WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2025 – 12:12 PM JST

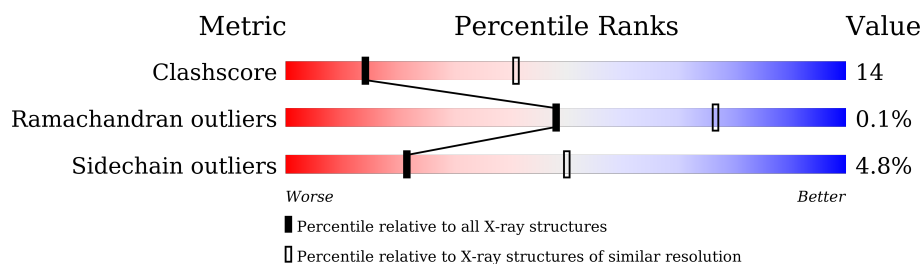|		
PDB ID	:	8XYE / pdb_00008xye
Title	:	Crystal structure of SARS-CoV-2 BA.4 RBD and human ACE2
Authors	:	Lan, J.; Wang, C.H.
Deposited on	:	2024-01-19
Resolution	:	3.32 Å(reported)

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 3.32 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.1%
Sidechain outliers		4.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1111 (3.34-3.30)
Ramachandran outliers	177936	1109 (3.34-3.30)
Sidechain outliers	177891	1108 (3.34-3.30)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	598	78% 20% •
1	B	598	72% 27% •
2	C	194	46% 47% 7% •
2	D	194	52% 41% 7% •
3	E	3	33% 67%
3	F	3	33% 67%
3	G	3	33% 67%
4	H	2	100%

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13101 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	598	Total 4884	C 3125	N 809	O 921	S 29	0	1	0
1	A	597	Total 4876	C 3121	N 808	O 918	S 29	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	ASP	-	expression tag	UNP Q9BYF1
B	18	PRO	-	expression tag	UNP Q9BYF1
A	17	ASP	-	expression tag	UNP Q9BYF1
A	18	PRO	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	194	Total 1549	C 997	N 262	O 282	S 8	0	0	0
2	D	194	Total 1549	C 997	N 262	O 282	S 8	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 3 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
3	E	3	Total 39	C 22	N 2	O 15	0	0	0
3	F	3	Total 39	C 22	N 2	O 15	0	0	0
3	G	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 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
4	H	2	Total 28	C 16	N 2	O 10	0	0	0

- 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	B	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0

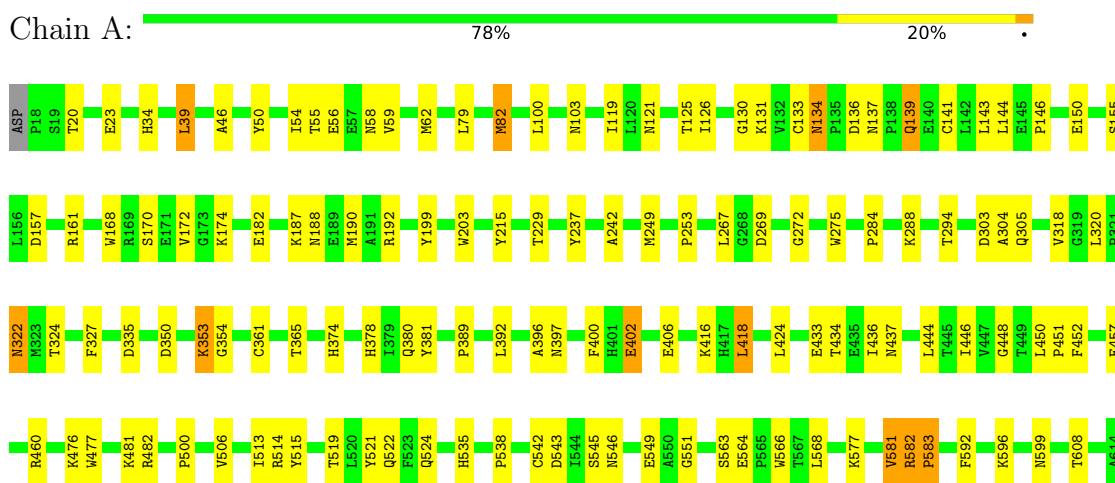# 3 Residue-property plots ⓘ

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. 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. 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.

Note EDS failed to run properly.

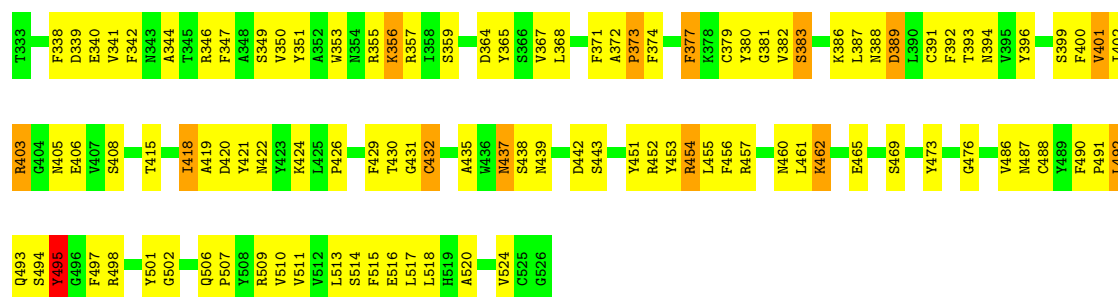• Molecule 1: Processed angiotensin-converting enzyme 2

Chain B:

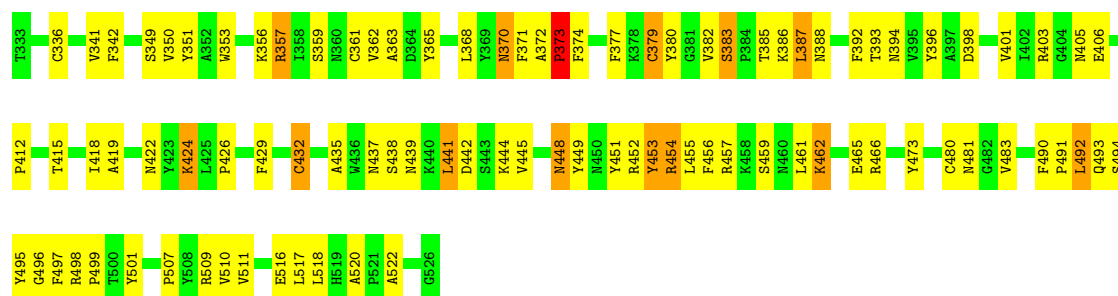• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

• Molecule 2: Spike protein S1

Chain C: 46% 47% 7% ·

T333 F338 D339 E340 V341 F342 N343 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 I358 S359 D364 Y365 S366 V367 L368 F371 A372 P373 F374 F377 K378 C379 Y380 G381 V382 S383 K386 L387 N388 D389 L390 C391 F392 T393 N394 V395 Y396 S399 F400 V401 I402

R403 G404 N405 E406 V407 S408 T415 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 F429 T430 G431 C432 A435 W436 N437 S438 N439 D442 S443 Y451 R452 Y453 R454 L455 F456 R457 N460 L461 K462 E465 S469 Y473 G476 V486 N487 C488 Y489 F490 F491 L492

Q493 S494 Y495 G496 F497 R498 Y501 G502 Q506 P507 Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 V524 C525 G526

• Molecule 2: Spike protein S1

Chain D: 52% 41% 7% ·

T333 C336 V341 F342 S349 V350 Y351 A352 W353 K356 R357 I358 S359 N360 C361 V362 A363 D364 Y365 L368 Y369 N370 F371 A372 P373 F374 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 F392 T393 N394 V395 Y396 A397 D398 V401 I402 R403 G404 N405 E406

P412 T415 I418 A419 N422 Y423 K424 L425 P426 F429 C432 A435 W436 N437 S438 N439 K440 L441 D442 S443 K444 V445 N448 Y449 N450 Y451 R452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 E465 R466 Y473 C480 N481 G482 V483 F490 P491 L492 Q493 S494

Y495 G496 F497 R498 P499 T500 Y501 P507 Y508 R509 V510 V511 E516 L517 L518 H519 A520 P521 A522 G526

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

Chain E: 33% 67%

NAG1 NAG2 BMA3

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

Chain F: 33% 67%

NAG1 NAG2 BMA3

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

Chain G: 33% 67%

NAG1 NAG2 BMA3

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

Chain H:

100%

NAG1
NAG2

4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.47Å 165.82Å 98.98Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	31.37 – 3.32	Depositor
% Data completeness (in resolution range)	98.3 (31.37-3.32)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.49 (at 3.31Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.191 , 0.242	Depositor
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.340	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13101	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	A	0.61	3/5018 (0.1%)	0.79	6/6818 (0.1%)
1	B	0.59	0/5026	0.79	6/6830 (0.1%)
2	C	0.74	1/1595 (0.1%)	0.94	4/2171 (0.2%)
2	D	0.63	0/1595	0.88	5/2171 (0.2%)
All	All	0.62	4/13234 (0.0%)	0.82	21/17990 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLU	CB-CG	7.80	1.67	1.52
1	A	203	TRP	CB-CG	-6.03	1.39	1.50
1	A	402	GLU	CG-CD	5.83	1.60	1.51
2	C	495	TYR	CE1-CZ	-5.39	1.31	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	492	LEU	CB-CG-CD2	-8.19	97.08	111.00
2	D	455	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	402	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	B	584	LEU	CB-CG-CD2	-6.12	100.59	111.00
2	C	373	PRO	N-CA-C	-6.10	96.24	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	GLU	CG-CD-OE2	6.07	130.44	118.30
1	B	382	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	39	LEU	CA-CB-CG	-5.84	101.86	115.30
2	D	361	CYS	CA-CB-SG	5.78	124.41	114.00
2	D	441	LEU	CA-CB-CG	5.68	128.37	115.30
2	D	373	PRO	N-CA-CB	-5.53	96.51	102.60
1	B	39	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	B	29	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	B	202	TYR	CA-CB-CG	5.35	123.56	113.40
1	A	350	ASP	CB-CG-OD1	5.28	123.05	118.30
2	C	346	ARG	CG-CD-NE	-5.21	100.86	111.80
1	A	100	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	418	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	B	143	LEU	CA-CB-CG	5.13	127.11	115.30
2	C	353	TRP	C-N-CA	-5.04	109.10	121.70
2	C	492	LEU	CB-CG-CD1	-5.01	102.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	495	TYR	Sidechain

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	4876	0	4649	87	0
1	B	4884	0	4650	99	0
2	C	1549	0	1472	98	0
2	D	1549	0	1472	76	0
3	E	39	0	34	0	0
3	F	39	0	34	3	0
3	G	39	0	34	0	0
4	H	28	0	25	1	0
5	A	42	0	39	1	0
5	B	56	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13101	0	12461	359	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 14.

