



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 AM UTC

PDB ID : 5I9Q / pdb_00005i9q
Title : Crystal structure of 3BNC55 Fab in complex with 426c.TM4deltaV1-3 gp120
Authors : Scharf, L.; Chen, C.; Bjorkman, P.J.
Deposited on : 2016-02-20
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

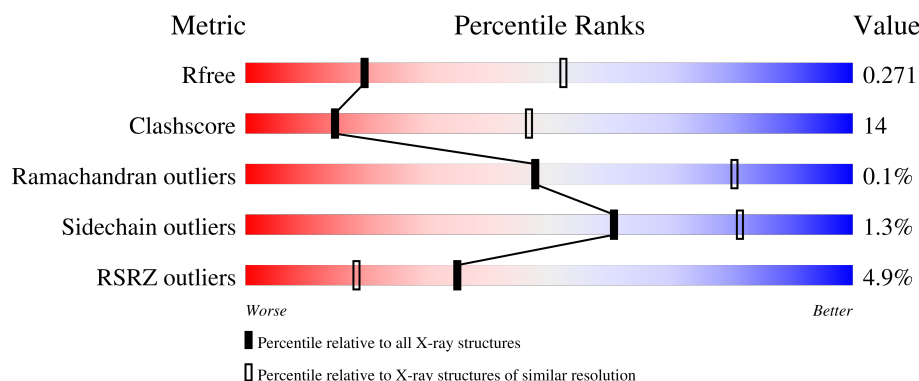
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	4% 76% 20% .
1	G	353	2% 78% 18% .
2	B	225	10% 62% 27% 10%
2	H	225	2% 78% 16% 5%
3	C	207	11% 60% 37% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	207	
4	D	6	
5	E	4	

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
7	EDO	G	605	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11445 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 426c.TM4dV1-3 p120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2497	1564	429	482	22			
1	G	339	Total	C	N	O	S	0	0	0
			2535	1594	435	484	22			

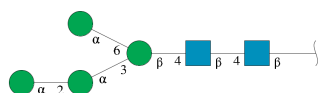
- Molecule 2 is a protein called 3BNC55 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	202	Total	C	N	O	S	0	0	0
			1497	954	251	285	7			
2	H	213	Total	C	N	O	S	0	0	0
			1630	1037	272	314	7			

- Molecule 3 is a protein called 3BNC55 light chain.

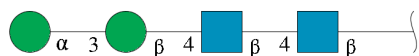
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1442	908	233	295	6			
3	L	206	Total	C	N	O	S	0	0	0
			1560	975	264	315	6			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



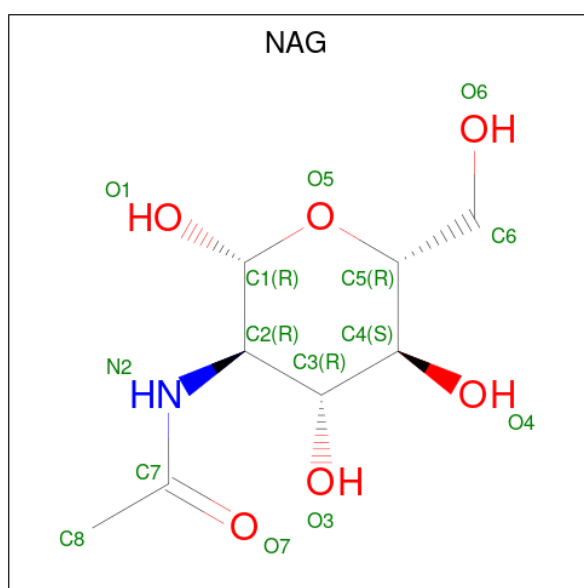
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
5	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



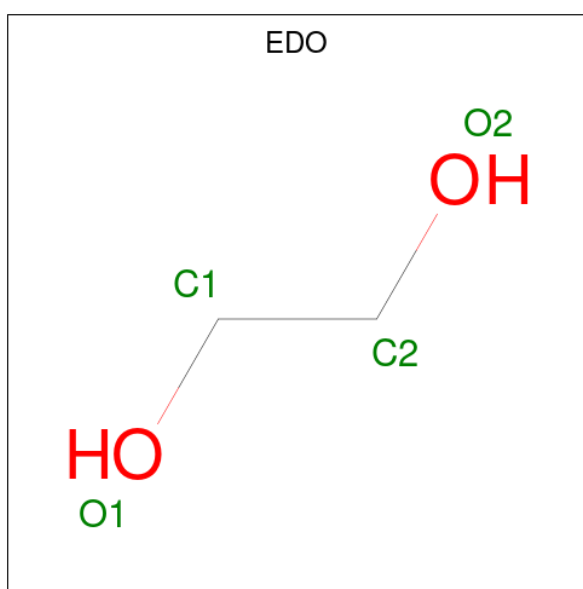
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

