



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:42 PM JST

PDB ID : 9JR5 / pdb\_00009jr5  
Title : Crystal structure of PCoV-GD receptor-binding domain complexed with squirrel ACE2  
Authors : Lan, J.; Nan, X.  
Deposited on : 2024-09-29  
Resolution : 3.41 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

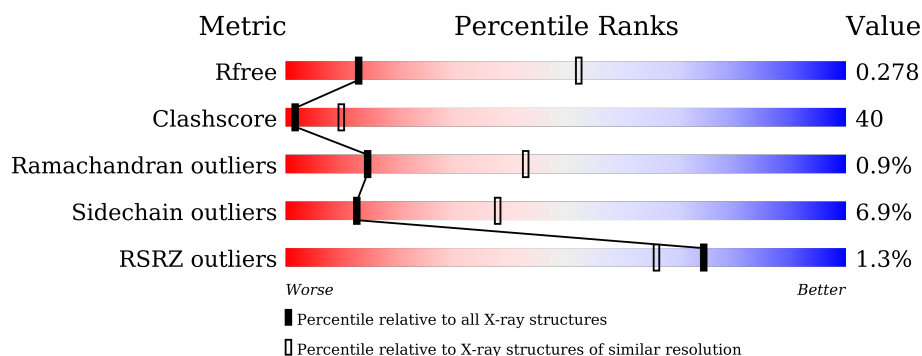
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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))
$R_{free}$	164625	1112 (3.48-3.36)
Clashscore	180529	1144 (3.48-3.36)
Ramachandran outliers	177936	1146 (3.48-3.36)
Sidechain outliers	177891	1146 (3.48-3.36)
RSRZ outliers	164620	1112 (3.48-3.36)

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  $\geq 3$ , 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	E	185	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>44%</div> <div>...</div> </div> </div>
2	A	598	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>47%</div> <div>6%</div> <div>.</div> </div> </div>
3	B	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div></div> <div>100%</div> </div>
4	C	3	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6408 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	181	Total	C	N	O	S	0	0	0
			1448	928	240	274	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	337	THR	PRO	conflict	UNP A0A7D6TQ96

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	592	Total	C	N	O	S	0	0	0
			4851	3095	817	909	30			

There is a discrepancy between the modelled and reference sequences:

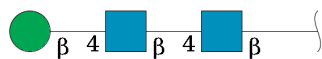
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PRO	-	expression tag	UNP A0A8D2KIZ1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



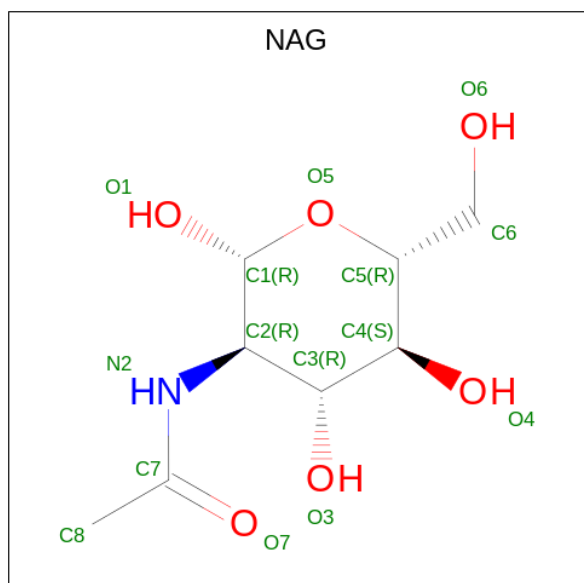
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



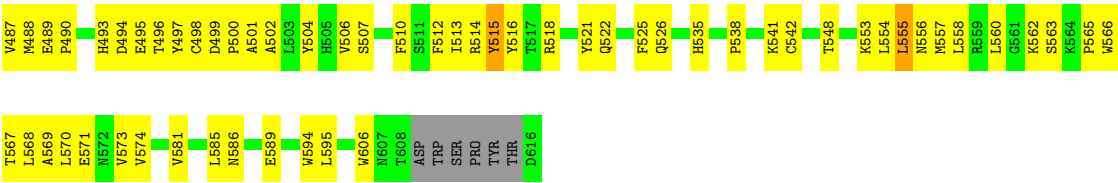
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

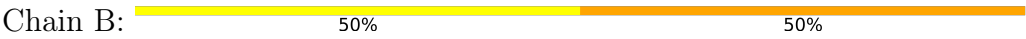


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		





● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.14Å 195.14Å 145.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.41 48.79 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.79-3.41) 98.9 (48.79-3.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.218 , 0.282 0.225 , 0.278	Depositor DCC
$R_{free}$ test set	963 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.8	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 92.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: NAG, BMA

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	E	0.70	0/1489	0.87	1/2026 (0.0%)
2	A	0.74	0/4982	0.90	8/6754 (0.1%)
All	All	0.73	0/6471	0.89	9/8780 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	406	GLU	N-CA-C	-6.41	106.00	113.88
2	A	374	HIS	CA-CB-CG	5.87	119.67	113.80
2	A	130	GLY	N-CA-C	-5.76	99.53	113.18
1	E	373	SER	N-CA-C	5.75	117.54	111.28
2	A	257	SER	CA-C-N	5.36	125.68	119.47
2	A	257	SER	C-N-CA	5.36	125.68	119.47
2	A	252	TYR	CA-C-N	5.22	124.72	119.19
2	A	252	TYR	C-N-CA	5.22	124.72	119.19
2	A	126	ILE	CB-CA-C	-5.01	105.54	111.81

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	E	1448	0	1363	104	0
2	A	4851	0	4660	400	0
3	B	28	0	25	1	0
3	D	28	0	25	0	0
4	C	39	0	34	4	0
5	E	14	0	13	1	0
All	All	6408	0	6120	501	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 40.

