



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:10 AM UTC

PDB ID : 4XNZ / pdb_00004xnz
Title : Crystal structure of broadly and potently neutralizing antibody VRC06B in complex with HIV-1 clade A/E strain 93TH057 gp120
Authors : Zhou, T.; Srivatsan, S.; Kwong, P.D.
Deposited on : 2015-01-16
Resolution : 3.39 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:

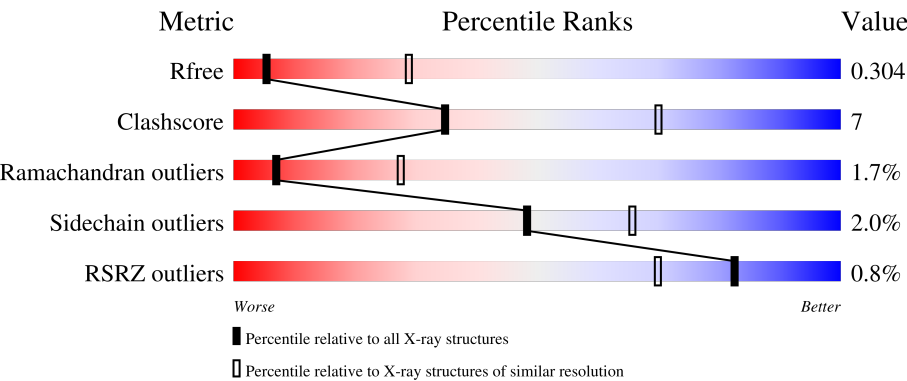
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.39 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.



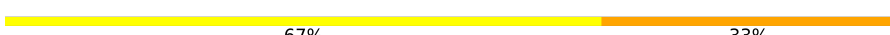
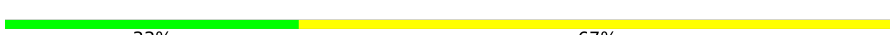
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	353	% 74% 22% ..
1	D	353	% 73% 20% 7%
1	G	353	2% 75% 22% .
2	B	234	79% 15% 5%
2	E	234	% 74% 18% 6%

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Mol	Chain	Length	Quality of chain
2	H	234	
3	C	209	
3	F	209	
3	L	209	
4	I	3	
4	J	3	
4	K	3	

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
4	FUC	K	3	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18134 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 gp160,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	340	Total	C	N	O	S	0	0	0
			2667	1674	463	509	21			
1	A	341	Total	C	N	O	S	0	0	0
			2665	1669	463	511	22			
1	D	330	Total	C	N	O	S	0	0	0
			2598	1634	452	492	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
D	124	GLY	-	linker	UNP Q0ED31
D	198	GLY	-	linker	UNP Q0ED31
D	318	GLY	-	linker	UNP Q0ED31
D	319	GLY	-	linker	UNP Q0ED31
D	320	SER	-	linker	UNP Q0ED31
D	321	GLY	-	linker	UNP Q0ED31
D	322	SER	-	linker	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	323	GLY	-	linker	UNP Q0ED31

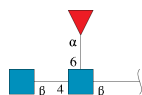
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY VRC06B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1686	1070	293	313	10			
2	B	222	Total	C	N	O	S	0	0	0
			1687	1071	294	312	10			
2	E	220	Total	C	N	O	S	0	0	0
			1670	1062	291	307	10			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY VRC06B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	207	Total	C	N	O	S	0	0	0
			1604	1006	276	318	4			
3	C	206	Total	C	N	O	S	0	0	0
			1596	999	275	318	4			
3	F	206	Total	C	N	O	S	0	0	0
			1595	1001	275	315	4			

- Molecule 4 is an oligosaccharide called 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
4	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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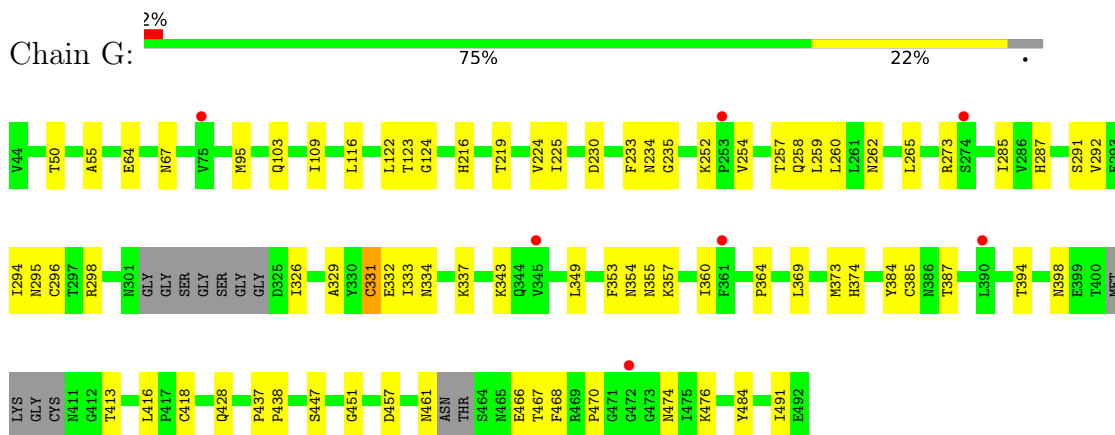
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

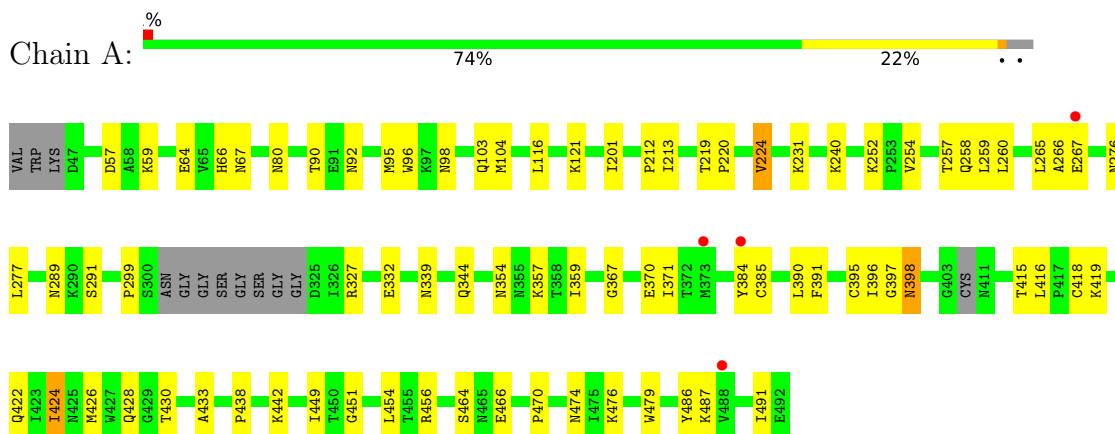
3 Residue-property plots [i](#)

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.

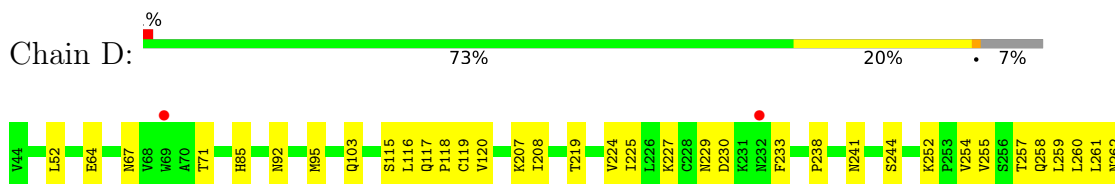
- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

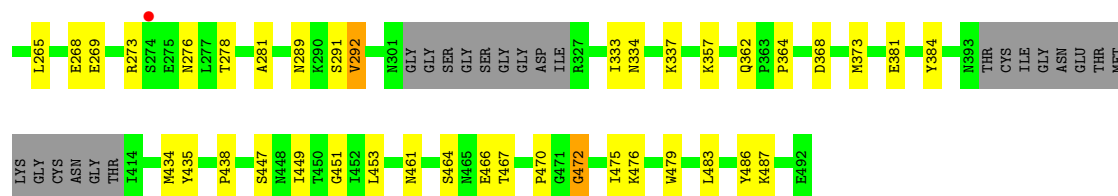


- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160



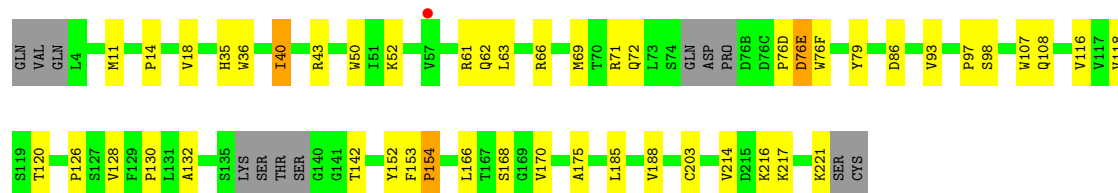
- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160





