E397	W474	
W267	A333	L398	E475	K565
F268	F334	T399	E476	
F269	M335	R400	K477	Q568
I270	R336	A401	E478	L569
E271	E337	L404	Q479	
D272	F338		R480	T572
F273	R339	Q411	R481	L573
P274	R340	G412	G482	R574
V275	L341	L413	L483	P575
S276	V342	W414	F484	Y576
K277	K343	N415	E485	Q577
T278	S344	L416	F486	G578
S279	L345	L417	Y487	M579
R280	M346	D418	K488	I580
T281		S419		L581
N282	A349	H420	I491	W582
Y283	L350		R492	N583
E284	I351		L493	G584
T285	V352	R424		R585
F286	G353	F425	R496	
A287	E354			
V288	M355	N432	G503	
Q289	W356	E433	M504	
V290	H357	A434	V505	
P291	D358	K435	R506	
A292		F436	S507	
M293	G361	R437		
P294	W362	L438	K512	
K295	L363	V440		
L296	M364	L441	L516	
	D365	F442		
E299	D366		R521	
N300	Q367	T445	T522	
		Y446	V523	
	S370	L447	Q524	
V303	V371			
Y306				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.45Å 118.50Å 114.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.71 – 3.10 47.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.5 (47.71-3.10) 92.6 (47.71-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.284 0.204 , 0.278	Depositor DCC
$R_{free}$ test set	2620 reflections (11.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.8	EDS
Estimated twinning fraction	0.025 for -h,l,k 0.032 for -k,-h,-l 0.025 for l,-k,h 0.007 for l,h,k 0.007 for k,l,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26435 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC

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	0.40	0/4906	0.67	0/6641
1	B	0.39	0/4906	0.64	0/6641
All	All	0.40	0/9812	0.66	0/13282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4776	0	4611	322	0
1	B	4776	0	4611	366	0
2	A	88	0	72	5	0
2	B	88	0	72	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	60	0	0	6	0
4	B	73	0	0	5	0
All	All	9863	0	9366	678	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (678) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.34	1.06
1:A:525:ASP:HB3	1:A:585:ARG:HD3	1.39	1.02
1:B:574:ARG:HH11	1:B:574:ARG:HB2	1.21	1.01
1:B:164:HIS:NE2	2:B:907:GLC:H2	1.81	0.96
1:B:158:LYS:HD2	1:B:478:GLU:HB3	1.47	0.94
1:B:259:GLY:HA2	1:B:275:VAL:HG21	1.49	0.93
1:A:210:LEU:HD22	1:A:313:PHE:HD1	1.34	0.92
1:A:392:GLU:HG3	1:A:512:LYS:HB3	1.49	0.92
1:A:223:ARG:NH1	1:A:223:ARG:HB3	1.84	0.92
1:B:146:PRO:HA	1:B:149:ASP:OD1	1.71	0.89
1:A:223:ARG:HB3	1:A:223:ARG:HH11	1.34	0.88
1:B:356:TRP:HD1	2:B:903:GLC:HO3	1.20	0.88
1:A:44:ARG:HA	1:A:81:LYS:HD3	1.53	0.88
1:B:382:ARG:CB	1:B:382:ARG:HH21	1.86	0.87
1:A:533:ASN:HB2	1:A:573:LEU:HD12	1.56	0.85
1:A:430:GLY:HA2	4:A:1031:HOH:O	1.77	0.85
1:A:535:ARG:HD3	1:A:539:GLN:HE22	1.43	0.84
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.57	0.84
1:B:435:LYS:HG2	1:B:576:TYR:CE2	2.14	0.82
1:B:197:ALA:HA	1:B:213:ASP:HA	1.59	0.82
1:B:475:GLU:HB3	1:B:478:GLU:HG2	1.62	0.82
1:A:164:HIS:HE1	2:A:805:GLC:O3	1.61	0.81
1:A:210:LEU:HD22	1:A:313:PHE:CD1	2.15	0.81
1:A:270:ILE:HG13	1:A:283:TYR:HB3	1.63	0.81
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.61	0.80
1:A:583:ASN:HD21	1:A:585:ARG:HD2	1.45	0.80
1:A:531:VAL:HG12	1:A:573:LEU:HD11	1.64	0.80
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.64	0.80
1:A:57:ALA:CA	1:A:71:ALA:HB2	2.13	0.79
1:B:271:GLU:HB2	1:B:283:TYR:HB2	1.64	0.79
1:B:286:PHE:HB3	1:B:290:VAL:HG11	1.63	0.79
1:A:270:ILE:HD11	1:A:275:VAL:HG11	1.65	0.79
1:A:523:VAL:HG13	1:A:524:GLN:H	1.48	0.79
1:B:381:ILE:HG13	1:B:425:PHE:CE1	2.19	0.78
1:A:130:GLU:HB3	1:A:501:THR:HG21	1.66	0.76
1:B:376:PHE:O	1:B:380:VAL:HG22	1.85	0.75
1:B:565:LYS:O	1:B:565:LYS:HD2	1.86	0.75
1:A:467:ASP:O	1:A:470:ARG:HG3	1.87	0.75
1:A:392:GLU:OE1	1:A:512:LYS:HG2	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:537:GLU:HA	1:B:575:PRO:HG3	1.67	0.74
1:B:381:ILE:HG13	1:B:425:PHE:HE1	1.51	0.74
1:A:390:HIS:HD2	1:A:392:GLU:H	1.36	0.74
1:B:390:HIS:CE1	1:B:512:LYS:HG3	2.24	0.73
1:B:424:ARG:HH11	1:B:424:ARG:HG2	1.53	0.73
1:B:137:PHE:HE1	1:B:469:ARG:HD3	1.53	0.73
1:A:92:GLU:O	1:A:92:GLU:HG2	1.87	0.73
1:A:131:ALA:O	1:A:132:VAL:HG23	1.89	0.73
1:A:535:ARG:HD3	1:A:539:GLN:NE2	2.03	0.73
1:B:63:ASP:HB3	1:B:66:PHE:H	1.53	0.73
1:B:328:ASN:N	1:B:328:ASN:HD22	1.84	0.72
1:A:523:VAL:HG13	1:A:524:GLN:N	2.04	0.72
1:A:222:PHE:O	1:A:226:VAL:HG23	1.88	0.72
1:B:202:HIS:ND1	1:B:202:HIS:O	2.23	0.72
1:B:504:ASN:HD22	1:B:504:ASN:C	1.93	0.72
1:B:168:TYR:HD2	1:B:168:TYR:N	1.87	0.71
1:A:89:PRO:HB2	1:A:90:GLN:OE1	1.91	0.71
1:B:135:GLN:HB2	1:B:451:LEU:HD21	1.73	0.71
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.21	0.71
1:B:270:ILE:HB	1:B:282:ASN:HD22	1.55	0.71
1:A:455:GLY:HA3	1:A:460:MET:HG3	1.72	0.70
1:A:392:GLU:HG3	1:A:512:LYS:CB	2.21	0.70
1:B:175:VAL:HG11	1:B:192:PHE:HZ	1.56	0.70
1:B:579:MET:HG2	1:B:581:LEU:HD21	1.74	0.70
