



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 1JL8 / pdb_00001jl8
Title : Complex of alpha-amylase II (TVA II) from Thermoactinomyces vulgaris R-47 with beta-cyclodextrin based on a co-crystallization with methyl beta-cyclodextrin
Authors : Yokota, T.; Tonozuka, T.; Shimura, Y.; Ichikawa, K.; Kamitori, S.; Sakano, Y.
Deposited on : 2001-07-16
Resolution : 3.20 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

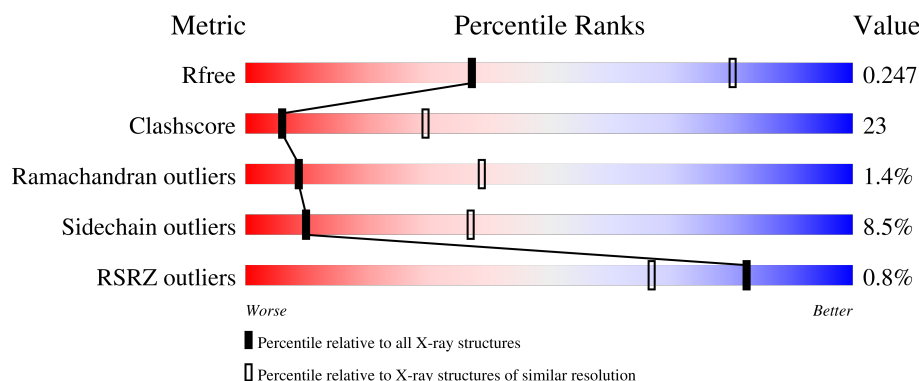
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	% 56% 38% 6%
1	B	585	% 57% 37% 5%
2	C	7	14% 86%
2	D	7	100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9706 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.

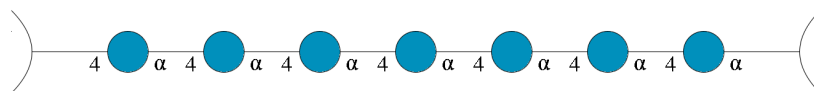
- Molecule 1 is a protein called ALPHA-AMYLASE II.

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 Cycloheptakis-(1-4)-(alpha-D-glucopyranose).

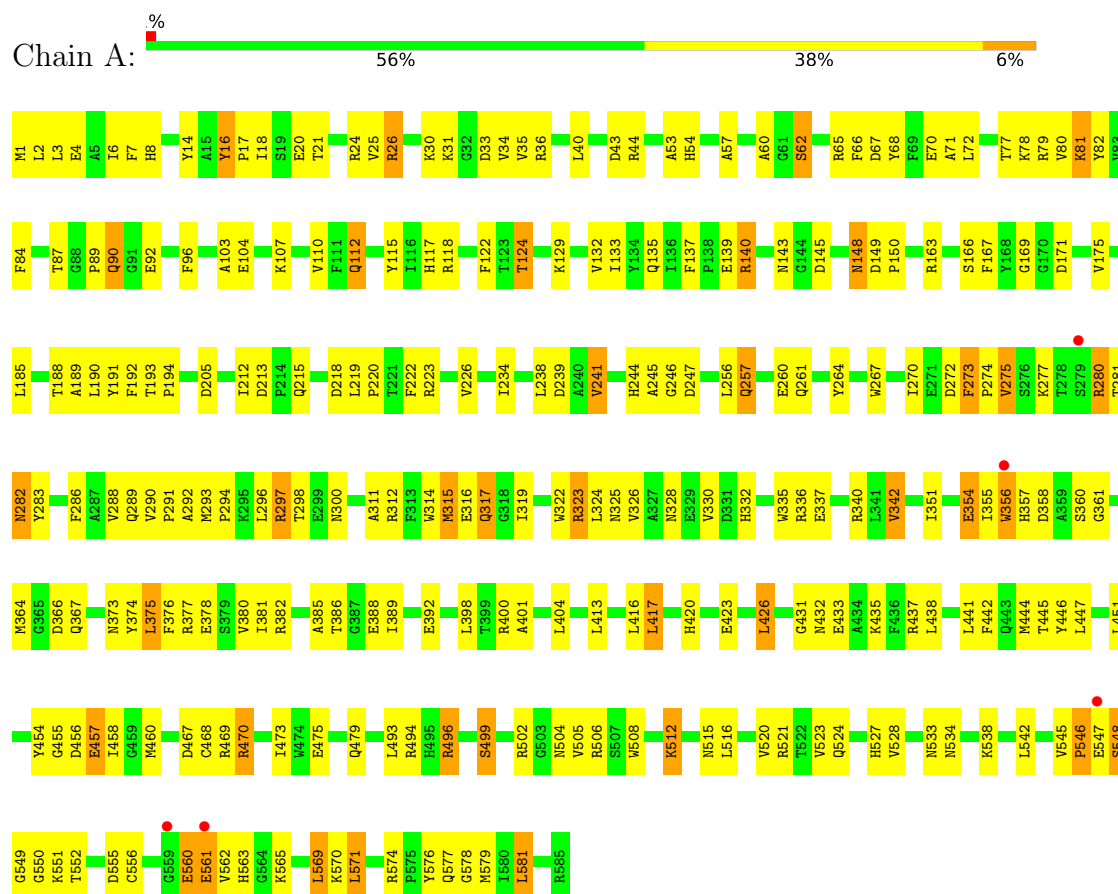


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			77	42	35			
2	D	7	Total	C	O	0	0	0
			77	42	35			

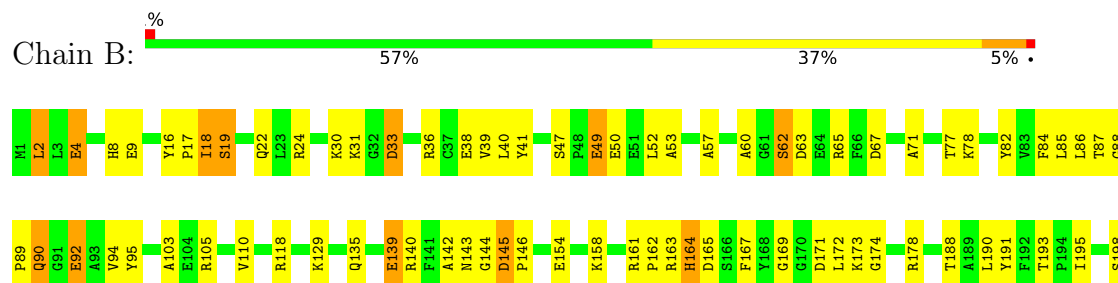
3 Residue-property plots [i](#)

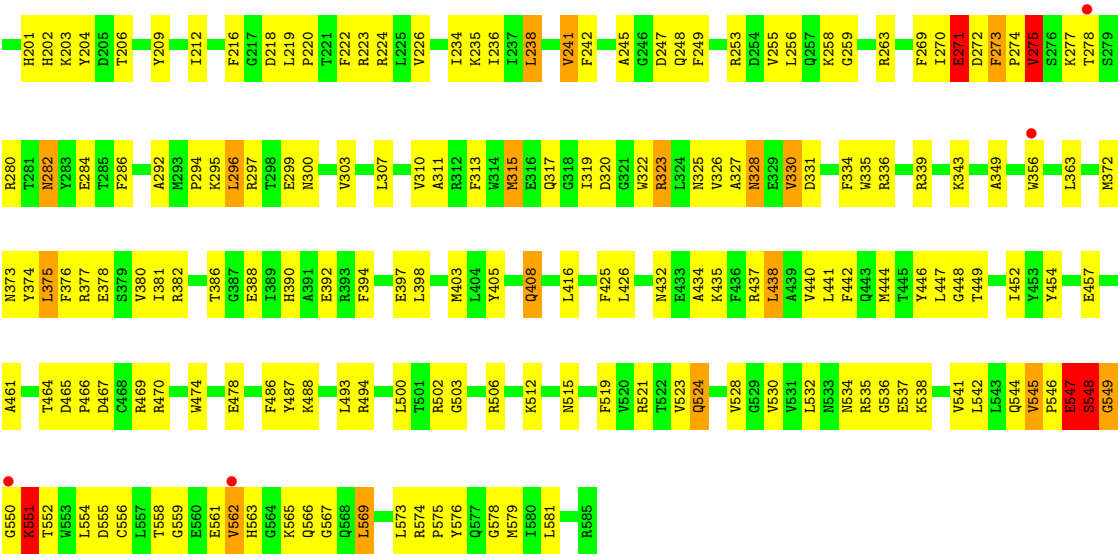
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

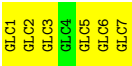


• Molecule 1: ALPHA-AMYLASE II

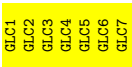
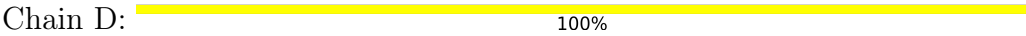




● Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.02Å 120.36Å 113.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.50 – 3.20 39.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.2 (39.50-3.20) 85.2 (39.50-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.255 0.187 , 0.247	Depositor DCC
R_{free} test set	2302 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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	0.60	0/4906	1.00	17/6641 (0.3%)
1	B	0.58	0/4906	1.00	16/6641 (0.2%)
All	All	0.59	0/9812	1.00	33/13282 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	VAL	CA-C-N	11.50	134.22	119.84
1	B	545	VAL	C-N-CA	11.50	134.22	119.84
1	B	18	ILE	N-CA-C	-8.34	104.33	113.43
1	A	18	ILE	N-CA-C	-8.30	104.93	112.90
1	B	551	LYS	N-CA-C	7.50	122.16	112.41
1	A	16	TYR	CA-C-N	7.39	127.15	119.76
1	A	16	TYR	C-N-CA	7.39	127.15	119.76
1	A	280	ARG	N-CA-C	-7.05	100.02	110.46
1	B	145	ASP	CA-C-N	6.88	126.50	119.56
1	B	145	ASP	C-N-CA	6.88	126.50	119.56
1	B	236	ILE	N-CA-C	6.83	117.73	107.75
1	B	275	VAL	N-CA-C	6.74	118.13	109.30
1	B	161	ARG	CA-C-N	6.71	128.23	119.84
1	B	161	ARG	C-N-CA	6.71	128.23	119.84
1	A	290	VAL	CA-C-N	6.31	126.79	119.47
1	A	290	VAL	C-N-CA	6.31	126.79	119.47
1	B	449	THR	CA-C-N	6.21	126.15	119.76
1	B	449	THR	C-N-CA	6.21	126.15	119.76
1	A	323	ARG	N-CA-C	-6.07	99.29	109.07
1	B	524	GLN	CB-CA-C	-6.01	109.63	116.54
1	A	80	VAL	N-CA-C	5.91	115.62	108.06
1	A	550	GLY	N-CA-C	5.89	118.92	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ALA	N-CA-C	-5.61	106.28	113.23
1	A	103	ALA	N-CA-C	-5.54	106.02	112.89
1	A	549	GLY	N-CA-C	5.49	125.17	115.61
1	A	148	ASN	N-CA-C	-5.43	104.91	112.45
1	B	545	VAL	N-CA-C	5.42	113.40	107.60
1	A	66	PHE	N-CA-C	5.39	118.49	110.14
1	A	524	GLN	CB-CA-C	-5.35	109.96	117.23
1	A	112	GLN	N-CA-C	5.24	117.62	108.76
1	A	342	VAL	N-CA-C	5.22	115.84	110.36
1	B	548	SER	N-CA-C	5.17	121.81	110.80
1	A	417	LEU	N-CA-C	-5.15	107.13	113.41

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	210	0
1	B	4776	0	4609	227	0
2	C	77	0	63	0	0
2	D	77	0	63	0	0
All	All	9706	0	9344	432	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 23.

