



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 PM UTC

PDB ID : 1JIB / pdb_00001jib
Title : Complex of Alpha-amylase II (TVA II) from Thermoactinomyces vulgaris R-47 with Maltotetraose Based on a Crystal Soaked with Maltohexaose.
Authors : Yokota, T.; Tonozuka, T.; Shimura, Y.; Ichikawa, K.; Kamitori, S.; Sakano, Y.
Deposited on : 2001-07-02
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

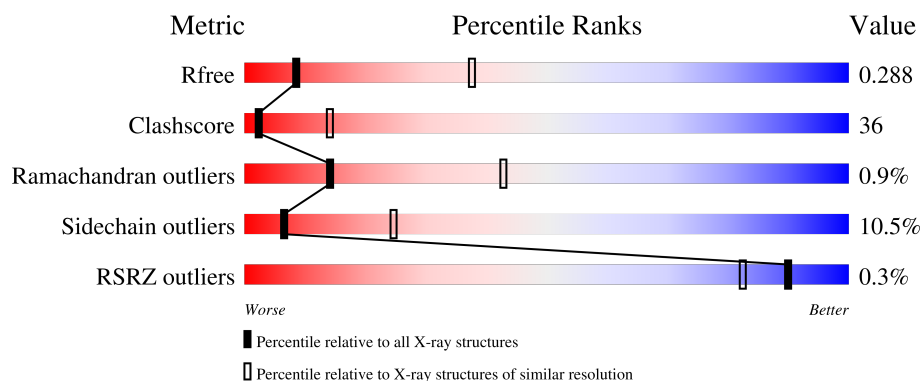
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

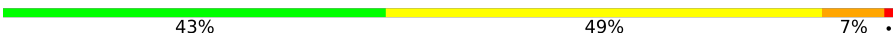
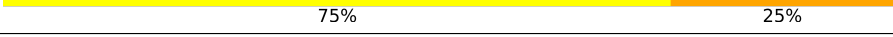
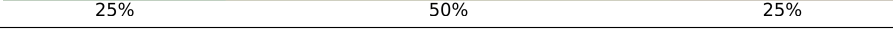
The reported resolution of this entry is 3.30 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 43% 49% 7% .
1	B	585	 39% 51% 10%
2	C	4	 75% 25%
2	D	4	 25% 50% 25%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9642 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	engineered mutation	UNP Q08751
B	325	ASN	ASP	engineered mutation	UNP Q08751

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

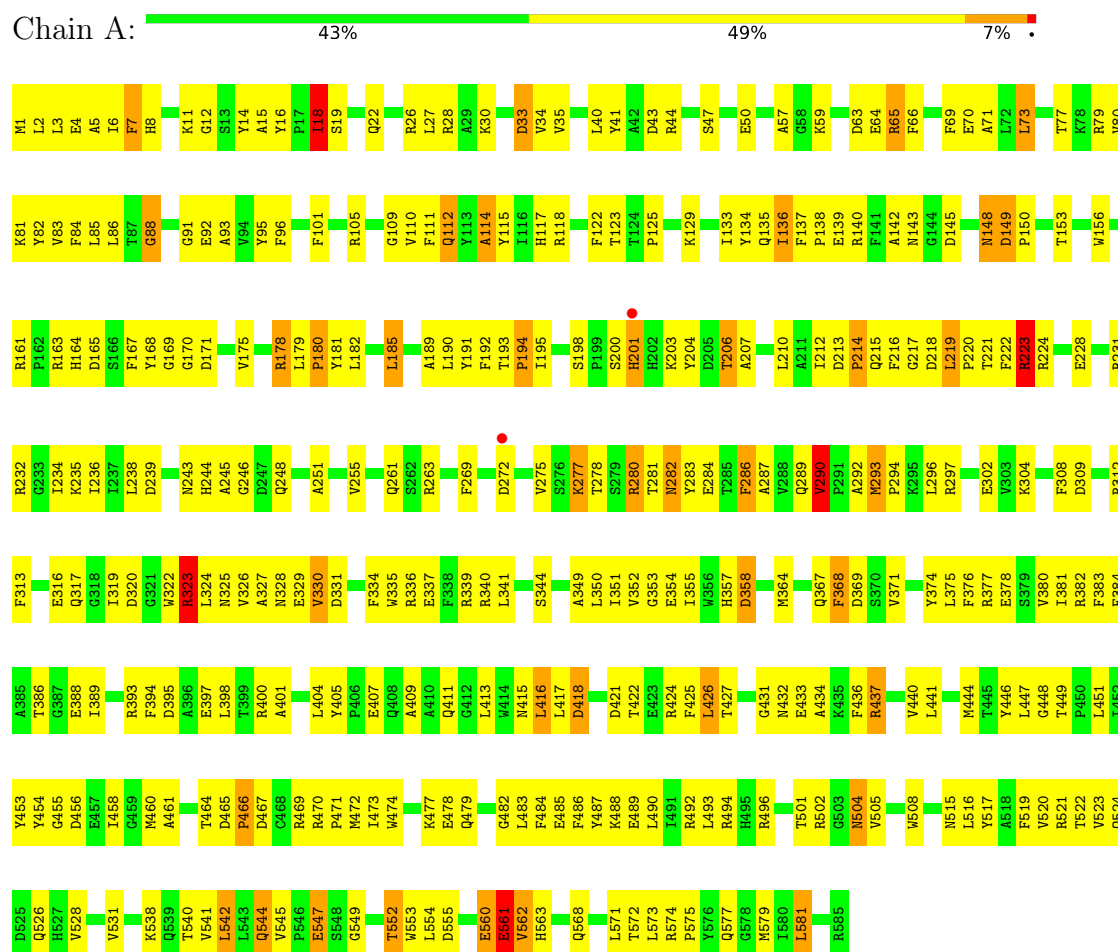


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			

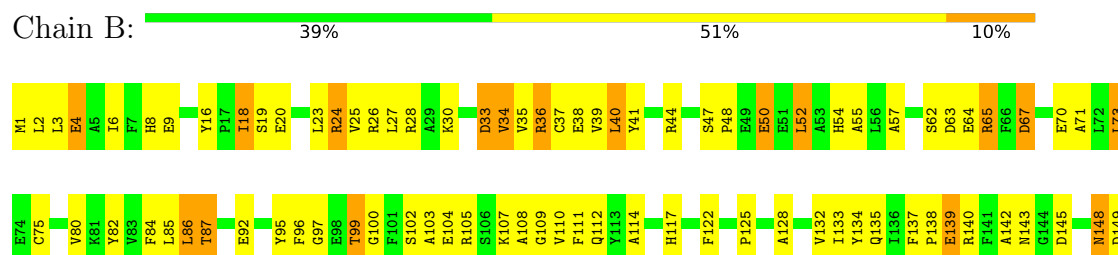
3 Residue-property plots

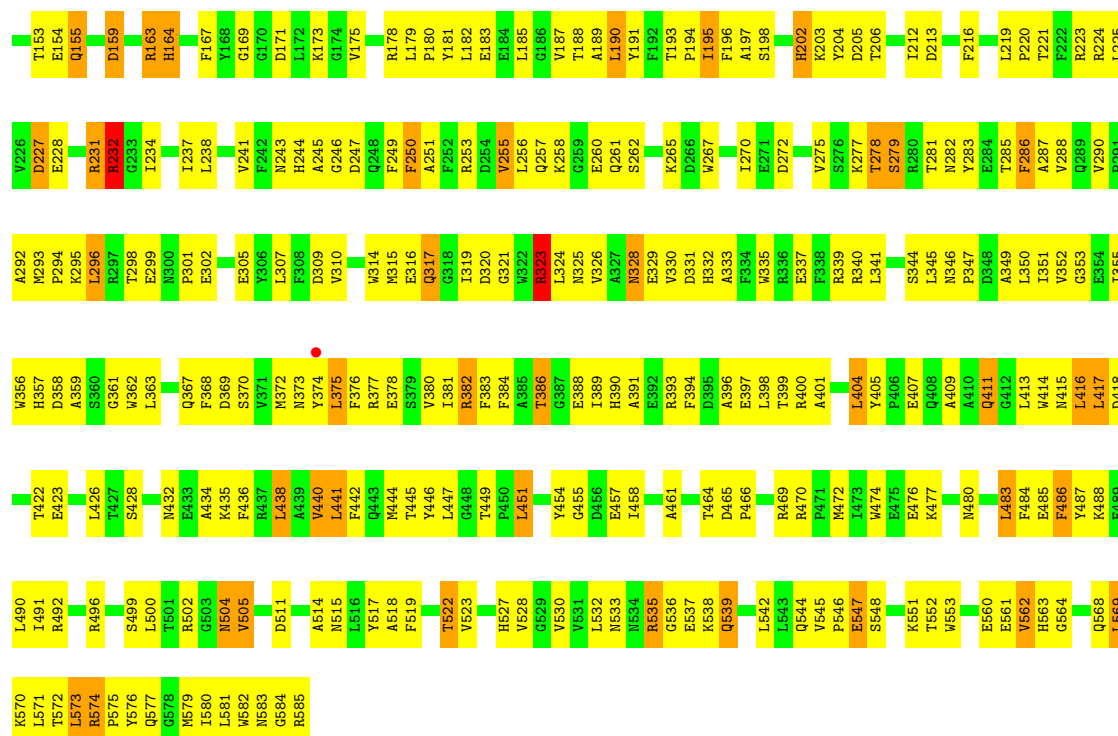
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: NEOPULLULANASE