All (501) 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)
2:A:252:TYR:CD2	2:A:266:LEU:HD23	1.44	1.47
2:A:418:LEU:HB2	2:A:423:LEU:CG	1.44	1.47
2:A:241:HIS:NE2	2:A:262:LEU:HD11	1.37	1.39
2:A:418:LEU:CB	2:A:423:LEU:HG	1.50	1.38
2:A:418:LEU:HD22	2:A:423:LEU:CD1	1.54	1.38
2:A:145:GLU:CG	2:A:146:PRO:HD3	1.55	1.36
2:A:145:GLU:HG3	2:A:146:PRO:CD	1.56	1.34
1:E:379:CYS:SG	1:E:432:CYS:SG	1.46	1.30
2:A:288:LYS:NZ	2:A:431:ASP:OD2	1.60	1.29
2:A:418:LEU:O	2:A:423:LEU:HB2	1.37	1.25
2:A:293:VAL:HG21	2:A:423:LEU:CD1	1.69	1.23
2:A:418:LEU:HB2	2:A:423:LEU:CB	1.68	1.22
2:A:241:HIS:NE2	2:A:262:LEU:CD1	2.03	1.20
2:A:407:ILE:CD1	2:A:526:GLN:HB2	1.72	1.20
2:A:293:VAL:CG2	2:A:423:LEU:HD13	1.71	1.18
2:A:424:LEU:HB2	2:A:425:PRO:HD2	1.18	1.13
2:A:418:LEU:CD2	2:A:423:LEU:HD12	1.79	1.12
2:A:152:MET:HE2	2:A:164:VAL:HG12	1.15	1.12
2:A:407:ILE:HD11	2:A:526:GLN:HB2	1.18	1.11
2:A:252:TYR:CD2	2:A:266:LEU:CD2	2.36	1.09
1:E:437:ASN:HA	1:E:508:TYR:CD1	1.88	1.08
2:A:418:LEU:C	2:A:423:LEU:HB2	1.78	1.08
2:A:421:ILE:HD11	2:A:423:LEU:HD23	1.37	1.03
1:E:337:THR:N	1:E:363:ALA:HB2	1.74	1.02
2:A:273:ARG:O	2:A:449:THR:OG1	1.75	1.02
2:A:352:GLN:HE22	2:A:393:ARG:HD2	1.21	1.01
2:A:152:MET:HE2	2:A:164:VAL:CG1	1.92	1.00
2:A:252:TYR:HD2	2:A:266:LEU:HD23	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:418:LEU:HB3	2:A:423:LEU:HG	1.45	0.96
2:A:293:VAL:HG11	2:A:423:LEU:HD11	1.45	0.96
2:A:418:LEU:HB2	2:A:423:LEU:HG	0.97	0.96
2:A:252:TYR:CE2	2:A:266:LEU:HD23	2.01	0.96
2:A:279:TYR:OH	2:A:437:ASN:OD1	1.84	0.95
2:A:127:TYR:CE2	2:A:504:TYR:HA	2.01	0.95
2:A:152:MET:CE	2:A:164:VAL:HG12	1.96	0.94
2:A:407:ILE:HD11	2:A:526:GLN:CB	1.97	0.94
2:A:424:LEU:HB2	2:A:425:PRO:CD	1.97	0.94
2:A:241:HIS:CD2	2:A:262:LEU:HD11	2.03	0.93
2:A:151:ILE:HG22	2:A:152:MET:N	1.81	0.93
2:A:166:GLU:OE2	2:A:497:TYR:CZ	2.25	0.90
1:E:357:ARG:NH1	1:E:394:ASN:OD1	2.03	0.90
2:A:45:LEU:O	2:A:49:ASN:OD1	1.88	0.89
2:A:471:ASP:HA	2:A:495:GLU:HG3	1.55	0.89
2:A:151:ILE:HG22	2:A:152:MET:H	1.35	0.88
1:E:403:ARG:HB2	1:E:406:GLU:HG3	1.54	0.88
2:A:418:LEU:CD2	2:A:423:LEU:CD1	2.44	0.87
2:A:151:ILE:CG2	2:A:152:MET:N	2.37	0.86
2:A:418:LEU:HB2	2:A:423:LEU:HB2	1.57	0.86
2:A:555:LEU:O	2:A:558:LEU:N	2.09	0.86
2:A:323:MET:HE1	2:A:379:ILE:HG21	1.58	0.85
1:E:394:ASN:HB2	1:E:516:GLU:HG3	1.59	0.84
2:A:418:LEU:O	2:A:423:LEU:CB	2.26	0.83
2:A:458:LYS:HE2	2:A:462:MET:HE3	1.61	0.82
1:E:379:CYS:SG	1:E:432:CYS:CB	2.67	0.82
1:E:365:TYR:HD2	1:E:387:LEU:HB3	1.44	0.82
1:E:365:TYR:CD2	1:E:387:LEU:HB3	2.13	0.82
2:A:161:ARG:HG2	2:A:265:HIS:HB2	1.62	0.82
2:A:44:SER:HB3	2:A:351:LEU:HD23	1.63	0.81
2:A:419:LYS:HB2	2:A:424:LEU:HD21	1.60	0.81
2:A:418:LEU:HD13	2:A:424:LEU:CD1	2.11	0.81
1:E:354:ASN:O	1:E:398:ASP:HA	1.81	0.81
2:A:184:VAL:O	2:A:188:ASN:ND2	2.14	0.81
2:A:156:THR:HA	2:A:252:TYR:OH	1.81	0.79
2:A:269:ASP:HB2	2:A:271:TRP:O	1.82	0.79
2:A:398:GLU:CD	2:A:514:ARG:HD2	2.07	0.79
1:E:428:ASP:OD1	1:E:428:ASP:N	2.15	0.79
2:A:398:GLU:OE2	2:A:514:ARG:HG2	1.83	0.78
2:A:81:LYS:NZ	2:A:101:GLN:O	2.15	0.78
2:A:288:LYS:CE	2:A:431:ASP:OD2	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:ILE:HD12	2:A:256:ILE:H	1.47	0.78
2:A:418:LEU:HD22	2:A:423:LEU:HD12	0.83	0.78
1:E:427:ASP:OD1	1:E:427:ASP:N	2.16	0.78
1:E:374:PHE:CD2	1:E:434:ILE:HG23	2.18	0.77
1:E:436:TRP:O	1:E:508:TYR:HB3	1.85	0.77
2:A:181:GLU:HG3	2:A:470:LYS:HD2	1.66	0.77
2:A:227:GLU:OE1	2:A:458:LYS:NZ	2.18	0.77
2:A:293:VAL:HG11	2:A:423:LEU:CD1	2.15	0.76
2:A:196:TYR:HE1	2:A:219:ARG:HH12	1.30	0.76
2:A:421:ILE:CD1	2:A:423:LEU:HD23	2.14	0.76
2:A:151:ILE:O	2:A:153:ALA:N	2.18	0.76
2:A:421:ILE:HD11	2:A:423:LEU:CD2	2.15	0.76
2:A:112:LYS:NZ	2:A:189:GLU:OE1	2.19	0.76
2:A:127:TYR:HD2	2:A:507:SER:HG	1.31	0.76
1:E:427:ASP:O	1:E:429:PHE:N	2.18	0.76
2:A:352:GLN:NE2	2:A:393:ARG:HD2	1.98	0.76
2:A:127:TYR:HD2	2:A:507:SER:OG	1.68	0.75
1:E:396:TYR:HB2	1:E:514:SER:HB3	1.68	0.75
2:A:168:TRP:HE1	2:A:502:ALA:HB1	1.51	0.74
1:E:374:PHE:CE2	1:E:434:ILE:HG21	2.23	0.74
1:E:401:VAL:HG11	1:E:451:TYR:CD2	2.23	0.74
2:A:177:ARG:NH1	2:A:470:LYS:O	2.21	0.73
1:E:437:ASN:ND2	1:E:508:TYR:HE1	1.86	0.73
1:E:487:ASN:CG	2:A:24:LEU:HD21	2.13	0.73
2:A:187:LYS:HG2	2:A:199:TYR:CE2	2.23	0.73
1:E:384:PRO:HA	1:E:387:LEU:HD23	1.70	0.73
2:A:263:PRO:HG2	2:A:266:LEU:HD13	1.70	0.73
2:A:288:LYS:HE2	2:A:433:GLU:HB2	1.71	0.73
2:A:423:LEU:HB3	2:A:424:LEU:HD13	1.69	0.73
2:A:418:LEU:CB	2:A:423:LEU:CB	2.61	0.72
2:A:166:GLU:OE2	2:A:497:TYR:CE1	2.41	0.72
2:A:418:LEU:CB	2:A:423:LEU:CG	2.29	0.72
1:E:437:ASN:HA	1:E:508:TYR:HD1	1.54	0.72
2:A:40:ASP:O	2:A:44:SER:OG	2.08	0.72
2:A:166:GLU:OE1	2:A:493:HIS:NE2	2.22	0.72
1:E:347:PHE:CE2	1:E:399:SER:HB2	2.24	0.72
1:E:374:PHE:CD2	1:E:434:ILE:CG2	2.73	0.72
2:A:407:ILE:CD1	2:A:526:GLN:CB	2.60	0.71
2:A:418:LEU:CD1	2:A:424:LEU:HD11	2.21	0.71
2:A:161:ARG:HD3	2:A:266:LEU:HA	1.72	0.71
5:E:601:NAG:O7	5:E:601:NAG:O3	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:226:VAL:HG21	2:A:513:ILE:HD11	1.71	0.71
2:A:276:THR:OG1	2:A:445:THR:HG22	1.91	0.70
2:A:417:HIS:O	2:A:420:SER:HB3	1.92	0.70
2:A:424:LEU:CB	2:A:425:PRO:HD2	2.11	0.70
2:A:127:TYR:HE2	2:A:504:TYR:HA	1.54	0.70
2:A:398:GLU:OE1	2:A:514:ARG:HD2	1.90	0.70
2:A:392:LEU:HD22	2:A:563:SER:HA	1.74	0.70
1:E:401:VAL:HG11	1:E:451:TYR:CE2	2.27	0.69
2:A:116:LEU:HD13	2:A:186:LEU:HD12	1.75	0.69
2:A:219:ARG:H	2:A:219:ARG:HD3	1.55	0.69
1:E:437:ASN:OD1	1:E:439:ASN:N	2.25	0.69
2:A:105:SER:O	2:A:113:ARG:CD	2.41	0.69
2:A:133:CYS:SG	2:A:141:CYS:N	2.66	0.69
2:A:249:MET:SD	2:A:258:PRO:HG3	2.33	0.69
2:A:482:ARG:NH2	2:A:489:GLU:OE1	2.26	0.69
2:A:420:SER:OG	4:C:1:NAG:H83	1.93	0.68
2:A:151:ILE:O	2:A:152:MET:C	2.35	0.68
2:A:103:SER:OG	2:A:194:ASN:OD1	2.08	0.68
2:A:323:MET:HE2	2:A:327:PHE:CD2	2.28	0.68
2:A:241:HIS:NE2	2:A:262:LEU:HD12	2.08	0.68
2:A:460:ARG:NH1	2:A:506:VAL:HA	2.09	0.68
2:A:418:LEU:O	2:A:423:LEU:N	2.24	0.67
2:A:160:GLU:HA	2:A:163:TRP:CD1	2.30	0.67
2:A:190:MET:HE1	2:A:202:TYR:CE2	2.30	0.67
2:A:256:ILE:HD12	2:A:256:ILE:N	2.06	0.67
2:A:554:LEU:HD12	2:A:554:LEU:O	1.95	0.67
2:A:95:ARG:NH1	2:A:563:SER:O	2.28	0.67
2:A:515:TYR:HD1	2:A:515:TYR:H	1.42	0.67
2:A:132:VAL:O	2:A:141:CYS:HA	1.94	0.67
1:E:394:ASN:HB2	1:E:516:GLU:CG	2.26	0.66
2:A:265:HIS:CE1	2:A:490:PRO:HG3	2.30	0.66
2:A:207:TYR:O	2:A:217:TYR:HD2	1.77	0.66
1:E:349:SER:OG	1:E:452:LEU:N	2.29	0.66
2:A:196:TYR:HE1	2:A:219:ARG:NH1	1.94	0.66
3:B:1:NAG:O7	3:B:1:NAG:O3	2.11	0.66
1:E:367:VAL:HG23	1:E:368:LEU:HD13	1.77	0.65
2:A:407:ILE:HD13	2:A:526:GLN:HB2	1.74	0.65
2:A:109:SER:HB3	2:A:112:LYS:HD2	1.79	0.65
2:A:407:ILE:HG22	2:A:408:MET:HE2	1.79	0.65
2:A:430:GLU:O	2:A:430:GLU:HG3	1.96	0.64
2:A:144:LEU:HD12	2:A:144:LEU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:TYR:HD1	2:A:127:TYR:O	1.81	0.64
2:A:318:VAL:O	2:A:548:THR:HA	1.98	0.64
1:E:378:LYS:HB3	1:E:380:TYR:CE1	2.32	0.64
2:A:122:THR:HA	2:A:125:THR:OG1	1.97	0.64
2:A:308:PHE:CE2	2:A:333:LEU:HD12	2.33	0.64
2:A:346:PRO:HB2	2:A:375:GLU:OE1	1.98	0.64
2:A:166:GLU:OE2	2:A:497:TYR:OH	2.16	0.63
2:A:418:LEU:CB	2:A:423:LEU:HB2	2.27	0.63
2:A:515:TYR:CD1	2:A:515:TYR:N	2.65	0.63
2:A:105:SER:O	2:A:113:ARG:HG3	1.97	0.63
2:A:424:LEU:N	2:A:424:LEU:HD22	2.14	0.63
1:E:503:VAL:HA	1:E:506:GLN:OE1	1.99	0.62
2:A:181:GLU:HG3	2:A:470:LYS:CD	2.28	0.62
2:A:156:THR:O	2:A:252:TYR:HE1	1.82	0.62
2:A:455:MET:HE2	2:A:485:VAL:HG21	1.80	0.62
2:A:504:TYR:HE1	2:A:510:PHE:CE2	2.18	0.62
1:E:443:SER:HB3	1:E:497:PHE:HB3	1.81	0.62
2:A:241:HIS:CE1	2:A:606:TRP:CD1	2.87	0.62
