



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:51 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

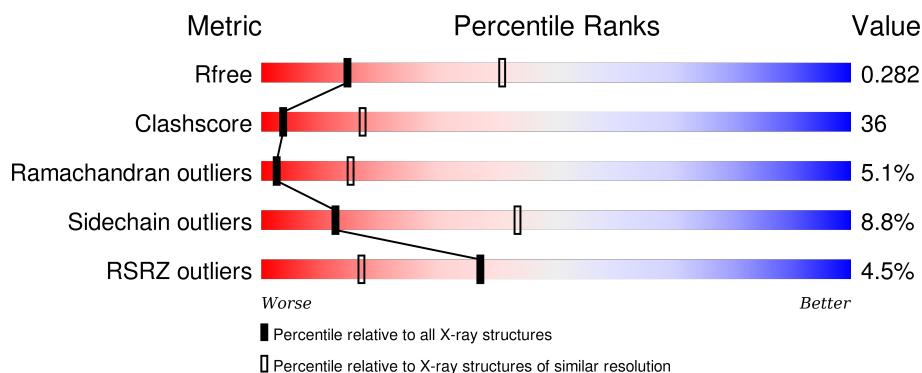
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>3%</div> <div>45%</div> <div>48%</div> <div>7%</div> </div>
1	B	585	<div> <div>6%</div> <div>43%</div> <div>49%</div> <div>8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9863 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 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		

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

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

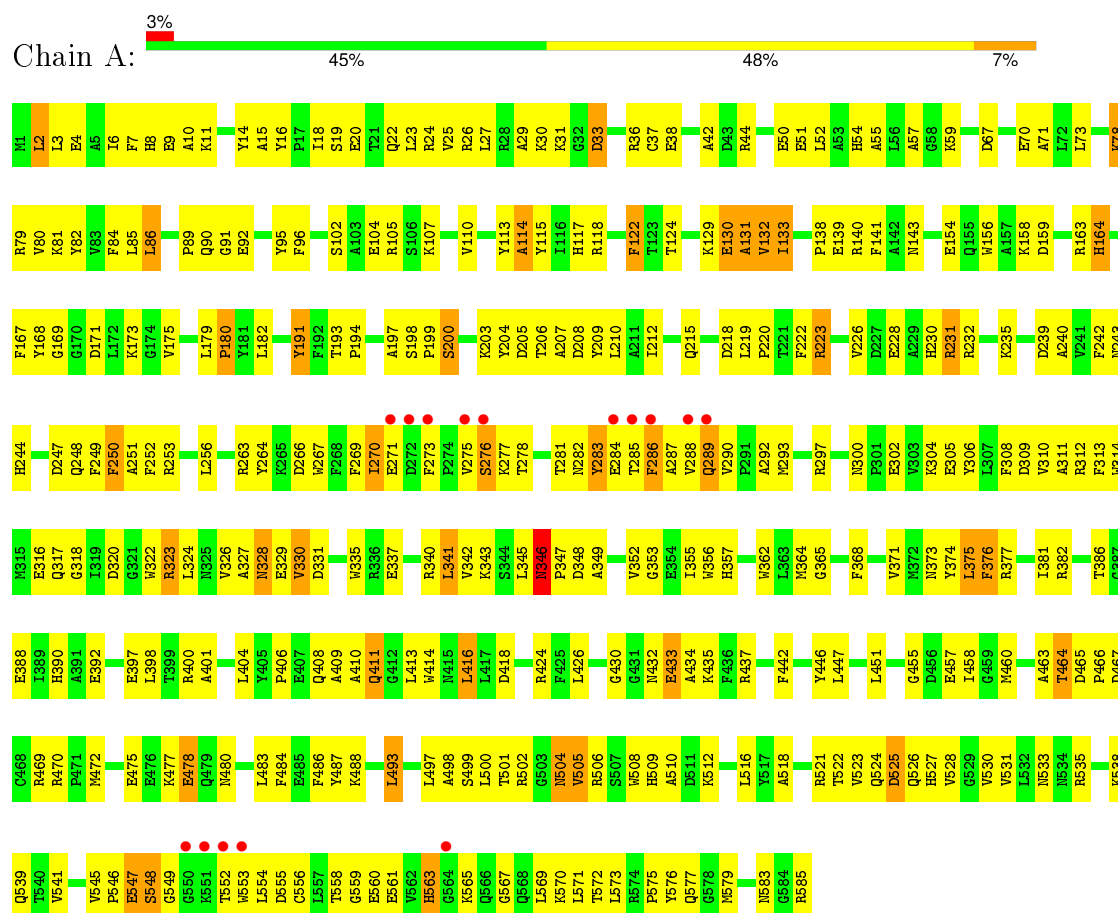
- Molecule 4 is water.