All (359) 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:D:453:TYR:CD2	2:D:495:TYR:HE1	1.85	0.95
1:A:378:HIS:NE2	1:A:402:GLU:OE2	2.02	0.92
2:C:393:THR:HG21	2:C:518:LEU:HD23	1.53	0.89
2:D:442:ASP:OD1	2:D:451:TYR:OH	1.93	0.86
2:D:453:TYR:CD2	2:D:495:TYR:CE1	2.65	0.85
2:C:340:GLU:O	2:C:344:ALA:HB2	1.81	0.81
2:D:495:TYR:HD2	2:D:497:PHE:CZ	1.98	0.81
2:C:453:TYR:CD2	2:C:495:TYR:HE1	2.00	0.79
2:C:453:TYR:HD2	2:C:495:TYR:CE1	2.02	0.77
2:C:453:TYR:CD2	2:C:495:TYR:CE1	2.72	0.77
1:A:134:ASN:HD21	1:A:137:ASN:HB3	1.51	0.75
2:C:392:PHE:HD1	2:C:517:LEU:HB2	1.50	0.75
2:C:495:TYR:HD2	2:C:497:PHE:CZ	2.04	0.74
2:D:349:SER:HB2	2:D:452:ARG:H	1.54	0.73
2:D:359:SER:OG	2:D:394:ASN:OD1	2.07	0.71
1:A:134:ASN:ND2	1:A:137:ASN:HB3	2.06	0.71
2:C:342:PHE:HE1	2:C:511:VAL:HG11	1.56	0.69
1:B:57:GLU:O	1:B:61:ASN:ND2	2.24	0.69
2:D:365:TYR:CD1	2:D:387:LEU:HD12	2.28	0.69
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.74	0.68
2:C:420:ASP:HB2	2:C:460:ASN:OD1	1.93	0.67
2:C:419:ALA:O	2:C:424:LYS:HB2	1.95	0.67
1:B:224:GLU:HB3	1:B:228[A]:HIS:CE1	2.30	0.66
2:C:365:TYR:HE1	2:C:388:ASN:HA	1.60	0.66
1:B:168:TRP:CZ3	1:B:172:VAL:HG21	2.30	0.66
1:A:187:LYS:HD2	1:A:199:TYR:CZ	2.30	0.66
1:B:21:ILE:HG21	1:B:84:PRO:HD2	1.78	0.66
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.78	0.66
2:D:422:ASN:HD21	2:D:453:TYR:HB2	1.59	0.65
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.32	0.65
2:C:381:GLY:HA3	2:C:430:THR:HA	1.78	0.65
1:B:20:THR:N	1:B:23:GLU:OE1	2.22	0.65
2:C:365:TYR:CE1	2:C:387:LEU:HG	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:448:ASN:HD21	2:D:451:TYR:HD1	1.42	0.64
2:C:453:TYR:HD2	2:C:495:TYR:HE1	1.40	0.64
3:F:2:NAG:H4	3:F:3:BMA:O2	1.97	0.63
1:B:131:LYS:HB3	1:B:143:LEU:HD23	1.79	0.63
2:C:453:TYR:CE1	2:C:493:GLN:HB3	2.32	0.63
2:D:453:TYR:CE1	2:D:493:GLN:HB3	2.33	0.63
2:C:365:TYR:CD1	2:C:387:LEU:HG	2.34	0.62
2:C:426:PRO:HD2	2:C:429:PHE:HD1	1.63	0.62
2:D:373:PRO:HD2	2:D:374:PHE:CD2	2.34	0.62
2:C:371:PHE:C	2:C:373:PRO:HD3	2.20	0.62
1:B:50:TYR:CE1	1:B:59:VAL:HG22	2.35	0.62
2:C:401:VAL:HG11	2:C:451:TYR:CD2	2.34	0.62
1:B:268:GLY:O	1:B:277:ASN:ND2	2.29	0.62
1:B:406:GLU:HG3	1:B:518:ARG:HH11	1.65	0.62
2:D:452:ARG:HG2	2:D:494:SER:HB3	1.80	0.62
1:A:564:GLU:HB3	1:A:568:LEU:HD23	1.82	0.62
2:C:456:PHE:HB3	2:C:473:TYR:CD2	2.35	0.61
2:C:435:ALA:HB2	2:C:510:VAL:HG12	1.81	0.61
2:C:377:PHE:HE1	2:C:432:CYS:SG	2.24	0.61
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.66	0.61
2:C:392:PHE:CD1	2:C:517:LEU:HB2	2.34	0.60
2:D:456:PHE:HB3	2:D:473:TYR:CD2	2.36	0.60
2:D:418:ILE:HG13	2:D:422:ASN:HD22	1.67	0.60
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.83	0.60
2:C:421:TYR:CD1	2:C:457:ARG:HB3	2.37	0.59
2:D:453:TYR:HD2	2:D:495:TYR:CE1	2.15	0.59
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.85	0.59
2:D:383:SER:O	2:D:387:LEU:HD23	2.02	0.59
1:A:121:ASN:O	1:A:125:THR:HG23	2.03	0.59
1:A:374:HIS:CE1	1:A:402:GLU:OE1	2.55	0.59
1:B:111:ASP:HA	1:B:114:LYS:HE3	1.83	0.58
1:B:458:LYS:HG2	1:B:462:MET:HE2	1.84	0.58
1:A:229:THR:HB	1:A:581:VAL:HG13	1.85	0.58
2:D:368:LEU:HA	2:D:371:PHE:CD1	2.38	0.58
1:A:50:TYR:HE1	1:A:54:ILE:HG23	1.69	0.58
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.67	0.58
1:B:247:LYS:HB2	1:B:282:THR:HG22	1.86	0.58
2:C:502:GLY:O	2:C:506:GLN:HG3	2.04	0.58
2:C:368:LEU:HA	2:C:371:PHE:CE1	2.40	0.57
1:B:312:GLU:OE2	1:B:322:ASN:HB2	2.04	0.57
2:D:415:THR:O	2:D:415:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:LEU:HD11	2:C:515:PHE:CZ	2.41	0.56
1:B:177:ARG:HH22	1:B:495:GLU:HG3	1.70	0.56
1:A:170:SER:O	1:A:174:LYS:HD2	2.06	0.56
1:B:187:LYS:HD2	1:B:199:TYR:CZ	2.41	0.56
1:B:229:THR:HB	1:B:581:VAL:HG13	1.88	0.56
2:C:403:ARG:HH21	2:C:405:ASN:CG	2.09	0.55
2:C:437:ASN:HD22	2:C:439:ASN:H	1.54	0.55
2:D:372:ALA:N	2:D:373:PRO:HD3	2.21	0.55
2:D:349:SER:CB	2:D:452:ARG:H	2.19	0.55
2:D:435:ALA:HB2	2:D:510:VAL:HG12	1.89	0.55
1:A:137:ASN:OD1	1:A:139:GLN:HB2	2.07	0.55
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.42	0.55
1:A:133:CYS:HA	1:A:141:CYS:HA	1.89	0.55
2:C:443:SER:HB3	2:C:507:PRO:HG3	1.89	0.54
2:D:415:THR:HG22	2:D:424:LYS:NZ	2.21	0.54
1:A:389:PRO:HG2	1:A:392:LEU:HD12	1.89	0.54
2:C:438:SER:OG	2:C:507:PRO:HB2	2.08	0.54
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.42	0.54
1:A:374:HIS:NE2	1:A:402:GLU:OE1	2.41	0.54
1:B:55:THR:O	1:B:58:ASN:N	2.40	0.54
2:C:396:TYR:HB2	2:C:514:SER:HB3	1.89	0.54
2:D:380:TYR:CD2	2:D:412:PRO:HD3	2.43	0.54
1:B:245:ARG:NH2	1:B:603:PHE:O	2.41	0.54
1:B:285:PHE:HE2	1:B:436:ILE:HB	1.73	0.54
1:B:81:GLN:HB3	3:F:2:NAG:H81	1.90	0.53
2:C:393:THR:HG22	2:C:517:LEU:HA	1.89	0.53
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.08	0.53
2:C:359:SER:OG	2:C:394:ASN:OD1	2.22	0.53
2:D:350:VAL:HG11	2:D:418:ILE:HD11	1.89	0.53
2:D:351:TYR:CZ	2:D:492:LEU:HD21	2.43	0.53
2:D:392:PHE:HA	2:D:517:LEU:HD13	1.91	0.53
2:D:349:SER:HB3	2:D:451:TYR:HA	1.90	0.53
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.91	0.53
2:C:387:LEU:CD1	2:C:515:PHE:CE2	2.92	0.53
2:D:498:ARG:HB2	2:D:501:TYR:CE1	2.44	0.53
2:D:462:LYS:O	2:D:465:GLU:HB2	2.09	0.52
1:B:145:GLU:OE2	1:B:146:PRO:HB3	2.09	0.52
2:D:379:CYS:HA	2:D:432:CYS:HA	1.91	0.52
2:C:438:SER:OG	2:C:442:ASP:HB2	2.10	0.52
2:C:476:GLY:H	2:C:487:ASN:HB3	1.74	0.52
2:D:393:THR:HG22	2:D:517:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:GLY:N	2:C:487:ASN:HB3	2.25	0.52
1:A:549:GLU:H	1:A:549:GLU:CD	2.13	0.52
2:C:502:GLY:HA3	1:A:354:GLY:HA3	1.92	0.52
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.46	0.51
2:C:373:PRO:HD2	2:C:374:PHE:CD1	2.45	0.51
2:C:497:PHE:CD1	2:C:507:PRO:HD3	2.46	0.51
2:D:481:ASN:N	2:D:483:VAL:HG23	2.25	0.51
1:A:242:ALA:HB3	1:A:599:ASN:ND2	2.26	0.51
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.93	0.51
1:A:582:ARG:HB3	1:A:583:PRO:HD3	1.91	0.51
2:D:461:LEU:HD22	2:D:465:GLU:HB3	1.93	0.50
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.46	0.50
1:B:248:LEU:HD12	1:B:262:LEU:HD22	1.93	0.50
2:C:393:THR:OG1	2:C:520:ALA:HB3	2.11	0.50
1:B:318:VAL:O	1:B:551:GLY:HA3	2.12	0.50
1:B:324:THR:OG1	1:B:327:PHE:N	2.39	0.50
1:A:452:PHE:CE2	1:A:481:LYS:NZ	2.80	0.50
2:D:441:LEU:HD11	2:D:509:ARG:NH1	2.27	0.50
2:D:449:TYR:OH	2:D:498:ARG:NH2	2.44	0.50
1:A:55:THR:O	1:A:58:ASN:N	2.44	0.50
1:B:270:MET:HB3	1:B:271:TRP:CZ3	2.47	0.50
1:B:482:ARG:HH21	1:B:489:GLU:CD	2.15	0.50
2:C:501:TYR:CE2	1:A:353:LYS:HD3	2.47	0.50
2:D:393:THR:HA	2:D:522:ALA:HA	1.94	0.50
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.46	0.49
2:C:415:THR:O	2:C:415:THR:OG1	2.30	0.49
2:D:351:TYR:CE2	2:D:492:LEU:HD21	2.47	0.49
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.12	0.49
1:A:581:VAL:O	1:A:582:ARG:C	2.50	0.49
1:B:55:THR:O	1:B:56:GLU:C	2.49	0.49
1:B:460:ARG:NH2	1:B:506:VAL:HA	2.27	0.49
2:C:372:ALA:C	2:C:374:PHE:H	2.16	0.49
1:B:108:LEU:HB2	1:B:113:SER:OG	2.11	0.49
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.47	0.49
2:C:387:LEU:HD12	2:C:387:LEU:O	2.12	0.49
1:A:519:THR:O	1:A:522:GLN:HG2	2.13	0.49
1:B:554:LEU:HG	1:B:558:LEU:HD11	1.94	0.48
1:B:192:ARG:NH1	1:B:197:GLU:O	2.46	0.48
1:B:347:THR:HB	1:B:349:TRP:NE1	2.28	0.48
2:D:393:THR:CG2	2:D:516:GLU:HG3	2.42	0.48
1:B:25:ALA:HB1	1:B:97:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:O	1:B:181:GLU:HG3	2.13	0.48
2:C:349:SER:HB3	2:C:451:TYR:HA	1.94	0.48
2:C:460:ASN:N	2:C:460:ASN:HD22	2.11	0.48
2:C:351:TYR:CD2	2:C:492:LEU:HD21	2.49	0.48
2:C:418:ILE:O	2:C:422:ASN:N	2.44	0.48
2:C:442:ASP:OD2	2:C:509:ARG:NE	2.45	0.48
2:C:452:ARG:HG2	2:C:494:SER:HB3	1.96	0.48
2:D:357:ARG:HG3	2:D:396:TYR:HE1	1.77	0.48
1:A:402:GLU:O	1:A:406:GLU:HG2	2.14	0.48
1:B:161:ARG:HE	1:B:266:LEU:HD23	1.79	0.48
1:B:375:GLU:O	1:B:378:HIS:HB2	2.14	0.48
1:B:424:LEU:HD12	1:B:424:LEU:HA	1.69	0.48
2:C:365:TYR:CZ	2:C:387:LEU:HG	2.49	0.48
2:D:392:PHE:HD1	2:D:517:LEU:HB2	1.79	0.48
1:A:46:ALA:HB1	1:A:62:MET:HA	1.95	0.48
1:A:188:ASN:O	1:A:192:ARG:HG3	2.14	0.48
1:A:582:ARG:O	1:A:583:PRO:C	2.51	0.48
2:C:461:LEU:HD22	2:C:465:GLU:HB3	1.95	0.47
2:D:373:PRO:HD2	2:D:374:PHE:CG	2.50	0.47
2:C:393:THR:CG2	2:C:516:GLU:HG3	2.44	0.47
2:C:462:LYS:O	2:C:465:GLU:HB2	2.14	0.47
1:A:249:MET:O	1:A:253:PRO:HA	2.14	0.47
1:A:374:HIS:NE2	1:A:402:GLU:OE2	2.47	0.47
2:C:460:ASN:HD22	2:C:460:ASN:H	1.63	0.47
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.28	0.47
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.27	0.47
1:B:288:LYS:HA	1:B:288:LYS:HD3	1.64	0.47