1:E:403:ARG:HD2	1:E:505:TYR:HA	1.81	0.62
2:A:330:ASN:HB2	2:A:357:ARG:HD3	1.81	0.62
2:A:424:LEU:HD22	2:A:424:LEU:H	1.65	0.62
1:E:374:PHE:CE2	1:E:434:ILE:CG2	2.83	0.62
1:E:400:PHE:CE2	1:E:423:TYR:CD2	2.87	0.61
2:A:326:GLY:O	2:A:330:ASN:ND2	2.33	0.61
2:A:432:ASN:OD1	2:A:432:ASN:N	2.17	0.61
2:A:513:ILE:HG12	2:A:513:ILE:O	2.00	0.61
2:A:122:THR:CA	2:A:125:THR:OG1	2.49	0.61
2:A:103:SER:HB2	2:A:107:ALA:HB2	1.83	0.60
2:A:155:SER:O	2:A:161:ARG:NH2	2.22	0.60
2:A:418:LEU:HD22	2:A:423:LEU:CG	2.28	0.60
2:A:229:THR:OG1	2:A:516:TYR:OH	2.18	0.60
2:A:482:ARG:NH1	2:A:489:GLU:OE2	2.35	0.60
1:E:493:GLN:OE1	2:A:31:LYS:NZ	2.35	0.60
2:A:419:LYS:HA	2:A:424:LEU:HD22	1.84	0.59
1:E:503:VAL:HG23	1:E:508:TYR:OH	2.02	0.59
2:A:134:ASN:HB3	2:A:163:TRP:CD2	2.36	0.59
2:A:406:GLU:HA	2:A:406:GLU:OE1	2.02	0.59
2:A:557:MET:HG2	2:A:573:VAL:HG21	1.84	0.59
2:A:144:LEU:HD12	2:A:144:LEU:C	2.27	0.59
2:A:279:TYR:CE1	2:A:441:LYS:HB2	2.38	0.59
2:A:489:GLU:OE2	2:A:489:GLU:N	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ASP:OD2	2:A:390:TYR:OH	2.09	0.59
2:A:215:TYR:OH	2:A:571:GLU:OE1	2.06	0.59
1:E:400:PHE:CE2	1:E:423:TYR:CE2	2.91	0.59
1:E:400:PHE:HE2	1:E:423:TYR:CE2	2.21	0.59
2:A:396:ALA:HB1	2:A:566:TRP:HB3	1.85	0.59
1:E:374:PHE:HD2	1:E:434:ILE:HG23	1.63	0.59
2:A:133:CYS:HA	2:A:141:CYS:HA	1.85	0.59
2:A:213:ASP:OD1	2:A:213:ASP:N	2.36	0.59
2:A:535:HIS:CE1	2:A:542:CYS:HA	2.37	0.59
1:E:403:ARG:HG3	1:E:495:TYR:HE1	1.68	0.58
2:A:501:ALA:O	2:A:507:SER:HB3	2.03	0.58
1:E:487:ASN:OD1	2:A:24:LEU:HD21	2.03	0.58
2:A:249:MET:HA	2:A:256:ILE:HG12	1.84	0.58
1:E:366:SER:HA	1:E:369:TYR:CZ	2.39	0.58
2:A:111:ASN:OD1	2:A:114:GLU:OE2	2.22	0.58
2:A:177:ARG:HB2	2:A:498:CYS:HB2	1.86	0.57
2:A:273:ARG:NH1	2:A:515:TYR:HE2	2.02	0.57
2:A:394:ASN:O	2:A:562:LYS:N	2.37	0.57
1:E:457:ARG:NE	1:E:467:ASP:OD2	2.34	0.57
1:E:394:ASN:H	1:E:516:GLU:HB2	1.70	0.57
1:E:400:PHE:HE2	1:E:423:TYR:HE2	1.52	0.57
2:A:418:LEU:CD1	2:A:424:LEU:CD1	2.80	0.57
1:E:412:PRO:HB3	1:E:427:ASP:HA	1.86	0.57
2:A:172:VAL:HG23	2:A:176:LEU:HD22	1.86	0.57
1:E:374:PHE:N	1:E:374:PHE:HD1	2.03	0.56
2:A:123:MET:O	2:A:124:SER:C	2.46	0.56
2:A:381:TYR:CD1	2:A:558:LEU:HD22	2.39	0.56
2:A:127:TYR:CE2	2:A:504:TYR:CA	2.82	0.56
1:E:487:ASN:ND2	2:A:24:LEU:HD21	2.21	0.56
2:A:126:ILE:HD13	2:A:175:GLN:OE1	2.06	0.56
2:A:227:GLU:HG2	2:A:454:TYR:OH	2.05	0.56
2:A:419:LYS:HA	2:A:424:LEU:CD2	2.36	0.55
2:A:342:VAL:HG22	2:A:343:VAL:O	2.06	0.55
2:A:504:TYR:HE1	2:A:510:PHE:HE2	1.53	0.55
2:A:273:ARG:NH1	2:A:515:TYR:CE2	2.75	0.55
1:E:374:PHE:N	1:E:374:PHE:CD1	2.75	0.55
2:A:204:ARG:HD2	2:A:219:ARG:O	2.07	0.55
2:A:418:LEU:CA	2:A:423:LEU:HB2	2.35	0.54
1:E:398:ASP:OD2	1:E:423:TYR:OH	2.21	0.54
1:E:439:ASN:ND2	1:E:506:GLN:HE21	2.06	0.54
2:A:151:ILE:C	2:A:153:ALA:N	2.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:330:ASN:CB	2:A:357:ARG:HD3	2.38	0.54
2:A:494:ASP:OD1	2:A:494:ASP:N	2.28	0.54
1:E:358:ILE:HG22	1:E:395:VAL:HG11	1.89	0.54
1:E:449:TYR:O	1:E:494:SER:HB2	2.07	0.54
2:A:477:TRP:CZ3	2:A:500:PRO:HB3	2.43	0.54
2:A:252:TYR:O	2:A:256:ILE:HG13	2.08	0.54
2:A:554:LEU:HD12	2:A:554:LEU:C	2.33	0.53
2:A:303:ASN:O	2:A:307:ILE:HG13	2.07	0.53
2:A:90:ASN:HB3	2:A:93:LEU:HB2	1.90	0.53
2:A:148:LEU:HD13	2:A:148:LEU:N	2.24	0.53
2:A:557:MET:CE	2:A:569:ALA:HB1	2.39	0.53
1:E:423:TYR:CD1	1:E:423:TYR:C	2.85	0.53
2:A:108:LEU:HD23	2:A:108:LEU:H	1.73	0.53
2:A:398:GLU:CD	2:A:514:ARG:CD	2.79	0.53
2:A:522:GLN:O	2:A:525:PHE:HB2	2.09	0.53
2:A:108:LEU:HD23	2:A:108:LEU:N	2.24	0.53
2:A:535:HIS:CD2	2:A:542:CYS:HB2	2.44	0.53
2:A:80:ALA:HB2	2:A:100:LEU:HD22	1.90	0.53
2:A:265:HIS:ND1	2:A:490:PRO:HG3	2.23	0.53
2:A:323:MET:HB3	2:A:327:PHE:HD2	1.73	0.53
2:A:166:GLU:CD	2:A:493:HIS:NE2	2.67	0.53
2:A:89:GLN:HA	2:A:89:GLN:NE2	2.24	0.52
2:A:419:LYS:CB	2:A:424:LEU:HD21	2.34	0.52
2:A:105:SER:O	2:A:113:ARG:CG	2.56	0.52
2:A:273:ARG:HH11	2:A:515:TYR:HE2	1.50	0.52
2:A:288:LYS:HD2	2:A:433:GLU:OE2	2.10	0.52
2:A:134:ASN:HB3	2:A:163:TRP:CE3	2.44	0.52
2:A:418:LEU:HD13	2:A:424:LEU:HD13	1.91	0.52
2:A:127:TYR:CD2	2:A:507:SER:OG	2.56	0.52
2:A:494:ASP:CG	2:A:496:THR:HG22	2.35	0.52
2:A:21:ILE:HD12	2:A:21:ILE:H	1.73	0.52
2:A:25:ALA:O	2:A:28:PHE:HB3	2.10	0.52
2:A:133:CYS:SG	2:A:141:CYS:CA	2.91	0.52
2:A:261:CYS:SG	2:A:606:TRP:HB3	2.50	0.51
1:E:458:LYS:NZ	1:E:474:GLN:O	2.43	0.51
2:A:108:LEU:N	2:A:108:LEU:CD2	2.72	0.51
2:A:84:PRO:HG2	2:A:87:GLU:HB2	1.91	0.51
2:A:293:VAL:HG21	2:A:423:LEU:HD13	0.75	0.51
2:A:315:PHE:CE2	2:A:376:MET:HG2	2.46	0.51
2:A:460:ARG:NH2	2:A:512:PHE:HB2	2.24	0.51
1:E:505:TYR:HD2	2:A:353:LYS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:ALA:HB2	1:E:510:VAL:HG22	1.93	0.51
2:A:394:ASN:OD1	2:A:395:GLY:N	2.42	0.51
2:A:418:LEU:HD13	2:A:423:LEU:HB3	1.93	0.51
2:A:538:PRO:CG	2:A:541:LYS:HE2	2.41	0.51
2:A:24:LEU:HD22	2:A:83:TYR:HE2	1.76	0.51
2:A:132:VAL:CG1	2:A:133:CYS:N	2.74	0.51
2:A:474:MET:HE2	2:A:474:MET:HA	1.93	0.51
2:A:557:MET:HG2	2:A:573:VAL:CG2	2.39	0.51
2:A:148:LEU:N	2:A:148:LEU:CD1	2.73	0.51
2:A:499:ASP:H	2:A:500:PRO:HD2	1.76	0.51
2:A:181:GLU:HG3	2:A:470:LYS:CE	2.41	0.50
2:A:49:ASN:OD1	2:A:49:ASN:N	2.43	0.50
2:A:400:PHE:HE2	2:A:557:MET:HE1	1.77	0.50
2:A:103:SER:CB	2:A:107:ALA:HB2	2.42	0.50
2:A:323:MET:HB3	2:A:327:PHE:CD2	2.46	0.50
1:E:355:ARG:HH21	1:E:398:ASP:CG	2.18	0.50
1:E:401:VAL:CG1	1:E:451:TYR:CD2	2.93	0.50
2:A:346:PRO:HA	2:A:360:MET:HB3	1.94	0.50
2:A:134:ASN:HB3	2:A:163:TRP:CE2	2.46	0.50
2:A:352:GLN:HE22	2:A:393:ARG:HH11	1.58	0.50
1:E:400:PHE:CE2	1:E:423:TYR:HD2	2.28	0.50
1:E:426:PRO:HD2	1:E:429:PHE:HB2	1.94	0.50
1:E:490:PHE:HE1	1:E:492:LEU:HB2	1.77	0.50
2:A:124:SER:O	2:A:128:SER:N	2.37	0.50
2:A:420:SER:CB	4:C:1:NAG:H83	2.42	0.50
2:A:398:GLU:CD	2:A:514:ARG:HG2	2.35	0.49
2:A:127:TYR:HE2	2:A:504:TYR:CA	2.22	0.49
2:A:288:LYS:HD3	2:A:433:GLU:HB3	1.94	0.49
1:E:474:GLN:OE1	1:E:479:PRO:HA	2.13	0.49
1:E:366:SER:HA	1:E:369:TYR:CE1	2.47	0.49
2:A:176:LEU:HD23	2:A:501:ALA:HB1	1.95	0.49
2:A:323:MET:CB	2:A:327:PHE:HD2	2.25	0.49
2:A:387:MET:HE2	2:A:387:MET:HA	1.93	0.49
2:A:314:PHE:HD2	2:A:373:HIS:HD2	1.59	0.49
1:E:493:GLN:HA	1:E:493:GLN:HE21	1.78	0.49
2:A:166:GLU:OE1	2:A:493:HIS:CE1	2.65	0.49
2:A:168:TRP:NE1	2:A:502:ALA:HB1	2.23	0.49
2:A:230:PHE:CE1	2:A:451:PRO:HA	2.48	0.49
2:A:246:ALA:HA	2:A:249:MET:HG3	1.94	0.49
2:A:555:LEU:HD12	2:A:558:LEU:HB2	1.93	0.49
1:E:439:ASN:ND2	1:E:506:GLN:NE2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:LEU:HA	1:E:494:SER:HA	1.93	0.49
2:A:291:ILE:HG13	2:A:291:ILE:O	2.12	0.49
1:E:350:VAL:HG22	1:E:422:ASN:OD1	2.12	0.49
1:E:427:ASP:C	1:E:429:PHE:N	2.69	0.49
1:E:426:PRO:O	1:E:429:PHE:HB2	2.13	0.48
2:A:352:GLN:OE1	2:A:393:ARG:NH1	2.45	0.48
1:E:503:VAL:HA	1:E:506:GLN:HB2	1.95	0.48
2:A:105:SER:O	2:A:113:ARG:HD3	2.13	0.48
2:A:515:TYR:HD1	2:A:515:TYR:N	2.06	0.48
1:E:403:ARG:HG3	1:E:495:TYR:CE1	2.48	0.48
2:A:48:TRP:CD1	2:A:48:TRP:C	2.90	0.48
2:A:187:LYS:HG2	2:A:199:TYR:CZ	2.48	0.48
1:E:374:PHE:HE2	1:E:434:ILE:HG21	1.75	0.48
2:A:187:LYS:HG2	2:A:199:TYR:CD2	2.47	0.48
2:A:416:LYS:NZ	4:C:1:NAG:H81	2.28	0.48
2:A:521:TYR:O	2:A:522:GLN:C	2.56	0.48
2:A:256:ILE:H	2:A:256:ILE:CD1	2.11	0.48
2:A:127:TYR:CD1	2:A:127:TYR:C	2.91	0.48
2:A:265:HIS:CD2	2:A:266:LEU:HD12	2.49	0.48
2:A:166:GLU:OE2	2:A:493:HIS:NE2	2.46	0.48
1:E:493:GLN:HA	1:E:493:GLN:NE2	2.29	0.48
2:A:144:LEU:C	2:A:144:LEU:CD1	2.85	0.48
2:A:145:GLU:CB	2:A:146:PRO:HD3	2.34	0.48
2:A:278:LEU:O	2:A:282:THR:HG23	2.14	0.48
2:A:259:THR:O	2:A:259:THR:OG1	2.25	0.47