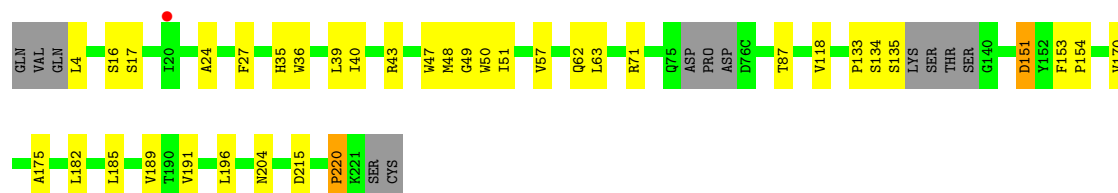
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain H: 74% 19% • 5%



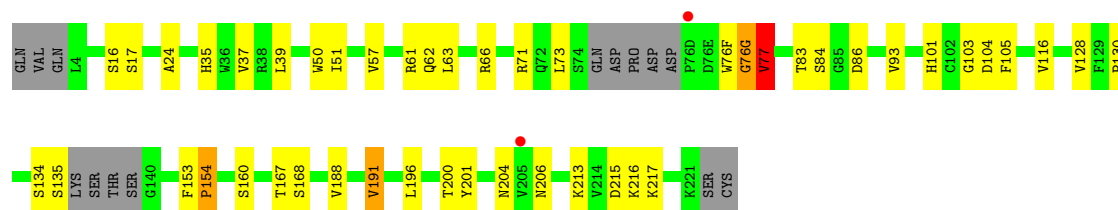
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain B: 79% 15% • 5%



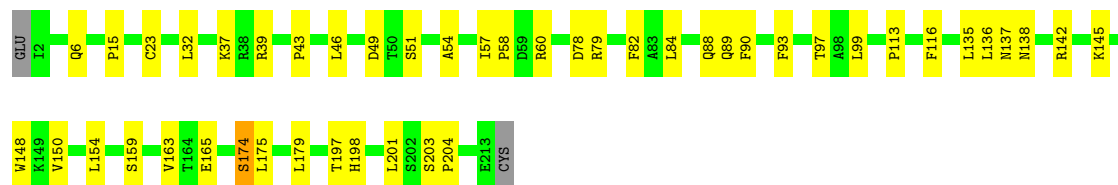
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain E: 74% 18% • 6%



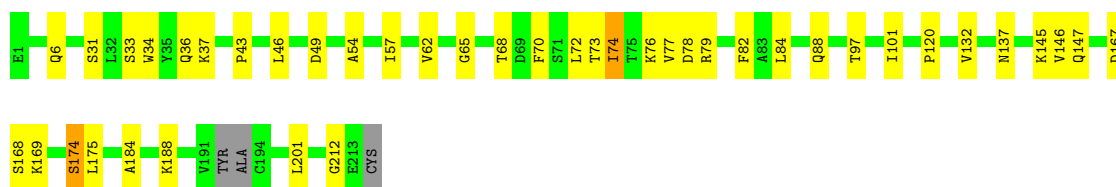
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain L: 77% 22% •



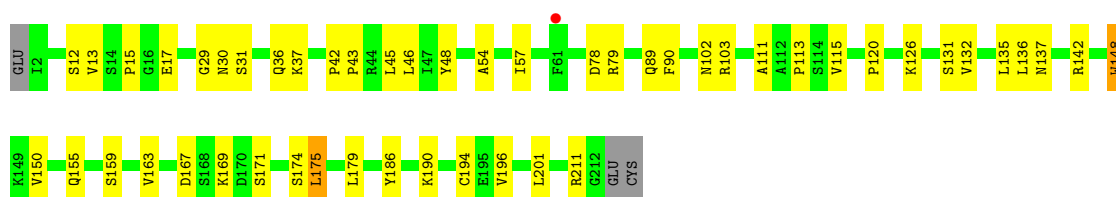
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain C:  78% 19% ..



- Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain F:  75% 23% ..



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

Chain I:  67% 33%

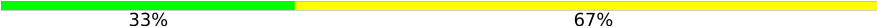


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%



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

Chain K:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 189.44Å 219.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 3.39 39.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	86.0 (39.90-3.39) 81.9 (39.90-3.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.301 0.249 , 0.304	Depositor DCC
R_{free} test set	1736 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18134	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: 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	0.25	0/2719	0.68	0/3689
1	D	0.26	0/2654	0.69	2/3603 (0.1%)
1	G	0.25	0/2722	0.67	0/3694
2	B	0.25	0/1735	0.68	0/2358
2	E	0.26	0/1718	0.71	2/2334 (0.1%)
2	H	0.26	0/1734	0.69	0/2357
3	C	0.26	0/1628	0.69	0/2203
3	F	0.27	0/1629	0.71	1/2207 (0.0%)
3	L	0.27	0/1638	0.70	0/2219
All	All	0.26	0/18177	0.69	5/24664 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	76(G)	GLY	CA-C-N	5.47	131.54	121.70
2	E	76(G)	GLY	C-N-CA	5.47	131.54	121.70
1	D	362	GLN	CA-C-N	5.45	123.64	119.66
1	D	362	GLN	C-N-CA	5.45	123.64	119.66
3	F	90	PHE	CB-CA-C	-5.14	110.24	117.23

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	2665	0	2601	47	0
1	D	2598	0	2540	40	0
1	G	2667	0	2601	43	0
2	B	1687	0	1638	24	0
2	E	1670	0	1627	24	0
2	H	1686	0	1634	24	0
3	C	1596	0	1553	20	1
3	F	1595	0	1553	29	0
3	L	1604	0	1559	23	0
4	I	38	0	34	0	1
4	J	38	0	34	1	0
4	K	38	0	34	1	0
5	A	98	0	91	1	0
5	D	70	0	65	2	0
5	G	84	0	78	0	0
All	All	18134	0	17642	267	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 7.