1:B:111:ASP:HA	1:B:114:LYS:CE	2.45	0.47
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.50	0.47
2:C:406:GLU:HG3	2:C:418:ILE:HG12	1.95	0.47
2:C:454:ARG:NH2	2:C:469:SER:O	2.34	0.47
2:D:426:PRO:HD2	2:D:429:PHE:HD2	1.80	0.47
2:D:438:SER:OG	2:D:507:PRO:HB2	2.15	0.47
1:A:55:THR:O	1:A:56:GLU:C	2.53	0.47
1:A:126:ILE:O	1:A:130:GLY:N	2.41	0.47
1:A:452:PHE:HE2	1:A:481:LYS:NZ	2.12	0.47
1:B:19:SER:HA	1:B:23:GLU:OE1	2.14	0.46
1:B:192:ARG:HA	1:B:196:TYR:O	2.15	0.46
2:C:431:GLY:HA3	2:C:513:LEU:O	2.15	0.46
2:C:453:TYR:OH	1:A:34:HIS:CD2	2.68	0.46
2:C:351:TYR:CE2	2:C:492:LEU:HD21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:PRO:HD2	2:C:429:PHE:CD1	2.46	0.46
2:D:439:ASN:HD21	2:D:499:PRO:HA	1.79	0.46
2:D:457:ARG:NH1	2:D:459:SER:O	2.45	0.46
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.51	0.46
1:B:206:ASP:OD2	1:B:397:ASN:HB2	2.16	0.46
1:B:41:TYR:HE2	1:B:45:LEU:HD22	1.80	0.46
2:C:371:PHE:HB3	2:C:373:PRO:HD3	1.97	0.46
2:C:498:ARG:HB2	2:C:501:TYR:CE1	2.51	0.46
2:C:422:ASN:HD21	2:C:453:TYR:HB2	1.80	0.46
2:C:342:PHE:CE1	2:C:511:VAL:HG11	2.45	0.46
2:D:353:TRP:NE1	2:D:466:ARG:HG3	2.30	0.46
2:C:350:VAL:HA	2:C:400:PHE:HB2	1.97	0.45
2:C:403:ARG:HG2	2:C:495:TYR:CE2	2.50	0.45
2:D:403:ARG:HH21	2:D:405:ASN:HB2	1.81	0.45
2:D:490:PHE:CD1	2:D:491:PRO:HD2	2.52	0.45
2:D:497:PHE:CE2	2:D:507:PRO:HB3	2.51	0.45
1:B:39:LEU:O	1:B:42:GLN:HB2	2.17	0.45
2:C:338:PHE:O	2:C:341:VAL:N	2.48	0.45
1:A:79:LEU:O	1:A:82:MET:HG3	2.15	0.45
1:B:389:PRO:HG2	1:B:392:LEU:HD12	1.97	0.45
1:B:521:TYR:O	1:B:524:GLN:N	2.49	0.45
1:B:525:PHE:O	1:B:526:GLN:C	2.54	0.45
1:B:346:PRO:HA	1:B:359:LEU:O	2.17	0.45
1:A:482:ARG:HD3	1:A:608:THR:O	2.17	0.45
1:A:535:HIS:HE1	1:A:538:PRO:O	2.00	0.45
2:C:401:VAL:HG11	2:C:451:TYR:HD2	1.79	0.45
2:D:370:ASN:C	2:D:372:ALA:N	2.69	0.45
2:C:391:CYS:HA	2:C:524:VAL:O	2.16	0.45
1:A:322:ASN:ND2	5:A:703:NAG:O7	2.44	0.45
1:A:397:ASN:ND2	1:A:400:PHE:HE1	2.15	0.45
4:H:1:NAG:H61	4:H:2:NAG:C7	2.46	0.45
1:B:446:ILE:O	1:B:449:THR:HG22	2.17	0.45
1:B:520:LEU:O	1:B:524:GLN:HG3	2.17	0.45
2:C:453:TYR:CE1	2:C:455:LEU:HB3	2.52	0.45
2:D:481:ASN:H	2:D:483:VAL:HG23	1.82	0.45
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.76	0.45
1:B:20:THR:OG1	1:B:23:GLU:HG3	2.17	0.45
1:B:110:GLU:O	1:B:114:LYS:HG3	2.17	0.45
2:C:347:PHE:CE2	2:C:399:SER:HB2	2.51	0.45
2:D:403:ARG:HE	2:D:403:ARG:HB2	1.57	0.44
1:B:455:MET:HE1	1:B:481:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:403:ARG:HG3	2:C:406:GLU:OE1	2.17	0.44
2:C:486:VAL:O	2:C:488:CYS:SG	2.75	0.44
1:A:119:ILE:HD11	1:A:182:GLU:CD	2.38	0.44
1:B:267:LEU:HA	1:B:278:LEU:HD11	1.98	0.44
2:D:495:TYR:CD2	2:D:497:PHE:CZ	2.91	0.44
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.52	0.44
1:A:397:ASN:ND2	1:A:521:TYR:OH	2.51	0.44
2:C:373:PRO:HD2	2:C:374:PHE:CE1	2.52	0.44
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.99	0.44
1:B:347:THR:CB	1:B:349:TRP:HE1	2.31	0.44
1:A:20:THR:HG23	1:A:23:GLU:OE1	2.17	0.44
1:A:545:SER:O	1:A:546:ASN:HB2	2.17	0.44
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.59	0.44
1:B:177:ARG:NH2	1:B:495:GLU:HG3	2.33	0.44
1:A:288:LYS:HE3	1:A:433:GLU:CG	2.48	0.44
1:A:320:LEU:HD13	1:A:380:GLN:HG2	2.00	0.44
1:B:430:GLU:OE1	1:B:541:LYS:NZ	2.51	0.44
2:D:368:LEU:HA	2:D:371:PHE:CE1	2.53	0.44
1:B:209:VAL:HG12	1:B:216:ASP:HA	2.00	0.43
2:C:342:PHE:CE2	2:C:368:LEU:HD21	2.53	0.43
1:B:48:TRP:CH2	1:B:357:ARG:HB3	2.53	0.43
2:C:387:LEU:HD11	2:C:515:PHE:CE2	2.52	0.43
2:D:419:ALA:O	2:D:424:LYS:HB2	2.18	0.43
2:D:495:TYR:HD2	2:D:497:PHE:CE2	2.36	0.43
1:A:155:SER:O	1:A:161:ARG:HD2	2.18	0.43
1:A:237:TYR:CE1	1:A:451:PRO:HG2	2.53	0.43
2:C:338:PHE:O	2:C:339:ASP:C	2.57	0.43
1:A:187:LYS:HD2	1:A:199:TYR:CE1	2.53	0.43
1:A:514:ARG:HG2	1:A:515:TYR:N	2.32	0.43
2:C:355:ARG:C	2:C:356:LYS:HD2	2.39	0.43
1:A:433:GLU:O	1:A:436:ILE:N	2.52	0.43
1:B:406:GLU:HG3	1:B:518:ARG:NH1	2.31	0.43
1:B:474:MET:HE1	1:B:499:ASP:HB2	2.01	0.43
2:C:372:ALA:N	2:C:373:PRO:HD3	2.34	0.43
2:D:422:ASN:OD1	2:D:454:ARG:HB2	2.19	0.43
1:B:378:HIS:NE2	1:B:402:GLU:OE2	2.45	0.43
1:B:460:ARG:HH21	1:B:506:VAL:HA	1.83	0.43
1:B:122:THR:O	1:B:126:ILE:HG13	2.18	0.43
2:C:380:TYR:O	2:C:431:GLY:O	2.37	0.43
2:C:420:ASP:O	2:C:460:ASN:HA	2.19	0.43
2:D:415:THR:HG22	2:D:424:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:CB	1:B:282:THR:HG22	2.49	0.43
2:D:444:LYS:O	2:D:444:LYS:HG3	2.19	0.43
1:B:81:GLN:CB	3:F:2:NAG:H81	2.49	0.42
1:B:227:GLU:HG2	1:B:454:TYR:OH	2.19	0.42
1:A:374:HIS:NE2	1:A:402:GLU:CD	2.73	0.42
1:A:215:TYR:CE1	1:A:577:LYS:HE2	2.54	0.42
1:B:315:PHE:O	1:B:318:VAL:HG22	2.19	0.42
1:B:320:LEU:HB3	1:B:380:GLN:OE1	2.19	0.42
2:C:401:VAL:CG1	2:C:451:TYR:HD2	2.32	0.42
2:C:442:ASP:OD1	2:C:451:TYR:OH	2.25	0.42
2:D:350:VAL:HG22	2:D:422:ASN:HB3	2.01	0.42
2:C:368:LEU:O	2:C:368:LEU:HD23	2.20	0.42
1:B:103:ASN:O	1:B:104:GLY:C	2.58	0.42
2:C:383:SER:O	2:C:387:LEU:N	2.49	0.42
1:A:275:TRP:O	1:A:444:LEU:HB3	2.19	0.42
1:B:80:ALA:C	1:B:82:MET:H	2.23	0.42
1:B:525:PHE:O	1:B:528:ALA:N	2.52	0.42
2:C:387:LEU:HD13	2:C:515:PHE:CE2	2.54	0.42
1:A:134:ASN:OD1	1:A:136:ASP:N	2.53	0.42
1:A:294:THR:HG23	1:A:365:THR:HA	2.01	0.42
1:B:475:LYS:HE2	1:B:479:GLU:OE2	2.20	0.42
2:C:365:TYR:CD1	2:C:388:ASN:OD1	2.73	0.42
2:C:386:LYS:HA	2:C:389:ASP:OD2	2.20	0.42
2:D:342:PHE:CE1	2:D:511:VAL:HG21	2.55	0.42
2:D:461:LEU:HA	2:D:461:LEU:HD23	1.55	0.42
1:B:41:TYR:CE2	1:B:45:LEU:HD22	2.54	0.42
2:C:473:TYR:O	2:C:488:CYS:HA	2.20	0.42
2:D:341:VAL:HG12	2:D:342:PHE:HD1	1.83	0.42
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.85	0.42
1:B:170:SER:O	1:B:174:LYS:HD2	2.20	0.42
1:B:316:VAL:HA	1:B:320:LEU:O	2.20	0.42
1:A:448:GLY:O	1:A:451:PRO:HD2	2.20	0.42
2:D:442:ASP:OD1	2:D:451:TYR:CZ	2.71	0.41
1:A:592:PHE:CZ	1:A:596:LYS:HD2	2.55	0.41
2:D:336:CYS:HB2	2:D:363:ALA:HA	2.01	0.41
1:A:318:VAL:O	1:A:551:GLY:HA3	2.20	0.41
2:C:382:VAL:HG22	2:C:383:SER:H	1.85	0.41
2:D:398:ASP:O	2:D:511:VAL:HA	2.21	0.41
2:D:452:ARG:HD2	2:D:492:LEU:HD23	2.01	0.41
1:A:457:GLU:HG2	1:A:513:ILE:HB	2.02	0.41
2:C:368:LEU:HA	2:C:371:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:TRP:O	2:D:466:ARG:NE	2.51	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.56	0.41
1:B:171:GLU:O	1:B:175:GLN:HG3	2.20	0.41
2:D:373:PRO:CD	2:D:374:PHE:CE2	3.03	0.41
2:D:386:LYS:C	2:D:388:ASN:N	2.74	0.41
1:A:269:ASP:OD1	1:A:272:GLY:N	2.54	0.41
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.03	0.41
1:B:286:GLY:O	1:B:287:GLN:C	2.59	0.41
2:C:403:ARG:HA	2:C:506:GLN:O	2.21	0.41
1:B:114:LYS:HE3	1:B:114:LYS:HB2	1.99	0.41
1:B:470:LYS:HA	1:B:473:TRP:CD1	2.56	0.41
1:B:485:VAL:HG12	1:B:487:VAL:HG23	2.03	0.41
2:D:387:LEU:H	2:D:387:LEU:HG	1.72	0.41
2:D:336:CYS:N	2:D:362:VAL:O	2.54	0.41
1:A:535:HIS:NE2	1:A:542:CYS:HA	2.36	0.41
1:B:478:TRP:CD2	1:B:489:GLU:HB3	2.56	0.41
1:B:557:MET:HE2	1:B:573:VAL:HG21	2.03	0.41
2:C:364:ASP:OD1	2:C:367:VAL:HG12	2.21	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.54	0.41
1:A:157:ASP:O	1:A:161:ARG:HG3	2.20	0.41
1:A:303:ASP:O	1:A:304:ALA:C	2.59	0.41
1:A:324:THR:O	1:A:327:PHE:HB3	2.21	0.41
1:A:392:LEU:HD13	1:A:563:SER:HA	2.03	0.41
1:B:46:ALA:HB1	1:B:62:MET:HA	2.01	0.41
1:B:305:GLN:O	1:B:309:LYS:HG2	2.21	0.41
1:B:535:HIS:CE1	1:B:542:CYS:HA	2.56	0.41
2:C:490:PHE:CD1	2:C:491:PRO:HD2	2.55	0.41
2:D:393:THR:OG1	2:D:520:ALA:HB3	2.21	0.41
2:D:438:SER:O	2:D:439:ASN:C	2.59	0.40
1:B:267:LEU:HA	1:B:267:LEU:HD23	1.79	0.40
1:A:146:PRO:O	1:A:150:GLU:HB2	2.20	0.40
1:A:284:PRO:HD2	1:A:437:ASN:OD1	2.21	0.40
1:A:446:ILE:O	1:A:450:LEU:HG	2.22	0.40
2:C:422:ASN:ND2	2:C:453:TYR:HB2	2.37	0.40
2:D:449:TYR:CE1	2:D:496:GLY:HA2	2.56	0.40
1:A:424:LEU:HD12	1:A:424:LEU:HA	1.62	0.40
2:D:480:CYS:SG	2:D:483:VAL:HB	2.61	0.40
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.57	0.40
1:A:433:GLU:O	1:A:434:THR:C	2.59	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	596/598 (100%)	568 (95%)	28 (5%)	0	100	100
1	B	597/598 (100%)	563 (94%)	34 (6%)	0	100	100
2	C	192/194 (99%)	172 (90%)	20 (10%)	0	100	100
2	D	192/194 (99%)	166 (86%)	25 (13%)	1 (0%)	25	57
All	All	1577/1584 (100%)	1469 (93%)	107 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	373	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	528/528 (100%)	515 (98%)	13 (2%)	42	67
1	B	529/528 (100%)	510 (96%)	19 (4%)	30	57
2	C	167/167 (100%)	152 (91%)	15 (9%)	8	28
2	D	167/167 (100%)	147 (88%)	20 (12%)	4	17
All	All	1391/1390 (100%)	1324 (95%)	67 (5%)	21	50