2:A:400:PHE:CE2	2:A:557:MET:HE1	2.49	0.47
1:E:453:TYR:HB3	1:E:495:TYR:CE2	2.49	0.47
2:A:20:THR:HG23	2:A:23:GLU:H	1.79	0.47
2:A:204:ARG:HG2	2:A:222:LEU:HD23	1.96	0.47
2:A:485:VAL:HG12	2:A:487:VAL:HG23	1.95	0.47
1:E:365:TYR:CE2	1:E:387:LEU:HB3	2.47	0.47
2:A:142:LEU:HD12	2:A:147:GLY:HA3	1.96	0.47
2:A:397:ASN:HD22	2:A:566:TRP:CG	2.33	0.47
2:A:555:LEU:HA	2:A:558:LEU:HB2	1.95	0.47
1:E:368:LEU:N	1:E:368:LEU:CD1	2.77	0.47
2:A:127:TYR:HD1	2:A:127:TYR:C	2.22	0.47
2:A:207:TYR:O	2:A:217:TYR:CD2	2.62	0.47
2:A:266:LEU:HD12	2:A:266:LEU:N	2.29	0.47
1:E:394:ASN:HD22	1:E:516:GLU:HG3	1.79	0.46
2:A:341:LYS:HD2	2:A:341:LYS:N	2.30	0.46
2:A:139:GLN:H	2:A:139:GLN:HG2	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:HIS:CD2	2:A:262:LEU:CD1	2.79	0.46
2:A:397:ASN:HD22	2:A:566:TRP:CD1	2.33	0.46
2:A:407:ILE:HD11	2:A:526:GLN:CA	2.44	0.46
1:E:369:TYR:OH	1:E:388:ASN:ND2	2.48	0.46
2:A:129:THR:O	2:A:129:THR:OG1	2.21	0.46
2:A:161:ARG:HD3	2:A:266:LEU:CA	2.43	0.46
2:A:30:ASP:OD1	2:A:30:ASP:N	2.48	0.46
2:A:233:ILE:CG1	2:A:581:VAL:HG21	2.46	0.46
2:A:288:LYS:CD	2:A:433:GLU:OE2	2.64	0.46
2:A:402:GLU:HB3	2:A:518:ARG:HD2	1.98	0.46
1:E:448:ASN:C	1:E:448:ASN:HD22	2.22	0.46
2:A:557:MET:HB2	2:A:557:MET:HE2	1.69	0.46
1:E:401:VAL:CG1	1:E:451:TYR:HD2	2.29	0.45
1:E:454:ARG:HD3	1:E:457:ARG:HD2	1.98	0.45
2:A:312:GLU:O	2:A:316:VAL:HG23	2.15	0.45
2:A:423:LEU:HD22	2:A:423:LEU:HA	1.77	0.45
2:A:173:GLY:O	2:A:174:LYS:C	2.57	0.45
2:A:451:PRO:O	2:A:452:PHE:C	2.59	0.45
2:A:455:MET:HE3	2:A:455:MET:HB3	1.59	0.45
2:A:560:LEU:O	2:A:563:SER:HB3	2.17	0.45
2:A:565:PRO:O	2:A:567:THR:N	2.49	0.45
1:E:422:ASN:HD21	1:E:454:ARG:H	1.64	0.45
2:A:241:HIS:CE1	2:A:606:TRP:HD1	2.33	0.45
1:E:365:TYR:O	1:E:369:TYR:CD2	2.69	0.45
2:A:209:ALA:HB1	2:A:565:PRO:HB3	1.98	0.45
2:A:288:LYS:HE2	2:A:431:ASP:OD2	2.12	0.45
1:E:400:PHE:CZ	1:E:423:TYR:HD2	2.35	0.45
1:E:437:ASN:ND2	1:E:508:TYR:CE1	2.75	0.45
2:A:288:LYS:HE3	2:A:434:THR:OG1	2.16	0.45
2:A:431:ASP:N	2:A:431:ASP:OD1	2.50	0.45
2:A:499:ASP:N	2:A:500:PRO:HD2	2.31	0.45
2:A:142:LEU:HD12	2:A:147:GLY:CA	2.46	0.45
2:A:180:TYR:O	2:A:184:VAL:HG23	2.17	0.45
2:A:448:GLY:O	2:A:451:PRO:HD2	2.17	0.45
2:A:137:LYS:O	2:A:140:GLU:HB2	2.17	0.44
2:A:161:ARG:HD3	2:A:265:HIS:C	2.42	0.44
2:A:163:TRP:CH2	2:A:164:VAL:HG23	2.52	0.44
2:A:283:VAL:HG13	2:A:286:PRO:HG3	1.99	0.44
2:A:297:MET:HG2	2:A:302:TRP:CE3	2.52	0.44
2:A:359:LYS:HB3	2:A:359:LYS:HE3	1.62	0.44
2:A:570:LEU:O	2:A:573:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:163:TRP:CZ2	2:A:164:VAL:HG23	2.52	0.44
2:A:311:ALA:O	2:A:312:GLU:C	2.60	0.44
2:A:374:HIS:O	2:A:377:GLY:N	2.51	0.44
2:A:418:LEU:CD2	2:A:423:LEU:CG	2.91	0.44
2:A:456:LEU:C	2:A:456:LEU:HD23	2.42	0.44
2:A:29:LEU:O	2:A:32:PHE:N	2.51	0.44
2:A:273:ARG:HH21	2:A:273:ARG:HD3	1.65	0.44
1:E:341:VAL:HG22	1:E:356:LYS:HD2	1.99	0.44
1:E:423:TYR:CD1	1:E:423:TYR:O	2.70	0.44
1:E:437:ASN:CA	1:E:508:TYR:CD1	2.80	0.44
2:A:476:LYS:NZ	2:A:479:GLU:OE2	2.48	0.44
2:A:313:LYS:O	2:A:314:PHE:C	2.58	0.44
2:A:48:TRP:CD1	2:A:48:TRP:O	2.70	0.44
2:A:311:ALA:O	2:A:314:PHE:N	2.51	0.44
2:A:447:VAL:O	2:A:448:GLY:C	2.61	0.44
2:A:486:GLY:HA3	2:A:606:TRP:CD1	2.52	0.44
2:A:100:LEU:HD23	2:A:100:LEU:O	2.18	0.44
2:A:352:GLN:NE2	2:A:393:ARG:HH11	2.16	0.43
2:A:557:MET:HE2	2:A:569:ALA:HB1	2.00	0.43
1:E:438:SER:O	1:E:438:SER:OG	2.36	0.43
1:E:425:LEU:HA	1:E:425:LEU:HD12	1.76	0.43
2:A:392:LEU:HD23	2:A:392:LEU:HA	1.58	0.43
2:A:79:LEU:O	2:A:82:ASP:HB2	2.19	0.43
2:A:375:GLU:OE2	2:A:375:GLU:HA	2.18	0.43
2:A:482:ARG:NH1	2:A:488:MET:HB2	2.33	0.43
2:A:424:LEU:CB	2:A:425:PRO:CD	2.75	0.43
2:A:494:ASP:OD2	2:A:496:THR:HG22	2.18	0.43
2:A:136:LYS:HD2	2:A:137:LYS:H	1.83	0.43
1:E:378:LYS:HD3	1:E:380:TYR:CZ	2.54	0.43
2:A:431:ASP:OD1	2:A:434:THR:HB	2.18	0.43
2:A:196:TYR:CD2	2:A:202:TYR:HD2	2.37	0.43
2:A:210:GLU:H	2:A:210:GLU:HG2	1.75	0.43
2:A:225:ASP:HA	2:A:228:ARG:NH1	2.33	0.43
1:E:353:TRP:H	1:E:353:TRP:CD1	2.36	0.43
2:A:148:LEU:HD13	2:A:148:LEU:H	1.84	0.43
2:A:565:PRO:O	2:A:568:LEU:N	2.50	0.43
2:A:287:GLU:H	2:A:287:GLU:CD	2.23	0.42
2:A:430:GLU:OE1	2:A:435:GLU:HB2	2.19	0.42
2:A:478:TRP:CZ2	2:A:489:GLU:HB3	2.54	0.42
2:A:109:SER:HB3	2:A:112:LYS:CD	2.47	0.42
2:A:138:PRO:C	2:A:140:GLU:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:GLY:O	2:A:208:GLU:N	2.52	0.42
2:A:293:VAL:CG1	2:A:423:LEU:CD1	2.91	0.42
2:A:55:THR:O	2:A:56:LYS:C	2.61	0.42
2:A:123:MET:C	2:A:125:THR:N	2.76	0.42
2:A:335:GLU:N	2:A:361:CYS:HB2	2.34	0.42
2:A:595:LEU:HD23	2:A:595:LEU:HA	1.88	0.42
2:A:142:LEU:HA	2:A:142:LEU:HD22	1.69	0.42
2:A:180:TYR:O	2:A:183:TYR:HB3	2.20	0.42
2:A:157:ASP:OD1	2:A:159:SER:N	2.52	0.42
2:A:198:ASP:OD1	2:A:198:ASP:N	2.52	0.42
2:A:568:LEU:HD23	2:A:568:LEU:O	2.19	0.42
2:A:72:PHE:CZ	2:A:76:GLN:HG3	2.55	0.42
2:A:196:TYR:CE1	2:A:219:ARG:NH1	2.74	0.42
2:A:398:GLU:H	2:A:398:GLU:HG2	1.69	0.42
1:E:410:ILE:O	1:E:410:ILE:HG22	2.19	0.42
2:A:416:LYS:HZ1	4:C:1:NAG:H81	1.84	0.42
2:A:119:ILE:O	2:A:122:THR:OG1	2.30	0.42
2:A:144:LEU:HB2	2:A:168:TRP:HZ3	1.48	0.42
1:E:417:ARG:NH1	1:E:453:TYR:HE2	2.16	0.42
2:A:145:GLU:HG3	2:A:146:PRO:HD3	0.63	0.42
2:A:518:ARG:O	2:A:522:GLN:HG3	2.20	0.42
2:A:20:THR:OG1	2:A:21:ILE:N	2.52	0.41
2:A:32:PHE:O	2:A:33:ASN:C	2.62	0.41
2:A:199:TYR:O	2:A:202:TYR:HB3	2.19	0.41
1:E:361:CYS:O	1:E:361:CYS:SG	2.78	0.41
2:A:43:ARG:O	2:A:46:ALA:HB3	2.20	0.41
2:A:215:TYR:CE2	2:A:568:LEU:HA	2.55	0.41
2:A:573:VAL:HG12	2:A:574:VAL:HG13	2.02	0.41
2:A:586:ASN:C	2:A:586:ASN:HD22	2.24	0.41
1:E:379:CYS:HA	1:E:432:CYS:HA	2.01	0.41
1:E:442:ASP:OD1	1:E:451:TYR:OH	2.20	0.41
2:A:172:VAL:O	2:A:176:LEU:HD13	2.20	0.41
2:A:190:MET:O	2:A:193:ALA:HB3	2.21	0.41
2:A:284:PRO:HB3	2:A:594:TRP:CH2	2.55	0.41
1:E:365:TYR:HD2	1:E:387:LEU:CB	2.25	0.41
2:A:151:ILE:HD12	2:A:151:ILE:HA	1.65	0.41
2:A:474:MET:HE1	2:A:500:PRO:CD	2.51	0.41
2:A:424:LEU:CD2	2:A:424:LEU:C	2.93	0.41
1:E:403:ARG:O	1:E:404:GLY:C	2.64	0.41
2:A:293:VAL:CB	2:A:423:LEU:CD1	2.99	0.41
2:A:418:LEU:CD2	2:A:423:LEU:HG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:585:LEU:O	2:A:589:GLU:N	2.54	0.41
1:E:462:LYS:O	1:E:463:PRO:C	2.63	0.41
2:A:77:SER:O	2:A:78:LYS:C	2.64	0.41
2:A:209:ALA:HB3	2:A:217:TYR:N	2.35	0.41
2:A:370:LEU:HD23	2:A:370:LEU:HA	1.65	0.41
2:A:134:ASN:O	2:A:135:PRO:C	2.64	0.40
2:A:398:GLU:OE1	2:A:514:ARG:CD	2.64	0.40
2:A:504:TYR:CE1	2:A:510:PHE:HE2	2.36	0.40
2:A:137:LYS:HD2	2:A:137:LYS:HA	1.82	0.40
2:A:242:ALA:O	2:A:243:TYR:C	2.64	0.40
1:E:400:PHE:CD1	1:E:400:PHE:C	3.00	0.40
2:A:77:SER:HA	2:A:100:LEU:CD2	2.52	0.40
2:A:160:GLU:HA	2:A:163:TRP:NE1	2.35	0.40
2:A:225:ASP:O	2:A:229:THR:HG23	2.21	0.40
2:A:424:LEU:N	2:A:424:LEU:CD2	2.84	0.40
2:A:522:GLN:HE21	2:A:522:GLN:HB2	1.64	0.40
2:A:39:LEU:O	2:A:39:LEU:HD12	2.21	0.40
2:A:88:ILE:HG21	2:A:93:LEU:HD12	2.03	0.40
2:A:308:PHE:CD2	2:A:333:LEU:HD12	2.57	0.40
2:A:407:ILE:CD1	2:A:526:GLN:CA	3.00	0.40
1:E:390:LEU:HD13	1:E:392:PHE:CZ	2.57	0.40
2:A:29:LEU:O	2:A:30:ASP:C	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	179/185 (97%)	163 (91%)	14 (8%)	2 (1%)	12	38
2	A	589/598 (98%)	527 (90%)	57 (10%)	5 (1%)	16	45
All	All	768/783 (98%)	690 (90%)	71 (9%)	7 (1%)	14	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	146	PRO
2	A	152	MET
2	A	556	ASN
1	E	428	ASP
2	A	51	ASN
2	A	473	TRP
1	E	507	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	158/162 (98%)	148 (94%)	10 (6%)	15	40
2	A	522/528 (99%)	485 (93%)	37 (7%)	12	37
All	All	680/690 (99%)	633 (93%)	47 (7%)	13	38

