



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:18 AM EDT

PDB ID : 1OAN / pdb_00001oan
Title : Crystal structure of the dengue 2 virus envelope protein
Authors : Modis, Y.; Harrison, S.C.
Deposited on : 2003-01-16
Resolution : 2.75 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:

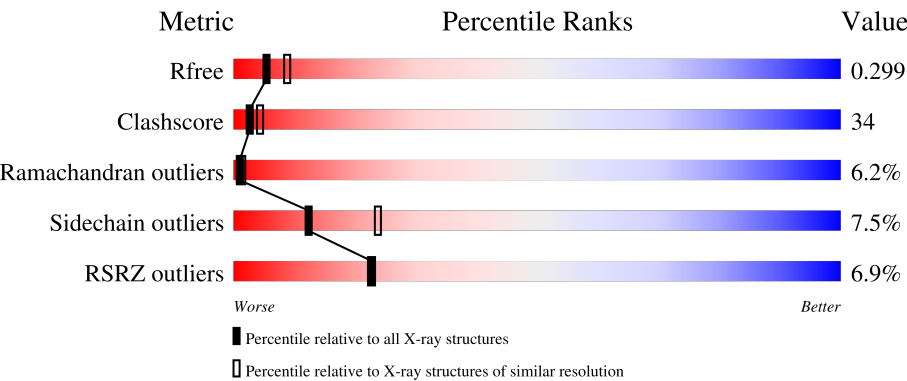
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	394	9% 47% 45% 7%
1	B	394	5% 43% 49% 6%
2	C	4	25% 50% 25%
2	D	4	25% 50% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	C	4	X	-	-	-
2	FUC	D	4	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6296 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.

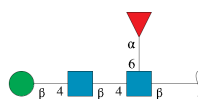
- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			
1	B	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLU	ASP	conflict	UNP P12823
A	390	ASN	ASP	conflict	UNP P12823
B	71	GLU	ASP	conflict	UNP P12823
B	390	ASN	ASP	conflict	UNP P12823

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

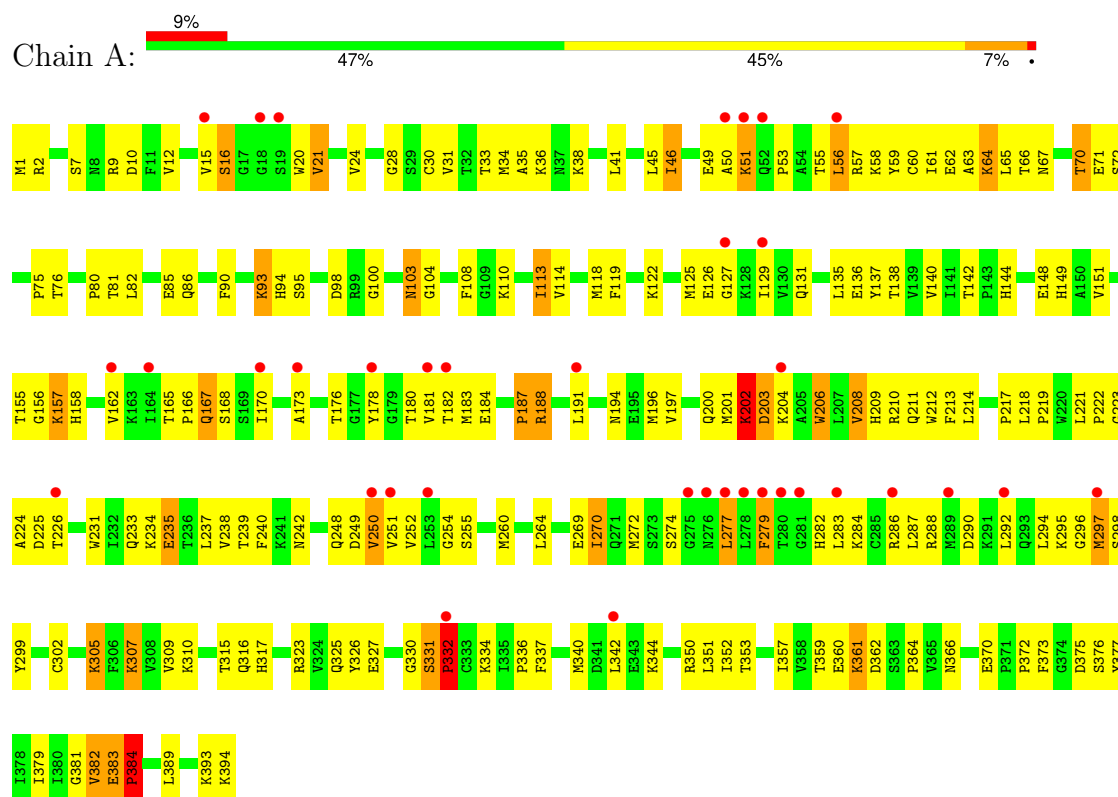
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	25	Total	O	0	0
			25	25		

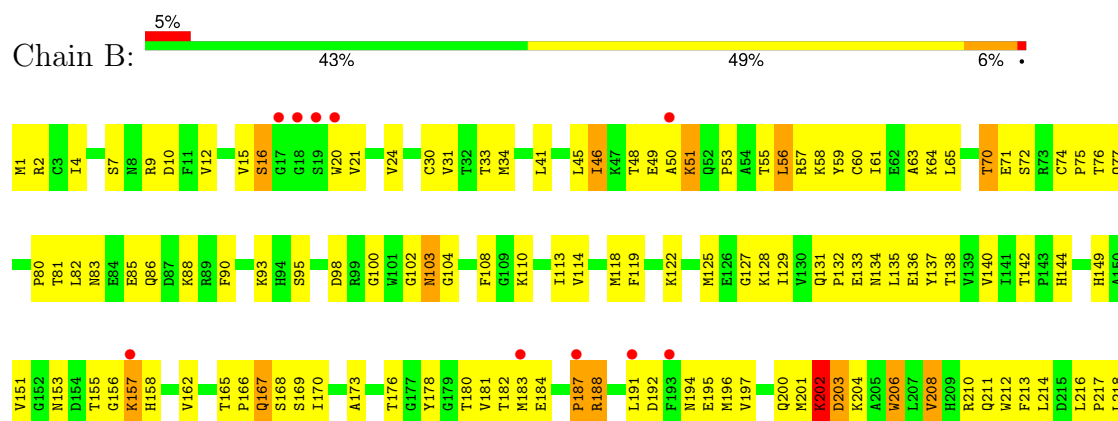
3 Residue-property plots [i](#)

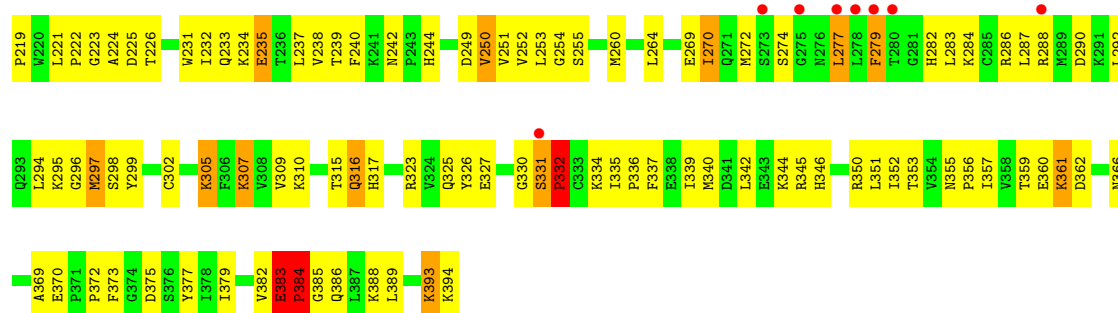
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ENVELOPE GLYCOPROTEIN





- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 25% 50% 25%



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 25% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.54Å 81.54Å 288.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.10 – 2.75 48.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.2 (48.10-2.75) 82.9 (48.10-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.261 , 0.296 0.265 , 0.299	Depositor DCC
R_{free} test set	1539 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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: BMA, NA, NAG, FUC