All (267) 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:D:95:MET:HE1	1:D:273:ARG:HB3	1.67	0.75
2:E:76(G):GLY:HA2	2:E:77:VAL:HB	1.70	0.72
1:G:95:MET:HE1	1:G:273:ARG:HB3	1.74	0.68
2:E:62:GLN:HG2	2:E:63:LEU:HD12	1.76	0.67
2:H:132:ALA:HB1	2:H:221:LYS:H	1.60	0.66
3:C:74:ILE:HD11	3:C:77:VAL:HG22	1.78	0.66
1:G:374:HIS:HB3	1:G:385:CYS:HB2	1.79	0.65
1:A:357:LYS:HD2	1:A:466:GLU:HG2	1.79	0.65
3:F:163:VAL:HB	3:F:175:LEU:HD12	1.80	0.64
1:D:85:HIS:NE2	1:D:241:ASN:OD1	2.31	0.64
1:D:120:VAL:HB	1:D:434:MET:HB3	1.79	0.64
3:C:82:PHE:HB3	3:C:101:ILE:HG12	1.80	0.64
2:H:36:TRP:HD1	2:H:69:MET:HE3	1.63	0.63
1:A:212:PRO:O	1:A:252:LYS:NZ	2.30	0.63
2:B:62:GLN:HG2	2:B:63:LEU:HD12	1.81	0.63
1:D:254:VAL:HG11	1:D:261:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:ALA:H	2:E:77:VAL:H	1.47	0.63
1:A:90:THR:HG22	1:A:240:LYS:HG2	1.81	0.62
1:A:92:ASN:O	1:A:487:LYS:NZ	2.31	0.62
1:G:333:ILE:O	1:G:413:THR:OG1	2.17	0.62
3:F:190:LYS:HD2	3:F:211:ARG:HB3	1.79	0.62
2:B:87:THR:HG22	2:B:118:VAL:H	1.63	0.62
3:F:113:PRO:HB2	3:F:136:LEU:HB2	1.80	0.62
1:G:295:ASN:HB3	1:G:332:GLU:HB3	1.82	0.61
1:G:353:PHE:O	1:G:355:ASN:N	2.33	0.61
1:A:424:ILE:O	1:A:433:ALA:N	2.31	0.61
1:G:294:ILE:HG22	1:G:333:ILE:HG12	1.83	0.61
1:A:426:MET:SD	1:A:430:THR:OG1	2.59	0.61
3:F:103:ARG:HD2	3:F:171:SER:HB2	1.81	0.60
1:A:426:MET:HE2	1:A:433:ALA:HB2	1.83	0.60
1:A:104:MET:HE3	1:A:479:TRP:HB3	1.83	0.60
1:G:343:LYS:HD3	1:G:398:ASN:HB3	1.84	0.59
1:A:357:LYS:HG3	1:A:464:SER:HB3	1.84	0.59
1:A:370:GLU:HA	1:A:384:TYR:HE2	1.67	0.59
2:E:35:HIS:HB2	2:E:93:VAL:HG23	1.83	0.59
2:H:175:ALA:HB2	2:H:185:LEU:HD23	1.86	0.58
3:C:79:ARG:NH1	3:C:168:SER:O	2.36	0.58
1:G:360:ILE:HG12	1:G:394:THR:HG23	1.86	0.57
1:D:357:LYS:HG3	1:D:464:SER:HB3	1.86	0.57
1:G:474:ASN:HD21	1:G:476:LYS:HE3	1.70	0.57
3:L:136:LEU:HD11	3:L:175:LEU:HD22	1.86	0.57
2:B:175:ALA:HB2	2:B:185:LEU:HD23	1.85	0.57
5:D:503:NAG:O4	3:F:29:GLY:O	2.22	0.57
3:C:33:SER:HB2	3:C:88:GLN:HB3	1.87	0.57
3:F:30:ASN:ND2	3:F:31:SER:O	2.38	0.57
3:F:37:LYS:HD2	3:F:43:PRO:HG3	1.85	0.57
1:A:265:LEU:HD21	1:A:291:SER:HB2	1.87	0.56
3:F:120:PRO:HB3	3:F:131:SER:H	1.70	0.56
1:G:64:GLU:HB3	1:G:67:ASN:HD22	1.69	0.56
3:L:159:SER:HB3	3:L:179:LEU:HD23	1.88	0.56
2:E:39:LEU:HD22	3:F:37:LYS:HE2	1.86	0.56
1:D:207:LYS:NZ	1:D:381:GLU:OE2	2.33	0.56
1:G:466:GLU:OE1	2:H:61:ARG:NH2	2.38	0.56
1:G:50:THR:O	1:G:103:GLN:NE2	2.37	0.56
2:B:24:ALA:HB1	2:B:27:PHE:HE1	1.69	0.56
1:D:453:LEU:HD22	1:D:472:GLY:HA2	1.88	0.55
2:H:36:TRP:CD1	2:H:69:MET:HE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:ARG:NH1	1:G:326:ILE:O	2.40	0.55
2:E:66:ARG:NH2	2:E:86:ASP:OD2	2.40	0.55
1:D:265:LEU:HD21	1:D:291:SER:HB3	1.89	0.55
3:C:137:ASN:HA	3:C:174:SER:HA	1.89	0.54
3:C:62:VAL:HB	3:C:73:THR:HG23	1.89	0.54
3:L:116:PHE:HD2	3:L:135:LEU:HD23	1.72	0.54
1:D:276:ASN:OD1	1:D:278:THR:OG1	2.23	0.54
1:A:332:GLU:HG2	1:A:415:THR:HG22	1.89	0.54
1:G:252:LYS:HD3	1:G:262:ASN:HB3	1.90	0.54
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.90	0.54
1:A:64:GLU:OE1	1:A:67:ASN:ND2	2.42	0.53
1:G:294:ILE:HD11	1:G:447:SER:HB2	1.90	0.53
1:D:92:ASN:O	1:D:487:LYS:NZ	2.40	0.53
3:F:78:ASP:OD1	3:F:79:ARG:N	2.38	0.53
3:F:12:SER:HB3	3:F:102:ASN:HB2	1.89	0.53
2:B:196:LEU:HD21	2:B:220:PRO:HG3	1.91	0.52
2:H:40:ILE:HG23	2:H:43:ARG:HB2	1.91	0.52
3:C:37:LYS:HD2	3:C:43:PRO:HG3	1.91	0.52
2:E:103:GLY:O	2:E:105:PHE:N	2.33	0.52
3:L:39:ARG:NH1	3:L:165:GLU:OE2	2.43	0.52
1:A:339:ASN:O	1:A:398:ASN:ND2	2.42	0.52
2:B:51:ILE:HD11	2:B:71:ARG:HD2	1.92	0.52
2:B:170:VAL:HG22	2:B:189:VAL:HG22	1.90	0.52
3:F:13:VAL:HG13	3:F:17:GLU:HB3	1.92	0.52
2:H:72:GLN:HB2	2:H:79:TYR:HE2	1.75	0.52
3:L:137:ASN:HA	3:L:174:SER:HA	1.90	0.52
1:A:367:GLY:HA3	1:A:371:ILE:HD11	1.91	0.52
3:C:31:SER:HB2	3:C:49:ASP:HA	1.91	0.52
3:F:148:TRP:HA	3:F:194:CYS:HA	1.92	0.52
1:G:457:ASP:HB3	1:G:467:THR:HB	1.91	0.52
1:D:52:LEU:O	1:D:103:GLN:NE2	2.41	0.51
1:D:64:GLU:OE1	1:D:67:ASN:ND2	2.36	0.51
3:F:159:SER:HB3	3:F:179:LEU:HG	1.92	0.51
1:D:268:GLU:HG2	1:D:269:GLU:HG2	1.93	0.51
3:F:137:ASN:HA	3:F:174:SER:HA	1.92	0.51
1:A:121:LYS:HB3	1:A:201:ILE:HB	1.92	0.51
1:D:227:LYS:NZ	1:D:229:ASN:OD1	2.44	0.51
1:D:257:THR:O	1:D:259:LEU:N	2.43	0.51
2:B:151:ASP:HA	2:B:182:LEU:HB3	1.92	0.51
2:E:200:THR:HG23	2:E:217:LYS:HE3	1.93	0.51
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:ASP:OD1	3:L:79:ARG:N	2.41	0.50
1:G:257:THR:O	1:G:259:LEU:N	2.43	0.50
2:H:98:SER:OG	2:H:108:GLN:OE1	2.26	0.50
3:C:54:ALA:HB3	3:C:57:ILE:HD12	1.93	0.50
2:H:35:HIS:HB2	2:H:93:VAL:HG23	1.93	0.50
1:A:390:LEU:HG	1:A:416:LEU:HD21	1.94	0.50
3:L:37:LYS:HD2	3:L:43:PRO:HG3	1.93	0.50
3:L:6:GLN:HE21	3:L:97:THR:HG23	1.76	0.50
1:A:231:LYS:HE2	1:A:267:GLU:HG3	1.94	0.50
2:H:107:TRP:HZ3	3:L:93:PHE:HZ	1.60	0.50
1:G:387:THR:HG22	1:G:416:LEU:HD13	1.94	0.49
3:L:54:ALA:H	3:L:57:ILE:HD12	1.77	0.49
3:L:163:VAL:HA	3:L:175:LEU:HA	1.94	0.49
1:G:265:LEU:HD21	1:G:291:SER:HB2	1.92	0.49
1:A:476:LYS:HA	1:A:479:TRP:CD1	2.47	0.49
1:D:483:LEU:HD12	1:D:486:TYR:HD2	1.78	0.49
1:A:224:VAL:HG23	1:A:491:ILE:HD11	1.93	0.49
1:A:257:THR:O	1:A:259:LEU:N	2.43	0.49
2:B:36:TRP:HB3	2:B:48:MET:HE3	1.93	0.49
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.95	0.49
1:A:64:GLU:HB3	1:A:67:ASN:HD22	1.78	0.49
1:G:64:GLU:OE1	1:G:67:ASN:ND2	2.46	0.48
2:E:71:ARG:HE	2:E:73:LEU:HD13	1.78	0.48
2:H:76(D):PRO:O	2:H:76(F):TRP:N	2.47	0.48
1:D:364:PRO:HD3	1:D:470:PRO:HG2	1.94	0.48
2:H:216:LYS:NZ	2:H:217:LYS:O	2.46	0.48
3:C:6:GLN:HE21	3:C:97:THR:HG23	1.78	0.48
3:C:145:LYS:NZ	3:C:147:GLN:OE1	2.45	0.48
1:G:230:ASP:HB3	1:G:233:PHE:HB2	1.94	0.48
1:A:98:ASN:ND2	1:A:486:TYR:O	2.47	0.48
1:D:252:LYS:HD3	1:D:262:ASN:HB3	1.95	0.48
3:F:163:VAL:HA	3:F:175:LEU:HA	1.94	0.48
3:C:78:ASP:OD1	3:C:79:ARG:N	2.46	0.48
1:D:118:PRO:HG3	1:D:435:TYR:CZ	2.48	0.48
1:D:357:LYS:NZ	1:D:466:GLU:OE2	2.44	0.48
1:G:234:ASN:O	1:G:273:ARG:NH2	2.42	0.48