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 75% 25%

GLC1
GLC2
GLC3
GLC4

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 25% 50% 25%

GLC1
GLC2
GLC3
GLC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.87Å 117.32Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 3.30 39.60 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.60-3.30) 95.7 (39.60-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.304 0.213 , 0.288	Depositor DCC
R_{free} test set	2182 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -k,-h,l 0.008 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9642	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.55	0/4906	1.09	36/6641 (0.5%)
1	B	0.55	0/4906	1.04	24/6641 (0.4%)
All	All	0.55	0/9812	1.06	60/13282 (0.5%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	VAL	CA-C-N	9.85	130.55	119.32
1	A	290	VAL	C-N-CA	9.85	130.55	119.32
1	A	323	ARG	N-CA-C	-9.39	93.94	109.07
1	A	88	GLY	CA-C-N	9.33	128.94	119.24
1	A	88	GLY	C-N-CA	9.33	128.94	119.24
1	A	18	ILE	N-CA-C	-8.62	104.74	113.10
1	B	163	ARG	N-CA-C	-8.24	97.65	110.42
1	A	212	ILE	N-CA-C	-7.97	99.30	109.58
1	A	148	ASN	N-CA-C	-7.54	102.41	111.69
1	B	18	ILE	N-CA-C	-7.44	105.96	113.47
1	A	482	GLY	N-CA-C	-7.11	104.25	112.50
1	B	486	PHE	N-CA-C	-7.11	103.46	111.14
1	A	149	ASP	CA-C-N	7.08	127.68	120.38
1	A	149	ASP	C-N-CA	7.08	127.68	120.38
1	A	7	PHE	N-CA-C	6.76	119.70	109.23
1	B	391	ALA	N-CA-C	6.71	119.16	111.11
1	B	323	ARG	N-CA-C	-6.65	97.69	108.52
1	B	270	ILE	N-CA-C	6.53	118.22	108.23
1	B	67	ASP	N-CA-C	-6.51	99.60	109.95
1	B	232	ARG	N-CA-C	-6.50	105.09	113.16
1	B	159	ASP	N-CA-C	6.38	119.99	112.72
1	B	560	GLU	N-CA-C	6.30	118.68	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	GLY	N-CA-C	-6.27	104.69	115.61
1	A	561	GLU	CA-C-N	6.08	127.37	121.65
1	A	561	GLU	C-N-CA	6.08	127.37	121.65
1	A	91	GLY	N-CA-C	6.08	123.45	115.36
1	B	202	HIS	N-CA-C	-6.07	99.31	108.96
1	A	515	ASN	N-CA-C	-6.04	103.59	111.74
1	B	227	ASP	N-CA-C	5.96	117.58	111.14
1	A	136	ILE	N-CA-C	5.95	116.42	107.80
1	B	100	GLY	N-CA-C	5.92	118.14	110.45
1	A	198	SER	CA-C-N	5.85	125.95	119.87
1	A	198	SER	C-N-CA	5.85	125.95	119.87
1	A	282	ASN	N-CA-C	-5.68	105.66	112.59
1	B	80	VAL	N-CA-C	5.64	115.79	108.35
1	A	185	LEU	N-CA-C	-5.59	105.18	111.28
1	B	290	VAL	CA-C-N	5.59	126.83	119.84
1	B	290	VAL	C-N-CA	5.59	126.83	119.84
1	A	320	ASP	N-CA-C	5.59	120.79	113.30
1	B	417	LEU	N-CA-C	-5.59	107.01	113.88
1	A	223	ARG	N-CA-C	-5.58	104.58	111.33
1	A	112	GLN	N-CA-C	5.57	117.48	108.34
1	A	161	ARG	CA-C-N	5.54	126.76	119.84
1	A	161	ARG	C-N-CA	5.54	126.76	119.84
1	A	280	ARG	N-CA-C	-5.41	102.15	109.95
1	A	417	LEU	N-CA-C	-5.40	106.86	113.50
1	A	562	VAL	N-CA-C	5.31	111.90	106.21
1	A	114	ALA	N-CA-C	5.26	119.99	111.37
1	A	41	TYR	N-CA-C	5.22	117.12	109.24
1	B	142	ALA	N-CA-C	5.19	116.83	108.32
1	B	320	ASP	N-CA-C	5.18	119.57	112.88
1	A	217	GLY	N-CA-C	5.18	117.19	110.45
1	B	103	ALA	N-CA-C	-5.17	106.81	113.23
1	A	349	ALA	N-CA-C	-5.13	102.69	110.28
1	A	206	THR	N-CA-C	5.13	117.74	110.10
1	B	309	ASP	N-CA-C	-5.08	105.83	111.36
1	A	524	GLN	CB-CA-C	-5.06	110.72	116.54
1	B	173	LYS	N-CA-C	-5.06	105.89	111.71
1	B	205	ASP	N-CA-C	-5.03	102.62	109.71
1	B	112	GLN	N-CA-C	5.00	117.30	108.75