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	358	ILE
1	E	359	SER
1	E	362	VAL
1	E	367	VAL
1	E	378	LYS
1	E	424	LYS
1	E	425	LEU
1	E	427	ASP
1	E	428	ASP
1	E	508	TYR
2	A	49	ASN
2	A	55	THR
2	A	108	LEU
2	A	109	SER
2	A	124	SER
2	A	125	THR

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Mol	Chain	Res	Type
2	A	126	ILE
2	A	132	VAL
2	A	133	CYS
2	A	137	LYS
2	A	142	LEU
2	A	144	LEU
2	A	148	LEU
2	A	149	ASP
2	A	150	GLU
2	A	151	ILE
2	A	164	VAL
2	A	169	ARG
2	A	172	VAL
2	A	254	SER
2	A	256	ILE
2	A	257	SER
2	A	259	THR
2	A	358	ILE
2	A	359	LYS
2	A	360	MET
2	A	407	ILE
2	A	421	ILE
2	A	423	LEU
2	A	424	LEU
2	A	427	ASP
2	A	429	ARG
2	A	430	GLU
2	A	432	ASN
2	A	515	TYR
2	A	553	LYS
2	A	555	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	388	ASN
1	E	414	GLN
1	E	439	ASN
1	E	448	ASN
1	E	460	ASN
2	A	63	ASN
2	A	89	GLN