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	B	92	THR
1	B	103	ASN
1	B	190	MET
1	B	287	GLN
1	B	305	GLN
1	B	317	SER
1	B	338	ASN
1	B	339	VAL
1	B	340	GLN
1	B	347	THR
1	B	381	TYR
1	B	385	TYR
1	B	409	SER
1	B	432	ASN
1	B	473	TRP
1	B	476	LYS
1	B	495	GLU
1	B	579	MET
2	C	356	LYS
2	C	357	ARG
2	C	377	PHE
2	C	379	CYS
2	C	383	SER
2	C	389	ASP
2	C	401	VAL
2	C	402	ILE
2	C	403	ARG
2	C	408	SER
2	C	418	ILE
2	C	432	CYS
2	C	437	ASN
2	C	454	ARG
2	C	462	LYS
2	D	356	LYS
2	D	357	ARG
2	D	370	ASN
2	D	377	PHE
2	D	379	CYS
2	D	382	VAL
2	D	383	SER
2	D	385	THR
2	D	387	LEU

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Mol	Chain	Res	Type
2	D	401	VAL
2	D	406	GLU
2	D	424	LYS
2	D	432	CYS
2	D	437	ASN
2	D	445	VAL
2	D	448	ASN
2	D	453	TYR
2	D	454	ARG
2	D	462	LYS
2	D	518	LEU
1	A	82	MET
1	A	103	ASN
1	A	134	ASN
1	A	139	GLN
1	A	190	MET
1	A	305	GLN
1	A	322	ASN
1	A	353	LYS
1	A	381	TYR
1	A	476	LYS
1	A	581	VAL
1	A	582	ARG
1	A	583	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	287	GLN
2	C	437	ASN
2	C	460	ASN
1	A	380	GLN
1	A	535	HIS