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	4609	339	0
1	B	4776	0	4609	357	0
2	C	45	0	39	2	0
2	D	45	0	39	1	0
All	All	9642	0	9296	675	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 (675) 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:275:VAL:HA	1:A:282:ASN:HD21	1.14	1.08
1:A:552:THR:HG23	1:A:562:VAL:HG11	1.19	1.06
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.38	1.03
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.40	1.01
1:B:552:THR:HG22	1:B:562:VAL:HG23	1.38	1.01
1:A:553:TRP:H	1:A:562:VAL:HG12	1.27	0.95
1:B:155:GLN:HA	1:B:155:GLN:HE21	1.31	0.94
1:B:416:LEU:HD23	1:B:416:LEU:H	1.32	0.93
1:A:540:THR:HG22	1:A:572:THR:HG23	1.49	0.93
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.49	0.93
1:B:426:LEU:HD23	1:B:461:ALA:HB2	1.47	0.93
1:A:165:ASP:HA	1:A:201:HIS:NE2	1.84	0.92
1:A:246:GLY:HA3	1:A:248:GLN:NE2	1.85	0.90
1:B:301:PRO:O	1:B:305:GLU:HG2	1.70	0.90
1:B:552:THR:CG2	1:B:562:VAL:HG23	2.01	0.90
1:A:207:ALA:HA	1:A:248:GLN:HG2	1.55	0.89
1:A:552:THR:HA	1:A:562:VAL:HB	1.53	0.89
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.54	0.89
1:B:190:LEU:HD22	1:B:234:ILE:HG21	1.57	0.87
1:A:328:ASN:HD22	1:A:355:ILE:HG23	1.39	0.87
1:B:356:TRP:HE3	1:B:374:TYR:HB2	1.38	0.86
1:A:455:GLY:HA3	1:A:460:MET:HE2	1.59	0.85
1:A:552:THR:HG23	1:A:562:VAL:CG1	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ALA:O	1:A:404:LEU:HB2	1.76	0.84
1:A:18:ILE:HD11	1:A:22:GLN:HB2	1.59	0.84
1:B:137:PHE:HD2	1:B:193:THR:HG21	1.41	0.84
1:B:26:ARG:HG2	1:B:70:GLU:HG3	1.60	0.84
1:A:377:ARG:NH1	1:A:381:ILE:HD11	1.92	0.83
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.58	0.83
1:A:552:THR:CG2	1:A:562:VAL:HG11	2.08	0.82
1:B:223:ARG:HD2	1:B:317:GLN:HG3	1.62	0.82
1:B:224:ARG:HH21	1:B:227:ASP:CB	1.92	0.82
1:B:488:LYS:HB3	1:B:492:ARG:HH11	1.45	0.81
1:B:394:PHE:CE2	1:B:398:LEU:HD11	2.15	0.81
1:A:246:GLY:HA3	1:A:248:GLN:HE22	1.43	0.80
1:A:275:VAL:HA	1:A:282:ASN:ND2	1.95	0.80
1:B:243:ASN:ND2	1:B:329:GLU:HB2	1.96	0.80
1:B:244:HIS:HD2	1:B:293:MET:HB3	1.46	0.80
1:A:309:ASP:HA	1:A:312:ARG:HD2	1.61	0.79
1:A:544:GLN:HE21	1:A:544:GLN:HA	1.47	0.79
1:B:36:ARG:HG2	1:B:36:ARG:HH21	1.46	0.79
1:A:145:ASP:O	1:A:148:ASN:ND2	2.12	0.79
1:A:340:ARG:NH1	1:B:340:ARG:HH22	1.80	0.78
1:A:140:ARG:HG2	1:A:469:ARG:O	1.84	0.78
1:A:553:TRP:N	1:A:562:VAL:HG12	1.96	0.78
1:A:538:LYS:HB2	1:A:573:LEU:O	1.82	0.78
1:A:562:VAL:HG23	1:A:562:VAL:O	1.83	0.78
1:B:416:LEU:H	1:B:416:LEU:CD2	1.95	0.78
1:A:182:LEU:N	1:A:182:LEU:HD12	1.99	0.77
1:A:337:GLU:HA	1:A:340:ARG:HD2	1.67	0.76
1:B:41:TYR:HB3	1:B:82:TYR:HB3	1.67	0.76
1:B:326:VAL:HG12	1:B:329:GLU:HG3	1.67	0.76
1:A:194:PRO:HD3	1:A:239:ASP:OD2	1.84	0.76
1:A:1:MET:HE2	1:A:6:ILE:HD11	1.67	0.76
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.68	0.76
1:A:330:VAL:HG13	1:A:335:TRP:NE1	2.02	0.75
1:A:382:ARG:NH2	1:A:397:GLU:OE1	2.19	0.75
1:B:411:GLN:OE1	1:B:502:ARG:HA	1.85	0.75
1:A:182:LEU:HD12	1:A:182:LEU:H	1.50	0.75
1:B:99:THR:HB	1:B:109:GLY:HA3	1.68	0.75
1:B:1:MET:HE1	1:B:86:LEU:HD13	1.68	0.75
1:A:340:ARG:HH12	1:B:340:ARG:HH22	1.33	0.75
1:B:352:VAL:HG22	1:B:370:SER:HB3	1.69	0.74
1:B:275:VAL:HG12	1:B:282:ASN:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.70	0.74
1:B:224:ARG:HH21	1:B:227:ASP:HB2	1.53	0.73
1:A:542:LEU:HD13	1:A:542:LEU:O	1.88	0.73
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.69	0.73
1:B:140:ARG:HD2	1:B:469:ARG:O	1.87	0.73
1:A:148:ASN:ND2	1:A:171:ASP:OD2	2.21	0.73
1:B:2:LEU:HD12	1:B:30:LYS:HD2	1.72	0.72
1:B:137:PHE:CD2	1:B:193:THR:HG21	2.24	0.72
1:B:212:ILE:HD12	1:B:212:ILE:H	1.54	0.72
1:B:573:LEU:N	1:B:573:LEU:HD22	2.05	0.72
1:B:135:GLN:HG3	1:B:191:TYR:CD2	2.24	0.72
1:B:355:ILE:HD13	1:B:362:TRP:CE3	2.24	0.72
1:B:175:VAL:HG12	1:B:225:LEU:HD11	1.72	0.72
1:B:180:PRO:HG3	1:B:232:ARG:NH2	2.05	0.71
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.73	0.71
1:A:340:ARG:HH12	1:B:340:ARG:HH12	1.36	0.71
1:B:193:THR:HB	1:B:194:PRO:HD2	1.71	0.71
1:A:277:LYS:HE2	1:A:278:THR:N	2.06	0.71
1:A:340:ARG:HH12	1:B:340:ARG:NH2	1.89	0.70
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.21	0.70
1:B:244:HIS:CD2	1:B:293:MET:HB3	2.26	0.70
1:B:547:GLU:HG2	1:B:551:LYS:HD3	1.71	0.70
1:A:193:THR:CG2	1:A:194:PRO:HD2	2.20	0.70
1:B:30:LYS:HB3	1:B:33:ASP:CG	2.17	0.70
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.27	0.69
1:B:238:LEU:HD11	1:B:319:ILE:HG21	1.73	0.69
1:A:182:LEU:HD23	1:A:190:LEU:HD21	1.73	0.69
1:B:584:GLY:O	1:B:585:ARG:HD2	1.91	0.69
1:B:204:TYR:HB3	1:B:293:MET:HE1	1.73	0.69
1:B:195:ILE:HG12	1:B:195:ILE:O	1.92	0.68
1:A:115:TYR:CE1	1:B:295:LYS:HE2	2.29	0.68
1:A:277:LYS:H	1:A:277:LYS:HD3	1.59	0.68
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.29	0.68
1:B:198:SER:HB2	1:B:203:LYS:HG3	1.76	0.68
1:B:350:LEU:HD12	1:B:351:ILE:H	1.59	0.68
1:A:340:ARG:HH12	1:B:340:ARG:NH1	1.91	0.68
1:B:164:HIS:CE1	1:B:466:PRO:HD3	2.30	0.67
1:A:164:HIS:H	1:A:164:HIS:CD2	2.11	0.67
1:A:246:GLY:HA2	1:A:292:ALA:O	1.95	0.67
1:B:436:PHE:O	1:B:440:VAL:HG13	1.94	0.67
1:B:454:TYR:HD1	1:B:472:MET:HE2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HG22	1:A:194:PRO:HD2	1.76	0.67
1:B:139:GLU:CD	1:B:140:ARG:HH12	2.03	0.67
1:B:432:ASN:OD1	1:B:434:ALA:HB3	1.94	0.66
1:B:562:VAL:HG22	1:B:562:VAL:O	1.95	0.66
1:A:394:PHE:O	1:A:398:LEU:HB2	1.95	0.66
1:B:585:ARG:HA	1:B:585:ARG:NE	2.11	0.66
1:B:458:ILE:HD11	1:B:472:MET:SD	2.37	0.65
1:B:536:GLY:HA2	1:B:576:TYR:CE1	2.31	0.65
1:B:6:ILE:HA	1:B:28:ARG:O	1.97	0.65
1:B:323:ARG:HD2	1:B:323:ARG:C	2.22	0.65
1:A:11:LYS:NZ	1:B:361:GLY:H	1.94	0.65
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.79	0.65
1:B:398:LEU:HD21	1:B:442:PHE:HZ	1.62	0.65
1:A:182:LEU:H	1:A:182:LEU:CD1	2.09	0.64
1:A:448:GLY:O	1:A:494:ARG:NH2	2.29	0.64
1:B:212:ILE:HD12	1:B:212:ILE:N	2.11	0.64
1:A:117:HIS:HB3	1:B:299:GLU:OE2	1.97	0.64
1:A:194:PRO:HD3	1:A:239:ASP:CG	2.22	0.64
1:A:381:ILE:HD13	1:A:425:PHE:HE1	1.62	0.64
1:A:143:ASN:HD21	1:A:148:ASN:ND2	1.95	0.64
1:A:508:TRP:HB2	1:A:520:VAL:HG23	1.80	0.64
1:B:551:LYS:HE3	1:B:564:GLY:O	1.98	0.64
1:A:331:ASP:HB3	1:B:117:HIS:CD2	2.33	0.64
1:A:427:THR:HG23	1:A:461:ALA:HB1	1.78	0.64
1:A:552:THR:HA	1:A:562:VAL:CB	2.28	0.63
1:A:374:TYR:CZ	1:A:375:LEU:HB2	2.33	0.63
1:B:134:TYR:HB2	1:B:187:VAL:HG11	1.81	0.63
1:A:374:TYR:CG	1:A:375:LEU:N	2.66	0.63
1:B:52:LEU:HD22	1:B:52:LEU:N	2.14	0.63
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.79	0.63
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.63	0.62
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.32	0.62
1:A:134:TYR:CE2	1:A:136:ILE:HD11	2.34	0.62
1:A:386:THR:OG1	1:A:388:GLU:HG2	1.99	0.62
1:A:251:ALA:O	1:A:255:VAL:HG23	1.99	0.62
1:A:377:ARG:O	1:A:381:ILE:HG12	1.99	0.62
1:A:18:ILE:HD13	1:A:18:ILE:H	1.63	0.62
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.35	0.62
1:A:2:LEU:HD11	1:B:2:LEU:CD1	2.30	0.62
1:B:441:LEU:HD23	1:B:441:LEU:C	2.23	0.61
1:A:375:LEU:O	1:A:376:PHE:C	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:PHE:CD1	1:A:415:ASN:HB3	2.35	0.61
1:A:263:ARG:NH2	1:A:302:GLU:OE1	2.34	0.61
1:B:135:GLN:O	1:B:454:TYR:HB3	2.01	0.61
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.36	0.61
1:A:4:GLU:OE1	1:B:30:LYS:HE2	2.01	0.60
1:B:135:GLN:HB2	1:B:451:LEU:HD21	1.82	0.60
1:A:191:TYR:CZ	1:A:323:ARG:HG3	2.36	0.60
1:B:455:GLY:N	1:B:472:MET:HE1	2.16	0.60
1:B:224:ARG:HH21	1:B:227:ASP:HB3	1.67	0.60
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.37	0.60
1:B:561:GLU:C	1:B:563:HIS:H	2.08	0.60
1:A:245:ALA:O	1:A:293:MET:HA	2.02	0.59
1:B:256:LEU:HD11	1:B:277:LYS:HG2	1.84	0.59
1:B:356:TRP:CE3	1:B:374:TYR:HB2	2.29	0.59
1:A:95:TYR:CE2	1:A:105:ARG:HB2	2.37	0.59
1:A:129:LYS:HD2	1:A:502:ARG:NH1	2.16	0.59
1:A:325:ASN:HA	1:A:354:GLU:OE2	2.01	0.59
1:A:330:VAL:HG13	1:A:335:TRP:HE1	1.65	0.59
1:A:418:ASP:N	1:A:418:ASP:OD2	2.33	0.59
1:A:458:ILE:HD12	1:A:473:ILE:HB	1.84	0.59
1:B:253:ARG:HB3	1:B:253:ARG:NH1	2.17	0.59
1:B:446:TYR:CE1	1:B:505:VAL:HG11	2.36	0.59
1:A:18:ILE:CD1	1:A:22:GLN:HB2	2.30	0.59
1:A:63:ASP:OD1	1:A:400:ARG:HD3	2.03	0.58
1:B:350:LEU:HD12	1:B:351:ILE:N	2.17	0.58
1:A:134:TYR:CD2	1:A:136:ILE:HD11	2.37	0.58
1:A:148:ASN:CG	1:A:171:ASP:OD2	2.46	0.58
1:B:30:LYS:O	1:B:33:ASP:HB2	2.03	0.58
1:A:135:GLN:O	1:A:454:TYR:HB3	2.04	0.58
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.38	0.58
1:A:504:ASN:C	1:A:504:ASN:ND2	2.62	0.58
1:B:394:PHE:CZ	1:B:398:LEU:HD11	2.38	0.58
1:A:281:THR:HG23	1:A:289:GLN:OE1	2.04	0.58
1:A:304:LYS:HG3	1:A:334:PHE:CD2	2.38	0.58
1:B:445:THR:HG21	1:B:580:ILE:HD12	1.85	0.58
1:B:523:VAL:O	1:B:523:VAL:HG13	2.04	0.58
1:B:574:ARG:O	1:B:577:GLN:HB2	2.04	0.58
1:B:40:LEU:HD11	1:B:54:HIS:HD1	1.68	0.58
1:B:202:HIS:O	1:B:202:HIS:ND1	2.37	0.58
1:B:328:ASN:N	1:B:328:ASN:HD22	2.01	0.57
1:A:182:LEU:N	1:A:182:LEU:CD1	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:CE2	1:B:105:ARG:HG3	2.38	0.57
1:A:340:ARG:HH12	1:B:340:ARG:CZ	2.17	0.57
1:A:538:LYS:HB3	1:A:575:PRO:HD3	1.84	0.57
1:A:224:ARG:HE	1:A:224:ARG:HA	1.68	0.57
1:A:277:LYS:HE2	1:A:277:LYS:C	2.28	0.57
1:A:337:GLU:O	1:A:340:ARG:HB2	2.05	0.57
1:B:137:PHE:CE1	1:B:469:ARG:HD3	2.38	0.57
1:B:148:ASN:HD22	1:B:149:ASP:N	2.02	0.57
1:A:30:LYS:O	1:A:33:ASP:HB2	2.05	0.57
1:A:277:LYS:H	1:A:277:LYS:CD	2.16	0.57
1:B:183:GLU:OE2	1:B:232:ARG:NH1	2.38	0.57
1:B:522:THR:HG23	1:B:527:HIS:CD2	2.39	0.57
1:A:83:VAL:HG22	1:A:109:GLY:O	2.04	0.57
1:A:290:VAL:HG22	1:A:293:MET:HG3	1.85	0.57
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.32	0.57
1:A:504:ASN:C	1:A:504:ASN:HD22	2.13	0.56
1:B:36:ARG:HH21	1:B:36:ARG:CG	2.15	0.56
1:B:197:ALA:HA	1:B:213:ASP:HA	1.87	0.56
1:B:542:LEU:HD11	1:B:568:GLN:NE2	2.20	0.56
1:A:368:PHE:N	1:A:368:PHE:CD2	2.72	0.56
1:A:178:ARG:HG2	1:A:474:TRP:CZ2	2.41	0.56
1:A:416:LEU:H	1:A:416:LEU:CD2	2.19	0.56
1:A:540:THR:HG22	1:A:572:THR:CG2	2.30	0.56
1:B:574:ARG:HG2	1:B:577:GLN:OE1	2.06	0.56
1:A:185:LEU:HD13	1:A:484:PHE:CE2	2.40	0.56
1:A:143:ASN:HD21	1:A:148:ASN:HD21	1.53	0.56
1:A:194:PRO:HG2	1:A:204:TYR:CD1	2.40	0.56
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.33	0.56
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.18	0.56
1:A:389:ILE:CG2	1:A:393:ARG:HG2	2.35	0.56
1:B:249:PHE:CE2	1:B:251:ALA:HB3	2.40	0.56