All (432) 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:44:ARG:HE	1:A:112:GLN:HE21	1.06	1.00
1:B:579:MET:HE2	1:B:581:LEU:HD11	1.46	0.97
1:B:408:GLN:H	1:B:408:GLN:HE21	1.06	0.95
1:A:378:GLU:OE2	1:A:382:ARG:HD3	1.69	0.93
1:B:558:THR:HG23	1:B:559:GLY:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:HG3	1:B:512:LYS:HB2	1.52	0.89
1:B:551:LYS:NZ	1:B:551:LYS:HB2	1.88	0.89
1:A:44:ARG:NE	1:A:112:GLN:HE21	1.71	0.88
1:B:408:GLN:H	1:B:408:GLN:NE2	1.72	0.88
1:A:282:ASN:H	1:A:282:ASN:HD22	1.15	0.88
1:A:44:ARG:HE	1:A:112:GLN:NE2	1.73	0.86
1:A:145:ASP:O	1:A:148:ASN:ND2	2.09	0.86
1:A:247:ASP:HB3	1:A:292:ALA:HA	1.60	0.84
1:A:382:ARG:HH11	1:A:389:ILE:HG21	1.42	0.83
1:B:282:ASN:HD22	1:B:282:ASN:H	1.25	0.83
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.60	0.83
1:B:548:SER:O	1:B:550:GLY:N	2.11	0.82
1:B:444:MET:HE1	1:B:452:ILE:HD11	1.60	0.82
1:B:380:VAL:HG23	1:B:381:ILE:HD12	1.63	0.80
1:B:546:PRO:O	1:B:548:SER:N	2.14	0.80
1:A:386:THR:OG1	1:A:388:GLU:HG3	1.82	0.80
1:B:158:LYS:O	1:B:158:LYS:HD3	1.82	0.79
1:B:546:PRO:C	1:B:548:SER:H	1.92	0.77
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.66	0.77
1:A:3:LEU:HA	1:A:6:ILE:HD12	1.66	0.76
1:A:288:VAL:HG23	1:A:289:GLN:H	1.48	0.76
1:B:282:ASN:HD22	1:B:282:ASN:N	1.84	0.76
1:B:280:ARG:NH1	1:B:280:ARG:HA	1.99	0.76
1:A:218:ASP:OD1	1:A:220:PRO:HD2	1.87	0.75
1:A:282:ASN:H	1:A:282:ASN:ND2	1.86	0.74
1:B:253:ARG:HG3	1:B:253:ARG:HH11	1.53	0.73
1:B:408:GLN:HE21	1:B:408:GLN:N	1.84	0.72
1:A:282:ASN:HD22	1:A:282:ASN:N	1.86	0.72
1:B:416:LEU:HD23	1:B:416:LEU:H	1.56	0.71
1:A:89:PRO:HG2	1:A:90:GLN:HE21	1.55	0.71
1:A:381:ILE:O	1:A:385:ALA:HB3	1.91	0.71
1:B:538:LYS:HG2	1:B:575:PRO:HD3	1.73	0.71
1:A:332:HIS:HD2	1:A:367:GLN:HE22	1.37	0.71
1:B:551:LYS:HB2	1:B:551:LYS:HZ2	1.55	0.70
1:A:24:ARG:HH21	1:A:72:LEU:HD23	1.56	0.70
1:B:2:LEU:HD23	1:B:4:GLU:HG2	1.73	0.69
1:A:280:ARG:HG2	1:A:281:THR:N	2.08	0.69
1:A:505:VAL:HG22	1:A:521:ARG:CD	2.22	0.68
1:B:296:LEU:HD23	1:B:307:LEU:HD11	1.74	0.68
1:B:143:ASN:CG	1:B:169:GLY:O	2.36	0.68
1:A:244:HIS:NE2	1:A:293:MET:HE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:OD1	1:A:148:ASN:ND2	2.27	0.67
1:A:373:ASN:ND2	1:A:376:PHE:HB2	2.10	0.67
1:B:253:ARG:HG3	1:B:253:ARG:NH1	2.07	0.67
1:A:496:ARG:HH11	1:A:496:ARG:HB2	1.60	0.67
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.59	0.66
1:A:311:ALA:O	1:A:315:MET:HG3	1.96	0.66
1:B:245:ALA:O	1:B:294:PRO:HD2	1.94	0.65
1:B:247:ASP:HB2	1:B:277:LYS:HE2	1.79	0.65
1:B:315:MET:HE3	1:B:322:TRP:NE1	2.11	0.65
1:A:377:ARG:HA	1:A:380:VAL:HG22	1.78	0.64
1:B:198:SER:HB3	1:B:203:LYS:HD2	1.80	0.64
1:B:373:ASN:ND2	1:B:376:PHE:HB2	2.14	0.63
1:A:2:LEU:HD13	1:B:2:LEU:HD21	1.79	0.63
1:A:193:THR:HB	1:A:194:PRO:HD2	1.80	0.62
1:A:274:PRO:O	1:A:275:VAL:C	2.42	0.62
1:A:20:GLU:OE1	1:A:118:ARG:HG2	2.00	0.62
1:B:558:THR:HG23	1:B:559:GLY:N	2.10	0.62
1:B:503:GLY:CA	1:B:523:VAL:HG23	2.29	0.62
1:B:198:SER:HB3	1:B:203:LYS:CD	2.29	0.62
1:A:515:ASN:ND2	1:A:534:ASN:HB3	2.14	0.61
1:B:435:LYS:HG2	1:B:576:TYR:CE2	2.35	0.61
1:A:190:LEU:HD13	1:A:234:ILE:HG21	1.82	0.61
1:A:104:GLU:OE2	1:A:107:LYS:HG3	2.01	0.61
1:B:381:ILE:HD12	1:B:425:PHE:HE1	1.65	0.61
1:B:546:PRO:C	1:B:548:SER:N	2.52	0.61
1:B:503:GLY:HA2	1:B:523:VAL:HG23	1.83	0.61
1:B:551:LYS:HB2	1:B:551:LYS:HZ3	1.66	0.60
1:B:140:ARG:HG2	1:B:469:ARG:O	2.01	0.60
1:B:275:VAL:HA	1:B:282:ASN:OD1	2.01	0.60
1:A:163:ARG:HB2	1:A:166:SER:OG	2.01	0.60
1:A:280:ARG:HG2	1:A:281:THR:H	1.66	0.60
1:B:62:SER:HB3	1:B:67:ASP:HA	1.83	0.60
1:B:202:HIS:HB2	1:B:204:TYR:HD2	1.67	0.60
1:B:89:PRO:HB2	1:B:90:GLN:OE1	2.02	0.60
1:B:255:VAL:HG12	1:B:275:VAL:HG21	1.84	0.60
1:A:433:GLU:HG2	1:A:437:ARG:HD2	1.83	0.59
1:B:273:PHE:HB3	1:B:274:PRO:HA	1.84	0.59
1:B:426:LEU:HD23	1:B:461:ALA:HB2	1.83	0.59
1:A:20:GLU:CD	1:A:118:ARG:HG2	2.27	0.59
1:A:273:PHE:CB	1:A:274:PRO:HA	2.33	0.58
1:B:282:ASN:H	1:B:282:ASN:ND2	1.98	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:MET:HE3	1:B:322:TRP:HE1	1.67	0.58
1:A:297:ARG:HG2	1:A:300:ASN:HB2	1.84	0.58
1:B:143:ASN:ND2	1:B:169:GLY:O	2.36	0.58
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.39	0.58
1:B:311:ALA:HA	1:B:322:TRP:CH2	2.38	0.57
1:A:317:GLN:N	1:A:317:GLN:HE21	2.03	0.57
1:B:144:GLY:HA3	1:B:173:LYS:HD2	1.86	0.57
1:A:273:PHE:HB3	1:A:274:PRO:HA	1.87	0.57
1:A:3:LEU:HA	1:A:6:ILE:CD1	2.35	0.57
1:A:273:PHE:CB	1:A:274:PRO:CA	2.82	0.57
1:A:117:HIS:HB3	1:B:299:GLU:OE2	2.05	0.57
1:A:241:VAL:CG1	1:A:325:ASN:HD22	2.18	0.57
1:A:373:ASN:HB2	1:A:413:LEU:HB3	1.87	0.57
1:B:500:LEU:CD2	1:B:528:VAL:HG21	2.35	0.57
1:A:190:LEU:HD13	1:A:234:ILE:CG2	2.35	0.57
1:B:273:PHE:CB	1:B:274:PRO:HA	2.35	0.57
1:B:47:SER:O	1:B:50:GLU:HG2	2.04	0.57
1:A:336:ARG:HD3	1:A:366:ASP:OD2	2.04	0.56
1:A:401:ALA:O	1:A:404:LEU:HB2	2.05	0.56
1:A:1:MET:HE2	1:A:34:VAL:HG22	1.88	0.56
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.40	0.56
1:B:398:LEU:HD21	1:B:442:PHE:HZ	1.70	0.56
1:B:273:PHE:CB	1:B:274:PRO:CA	2.83	0.56
1:B:408:GLN:NE2	1:B:408:GLN:N	2.50	0.56
1:B:538:LYS:HA	1:B:573:LEU:O	2.06	0.56
1:B:377:ARG:HG2	1:B:381:ILE:HD13	1.87	0.56
1:B:467:ASP:CG	1:B:470:ARG:HH21	2.13	0.56
1:B:547:GLU:O	1:B:549:GLY:N	2.34	0.56
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.87	0.55
1:A:467:ASP:OD2	1:A:470:ARG:HD3	2.07	0.55
1:A:270:ILE:HG21	1:A:273:PHE:CD1	2.41	0.55
1:A:328:ASN:HB3	1:A:355:ILE:HG13	1.87	0.55
1:B:235:LYS:HG2	1:B:320:ASP:CG	2.31	0.55
1:A:281:THR:HG23	1:A:289:GLN:HE21	1.71	0.55
1:A:545:VAL:CG1	1:A:569:LEU:HD13	2.37	0.55
1:A:223:ARG:HD3	1:A:317:GLN:HG3	1.88	0.55
1:B:386:THR:OG1	1:B:388:GLU:HG3	2.08	0.55
1:A:523:VAL:O	1:A:523:VAL:HG13	2.07	0.54
1:B:503:GLY:HA2	1:B:523:VAL:CG2	2.36	0.54
1:B:555:ASP:CG	1:B:558:THR:HG22	2.32	0.54
1:A:354:GLU:C	1:A:355:ILE:HD12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:VAL:O	1:A:545:VAL:HG23	2.06	0.54
1:B:271:GLU:HB2	1:B:282:ASN:O	2.08	0.54
1:B:537:GLU:CA	1:B:575:PRO:HG3	2.38	0.54
1:B:562:VAL:HG22	1:B:562:VAL:O	2.08	0.54
1:A:245:ALA:O	1:A:294:PRO:HD2	2.08	0.54
1:B:41:TYR:HB3	1:B:82:TYR:HB3	1.90	0.54
1:B:86:LEU:HB2	1:B:94:VAL:HG23	1.90	0.54
1:B:191:TYR:CZ	1:B:323:ARG:HD3	2.43	0.53
1:A:21:THR:CG2	1:A:21:THR:O	2.56	0.53
1:A:148:ASN:ND2	1:A:171:ASP:OD2	2.41	0.53
1:A:14:TYR:HD1	1:A:26:ARG:HB3	1.74	0.53
1:A:21:THR:O	1:A:21:THR:HG22	2.08	0.53
1:B:143:ASN:ND2	1:B:171:ASP:OD2	2.42	0.53
1:A:528:VAL:HA	1:A:581:LEU:O	2.08	0.53
1:A:432:ASN:OD1	1:A:435:LYS:HG3	2.08	0.52
1:B:129:LYS:HD2	1:B:502:ARG:NH1	2.24	0.52