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	0.54	0/3124	1.03	14/4219 (0.3%)
1	B	0.55	0/3124	1.02	14/4219 (0.3%)
All	All	0.54	0/6248	1.02	28/8438 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	B	167	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	B	352	ILE	N-CA-C	-8.49	102.58	111.58
1	A	352	ILE	N-CA-C	-8.44	102.64	111.58
1	A	131	GLN	CA-C-N	8.34	130.27	119.84
1	A	131	GLN	C-N-CA	8.34	130.27	119.84
1	A	384	PRO	CA-N-CD	-7.27	101.83	112.00
1	B	167	GLN	CG-CD-NE2	7.18	127.17	116.40
1	A	167	GLN	CG-CD-NE2	6.97	126.85	116.40
1	A	51	LYS	N-CA-C	6.88	118.47	110.97
1	A	242	ASN	CA-C-N	6.69	126.47	119.05
1	A	242	ASN	C-N-CA	6.69	126.47	119.05
1	A	104	GLY	N-CA-C	6.29	123.10	114.92
1	B	242	ASN	CA-C-N	6.22	125.95	119.05
1	B	242	ASN	C-N-CA	6.22	125.95	119.05
1	B	226	THR	N-CA-C	-6.21	107.54	114.62
1	B	104	GLY	N-CA-C	6.11	122.86	114.92
1	B	384	PRO	CA-N-CD	-6.01	103.59	112.00
1	A	226	THR	N-CA-C	-5.96	107.82	114.62
1	B	51	LYS	N-CA-C	5.94	117.44	110.97
1	A	49	GLU	N-CA-C	5.83	118.03	108.52
1	B	49	GLU	N-CA-C	5.81	117.99	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	PHE	N-CA-C	-5.80	101.90	110.48
1	B	335	ILE	N-CA-C	5.35	113.16	107.76
1	B	194	ASN	N-CA-C	-5.26	106.92	113.55
1	A	194	ASN	N-CA-C	-5.18	107.03	113.55
1	B	373	PHE	N-CA-C	-5.13	102.89	110.48
1	B	393	LYS	N-CA-C	5.03	117.95	109.95

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	3062	0	3065	213	0
1	B	3062	0	3065	214	0
2	C	49	0	43	2	0
2	D	49	0	43	2	0
3	A	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	20	0	0	5	0
5	B	25	0	0	5	1
All	All	6296	0	6242	421	1

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 34.