1:A:122:PHE:CE2	1:A:365:GLY:HA2	2.27	0.70
1:A:50:GLU:HG2	1:A:51:GLU:H	1.56	0.70
1:A:493:LEU:HD11	1:A:556:CYS:HB3	1.74	0.70
1:B:168:TYR:CD2	1:B:168:TYR:N	2.60	0.69
1:B:382:ARG:HH21	1:B:382:ARG:HB3	1.57	0.69
1:B:202:HIS:CG	2:B:908:GLC:H2	2.28	0.69
1:B:270:ILE:HD13	1:B:270:ILE:H	1.56	0.69
1:B:553:TRP:CE3	1:B:569:LEU:HD11	2.28	0.69
1:A:256:LEU:HD21	1:A:276:SER:HB2	1.75	0.69
1:A:275:VAL:HA	1:A:282:ASN:HB2	1.73	0.68
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.28	0.68
1:A:163:ARG:C	1:A:466:PRO:HG3	2.13	0.68
1:A:164:HIS:N	1:A:466:PRO:HG3	2.09	0.68
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.28	0.68
1:A:24:ARG:HD2	1:A:70:GLU:OE1	1.92	0.68
1:B:565:LYS:HE2	1:B:568:GLN:HB2	1.75	0.68
1:B:43:ASP:OD1	1:B:77:THR:HG21	1.94	0.68
1:A:504:ASN:O	1:A:521:ARG:HA	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:PHE:HE2	1:A:297:ARG:HA	1.58	0.67
1:A:504:ASN:C	1:A:504:ASN:HD22	1.98	0.67
1:B:275:VAL:HB	4:B:1066:HOH:O	1.94	0.66
1:B:250:PHE:CG	1:B:251:ALA:N	2.63	0.66
1:B:49:GLU:HG2	1:B:50:GLU:N	2.08	0.66
1:B:393:ARG:NH2	1:B:397:GLU:HG2	2.10	0.66
1:B:138:PRO:HD2	1:B:193:THR:HG22	1.78	0.66
1:B:166:SER:HB3	1:B:168:TYR:HE2	1.60	0.66
1:A:373:ASN:HB2	1:A:413:LEU:HB3	1.78	0.66
1:A:285:THR:HG23	1:A:293:MET:O	1.96	0.66
1:A:583:ASN:ND2	1:A:585:ARG:HD2	2.11	0.65
1:B:473:ILE:CG2	1:B:478:GLU:HB2	2.25	0.65
1:B:382:ARG:HH21	1:B:382:ARG:HB2	1.62	0.65
1:A:38:GLU:OE1	1:A:54:HIS:HB3	1.97	0.65
1:A:8:HIS:HD2	1:A:26:ARG:O	1.78	0.65
1:B:384:PHE:HE2	1:B:438:LEU:HD12	1.60	0.65
1:B:204:TYR:HB3	2:B:901:GLC:H61	1.77	0.65
1:B:545:VAL:HB	1:B:553:TRP:HH2	1.61	0.65
1:A:133:ILE:HG12	1:A:451:LEU:HD13	1.77	0.65
1:A:42:ALA:O	1:A:81:LYS:HG2	1.97	0.65
1:A:509:HIS:HD2	1:A:516:LEU:HD22	1.62	0.65
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.78	0.65
1:A:31:LYS:HA	1:A:67:ASP:OD1	1.96	0.65
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.79	0.65
1:A:27:LEU:HD13	1:A:84:PHE:CD2	2.32	0.64
1:B:553:TRP:CD1	1:B:583:ASN:HA	2.33	0.64
1:A:398:LEU:HD21	1:A:442:PHE:CZ	2.31	0.64
1:B:573:LEU:N	1:B:573:LEU:HD22	2.13	0.64
2:A:807:GLC:C5	2:A:808:GLC:H62	2.28	0.64
1:B:390:HIS:HE1	1:B:512:LYS:HG3	1.62	0.64
1:A:288:VAL:HG22	1:B:45:TYR:HB3	1.78	0.64
1:B:366:ASP:OD1	1:B:367:GLN:HG3	1.96	0.64
1:A:416:LEU:HD12	1:A:416:LEU:H	1.61	0.64
1:A:3:LEU:H	1:A:3:LEU:HD12	1.63	0.64
1:B:574:ARG:HB2	1:B:574:ARG:NH1	2.05	0.63
1:B:390:HIS:CD2	1:B:390:HIS:H	2.15	0.63
1:B:270:ILE:HD13	1:B:270:ILE:N	2.12	0.63
1:A:352:VAL:HG21	1:A:414:TRP:CZ2	2.33	0.63
1:A:270:ILE:CD1	1:A:275:VAL:HG21	2.29	0.63
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.81	0.63
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.13	0.63
1:B:572:THR:C	1:B:573:LEU:HD22	2.19	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:ASN:HB3	1:A:355:ILE:HG23	1.82	0.62
1:B:308:PHE:HE2	1:B:334:PHE:CE2	2.18	0.62
1:B:536:GLY:HA2	1:B:576:TYR:CE1	2.35	0.62
1:A:270:ILE:HD11	1:A:275:VAL:HG21	1.81	0.62
1:A:210:LEU:CD2	1:A:313:PHE:HD1	2.11	0.62
1:B:260:GLU:HA	1:B:265:LYS:HD3	1.82	0.62
1:A:505:VAL:O	1:A:506:ARG:HG2	2.00	0.62
1:A:463:ALA:O	1:A:464:THR:O	2.18	0.62
1:B:277:LYS:HB3	1:B:282:ASN:OD1	1.99	0.62
1:B:320:ASP:O	1:B:349:ALA:HA	2.00	0.61
1:A:390:HIS:CD2	1:A:392:GLU:HB2	2.36	0.61
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.30	0.61
1:B:382:ARG:HH22	1:B:389:ILE:HG23	1.65	0.61
1:B:492:ARG:O	1:B:496:ARG:HG3	2.00	0.61
1:A:31:LYS:HG3	1:A:67:ASP:OD2	1.99	0.61
1:A:560:GLU:HG2	1:A:561:GLU:N	2.16	0.61
1:B:274:PRO:C	1:B:276:SER:H	2.04	0.61
1:B:323:ARG:HD2	1:B:323:ARG:C	2.21	0.61
1:B:245:ALA:O	1:B:294:PRO:HD2	2.01	0.61
1:B:263:ARG:O	1:B:263:ARG:NE	2.31	0.61
1:A:343:LYS:HE2	1:A:349:ALA:O	2.01	0.61
1:A:206:THR:HG21	1:A:209:TYR:CG	2.36	0.61
1:B:197:ALA:HA	1:B:213:ASP:CA	2.31	0.61
1:A:382:ARG:NH1	1:A:397:GLU:OE2	2.34	0.61
1:B:536:GLY:O	1:B:537:GLU:HB2	2.00	0.60
1:B:437:ARG:HE	1:B:483:LEU:CD1	2.14	0.60
1:A:289:GLN:O	1:A:289:GLN:CG	2.49	0.60
1:B:331:ASP:OD2	1:B:333:ALA:HB3	2.00	0.60
1:B:574:ARG:HH11	1:B:574:ARG:CB	2.07	0.60
1:B:393:ARG:HH22	1:B:397:GLU:HG2	1.67	0.60
1:A:398:LEU:HD21	1:A:442:PHE:HZ	1.66	0.60
1:B:441:LEU:HD13	1:B:578:GLY:HA3	1.83	0.60
1:A:516:LEU:C	1:A:516:LEU:HD23	2.23	0.60
1:B:350:LEU:HD12	1:B:351:ILE:H	1.66	0.60
1:A:140:ARG:HG2	1:A:469:ARG:O	2.02	0.59
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.37	0.59
1:A:130:GLU:HB3	1:A:501:THR:CG2	2.31	0.59
1:B:240:ALA:HB1	1:B:242:PHE:CE1	2.37	0.59
1:B:259:GLY:CA	1:B:275:VAL:HG21	2.27	0.59
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.02	0.59
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.18	0.59
1:B:137:PHE:CE1	1:B:469:ARG:HD3	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:390:HIS:HD2	1:B:390:HIS:H	1.49	0.59