1:B:548:SER:O	1:B:549:GLY:C	2.52	0.52
1:A:44:ARG:HH21	1:A:112:GLN:NE2	2.07	0.52
1:A:40:LEU:HA	1:A:53:ALA:O	2.09	0.52
1:A:44:ARG:HA	1:A:81:LYS:HG2	1.90	0.52
1:A:185:LEU:O	1:A:185:LEU:HD12	2.10	0.52
1:A:246:GLY:HA2	1:A:292:ALA:O	2.09	0.52
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.91	0.52
1:B:313:PHE:O	1:B:317:GLN:HG2	2.09	0.52
1:B:378:GLU:O	1:B:382:ARG:HG3	2.09	0.52
1:A:545:VAL:HG11	1:A:569:LEU:HD13	1.90	0.52
1:A:562:VAL:O	1:A:562:VAL:HG13	2.09	0.52
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.92	0.52
1:B:437:ARG:O	1:B:440:VAL:HG22	2.09	0.52
1:B:154:GLU:OE1	1:B:163:ARG:NH1	2.43	0.52
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.90	0.52
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.25	0.52
1:B:19:SER:OG	1:B:22:GLN:HG2	2.09	0.52
1:A:542:LEU:HD23	1:A:570:LYS:HA	1.91	0.51
1:A:257:GLN:HE21	1:A:257:GLN:HA	1.75	0.51
1:B:561:GLU:C	1:B:563:HIS:H	2.17	0.51
1:B:256:LEU:HD11	1:B:277:LYS:HD2	1.92	0.51
1:A:446:TYR:CG	1:A:447:LEU:N	2.79	0.51
1:B:273:PHE:HB3	1:B:275:VAL:H	1.76	0.51
1:B:325:ASN:HD22	1:B:326:VAL:H	1.59	0.51
1:B:135:GLN:HG3	1:B:191:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:HG2	1:B:381:ILE:CD1	2.41	0.51
1:A:77:THR:O	1:A:78:LYS:HB2	2.11	0.50
1:A:245:ALA:O	1:A:293:MET:HA	2.11	0.50
1:A:26:ARG:HD2	1:A:70:GLU:OE2	2.12	0.50
1:A:426:LEU:CD2	1:A:431:GLY:HA2	2.41	0.50
1:A:455:GLY:N	1:A:457:GLU:OE1	2.42	0.50
1:A:508:TRP:HB2	1:A:520:VAL:HG23	1.94	0.50
1:B:330:VAL:HG21	1:B:334:PHE:HD1	1.77	0.50
1:A:245:ALA:HB2	1:A:296:LEU:HD11	1.94	0.50
1:B:273:PHE:HB3	1:B:274:PRO:CA	2.41	0.50
1:A:14:TYR:CD1	1:A:26:ARG:HB3	2.46	0.50
1:B:8:HIS:CG	1:B:9:GLU:N	2.80	0.50
1:A:122:PHE:HE2	1:A:124:THR:HG22	1.76	0.50
1:B:328:ASN:N	1:B:328:ASN:HD22	2.09	0.50
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.47	0.50
1:A:273:PHE:HB3	1:A:275:VAL:H	1.76	0.49
1:A:277:LYS:HG2	1:A:291:PRO:HB3	1.94	0.49
1:B:202:HIS:HB2	1:B:204:TYR:CD2	2.46	0.49
1:B:382:ARG:HH12	1:B:397:GLU:CD	2.20	0.49
1:B:87:THR:HA	1:B:92:GLU:O	2.12	0.49
1:B:139:GLU:OE2	1:B:167:PHE:HA	2.12	0.49
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.92	0.49
1:B:325:ASN:ND2	1:B:326:VAL:N	2.60	0.49
1:B:515:ASN:ND2	1:B:534:ASN:HB3	2.27	0.49
1:B:444:MET:O	1:B:494:ARG:NH1	2.45	0.49
1:A:342:VAL:HG11	1:A:351:ILE:HD11	1.95	0.49
1:B:2:LEU:CD2	1:B:4:GLU:HG2	2.42	0.49
1:A:192:PHE:O	1:A:239:ASP:HB2	2.13	0.49
1:B:158:LYS:HD3	1:B:158:LYS:C	2.37	0.49
1:B:209:TYR:HB3	1:B:310:VAL:HG11	1.95	0.49
1:B:467:ASP:OD2	1:B:470:ARG:NE	2.46	0.49
1:A:137:PHE:CE1	1:A:469:ARG:HD3	2.47	0.49
1:A:533:ASN:O	1:A:576:TYR:HA	2.13	0.49
1:B:38:GLU:HB2	1:B:85:LEU:HB3	1.94	0.49
1:B:241:VAL:HG13	1:B:325:ASN:HB3	1.95	0.49
1:B:500:LEU:HD21	1:B:528:VAL:HG21	1.95	0.49
1:A:82:TYR:O	1:A:110:VAL:HG23	2.13	0.48
1:B:545:VAL:HG23	1:B:567:GLY:C	2.38	0.48
1:A:551:LYS:O	1:A:562:VAL:HG23	2.14	0.48
1:A:35:VAL:HG22	1:A:87:THR:O	2.13	0.48
1:A:117:HIS:CD2	1:B:331:ASP:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:HIS:HD1	1:B:466:PRO:HG3	1.77	0.48
1:A:135:GLN:O	1:A:454:TYR:HB3	2.13	0.48
1:B:538:LYS:CG	1:B:575:PRO:HD3	2.43	0.48
1:B:377:ARG:HA	1:B:380:VAL:HG22	1.96	0.48
1:A:2:LEU:HD12	1:A:30:LYS:HD2	1.95	0.48
1:A:475:GLU:O	1:A:479:GLN:HG3	2.12	0.48
1:A:213:ASP:OD1	1:A:215:GLN:HB3	2.14	0.48
1:A:458:ILE:HG13	1:A:460:MET:HG3	1.95	0.48
1:A:493:LEU:HD21	1:A:556:CYS:HB3	1.96	0.48
1:B:256:LEU:CD1	1:B:277:LYS:HD2	2.44	0.48
1:A:82:TYR:C	1:A:110:VAL:HG23	2.39	0.48
1:B:195:ILE:HG13	1:B:195:ILE:O	2.13	0.48
1:B:297:ARG:HD2	1:B:300:ASN:HB2	1.96	0.48
1:B:139:GLU:C	1:B:140:ARG:HD2	2.39	0.48
1:B:248:GLN:O	1:B:253:ARG:HD3	2.14	0.48
1:B:403:MET:HE2	1:B:403:MET:HA	1.95	0.48
1:B:441:LEU:HD13	1:B:578:GLY:HA3	1.96	0.48
1:A:132:VAL:H	1:A:188:THR:HB	1.79	0.47
1:B:270:ILE:HD12	1:B:275:VAL:HG11	1.96	0.47
1:A:8:HIS:HD2	1:A:26:ARG:O	1.96	0.47
1:A:175:VAL:HG11	1:A:192:PHE:HZ	1.78	0.47
1:A:355:ILE:HG22	1:A:357:HIS:H	1.79	0.47
1:A:324:LEU:HD22	1:A:335:TRP:CH2	2.49	0.47
1:B:30:LYS:O	1:B:33:ASP:HB2	2.15	0.47
1:B:129:LYS:HD2	1:B:502:ARG:HH12	1.79	0.47
1:A:273:PHE:HB3	1:A:274:PRO:CA	2.44	0.47
1:A:191:TYR:CZ	1:A:323:ARG:HD3	2.50	0.47
1:A:504:ASN:O	1:A:521:ARG:HA	2.15	0.47
1:B:40:LEU:HA	1:B:53:ALA:O	2.15	0.47
1:A:245:ALA:CB	1:A:296:LEU:HD11	2.44	0.47
1:A:260:GLU:OE1	1:A:260:GLU:N	2.46	0.47
1:B:555:ASP:OD1	1:B:558:THR:HG22	2.15	0.47
1:B:435:LYS:HG2	1:B:576:TYR:HE2	1.78	0.47
1:B:544:GLN:O	1:B:546:PRO:HD3	2.15	0.47
1:B:249:PHE:O	1:B:253:ARG:HG2	2.14	0.47
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.49	0.47
1:B:432:ASN:OD1	1:B:434:ALA:HB3	2.15	0.47
1:A:277:LYS:HG2	1:A:277:LYS:O	2.14	0.47
1:B:193:THR:O	1:B:195:ILE:HG23	2.15	0.46
1:A:560:GLU:C	1:A:561:GLU:HG2	2.41	0.46
1:B:452:ILE:HD12	1:B:487:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HB3	1:A:107:LYS:HB2	1.97	0.46
1:B:49:GLU:H	1:B:49:GLU:HG2	1.57	0.46
1:B:390:HIS:CD2	1:B:512:LYS:HG3	2.50	0.46
1:B:519:PHE:CE1	1:B:530:VAL:HB	2.50	0.46
1:B:195:ILE:HD12	1:B:212:ILE:HD12	1.97	0.46
1:B:273:PHE:HB3	1:B:275:VAL:N	2.30	0.46
1:A:35:VAL:HG23	1:A:36:ARG:HG2	1.98	0.46
1:B:18:ILE:HG13	1:B:22:GLN:HG3	1.98	0.46
1:B:172:LEU:O	1:B:173:LYS:C	2.58	0.46
1:A:336:ARG:CD	1:A:366:ASP:OD2	2.64	0.46
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.51	0.46
1:B:536:GLY:HA2	1:B:575:PRO:HB3	1.98	0.46
1:A:458:ILE:HD12	1:A:473:ILE:HB	1.98	0.46
1:B:377:ARG:O	1:B:381:ILE:HD13	2.16	0.46
1:A:60:ALA:HB1	1:A:506:ARG:NH2	2.31	0.45
1:A:398:LEU:HD21	1:A:442:PHE:CZ	2.51	0.45
1:B:523:VAL:HG12	1:B:524:GLN:HG2	1.98	0.45
1:A:244:HIS:HE2	1:A:293:MET:CE	2.29	0.45
1:B:202:HIS:O	1:B:202:HIS:ND1	2.49	0.45
1:B:327:ALA:O	1:B:330:VAL:HG13	2.16	0.45
1:B:247:ASP:HB3	1:B:292:ALA:HA	1.99	0.45
1:B:574:ARG:HE	1:B:574:ARG:HB3	1.53	0.45
1:A:31:LYS:HA	1:A:67:ASP:OD2	2.15	0.45
1:B:537:GLU:HA	1:B:575:PRO:HG3	1.99	0.45
1:A:140:ARG:HG2	1:A:469:ARG:O	2.17	0.45
1:B:392:GLU:HG3	1:B:512:LYS:CB	2.35	0.45
1:B:565:LYS:HG2	1:B:566:GLN:HG2	1.98	0.45
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.52	0.45
1:A:552:THR:HG23	1:A:562:VAL:HB	1.99	0.45
1:B:300:ASN:HB3	1:B:303:VAL:HG23	1.98	0.45
1:A:122:PHE:CE2	1:A:124:THR:HG22	2.52	0.45
1:A:355:ILE:HD12	1:A:355:ILE:N	2.32	0.45
1:A:445:THR:O	1:A:521:ARG:NH2	2.49	0.45
1:B:88:GLY:HA3	1:B:92:GLU:OE1	2.17	0.45
1:B:253:ARG:HH11	1:B:253:ARG:CG	2.22	0.45
1:B:416:LEU:H	1:B:416:LEU:CD2	2.28	0.45
1:A:244:HIS:HE2	1:A:293:MET:HE2	1.82	0.44
1:B:535:ARG:NE	1:B:535:ARG:HA	2.31	0.44