All (421) 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:383:GLU:HB3	1:A:384:PRO:HD2	1.43	1.01
1:B:191:LEU:HD13	1:B:196:MET:HE3	1.44	0.99
1:B:323:ARG:HE	1:B:366:ASN:HD21	1.13	0.96
1:A:323:ARG:HE	1:A:366:ASN:HD21	1.09	0.95
1:A:191:LEU:HD13	1:A:196:MET:HE3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:HG22	1:B:288:ARG:HB2	1.56	0.87
1:B:344:LYS:HG3	5:B:2017:HOH:O	1.77	0.85
1:A:182:THR:HG22	1:A:288:ARG:HB2	1.57	0.85
1:A:71:GLU:HG2	1:A:81:THR:H	1.40	0.84
1:B:71:GLU:HG2	1:B:81:THR:H	1.41	0.84
1:A:323:ARG:NE	1:A:366:ASN:HD21	1.75	0.83
1:B:202:LYS:O	1:B:203:ASP:CG	2.25	0.79
1:B:345:ARG:HG2	1:B:346:HIS:CD2	2.17	0.79
1:A:125:MET:SD	1:A:260:MET:HE2	2.22	0.79
1:B:323:ARG:NE	1:B:366:ASN:HD21	1.79	0.79
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.13	0.79
1:A:342:LEU:HA	1:A:377:TYR:CE1	2.18	0.79
1:A:342:LEU:HD23	1:A:377:TYR:CE1	2.17	0.79
1:A:305:LYS:H	1:A:305:LYS:HZ2	1.32	0.77
1:A:56:LEU:HD22	1:A:213:PHE:HE2	1.49	0.77
1:A:269:GLU:O	1:A:270:ILE:HG13	1.85	0.77
1:A:56:LEU:HD21	1:A:214:LEU:HD21	1.68	0.75
1:B:296:GLY:C	1:B:298:SER:H	1.94	0.75
1:A:277:LEU:HB2	1:A:279:PHE:CE1	2.22	0.75
1:A:394:LYS:OXT	1:A:394:LYS:HD3	1.86	0.74
1:B:394:LYS:OXT	1:B:394:LYS:HD3	1.87	0.74
1:B:277:LEU:HB2	1:B:279:PHE:CE1	2.23	0.74
1:B:383:GLU:HB3	1:B:384:PRO:HD2	1.67	0.74
1:B:269:GLU:O	1:B:270:ILE:HG13	1.88	0.74
1:B:56:LEU:HD21	1:B:214:LEU:HD21	1.70	0.73
1:B:56:LEU:HD22	1:B:213:PHE:HE2	1.53	0.73
1:A:305:LYS:H	1:A:305:LYS:NZ	1.86	0.72
1:B:56:LEU:HD23	1:B:56:LEU:C	2.14	0.72
1:B:383:GLU:OE1	5:B:2022:HOH:O	2.07	0.72
1:A:165:THR:HB	1:A:168:SER:OG	1.89	0.72
1:B:217:PRO:O	1:B:218:LEU:HD23	1.90	0.71
1:B:125:MET:SD	1:B:260:MET:HE2	2.30	0.71
1:B:192:ASP:OD2	1:B:195:GLU:HG2	1.90	0.71
1:B:336:PRO:HG2	1:B:382:VAL:HG23	1.70	0.71
1:B:305:LYS:H	1:B:305:LYS:CE	2.03	0.71
1:A:359:THR:O	1:A:360:GLU:HG3	1.91	0.71
1:B:100:GLY:H	1:B:103:ASN:HD21	1.37	0.71
1:A:342:LEU:HD23	1:A:377:TYR:HE1	1.54	0.70
1:B:165:THR:HB	1:B:168:SER:OG	1.90	0.70
1:B:155:THR:HG22	1:B:157:LYS:H	1.57	0.70
1:A:20:TRP:HA	1:A:287:LEU:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:C	1:A:56:LEU:HD23	2.17	0.69
1:A:296:GLY:C	1:A:298:SER:H	1.99	0.69
1:B:240:PHE:CE1	1:B:250:VAL:HG22	2.27	0.69
1:A:98:ASP:OD2	1:B:7:SER:HB2	1.93	0.69
1:B:240:PHE:HE1	1:B:250:VAL:HG22	1.57	0.69
1:A:305:LYS:H	1:A:305:LYS:CE	2.05	0.69
1:B:305:LYS:H	1:B:305:LYS:NZ	1.90	0.69
1:A:155:THR:HG22	1:A:157:LYS:H	1.58	0.69
1:B:20:TRP:HA	1:B:287:LEU:O	1.92	0.68
1:A:100:GLY:H	1:A:103:ASN:HD21	1.39	0.68
1:A:204:LYS:HB3	1:A:206:TRP:CH2	2.28	0.68
1:B:305:LYS:N	1:B:305:LYS:HE3	2.08	0.67
1:B:206:TRP:H	1:B:206:TRP:HE3	1.43	0.67
1:B:359:THR:O	1:B:360:GLU:HG3	1.94	0.67
1:A:173:ALA:HB3	1:A:181:VAL:HG13	1.77	0.67
1:A:376:SER:C	1:A:377:TYR:CD1	2.73	0.67
1:A:71:GLU:HG3	1:A:80:PRO:HB3	1.75	0.67
1:B:20:TRP:CE3	1:B:286:ARG:HD2	2.30	0.67
1:A:20:TRP:CE3	1:A:286:ARG:HD2	2.31	0.66
1:B:344:LYS:NZ	1:B:344:LYS:HB3	2.10	0.66
1:B:71:GLU:HG3	1:B:80:PRO:HB3	1.76	0.66
1:B:206:TRP:N	1:B:206:TRP:CE3	2.64	0.66
1:B:337:PHE:CD2	1:B:351:LEU:HD21	2.31	0.66
1:B:344:LYS:HE3	1:B:388:LYS:HE3	1.77	0.66
1:B:170:ILE:HG13	1:B:184:GLU:HG3	1.77	0.66
1:A:305:LYS:HE3	1:A:305:LYS:N	2.11	0.65
1:B:305:LYS:H	1:B:305:LYS:HZ2	1.42	0.65
1:A:316:GLN:HE22	1:B:110:LYS:HE2	1.60	0.65
1:B:170:ILE:CG1	1:B:184:GLU:HG3	2.27	0.65
1:A:382:VAL:HG22	5:A:2018:HOH:O	1.96	0.64
1:B:82:LEU:O	1:B:85:GLU:HB2	1.97	0.64
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.27	0.64
1:A:240:PHE:CE1	1:A:250:VAL:HG22	2.32	0.64
1:A:206:TRP:CE3	1:A:206:TRP:N	2.67	0.63
1:B:286:ARG:HE	1:B:288:ARG:HH21	1.44	0.63
1:A:162:VAL:HG11	1:A:183:MET:CE	2.28	0.63
1:B:173:ALA:HB3	1:B:181:VAL:HG13	1.80	0.63
1:B:202:LYS:O	1:B:203:ASP:OD2	2.17	0.63
1:B:162:VAL:HG11	1:B:183:MET:CE	2.29	0.63
1:A:217:PRO:O	1:A:218:LEU:HD23	1.99	0.63
1:B:240:PHE:CE1	1:B:250:VAL:HG13	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CD2	1:B:283:LEU:HD22	2.34	0.63
1:A:206:TRP:HE3	1:A:206:TRP:H	1.47	0.63
1:A:286:ARG:HE	1:A:288:ARG:HH21	1.47	0.63
2:C:2:NAG:H4	2:C:3:BMA:O2	1.98	0.62
1:A:383:GLU:CB	1:A:384:PRO:CD	2.77	0.62
1:B:296:GLY:HA3	1:B:299:TYR:CE2	2.34	0.62
1:B:100:GLY:H	1:B:103:ASN:ND2	1.96	0.62
1:B:166:PRO:CG	1:B:187:PRO:HG3	2.30	0.62
1:A:240:PHE:HE1	1:A:250:VAL:HG22	1.65	0.62
1:B:297:MET:HA	1:B:334:LYS:NZ	2.15	0.61
1:A:24:VAL:HG22	1:A:284:LYS:HG2	1.81	0.61
1:A:100:GLY:H	1:A:103:ASN:ND2	1.98	0.61
1:A:127:GLY:HA3	1:A:213:PHE:CZ	2.35	0.61
1:B:24:VAL:HG22	1:B:284:LYS:HG2	1.81	0.61
1:B:127:GLY:HA3	1:B:213:PHE:CZ	2.35	0.61
1:A:170:ILE:CG1	1:A:184:GLU:HG3	2.31	0.61
2:D:2:NAG:H4	2:D:3:BMA:O2	1.99	0.61
1:A:166:PRO:CG	1:A:187:PRO:HG3	2.31	0.61
1:A:221:LEU:HD13	1:A:225:ASP:OD2	2.01	0.60
1:A:137:TYR:CD2	1:A:283:LEU:HD22	2.36	0.60
1:A:270:ILE:HG22	1:A:270:ILE:O	2.02	0.60
1:B:206:TRP:HE3	1:B:206:TRP:N	1.97	0.60
1:A:82:LEU:O	1:A:85:GLU:HB2	2.01	0.60
1:A:206:TRP:N	1:A:206:TRP:HE3	1.98	0.60
1:A:340:MET:HG3	1:A:379:ILE:HG13	1.82	0.60
1:B:182:THR:CG2	1:B:288:ARG:HB2	2.31	0.60
1:B:204:LYS:HB3	1:B:206:TRP:CH2	2.36	0.60
1:B:340:MET:HG3	1:B:379:ILE:HG13	1.84	0.60
1:A:20:TRP:HE3	1:A:286:ARG:HD2	1.67	0.60
1:B:56:LEU:HD23	1:B:56:LEU:O	2.02	0.60
1:A:71:GLU:HG2	1:A:81:THR:N	2.16	0.59
1:B:270:ILE:O	1:B:270:ILE:HG22	2.02	0.59
1:A:383:GLU:HA	1:A:383:GLU:OE1	2.03	0.58
1:B:162:VAL:HG11	1:B:183:MET:HE1	1.86	0.58
1:A:182:THR:CG2	1:A:288:ARG:HB2	2.30	0.58
1:A:323:ARG:HE	1:A:366:ASN:ND2	1.91	0.58
1:A:129:ILE:CD1	1:A:210:ARG:HH22	2.16	0.58
1:A:162:VAL:HG11	1:A:183:MET:HE1	1.85	0.58
1:A:206:TRP:NE1	1:A:264:LEU:HB3	2.18	0.58
1:B:383:GLU:OE1	1:B:383:GLU:HA	2.03	0.57
1:B:221:LEU:HD13	1:B:225:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:HE3	1:B:286:ARG:HD2	1.67	0.57
1:A:55:THR:O	1:A:223:GLY:HA3	2.04	0.57
1:A:297:MET:HA	1:A:334:LYS:NZ	2.19	0.57
1:A:50:ALA:HA	1:A:135:LEU:HD23	1.87	0.57
1:A:34:MET:SD	1:A:350:ARG:NH2	2.78	0.57
1:A:200:GLN:NE2	1:A:272:MET:HE3	2.20	0.57
1:B:296:GLY:HA3	1:B:299:TYR:CD2	2.40	0.57
1:B:50:ALA:HA	1:B:135:LEU:HD23	1.85	0.57
1:A:56:LEU:HD12	1:A:129:ILE:HD11	1.86	0.57
1:B:221:LEU:CD2	1:B:231:TRP:HA	2.35	0.57
1:A:53:PRO:HB3	1:A:129:ILE:O	2.04	0.56
1:A:65:LEU:HG	1:A:252:VAL:HG22	1.87	0.56