1:G:428:GLN:OE1	1:G:428:GLN:N	2.45	0.48
1:G:273:ARG:HB2	1:G:285:ILE:HB	1.96	0.47
1:G:55:ALA:N	1:G:216:HIS:O	2.39	0.47
1:A:428:GLN:N	1:A:428:GLN:OE1	2.47	0.47
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ASP:CG	2:E:71:ARG:HH12	2.23	0.47
2:E:130:PRO:HD3	2:E:216:LYS:HE3	1.95	0.47
2:B:189:VAL:HG12	2:B:191:VAL:HG23	1.97	0.47
2:E:51:ILE:HG22	2:E:57:VAL:HG12	1.95	0.47
1:G:329:ALA:HB3	1:G:418:CYS:HB2	1.96	0.47
3:F:142:ARG:HE	3:F:163:VAL:HG21	1.79	0.47
1:G:292:VAL:HG13	1:G:337:LYS:HE3	1.97	0.47
2:H:14:PRO:HG3	2:H:120:THR:HG22	1.97	0.47
1:G:122:LEU:HG	1:G:124:GLY:H	1.80	0.47
2:H:11:MET:SD	2:H:154:PRO:HG3	2.54	0.47
3:L:82:PHE:HA	3:L:99:LEU:HB3	1.97	0.46
2:B:40:ILE:HB	2:B:43:ARG:HB3	1.96	0.46
3:F:103:ARG:HH12	3:F:111:ALA:HB2	1.80	0.46
1:D:92:ASN:HA	1:D:238:PRO:HA	1.97	0.46
1:D:373:MET:SD	1:D:384:TYR:HB3	2.55	0.46
2:E:206:ASN:HD21	2:E:213:LYS:HE3	1.80	0.46
3:L:113:PRO:HD3	3:L:198:HIS:HD2	1.81	0.46
1:A:277:LEU:O	1:A:456:ARG:NH1	2.48	0.46
2:E:191:VAL:HG11	2:E:201:TYR:CE2	2.50	0.46
1:G:461:ASN:OD1	1:G:461:ASN:N	2.45	0.46
1:D:230:ASP:HB2	1:D:233:PHE:HB2	1.98	0.46
3:L:32:LEU:HD12	3:L:89:GLN:HG3	1.98	0.46
1:A:384:TYR:CZ	1:A:424:ILE:HD11	2.51	0.45
3:F:54:ALA:H	3:F:57:ILE:HD12	1.81	0.45
1:G:373:MET:SD	1:G:384:TYR:HB3	2.56	0.45
4:K:2:NAG:C8	4:K:3:FUC:H2	2.45	0.45
1:A:327:ARG:HD3	1:A:419:LYS:HE3	1.99	0.45
2:B:39:LEU:HD22	3:C:37:LYS:HE2	1.98	0.45
2:E:204:ASN:ND2	2:E:215:ASP:OD1	2.42	0.45
1:G:219:THR:HG23	1:G:225:ILE:HG13	1.99	0.45
1:G:334:ASN:HB3	1:G:337:LYS:HG2	1.99	0.45
1:G:357:LYS:HD2	1:G:466:GLU:HG2	1.99	0.45
2:H:130:PRO:HD3	2:H:216:LYS:HE3	1.99	0.45
2:B:16:SER:OG	2:B:17:SER:N	2.48	0.45
3:C:167:ASP:C	3:C:169:LYS:H	2.25	0.45
1:D:67:ASN:O	1:D:71:THR:OG1	2.27	0.45
1:D:292:VAL:HG13	1:D:449:ILE:HD11	1.98	0.44
2:B:24:ALA:HB1	2:B:27:PHE:CE1	2.49	0.44
2:E:83:THR:OG1	2:E:84:SER:N	2.47	0.44
3:L:142:ARG:HH21	3:L:163:VAL:HG11	1.82	0.44
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ALA:HA	2:E:50:TRP:CZ2	2.52	0.44
3:F:30:ASN:OD1	3:F:89:GLN:NE2	2.50	0.44
1:A:424:ILE:HD12	1:A:424:ILE:HA	1.76	0.44
2:E:16:SER:OG	2:E:17:SER:N	2.49	0.44
3:C:65:GLY:HA3	3:C:70:PHE:HA	2.00	0.44
2:E:188:VAL:HG21	3:F:135:LEU:HD11	1.99	0.44
1:A:299:PRO:HA	1:A:442:LYS:HD2	1.98	0.44
1:A:344:GLN:HB3	5:A:505:NAG:H62	2.00	0.44
1:A:474:ASN:HD21	1:A:476:LYS:HE2	1.82	0.44
1:D:260:LEU:HD12	1:D:451:GLY:HA3	1.99	0.44
1:G:224:VAL:HG23	1:G:491:ILE:HD11	2.00	0.44
1:A:57:ASP:O	1:A:59:LYS:NZ	2.48	0.44
3:C:34:TRP:CD2	3:C:72:LEU:HB2	2.53	0.44
3:F:45:LEU:HD21	3:F:48:TYR:HB3	2.00	0.44
3:C:34:TRP:CE2	3:C:72:LEU:HB2	2.53	0.44
2:H:203:CYS:SG	2:H:216:LYS:HB3	2.58	0.44
1:D:219:THR:HG23	1:D:225:ILE:HG12	2.00	0.44
1:D:269:GLU:HA	1:D:289:ASN:HD22	1.83	0.43
3:F:79:ARG:NH1	3:F:169:LYS:O	2.50	0.43
2:H:50:TRP:CZ3	2:H:52:LYS:HG2	2.52	0.43
3:L:145:LYS:HE2	3:L:197:THR:HB	1.99	0.43
1:G:349:LEU:HD13	1:G:468:PHE:CE2	2.54	0.43
2:B:153:PHE:HA	2:B:154:PRO:HA	1.71	0.43
2:H:128:VAL:HG21	2:H:214:VAL:HG11	1.99	0.43
1:A:266:ALA:HB3	1:A:289:ASN:HB3	2.00	0.43
1:D:476:LYS:HA	1:D:479:TRP:CD1	2.54	0.43
3:F:150:VAL:HB	3:F:155:GLN:HE22	1.84	0.43
3:F:167:ASP:C	3:F:169:LYS:H	2.25	0.43
1:A:80:ASN:OD1	1:A:80:ASN:N	2.51	0.43
2:B:35:HIS:CG	2:B:50:TRP:HB3	2.54	0.43
2:B:40:ILE:HG21	2:B:43:ARG:HE	1.84	0.43
1:D:447:SER:HB3	5:D:502:NAG:HN2	1.84	0.43
2:H:76(E):ASP:OD1	2:H:76(F):TRP:N	2.51	0.43
2:E:76(G):GLY:CA	2:E:77:VAL:HB	2.46	0.43
2:H:62:GLN:HG2	2:H:63:LEU:HD12	2.01	0.42
2:B:35:HIS:ND1	2:B:50:TRP:HB3	2.33	0.42
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.52	0.42
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.54	0.42
3:F:186:TYR:O	3:F:211:ARG:NH2	2.52	0.42
3:L:46:LEU:HA	3:L:57:ILE:HD13	2.01	0.42
1:A:422:GLN:HE21	1:A:438:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:115:VAL:HG22	3:F:136:LEU:HB3	2.01	0.42
2:E:134:SER:OG	2:E:135:SER:N	2.52	0.42
2:E:153:PHE:HA	2:E:154:PRO:HA	1.74	0.42
1:G:260:LEU:HD12	1:G:451:GLY:HA3	2.01	0.42
3:L:88:GLN:NE2	3:L:90:PHE:O	2.53	0.42
1:A:474:ASN:OD1	1:A:476:LYS:HB2	2.18	0.42
3:F:42:PRO:HA	3:F:43:PRO:HD3	1.91	0.42
1:G:364:PRO:HD3	1:G:470:PRO:HG2	2.00	0.42
2:H:126:PRO:HB3	2:H:152:TYR:HB3	2.02	0.42
1:A:454:LEU:HA	1:A:470:PRO:HA	2.01	0.42
3:L:203:SER:HA	3:L:204:PRO:HD3	1.94	0.42
2:B:134:SER:OG	2:B:135:SER:N	2.53	0.42
1:A:252:LYS:HB3	1:A:254:VAL:HG23	2.02	0.41
1:G:109:ILE:HG13	1:G:428:GLN:HG3	2.01	0.41
1:G:296:CYS:HA	1:G:331:CYS:HA	2.01	0.41
2:B:133:PRO:HD2	2:B:220:PRO:HA	2.02	0.41
1:A:219:THR:HA	1:A:220:PRO:HD3	1.91	0.41
1:D:381:GLU:OE2	1:D:438:PRO:HA	2.20	0.41
3:L:58:PRO:HB2	3:L:60:ARG:HG2	2.03	0.41
1:A:95:MET:HE3	1:A:96:TRP:CH2	2.56	0.41
1:A:385:CYS:HA	1:A:418:CYS:HA	2.02	0.41
1:G:437:PRO:HA	1:G:438:PRO:HD3	1.96	0.41
3:C:184:ALA:O	3:C:188:LYS:HG2	2.21	0.41
2:B:35:HIS:HA	2:B:50:TRP:HA	2.03	0.41
1:D:224:VAL:HG11	1:D:244:SER:HB2	2.03	0.41
3:F:36:GLN:HB2	3:F:46:LEU:HD11	2.02	0.41
1:G:95:MET:HB3	1:G:484:TYR:HA	2.03	0.41
1:G:369:LEU:O	1:G:373:MET:HG2	2.20	0.41
2:H:188:VAL:HG21	3:L:135:LEU:HD11	2.03	0.41
1:A:121:LYS:O	1:A:201:ILE:N	2.44	0.41
3:C:36:GLN:HB2	3:C:46:LEU:HD11	2.03	0.41
1:D:254:VAL:HG21	1:D:262:ASN:HB2	2.03	0.41
2:E:160:SER:O	2:E:204:ASN:N	2.42	0.41
2:H:153:PHE:HA	2:H:154:PRO:HA	1.78	0.41
3:L:49:ASP:O	3:L:51:SER:N	2.51	0.40
4:J:1:NAG:H61	4:J:2:NAG:HN2	1.86	0.40
1:D:334:ASN:HD21	1:D:337:LYS:HD3	1.87	0.40
1:D:475:ILE:H	1:D:475:ILE:HG12	1.71	0.40
1:G:234:ASN:OD1	1:G:235:GLY:N	2.54	0.40
3:L:6:GLN:HE21	3:L:6:GLN:HB3	1.70	0.40
1:A:259:LEU:HD13	1:A:449:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HB	2:B:57:VAL:HG12	2.02	0.40
1:D:115:SER:O	1:D:117:GLN:N	2.55	0.40
1:D:333:ILE:HG23	1:D:337:LYS:HZ1	1.87	0.40
1:D:466:GLU:CD	2:E:61:ARG:HH22	2.29	0.40
1:A:359:ILE:HB	1:A:395:CYS:SG	2.61	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)
3:C:68:THR:OG1	4:I:3:FUC:O4[3_545]	1.86	0.34