1:B:356:TRP:NE1	2:B:902:GLC:O2	2.35	0.59
1:B:139:GLU:OE2	1:B:169:GLY:HA2	2.02	0.59
1:A:373:ASN:ND2	1:A:376:PHE:HB2	2.18	0.59
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.85	0.59
1:A:164:HIS:CE1	2:A:805:GLC:O3	2.50	0.59
1:B:432:ASN:OD1	1:B:434:ALA:HB3	2.03	0.59
1:B:503:GLY:HA2	1:B:523:VAL:HG23	1.83	0.59
1:A:304:LYS:NZ	1:A:337:GLU:OE1	2.35	0.59
1:B:477:LYS:HA	4:B:1041:HOH:O	2.02	0.59
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.85	0.59
1:B:253:ARG:HH11	1:B:253:ARG:CB	2.16	0.58
1:B:253:ARG:C	1:B:255:VAL:H	2.06	0.58
1:B:255:VAL:O	1:B:275:VAL:HG21	2.02	0.58
1:B:536:GLY:HA2	1:B:576:TYR:HE1	1.68	0.58
1:B:224:ARG:HA	1:B:224:ARG:HE	1.68	0.58
1:A:244:HIS:CE1	1:A:293:MET:SD	2.97	0.58
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.39	0.58
1:B:533:ASN:O	1:B:576:TYR:HA	2.04	0.58
1:B:473:ILE:HG21	1:B:478:GLU:HB2	1.86	0.58
1:B:389:ILE:HB	1:B:393:ARG:HB3	1.86	0.57
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.39	0.57
1:A:218:ASP:HB2	1:A:220:PRO:HD2	1.87	0.57
1:B:357:HIS:HA	1:B:374:TYR:OH	2.05	0.57
1:B:382:ARG:HH22	1:B:389:ILE:CG2	2.18	0.57
1:B:435:LYS:HG2	1:B:576:TYR:HE2	1.68	0.57
1:B:270:ILE:H	1:B:270:ILE:CD1	2.16	0.57
1:A:353:GLY:O	1:A:371:VAL:HA	2.04	0.57
1:A:458:ILE:HG22	1:A:484:PHE:HB2	1.85	0.57
1:B:479:GLN:OE1	1:B:481:ARG:NH1	2.36	0.57
1:B:393:ARG:NH2	1:B:397:GLU:CG	2.68	0.57
1:B:122:PHE:HB2	4:B:1003:HOH:O	2.05	0.57
1:A:219:LEU:HD21	1:A:317:GLN:OE1	2.03	0.57
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.86	0.57
1:A:78:LYS:HB2	1:A:115:TYR:CE2	2.40	0.57
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.37	0.57
1:A:50:GLU:HG2	1:A:51:GLU:N	2.20	0.56
1:A:416:LEU:CD1	1:A:416:LEU:H	2.18	0.56
1:B:384:PHE:CE2	1:B:438:LEU:HD12	2.38	0.56
1:B:139:GLU:CD	1:B:169:GLY:HA2	2.26	0.56
1:B:139:GLU:HG2	1:B:216:PHE:CE1	2.40	0.56
1:A:357:HIS:CD2	1:B:112:GLN:HB2	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:545:VAL:HG21	1:A:569:LEU:HB2	1.86	0.56
1:A:504:ASN:ND2	1:A:504:ASN:C	2.58	0.56
1:B:475:GLU:CB	1:B:478:GLU:HG2	2.35	0.56
1:B:43:ASP:O	1:B:81:LYS:HE2	2.06	0.56
1:A:316:GLU:HB3	1:A:317:GLN:HE21	1.70	0.56
1:B:286:PHE:HE2	2:B:902:GLC:H62	1.70	0.56
1:B:138:PRO:CD	1:B:193:THR:HG22	2.35	0.56
1:B:275:VAL:HG22	1:B:275:VAL:O	2.06	0.56
1:B:258:LYS:HB2	1:B:262:SER:HB2	1.86	0.56
1:B:154:GLU:O	1:B:155:GLN:HB3	2.05	0.56
1:A:193:THR:HB	1:A:194:PRO:CD	2.35	0.56
1:A:110:VAL:O	1:A:110:VAL:HG13	2.07	0.55
1:A:230:HIS:C	1:A:232:ARG:H	2.09	0.55
1:B:143:ASN:ND2	1:B:169:GLY:O	2.38	0.55
1:B:445:THR:O	1:B:521:ARG:NH1	2.38	0.55
1:A:326:VAL:O	1:A:326:VAL:HG12	2.06	0.55
1:B:314:TRP:HA	1:B:314:TRP:CE3	2.40	0.55
1:A:510:ALA:O	4:A:1056:HOH:O	2.18	0.55
1:B:253:ARG:HH11	1:B:253:ARG:HB3	1.72	0.55
1:A:553:TRP:CZ3	1:A:569:LEU:HD22	2.41	0.55
1:B:41:TYR:CD2	1:B:73:LEU:HG	2.41	0.55
1:A:11:LYS:N	1:A:15:ALA:HB3	2.22	0.55
1:A:552:THR:HA	1:A:563:HIS:HA	1.88	0.55
1:B:27:LEU:C	1:B:27:LEU:HD23	2.27	0.55
1:B:213:ASP:CG	1:B:214:PRO:HD2	2.27	0.55
1:B:315:MET:SD	1:B:342:VAL:HG22	2.47	0.55
1:B:227:ASP:O	1:B:231:ARG:HG2	2.06	0.55
1:A:390:HIS:CD2	1:A:392:GLU:H	2.20	0.55
1:A:218:ASP:CB	1:A:220:PRO:HD2	2.37	0.55
1:B:97:GLY:HA3	1:B:108:ALA:O	2.07	0.55
1:A:269:PHE:HB2	1:A:284:GLU:HB2	1.90	0.54
1:B:241:VAL:C	1:B:242:PHE:HD1	2.11	0.54
1:B:538:LYS:HA	1:B:573:LEU:O	2.07	0.54
1:A:171:ASP:O	1:A:175:VAL:HG23	2.07	0.54
1:A:80:VAL:HG22	1:A:81:LYS:N	2.22	0.54
1:B:271:GLU:N	1:B:283:TYR:HB2	2.23	0.54
1:A:401:ALA:O	1:A:404:LEU:HB2	2.07	0.54
1:A:437:ARG:HG2	1:A:486:PHE:CD1	2.43	0.54
1:B:356:TRP:HA	1:B:356:TRP:CE3	2.41	0.54
1:B:242:PHE:CD2	1:B:307:LEU:HD22	2.43	0.54
1:B:271:GLU:HB2	1:B:283:TYR:CB	2.37	0.54
1:B:545:VAL:HB	1:B:553:TRP:CH2	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:285:THR:HG21	1:A:290:VAL:O	2.08	0.54
1:A:250:PHE:HE2	1:A:306:TYR:CE2	2.26	0.54
1:B:580:ILE:HG22	1:B:580:ILE:O	2.08	0.53
1:A:139:GLU:OE2	1:A:140:ARG:HD2	2.07	0.53
1:B:206:THR:HB	1:B:209:TYR:CZ	2.43	0.53
1:B:83:VAL:HG23	1:B:96:PHE:O	2.07	0.53
1:A:570:LYS:O	1:A:571:LEU:HD12	2.08	0.53
1:B:27:LEU:HD23	1:B:28:ARG:N	2.24	0.53
1:B:22:GLN:HB3	1:B:72:LEU:HD11	1.90	0.53
1:B:92:GLU:CD	1:B:92:GLU:H	2.11	0.53
1:B:542:LEU:HD21	1:B:568:GLN:HE22	1.74	0.53
1:B:346:ASN:HB3	1:B:349:ALA:HB2	1.89	0.53
1:B:287:ALA:H	1:B:290:VAL:HG21	1.74	0.53
1:A:122:PHE:O	1:A:408:GLN:HG2	2.09	0.53
1:B:104:GLU:HB3	4:B:1050:HOH:O	2.08	0.53
1:B:253:ARG:HB2	1:B:253:ARG:NH1	2.24	0.53
1:A:531:VAL:CG1	1:A:573:LEU:HD11	2.36	0.53
1:A:85:LEU:HD23	1:A:95:TYR:CE2	2.44	0.53
1:A:357:HIS:HB3	1:B:112:GLN:NE2	2.23	0.53
1:A:248:GLN:OE1	1:A:253:ARG:HD3	2.09	0.53
1:B:1:MET:HA	1:B:33:ASP:OD1	2.08	0.52
1:B:516:LEU:HD12	1:B:533:ASN:HA	1.90	0.52
1:B:138:PRO:HB2	1:B:216:PHE:CE1	2.44	0.52
1:B:382:ARG:NH2	1:B:382:ARG:CB	2.66	0.52