1:A:251:VAL:HG21	1:B:204:LYS:HE3	1.86	0.56
1:A:350:ARG:HD3	1:A:370:GLU:OE1	2.05	0.56
1:B:61:ILE:CG2	1:B:125:MET:HE2	2.35	0.56
1:A:7:SER:HB2	1:B:98:ASP:OD2	2.06	0.56
1:A:200:GLN:HE21	1:A:272:MET:HE3	1.68	0.56
1:B:55:THR:O	1:B:223:GLY:HA3	2.05	0.56
1:B:235:GLU:CD	1:B:235:GLU:H	2.12	0.56
1:B:202:LYS:HE2	1:B:202:LYS:HA	1.88	0.56
1:A:61:ILE:CG2	1:A:125:MET:HE2	2.36	0.56
1:A:235:GLU:H	1:A:235:GLU:CD	2.13	0.56
1:B:307:LYS:NZ	1:B:307:LYS:HB3	2.21	0.56
1:A:296:GLY:HA3	1:A:299:TYR:CE2	2.41	0.56
1:A:383:GLU:HG3	1:A:384:PRO:HD3	1.88	0.56
1:B:286:ARG:NE	1:B:288:ARG:HH21	2.04	0.56
1:B:296:GLY:C	1:B:298:SER:N	2.63	0.56
1:B:350:ARG:HD3	1:B:370:GLU:OE1	2.06	0.56
1:B:191:LEU:CD1	1:B:196:MET:HE3	2.28	0.55
1:B:305:LYS:CE	1:B:305:LYS:N	2.68	0.55
1:A:221:LEU:CD2	1:A:231:TRP:HA	2.37	0.55
1:B:129:ILE:CD1	1:B:210:ARG:HH22	2.18	0.55
1:A:98:ASP:CG	1:B:7:SER:HB2	2.31	0.55
1:B:9:ARG:HB3	1:B:317:HIS:CE1	2.41	0.55
1:A:151:VAL:HB	5:A:2009:HOH:O	2.07	0.55
1:A:202:LYS:O	1:A:203:ASP:CG	2.48	0.55
1:B:206:TRP:NE1	1:B:264:LEU:HB3	2.22	0.55
1:B:342:LEU:HD21	1:B:375:ASP:CB	2.37	0.55
1:A:305:LYS:CE	1:A:305:LYS:N	2.68	0.55
1:A:337:PHE:CD2	1:A:351:LEU:HD21	2.41	0.55
1:A:197:VAL:HG23	1:A:210:ARG:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG23	1:B:210:ARG:HA	1.88	0.54
1:A:307:LYS:HB3	1:A:307:LYS:NZ	2.22	0.54
1:A:234:LYS:O	1:A:238:VAL:HG23	2.07	0.54
1:A:240:PHE:CE1	1:A:250:VAL:HG13	2.43	0.54
1:A:70:THR:HA	1:A:82:LEU:HD11	1.90	0.54
1:A:165:THR:HB	1:A:168:SER:CB	2.38	0.54
1:B:53:PRO:HB3	1:B:129:ILE:O	2.07	0.54
1:B:344:LYS:HE3	1:B:388:LYS:CE	2.38	0.54
1:B:200:GLN:HE21	1:B:272:MET:HE3	1.72	0.53
1:A:1:MET:HG3	1:A:144:HIS:HA	1.90	0.53
1:B:221:LEU:HD21	1:B:231:TRP:HA	1.90	0.53
1:A:286:ARG:NE	1:A:288:ARG:HH21	2.06	0.53
1:A:342:LEU:HD23	1:A:377:TYR:OH	2.09	0.53
1:B:223:GLY:C	1:B:225:ASP:H	2.17	0.53
1:B:65:LEU:HG	1:B:252:VAL:HG22	1.91	0.53
1:B:80:PRO:HG2	1:B:113:ILE:CA	2.39	0.53
1:B:34:MET:SD	1:B:350:ARG:NH2	2.82	0.53
1:A:155:THR:CG2	1:A:157:LYS:HG3	2.39	0.53
1:B:1:MET:HG3	1:B:144:HIS:HA	1.90	0.53
1:B:56:LEU:HD12	1:B:129:ILE:HD11	1.90	0.52
1:B:165:THR:HB	1:B:168:SER:HG	1.74	0.52
1:B:344:LYS:HB3	1:B:344:LYS:HZ3	1.73	0.52
1:B:165:THR:HB	1:B:168:SER:CB	2.39	0.52
1:A:165:THR:HG22	1:A:167:GLN:H	1.75	0.52
1:A:223:GLY:C	1:A:225:ASP:H	2.17	0.52
1:B:336:PRO:HG2	1:B:382:VAL:CG2	2.37	0.52
1:A:204:LYS:HE3	1:B:251:VAL:HG21	1.92	0.52
1:B:64:LYS:HB2	1:B:122:LYS:HD2	1.91	0.52
1:A:202:LYS:O	1:A:203:ASP:OD2	2.27	0.52
1:B:90:PHE:CZ	1:B:118:MET:HB2	2.44	0.52
1:B:114:VAL:O	1:B:114:VAL:HG13	2.10	0.52
1:A:64:LYS:HB2	1:A:122:LYS:HD2	1.92	0.51
1:B:155:THR:CG2	1:B:157:LYS:HG3	2.39	0.51
1:A:80:PRO:HG2	1:A:113:ILE:CA	2.41	0.51
1:A:296:GLY:HA3	1:A:299:TYR:CD2	2.46	0.51
1:B:165:THR:HG22	1:B:167:GLN:H	1.75	0.51
1:B:57:ARG:HG2	1:B:58:LYS:N	2.26	0.51
1:B:331:SER:CB	1:B:332:PRO:CD	2.88	0.51
1:A:296:GLY:C	1:A:298:SER:N	2.68	0.51
1:A:221:LEU:HD21	1:A:231:TRP:HA	1.92	0.51
1:A:381:GLY:HA2	5:A:2018:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD12	1:B:138:THR:O	2.11	0.51
1:B:70:THR:HA	1:B:82:LEU:HD11	1.93	0.51
1:B:166:PRO:HG2	1:B:187:PRO:HG3	1.93	0.51
1:A:166:PRO:HB3	1:A:187:PRO:HD3	1.92	0.51
1:A:170:ILE:HG13	1:A:184:GLU:HG3	1.93	0.51
1:B:56:LEU:C	1:B:56:LEU:CD2	2.82	0.51
1:A:56:LEU:HD23	1:A:56:LEU:O	2.11	0.50
1:B:234:LYS:O	1:B:238:VAL:HG23	2.11	0.50
1:A:28:GLY:HA3	1:B:244:HIS:CD2	2.46	0.50
1:A:166:PRO:HG2	1:A:187:PRO:HG3	1.93	0.50
1:A:342:LEU:HD23	1:A:377:TYR:CZ	2.45	0.50
1:A:90:PHE:CZ	1:A:118:MET:HB2	2.47	0.50
1:A:9:ARG:HB3	1:A:317:HIS:CE1	2.47	0.50
1:A:80:PRO:HB2	1:A:114:VAL:HG12	1.94	0.50
1:A:239:THR:HB	1:A:251:VAL:CG1	2.42	0.50
1:A:342:LEU:HD21	1:A:375:ASP:CB	2.41	0.50
1:A:45:LEU:HD12	1:A:138:THR:O	2.11	0.50
1:B:71:GLU:HG2	1:B:81:THR:N	2.18	0.50
1:A:63:ALA:O	1:A:252:VAL:HG11	2.12	0.50
1:A:100:GLY:HA3	1:A:108:PHE:CD1	2.47	0.50
1:A:114:VAL:HG13	1:A:114:VAL:O	2.12	0.50
1:B:100:GLY:HA3	1:B:108:PHE:CD1	2.46	0.50
1:B:239:THR:HB	1:B:251:VAL:CG1	2.42	0.50
1:A:307:LYS:HB3	1:A:307:LYS:HZ3	1.76	0.49
1:A:219:PRO:HG2	1:A:237:LEU:HD12	1.95	0.49
1:B:170:ILE:HD12	1:B:170:ILE:N	2.28	0.49
1:B:46:ILE:CG1	1:B:140:VAL:HG23	2.43	0.49
1:A:202:LYS:HE2	1:A:202:LYS:HA	1.95	0.48
1:B:166:PRO:HB3	1:B:187:PRO:HD3	1.94	0.48
1:B:173:ALA:O	1:B:180:THR:HG23	2.12	0.48
1:B:200:GLN:NE2	1:B:272:MET:HE3	2.29	0.48
1:A:277:LEU:HD12	1:A:277:LEU:H	1.79	0.48
1:A:46:ILE:CG1	1:A:140:VAL:HG23	2.44	0.48
1:B:95:SER:HB3	1:B:113:ILE:CG2	2.43	0.48
1:A:56:LEU:C	1:A:56:LEU:CD2	2.85	0.48
1:A:57:ARG:HG2	1:A:58:LYS:N	2.29	0.48
1:A:340:MET:HE3	1:A:344:LYS:C	2.38	0.48
1:B:131:GLN:HG3	1:B:134:ASN:HD22	1.78	0.48
1:B:197:VAL:CG2	1:B:210:ARG:HA	2.44	0.48
1:B:202:LYS:HE2	1:B:202:LYS:CA	2.44	0.48
1:A:110:LYS:HE2	1:B:316:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:HG12	1:B:140:VAL:HG23	1.96	0.48
1:A:331:SER:CB	1:A:332:PRO:CD	2.92	0.48
1:A:75:PRO:O	1:A:76:THR:OG1	2.23	0.47
1:B:131:GLN:HB2	1:B:133:GLU:OE1	2.14	0.47
1:B:277:LEU:HD12	1:B:277:LEU:H	1.79	0.47
1:A:173:ALA:HB3	1:A:181:VAL:CG1	2.43	0.47
1:A:309:VAL:CG2	1:A:325:GLN:HB2	2.44	0.47
1:B:233:GLN:HA	1:B:235:GLU:OE2	2.14	0.47
1:A:95:SER:HB3	1:A:113:ILE:CG2	2.44	0.47
1:A:197:VAL:CG2	1:A:210:ARG:HA	2.45	0.47
1:B:201:MET:O	1:B:203:ASP:N	2.47	0.47
1:B:342:LEU:HD21	1:B:375:ASP:HB2	1.95	0.47
1:B:345:ARG:NH1	1:B:345:ARG:HB2	2.29	0.47
1:B:251:VAL:HG22	1:B:252:VAL:N	2.30	0.47
1:A:56:LEU:HB2	1:A:129:ILE:HG13	1.97	0.47
1:A:51:LYS:HE3	1:A:136:GLU:HB2	1.96	0.47
1:B:309:VAL:CG2	1:B:325:GLN:HB2	2.44	0.47
1:B:383:GLU:O	1:B:385:GLY:N	2.48	0.47
1:A:59:TYR:HB2	1:A:125:MET:HE3	1.96	0.47
1:A:204:LYS:HB3	1:A:206:TRP:CZ3	2.49	0.47
1:A:233:GLN:HA	1:A:235:GLU:OE2	2.14	0.47
1:A:269:GLU:C	1:A:270:ILE:HG13	2.40	0.47
1:B:51:LYS:HE3	1:B:136:GLU:HB2	1.96	0.47
1:A:309:VAL:HG21	1:A:325:GLN:HB2	1.97	0.47
1:B:307:LYS:HB3	1:B:307:LYS:HZ3	1.78	0.47
1:A:208:VAL:HG21	1:A:212:TRP:CZ3	2.50	0.46
1:A:342:LEU:HD21	1:A:375:ASP:HB2	1.97	0.46
1:B:59:TYR:HB2	1:B:125:MET:HE3	1.97	0.46
1:B:156:GLY:C	1:B:158:HIS:H	2.24	0.46
1:A:377:TYR:CD1	1:A:377:TYR:N	2.83	0.46
1:B:72:SER:HB3	1:B:113:ILE:HG13	1.96	0.46
1:B:372:PRO:O	5:B:2020:HOH:O	2.21	0.46
1:A:155:THR:HG22	1:A:157:LYS:HG3	1.96	0.46