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	335/353 (95%)	311 (93%)	18 (5%)	6 (2%)	6	26
1	D	324/353 (92%)	309 (95%)	12 (4%)	3 (1%)	14	41
1	G	332/353 (94%)	306 (92%)	23 (7%)	3 (1%)	14	41
2	B	216/234 (92%)	195 (90%)	19 (9%)	2 (1%)	14	41
2	E	214/234 (92%)	193 (90%)	16 (8%)	5 (2%)	5	23
2	H	216/234 (92%)	194 (90%)	17 (8%)	5 (2%)	5	23
3	C	202/209 (97%)	178 (88%)	19 (9%)	5 (2%)	4	21
3	F	204/209 (98%)	176 (86%)	24 (12%)	4 (2%)	6	24
3	L	205/209 (98%)	176 (86%)	24 (12%)	5 (2%)	4	22
All	All	2248/2388 (94%)	2038 (91%)	172 (8%)	38 (2%)	7	27

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	354	ASN
2	H	76(E)	ASP
1	A	354	ASN
1	A	396	ILE
2	E	76(F)	TRP
2	H	168	SER
2	B	151	ASP
2	E	104	ASP
2	E	168	SER
1	G	116	LEU
3	L	148	TRP
3	L	201	LEU
1	A	398	ASN
2	B	220	PRO
3	C	76	LYS
3	C	201	LEU
1	D	116	LEU
2	E	77	VAL
3	F	148	TRP
3	F	201	LEU
1	G	258	GLN
2	H	142	THR
3	F	175	LEU
3	L	138	ASN
1	A	116	LEU
1	A	258	GLN
1	D	258	GLN
3	L	174	SER
3	C	174	SER
3	C	175	LEU
3	C	212	GLY
3	F	15	PRO
3	L	15	PRO
1	A	397	GLY
2	H	97	PRO
1	D	472	GLY
2	E	154	PRO
2	H	154	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	A	304/311 (98%)	300 (99%)	4 (1%)	61	71
1	D	296/311 (95%)	290 (98%)	6 (2%)	48	66
1	G	304/311 (98%)	300 (99%)	4 (1%)	61	71
2	B	186/198 (94%)	185 (100%)	1 (0%)	81	80
2	E	184/198 (93%)	176 (96%)	8 (4%)	26	51
2	H	186/198 (94%)	179 (96%)	7 (4%)	29	54
3	C	180/182 (99%)	177 (98%)	3 (2%)	53	67
3	F	179/182 (98%)	176 (98%)	3 (2%)	53	67
3	L	180/182 (99%)	176 (98%)	4 (2%)	45	63
All	All	1999/2073 (96%)	1959 (98%)	40 (2%)	48	66

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	123	THR
1	G	254	VAL
1	G	287	HIS
1	G	331	CYS
2	H	18	VAL
2	H	40	ILE
2	H	71	ARG
2	H	116	VAL
2	H	118	VAL
2	H	166	LEU
2	H	170	VAL
3	L	23	CYS
3	L	84	LEU
3	L	150	VAL
3	L	154	LEU
1	A	103	GLN
1	A	224	VAL
1	A	276	ASN
1	A	424	ILE
2	B	4	LEU
3	C	74	ILE
3	C	84	LEU

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Mol	Chain	Res	Type
3	C	146	VAL
1	D	119	CYS
1	D	208	ILE
1	D	255	VAL
1	D	292	VAL
1	D	461	ASN
1	D	467	THR
2	E	37	VAL
2	E	77	VAL
2	E	101	HIS
2	E	116	VAL
2	E	128	VAL
2	E	167	THR
2	E	191	VAL
2	E	196	LEU
3	F	126	LYS
3	F	132	VAL
3	F	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	67	ASN
1	G	99	ASN
1	G	374	HIS
1	G	377	ASN
1	G	432	GLN
1	G	474	ASN
2	H	211	ASN
3	L	160	GLN
3	L	198	HIS
1	A	72	HIS
1	A	352	HIS
1	A	422	GLN
1	A	462	ASN
2	B	108	GLN
3	C	30	ASN
1	D	354	ASN
1	D	448	ASN
1	D	461	ASN
3	F	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	$\# Z > 2$
4	NAG	I	1	3,4	14,14,15	0.56	0	17,19,21	0.80	1 (5%)
4	NAG	I	2	4	14,14,15	0.35	0	17,19,21	0.68	1 (5%)
4	FUC	I	3	4	10,10,11	0.43	0	14,14,16	1.35	1 (7%)
4	NAG	J	1	3,4	14,14,15	0.27	0	17,19,21	0.72	1 (5%)
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.33	0
4	FUC	J	3	4	10,10,11	0.88	1 (10%)	14,14,16	1.27	1 (7%)
4	NAG	K	1	3,4	14,14,15	0.27	0	17,19,21	0.52	0
4	NAG	K	2	4	14,14,15	0.35	0	17,19,21	0.67	0
4	FUC	K	3	4	10,10,11	0.71	0	14,14,16	0.90	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	I	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
4	NAG	K	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	FUC	K	3	4	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	O5-C1	-2.14	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	FUC	C1-O5-C5	3.13	120.34	112.97
4	I	3	FUC	C3-C4-C5	2.88	114.18	109.81
4	I	2	NAG	C1-O5-C5	2.36	115.35	112.19
4	J	1	NAG	C1-O5-C5	2.36	115.35	112.19
4	I	1	NAG	O4-C4-C5	-2.03	104.31	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	3	FUC	C1

All (11) torsion outliers are listed below:

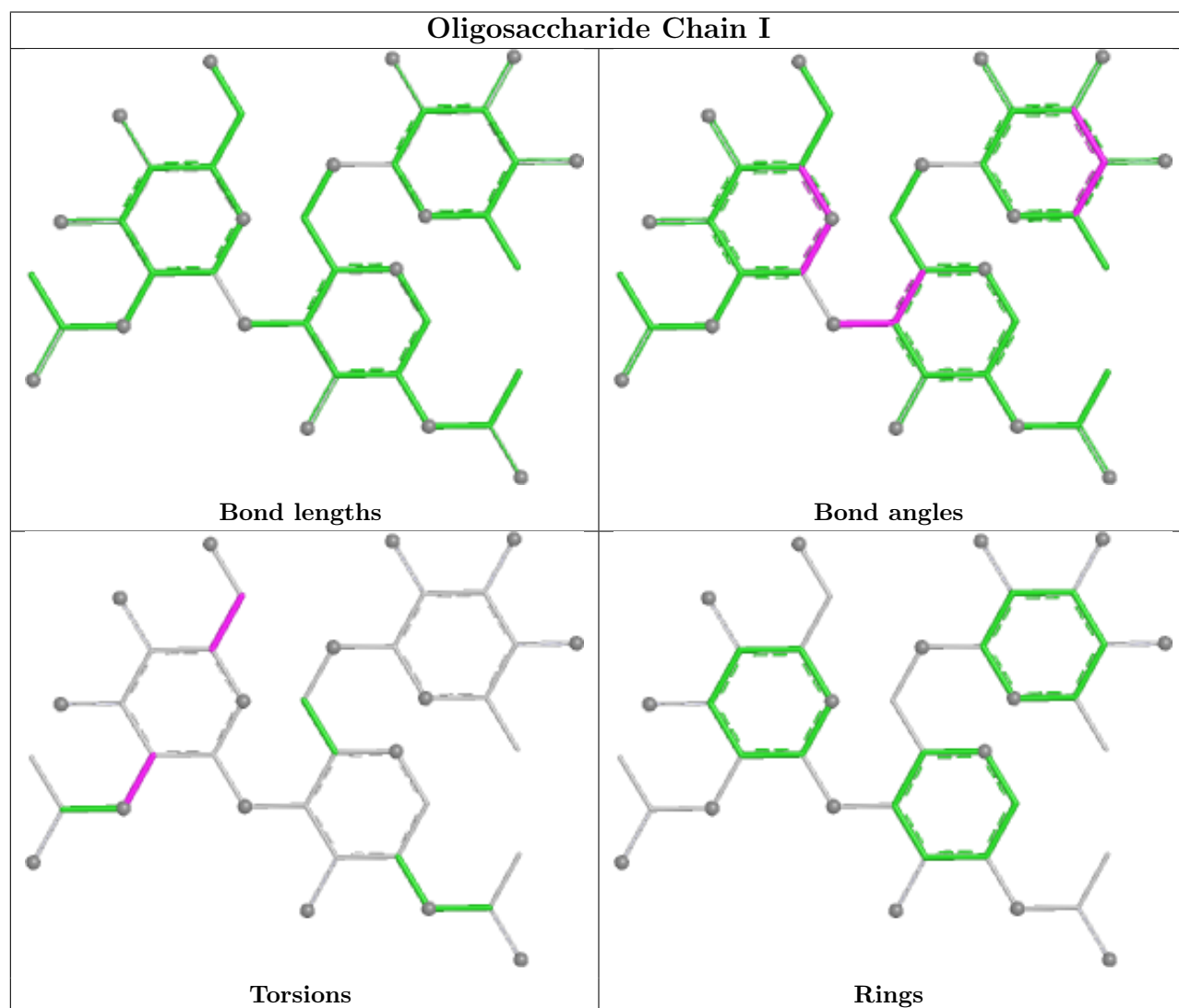
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7

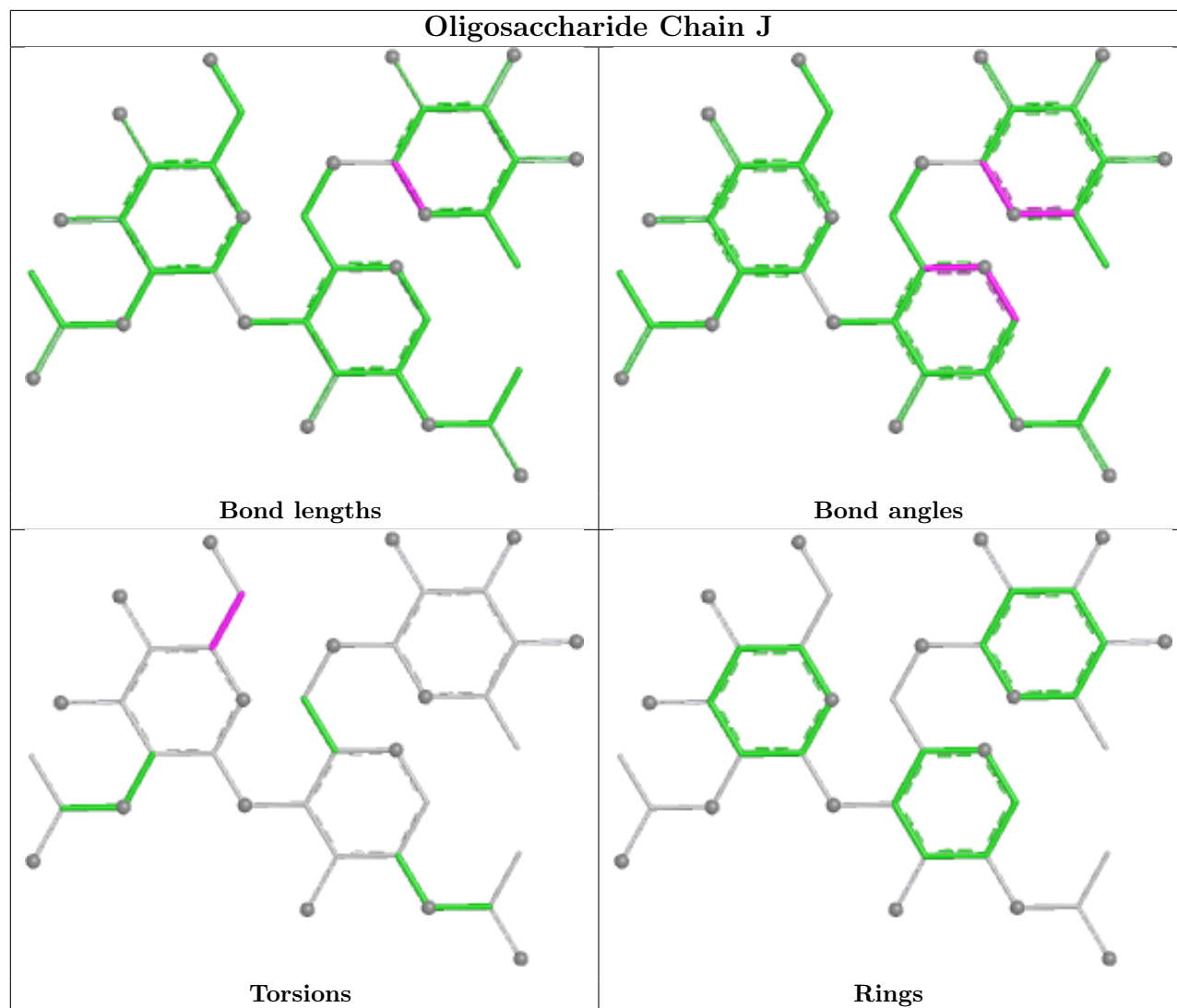
There are no ring outliers.