1:B:538:LYS:HG2	1:B:574:ARG:HA	1.98	0.44
1:B:398:LEU:HG	1:B:446:TYR:OH	2.16	0.44
1:B:325:ASN:CG	1:B:326:VAL:HG23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLY:O	1:B:494:ARG:NH2	2.51	0.44
1:B:561:GLU:OE1	1:B:561:GLU:HA	2.18	0.44
1:A:326:VAL:HG12	1:A:326:VAL:O	2.17	0.44
1:A:420:HIS:O	1:A:468:CYS:SG	2.75	0.44
1:A:416:LEU:H	1:A:416:LEU:HD23	1.82	0.44
1:B:18:ILE:CG1	1:B:22:GLN:HG3	2.47	0.44
1:B:320:ASP:O	1:B:349:ALA:HA	2.18	0.44
1:B:382:ARG:NH1	1:B:397:GLU:OE1	2.49	0.44
1:B:579:MET:HB3	1:B:581:LEU:CD1	2.48	0.44
1:A:133:ILE:HD13	1:A:189:ALA:HB3	1.99	0.44
1:A:330:VAL:HB	1:A:335:TRP:NE1	2.33	0.44
1:A:332:HIS:CD2	1:A:367:GLN:HE22	2.27	0.44
1:B:503:GLY:CA	1:B:523:VAL:CG2	2.95	0.44
1:B:562:VAL:O	1:B:562:VAL:HG13	2.17	0.44
1:A:241:VAL:HG12	1:A:325:ASN:HD22	1.82	0.44
1:B:325:ASN:HD22	1:B:326:VAL:N	2.16	0.44
1:A:25:VAL:CG1	1:A:84:PHE:HZ	2.31	0.44
1:A:256:LEU:HD11	1:A:277:LYS:HE3	2.00	0.44
1:B:552:THR:HG22	1:B:562:VAL:HG23	2.00	0.44
1:A:65:ARG:NH1	1:A:65:ARG:HG3	2.33	0.43
1:A:205:ASP:HB2	1:A:246:GLY:HA2	2.01	0.43
1:B:271:GLU:HB3	1:B:272:ASP:H	1.60	0.43
1:B:446:TYR:CG	1:B:447:LEU:N	2.86	0.43
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.53	0.43
1:A:392:GLU:HG3	1:A:512:LYS:N	2.34	0.43
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.47	0.43
1:B:164:HIS:ND1	1:B:466:PRO:HG3	2.32	0.43
1:B:515:ASN:HD22	1:B:534:ASN:HB3	1.84	0.43
1:A:2:LEU:HD11	1:B:2:LEU:HD11	2.01	0.43
1:B:374:TYR:CE2	1:B:375:LEU:HD22	2.53	0.43
1:A:7:PHE:HE2	1:A:14:TYR:CE2	2.35	0.43
1:A:282:ASN:ND2	1:A:282:ASN:N	2.51	0.43
1:A:444:MET:O	1:A:494:ARG:NH1	2.49	0.43
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.84	0.43
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.18	0.43
1:A:16:TYR:HA	1:A:17:PRO:HD3	1.74	0.43
1:A:288:VAL:HG23	1:A:289:GLN:N	2.25	0.43
1:A:438:LEU:HD12	1:A:441:LEU:HD23	2.01	0.43
1:A:274:PRO:O	1:A:274:PRO:HG2	2.19	0.43
1:B:382:ARG:HH22	1:B:397:GLU:CD	2.26	0.43
1:B:547:GLU:C	1:B:549:GLY:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LYS:NZ	1:B:551:LYS:CB	2.71	0.43
1:A:145:ASP:OD1	1:A:145:ASP:C	2.62	0.43
1:A:357:HIS:O	1:A:358:ASP:C	2.61	0.43
1:B:440:VAL:CG2	1:B:486:PHE:HE1	2.31	0.43
1:A:281:THR:HG23	1:A:289:GLN:NE2	2.33	0.42
1:A:205:ASP:HB2	1:A:246:GLY:CA	2.49	0.42
1:A:563:HIS:O	1:A:565:LYS:N	2.52	0.42
1:B:377:ARG:O	1:B:380:VAL:HG22	2.19	0.42
1:B:394:PHE:O	1:B:398:LEU:HB2	2.19	0.42
1:A:40:LEU:HD22	1:A:54:HIS:ND1	2.34	0.42
1:A:247:ASP:N	1:A:292:ALA:O	2.52	0.42
1:A:382:ARG:HB3	1:A:389:ILE:HG12	2.01	0.42
1:B:536:GLY:HA2	1:B:576:TYR:CE1	2.54	0.42
1:A:62:SER:HB3	1:A:67:ASP:OD1	2.20	0.42
1:A:457:GLU:H	1:A:457:GLU:HG3	1.52	0.42
1:A:149:ASP:HA	1:A:150:PRO:HD3	1.83	0.42
1:A:222:PHE:O	1:A:226:VAL:HG23	2.19	0.42
1:A:527:HIS:CE1	1:A:548:SER:HG	2.35	0.42
1:B:464:THR:O	1:B:465:ASP:C	2.62	0.42
1:A:143:ASN:OD1	1:A:169:GLY:O	2.37	0.42
1:A:361:GLY:HA2	1:A:364:MET:HE2	2.00	0.42
1:A:377:ARG:HD2	1:A:417:LEU:O	2.20	0.42
1:A:454:TYR:O	1:A:454:TYR:CG	2.72	0.42
1:B:95:TYR:CE2	1:B:105:ARG:HB2	2.54	0.42
1:B:493:LEU:HD21	1:B:556:CYS:HB3	2.00	0.42
1:A:43:ASP:OD2	1:A:79:ARG:NH2	2.52	0.42
1:A:82:TYR:N	1:A:82:TYR:CD2	2.88	0.42
1:B:381:ILE:CD1	1:B:425:PHE:HE1	2.32	0.42
1:B:454:TYR:O	1:B:454:TYR:CG	2.71	0.42
1:A:374:TYR:CZ	1:A:375:LEU:HD22	2.55	0.42
1:A:505:VAL:HG22	1:A:521:ARG:NE	2.35	0.42
1:B:52:LEU:HD11	1:B:105:ARG:HE	1.84	0.42
1:B:541:VAL:HG22	1:B:542:LEU:N	2.34	0.42
1:A:212:ILE:CD1	1:A:222:PHE:HB2	2.50	0.42
1:A:277:LYS:HG3	1:A:283:TYR:OH	2.20	0.42
1:B:190:LEU:HD13	1:B:234:ILE:HG21	2.01	0.41
1:B:438:LEU:HD22	1:B:532:LEU:HD23	2.01	0.41
1:A:505:VAL:HG22	1:A:521:ARG:HD3	2.00	0.41
1:B:218:ASP:OD2	1:B:220:PRO:HD2	2.20	0.41
1:A:149:ASP:OD2	1:A:149:ASP:N	2.53	0.41
1:A:312:ARG:O	1:A:316:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:O	1:B:343:LYS:HG2	2.20	0.41
1:A:264:TYR:O	1:A:267:TRP:HB2	2.21	0.41
1:A:273:PHE:HB3	1:A:275:VAL:N	2.35	0.41
1:A:311:ALA:HA	1:A:322:TRP:CZ2	2.55	0.41
1:A:377:ARG:O	1:A:380:VAL:HG22	2.20	0.41
1:A:542:LEU:HD21	1:A:570:LYS:HG3	2.03	0.41
1:A:545:VAL:O	1:A:546:PRO:C	2.63	0.41
1:A:577:GLN:HG2	1:A:578:GLY:N	2.35	0.41
1:B:144:GLY:C	1:B:173:LYS:HD2	2.45	0.41
1:B:206:THR:HG21	1:B:209:TYR:CG	2.55	0.41
1:B:548:SER:C	1:B:550:GLY:N	2.77	0.41
1:B:16:TYR:HA	1:B:17:PRO:HD3	1.94	0.41
1:A:84:PHE:HB2	1:A:96:PHE:HB3	2.02	0.41
1:A:257:GLN:HA	1:A:257:GLN:NE2	2.36	0.41
1:B:381:ILE:HD12	1:B:381:ILE:N	2.36	0.41
1:B:579:MET:CE	1:B:581:LEU:HD11	2.34	0.41
1:A:314:TRP:O	1:A:319:ILE:HG23	2.21	0.41
1:B:323:ARG:HH21	1:B:372:MET:HE2	1.85	0.41
1:B:545:VAL:HG22	1:B:569:LEU:HD13	2.02	0.41
1:B:242:PHE:CD1	1:B:307:LEU:HD22	2.56	0.41
1:A:256:LEU:HD23	1:A:256:LEU:O	2.21	0.41
1:A:571:LEU:HD22	1:A:579:MET:HE1	2.03	0.41
1:B:36:ARG:HG3	1:B:36:ARG:HH11	1.86	0.41
1:B:39:VAL:HG22	1:B:84:PHE:CD2	2.56	0.41
1:B:85:LEU:HD13	1:B:95:TYR:CE2	2.55	0.41
1:B:238:LEU:HD22	1:B:319:ILE:HG21	2.02	0.41
1:B:325:ASN:ND2	1:B:326:VAL:H	2.18	0.41
1:B:547:GLU:H	1:B:547:GLU:HG3	1.60	0.41
1:B:579:MET:HE2	1:B:581:LEU:CD1	2.33	0.41
1:A:516:LEU:HD23	1:A:516:LEU:C	2.46	0.41
1:A:542:LEU:CD2	1:A:570:LYS:HG3	2.51	0.41
1:B:258:LYS:O	1:B:259:GLY:C	2.62	0.41
1:B:488:LYS:HB3	1:B:488:LYS:HE2	1.75	0.41
1:A:222:PHE:O	1:A:223:ARG:C	2.65	0.40
1:A:455:GLY:O	1:A:456:ASP:C	2.62	0.40
1:A:528:VAL:HG23	1:A:528:VAL:O	2.20	0.40
1:B:330:VAL:HG21	1:B:334:PHE:CD1	2.54	0.40
1:B:330:VAL:HG22	1:B:335:TRP:NE1	2.35	0.40
1:B:438:LEU:HD23	1:B:438:LEU:HA	1.86	0.40
1:A:499:SER:HB2	1:A:528:VAL:HG22	2.04	0.40
1:A:555:ASP:OD2	1:A:555:ASP:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HG3	1:B:118:ARG:HH11	1.87	0.40
1:B:198:SER:HB3	1:B:203:LYS:HD3	2.02	0.40
1:B:272:ASP:C	1:B:273:PHE:O	2.63	0.40
1:B:558:THR:CG2	1:B:559:GLY:N	2.80	0.40
1:A:257:GLN:HE21	1:A:257:GLN:CA	2.35	0.40
1:A:272:ASP:O	1:A:272:ASP:CG	2.63	0.40
1:A:326:VAL:H	1:A:354:GLU:HG2	1.87	0.40
1:A:382:ARG:HH11	1:A:389:ILE:HD13	1.85	0.40
1:B:171:ASP:HB2	1:B:216:PHE:O	2.21	0.40
1:A:60:ALA:N	1:A:68:TYR:O	2.52	0.40
1:A:552:THR:HA	1:A:562:VAL:HG23	2.04	0.40
1:B:31:LYS:HE2	1:B:63:ASP:O	2.21	0.40
1:B:60:ALA:HA	1:B:506:ARG:CZ	2.50	0.40
1:B:222:PHE:O	1:B:226:VAL:HG23	2.21	0.40
1:B:142:ALA:O	1:B:174:GLY:HA3	2.22	0.40
1:B:145:ASP:HA	1:B:146:PRO:HD2	1.88	0.40
1:B:561:GLU:C	1:B:563:HIS:N	2.80	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%)	542 (93%)	33 (6%)	8 (1%)	9	39
1	B	583/585 (100%)	534 (92%)	41 (7%)	8 (1%)	9	39
All	All	1166/1170 (100%)	1076 (92%)	74 (6%)	16 (1%)	9	39