1:B:328:ASN:ND2	1:B:328:ASN:N	2.56	0.52
1:A:219:LEU:N	1:A:220:PRO:CD	2.71	0.52
1:B:253:ARG:O	1:B:255:VAL:N	2.41	0.52
1:A:206:THR:HG21	1:A:209:TYR:CD1	2.44	0.52
1:B:373:ASN:ND2	1:B:376:PHE:HB2	2.25	0.52
1:B:339:ARG:HD2	1:B:367:GLN:O	2.10	0.52
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.44	0.52
1:B:173:LYS:HD2	1:B:176:ILE:HD12	1.92	0.52
1:B:267:TRP:N	1:B:267:TRP:CD1	2.76	0.52
1:A:377:ARG:NH2	1:A:381:ILE:HD11	2.25	0.52
1:B:146:PRO:C	1:B:148:ASN:H	2.13	0.52
1:B:356:TRP:HE3	1:B:356:TRP:HA	1.75	0.52
1:A:122:PHE:HB3	1:A:408:GLN:HG2	1.92	0.52
1:B:504:ASN:ND2	1:B:504:ASN:C	2.59	0.52
1:B:168:TYR:CD1	1:B:471:PRO:HG3	2.45	0.52
1:B:382:ARG:NH2	1:B:382:ARG:HB3	2.22	0.51
1:B:438:LEU:HD11	1:B:532:LEU:HB3	1.92	0.51
1:A:283:TYR:N	1:A:283:TYR:CD2	2.78	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:117:HIS:CD2	1:B:331:ASP:HB3	2.44	0.51
1:A:357:HIS:HB3	1:B:112:GLN:HE21	1.75	0.51
1:A:346:ASN:HD22	1:A:346:ASN:C	2.12	0.51
1:A:523:VAL:CG1	1:A:524:GLN:H	2.19	0.51
1:A:130:GLU:HA	1:A:501:THR:HG23	1.91	0.51
1:B:324:LEU:HD22	1:B:335:TRP:CH2	2.46	0.51
1:A:9:GLU:O	1:A:11:LYS:N	2.34	0.51
1:A:250:PHE:CG	1:A:251:ALA:N	2.77	0.51
1:A:52:LEU:HD11	1:A:105:ARG:CZ	2.41	0.51
1:B:424:ARG:HG2	1:B:424:ARG:NH1	2.24	0.51
1:A:228:GLU:OE2	1:A:231:ARG:HD3	2.10	0.51
1:B:158:LYS:HD2	1:B:478:GLU:CB	2.31	0.51
1:A:133:ILE:CG1	1:A:451:LEU:HD13	2.40	0.51
1:A:79:ARG:HG2	1:A:115:TYR:HD2	1.76	0.51
1:A:345:LEU:O	1:A:346:ASN:HB2	2.10	0.51
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.93	0.51
1:A:552:THR:OG1	1:A:563:HIS:HB3	2.10	0.51
1:B:253:ARG:HA	1:B:256:LEU:HG	1.92	0.51
1:A:424:ARG:NH1	1:A:460:MET:HB2	2.26	0.51
1:A:92:GLU:O	1:A:92:GLU:CG	2.55	0.51
1:A:414:TRP:CE3	1:A:451:LEU:HD22	2.46	0.51
1:A:249:PHE:CE2	1:A:251:ALA:HB3	2.46	0.51
1:B:271:GLU:CB	1:B:283:TYR:HB2	2.38	0.50
1:B:437:ARG:HE	1:B:483:LEU:HD12	1.76	0.50
1:B:152:GLY:O	1:B:153:THR:C	2.50	0.50
1:A:413:LEU:HD22	1:A:413:LEU:H	1.76	0.50
1:B:324:LEU:HD22	1:B:335:TRP:CZ3	2.46	0.50
1:A:248:GLN:HA	1:A:248:GLN:OE1	2.11	0.50
1:B:91:GLY:N	1:B:92:GLU:OE2	2.44	0.50
1:A:7:PHE:CG	1:A:8:HIS:N	2.80	0.50
1:A:289:GLN:O	1:A:289:GLN:HG3	2.11	0.50
1:A:78:LYS:N	1:A:78:LYS:HD2	2.26	0.50
1:B:253:ARG:NH1	1:B:253:ARG:CB	2.74	0.50
1:A:139:GLU:OE1	1:A:168:TYR:N	2.29	0.50
1:A:500:LEU:HD21	1:A:528:VAL:HG11	1.92	0.50
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.47	0.50
1:B:78:LYS:O	1:B:115:TYR:HA	2.11	0.50
1:A:230:HIS:HE1	1:A:318:GLY:O	1.95	0.50
1:B:175:VAL:HG11	1:B:192:PHE:CZ	2.43	0.50
1:B:173:LYS:HA	1:B:176:ILE:HD12	1.93	0.50
1:B:544:GLN:HA	1:B:544:GLN:HE21	1.77	0.50
1:B:352:VAL:HG21	1:B:414:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:531:VAL:HB	1:A:579:MET:HB2	1.93	0.50
1:B:573:LEU:N	1:B:573:LEU:CD2	2.74	0.50
1:A:31:LYS:HA	1:A:67:ASP:CG	2.32	0.50
1:A:386:THR:OG1	1:A:388:GLU:HG3	2.12	0.50
1:A:526:GLN:HA	1:A:585:ARG:HB2	1.93	0.49
1:B:475:GLU:O	1:B:477:LYS:N	2.45	0.49
1:B:573:LEU:HD13	1:B:579:MET:CE	2.42	0.49
1:B:153:THR:HA	1:B:167:PHE:O	2.13	0.49
1:A:327:ALA:HB1	1:A:368:PHE:CZ	2.47	0.49
1:A:124:THR:O	1:A:129:LYS:NZ	2.46	0.49
1:A:497:LEU:C	1:A:499:SER:H	2.16	0.49
1:A:240:ALA:HB1	1:A:242:PHE:CE1	2.47	0.49
1:B:167:PHE:HZ	1:B:215:GLN:HE22	1.57	0.49
1:A:331:ASP:OD1	1:A:331:ASP:N	2.45	0.49
1:A:285:THR:HG22	1:A:287:ALA:H	1.77	0.49
1:B:547:GLU:HG2	1:B:551:LYS:CE	2.42	0.49
1:A:308:PHE:O	1:A:311:ALA:HB3	2.13	0.49
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.48	0.49
1:B:475:GLU:C	1:B:477:LYS:N	2.64	0.49
1:B:64:GLU:HB3	1:B:396:ALA:HB1	1.95	0.49
1:A:516:LEU:HD13	1:A:541:VAL:CG1	2.39	0.49
1:B:484:PHE:O	1:B:488:LYS:HG3	2.13	0.49
1:B:183:GLU:CD	1:B:232:ARG:HG3	2.33	0.49
1:B:140:ARG:HD2	1:B:469:ARG:O	2.12	0.48
1:B:488:LYS:HB3	1:B:492:ARG:HH11	1.78	0.48
1:B:133:ILE:HG22	1:B:134:TYR:N	2.27	0.48
1:B:306:TYR:O	1:B:310:VAL:HG23	2.13	0.48
1:B:258:LYS:HD3	1:B:261:GLN:O	2.12	0.48
1:A:316:GLU:HB3	1:A:317:GLN:NE2	2.28	0.48
1:B:172:LEU:O	1:B:176:ILE:HG13	2.13	0.48
1:B:202:HIS:CB	2:B:908:GLC:H2	2.43	0.48
1:A:288:VAL:CG2	1:B:45:TYR:HB3	2.41	0.48
1:B:205:ASP:HB3	1:B:293:MET:CE	2.43	0.48
1:B:181:TYR:OH	1:B:458:ILE:HG23	2.13	0.48
1:A:247:ASP:OD2	1:A:292:ALA:HA	2.12	0.48
1:A:23:LEU:HD23	1:A:25:VAL:HG13	1.94	0.48
1:B:393:ARG:O	1:B:397:GLU:HG3	2.14	0.48
1:B:401:ALA:O	1:B:404:LEU:HB2	2.13	0.48
1:A:230:HIS:O	1:A:232:ARG:N	2.47	0.48
1:B:504:ASN:O	1:B:521:ARG:HA	2.13	0.48
1:A:235:LYS:HB3	1:A:320:ASP:OD2	2.14	0.48
1:B:253:ARG:C	1:B:255:VAL:N	2.67	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:463:ALA:H	1:A:467:ASP:HB3	1.79	0.48
1:B:545:VAL:HG21	1:B:553:TRP:CZ3	2.49	0.48
1:A:565:LYS:HZ1	1:A:570:LYS:HD2	1.78	0.48
1:A:219:LEU:O	1:A:219:LEU:HD13	2.14	0.48
1:B:114:ALA:O	1:B:115:TYR:HB2	2.14	0.48