1:B:155:THR:HG22	1:B:157:LYS:HG3	1.98	0.46
1:A:119:PHE:CB	1:A:234:LYS:HD2	2.45	0.46
1:A:156:GLY:C	1:A:158:HIS:H	2.23	0.46
1:B:57:ARG:CG	1:B:58:LYS:N	2.79	0.46
1:B:65:LEU:HD11	1:B:238:VAL:HG13	1.98	0.46
1:B:83:ASN:ND2	5:B:2003:HOH:O	2.47	0.46
1:A:208:VAL:HG21	1:A:212:TRP:HZ3	1.81	0.46
1:B:309:VAL:HG21	1:B:325:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HB	1:A:251:VAL:HG12	1.98	0.46
1:A:360:GLU:O	1:A:362:ASP:N	2.49	0.46
1:B:60:CYS:HB2	1:B:231:TRP:CZ3	2.51	0.46
1:B:169:SER:C	1:B:170:ILE:HD12	2.41	0.46
1:A:60:CYS:HB2	1:A:231:TRP:CZ3	2.51	0.45
1:B:221:LEU:HG	1:B:231:TRP:CE3	2.51	0.45
1:A:170:ILE:HG12	1:A:184:GLU:HG3	1.98	0.45
1:B:119:PHE:CB	1:B:234:LYS:HD2	2.45	0.45
1:A:173:ALA:O	1:A:180:THR:HG23	2.15	0.45
1:A:206:TRP:CD1	1:A:264:LEU:HB3	2.50	0.45
1:A:296:GLY:O	1:A:299:TYR:HD2	2.00	0.45
1:B:15:VAL:O	1:B:16:SER:C	2.59	0.45
1:B:173:ALA:HB3	1:B:181:VAL:CG1	2.46	0.45
1:A:310:LYS:HB3	1:A:323:ARG:HB3	1.97	0.45
1:B:131:GLN:O	1:B:132:PRO:C	2.60	0.45
1:B:63:ALA:O	1:B:252:VAL:HG11	2.17	0.45
1:A:201:MET:O	1:A:203:ASP:N	2.50	0.45
1:B:269:GLU:C	1:B:270:ILE:HG13	2.42	0.45
1:B:323:ARG:HE	1:B:366:ASN:ND2	1.96	0.45
1:B:339:ILE:HA	1:B:377:TYR:O	2.17	0.45
1:A:36:LYS:O	1:A:38:LYS:HG2	2.17	0.45
1:A:65:LEU:HD11	1:A:238:VAL:HG13	1.99	0.45
1:A:251:VAL:HG22	1:A:252:VAL:N	2.32	0.45
1:B:208:VAL:HG21	1:B:212:TRP:HZ3	1.82	0.45
1:A:95:SER:HB2	1:A:248:GLN:NE2	2.32	0.44
1:A:302:CYS:HB3	1:A:326:TYR:CZ	2.52	0.44
1:B:41:LEU:HD11	1:B:292:LEU:HD11	1.99	0.44
1:A:360:GLU:O	1:A:361:LYS:C	2.61	0.44
1:B:208:VAL:HG21	1:B:212:TRP:CZ3	2.52	0.44
1:A:296:GLY:O	1:A:299:TYR:CD2	2.70	0.44
1:A:336:PRO:HG2	5:A:2018:HOH:O	2.17	0.44
1:B:7:SER:O	1:B:317:HIS:CE1	2.71	0.44
1:B:372:PRO:O	1:B:393:LYS:HB3	2.18	0.44
1:A:35:ALA:O	1:A:36:LYS:C	2.60	0.44
1:B:219:PRO:HG2	1:B:237:LEU:HD12	2.00	0.44
1:B:240:PHE:HA	1:B:249:ASP:O	2.18	0.44
1:A:302:CYS:SG	1:A:334:LYS:O	2.75	0.44
1:B:178:TYR:CE1	1:B:295:LYS:HE3	2.52	0.44
1:B:239:THR:HB	1:B:251:VAL:HG12	1.99	0.43
1:B:377:TYR:HB3	1:B:379:ILE:HD11	2.00	0.43
1:A:93:LYS:NZ	5:A:2007:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:HG2	1:A:122:LYS:HB2	2.01	0.43
1:B:360:GLU:O	1:B:361:LYS:C	2.62	0.43
1:A:46:ILE:HG12	1:A:140:VAL:HG23	2.01	0.43
1:A:334:LYS:HG2	1:A:357:ILE:HG22	2.00	0.43
1:A:210:ARG:O	1:A:213:PHE:HB3	2.19	0.43
1:A:72:SER:HB3	1:A:113:ILE:HG13	2.01	0.43
1:A:353:THR:O	1:A:353:THR:HG22	2.19	0.43
1:A:12:VAL:O	1:A:33:THR:HA	2.18	0.43
1:A:221:LEU:HG	1:A:231:TRP:CE3	2.54	0.43
1:B:12:VAL:O	1:B:33:THR:HA	2.18	0.43
1:B:80:PRO:HB2	1:B:114:VAL:HG12	2.00	0.43
1:B:151:VAL:HB	5:B:2010:HOH:O	2.18	0.43
1:A:327:GLU:C	1:A:361:LYS:HE3	2.44	0.43
1:B:59:TYR:CD1	1:B:218:LEU:HB2	2.53	0.43
1:A:191:LEU:CD1	1:A:196:MET:HE3	2.35	0.42
1:A:10:ASP:O	1:A:31:VAL:HA	2.18	0.42
1:A:41:LEU:HD11	1:A:292:LEU:HD11	2.00	0.42
1:A:327:GLU:O	1:A:361:LYS:HE3	2.19	0.42
1:B:10:ASP:O	1:B:31:VAL:HA	2.19	0.42
1:B:383:GLU:CB	1:B:384:PRO:CD	2.96	0.42
1:B:302:CYS:HB3	1:B:326:TYR:CZ	2.54	0.42
1:B:310:LYS:HB3	1:B:323:ARG:HB3	2.00	0.42
1:B:331:SER:HB2	1:B:332:PRO:CD	2.49	0.42
1:A:218:LEU:O	1:A:219:PRO:C	2.63	0.42
1:B:74:CYS:HB2	1:B:77:GLN:HG3	2.01	0.42
1:B:201:MET:C	1:B:203:ASP:H	2.27	0.42
1:B:360:GLU:O	1:B:362:ASP:N	2.52	0.42
1:A:95:SER:C	1:A:113:ILE:HG22	2.45	0.42
1:A:222:PRO:O	1:A:225:ASP:HB2	2.20	0.42
1:B:75:PRO:O	1:B:76:THR:OG1	2.28	0.42
1:B:327:GLU:C	1:B:361:LYS:HE3	2.45	0.42
1:B:355:ASN:N	1:B:356:PRO:HD3	2.34	0.42
1:A:206:TRP:CD2	1:A:264:LEU:HD13	2.55	0.42
1:A:57:ARG:CG	1:A:58:LYS:N	2.83	0.42
1:A:85:GLU:OE1	1:A:94:HIS:NE2	2.31	0.42
1:A:178:TYR:CE1	1:A:295:LYS:HE3	2.54	0.42
1:A:331:SER:O	1:A:332:PRO:C	2.61	0.42
1:A:148:GLU:CD	1:A:364:PRO:HD2	2.45	0.42
1:A:188:ARG:CZ	1:A:284:LYS:HD2	2.50	0.42
1:A:360:GLU:C	1:A:362:ASP:N	2.77	0.42
1:B:296:GLY:O	1:B:299:TYR:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ILE:HD11	1:B:369:ALA:HB1	2.02	0.42
1:B:56:LEU:HB2	1:B:129:ILE:HG13	2.02	0.42
1:B:57:ARG:CG	1:B:58:LYS:H	2.32	0.42
1:A:15:VAL:O	1:A:16:SER:C	2.63	0.42
1:A:59:TYR:CD1	1:A:218:LEU:HB2	2.55	0.42
1:B:327:GLU:O	1:B:361:LYS:HE3	2.20	0.42
1:B:331:SER:CB	1:B:332:PRO:HD2	2.49	0.42
1:A:12:VAL:HG12	1:A:21:VAL:HG11	2.01	0.41
1:A:119:PHE:HB3	1:A:234:LYS:HD2	2.02	0.41
1:B:149:HIS:O	1:B:153:ASN:HB2	2.20	0.41
1:B:188:ARG:CZ	1:B:284:LYS:HD2	2.50	0.41
1:A:170:ILE:N	1:A:170:ILE:HD12	2.36	0.41
1:B:119:PHE:HB3	1:B:234:LYS:HD2	2.02	0.41
1:B:149:HIS:HB3	2:D:1:NAG:H2	2.01	0.41
1:B:334:LYS:HG2	1:B:357:ILE:HG22	2.03	0.41
1:A:66:THR:O	1:A:67:ASN:C	2.64	0.41
1:A:315:THR:C	1:A:317:HIS:H	2.29	0.41
1:B:315:THR:C	1:B:317:HIS:H	2.28	0.41
1:B:48:THR:O	1:B:279:PHE:CE1	2.73	0.41
1:B:206:TRP:CD1	1:B:264:LEU:HB3	2.56	0.41
1:B:232:ILE:HG22	1:B:233:GLN:HG3	2.02	0.41
1:B:331:SER:O	1:B:332:PRO:C	2.63	0.41
1:B:379:ILE:CG2	1:B:386:GLN:CD	2.94	0.41
1:A:202:LYS:HE2	1:A:202:LYS:CA	2.51	0.41
1:A:240:PHE:HA	1:A:249:ASP:O	2.21	0.41
1:A:331:SER:CB	1:A:332:PRO:HD2	2.51	0.41
1:A:359:THR:O	1:A:360:GLU:CG	2.65	0.41
1:B:206:TRP:CD2	1:B:264:LEU:HD13	2.56	0.41
1:B:210:ARG:O	1:B:213:PHE:HB3	2.20	0.41
1:B:238:VAL:CG1	1:B:250:VAL:HG12	2.51	0.41
1:B:296:GLY:O	1:B:299:TYR:CD2	2.74	0.41
1:A:173:ALA:O	1:A:180:THR:HA	2.21	0.41
1:A:372:PRO:O	1:A:393:LYS:HB3	2.21	0.41
1:B:184:GLU:HB3	1:B:286:ARG:HB3	2.02	0.41
1:B:213:PHE:O	1:B:216:LEU:HG	2.20	0.41
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.96	0.41
1:A:66:THR:OG1	1:A:118:MET:HE2	2.21	0.40
1:A:51:LYS:HE3	1:A:136:GLU:CB	2.51	0.40
1:A:382:VAL:O	1:A:383:GLU:C	2.65	0.40
1:B:128:LYS:O	1:B:197:VAL:HG13	2.21	0.40
1:A:129:ILE:HD11	1:A:210:ARG:HH22	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:N	1:A:103:ASN:HD21	2.14	0.40
1:A:149:HIS:HB3	2:C:1:NAG:H2	2.03	0.40
1:A:188:ARG:HH11	1:A:188:ARG:HB2	1.86	0.40
1:A:221:LEU:HD23	1:A:231:TRP:HA	2.04	0.40
1:B:222:PRO:O	1:B:225:ASP:HB2	2.22	0.40
1:B:353:THR:O	1:B:353:THR:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2003:HOH:O	5:B:2003:HOH:O[6_555]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/394 (100%)	321 (82%)	48 (12%)	23 (6%)	1	1
1	B	392/394 (100%)	318 (81%)	48 (12%)	26 (7%)	1	1
All	All	784/788 (100%)	639 (82%)	96 (12%)	49 (6%)	1	1