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	PHE

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Mol	Chain	Res	Type
1	A	286	PHE
1	A	560	GLU
1	B	273	PHE
1	B	286	PHE
1	B	547	GLU
1	B	548	SER
1	B	549	GLY
1	B	562	VAL
1	A	275	VAL
1	A	547	GLU
1	B	271	GLU
1	B	278	THR
1	A	561	GLU
1	A	548	SER
1	A	546	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%)	453 (92%)	40 (8%)	11	39
1	B	493/493 (100%)	449 (91%)	44 (9%)	9	34
All	All	986/986 (100%)	902 (92%)	84 (8%)	10	37

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	26	ARG
1	A	33	ASP
1	A	62	SER
1	A	81	LYS
1	A	90	GLN
1	A	92	GLU
1	A	124	THR

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Mol	Chain	Res	Type
1	A	139	GLU
1	A	140	ARG
1	A	167	PHE
1	A	219	LEU
1	A	238	LEU
1	A	241	VAL
1	A	257	GLN
1	A	261	GLN
1	A	282	ASN
1	A	297	ARG
1	A	298	THR
1	A	315	MET
1	A	317	GLN
1	A	337	GLU
1	A	340	ARG
1	A	354	GLU
1	A	356	TRP
1	A	360	SER
1	A	375	LEU
1	A	400	ARG
1	A	423	GLU
1	A	426	LEU
1	A	457	GLU
1	A	470	ARG
1	A	496	ARG
1	A	499	SER
1	A	512	LYS
1	A	538	LYS
1	A	569	LEU
1	A	571	LEU
1	A	574	ARG
1	A	581	LEU
1	B	2	LEU
1	B	4	GLU
1	B	19	SER
1	B	24	ARG
1	B	33	ASP
1	B	49	GLU
1	B	62	SER
1	B	65	ARG
1	B	77	THR
1	B	78	LYS

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Mol	Chain	Res	Type
1	B	90	GLN
1	B	92	GLU
1	B	110	VAL
1	B	139	GLU
1	B	164	HIS
1	B	165	ASP
1	B	188	THR
1	B	201	HIS
1	B	223	ARG
1	B	238	LEU
1	B	241	VAL
1	B	263	ARG
1	B	271	GLU
1	B	275	VAL
1	B	282	ASN
1	B	296	LEU
1	B	315	MET
1	B	323	ARG
1	B	328	ASN
1	B	330	VAL
1	B	336	ARG
1	B	356	TRP
1	B	363	LEU
1	B	375	LEU
1	B	405	TYR
1	B	408	GLN
1	B	438	LEU
1	B	457	GLU
1	B	478	GLU
1	B	521	ARG
1	B	547	GLU
1	B	551	LYS
1	B	554	LEU
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	90	GLN
1	A	112	GLN
1	A	135	GLN

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Mol	Chain	Res	Type
1	A	164	HIS
1	A	215	GLN
1	A	243	ASN
1	A	257	GLN
1	A	261	GLN
1	A	282	ASN
1	A	289	GLN
1	A	317	GLN
1	A	325	ASN
1	A	332	HIS
1	A	390	HIS
1	A	411	GLN
1	A	443	GLN
1	A	479	GLN
1	A	513	GLN
1	A	534	ASN
1	B	22	GLN
1	B	135	GLN
1	B	143	ASN
1	B	155	GLN
1	B	257	GLN
1	B	261	GLN
1	B	289	GLN
1	B	325	ASN
1	B	328	ASN
1	B	373	ASN
1	B	390	HIS
1	B	408	GLN
1	B	415	ASN
1	B	509	HIS
1	B	515	ASN
1	B	539	GLN
1	B	566	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 ⓘ

14 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	11,11,12	1.66	3 (27%)	15,15,17	1.49	3 (20%)
2	GLC	C	2	2	11,11,12	1.61	3 (27%)	15,15,17	0.73	0
2	GLC	C	3	2	11,11,12	1.54	3 (27%)	15,15,17	1.16	1 (6%)
2	GLC	C	4	2	11,11,12	1.23	0	15,15,17	0.61	0
2	GLC	C	5	2	11,11,12	1.34	1 (9%)	15,15,17	1.09	1 (6%)
2	GLC	C	6	2	11,11,12	1.65	2 (18%)	15,15,17	0.98	1 (6%)
2	GLC	C	7	2	11,11,12	1.88	5 (45%)	15,15,17	0.82	1 (6%)
2	GLC	D	1	2	11,11,12	1.52	2 (18%)	15,15,17	1.44	2 (13%)
2	GLC	D	2	2	11,11,12	1.52	3 (27%)	15,15,17	0.81	1 (6%)
2	GLC	D	3	2	11,11,12	1.56	3 (27%)	15,15,17	1.23	2 (13%)
2	GLC	D	4	2	11,11,12	1.52	3 (27%)	15,15,17	0.62	0
2	GLC	D	5	2	11,11,12	1.29	1 (9%)	15,15,17	0.99	1 (6%)
2	GLC	D	6	2	11,11,12	1.56	3 (27%)	15,15,17	1.03	1 (6%)
2	GLC	D	7	2	11,11,12	1.61	2 (18%)	15,15,17	0.79	1 (6%)