1:A:565:LYS:NZ	1:A:570:LYS:HD2	2.29	0.48
1:A:558:THR:O	1:A:560:GLU:N	2.47	0.48
1:B:181:TYR:CE1	1:B:484:PHE:CE2	3.02	0.47
1:A:416:LEU:N	1:A:416:LEU:HD12	2.29	0.47
1:A:129:LYS:HA	1:A:411:GLN:OE1	2.14	0.47
1:A:82:TYR:H	1:A:110:VAL:HG22	1.79	0.47
1:B:313:PHE:O	1:B:316:GLU:CB	2.62	0.47
1:A:23:LEU:CD2	1:A:25:VAL:HG13	2.44	0.47
1:B:259:GLY:C	1:B:261:GLN:N	2.68	0.47
1:A:44:ARG:HG3	1:A:80:VAL:C	2.34	0.47
1:B:154:GLU:OE1	1:B:166:SER:HA	2.14	0.47
1:B:441:LEU:CD1	1:B:578:GLY:HA3	2.45	0.47
1:B:315:MET:HG3	1:B:322:TRP:HZ2	1.78	0.47
1:A:122:PHE:HB3	1:A:408:GLN:CG	2.44	0.47
1:A:547:GLU:HG3	1:A:567:GLY:HA2	1.97	0.47
1:A:426:LEU:HD13	1:A:426:LEU:O	2.14	0.47
1:B:95:TYR:CE2	1:B:105:ARG:HD3	2.49	0.47
1:B:425:PHE:HB3	1:B:436:PHE:CE1	2.49	0.47
1:B:415:ASN:HD21	1:B:448:GLY:HA3	1.79	0.47
1:B:545:VAL:HG21	1:B:569:LEU:HG	1.95	0.47
1:B:544:GLN:HA	1:B:544:GLN:NE2	2.28	0.47
1:A:400:ARG:HH12	1:B:99:THR:C	2.18	0.47
1:A:465:ASP:HA	1:A:466:PRO:HA	1.23	0.47
1:A:4:GLU:HG2	1:B:30:LYS:HG3	1.97	0.47
1:B:363:LEU:HD11	1:B:371:VAL:HG22	1.97	0.47
1:A:335:TRP:HA	1:A:335:TRP:HE3	1.78	0.47
1:A:199:PRO:HG2	1:A:200:SER:H	1.79	0.47
1:A:410:ALA:HA	1:A:413:LEU:CD2	2.45	0.47
1:A:235:LYS:HB3	1:A:320:ASP:CG	2.35	0.47
1:B:280:ARG:HE	1:B:280:ARG:HA	1.80	0.47
1:A:266:ASP:O	1:A:300:ASN:ND2	2.48	0.47
1:A:264:TYR:O	1:A:267:TRP:HB2	2.14	0.47
1:B:204:TYR:HE2	1:B:420:HIS:HE2	1.63	0.47
1:A:36:ARG:NH2	1:A:38:GLU:OE2	2.48	0.47
1:B:17:PRO:HB3	1:B:116:ILE:HG23	1.96	0.47
1:B:132:VAL:HG11	1:B:491:ILE:HD12	1.95	0.47
1:A:158:LYS:O	1:A:158:LYS:HG2	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:PRO:HG3	4:A:1047:HOH:O	2.14	0.46
2:A:807:GLC:O5	2:A:808:GLC:H62	2.15	0.46
1:A:416:LEU:CD1	1:A:416:LEU:N	2.78	0.46
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.97	0.46
1:A:194:PRO:HG2	1:A:204:TYR:CD1	2.50	0.46
1:A:37:CYS:O	1:A:57:ALA:HB3	2.16	0.46
1:B:255:VAL:CG2	1:B:264:TYR:HB2	2.45	0.46
1:B:356:TRP:CZ3	1:B:372:MET:HB2	2.51	0.46
1:B:43:ASP:CG	1:B:77:THR:HG21	2.35	0.46
1:B:439:ALA:O	1:B:442:PHE:N	2.48	0.46
1:A:141:PHE:O	1:A:472:MET:HB3	2.15	0.46
1:B:357:HIS:O	1:B:358:ASP:C	2.54	0.46
1:A:572:THR:C	1:A:573:LEU:HD23	2.36	0.46
1:B:553:TRP:CE3	1:B:569:LEU:HD21	2.51	0.46
1:A:521:ARG:HH21	1:A:521:ARG:HG3	1.80	0.46
1:B:205:ASP:O	1:B:246:GLY:HA3	2.16	0.46
1:A:143:ASN:ND2	1:A:169:GLY:HA3	2.31	0.46
1:B:537:GLU:CA	1:B:575:PRO:HG3	2.41	0.46
1:B:274:PRO:HG2	1:B:276:SER:O	2.16	0.46
1:B:516:LEU:HD12	1:B:532:LEU:O	2.16	0.46
1:A:115:TYR:HB3	1:A:117:HIS:CE1	2.51	0.46
1:A:546:PRO:C	1:A:548:SER:H	2.19	0.46
1:A:455:GLY:HA3	1:A:460:MET:CG	2.45	0.46
2:A:807:GLC:H5	2:A:808:GLC:H62	1.98	0.45
1:B:315:MET:HG3	1:B:322:TRP:CZ2	2.51	0.45
1:A:386:THR:CB	1:A:388:GLU:HG3	2.46	0.45
1:A:575:PRO:O	1:A:577:GLN:N	2.49	0.45
1:B:63:ASP:HB2	1:B:68:TYR:HE1	1.80	0.45
1:A:310:VAL:O	1:A:314:TRP:HD1	2.00	0.45
1:B:242:PHE:CG	1:B:307:LEU:HD22	2.51	0.45
1:B:259:GLY:C	1:B:261:GLN:H	2.20	0.45
1:B:290:VAL:HG12	1:B:290:VAL:O	2.16	0.45
1:A:283:TYR:HD2	1:A:283:TYR:N	2.14	0.45
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.50	0.45
1:B:194:PRO:HG2	1:B:204:TYR:CD1	2.51	0.45
1:B:64:GLU:C	1:B:65:ARG:HG3	2.37	0.45
1:B:77:THR:HG22	1:B:77:THR:O	2.17	0.45
1:A:218:ASP:CG	1:A:220:PRO:HD2	2.35	0.45
1:A:323:ARG:C	1:A:323:ARG:HD2	2.37	0.45
1:B:183:GLU:OE2	1:B:232:ARG:HD2	2.16	0.45
1:A:305:GLU:HG3	4:A:1033:HOH:O	2.16	0.45
1:B:565:LYS:HE3	1:B:568:GLN:HE21	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:ARG:HH21	1:B:36:ARG:HG3	1.81	0.45
1:B:178:ARG:O	1:B:181:TYR:HB3	2.17	0.45
1:A:554:LEU:HD23	1:A:555:ASP:N	2.31	0.45
1:A:525:ASP:O	1:A:585:ARG:HD2	2.17	0.45
1:B:138:PRO:CG	1:B:193:THR:HG22	2.47	0.45
1:B:308:PHE:CE2	1:B:334:PHE:CE2	3.02	0.45
1:B:341:LEU:O	1:B:344:SER:OG	2.21	0.45
1:A:113:TYR:O	1:A:114:ALA:C	2.54	0.45
1:B:425:PHE:HB3	1:B:436:PHE:HE1	1.81	0.45
1:B:202:HIS:O	1:B:204:TYR:N	2.50	0.45
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.52	0.45
1:B:541:VAL:HG22	1:B:542:LEU:N	2.31	0.45
1:A:484:PHE:O	1:A:488:LYS:HG3	2.17	0.45
1:A:7:PHE:HE2	1:A:14:TYR:CD2	2.35	0.45
1:B:583:ASN:HD21	1:B:585:ARG:HB2	1.81	0.45
1:B:472:MET:HG2	1:B:474:TRP:CZ2	2.52	0.45
1:A:457:GLU:HG2	1:A:458:ILE:HG23	1.99	0.45
1:A:2:LEU:N	1:A:33:ASP:OD2	2.50	0.45
1:A:446:TYR:CG	1:A:447:LEU:N	2.85	0.45
1:B:146:PRO:C	1:B:148:ASN:N	2.71	0.44
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.98	0.44
1:B:165:ASP:O	1:B:166:SER:O	2.35	0.44
1:B:193:THR:O	1:B:195:ILE:HG23	2.17	0.44
1:A:226:VAL:HG12	1:A:230:HIS:CE1	2.52	0.44
1:A:409:ALA:O	1:A:413:LEU:HD22	2.18	0.44
1:A:346:ASN:ND2	1:A:348:ASP:H	2.15	0.44
1:A:386:THR:HB	1:A:388:GLU:HG3	1.99	0.44
1:A:179:LEU:N	1:A:180:PRO:CD	2.80	0.44
1:A:488:LYS:HB2	4:A:1029:HOH:O	2.17	0.44
1:B:82:TYR:N	1:B:110:VAL:CG2	2.80	0.44