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	THR
1	A	187	PRO
1	A	202	LYS
1	A	383	GLU
1	B	176	THR
1	B	187	PRO
1	B	202	LYS

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Mol	Chain	Res	Type
1	B	383	GLU
1	A	16	SER
1	A	203	ASP
1	A	224	ALA
1	A	254	GLY
1	A	270	ILE
1	A	279	PHE
1	A	330	GLY
1	A	331	SER
1	A	361	LYS
1	B	16	SER
1	B	203	ASP
1	B	224	ALA
1	B	254	GLY
1	B	270	ILE
1	B	279	PHE
1	B	330	GLY
1	B	331	SER
1	A	274	SER
1	A	282	HIS
1	A	332	PRO
1	A	384	PRO
1	B	274	SER
1	B	282	HIS
1	B	332	PRO
1	B	361	LYS
1	B	384	PRO
1	A	157	LYS
1	A	255	SER
1	A	294	LEU
1	B	46	ILE
1	B	157	LYS
1	B	294	LEU
1	B	297	MET
1	A	46	ILE
1	A	297	MET
1	B	88	LYS
1	A	126	GLU
1	B	255	SER
1	B	316	GLN
1	B	102	GLY
1	B	4	ILE

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	342/342 (100%)	315 (92%)	27 (8%)	11	21
1	B	342/342 (100%)	318 (93%)	24 (7%)	14	26
All	All	684/684 (100%)	633 (92%)	51 (8%)	12	24

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	21	VAL
1	A	30	CYS
1	A	56	LEU
1	A	64	LYS
1	A	70	THR
1	A	86	GLN
1	A	93	LYS
1	A	103	ASN
1	A	113	ILE
1	A	142	THR
1	A	188	ARG
1	A	202	LYS
1	A	206	TRP
1	A	208	VAL
1	A	209	HIS
1	A	211	GLN
1	A	235	GLU
1	A	250	VAL
1	A	277	LEU
1	A	290	ASP
1	A	305	LYS
1	A	307	LYS
1	A	332	PRO
1	A	382	VAL
1	A	384	PRO
1	A	389	LEU

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Mol	Chain	Res	Type
1	B	2	ARG
1	B	21	VAL
1	B	30	CYS
1	B	56	LEU
1	B	70	THR
1	B	86	GLN
1	B	93	LYS
1	B	103	ASN
1	B	142	THR
1	B	188	ARG
1	B	202	LYS
1	B	206	TRP
1	B	208	VAL
1	B	211	GLN
1	B	235	GLU
1	B	250	VAL
1	B	277	LEU
1	B	290	ASP
1	B	305	LYS
1	B	307	LYS
1	B	332	PRO
1	B	383	GLU
1	B	384	PRO
1	B	389	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	77	GLN
1	A	86	GLN
1	A	103	ASN
1	A	131	GLN
1	A	149	HIS
1	A	167	GLN
1	A	200	GLN
1	A	244	HIS
1	A	248	GLN
1	A	256	GLN
1	A	276	ASN
1	A	316	GLN
1	A	366	ASN