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

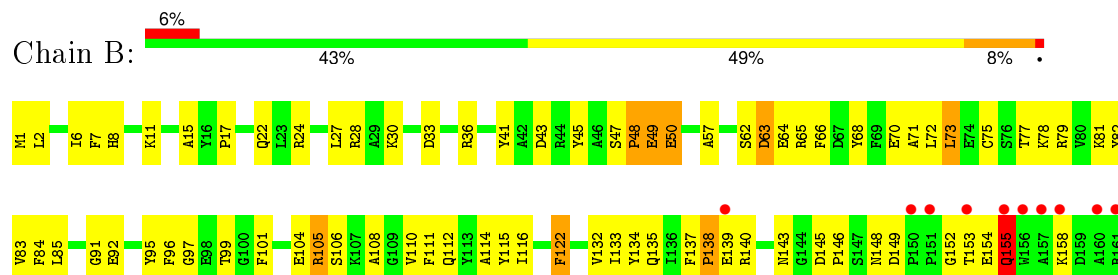
3 Residue-property plots

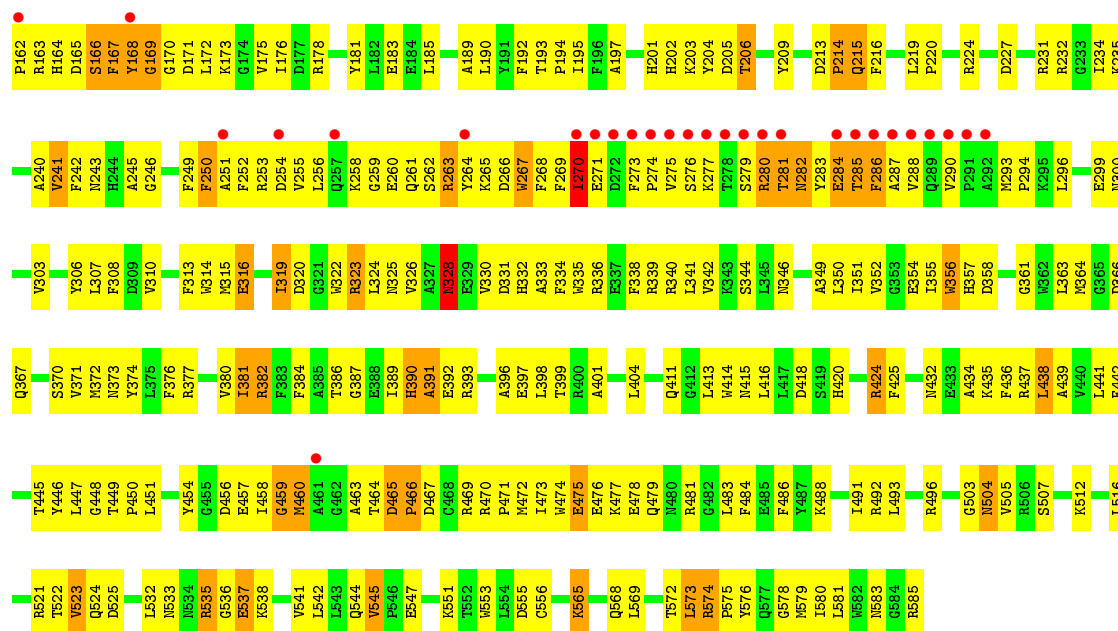
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



• Molecule 1: Neopullulanase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.284 0.210 , 0.282	Depositor DCC
R_{free} test set	2620 reflections (9.91%)	DCC
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.7	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 ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

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

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 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	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

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 36.

All (678) 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: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
1:B:537:GLU:HA	1:B:575:PRO:HG3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:THR:C	1:B:573:LEU:HD22	2.19	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	583/585 (100%)	472 (81%)	84 (14%)	27 (5%)	3	17
1	B	583/585 (100%)	479 (82%)	72 (12%)	32 (6%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1166/1170 (100%)	951 (82%)	156 (13%)	59 (5%)	2 15

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
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

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Mol	Chain	Res	Type
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
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%)	14	46
1	B	493/493 (100%)	447 (91%)	46 (9%)	11	39
All	All	986/986 (100%)	899 (91%)	87 (9%)	12	43

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

Mol	Chain	Res	Type
1	A	20	GLU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 ⓘ