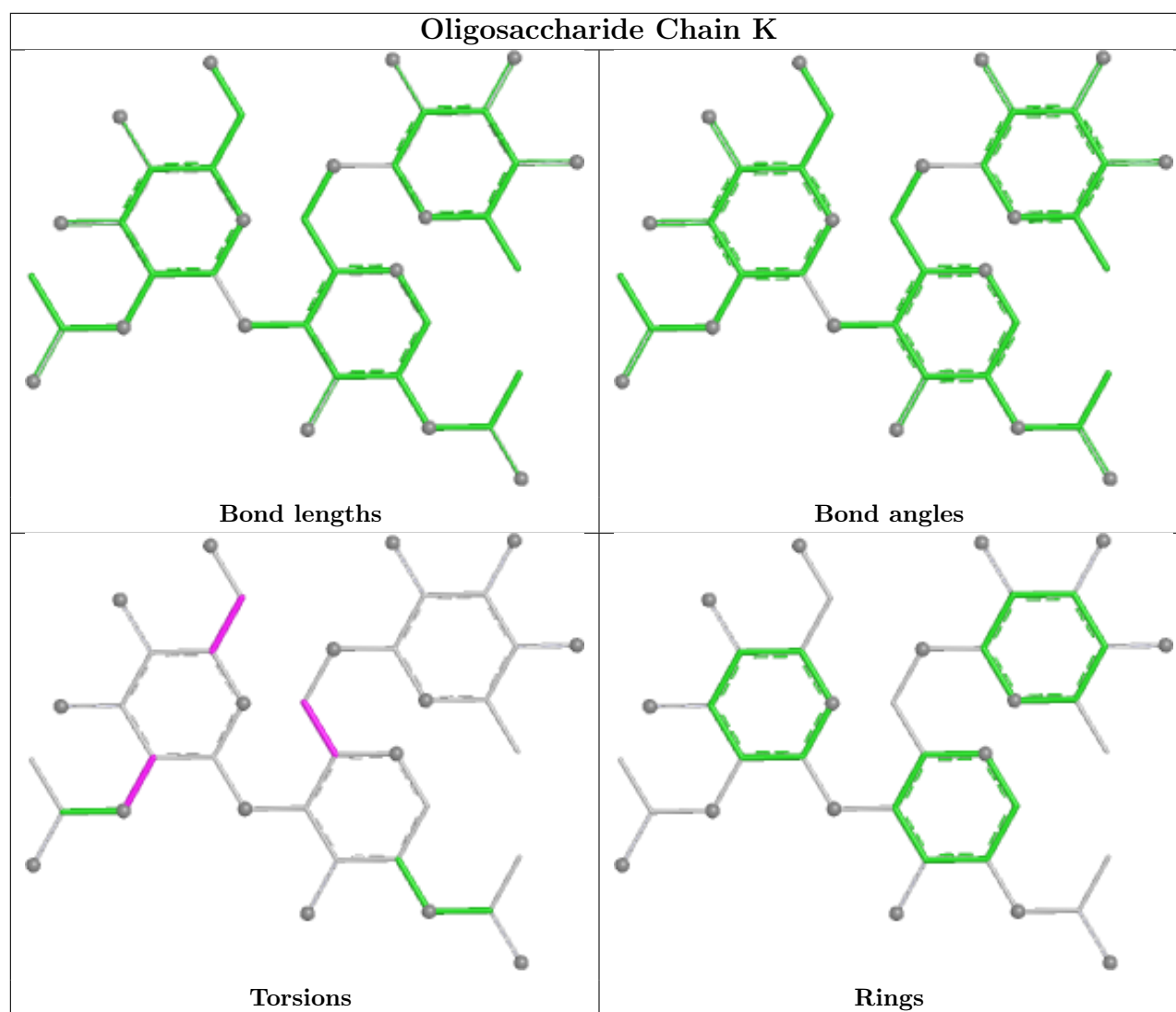
5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	3	FUC	1	0
4	I	3	FUC	0	1
4	K	2	NAG	1	0
4	J	2	NAG	1	0
4	J	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](#)

18 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	504	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	G	506	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	G	505	1	14,14,15	0.29	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	502	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	A	507	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	G	504	1	14,14,15	0.23	0	17,19,21	0.38	0
5	NAG	A	503	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	A	501	1	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	A	505	1	14,14,15	0.20	0	17,19,21	0.46	0
5	NAG	D	501	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	D	503	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	D	504	1	14,14,15	0.29	0	17,19,21	0.45	0
5	NAG	D	505	1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	D	502	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	G	501	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	A	506	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	G	503	1	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	A	502	1	14,14,15	0.33	0	17,19,21	0.46	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	504	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	4/6/23/26	0/1/1/1
5	NAG	G	505	1	-	3/6/23/26	0/1/1/1
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
5	NAG	A	507	1	-	4/6/23/26	0/1/1/1
5	NAG	G	504	1	-	2/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	503	1	-	1/6/23/26	0/1/1/1
5	NAG	D	504	1	-	2/6/23/26	0/1/1/1
5	NAG	D	505	1	-	2/6/23/26	0/1/1/1
5	NAG	D	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	4/6/23/26	0/1/1/1
5	NAG	G	503	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	NAG	O5-C5-C6-O6
5	G	502	NAG	O5-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	D	505	NAG	O5-C5-C6-O6
5	A	506	NAG	O5-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	A	506	NAG	C4-C5-C6-O6
5	A	504	NAG	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6
5	G	506	NAG	O5-C5-C6-O6
5	G	502	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	D	505	NAG	C4-C5-C6-O6
5	G	505	NAG	C8-C7-N2-C2
5	G	505	NAG	O7-C7-N2-C2
5	G	506	NAG	C8-C7-N2-C2
5	G	506	NAG	O7-C7-N2-C2
5	A	506	NAG	C8-C7-N2-C2
5	A	506	NAG	O7-C7-N2-C2
5	A	507	NAG	C8-C7-N2-C2
5	A	507	NAG	O7-C7-N2-C2
5	D	504	NAG	C8-C7-N2-C2
5	D	504	NAG	O7-C7-N2-C2
5	G	503	NAG	O5-C5-C6-O6
5	A	507	NAG	O5-C5-C6-O6
5	G	503	NAG	C4-C5-C6-O6
5	G	504	NAG	O5-C5-C6-O6
5	G	506	NAG	C4-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	507	NAG	C4-C5-C6-O6
5	D	503	NAG	O5-C5-C6-O6
5	D	502	NAG	O5-C5-C6-O6
5	G	504	NAG	C4-C5-C6-O6
5	G	505	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	NAG	1	0
5	D	503	NAG	1	0
5	D	502	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

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	341/353 (96%)	-0.19	4 (1%) 76 62	86, 142, 228, 331	0
1	D	330/353 (93%)	-0.27	3 (0%) 81 68	92, 148, 217, 300	0
1	G	340/353 (96%)	-0.19	7 (2%) 63 47	93, 151, 224, 305	0
2	B	222/234 (94%)	-0.35	1 (0%) 87 77	77, 145, 225, 262	0
2	E	220/234 (94%)	-0.28	2 (0%) 81 68	86, 128, 221, 268	0
2	H	222/234 (94%)	-0.35	1 (0%) 87 77	82, 133, 224, 285	0
3	C	206/209 (98%)	-0.32	0 100 100	69, 140, 212, 269	0
3	F	206/209 (98%)	-0.42	1 (0%) 87 77	95, 143, 202, 265	0
3	L	207/209 (99%)	-0.42	0 100 100	67, 114, 173, 230	0
All	All	2294/2388 (96%)	-0.29	19 (0%) 82 70	67, 141, 219, 331	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	390	LEU	4.5
1	G	75	VAL	4.0
1	G	253	PRO	3.1
1	A	373	MET	3.1
1	D	232	ASN	2.8
1	A	384	TYR	2.7
1	D	69	TRP	2.4
1	G	274	SER	2.4
3	F	61	PHE	2.3
2	E	76(D)	PRO	2.3
1	G	472	GLY	2.3
2	E	205	VAL	2.2
1	D	274	SER	2.1
1	G	361	PHE	2.1
1	A	267	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	345	VAL	2.1
2	B	20	ILE	2.0
2	H	57	VAL	2.0
1	A	488	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

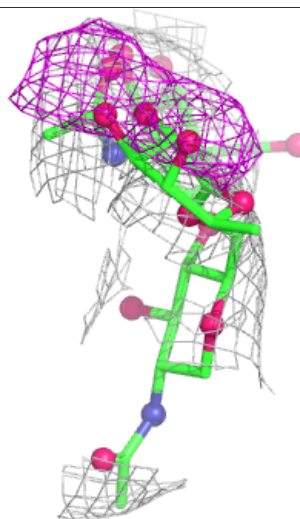
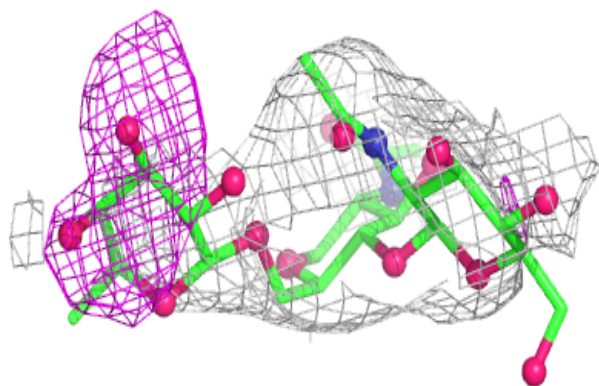
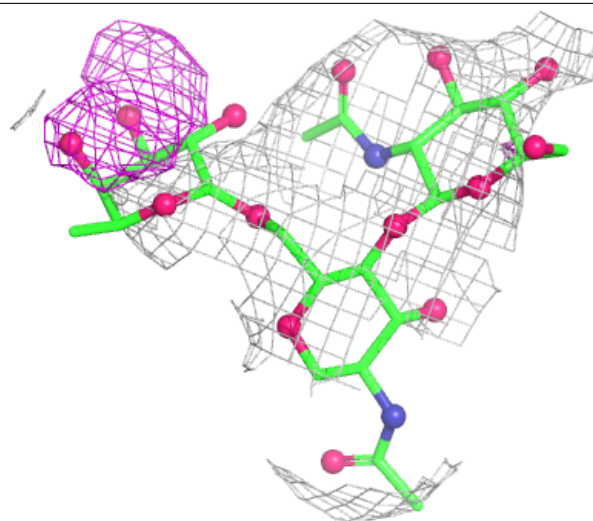
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	-	-	100,114,129,133	0
4	NAG	I	2	14/15	-	-	145,151,158,159	0
4	FUC	I	3	10/11	-	-	139,161,170,180	0
4	NAG	J	2	14/15	0.41	0.09	164,167,172,174	0
4	NAG	K	2	14/15	0.58	0.08	217,223,230,232	0
4	NAG	K	1	14/15	0.65	0.09	164,175,184,199	0
4	NAG	J	1	14/15	0.72	0.09	124,140,151,155	0
4	FUC	J	3	10/11	0.75	0.14	156,161,162,162	0
4	FUC	K	3	10/11	0.78	0.10	159,165,169,173	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.