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	83	ASN
1	B	86	GLN
1	B	103	ASN
1	B	131	GLN
1	B	134	ASN
1	B	149	HIS
1	B	200	GLN
1	B	244	HIS
1	B	248	GLN
1	B	256	GLN
1	B	316	GLN
1	B	317	HIS
1	B	366	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.70	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	1.02	1 (5%)
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	0.37	0
2	FUC	C	4	2	10,10,11	0.40	0	14,14,16	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2,1	14,14,15	0.63	0	17,19,21	0.63	0
2	NAG	D	2	2	14,14,15	0.75	0	17,19,21	1.03	1 (5%)
2	BMA	D	3	2	11,11,12	0.63	0	15,15,17	0.34	0
2	FUC	D	4	2	10,10,11	0.47	0	14,14,16	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	1/1/4/5	-	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	1/1/4/5	-	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(°)	Ideal(°)
2	C	2	NAG	C4-C3-C2	2.54	114.73	111.02
2	D	2	NAG	C4-C3-C2	2.45	114.61	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	4	FUC	C1
2	D	4	FUC	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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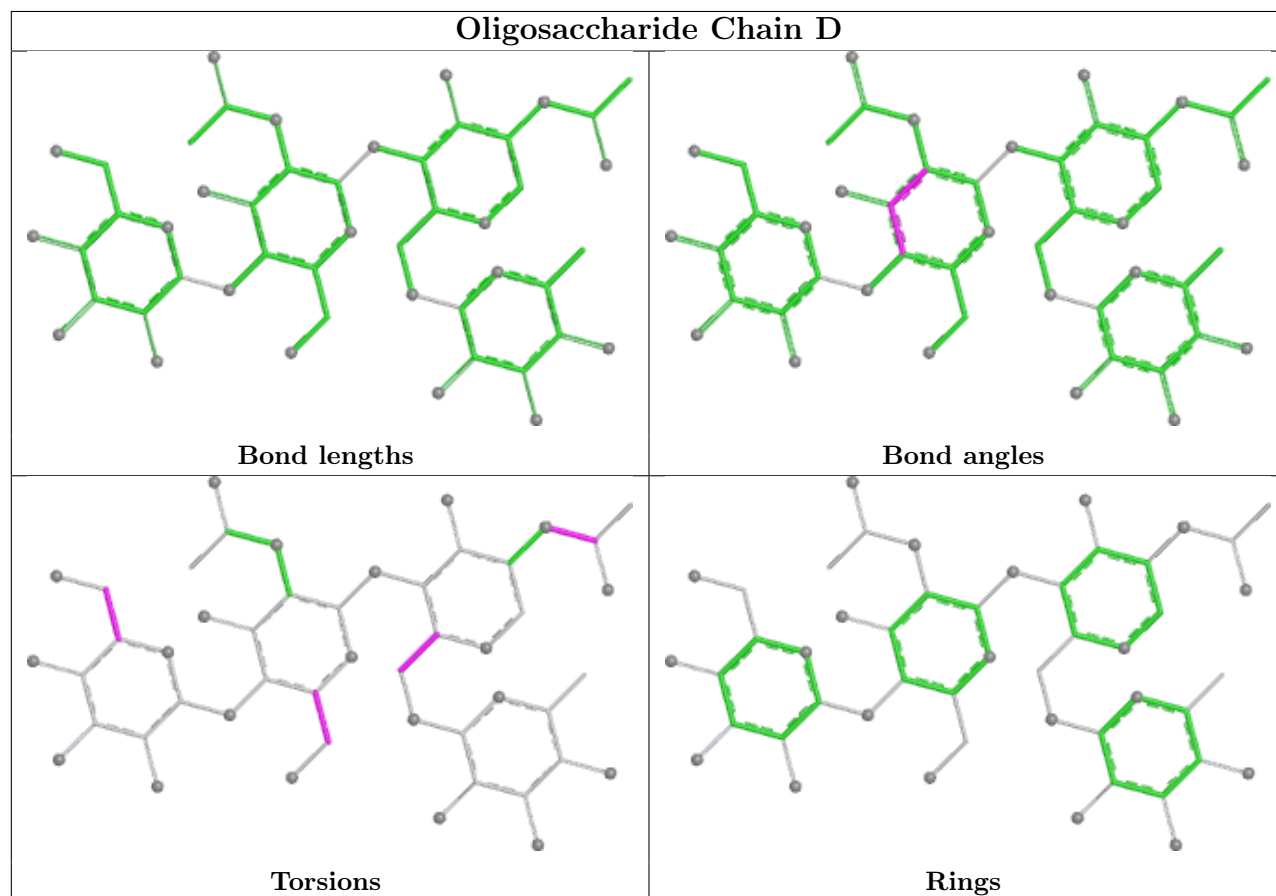
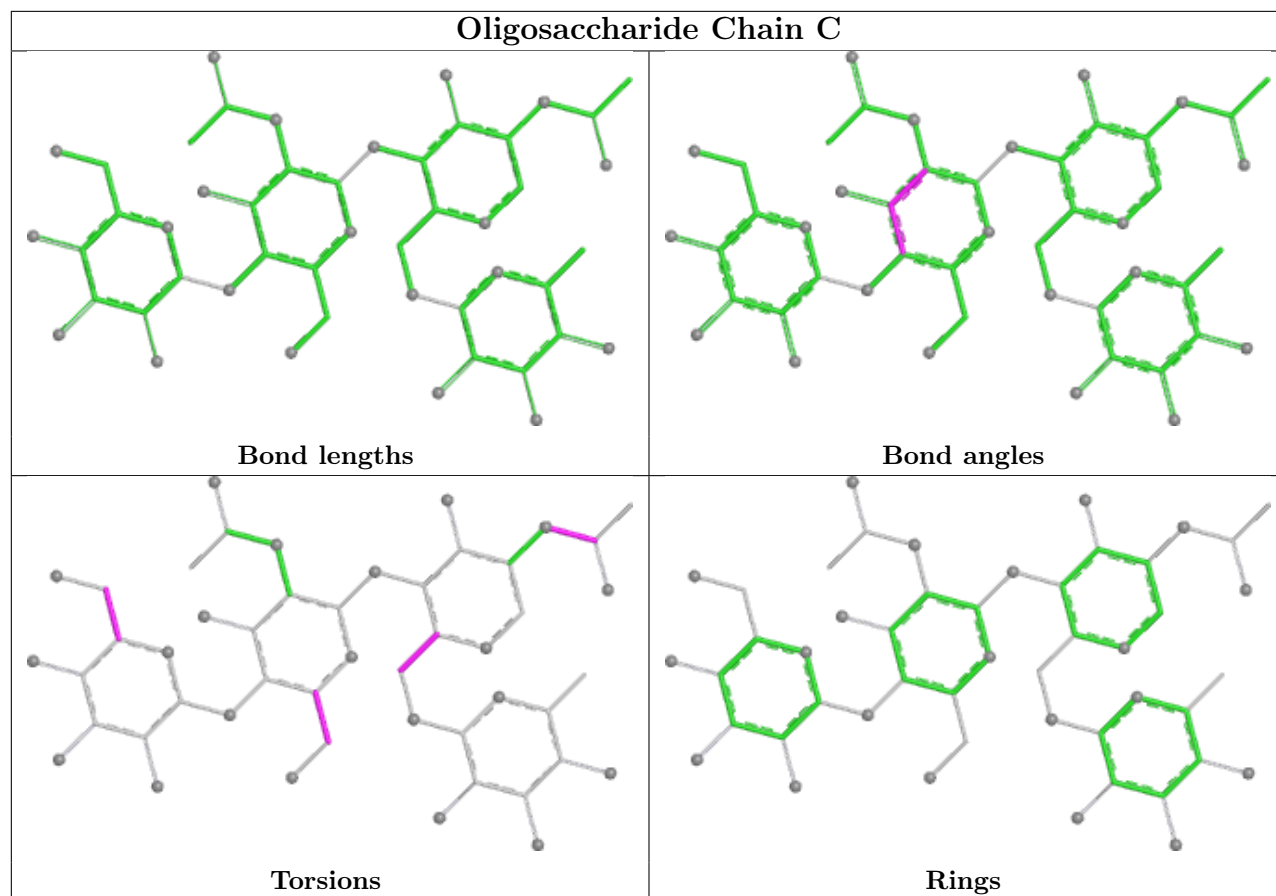
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 4 short contacts:

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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	NAG	A	1396	1	14,14,15	0.85	1 (7%)	17,19,21	0.60	0
4	NAG	B	1395	1	14,14,15	0.70	0	17,19,21	0.62	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
4	NAG	A	1396	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1395	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1396	NAG	C1-C2	2.19	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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	394/394 (100%)	0.54	36 (9%) 15 14	29, 73, 131, 149	0
1	B	394/394 (100%)	0.38	18 (4%) 37 36	24, 69, 116, 149	0
All	All	788/788 (100%)	0.46	54 (6%) 23 22	24, 71, 126, 149	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	5.0
1	A	276	ASN	3.9
1	A	162	VAL	3.4
1	B	19	SER	3.3
1	A	286	ARG	3.3
1	A	277	LEU	3.2
1	B	20	TRP	3.2
1	B	275	GLY	3.1
1	A	173	ALA	3.0
1	A	279	PHE	2.9
1	A	127	GLY	2.9
1	A	50	ALA	2.9
1	A	275	GLY	2.9
1	A	280	THR	2.9
1	A	278	LEU	2.8
1	A	18	GLY	2.8
1	A	129	ILE	2.7
1	B	191	LEU	2.6
1	B	278	LEU	2.6
1	A	164	ILE	2.6
1	A	191	LEU	2.5
1	A	51	LYS	2.5
1	B	280	THR	2.5
1	B	157	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	170	ILE	2.4
1	A	283	LEU	2.4
1	A	15	VAL	2.4
1	A	250	VAL	2.4
1	B	17	GLY	2.4
1	A	182	THR	2.3
1	A	226	THR	2.3
1	B	331	SER	2.3
1	B	277	LEU	2.3
1	A	251	VAL	2.3
1	B	18	GLY	2.3
1	B	193	PHE	2.3
1	B	183	MET	2.2
1	A	281	GLY	2.2
1	A	204	LYS	2.2
1	A	332	PRO	2.2
1	B	273	SER	2.2
1	A	178	TYR	2.2
1	A	19	SER	2.2
1	A	56	LEU	2.2
1	A	289	MET	2.2
1	B	279	PHE	2.2
1	B	288	ARG	2.1
1	B	187	PRO	2.1
1	A	292	LEU	2.1
1	A	297	MET	2.1
1	A	342	LEU	2.1
1	A	181	VAL	2.1
1	A	52	GLN	2.0
1	A	253	LEU	2.0