1:B:134:TYR:HB3	1:B:190:LEU:CD1	2.36	0.56
1:B:390:HIS:HA	1:B:515:ASN:OD1	2.06	0.56
1:A:221:THR:O	1:A:224:ARG:HB3	2.05	0.56
1:A:375:LEU:HD23	1:A:401:ALA:HB2	1.88	0.56
1:B:487:TYR:O	1:B:491:ILE:HG12	2.06	0.56
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.70	0.56
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.69	0.56
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.70	0.56
1:A:178:ARG:HG2	1:A:474:TRP:CH2	2.41	0.55
1:A:409:ALA:O	1:A:413:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ALA:O	1:B:363:LEU:HD22	2.06	0.55
1:B:377:ARG:HA	1:B:380:VAL:CG2	2.36	0.55
1:B:84:PHE:O	1:B:95:TYR:HA	2.06	0.55
1:B:492:ARG:O	1:B:496:ARG:HG3	2.05	0.55
1:A:207:ALA:CA	1:A:248:GLN:HG2	2.31	0.55
1:B:377:ARG:HA	1:B:380:VAL:HG22	1.89	0.55
1:B:442:PHE:HB2	1:B:532:LEU:HD11	1.88	0.55
1:A:341:LEU:O	1:A:344:SER:HB3	2.07	0.55
1:B:537:GLU:O	1:B:539:GLN:HG2	2.06	0.55
1:B:569:LEU:HD22	1:B:571:LEU:HG	1.88	0.55
1:B:256:LEU:C	1:B:256:LEU:HD23	2.32	0.55
1:A:453:TYR:HB3	1:A:456:ASP:OD2	2.06	0.55
1:B:286:PHE:CG	1:B:287:ALA:N	2.73	0.55
1:B:324:LEU:HD22	1:B:335:TRP:CH2	2.42	0.55
1:B:356:TRP:O	1:B:374:TYR:CD2	2.60	0.55
1:A:272:ASP:O	1:A:282:ASN:ND2	2.38	0.54
1:B:39:VAL:HB	1:B:55:ALA:HB3	1.89	0.54
1:B:185:LEU:HD23	1:B:187:VAL:HG13	1.88	0.54
1:A:340:ARG:NH1	1:B:340:ARG:HH12	2.04	0.54
1:B:454:TYR:CD1	1:B:472:MET:HE2	2.41	0.54
1:A:2:LEU:HD21	1:B:2:LEU:HD13	1.88	0.54
1:B:47:SER:O	1:B:50:GLU:HB3	2.07	0.54
1:B:256:LEU:HD11	1:B:277:LYS:CG	2.38	0.54
1:A:63:ASP:OD2	1:A:63:ASP:C	2.48	0.54
1:A:544:GLN:HA	1:A:544:GLN:NE2	2.18	0.54
1:B:286:PHE:C	1:B:286:PHE:CD2	2.85	0.54
1:B:376:PHE:O	1:B:380:VAL:HG22	2.08	0.54
1:A:44:ARG:NH2	1:A:114:ALA:HA	2.23	0.54
1:A:193:THR:HG22	1:A:194:PRO:CD	2.36	0.54
1:A:380:VAL:HG13	1:A:384:PHE:CD1	2.43	0.54
1:B:178:ARG:O	1:B:181:TYR:HB3	2.08	0.54
1:B:384:PHE:HE2	1:B:438:LEU:HD22	1.73	0.54
1:B:394:PHE:O	1:B:398:LEU:HD12	2.08	0.54
1:A:374:TYR:CD2	1:A:375:LEU:N	2.74	0.54
1:B:135:GLN:HG3	1:B:191:TYR:CE2	2.43	0.54
1:A:30:LYS:HD3	1:A:33:ASP:OD1	2.09	0.53
1:A:193:THR:CG2	1:A:194:PRO:CD	2.85	0.53
1:A:245:ALA:HB2	1:A:296:LEU:HD11	1.90	0.53
1:B:87:THR:HA	1:B:92:GLU:O	2.08	0.53
1:B:267:TRP:CZ2	1:B:302:GLU:HB3	2.43	0.53
1:B:4:GLU:CD	1:B:4:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:O	1:B:294:PRO:HD2	2.09	0.53
1:B:148:ASN:OD1	1:B:171:ASP:OD2	2.25	0.53
1:A:542:LEU:HD23	1:A:568:GLN:CD	2.34	0.53
1:A:27:LEU:C	1:A:27:LEU:HD23	2.32	0.53
1:A:193:THR:HG23	1:A:194:PRO:HD2	1.90	0.53
1:A:218:ASP:OD2	1:A:220:PRO:HD2	2.09	0.53
1:B:326:VAL:HG12	1:B:326:VAL:O	2.08	0.53
1:B:504:ASN:C	1:B:504:ASN:HD22	2.16	0.53
1:A:210:LEU:N	1:A:210:LEU:HD12	2.22	0.53
1:A:496:ARG:HD3	1:A:496:ARG:C	2.34	0.53
1:B:16:TYR:OH	1:B:407:GLU:HG2	2.09	0.53
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.43	0.53
1:B:148:ASN:HD22	1:B:148:ASN:C	2.17	0.53
1:A:467:ASP:O	1:A:470:ARG:HG3	2.10	0.52
1:B:139:GLU:OE2	1:B:167:PHE:HA	2.09	0.52
1:B:1:MET:HE2	1:B:6:ILE:HD11	1.92	0.52
1:A:44:ARG:HG3	1:A:80:VAL:N	2.24	0.52
1:A:153:THR:HG23	1:A:168:TYR:HA	1.90	0.52
1:A:376:PHE:CE1	1:A:415:ASN:HB3	2.45	0.52
1:B:247:ASP:HB3	1:B:292:ALA:HA	1.90	0.52
1:B:97:GLY:HA3	1:B:108:ALA:O	2.10	0.52
1:B:326:VAL:CG1	1:B:329:GLU:HG3	2.38	0.52
1:A:19:SER:OG	1:A:22:GLN:HG3	2.10	0.52
1:B:250:PHE:CG	1:B:251:ALA:N	2.78	0.52
1:A:59:LYS:HG2	1:A:69:PHE:CE1	2.45	0.52
1:A:350:LEU:HG	1:A:352:VAL:HG23	1.90	0.52
1:B:250:PHE:CD1	1:B:250:PHE:C	2.86	0.52
1:A:206:THR:C	1:A:248:GLN:HE21	2.18	0.52
1:A:447:LEU:HB2	1:A:505:VAL:HG23	1.92	0.52
1:B:212:ILE:HD11	1:B:314:TRP:HH2	1.74	0.52
1:A:44:ARG:HH21	1:A:114:ALA:HA	1.74	0.51
1:B:377:ARG:NH2	1:B:422:THR:HB	2.25	0.51
1:B:571:LEU:HD11	1:B:581:LEU:HD11	1.91	0.51
1:A:331:ASP:HB3	1:B:117:HIS:HD2	1.76	0.51
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.42	0.51
1:B:401:ALA:O	1:B:404:LEU:HB2	2.09	0.51
1:A:489:GLU:O	1:A:493:LEU:HG	2.11	0.51
1:B:155:GLN:HA	1:B:155:GLN:NE2	2.13	0.51
1:B:227:ASP:O	1:B:231:ARG:HG2	2.10	0.51
1:A:11:LYS:HZ2	1:B:361:GLY:H	1.58	0.51
1:B:16:TYR:C	1:B:23:LEU:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLN:O	1:B:258:LYS:HD3	2.11	0.51
1:B:440:VAL:O	1:B:444:MET:HG2	2.11	0.51
1:B:545:VAL:HG21	1:B:569:LEU:HB2	1.92	0.51
1:A:219:LEU:HD11	1:A:317:GLN:OE1	2.10	0.51
1:A:523:VAL:O	1:A:523:VAL:HG13	2.11	0.51
1:B:488:LYS:CB	1:B:492:ARG:HH11	2.21	0.51
1:A:287:ALA:H	1:A:290:VAL:HG11	1.76	0.51
1:A:367:GLN:C	1:A:368:PHE:HD2	2.19	0.51
1:B:212:ILE:H	1:B:212:ILE:CD1	2.21	0.51
1:B:404:LEU:HB3	1:B:405:TYR:CD2	2.46	0.51
1:A:88:GLY:HA3	1:A:92:GLU:OE2	2.10	0.51
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.92	0.51
1:B:44:ARG:HD2	1:B:114:ALA:HA	1.93	0.51
1:B:244:HIS:HB3	1:B:295:LYS:HA	1.93	0.51
1:B:373:ASN:HB3	1:B:376:PHE:HB3	1.91	0.51
1:A:57:ALA:HB1	1:A:70:GLU:C	2.36	0.50
1:A:494:ARG:HG2	1:A:501:THR:HG22	1.93	0.50
1:B:386:THR:HB	1:B:388:GLU:HG3	1.92	0.50
1:B:1:MET:CE	1:B:86:LEU:HD13	2.38	0.50
1:B:536:GLY:CA	1:B:576:TYR:CE1	2.93	0.50
1:A:148:ASN:ND2	1:A:169:GLY:O	2.39	0.50
1:A:178:ARG:O	1:A:182:LEU:HD13	2.11	0.50
1:A:424:ARG:NH2	1:A:454:TYR:O	2.42	0.50
1:B:85:LEU:HD13	1:B:95:TYR:CE2	2.47	0.50
1:B:569:LEU:HD23	1:B:570:LYS:N	2.25	0.50
1:A:269:PHE:HB2	1:A:284:GLU:HB3	1.92	0.50
1:B:243:ASN:ND2	1:B:295:LYS:NZ	2.59	0.50
1:B:253:ARG:HB3	1:B:253:ARG:CZ	2.41	0.50
1:A:133:ILE:HD13	1:A:449:THR:HG21	1.93	0.50
1:A:304:LYS:HG3	1:A:334:PHE:CE2	2.46	0.50
1:B:27:LEU:HD23	1:B:27:LEU:C	2.37	0.50
1:B:40:LEU:HD11	1:B:54:HIS:ND1	2.27	0.50
1:B:582:TRP:CE3	1:B:584:GLY:HA2	2.47	0.50
1:A:330:VAL:HG11	1:A:335:TRP:CZ2	2.46	0.50
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.77	0.50
1:A:26:ARG:HD3	1:A:70:GLU:HG3	1.93	0.50
1:A:421:ASP:OD2	2:C:3:GLC:O2	2.27	0.50
1:B:255:VAL:HA	1:B:262:SER:CB	2.42	0.50
1:A:140:ARG:HH12	1:A:201:HIS:HB3	1.77	0.50
1:A:573:LEU:CD2	1:A:579:MET:HG3	2.42	0.49
1:B:133:ILE:HG13	1:B:414:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:CG1	1:B:225:LEU:HD11	2.41	0.49
1:B:455:GLY:N	1:B:457:GLU:OE1	2.46	0.49
1:A:353:GLY:O	1:A:371:VAL:HA	2.11	0.49
1:B:283:TYR:CD1	1:B:285:THR:HG22	2.48	0.49
1:B:573:LEU:N	1:B:573:LEU:CD2	2.75	0.49
1:B:307:LEU:O	1:B:310:VAL:HB	2.12	0.49
1:B:202:HIS:O	1:B:202:HIS:CG	2.65	0.49
1:B:238:LEU:CD1	1:B:319:ILE:HG21	2.41	0.49
1:A:441:LEU:C	1:A:441:LEU:HD23	2.38	0.49
1:B:569:LEU:HD23	1:B:569:LEU:C	2.38	0.49
1:B:64:GLU:H	1:B:396:ALA:HB1	1.78	0.49
1:A:263:ARG:HD2	1:A:263:ARG:O	2.13	0.49
1:B:48:PRO:C	1:B:50:GLU:H	2.20	0.49
1:B:219:LEU:HD11	1:B:317:GLN:CD	2.38	0.49
1:B:237:ILE:HG23	1:B:321:GLY:C	2.37	0.49
1:B:314:TRP:CE3	1:B:314:TRP:HA	2.48	0.49
1:A:483:LEU:HD21	1:A:487:TYR:CE1	2.47	0.49
1:A:337:GLU:HG2	1:A:340:ARG:HH11	1.77	0.49
1:A:395:ASP:HB2	1:A:517:TYR:CE2	2.48	0.49
1:B:125:PRO:HD3	1:B:369:ASP:OD2	2.13	0.49
1:A:422:THR:C	1:A:464:THR:HA	2.38	0.48
1:A:277:LYS:HE2	1:A:277:LYS:N	2.29	0.48
1:B:435:LYS:HG2	1:B:576:TYR:CE2	2.48	0.48
1:B:485:GLU:OE2	1:B:485:GLU:HA	2.13	0.48
1:A:16:TYR:OH	1:A:407:GLU:HG2	2.12	0.48
1:B:203:LYS:HE3	1:B:216:PHE:CE2	2.48	0.48
1:B:533:ASN:HD22	1:B:573:LEU:HB2	1.77	0.48
1:A:562:VAL:O	1:A:562:VAL:CG2	2.54	0.48
1:B:104:GLU:OE1	1:B:107:LYS:NZ	2.38	0.48
1:B:256:LEU:HD21	1:B:277:LYS:HG3	1.95	0.48
1:B:1:MET:HE3	1:B:34:VAL:HG12	1.95	0.48
1:A:105:ARG:O	1:A:105:ARG:HG2	2.13	0.48
1:A:519:PHE:HE2	1:A:521:ARG:HD3	1.79	0.48
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.42	0.48
1:A:516:LEU:HD21	1:A:541:VAL:HG11	1.96	0.48
1:B:24:ARG:CG	1:B:24:ARG:HH11	2.25	0.48
1:B:41:TYR:CE2	1:B:73:LEU:HD12	2.49	0.48
1:B:196:PHE:CZ	1:B:314:TRP:NE1	2.82	0.48
1:B:204:TYR:O	1:B:241:VAL:HG11	2.13	0.48
1:B:417:LEU:HD11	1:B:440:VAL:HG12	1.94	0.48
1:A:122:PHE:HD2	1:A:123:THR:N	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:HG3	1:B:65:ARG:HB2	1.96	0.48
1:A:137:PHE:CZ	1:A:469:ARG:HD3	2.49	0.48
1:A:355:ILE:HG22	1:A:357:HIS:CD2	2.48	0.48
1:B:245:ALA:HB2	1:B:296:LEU:HD21	1.95	0.48
1:B:44:ARG:HH11	1:B:114:ALA:C	2.22	0.47
1:B:128:ALA:O	1:B:449:THR:HG21	2.13	0.47
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.44	0.47
1:B:411:GLN:HG2	1:B:447:LEU:HD11	1.96	0.47
1:A:339:ARG:NH2	1:A:369:ASP:OD1	2.46	0.47
1:B:330:VAL:HB	1:B:335:TRP:HE1	1.79	0.47
1:B:398:LEU:CD2	1:B:442:PHE:HZ	2.24	0.47
1:B:585:ARG:NE	1:B:585:ARG:CA	2.76	0.47
1:A:178:ARG:O	1:A:181:TYR:HB3	2.14	0.47
1:A:528:VAL:HA	1:A:581:LEU:O	2.14	0.47
1:B:455:GLY:CA	1:B:472:MET:HE1	2.45	0.47
1:A:134:TYR:HB3	1:A:190:LEU:HD23	1.97	0.47
1:A:223:ARG:CG	1:A:223:ARG:NH1	2.77	0.47
1:A:540:THR:HA	1:A:572:THR:HA	1.96	0.47
1:B:221:THR:O	1:B:224:ARG:HB3	2.14	0.47
1:B:511:ASP:HB3	1:B:514:ALA:HB3	1.97	0.47
1:A:26:ARG:CG	1:A:70:GLU:HG3	2.43	0.47
1:A:143:ASN:ND2	1:A:148:ASN:HD21	2.13	0.47
1:A:148:ASN:OD1	1:A:215:GLN:O	2.33	0.47
1:A:437:ARG:HA	1:A:440:VAL:HG22	1.96	0.47
1:B:16:TYR:HE1	1:B:18:ILE:HG22	1.79	0.47
1:B:283:TYR:CE1	1:B:285:THR:HG22	2.49	0.47
1:B:445:THR:HB	1:B:530:VAL:HG21	1.96	0.47
1:B:530:VAL:HA	1:B:579:MET:O	2.15	0.47
1:A:95:TYR:CD2	1:A:105:ARG:HA	2.50	0.47
1:A:286:PHE:CE2	2:C:3:GLC:H62	2.50	0.47
1:A:458:ILE:HD11	1:A:472:MET:SD	2.55	0.47
1:A:464:THR:O	1:A:465:ASP:C	2.56	0.47
1:B:546:PRO:O	1:B:548:SER:N	2.48	0.47
1:A:148:ASN:ND2	1:A:149:ASP:OD2	2.47	0.47
1:B:36:ARG:HG2	1:B:36:ARG:NH2	2.24	0.47
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.30	0.47
1:B:476:GLU:HG2	1:B:477:LYS:N	2.30	0.47
1:B:8:HIS:CG	1:B:9:GLU:N	2.84	0.46
1:B:85:LEU:HD13	1:B:95:TYR:CZ	2.50	0.46
1:B:285:THR:O	1:B:286:PHE:C	2.58	0.46
1:A:236:ILE:CG2	1:A:238:LEU:HD21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:O	1:A:416:LEU:HD23	2.15	0.46
1:A:11:LYS:HZ3	1:B:361:GLY:H	1.62	0.46
1:A:313:PHE:O	1:A:316:GLU:HB2	2.14	0.46
1:B:346:ASN:HD22	1:B:349:ALA:HB2	1.80	0.46
1:A:134:TYR:CE2	1:A:136:ILE:CD1	2.99	0.46
1:A:179:LEU:HB3	1:A:232:ARG:HD2	1.98	0.46
1:A:369:ASP:OD1	1:A:369:ASP:N	2.48	0.46
1:A:554:LEU:C	1:A:554:LEU:HD23	2.40	0.46
1:A:554:LEU:HD23	1:A:555:ASP:N	2.30	0.46
1:A:65:ARG:HG2	1:B:4:GLU:HG3	1.96	0.46
1:A:138:PRO:HG3	1:A:195:ILE:HG22	1.97	0.46
1:A:331:ASP:OD1	1:A:331:ASP:N	2.47	0.46
1:A:389:ILE:HG21	1:A:393:ARG:HG2	1.97	0.46
1:A:485:GLU:OE2	1:A:488:LYS:HD3	2.15	0.46
1:B:134:TYR:HB3	1:B:190:LEU:HD12	1.95	0.46
1:B:182:LEU:O	1:B:187:VAL:HG22	2.16	0.46