1:A:81:LYS:O	1:A:82:TYR:HB3	2.17	0.44
1:A:518:ALA:HA	1:A:530:VAL:O	2.17	0.44
1:A:464:THR:HG22	1:A:465:ASP:N	2.32	0.44
1:A:95:TYR:CD2	1:A:105:ARG:HA	2.52	0.44
1:A:433:GLU:HG2	1:A:433:GLU:O	2.17	0.44
1:A:522:THR:HG23	1:A:527:HIS:HD2	1.81	0.44
1:B:252:PHE:CE2	1:B:256:LEU:HD21	2.52	0.44
1:B:435:LYS:O	1:B:436:PHE:C	2.54	0.44
1:B:193:THR:OG1	1:B:194:PRO:CD	2.65	0.44
1:B:542:LEU:HD11	1:B:568:GLN:HB3	2.00	0.44
1:B:346:ASN:ND2	1:B:349:ALA:N	2.66	0.44
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:435:LYS:HE2	1:B:576:TYR:OH	2.18	0.44
1:B:171:ASP:HB2	1:B:216:PHE:O	2.17	0.44
1:B:64:GLU:O	1:B:65:ARG:HG3	2.17	0.44
1:B:77:THR:HG21	1:B:79:ARG:HH21	1.83	0.44
1:A:133:ILE:HD11	1:A:414:TRP:CZ3	2.52	0.44
1:B:547:GLU:HG2	1:B:551:LYS:NZ	2.32	0.44
1:B:354:GLU:C	1:B:355:ILE:HD12	2.38	0.44
1:B:493:LEU:HD21	1:B:556:CYS:HB3	2.00	0.44
1:A:243:ASN:ND2	1:A:286:PHE:HB2	2.33	0.44
1:B:250:PHE:C	1:B:250:PHE:CD1	2.89	0.44
1:B:390:HIS:CD2	1:B:390:HIS:N	2.83	0.44
1:B:390:HIS:O	1:B:391:ALA:C	2.55	0.44
1:A:327:ALA:C	1:A:329:GLU:H	2.21	0.44
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.99	0.44
1:A:432:ASN:OD1	1:A:434:ALA:HB3	2.18	0.44
1:A:80:VAL:CG2	1:A:81:LYS:N	2.81	0.44
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.83	0.44
1:A:545:VAL:O	1:A:545:VAL:HG23	2.18	0.44
1:A:209:TYR:HB3	1:A:310:VAL:HG11	2.00	0.44
1:A:572:THR:O	1:A:573:LEU:HD23	2.18	0.43
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.33	0.43
1:A:240:ALA:HB2	1:A:322:TRP:HE3	1.83	0.43
1:B:255:VAL:HG22	1:B:264:TYR:HB2	2.00	0.43
1:B:377:ARG:HG2	1:B:377:ARG:NH1	2.32	0.43
1:B:283:TYR:CG	1:B:284:GLU:N	2.85	0.43
1:B:459:GLY:O	1:B:460:MET:HB2	2.18	0.43
1:A:84:PHE:HB3	1:A:86:LEU:HD21	1.99	0.43
1:B:446:TYR:CG	1:B:447:LEU:N	2.86	0.43
1:B:296:LEU:HD13	1:B:307:LEU:HD11	2.00	0.43
1:B:377:ARG:O	1:B:381:ILE:HB	2.19	0.43
1:B:390:HIS:O	1:B:392:GLU:N	2.51	0.43
1:B:424:ARG:NH2	1:B:454:TYR:O	2.51	0.43
1:A:156:TRP:CE3	1:A:168:TYR:HB3	2.53	0.43
1:A:346:ASN:HD22	1:A:347:PRO:N	2.16	0.43
1:B:555:ASP:OD1	1:B:579:MET:HG3	2.19	0.43
1:A:285:THR:HG21	1:A:290:VAL:HB	2.01	0.43
1:B:213:ASP:HB3	1:B:216:PHE:HD2	1.83	0.43
1:A:270:ILE:HG13	1:A:283:TYR:CB	2.42	0.43
1:B:579:MET:HG2	1:B:581:LEU:CD2	2.47	0.43
1:B:472:MET:HG3	1:B:474:TRP:CE2	2.53	0.43
1:A:197:ALA:O	1:A:207:ALA:HB3	2.19	0.43
1:B:185:LEU:HD22	1:B:457:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:530:VAL:HA	1:A:579:MET:O	2.18	0.43
1:A:328:ASN:O	1:B:114:ALA:HB1	2.18	0.43
1:B:57:ALA:HA	1:B:70:GLU:O	2.18	0.43
1:A:198:SER:HB3	1:A:203:LYS:CD	2.49	0.43
1:B:300:ASN:HB3	1:B:303:VAL:CG2	2.49	0.43
1:B:285:THR:OG1	1:B:286:PHE:N	2.52	0.43
1:A:538:LYS:HE2	1:A:572:THR:HG21	2.01	0.43
1:A:463:ALA:C	1:A:464:THR:O	2.56	0.43
1:A:376:PHE:CD1	1:A:376:PHE:C	2.91	0.43
1:B:463:ALA:HB3	1:B:467:ASP:HB3	1.99	0.43
1:A:483:LEU:O	1:A:486:PHE:N	2.52	0.43
1:B:535:ARG:HG2	1:B:535:ARG:NH1	2.34	0.43
1:B:63:ASP:OD2	1:B:64:GLU:N	2.52	0.43
1:A:27:LEU:HD13	1:A:84:PHE:CE2	2.54	0.43
1:B:245:ALA:O	1:B:293:MET:HA	2.19	0.43
1:B:315:MET:HA	1:B:319:ILE:HG12	1.99	0.43
1:B:416:LEU:H	1:B:416:LEU:HD23	1.84	0.43
1:B:277:LYS:HD2	1:B:282:ASN:HB3	2.00	0.42
1:A:324:LEU:HD12	1:A:368:PHE:CE2	2.54	0.42
1:B:213:ASP:OD1	1:B:214:PRO:HD2	2.18	0.42
1:B:274:PRO:C	1:B:276:SER:N	2.71	0.42
1:B:110:VAL:HG22	1:B:111:PHE:O	2.20	0.42
1:B:82:TYR:C	1:B:110:VAL:HG23	2.40	0.42
1:B:458:ILE:HG12	1:B:472:MET:CE	2.49	0.42
1:A:287:ALA:HB3	1:A:290:VAL:HG23	2.01	0.42
1:A:273:PHE:N	1:A:273:PHE:CD1	2.87	0.42
1:B:483:LEU:O	1:B:486:PHE:N	2.53	0.42
1:B:324:LEU:HD21	1:B:338:PHE:HE2	1.84	0.42
1:A:480:ASN:O	1:A:483:LEU:HB2	2.20	0.42
1:A:4:GLU:OE1	1:B:30:LYS:HE2	2.19	0.42
1:B:249:PHE:HZ	1:B:306:TYR:CE1	2.37	0.42
1:B:145:ASP:HB3	1:B:148:ASN:HD21	1.85	0.42
1:B:377:ARG:CZ	1:B:381:ILE:HD12	2.50	0.42
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.83	0.42
1:A:424:ARG:NH1	1:A:460:MET:CB	2.82	0.42
1:B:464:THR:O	1:B:465:ASP:C	2.57	0.42
1:A:25:VAL:HG22	1:A:71:ALA:O	2.18	0.42
1:B:251:ALA:O	1:B:255:VAL:HG23	2.18	0.42
1:A:424:ARG:NH1	1:A:460:MET:HG3	2.35	0.42
1:B:458:ILE:HD12	1:B:459:GLY:O	2.20	0.42
1:B:24:ARG:HD2	1:B:70:GLU:CG	2.50	0.42
1:A:330:VAL:HG11	1:A:335:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:GLU:CG	1:B:30:LYS:HG3	2.49	0.42
1:B:202:HIS:C	1:B:204:TYR:H	2.22	0.42
1:A:36:ARG:HH12	1:A:85:LEU:HD12	1.85	0.42
1:A:159:ASP:HA	4:A:1037:HOH:O	2.18	0.42
1:A:23:LEU:HD23	1:A:23:LEU:C	2.40	0.42
1:A:475:GLU:CD	1:A:478:GLU:HG3	2.40	0.42
1:A:525:ASP:O	1:A:585:ARG:CD	2.68	0.42
1:A:390:HIS:NE2	1:A:392:GLU:HB2	2.34	0.42
1:A:553:TRP:HZ3	1:A:569:LEU:HD13	1.83	0.42
1:A:330:VAL:HG13	1:A:335:TRP:HE1	1.84	0.42
1:B:352:VAL:HA	1:B:370:SER:O	2.20	0.42
1:A:424:ARG:HH11	1:A:460:MET:HB2	1.85	0.42
1:A:104:GLU:O	1:A:105:ARG:C	2.58	0.42