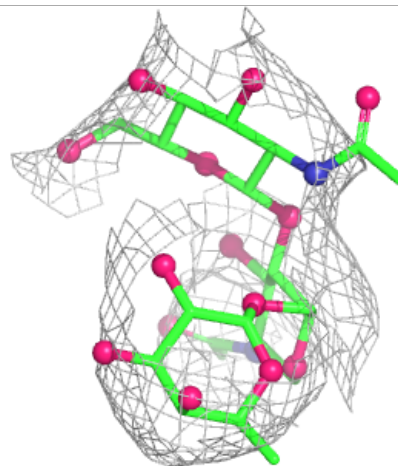
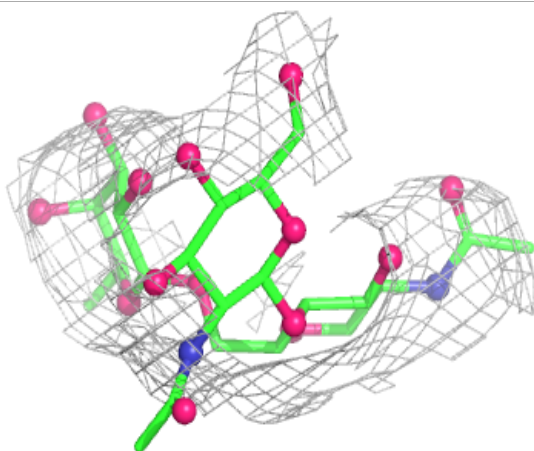
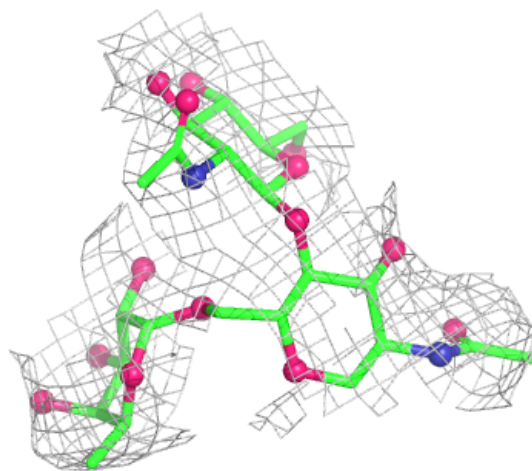
Electron density around Chain I:

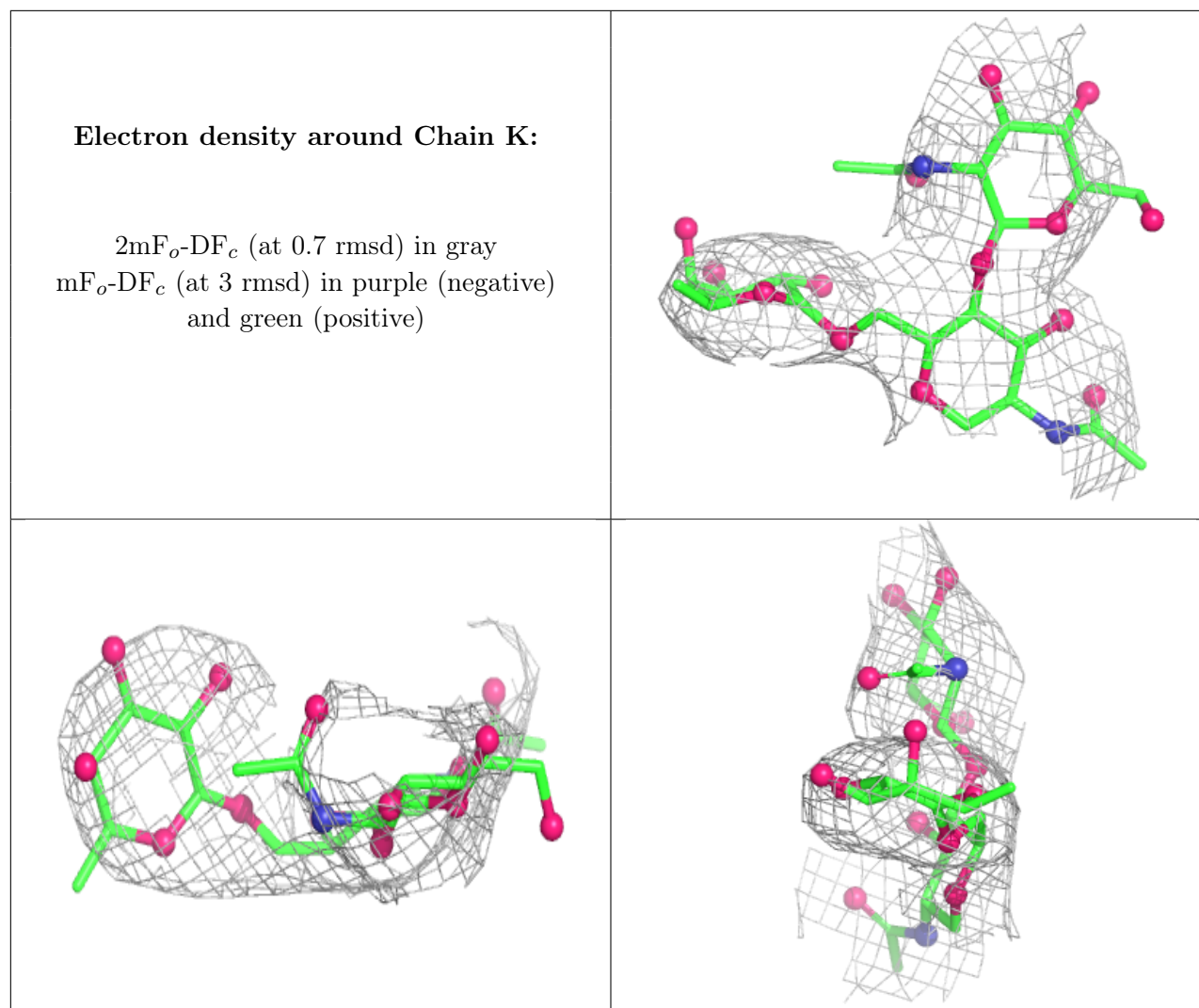
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	506	14/15	0.19	0.11	130,149,155,160	0
5	NAG	A	505	14/15	0.50	0.08	120,133,138,145	0
5	NAG	A	507	14/15	0.51	0.09	121,135,143,145	0
5	NAG	G	504	14/15	0.55	0.12	152,171,173,176	0
5	NAG	D	505	14/15	0.63	0.07	120,132,135,137	0
5	NAG	G	503	14/15	0.67	0.11	112,124,129,131	0
5	NAG	D	503	14/15	0.68	0.09	137,156,159,161	0
5	NAG	D	504	14/15	0.73	0.08	121,127,131,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	502	14/15	0.73	0.10	143,155,165,167	0
5	NAG	A	504	14/15	0.74	0.09	136,151,170,175	0
5	NAG	A	506	14/15	0.76	0.07	100,109,113,114	0
5	NAG	G	505	14/15	0.80	0.06	107,116,125,126	0
5	NAG	G	502	14/15	0.80	0.06	131,144,150,152	0
5	NAG	D	501	14/15	0.82	0.07	138,144,146,147	0
5	NAG	A	501	14/15	0.86	0.06	123,134,138,138	0
5	NAG	G	501	14/15	0.87	0.08	113,121,124,125	0
5	NAG	D	502	14/15	0.94	0.08	113,119,136,139	0
5	NAG	A	503	14/15	0.94	0.06	93,98,100,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.