1:B:245:ALA:CB	1:B:296:LEU:HD11	2.45	0.46
1:A:204:TYR:OH	1:A:323:ARG:NH1	2.48	0.46
1:A:324:LEU:HB2	1:A:327:ALA:HB2	1.98	0.46
1:A:574:ARG:HD2	1:A:577:GLN:HG3	1.98	0.46
1:B:256:LEU:HD23	1:B:256:LEU:O	2.16	0.46
1:B:519:PHE:CE1	1:B:530:VAL:HB	2.51	0.46
1:A:207:ALA:HB2	1:A:248:GLN:HG3	1.98	0.46
1:A:440:VAL:O	1:A:444:MET:HB2	2.16	0.45
1:A:542:LEU:HD23	1:A:568:GLN:NE2	2.31	0.45
1:A:11:LYS:N	1:A:15:ALA:HB3	2.32	0.45
1:A:134:TYR:HB3	1:A:190:LEU:CD2	2.46	0.45
1:A:137:PHE:CE2	1:A:469:ARG:HD3	2.51	0.45
1:A:290:VAL:CG2	1:A:293:MET:HG3	2.46	0.45
1:B:315:MET:HA	1:B:319:ILE:HG12	1.97	0.45
1:B:359:ALA:O	1:B:363:LEU:CD2	2.64	0.45
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.15	0.45
1:B:535:ARG:HB3	1:B:539:GLN:OE1	2.15	0.45
1:A:319:ILE:HD11	1:A:322:TRP:CZ2	2.52	0.45
1:B:257:GLN:C	1:B:258:LYS:HD3	2.41	0.45
1:B:339:ARG:NH2	1:B:369:ASP:OD1	2.43	0.45
1:A:290:VAL:HG22	1:A:290:VAL:O	2.16	0.45
1:A:405:TYR:CE1	1:A:413:LEU:HD21	2.52	0.45
1:B:24:ARG:CG	1:B:24:ARG:NH1	2.80	0.45
1:B:245:ALA:HB2	1:B:296:LEU:HD11	1.99	0.45
1:B:538:LYS:HA	1:B:573:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:HD12	1:A:133:ILE:N	2.32	0.45
1:A:190:LEU:HG	1:A:234:ILE:CG2	2.47	0.45
1:A:213:ASP:OD2	1:A:214:PRO:HD2	2.17	0.45
1:A:357:HIS:HA	1:A:374:TYR:CD1	2.52	0.45
1:B:52:LEU:HD22	1:B:52:LEU:H	1.81	0.45
1:B:224:ARG:HE	1:B:224:ARG:HA	1.82	0.45
1:B:275:VAL:HG12	1:B:282:ASN:CB	2.41	0.45
1:A:374:TYR:CE2	1:A:375:LEU:HB2	2.52	0.45
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.52	0.45
1:B:143:ASN:ND2	1:B:169:GLY:O	2.49	0.45
1:B:224:ARG:HA	1:B:224:ARG:NE	2.31	0.45
1:B:464:THR:OG1	1:B:465:ASP:N	2.50	0.45
1:B:561:GLU:C	1:B:563:HIS:N	2.75	0.45
1:A:432:ASN:OD1	1:A:434:ALA:HB3	2.16	0.44
1:B:228:GLU:O	1:B:232:ARG:HD3	2.16	0.44
1:B:465:ASP:HA	1:B:466:PRO:HA	1.70	0.44
1:A:150:PRO:HB3	1:A:215:GLN:OE1	2.17	0.44
1:A:416:LEU:H	1:A:416:LEU:HD23	1.82	0.44
1:B:357:HIS:O	1:B:358:ASP:C	2.61	0.44
1:B:416:LEU:CD2	1:B:416:LEU:N	2.67	0.44
1:B:523:VAL:O	1:B:523:VAL:CG1	2.65	0.44
1:A:43:ASP:OD1	1:A:79:ARG:NH1	2.50	0.44
1:A:85:LEU:HD13	1:A:85:LEU:C	2.42	0.44
1:A:175:VAL:HG11	1:A:192:PHE:HZ	1.83	0.44
1:A:336:ARG:O	1:A:340:ARG:HG3	2.16	0.44
1:A:496:ARG:HD3	1:A:496:ARG:O	2.17	0.44
1:B:26:ARG:CG	1:B:70:GLU:HG3	2.37	0.44
1:B:35:VAL:HG22	1:B:87:THR:O	2.17	0.44
1:B:62:SER:N	1:B:399:THR:HG21	2.32	0.44
1:B:110:VAL:O	1:B:110:VAL:HG13	2.17	0.44
1:B:281:THR:CG2	1:B:283:TYR:O	2.65	0.44
1:B:324:LEU:HB2	1:B:353:GLY:HA2	1.99	0.44
1:A:117:HIS:CE1	1:B:331:ASP:N	2.86	0.44
1:B:145:ASP:O	1:B:148:ASN:CG	2.60	0.44
1:B:272:ASP:HB2	1:B:282:ASN:ND2	2.32	0.44
1:B:573:LEU:HD11	1:B:579:MET:SD	2.57	0.44
1:A:357:HIS:O	1:A:358:ASP:C	2.61	0.44
1:A:394:PHE:CE2	1:A:398:LEU:HD13	2.53	0.44
1:A:454:TYR:CD1	1:A:454:TYR:C	2.95	0.44
1:B:175:VAL:HG12	1:B:225:LEU:CD1	2.45	0.44
1:B:195:ILE:HD13	1:B:195:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:HB	1:B:393:ARG:CG	2.47	0.44
1:A:191:TYR:OH	1:A:323:ARG:NE	2.51	0.44
1:A:277:LYS:CD	1:A:277:LYS:N	2.80	0.44
1:B:52:LEU:N	1:B:52:LEU:CD2	2.79	0.44
1:A:133:ILE:HG22	1:A:451:LEU:HD13	1.99	0.44
1:A:143:ASN:ND2	1:A:148:ASN:ND2	2.63	0.44
1:A:433:GLU:HG2	1:A:437:ARG:HD2	1.99	0.44
1:B:122:PHE:CD1	1:B:122:PHE:C	2.95	0.44
1:B:231:ARG:HB2	1:B:231:ARG:HH11	1.83	0.44
1:B:517:TYR:CD2	1:B:518:ALA:N	2.86	0.44
1:A:236:ILE:HG21	1:A:319:ILE:HG22	2.00	0.44
1:B:41:TYR:CD2	1:B:73:LEU:HD12	2.53	0.44
1:B:154:GLU:OE2	1:B:163:ARG:NH1	2.50	0.44
1:B:341:LEU:HD11	1:B:345:LEU:HD11	1.99	0.44
1:B:483:LEU:O	1:B:486:PHE:HB3	2.17	0.44
1:A:83:VAL:HG12	1:A:84:PHE:N	2.31	0.43
1:A:508:TRP:HZ2	1:A:545:VAL:HG22	1.82	0.43
1:B:246:GLY:HA2	1:B:292:ALA:O	2.18	0.43
1:B:278:THR:OG1	1:B:279:SER:N	2.50	0.43
1:B:346:ASN:HA	1:B:347:PRO:HD2	1.83	0.43
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.53	0.43
1:B:582:TRP:CZ3	1:B:584:GLY:HA2	2.52	0.43
1:A:125:PRO:HD3	1:A:369:ASP:OD2	2.17	0.43
1:A:378:GLU:O	1:A:382:ARG:HG3	2.18	0.43
1:A:383:PHE:CD2	1:A:394:PHE:CD1	3.07	0.43
1:A:189:ALA:CB	1:A:235:LYS:HB2	2.47	0.43
1:A:458:ILE:CG2	1:A:479:GLN:HG2	2.48	0.43
1:B:191:TYR:CD1	1:B:191:TYR:C	2.94	0.43
1:B:480:ASN:CG	1:B:483:LEU:HB2	2.43	0.43
1:A:248:GLN:H	1:A:248:GLN:CD	2.26	0.43
1:B:132:VAL:HG11	1:B:491:ILE:HD12	2.01	0.43
1:A:14:TYR:OH	1:A:28:ARG:HD3	2.19	0.43
1:A:86:LEU:O	1:A:93:ALA:HA	2.17	0.43
1:B:63:ASP:HA	1:B:396:ALA:HA	2.01	0.43
1:B:95:TYR:CD2	1:B:105:ARG:HG3	2.53	0.43
1:B:238:LEU:HD12	1:B:319:ILE:HD13	2.01	0.43
1:B:332:HIS:O	1:B:333:ALA:C	2.59	0.43
1:B:377:ARG:NH2	1:B:381:ILE:HD11	2.33	0.43
1:A:426:LEU:HD12	1:A:431:GLY:HA2	2.01	0.43
1:B:243:ASN:ND2	1:B:295:LYS:HZ3	2.16	0.43
1:B:375:LEU:HD21	1:B:400:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD23	1:B:442:PHE:N	2.32	0.43
1:B:444:MET:HG3	1:B:490:LEU:HB3	2.01	0.43
1:A:193:THR:O	1:A:195:ILE:HG23	2.19	0.43
1:A:3:LEU:HD13	1:A:101:PHE:CD1	2.54	0.43
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.83	0.43
1:B:572:THR:C	1:B:573:LEU:HD22	2.44	0.43
1:A:1:MET:CE	1:A:34:VAL:HG22	2.49	0.43
1:A:190:LEU:HG	1:A:234:ILE:HG21	2.00	0.43
1:A:415:ASN:HD21	1:A:448:GLY:HA3	1.83	0.43
1:B:122:PHE:C	1:B:122:PHE:HD1	2.27	0.43
1:A:7:PHE:CG	1:A:8:HIS:N	2.87	0.42
1:A:134:TYR:HE2	1:A:136:ILE:HD11	1.82	0.42
1:A:203:LYS:HG3	1:A:216:PHE:CE2	2.54	0.42
1:A:560:GLU:HG3	1:A:562:VAL:HG13	2.00	0.42
1:B:193:THR:O	1:B:195:ILE:HG23	2.19	0.42
1:B:260:GLU:O	1:B:265:LYS:HD3	2.19	0.42
1:B:409:ALA:O	1:B:413:LEU:HG	2.19	0.42
1:B:332:HIS:CD2	1:B:367:GLN:OE1	2.72	0.42
1:A:179:LEU:HB2	1:A:180:PRO:HD3	2.02	0.42
1:B:219:LEU:N	1:B:220:PRO:CD	2.82	0.42
1:B:223:ARG:HH21	1:B:223:ARG:HG3	1.84	0.42
1:B:398:LEU:HD12	1:B:398:LEU:H	1.85	0.42
1:A:269:PHE:O	1:A:283:TYR:HA	2.18	0.42
1:A:277:LYS:N	1:A:277:LYS:CE	2.83	0.42
1:B:8:HIS:CD2	1:B:84:PHE:HE1	2.38	0.42
1:A:64:GLU:OE2	1:A:64:GLU:HA	2.20	0.42
1:A:178:ARG:O	1:A:182:LEU:CD1	2.67	0.42
1:A:377:ARG:C	1:A:377:ARG:HD3	2.44	0.42
1:A:433:GLU:O	1:A:436:PHE:HB3	2.20	0.42
1:A:523:VAL:O	1:A:523:VAL:CG1	2.67	0.42
1:B:19:SER:OG	1:B:20:GLU:N	2.53	0.42
1:B:203:LYS:NZ	1:B:213:ASP:OD2	2.38	0.42
1:A:12:GLY:HA2	1:A:364:MET:CE	2.49	0.42
1:B:47:SER:HA	1:B:48:PRO:HD3	1.94	0.42
1:B:337:GLU:O	1:B:340:ARG:HB3	2.19	0.42
1:B:411:GLN:HE21	1:B:411:GLN:HB3	1.64	0.42
1:A:200:SER:O	1:A:203:LYS:HE2	2.20	0.42
1:A:326:VAL:HG12	1:A:326:VAL:O	2.20	0.42
1:B:382:ARG:HH22	1:B:397:GLU:CD	2.27	0.42
1:B:423:GLU:HG3	1:B:428:SER:OG	2.20	0.42
1:A:193:THR:HG22	1:A:194:PRO:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HA	1:A:28:ARG:O	2.20	0.42
1:A:179:LEU:N	1:A:180:PRO:CD	2.83	0.42
1:A:574:ARG:HD2	1:A:577:GLN:CD	2.45	0.42
1:B:97:GLY:C	1:B:111:PHE:CE1	2.98	0.42
1:A:222:PHE:O	1:A:223:ARG:C	2.61	0.41
1:B:383:PHE:HD2	1:B:384:PHE:CE1	2.38	0.41
1:B:416:LEU:HD23	1:B:416:LEU:N	2.10	0.41
1:A:73:LEU:HD12	1:A:73:LEU:N	2.35	0.41
1:A:81:LYS:HA	1:A:111:PHE:O	2.19	0.41
1:A:82:TYR:N	1:A:110:VAL:HG22	2.35	0.41
1:A:171:ASP:HB3	1:A:215:GLN:O	2.20	0.41
1:A:351:ILE:HB	1:A:369:ASP:OD1	2.20	0.41
1:A:411:GLN:OE1	1:A:502:ARG:HA	2.20	0.41
1:A:148:ASN:CG	1:A:149:ASP:N	2.78	0.41
1:A:1:MET:HE1	1:A:34:VAL:HG22	2.01	0.41
1:B:253:ARG:O	1:B:257:GLN:HG3	2.19	0.41
1:B:378:GLU:O	1:B:382:ARG:HG3	2.21	0.41
1:B:442:PHE:HB2	1:B:532:LEU:CD1	2.51	0.41
1:B:553:TRP:CZ3	1:B:583:ASN:HB3	2.55	0.41
1:A:297:ARG:HG3	1:A:297:ARG:NH1	2.35	0.41
1:B:499:SER:HB3	1:B:523:VAL:HG12	2.03	0.41
1:A:287:ALA:H	1:A:290:VAL:CG1	2.34	0.41
1:A:446:TYR:CD2	1:A:447:LEU:N	2.89	0.41
1:B:44:ARG:HD3	1:B:114:ALA:O	2.21	0.41
1:A:5:ALA:HB1	1:A:66:PHE:HE2	1.86	0.41
1:A:133:ILE:HD13	1:A:449:THR:CG2	2.50	0.41
1:A:193:THR:O	1:A:194:PRO:C	2.61	0.41
1:A:228:GLU:OE2	1:A:231:ARG:NH1	2.53	0.41
1:A:243:ASN:ND2	1:A:244:HIS:HD2	2.19	0.41
1:B:447:LEU:HD22	1:B:505:VAL:CG2	2.50	0.41
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.56	0.41
1:A:142:ALA:O	1:A:170:GLY:HA2	2.21	0.41
1:A:143:ASN:ND2	1:A:169:GLY:O	2.53	0.41
1:A:150:PRO:HG3	1:A:167:PHE:CD2	2.56	0.41
1:A:165:ASP:HA	1:A:201:HIS:CD2	2.54	0.41
1:A:308:PHE:HB3	1:A:341:LEU:HD22	2.02	0.41
1:A:386:THR:CB	1:A:388:GLU:HG2	2.50	0.41
1:A:444:MET:HG2	1:A:490:LEU:HB3	2.03	0.41
1:A:454:TYR:CE1	1:A:460:MET:HE1	2.55	0.41
1:A:531:VAL:HG11	1:A:573:LEU:HD11	2.03	0.41
1:B:3:LEU:CD1	1:B:3:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:OE1	1:B:54:HIS:ND1	2.54	0.41
1:B:73:LEU:H	1:B:73:LEU:HD22	1.85	0.41
1:B:185:LEU:HD23	1:B:187:VAL:CG1	2.49	0.41
1:B:362:TRP:O	1:B:363:LEU:HD13	2.21	0.41
1:B:363:LEU:HB3	1:B:409:ALA:HB2	2.03	0.41
1:B:368:PHE:N	1:B:368:PHE:CD1	2.88	0.41
1:B:455:GLY:CA	1:B:457:GLU:OE1	2.68	0.41
1:B:538:LYS:HB2	1:B:575:PRO:HD3	2.02	0.41
1:A:377:ARG:NH1	1:A:381:ILE:CD1	2.76	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.84	0.41
1:B:432:ASN:CG	1:B:435:LYS:HG3	2.46	0.41
1:A:404:LEU:HB3	1:A:405:TYR:CD2	2.56	0.40
1:B:36:ARG:CG	1:B:36:ARG:NH2	2.76	0.40
1:B:243:ASN:HD21	1:B:295:LYS:NZ	2.19	0.40
1:B:394:PHE:CD2	1:B:398:LEU:HD11	2.53	0.40
1:B:447:LEU:HB2	1:B:505:VAL:HG22	2.04	0.40
1:A:27:LEU:HD23	1:A:28:ARG:N	2.35	0.40
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.36	0.40
1:A:488:LYS:HE2	1:A:492:ARG:HH22	1.87	0.40
1:B:3:LEU:N	1:B:3:LEU:HD12	2.36	0.40
1:B:134:TYR:HB2	1:B:187:VAL:CG1	2.50	0.40
1:B:298:THR:OG1	1:B:330:VAL:HG13	2.21	0.40
1:B:358:ASP:C	1:B:358:ASP:OD1	2.64	0.40
1:B:500:LEU:HD21	1:B:528:VAL:HG11	2.02	0.40
1:A:238:LEU:HD11	1:A:319:ILE:HG21	2.04	0.40
1:A:377:ARG:HH12	1:A:381:ILE:HD11	1.77	0.40
1:A:382:ARG:HA	1:A:386:THR:OG1	2.22	0.40
1:B:398:LEU:HD23	1:B:446:TYR:CZ	2.57	0.40
1:B:528:VAL:HG22	1:B:582:TRP:HD1	1.86	0.40
1:A:400:ARG:NH1	1:B:99:THR:O	2.54	0.40
1:A:436:PHE:CE2	1:A:483:LEU:HD11	2.56	0.40
1:B:132:VAL:H	1:B:188:THR:HG1	1.70	0.40
1:B:286:PHE:CZ	2:D:3:GLC:H62	2.56	0.40
1:B:363:LEU:HD22	1:B:363:LEU:N	2.36	0.40
1:A:245:ALA:O	1:A:294:PRO:HD2	2.21	0.40
1:A:519:PHE:CE2	1:A:521:ARG:HD3	2.56	0.40
1:A:522:THR:HG23	1:A:526:GLN:O	2.22	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%)	537 (92%)	41 (7%)	5 (1%)	14	43
1	B	583/585 (100%)	534 (92%)	43 (7%)	6 (1%)	12	40
All	All	1166/1170 (100%)	1071 (92%)	84 (7%)	11 (1%)	14	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	GLU
1	B	286	PHE
1	B	547	GLU
1	B	562	VAL
1	B	278	THR
1	A	358	ASP
1	A	547	GLU
1	B	279	SER
1	A	286	PHE
1	A	560	GLU
1	B	288	VAL