1:A:545:VAL:HG22	1:A:569:LEU:N	2.34	0.42
1:B:27:LEU:HD12	1:B:84:PHE:CD2	2.55	0.42
1:A:497:LEU:O	1:A:499:SER:N	2.53	0.42
1:A:6:ILE:HG12	1:A:29:ALA:CB	2.50	0.42
1:B:467:ASP:CG	1:B:470:ARG:HH11	2.22	0.41
1:B:340:ARG:O	1:B:344:SER:HB3	2.20	0.41
1:B:268:PHE:O	1:B:269:PHE:HD2	2.03	0.41
1:B:449:THR:HA	1:B:450:PRO:HD3	1.89	0.41
1:B:62:SER:O	1:B:399:THR:HG21	2.20	0.41
1:A:252:PHE:CZ	1:A:283:TYR:CE1	3.08	0.41
1:A:424:ARG:HH12	1:A:455:GLY:HA3	1.84	0.41
1:A:497:LEU:C	1:A:499:SER:N	2.74	0.41
1:B:47:SER:HA	1:B:48:PRO:HD3	1.90	0.41
1:A:410:ALA:HA	1:A:413:LEU:HD21	2.02	0.41
1:A:267:TRP:HE1	1:A:302:GLU:HB2	1.84	0.41
1:A:546:PRO:O	1:A:548:SER:N	2.53	0.41
1:B:164:HIS:CE1	2:B:907:GLC:H2	2.48	0.41
1:A:569:LEU:CG	1:A:571:LEU:HD13	2.49	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.89	0.41
1:A:432:ASN:HB3	1:A:435:LYS:HD2	2.02	0.41
1:A:477:LYS:O	1:A:478:GLU:CG	2.67	0.41
1:A:212:ILE:HD11	1:A:314:TRP:CZ3	2.56	0.41
1:B:167:PHE:CE1	1:B:201:HIS:CD2	3.09	0.41
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.51	0.41
1:B:266:ASP:O	1:B:268:PHE:N	2.53	0.41
1:B:163:ARG:C	1:B:466:PRO:HG3	2.41	0.41
1:A:18:ILE:HD13	1:A:24:ARG:NH1	2.36	0.41
1:A:117:HIS:HB3	1:B:299:GLU:OE2	2.21	0.41
1:A:330:VAL:HG13	1:A:335:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:437:ARG:HG2	1:A:486:PHE:CE1	2.56	0.41
1:B:363:LEU:HD11	1:B:371:VAL:CG2	2.51	0.41
1:B:280:ARG:O	1:B:281:THR:C	2.58	0.41
1:B:268:PHE:CD1	1:B:268:PHE:N	2.89	0.41
1:A:549:GLY:HA2	1:A:585:ARG:NH2	2.35	0.41
1:A:535:ARG:HH21	1:A:539:GLN:CD	2.24	0.41
1:B:137:PHE:HA	1:B:138:PRO:HD2	1.68	0.41
1:B:139:GLU:O	1:B:170:GLY:N	2.53	0.41
1:B:202:HIS:O	1:B:202:HIS:CG	2.74	0.41
1:B:553:TRP:HD1	1:B:583:ASN:HA	1.83	0.41
1:B:386:THR:OG1	1:B:387:GLY:N	2.54	0.41
1:B:356:TRP:CZ3	1:B:374:TYR:HB3	2.56	0.41
1:B:49:GLU:CB	4:B:1061:HOH:O	2.68	0.41
1:A:414:TRP:HE3	1:A:451:LEU:HD22	1.85	0.41
1:A:19:SER:OG	1:A:22:GLN:HG3	2.20	0.41
1:B:251:ALA:HB1	1:B:264:TYR:CD2	2.56	0.41
1:B:286:PHE:HD1	1:B:290:VAL:HG21	1.86	0.41
1:A:535:ARG:NH2	1:A:539:GLN:CD	2.75	0.41
1:A:281:THR:HG22	1:A:283:TYR:HE2	1.84	0.41
1:B:265:LYS:HG2	1:B:265:LYS:O	2.20	0.41
1:B:30:LYS:HD3	1:B:33:ASP:OD2	2.20	0.41
1:A:59:LYS:HB2	1:A:59:LYS:HE3	1.76	0.41
1:A:82:TYR:C	1:A:110:VAL:HG23	2.41	0.41
1:B:373:ASN:HB2	1:B:413:LEU:HB3	2.02	0.41
1:B:565:LYS:CE	1:B:568:GLN:HE21	2.32	0.41
1:A:2:LEU:HD12	1:A:30:LYS:CD	2.51	0.41
1:A:8:HIS:HE1	1:A:82:TYR:OH	2.04	0.40
1:A:306:TYR:C	1:A:306:TYR:CD1	2.94	0.40
1:B:133:ILE:HD13	1:B:189:ALA:HB3	2.03	0.40
1:B:332:HIS:O	1:B:336:ARG:HB2	2.21	0.40
1:B:393:ARG:NH2	1:B:397:GLU:OE1	2.54	0.40
1:A:95:TYR:HB2	1:A:102:SER:O	2.22	0.40
1:A:102:SER:OG	1:A:107:LYS:HB2	2.21	0.40
1:B:346:ASN:HD22	1:B:349:ALA:HB2	1.86	0.40
1:B:324:LEU:HD11	1:B:351:ILE:CG2	2.52	0.40
1:B:267:TRP:HD1	1:B:267:TRP:N	2.18	0.40
1:B:11:LYS:N	1:B:15:ALA:HB3	2.36	0.40
1:B:256:LEU:N	1:B:256:LEU:HD23	2.37	0.40
1:B:435:LYS:O	1:B:438:LEU:N	2.54	0.40
1:A:362:TRP:HB3	1:A:368:PHE:CD1	2.55	0.40
1:A:277:LYS:O	1:A:278:THR:C	2.59	0.40
1:A:85:LEU:HD23	1:A:95:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:VAL:HG22	1:B:45:TYR:CB	2.48	0.40
1:A:508:TRP:HZ2	1:A:545:VAL:CG1	2.35	0.40
1:B:314:TRP:HB2	1:B:322:TRP:HH2	1.87	0.40
1:B:6:ILE:HB	1:B:101:PHE:HZ	1.85	0.40
1:A:313:PHE:CD2	1:A:313:PHE:C	2.94	0.40
1:A:373:ASN:ND2	1:A:376:PHE:CB	2.85	0.40
1:B:133:ILE:CG2	1:B:134:TYR:N	2.85	0.40
1:B:7:PHE:CD2	1:B:8:HIS:N	2.90	0.40
1:A:16:TYR:CE2	1:A:406:PRO:HA	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	472 (81%)	84 (14%)	27 (5%)	4	24
1	B	583/585 (100%)	479 (82%)	72 (12%)	32 (6%)	3	19
All	All	1166/1170 (100%)	951 (82%)	156 (13%)	59 (5%)	3	22

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	200	SER
1	A	289	GLN
1	A	464	THR
1	B	138	PRO
1	B	166	SER
1	B	319	ILE
1	A	2	LEU
1	A	10	ALA
1	A	91	GLY
1	A	154	GLU

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Mol	Chain	Res	Type
1	A	164	HIS
1	A	231	ARG
1	A	271	GLU
1	A	328	ASN
1	A	433	GLU
1	A	548	SER
1	A	559	GLY
1	A	576	TYR
1	B	2	LEU
1	B	169	GLY
1	B	203	LYS
1	B	254	ASP
1	B	270	ILE
1	B	284	GLU
1	B	286	PHE
1	B	288	VAL
1	B	328	ASN
1	A	114	ALA
1	A	341	LEU
1	A	498	ALA
1	A	547	GLU
1	B	50	GLU
1	B	105	ARG
1	B	215	GLN
1	B	267	TRP
1	B	281	THR
1	B	391	ALA
1	B	459	GLY
1	B	476	GLU
1	A	131	ALA
1	A	478	GLU
1	B	48	PRO
1	B	206	THR
1	B	214	PRO
1	B	460	MET
1	B	537	GLU
1	A	55	ALA
1	A	215	GLN
1	B	63	ASP
1	B	155	GLN
1	A	346	ASN
1	B	106	SER

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Mol	Chain	Res	Type
1	B	279	SER
1	A	342	VAL
1	B	361	GLY
1	B	465	ASP
1	B	326	VAL
1	A	138	PRO

### 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	493/493 (100%)	452 (92%)	41 (8%)	16	53
1	B	493/493 (100%)	447 (91%)	46 (9%)	13	44