5.3.3 RNA (i)

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 ⓘ

11 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	E	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.67	0
3	BMA	E	3	3	11,11,12	3.30	8 (72%)	15,15,17	1.78	5 (33%)
3	NAG	F	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	F	2	3	14,14,15	0.80	1 (7%)	17,19,21	1.18	1 (5%)
3	BMA	F	3	3	11,11,12	3.81	9 (81%)	15,15,17	2.21	6 (40%)
3	NAG	G	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	0.55	0
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	0.94	0
3	BMA	G	3	3	11,11,12	2.80	8 (72%)	15,15,17	1.58	3 (20%)
4	NAG	H	1	4,1	14,14,15	1.17	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	H	2	4	14,14,15	0.93	1 (7%)	17,19,21	0.72	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	O5-C1	7.06	1.55	1.43
3	E	3	BMA	C4-C3	5.06	1.65	1.52
3	F	3	BMA	C1-C2	4.72	1.63	1.52
3	F	3	BMA	O5-C5	4.71	1.53	1.43
3	F	3	BMA	C4-C5	4.58	1.62	1.53
3	E	3	BMA	C1-C2	4.41	1.62	1.52
3	E	3	BMA	O5-C1	4.33	1.50	1.43
4	H	1	NAG	O5-C1	4.04	1.50	1.43
3	G	3	BMA	C1-C2	4.01	1.61	1.52
3	G	3	BMA	C4-C3	3.97	1.62	1.52
3	E	3	BMA	C4-C5	3.85	1.61	1.53
3	G	1	NAG	O5-C1	-3.67	1.37	1.43
3	G	3	BMA	O3-C3	3.65	1.51	1.43
3	F	1	NAG	C1-C2	3.64	1.57	1.52
3	E	3	BMA	O3-C3	3.56	1.51	1.43
3	F	3	BMA	C4-C3	3.51	1.61	1.52
3	G	3	BMA	C4-C5	3.48	1.60	1.53
3	G	3	BMA	C2-C3	3.34	1.57	1.52
3	E	3	BMA	O4-C4	3.06	1.50	1.43
4	H	2	NAG	O5-C1	3.00	1.48	1.43
3	F	3	BMA	O4-C4	2.89	1.49	1.43
3	F	3	BMA	O2-C2	2.82	1.49	1.43
3	F	3	BMA	C6-C5	2.81	1.61	1.51
3	E	3	BMA	O5-C5	2.78	1.49	1.43
3	F	3	BMA	O3-C3	2.71	1.49	1.43
3	E	3	BMA	C6-C5	2.55	1.60	1.51
3	E	1	NAG	O5-C1	2.54	1.47	1.43
3	G	3	BMA	O4-C4	2.49	1.48	1.43
3	G	3	BMA	O2-C2	2.20	1.48	1.43
3	G	3	BMA	O5-C1	2.17	1.47	1.43
3	F	2	NAG	C1-C2	2.15	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	BMA	O5-C5-C6	4.87	114.84	107.20
3	E	3	BMA	C1-O5-C5	3.56	117.02	112.19
3	F	2	NAG	O4-C4-C3	-3.20	102.95	110.35
3	F	3	BMA	O5-C1-C2	3.11	115.56	110.77
3	E	3	BMA	O3-C3-C4	3.10	117.52	110.35
3	F	3	BMA	O2-C2-C1	3.05	115.39	109.15
3	G	3	BMA	C1-C2-C3	3.04	113.41	109.67
3	E	3	BMA	O5-C1-C2	2.97	115.36	110.77
3	G	3	BMA	C1-O5-C5	2.67	115.81	112.19
3	G	3	BMA	O5-C1-C2	2.59	114.76	110.77
4	H	1	NAG	O3-C3-C2	-2.35	104.60	109.47
3	F	1	NAG	O3-C3-C2	-2.33	104.64	109.47
3	F	3	BMA	O4-C4-C3	2.26	115.58	110.35
3	E	3	BMA	O5-C5-C6	2.22	110.69	107.20
3	E	3	BMA	O4-C4-C3	2.20	115.44	110.35
3	F	3	BMA	C2-C3-C4	-2.18	107.12	110.89
3	F	1	NAG	C2-N2-C7	2.16	125.97	122.90
3	F	3	BMA	O3-C3-C2	2.01	113.83	109.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	1	0
4	H	1	NAG	1	0
4	H	2	NAG	1	0
3	F	2	NAG	3	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H
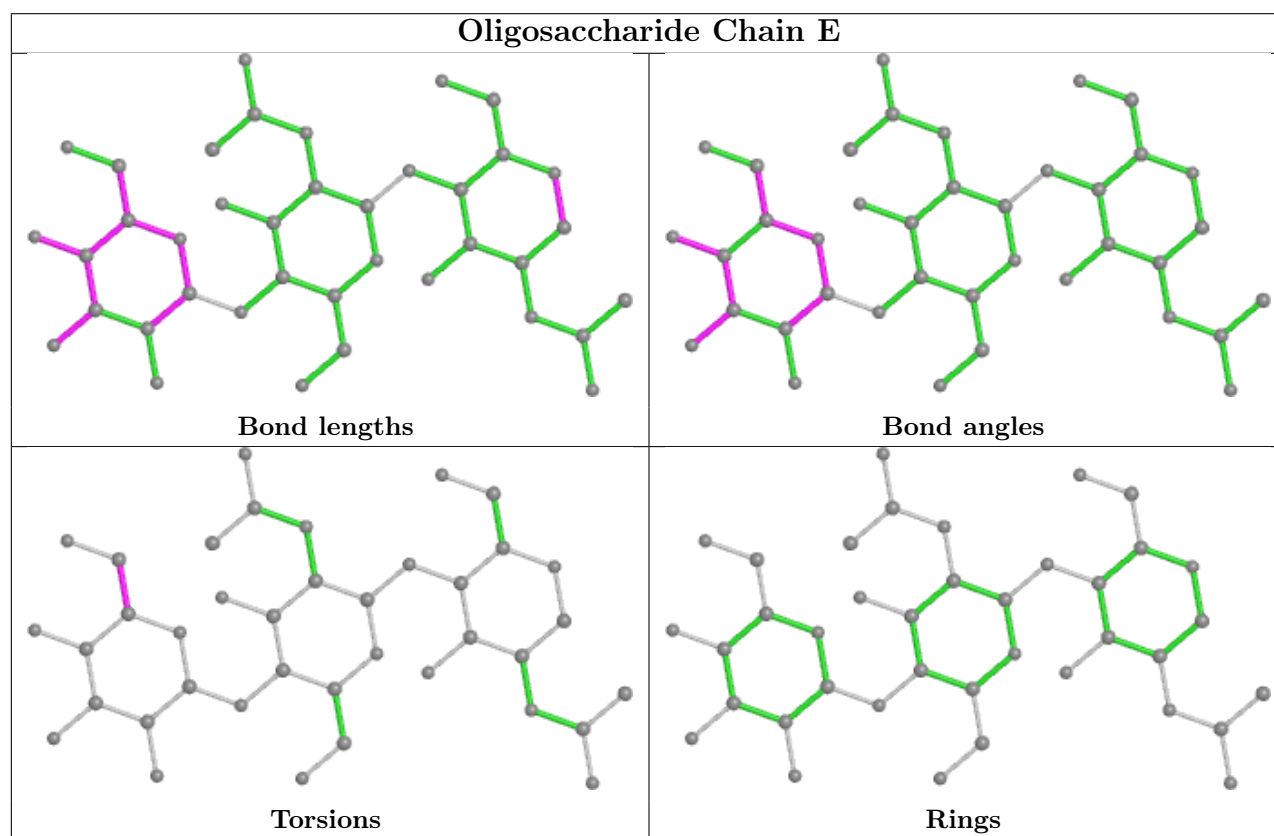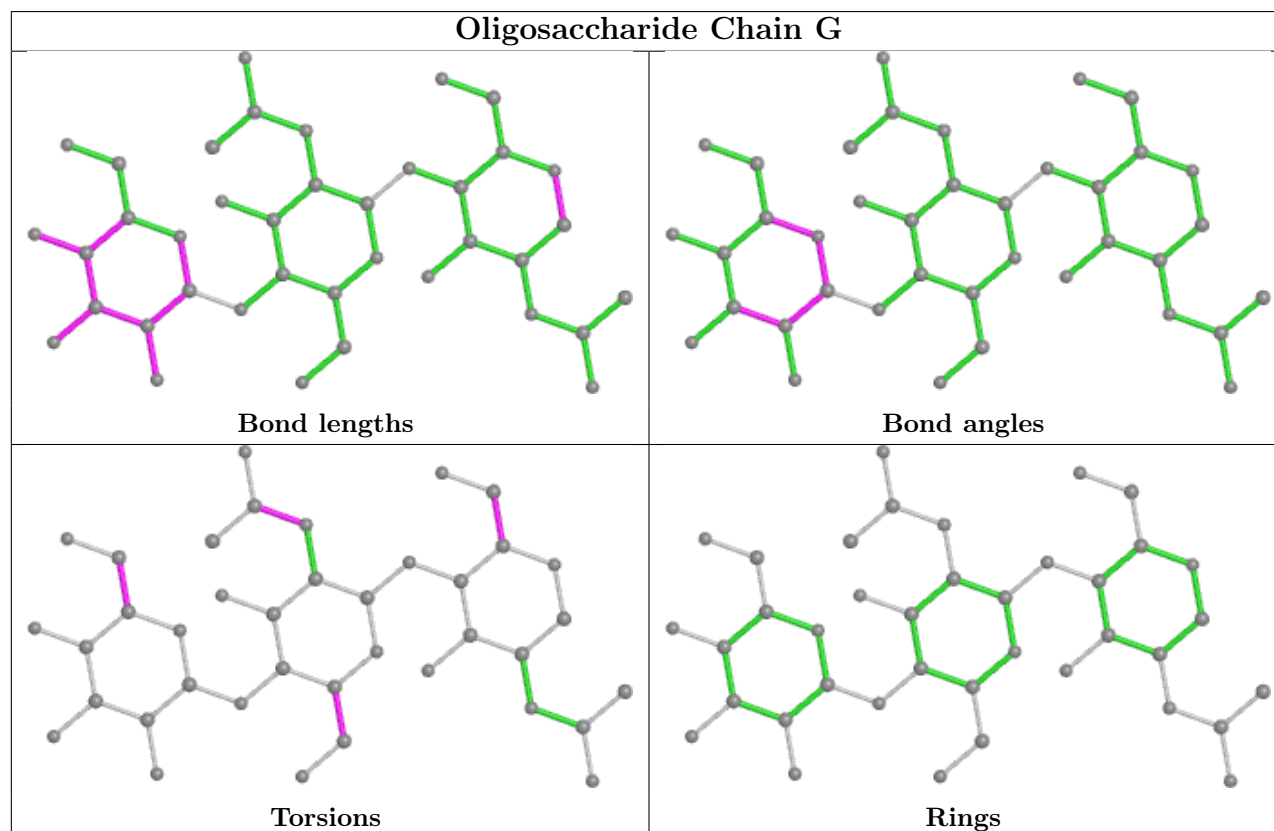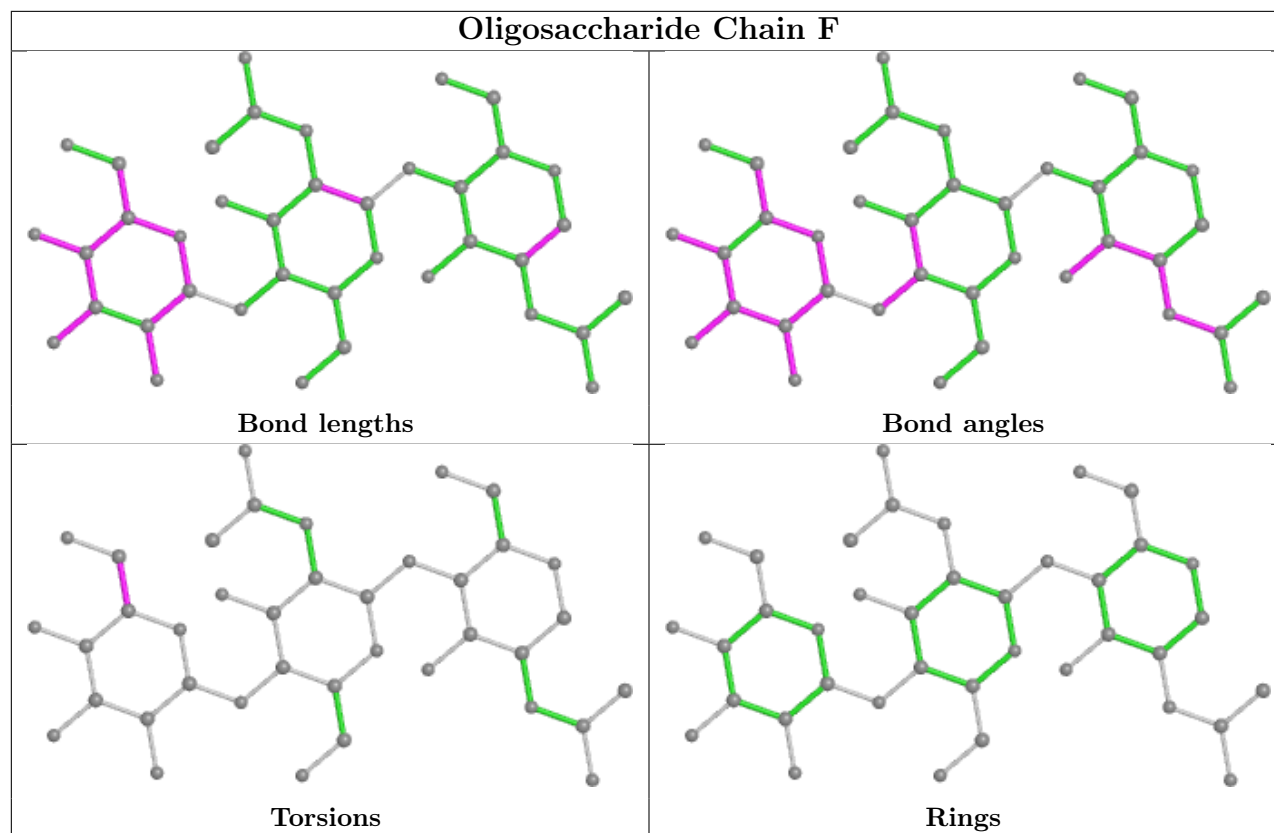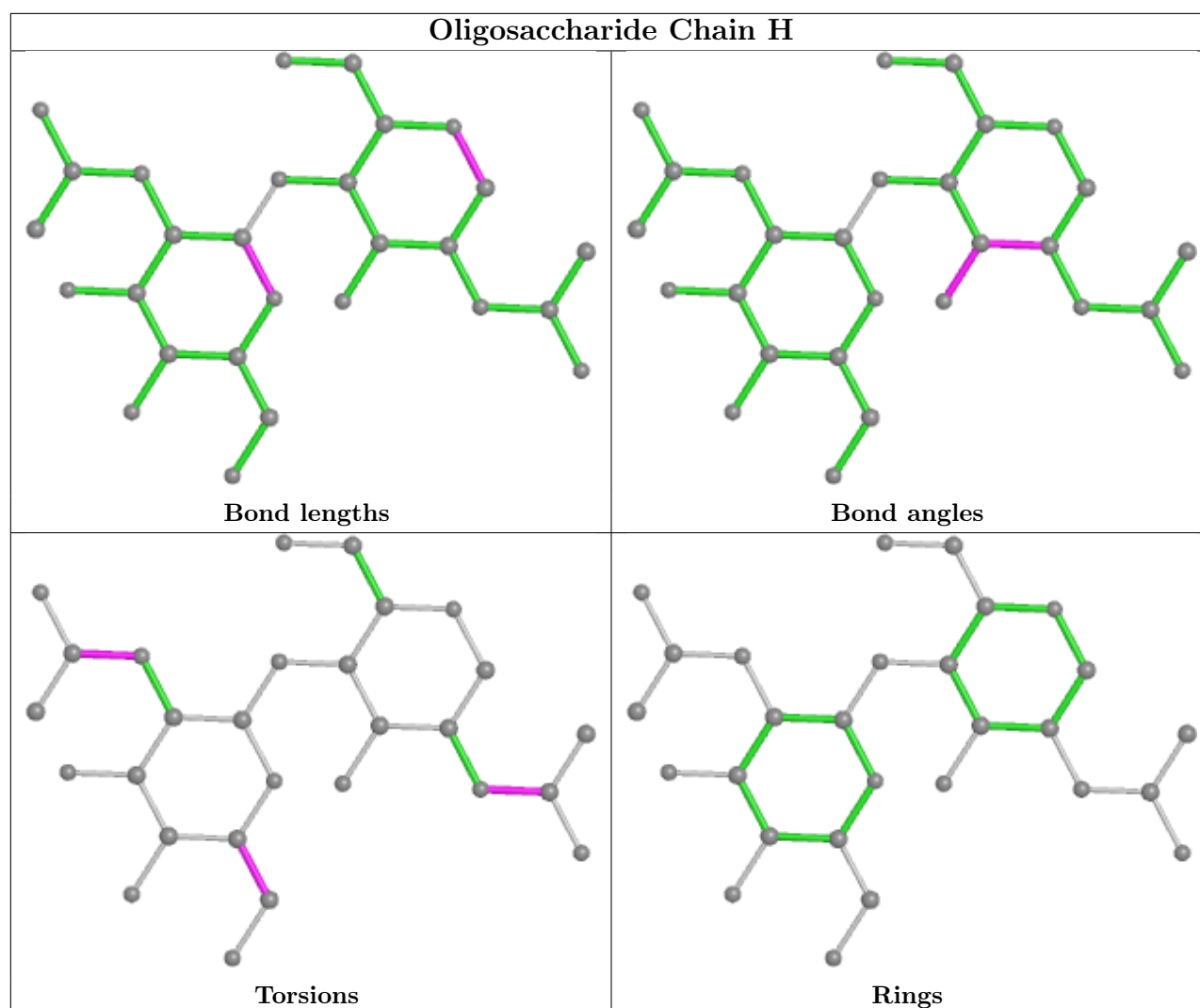
5.6　Ligand geometry (i)