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

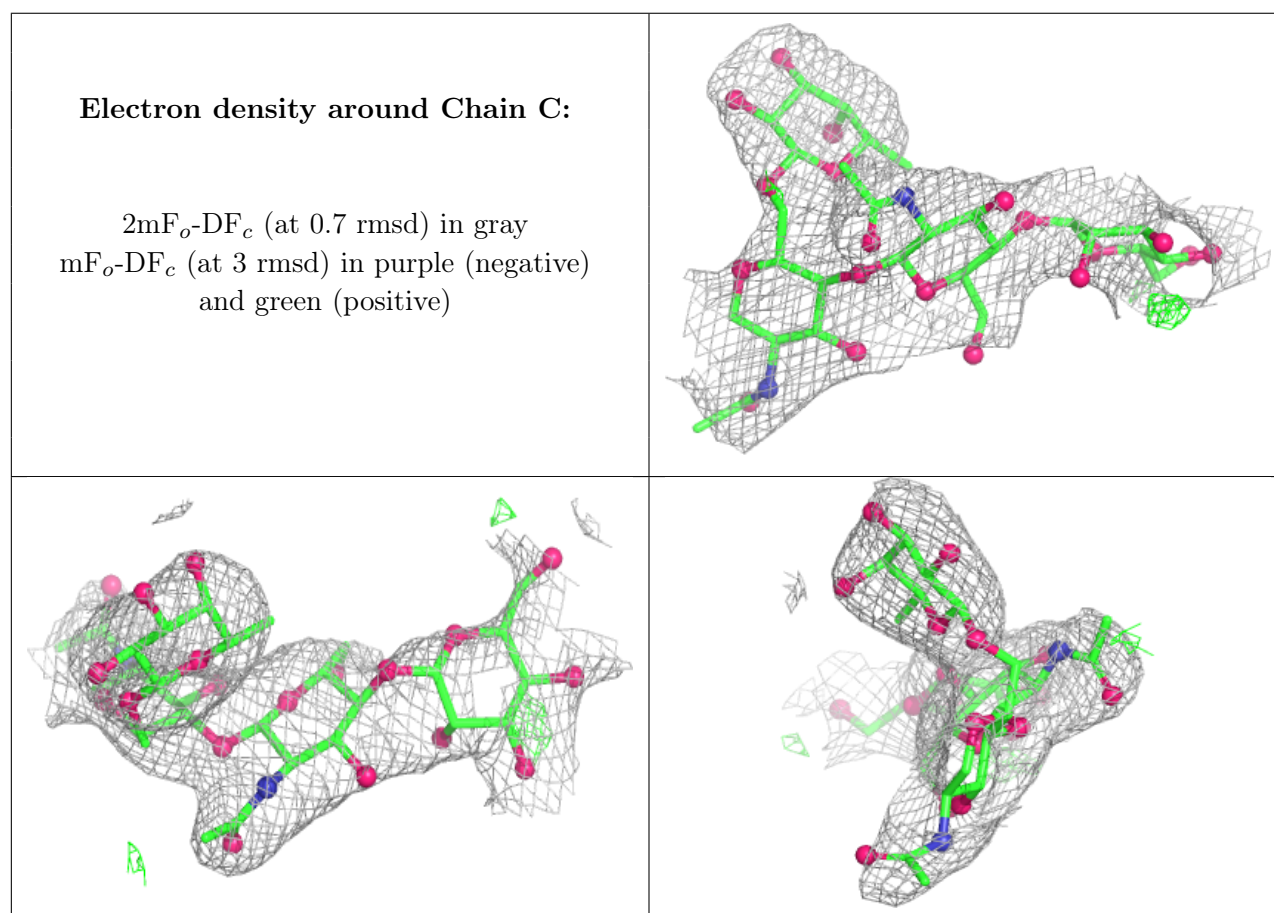
There are no non-standard protein/DNA/RNA residues in this entry.

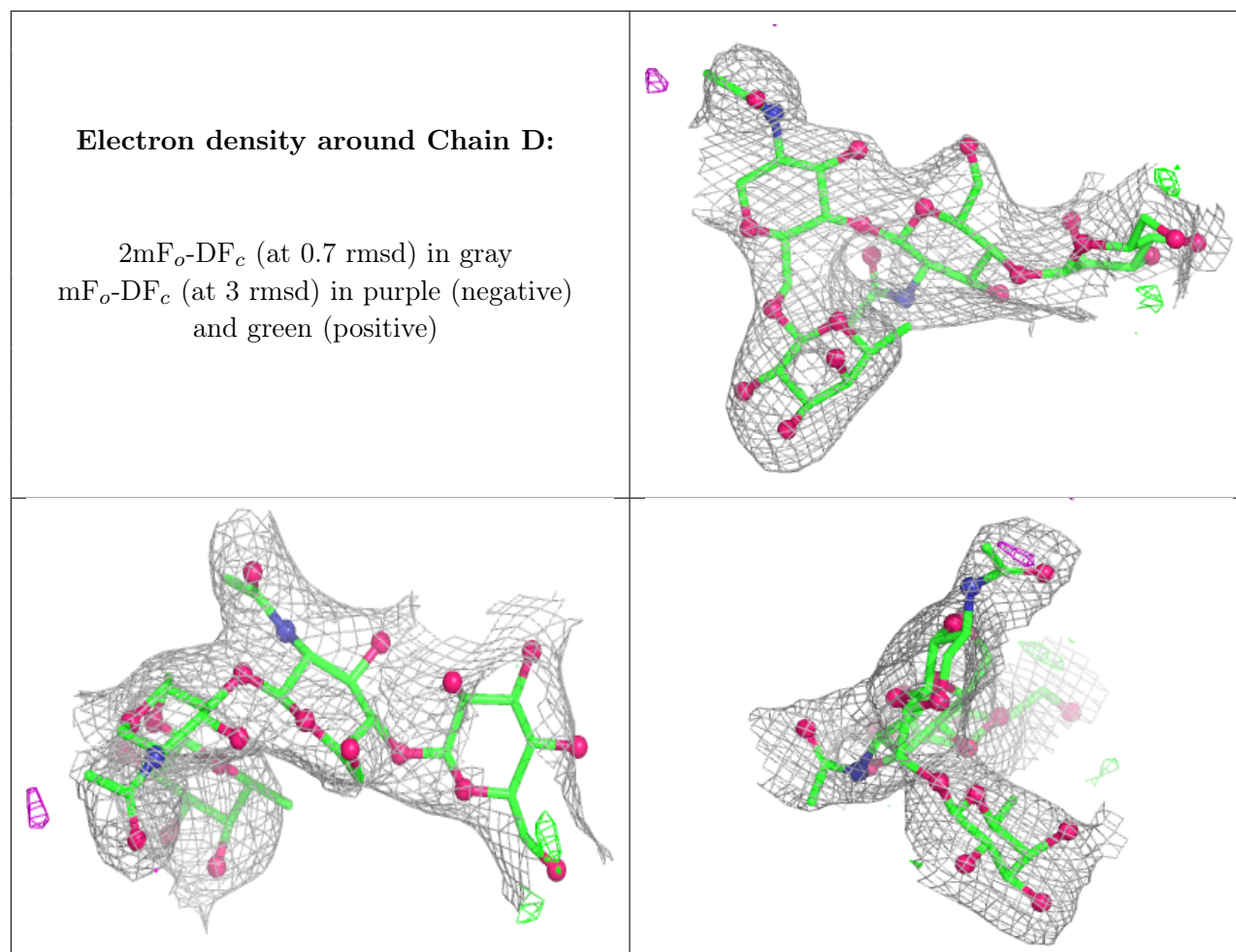
6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
2	BMA	D	3	11/12	0.22	0.15	108,121,127,129	0
2	BMA	C	3	11/12	0.32	0.16	124,127,129,131	0
2	NAG	C	2	14/15	0.84	0.11	82,94,105,119	0
2	NAG	D	2	14/15	0.87	0.10	58,80,95,105	0
2	FUC	D	4	10/11	0.87	0.10	63,71,77,81	0
2	NAG	D	1	14/15	0.91	0.11	45,67,72,74	0
2	FUC	C	4	10/11	0.91	0.09	70,75,78,88	0
2	NAG	C	1	14/15	0.92	0.12	75,81,89,90	0

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





6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	1396	14/15	0.67	0.13	88,98,103,104	0
4	NAG	B	1395	14/15	0.69	0.12	74,91,101,105	0
3	NA	A	1395	1/1	0.98	0.17	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.