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Mol	Chain	Res	Type
2	A	117	ASN
2	A	188	ASN
2	A	218	ASN
2	A	221	GLN
2	A	508	ASN
2	A	522	GLN
2	A	586	ASN
2	A	601	ASN

### 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 ⓘ

7 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	$\# Z  > 2$
3	NAG	B	1	3,2	14,14,15	0.65	1 (7%)	17,19,21	1.37	3 (17%)
3	NAG	B	2	3	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	NAG	C	1	4,2	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	C	2	4	14,14,15	0.91	1 (7%)	17,19,21	1.21	3 (17%)
4	BMA	C	3	4	11,11,12	0.75	0	15,15,17	0.91	1 (6%)
3	NAG	D	1	3,2	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	D	2	3	14,14,15	0.39	0	17,19,21	0.38	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
3	NAG	B	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1
4	NAG	C	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	NAG	O5-C1	-3.32	1.38	1.43
3	B	1	NAG	C1-C2	-2.07	1.49	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C3-C4-C5	3.09	115.75	110.24
3	B	1	NAG	C1-O5-C5	2.97	116.22	112.19
3	B	1	NAG	C4-C3-C2	-2.82	106.88	111.02
4	C	3	BMA	C1-O5-C5	2.56	115.66	112.19
3	B	2	NAG	C1-O5-C5	2.43	115.48	112.19
4	C	2	NAG	O4-C4-C5	-2.39	103.36	109.30
3	B	1	NAG	C2-N2-C7	2.18	126.01	122.90
4	C	2	NAG	C4-C3-C2	2.16	114.19	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
4	C	1	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C1-C2-N2-C7

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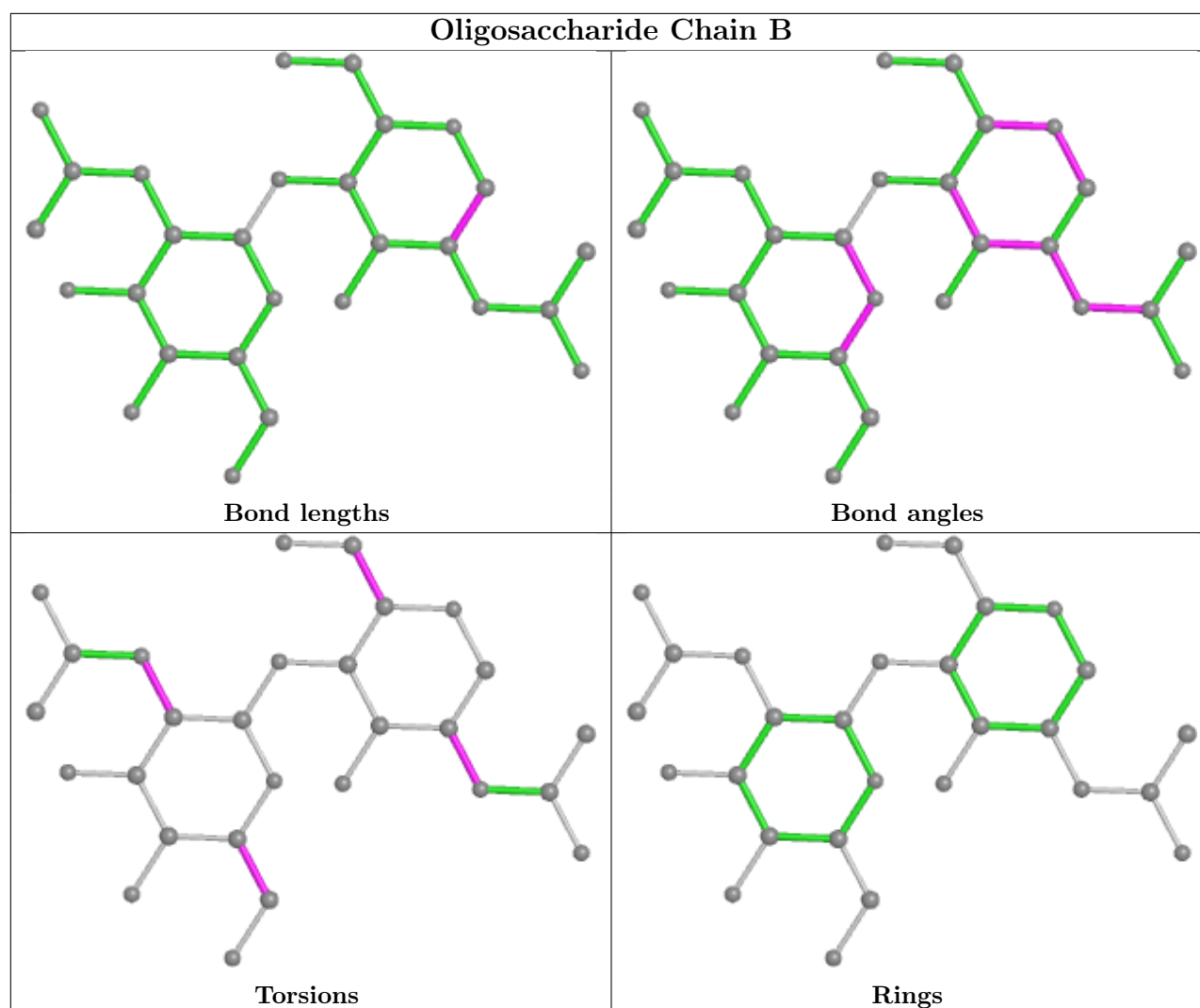
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C3-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7