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%)	451 (92%)	42 (8%)	10	33
1	B	493/493 (100%)	431 (87%)	62 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	986/986 (100%)	882 (90%)	104 (10%)	6 25

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	33	ASP
1	A	35	VAL
1	A	40	LEU
1	A	65	ARG
1	A	73	LEU
1	A	77	THR
1	A	112	GLN
1	A	118	ARG
1	A	139	GLU
1	A	163	ARG
1	A	178	ARG
1	A	180	PRO
1	A	194	PRO
1	A	201	HIS
1	A	214	PRO
1	A	219	LEU
1	A	223	ARG
1	A	261	GLN
1	A	277	LYS
1	A	280	ARG
1	A	290	VAL
1	A	293	MET
1	A	323	ARG
1	A	330	VAL
1	A	368	PHE
1	A	416	LEU
1	A	418	ASP
1	A	426	LEU
1	A	437	ARG
1	A	466	PRO
1	A	477	LYS
1	A	478	GLU
1	A	504	ASN
1	A	542	LEU
1	A	544	GLN
1	A	547	GLU

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Mol	Chain	Res	Type
1	A	552	THR
1	A	561	GLU
1	A	563	HIS
1	A	571	LEU
1	A	581	LEU
1	B	4	GLU
1	B	24	ARG
1	B	25	VAL
1	B	33	ASP
1	B	34	VAL
1	B	36	ARG
1	B	37	CYS
1	B	40	LEU
1	B	50	GLU
1	B	52	LEU
1	B	65	ARG
1	B	67	ASP
1	B	73	LEU
1	B	75	CYS
1	B	86	LEU
1	B	87	THR
1	B	99	THR
1	B	102	SER
1	B	139	GLU
1	B	148	ASN
1	B	153	THR
1	B	155	GLN
1	B	159	ASP
1	B	164	HIS
1	B	190	LEU
1	B	195	ILE
1	B	206	THR
1	B	231	ARG
1	B	232	ARG
1	B	250	PHE
1	B	255	VAL
1	B	261	GLN
1	B	296	LEU
1	B	316	GLU
1	B	317	GLN
1	B	323	ARG
1	B	325	ASN