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	-	1/2/19/22	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	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	1/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	7	2	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GLC	C4-C5	3.39	1.60	1.53
2	C	6	GLC	O5-C5	3.08	1.49	1.43
2	D	1	GLC	C4-C5	3.03	1.59	1.53
2	C	7	GLC	O5-C5	3.03	1.49	1.43
2	D	3	GLC	C4-C5	2.84	1.59	1.53
2	C	3	GLC	C4-C5	2.58	1.58	1.53
2	D	6	GLC	C4-C5	2.58	1.58	1.53
2	C	7	GLC	O5-C1	2.56	1.48	1.43
2	C	5	GLC	O5-C5	2.55	1.48	1.43
2	D	6	GLC	O5-C5	2.55	1.48	1.43
2	C	3	GLC	O5-C5	2.55	1.48	1.43
2	D	5	GLC	O5-C5	2.55	1.48	1.43
2	D	4	GLC	O5-C5	2.54	1.48	1.43
2	C	7	GLC	C4-C5	2.50	1.58	1.53
2	D	4	GLC	C2-C3	2.47	1.56	1.52
2	D	7	GLC	C4-C5	2.45	1.58	1.53
2	C	2	GLC	O5-C5	2.42	1.48	1.43
2	C	2	GLC	C4-C5	2.42	1.58	1.53
2	D	3	GLC	C2-C3	2.38	1.56	1.52
2	C	6	GLC	C4-C5	2.34	1.58	1.53
2	D	7	GLC	O5-C5	2.29	1.47	1.43
2	D	3	GLC	O5-C5	2.29	1.47	1.43
2	C	1	GLC	O5-C5	2.28	1.47	1.43
2	D	2	GLC	O5-C5	2.27	1.47	1.43
2	C	7	GLC	C2-C3	2.20	1.55	1.52
2	C	3	GLC	C4-C3	2.20	1.58	1.52
2	D	6	GLC	C1-C2	2.14	1.57	1.52
2	C	2	GLC	O5-C1	2.13	1.47	1.43
2	D	1	GLC	C2-C3	2.08	1.55	1.52
2	C	7	GLC	C1-C2	2.07	1.57	1.52
2	D	4	GLC	O5-C1	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GLC	C1-C2	2.05	1.57	1.52
2	D	2	GLC	O5-C1	2.01	1.47	1.43
2	D	2	GLC	C2-C3	2.00	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-O5-C5	4.20	117.82	112.19
2	C	1	GLC	C1-O5-C5	4.08	117.66	112.19
2	C	5	GLC	C1-O5-C5	3.42	116.77	112.19
2	D	6	GLC	C1-O5-C5	3.16	116.42	112.19
2	D	5	GLC	C1-O5-C5	3.13	116.38	112.19
2	C	6	GLC	C1-O5-C5	3.02	116.24	112.19
2	C	3	GLC	C1-O5-C5	2.81	115.95	112.19
2	D	3	GLC	C1-O5-C5	2.56	115.62	112.19
2	D	2	GLC	C1-O5-C5	2.42	115.43	112.19
2	D	3	GLC	O4-C4-C3	-2.31	104.93	110.38
2	D	7	GLC	C1-O5-C5	2.26	115.22	112.19
2	C	7	GLC	C1-O5-C5	2.26	115.22	112.19
2	C	1	GLC	O4-C4-C3	-2.09	105.46	110.38
2	C	1	GLC	O5-C5-C6	-2.03	103.72	107.66
2	D	1	GLC	O5-C5-C6	-2.01	103.75	107.66

There are no chirality outliers.

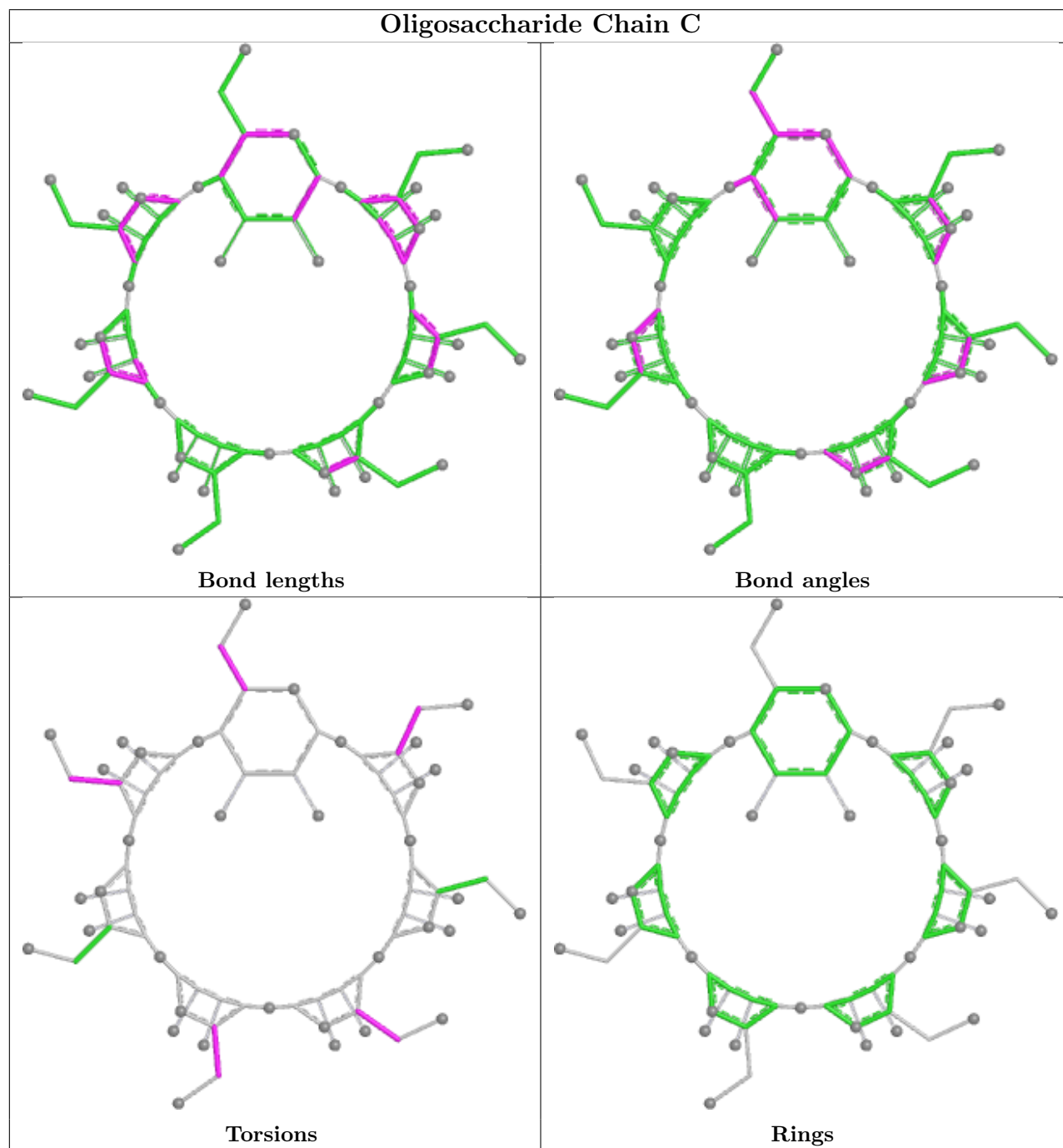
All (12) torsion outliers are listed below:

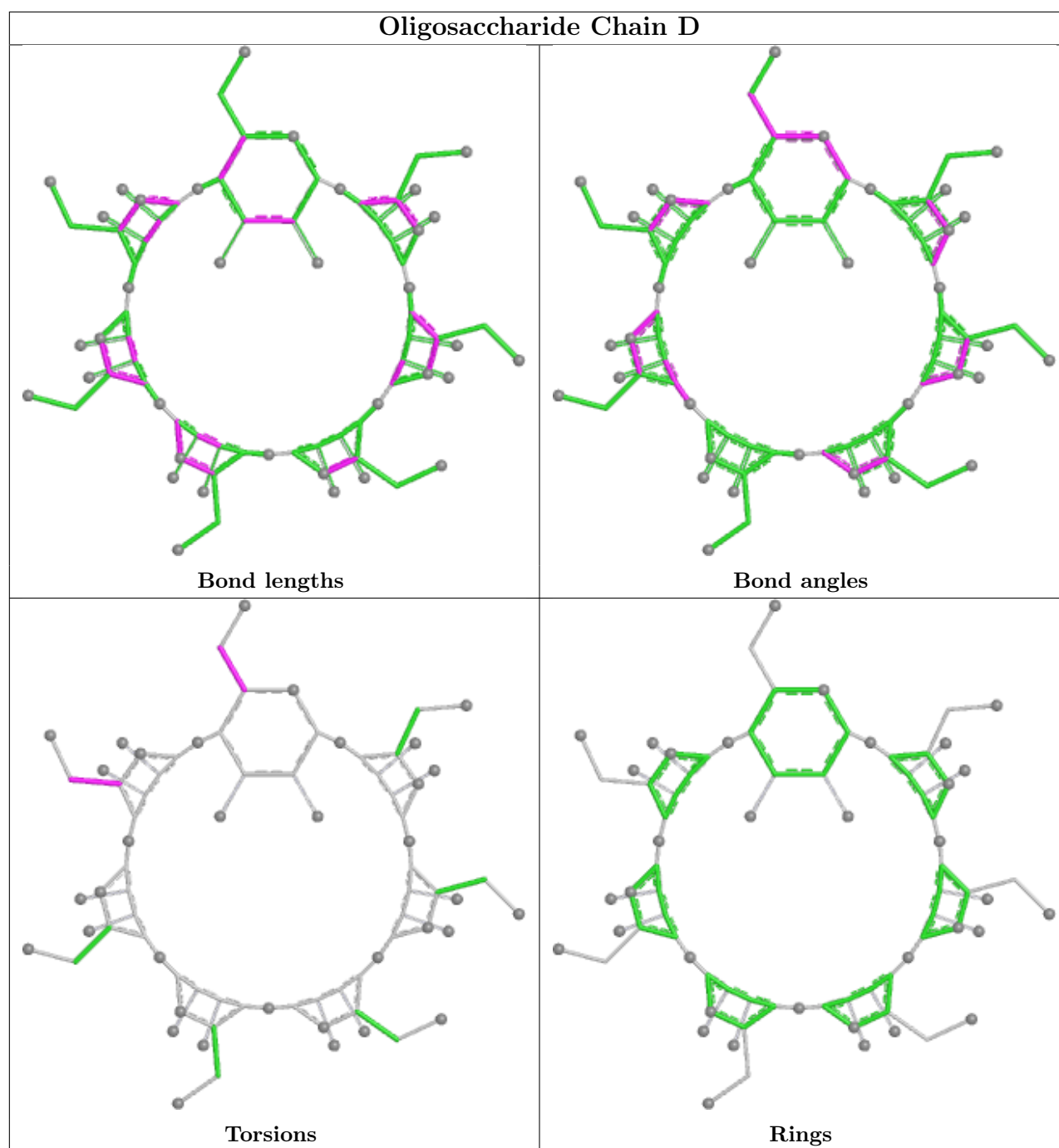
Mol	Chain	Res	Type	Atoms
2	C	5	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	C	5	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	7	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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%)	-0.42	5 (0%) 81 64	11, 33, 69, 86	0
1	B	585/585 (100%)	-0.31	4 (0%) 84 69	10, 37, 72, 87	0
All	All	1170/1170 (100%)	-0.37	9 (0%) 82 67	10, 36, 71, 87	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	THR	3.2
1	A	279	SER	3.0
1	B	562	VAL	2.7
1	A	356	TRP	2.7
1	B	550	GLY	2.4
1	A	561	GLU	2.2
1	A	559	GLY	2.2
1	A	547	GLU	2.2
1	B	356	TRP	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	7	11/12	0.43	0.16	100,101,101,101	0

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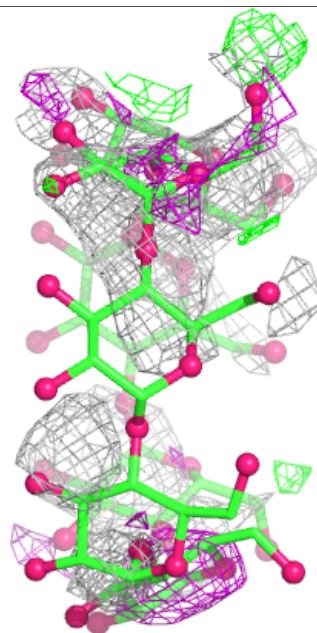
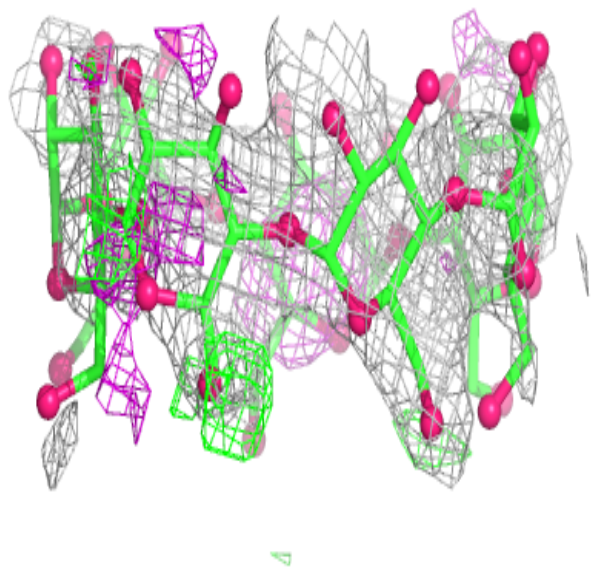
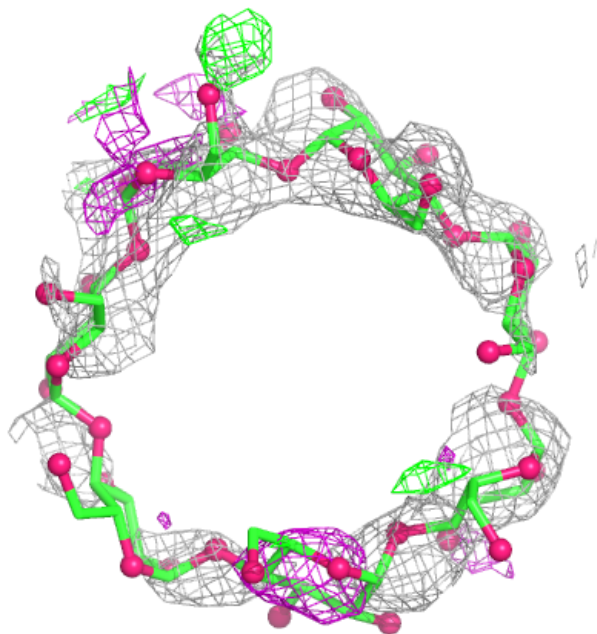
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	3	11/12	0.51	0.22	84,87,89,90	0
2	GLC	D	5	11/12	0.51	0.13	93,94,94,94	0
2	GLC	C	6	11/12	0.61	0.15	94,96,97,99	0
2	GLC	D	3	11/12	0.62	0.14	93,94,95,95	0
2	GLC	D	4	11/12	0.64	0.13	92,94,95,95	0
2	GLC	D	2	11/12	0.71	0.12	87,89,90,91	0
2	GLC	C	2	11/12	0.78	0.17	92,94,95,95	0
2	GLC	C	1	11/12	0.79	0.13	96,98,99,99	0
2	GLC	D	7	11/12	0.79	0.16	88,90,91,91	0
2	GLC	D	6	11/12	0.80	0.13	91,93,94,94	0
2	GLC	C	5	11/12	0.80	0.14	88,90,91,92	0
2	GLC	D	1	11/12	0.81	0.14	86,88,89,89	0
2	GLC	C	4	11/12	0.88	0.15	83,86,86,87	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.

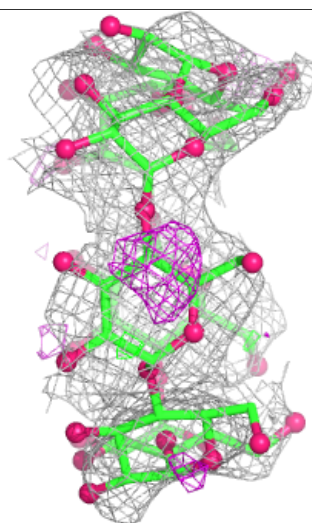
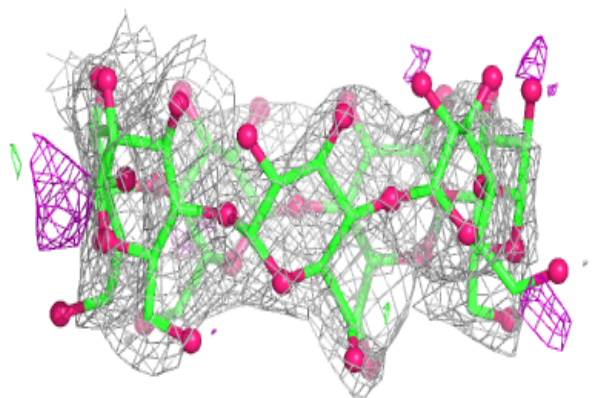
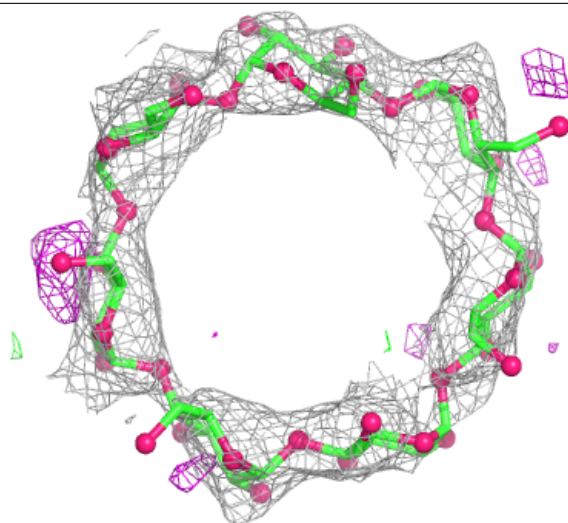
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**6.4 Ligands** [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.