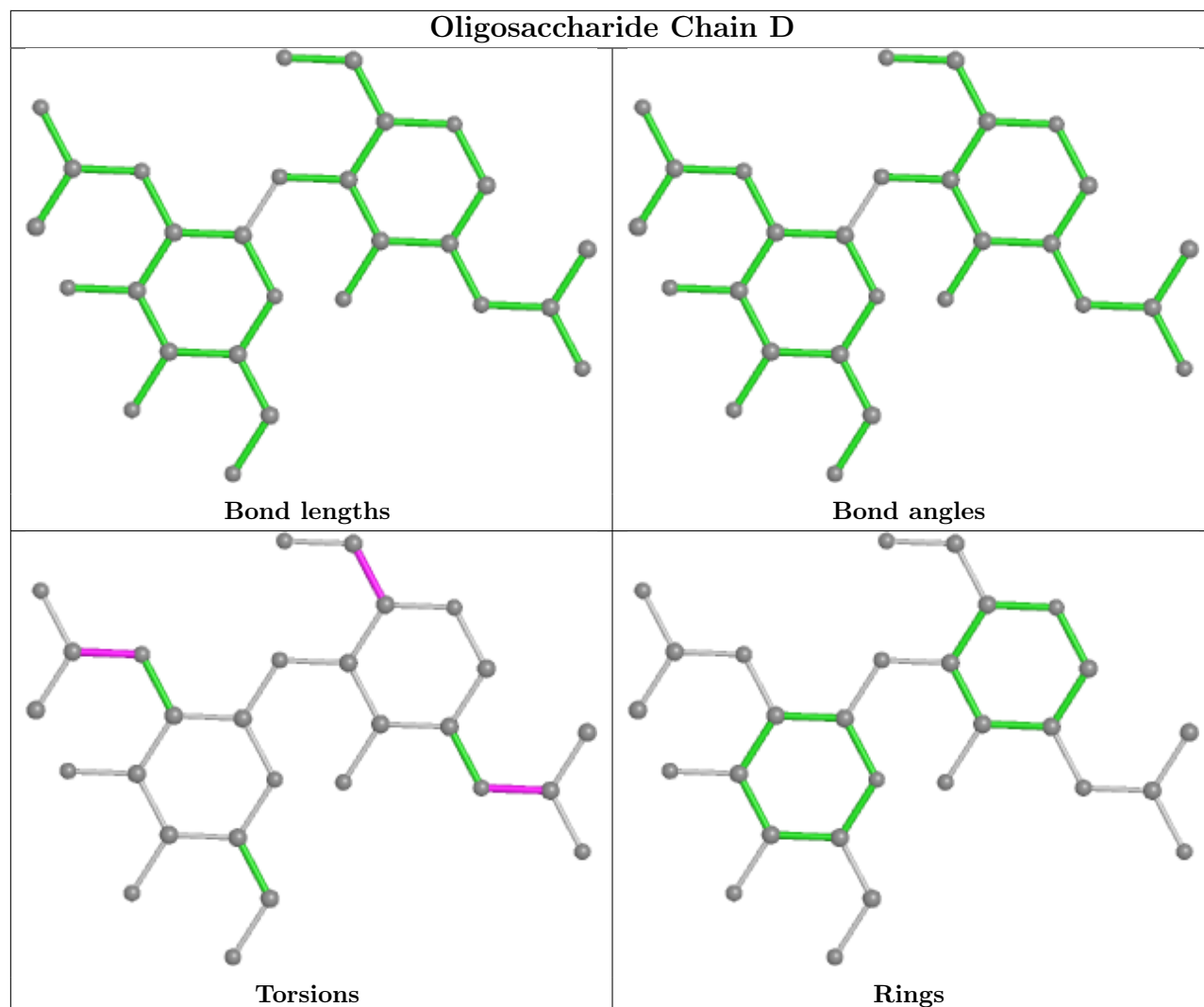
There are no ring outliers.

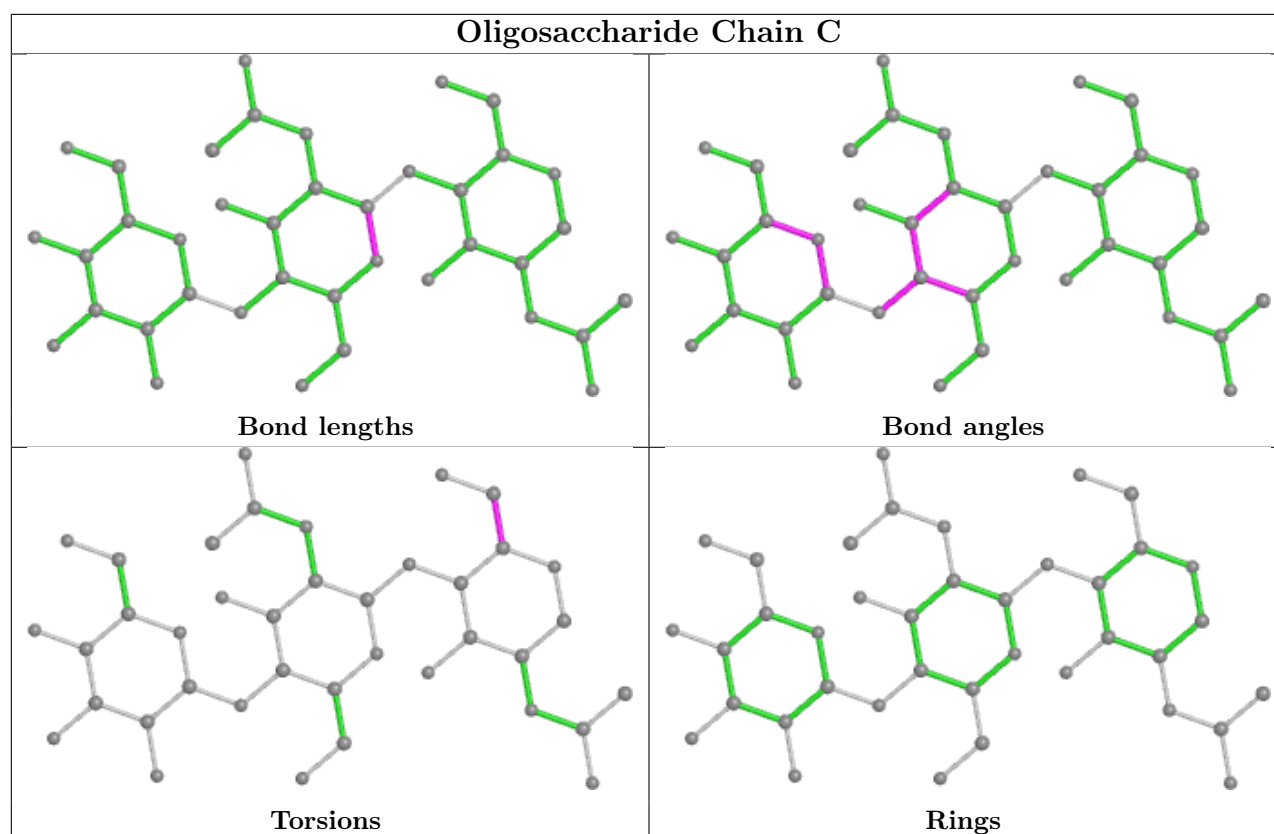
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	4	0
3	B	1	NAG	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](#)

1 ligand is 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	$\# Z  > 2$
5	NAG	E	601	1	14,14,15	0.35	0	17,19,21	1.44	2 (11%)

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
5	NAG	E	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	E	601	NAG	C2-N2-C7	4.16	128.82	122.90
5	E	601	NAG	C1-O5-C5	3.02	116.28	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	C3-C2-N2-C7
5	E	601	NAG	C4-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	NAG	1	0

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	181/185 (97%)	-0.06	3 (1%) 69 60	53, 89, 168, 225	0
2	A	592/598 (98%)	-0.17	7 (1%) 76 68	30, 83, 141, 183	0
All	All	773/783 (98%)	-0.15	10 (1%) 74 66	30, 84, 150, 225	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	423	LEU	3.7
2	A	210	GLU	3.1
2	A	359	LYS	2.8
2	A	168	TRP	2.6
2	A	149	ASP	2.4
1	E	365	TYR	2.3
1	E	362	VAL	2.3
2	A	343	VAL	2.2
1	E	508	TYR	2.1
2	A	399	GLY	2.1