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Mol	Chain	Res	Type
1	B	328	ASN
1	B	344	SER
1	B	372	MET
1	B	375	LEU
1	B	382	ARG
1	B	386	THR
1	B	404	LEU
1	B	411	GLN
1	B	416	LEU
1	B	418	ASP
1	B	438	LEU
1	B	440	VAL
1	B	441	LEU
1	B	451	LEU
1	B	470	ARG
1	B	483	LEU
1	B	504	ASN
1	B	505	VAL
1	B	522	THR
1	B	535	ARG
1	B	539	GLN
1	B	544	GLN
1	B	569	LEU
1	B	573	LEU
1	B	574	ARG

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

Mol	Chain	Res	Type
1	A	22	GLN
1	A	112	GLN
1	A	117	HIS
1	A	143	ASN
1	A	148	ASN
1	A	164	HIS
1	A	215	GLN
1	A	248	GLN
1	A	346	ASN
1	A	408	GLN
1	A	411	GLN
1	A	415	ASN
1	A	443	GLN

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Mol	Chain	Res	Type
1	A	504	ASN
1	A	527	HIS
1	A	544	GLN
1	A	566	GLN
1	A	568	GLN
1	B	143	ASN
1	B	148	ASN
1	B	155	GLN
1	B	243	ASN
1	B	328	ASN
1	B	332	HIS
1	B	346	ASN
1	B	357	HIS
1	B	408	GLN
1	B	495	HIS
1	B	504	ASN
1	B	509	HIS
1	B	513	GLN
1	B	526	GLN
1	B	527	HIS
1	B	544	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	1	2	12,12,12	0.75	0	17,17,17	2.30	4 (23%)
2	GLC	C	2	2	11,11,12	0.46	0	15,15,17	1.23	1 (6%)
2	GLC	C	3	2	11,11,12	1.02	1 (9%)	15,15,17	0.99	1 (6%)
2	GLC	C	4	2	11,11,12	0.97	0	15,15,17	1.26	3 (20%)
2	GLC	D	1	2	12,12,12	0.77	0	17,17,17	2.56	5 (29%)
2	GLC	D	2	2	11,11,12	0.51	0	15,15,17	1.59	1 (6%)
2	GLC	D	3	2	11,11,12	0.89	1 (9%)	15,15,17	0.93	1 (6%)
2	GLC	D	4	2	11,11,12	0.97	0	15,15,17	0.94	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	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	GLC	O5-C1	2.57	1.48	1.43
2	D	3	GLC	O5-C1	2.30	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-O5-C5	7.22	127.62	113.65
2	C	1	GLC	C1-O5-C5	6.10	125.46	113.65
2	D	2	GLC	C1-O5-C5	5.25	119.22	112.19
2	D	1	GLC	C4-C3-C2	4.30	118.37	110.83
2	C	2	GLC	C1-O5-C5	4.06	117.63	112.19
2	D	1	GLC	C1-C2-C3	3.99	118.49	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-C2-C3	3.99	118.48	110.36
2	C	1	GLC	C4-C3-C2	3.90	117.67	110.83
2	C	4	GLC	C1-O5-C5	2.85	116.01	112.19
2	D	1	GLC	O5-C1-C2	2.81	115.24	110.30
2	C	3	GLC	C1-O5-C5	2.70	115.80	112.19
2	C	1	GLC	O5-C1-C2	2.61	114.89	110.30
2	D	1	GLC	C3-C4-C5	2.41	114.61	110.23
2	C	4	GLC	C1-C2-C3	2.21	112.87	109.64
2	D	3	GLC	C1-O5-C5	2.17	115.09	112.19
2	C	4	GLC	C2-C3-C4	-2.09	107.18	110.86

There are no chirality outliers.