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	11,11,12	0.56	0	14,15,17	0.88	0
2	GLC	A	802	2	11,11,12	0.48	0	14,15,17	0.63	0
2	GLC	A	803	2	11,11,12	0.59	0	14,15,17	0.81	0
2	GLC	A	804	2	11,11,12	0.71	0	14,15,17	0.62	0
2	GLC	A	805	2	11,11,12	0.58	0	14,15,17	0.71	1 (7%)
2	GLC	A	806	2	11,11,12	0.56	0	14,15,17	0.74	1 (7%)
2	GLC	A	807	2	11,11,12	0.48	0	14,15,17	0.60	0
2	GLC	A	808	2	11,11,12	0.53	0	14,15,17	0.66	0
2	GLC	B	901	2	11,11,12	0.67	0	14,15,17	0.74	0
2	GLC	B	902	2	11,11,12	0.56	0	14,15,17	1.08	2 (14%)
2	GLC	B	903	2	11,11,12	0.67	0	14,15,17	0.77	1 (7%)
2	GLC	B	904	2	11,11,12	0.72	0	14,15,17	0.83	0
2	GLC	B	905	2	11,11,12	0.65	0	14,15,17	0.93	2 (14%)
2	GLC	B	906	2	11,11,12	0.69	0	14,15,17	0.74	1 (7%)
2	GLC	B	907	2	11,11,12	0.67	0	14,15,17	0.79	1 (7%)
2	GLC	B	908	2	11,11,12	0.70	0	14,15,17	0.78	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	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.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	905	GLC	C1-C2-C3	2.05	111.97	109.54
2	B	902	GLC	C1-O5-C5	2.10	114.91	112.25
2	A	806	GLC	C1-O5-C5	2.11	114.92	112.25
2	B	907	GLC	C1-O5-C5	2.16	114.99	112.25
2	B	906	GLC	C1-O5-C5	2.18	115.01	112.25
2	A	805	GLC	C1-O5-C5	2.18	115.02	112.25
2	B	903	GLC	C1-O5-C5	2.20	115.03	112.25
2	B	908	GLC	C1-O5-C5	2.28	115.15	112.25
2	B	905	GLC	C1-O5-C5	2.41	115.30	112.25
2	B	902	GLC	C1-C2-C3	3.00	113.09	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	805	GLC	2	0
2	A	807	GLC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	808	GLC	3	0
2	B	901	GLC	1	0
2	B	902	GLC	2	0
2	B	903	GLC	1	0
2	B	907	GLC	2	0
2	B	908	GLC	2	0

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/585 (100%)	-0.21	15 (2%) 59 35	23, 54, 104, 111	0
1	B	585/585 (100%)	-0.04	38 (6%) 22 8	31, 63, 110, 111	0
All	All	1170/1170 (100%)	-0.13	53 (4%) 37 17	23, 58, 109, 111	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	GLN	7.8
1	B	276	SER	7.1
1	B	287	ALA	5.8
1	A	272	ASP	5.1
1	B	272	ASP	4.8
1	B	291	PRO	4.4
1	A	553	TRP	4.1
1	A	271	GLU	4.0
1	B	157	ALA	4.0
1	A	273	PHE	4.0
1	B	277	LYS	4.0
1	B	286	PHE	3.8
1	B	156	TRP	3.7
1	B	279	SER	3.7
1	B	288	VAL	3.7
1	A	551	LYS	3.4
1	B	275	VAL	3.4
1	A	276	SER	3.3
1	B	162	PRO	3.3
1	B	155	GLN	3.3
1	B	278	THR	3.1
1	B	281	THR	3.1
1	A	285	THR	3.0
1	B	160	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	257	GLN	3.0
1	A	286	PHE	2.9
1	B	264	TYR	2.9
1	B	150	PRO	2.9
1	B	274	PRO	2.9
1	B	161	ARG	2.7
1	B	273	PHE	2.6
1	B	290	VAL	2.6
1	B	153	THR	2.6
1	B	168	TYR	2.6
1	B	461	ALA	2.5
1	A	288	VAL	2.5
1	A	289	GLN	2.5
1	A	552	THR	2.4
1	A	550	GLY	2.3
1	A	284	GLU	2.3
1	B	251	ALA	2.3
1	B	270	ILE	2.2
1	B	254	ASP	2.2
1	B	285	THR	2.2
1	B	158	LYS	2.2
1	B	284	GLU	2.1
1	A	275	VAL	2.1
1	B	139	GLU	2.1
1	B	271	GLU	2.1
1	B	151	PRO	2.1
1	B	280	ARG	2.1
1	B	292	ALA	2.1
1	A	564	GLY	2.0

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, 95th 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	A	802	11/12	0.85	0.19	0.93	109,110,111,111	0
2	GLC	A	807	11/12	0.95	0.20	-0.28	106,107,108,109	0
2	GLC	A	808	11/12	0.86	0.22	-0.29	108,109,110,110	0
2	GLC	B	902	11/12	0.91	0.25	-0.33	107,108,109,110	0
2	GLC	A	806	11/12	0.92	0.17	-0.62	105,106,106,108	0
2	GLC	B	901	11/12	0.90	0.18	-0.78	109,110,111,111	0
2	GLC	B	908	11/12	0.89	0.18	-0.97	106,111,111,111	0
2	GLC	A	805	11/12	0.82	0.29	-	108,110,110,110	0
2	GLC	B	907	11/12	0.85	0.22	-	109,111,111,111	0
2	GLC	A	803	11/12	0.73	0.40	-	108,110,111,111	0
2	GLC	B	905	11/12	0.70	0.28	-	110,111,111,111	0
2	GLC	B	904	11/12	0.84	0.22	-	108,111,111,111	0
2	GLC	A	804	11/12	0.59	0.44	-	109,111,111,111	0
2	GLC	B	906	11/12	0.74	0.25	-	108,111,111,111	0
2	GLC	A	801	11/12	0.89	0.22	-	109,110,111,111	0
2	GLC	B	903	11/12	0.85	0.23	-	109,110,111,111	0

6.4 Ligands [i](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	A	1001	1/1	0.99	0.10	-1.47	32,32,32,32	0
3	CA	B	1002	1/1	0.90	0.07	-2.53	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.