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

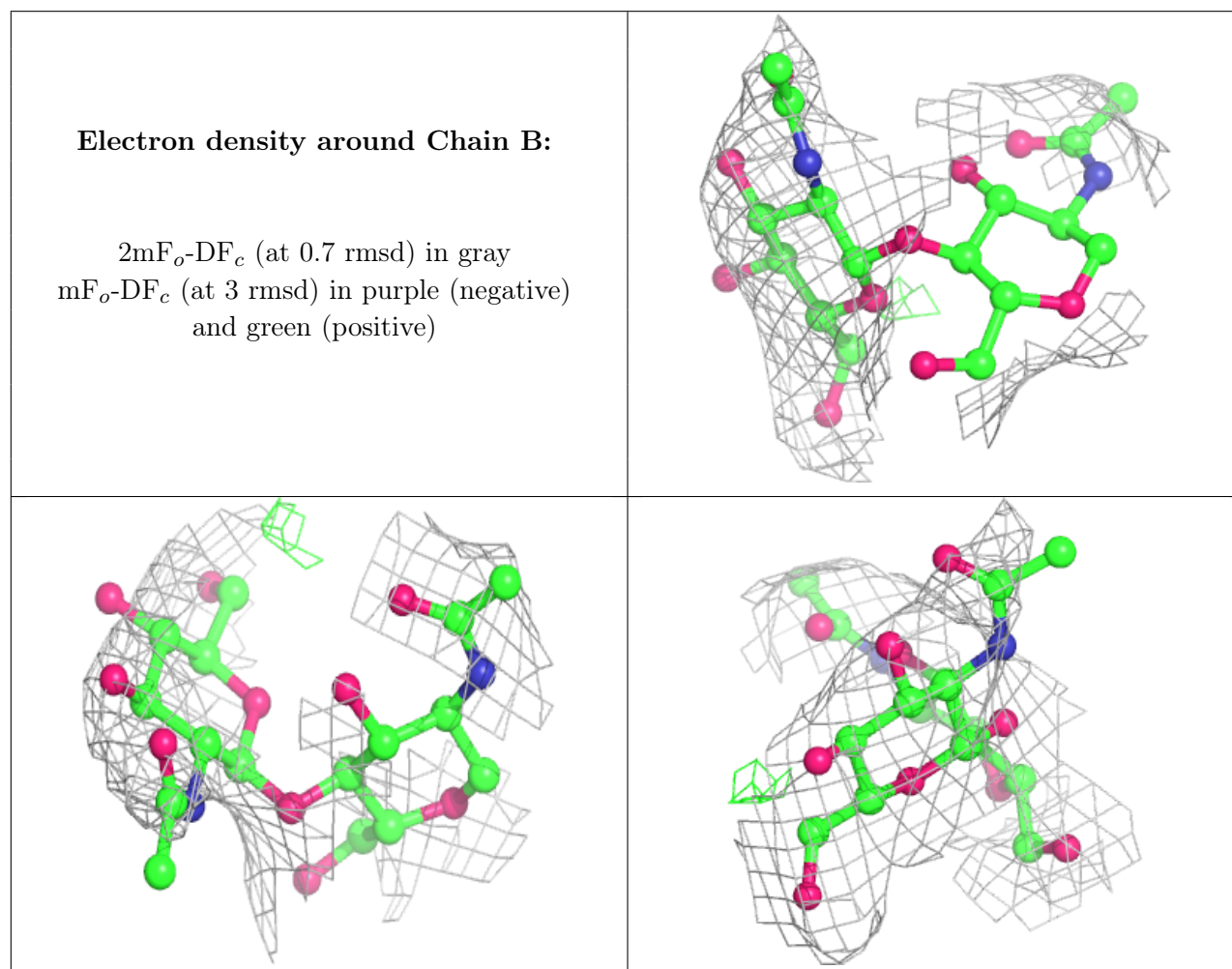
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	1	14/15	-	-	108,125,149,161	0
3	NAG	B	2	14/15	-	-	118,137,149,151	0
4	NAG	C	2	14/15	0.33	0.14	119,136,152,163	0
4	NAG	C	1	14/15	0.64	0.12	81,103,117,126	0
3	NAG	D	2	14/15	0.70	0.10	30,30,30,30	0
3	NAG	D	1	14/15	0.84	0.09	30,30,30,30	0
4	BMA	C	3	11/12	-	-	110,148,157,163	0

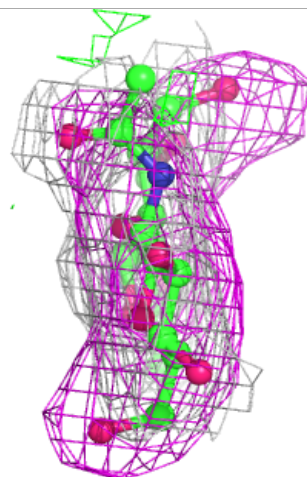
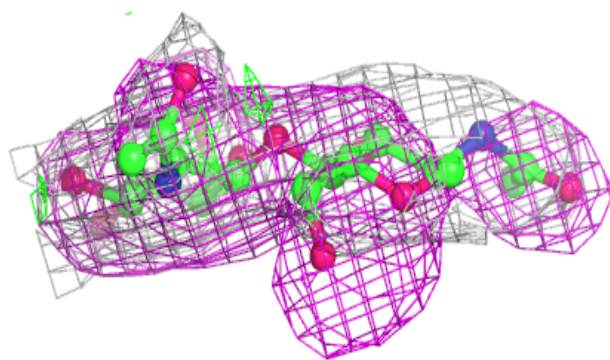
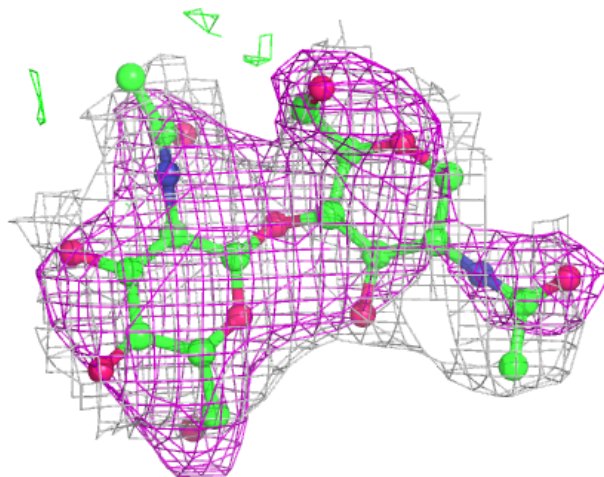
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

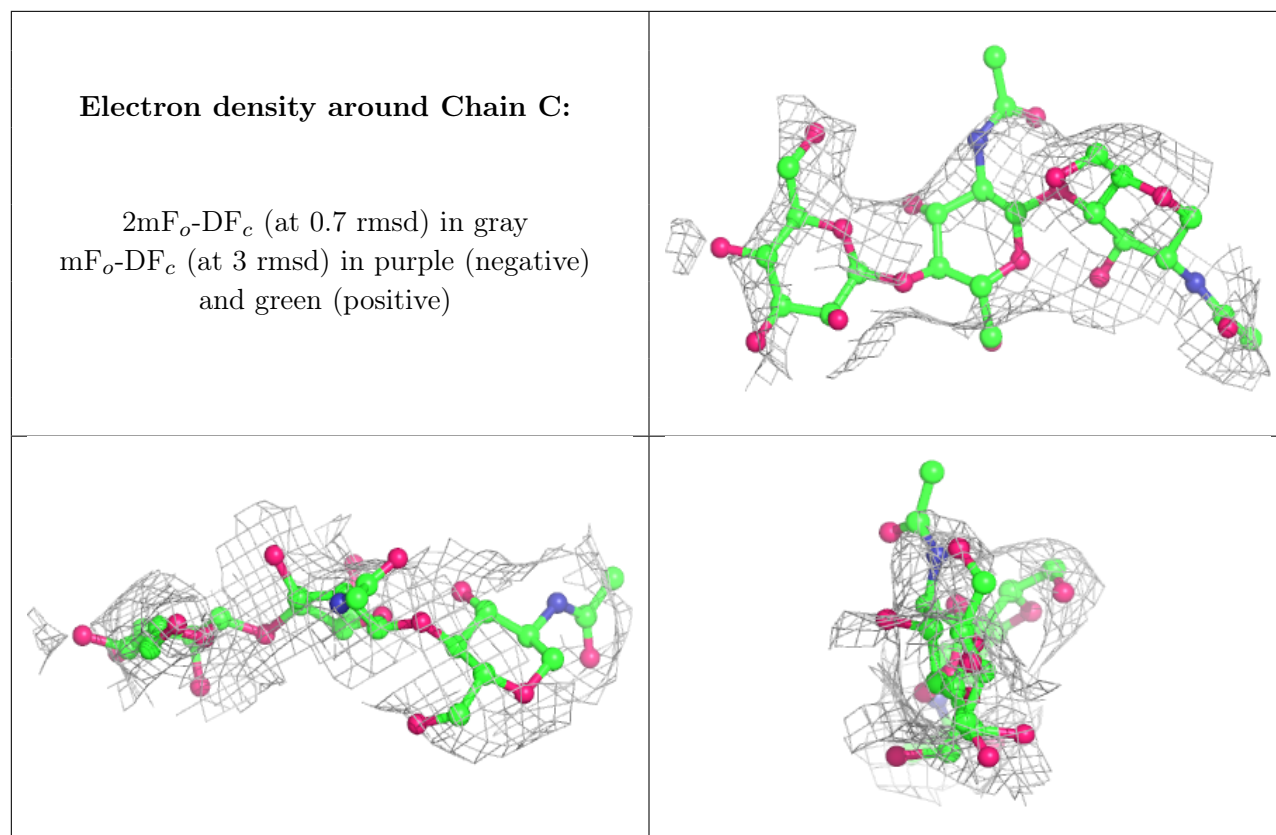




**Electron density around Chain D:**

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





## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	601	14/15	0.73	0.11	120,140,145,152	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.