All	All	986/986 (100%)	899 (91%)	87 (9%)	14	49

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	33	ASP
1	A	73	LEU
1	A	78	LYS
1	A	86	LEU
1	A	118	ARG
1	A	122	PHE
1	A	130	GLU
1	A	133	ILE
1	A	167	PHE
1	A	173	LYS
1	A	180	PRO
1	A	182	LEU
1	A	191	TYR
1	A	205	ASP
1	A	223	ARG
1	A	239	ASP
1	A	250	PHE
1	A	263	ARG

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Mol	Chain	Res	Type
1	A	270	ILE
1	A	276	SER
1	A	283	TYR
1	A	286	PHE
1	A	323	ARG
1	A	330	VAL
1	A	340	ARG
1	A	341	LEU
1	A	346	ASN
1	A	356	TRP
1	A	364	MET
1	A	375	LEU
1	A	376	PHE
1	A	411	GLN
1	A	416	LEU
1	A	418	ASP
1	A	493	LEU
1	A	502	ARG
1	A	504	ASN
1	A	505	VAL
1	A	525	ASP
1	A	563	HIS
1	B	49	GLU
1	B	73	LEU
1	B	75	CYS
1	B	85	LEU
1	B	122	PHE
1	B	155	GLN
1	B	167	PHE
1	B	168	TYR
1	B	235	LYS
1	B	241	VAL
1	B	243	ASN
1	B	250	PHE
1	B	263	ARG
1	B	270	ILE
1	B	273	PHE
1	B	280	ARG
1	B	282	ASN
1	B	285	THR
1	B	316	GLU
1	B	323	ARG

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Mol	Chain	Res	Type
1	B	325	ASN
1	B	328	ASN
1	B	356	TRP
1	B	364	MET
1	B	381	ILE
1	B	382	ARG
1	B	390	HIS
1	B	398	LEU
1	B	411	GLN
1	B	418	ASP
1	B	424	ARG
1	B	438	LEU
1	B	456	ASP
1	B	466	PRO
1	B	475	GLU
1	B	504	ASN
1	B	507	SER
1	B	522	THR
1	B	523	VAL
1	B	524	GLN
1	B	525	ASP
1	B	535	ARG
1	B	545	VAL
1	B	565	LYS
1	B	573	LEU
1	B	574	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	135	GLN
1	A	155	GLN
1	A	164	HIS
1	A	230	HIS
1	A	243	ASN
1	A	244	HIS
1	A	282	ASN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS

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Mol	Chain	Res	Type
1	A	504	ASN
1	A	509	HIS
1	A	527	HIS
1	A	539	GLN
1	B	90	GLN
1	B	112	GLN
1	B	135	GLN
1	B	201	HIS
1	B	243	ASN
1	B	317	GLN
1	B	328	ASN
1	B	332	HIS
1	B	346	ASN
1	B	367	GLN
1	B	390	HIS
1	B	411	GLN
1	B	495	HIS
1	B	504	ASN
1	B	534	ASN
1	B	563	HIS
1	B	566	GLN
1	B	568	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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	GLC	A	801	2	10,11,12	0.50	0	11,15,17	0.66	0
2	GLC	A	802	2	10,11,12	0.48	0	11,15,17	0.56	0
2	GLC	A	803	2	10,11,12	0.53	0	11,15,17	0.75	0
2	GLC	A	804	2	10,11,12	0.62	0	11,15,17	0.35	0
2	GLC	A	805	2	10,11,12	0.43	0	11,15,17	0.39	0
2	GLC	A	806	2	10,11,12	0.53	0	11,15,17	0.52	0
2	GLC	A	807	2	10,11,12	0.43	0	11,15,17	0.23	0
2	GLC	A	808	2	10,11,12	0.45	0	11,15,17	0.48	0
2	GLC	B	901	2	10,11,12	0.59	0	11,15,17	0.51	0
2	GLC	B	902	2	10,11,12	0.47	0	11,15,17	0.66	0
2	GLC	B	903	2	10,11,12	0.55	0	11,15,17	0.48	0
2	GLC	B	904	2	10,11,12	0.67	0	11,15,17	0.82	0
2	GLC	B	905	2	10,11,12	0.53	0	11,15,17	0.56	0
2	GLC	B	906	2	10,11,12	0.63	0	11,15,17	0.46	0
2	GLC	B	907	2	10,11,12	0.54	0	11,15,17	0.29	0
2	GLC	B	908	2	10,11,12	0.59	0	11,15,17	0.43	0

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	GLC	A	801	2	-	0/2/19/22	0/1/1/1
2	GLC	A	802	2	-	0/2/19/22	0/1/1/1
2	GLC	A	803	2	-	0/2/19/22	0/1/1/1
2	GLC	A	804	2	-	0/2/19/22	0/1/1/1
2	GLC	A	805	2	-	0/2/19/22	0/1/1/1
2	GLC	A	806	2	-	0/2/19/22	0/1/1/1
2	GLC	A	807	2	-	0/2/19/22	0/1/1/1
2	GLC	A	808	2	-	0/2/19/22	0/1/1/1
2	GLC	B	901	2	-	0/2/19/22	0/1/1/1
2	GLC	B	902	2	-	0/2/19/22	0/1/1/1
2	GLC	B	903	2	-	0/2/19/22	0/1/1/1
2	GLC	B	904	2	-	0/2/19/22	0/1/1/1
2	GLC	B	905	2	-	0/2/19/22	0/1/1/1
2	GLC	B	906	2	-	0/2/19/22	0/1/1/1
2	GLC	B	907	2	-	0/2/19/22	0/1/1/1
2	GLC	B	908	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	585/585 (100%)	-0.14	4 (0%) 84 32	23, 54, 104, 111	0
1	B	585/585 (100%)	-0.08	5 (0%) 81 25	31, 63, 110, 111	0
All	All	1170/1170 (100%)	-0.11	9 (0%) 83 28	23, 58, 109, 111	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	GLN	4.3
1	B	287	ALA	3.6
1	A	551	LYS	3.1
1	B	139	GLU	2.7
1	B	286	PHE	2.3
1	A	273	PHE	2.3
1	A	272	ASP	2.2
1	B	291	PRO	2.2
1	A	271	GLU	2.1

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	A	803	11/12	0.47	7.48	108,110,111,111	0
2	GLC	A	804	11/12	0.49	6.08	109,111,111,111	0
2	GLC	B	906	11/12	0.24	3.89	108,111,111,111	0
2	GLC	A	802	11/12	0.24	2.74	109,110,111,111	0
2	GLC	A	801	11/12	0.25	1.89	109,110,111,111	0
2	GLC	A	805	11/12	0.37	1.59	108,110,110,110	0
2	GLC	B	904	11/12	0.20	-0.12	108,111,111,111	0
2	GLC	A	808	11/12	0.23	-0.19	108,109,110,110	0
2	GLC	A	807	11/12	0.22	-0.24	106,107,108,109	0
2	GLC	A	806	11/12	0.20	-0.47	105,106,106,108	0
2	GLC	B	908	11/12	0.22	-0.49	106,111,111,111	0
2	GLC	B	902	11/12	0.18	-0.58	107,108,109,110	0
2	GLC	B	903	11/12	0.23	-0.67	109,110,111,111	0
2	GLC	B	901	11/12	0.17	-0.72	109,110,111,111	0
2	GLC	B	907	11/12	0.22	-0.96	109,111,111,111	0
2	GLC	B	905	11/12	0.28	-	110,111,111,111	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	1001	1/1	0.12	-1.21	32,32,32,32	0
3	CA	B	1002	1/1	0.07	-2.26	85,85,85,85	0

## 6.5 Other polymers

There are no such residues in this entry.