7 ligands 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	$\#|Z| > 2$
5	NAG	A	701	1	14,14,15	2.18	1 (7%)	17,19,21	1.18	1 (5%)
5	NAG	B	701	1	14,14,15	1.60	1 (7%)	17,19,21	1.73	1 (5%)
5	NAG	A	703	1	14,14,15	1.96	2 (14%)	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
5	NAG	B	703	1	14,14,15	1.43	1 (7%)	17,19,21	0.74	0
5	NAG	A	702	1	14,14,15	1.40	2 (14%)	17,19,21	1.10	1 (5%)
5	NAG	B	702	1	14,14,15	1.67	1 (7%)	17,19,21	1.36	3 (17%)
5	NAG	B	704	1	14,14,15	1.28	1 (7%)	17,19,21	0.89	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
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	B	701	1	-	1/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	B	703	1	-	1/6/23/26	0/1/1/1
5	NAG	A	702	1	-	4/6/23/26	0/1/1/1
5	NAG	B	702	1	-	3/6/23/26	0/1/1/1
5	NAG	B	704	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	NAG	O5-C1	7.86	1.56	1.43
5	A	703	NAG	O5-C1	6.39	1.53	1.43
5	B	702	NAG	O5-C1	5.74	1.52	1.43
5	B	701	NAG	O5-C1	5.65	1.52	1.43
5	B	703	NAG	O5-C1	5.04	1.51	1.43
5	B	704	NAG	O5-C1	4.23	1.50	1.43
5	A	702	NAG	O5-C1	4.15	1.50	1.43
5	A	703	NAG	C1-C2	3.17	1.57	1.52
5	A	702	NAG	C1-C2	2.82	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	701	NAG	C1-O5-C5	6.33	120.76	112.19
5	A	701	NAG	C1-O5-C5	3.75	117.27	112.19
5	A	702	NAG	C1-O5-C5	3.68	117.18	112.19
5	B	702	NAG	C1-O5-C5	3.48	116.91	112.19
5	B	702	NAG	C2-N2-C7	2.25	126.11	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	702	NAG	O6-C6-C5	2.01	118.19	111.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	NAG	O5-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6
5	B	704	NAG	C8-C7-N2-C2
5	B	704	NAG	O7-C7-N2-C2
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	B	701	NAG	C1-C2-N2-C7
5	A	703	NAG	C4-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	A	702	NAG	C1-C2-N2-C7
5	B	702	NAG	O5-C5-C6-O6
5	B	703	NAG	O5-C5-C6-O6
5	B	702	NAG	C1-C2-N2-C7
5	B	702	NAG	C3-C2-N2-C7
5	A	702	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