All (9) torsion outliers are listed below:

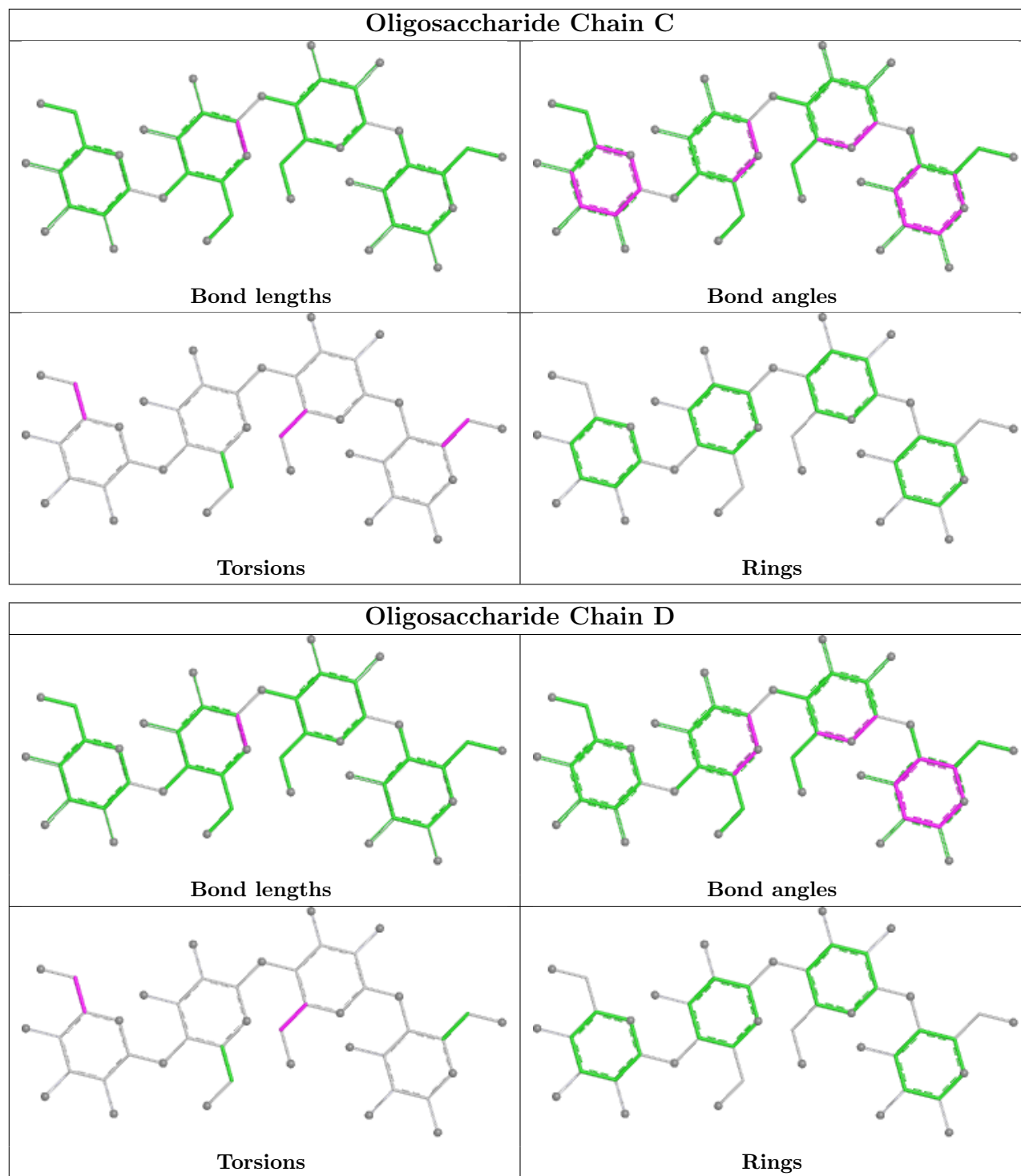
Mol	Chain	Res	Type	Atoms
2	C	4	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	GLC	2	0
2	D	3	GLC	1	0

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



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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%)	-0.33	2 (0%) 90 82	9, 30, 53, 72	0
1	B	585/585 (100%)	-0.36	1 (0%) 91 86	11, 32, 59, 88	0
All	All	1170/1170 (100%)	-0.34	3 (0%) 90 82	9, 31, 57, 88	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	TYR	3.1
1	A	272	ASP	2.0
1	A	201	HIS	2.0

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

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

6.3 Carbohydrates [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. 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.

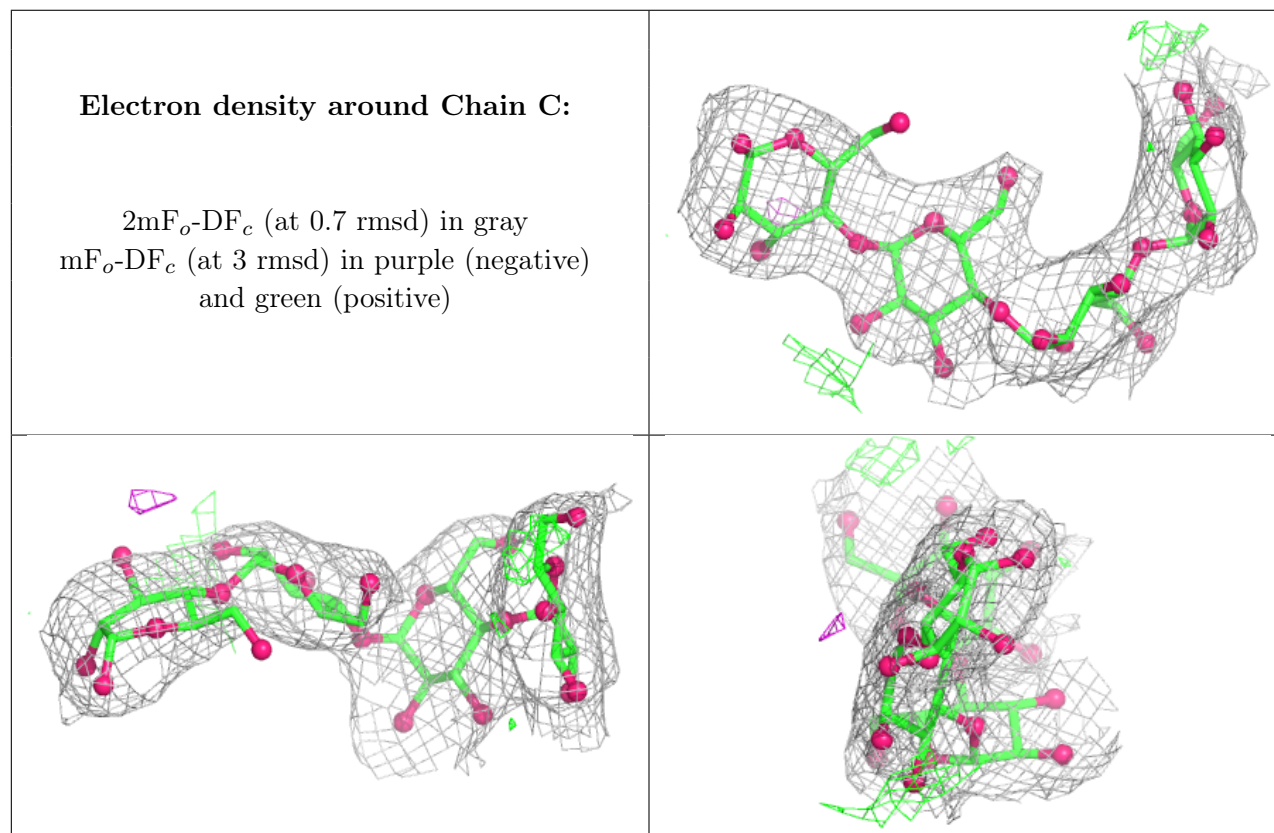
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	1	12/12	0.85	0.14	36,41,45,46	0
2	GLC	D	2	11/12	0.90	0.10	40,41,44,46	0
2	GLC	D	4	11/12	0.90	0.12	48,49,51,53	0
2	GLC	C	4	11/12	0.91	0.08	23,23,27,29	0
2	GLC	D	1	12/12	0.91	0.10	38,39,43,46	0
2	GLC	D	3	11/12	0.93	0.10	42,45,47,47	0

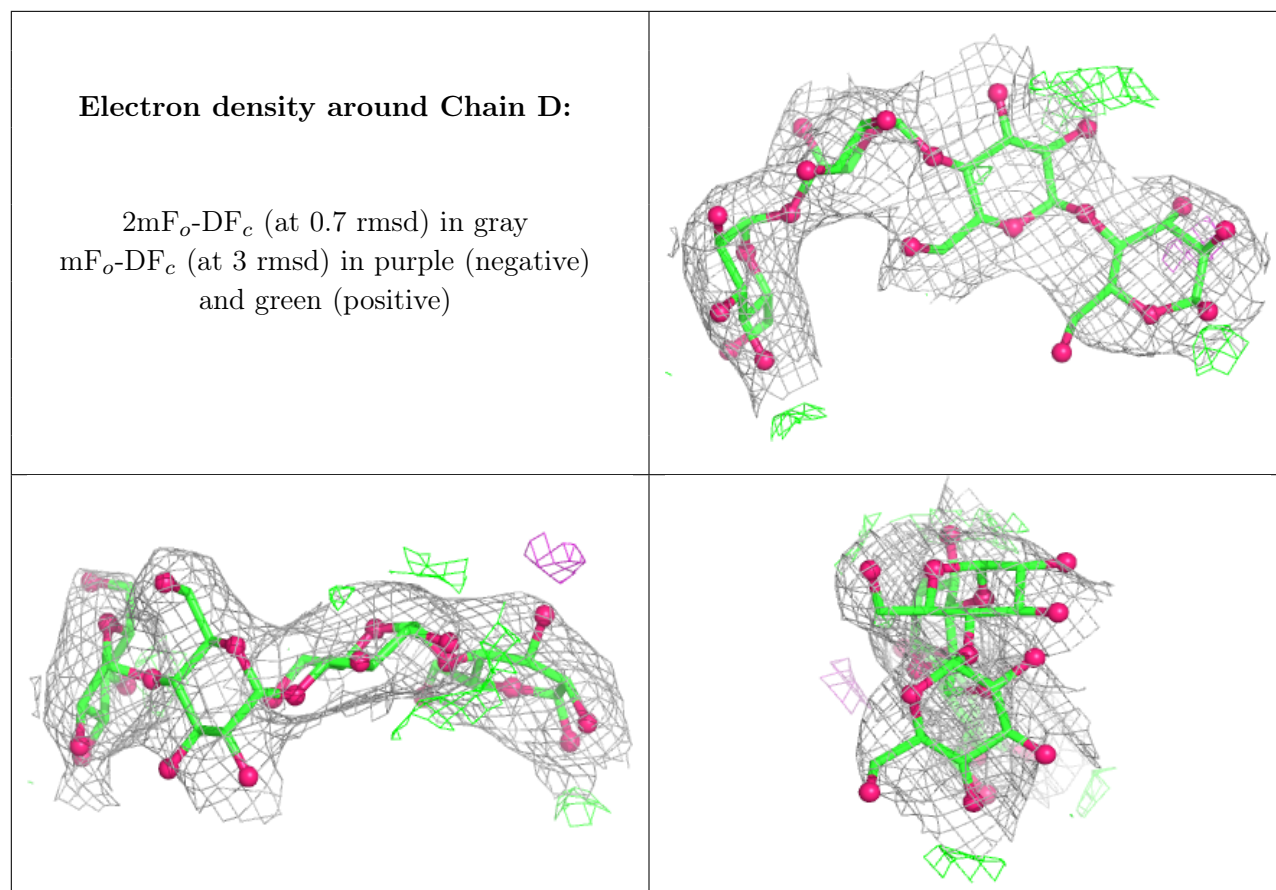
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	2	11/12	0.95	0.08	28,30,34,34	0
2	GLC	C	3	11/12	0.97	0.06	13,21,23,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.