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 E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
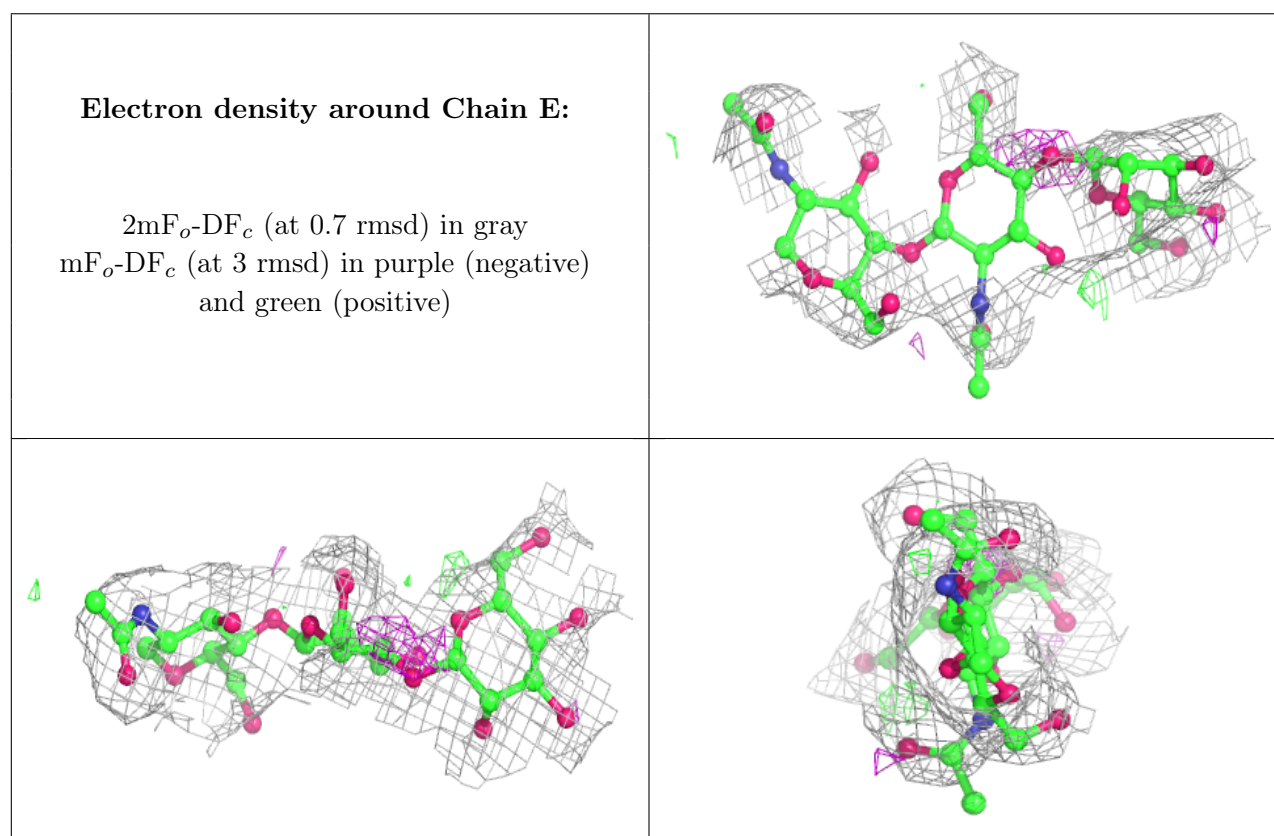
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
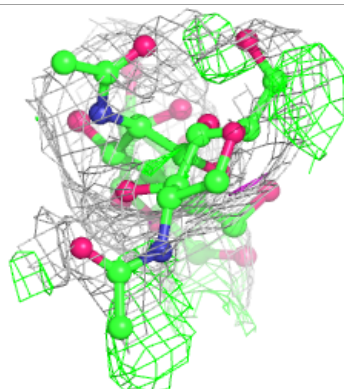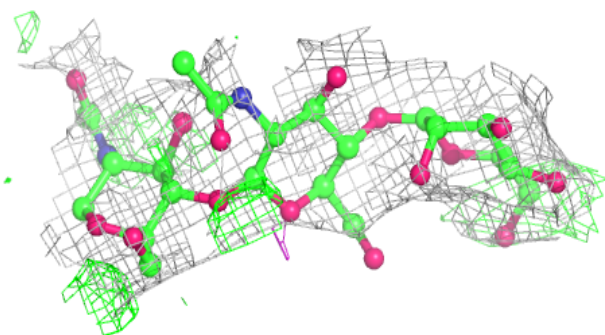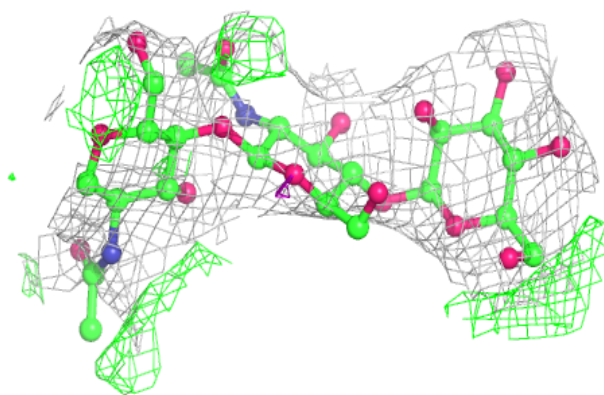
Electron density around Chain G:

$2mF_o$-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 H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
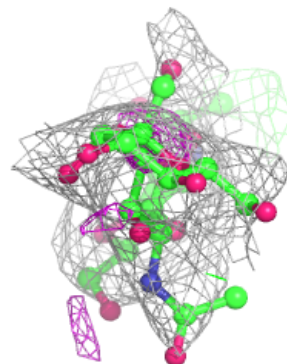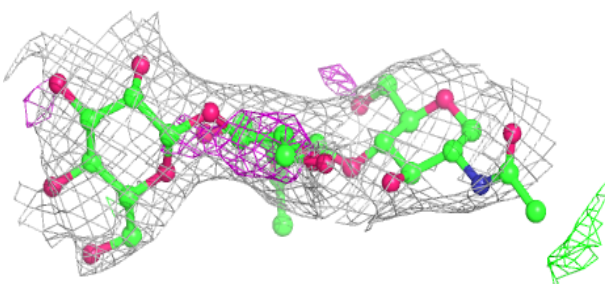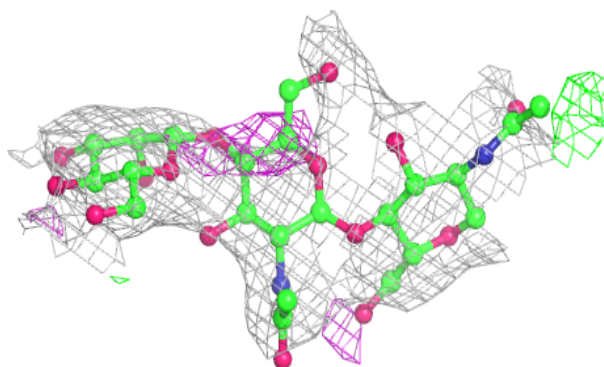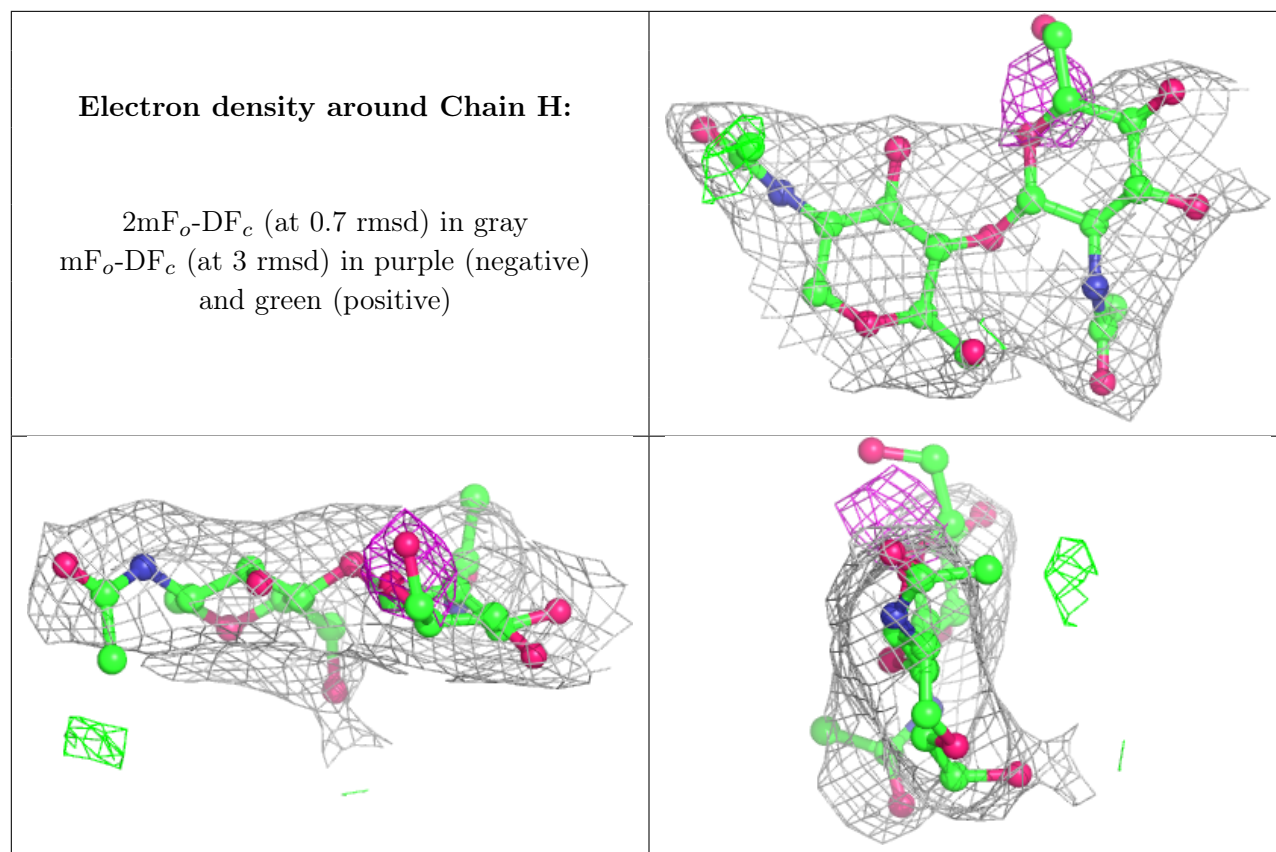
6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.