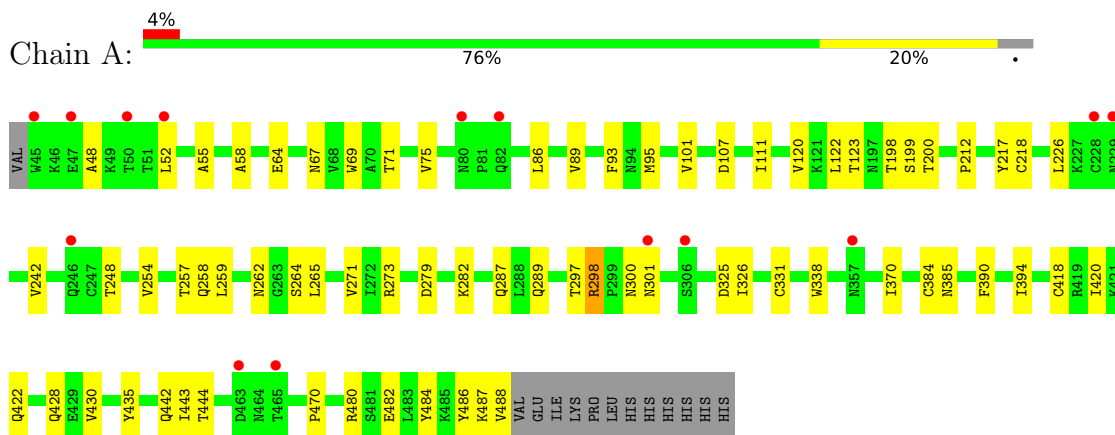


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			10	6	4		

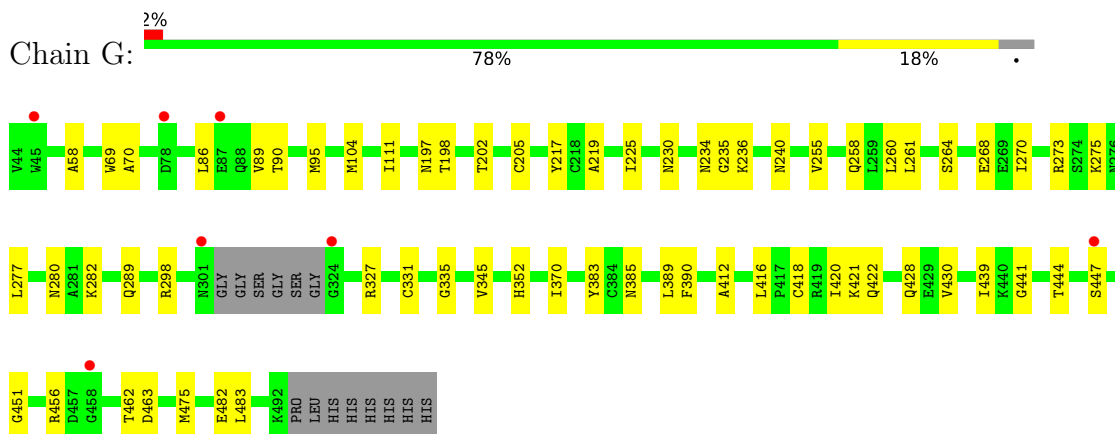
3 Residue-property plots [i](#)

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.

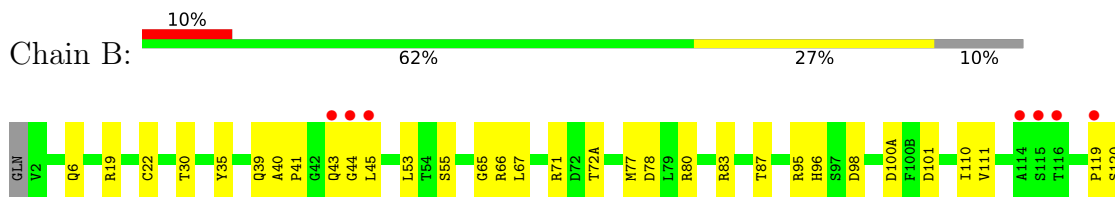
- Molecule 1: 426c.TM4dV1-3 p120

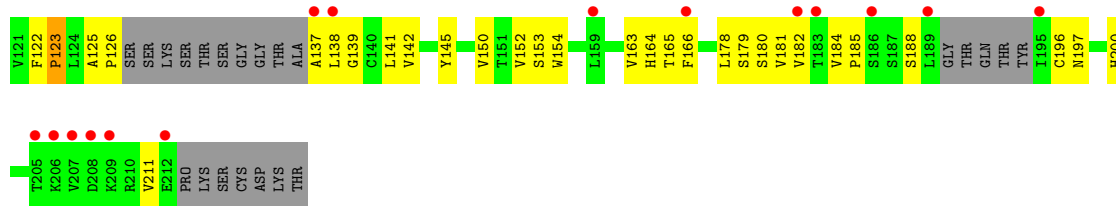


- Molecule 1: 426c.TM4dV1-3 p120

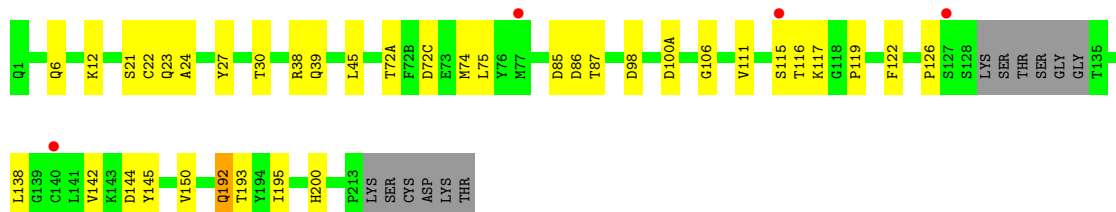
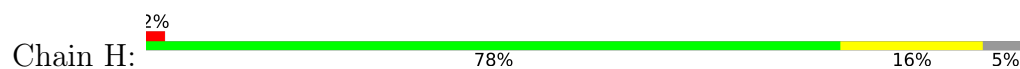


- Molecule 2: 3BNC55 Fab heavy chain

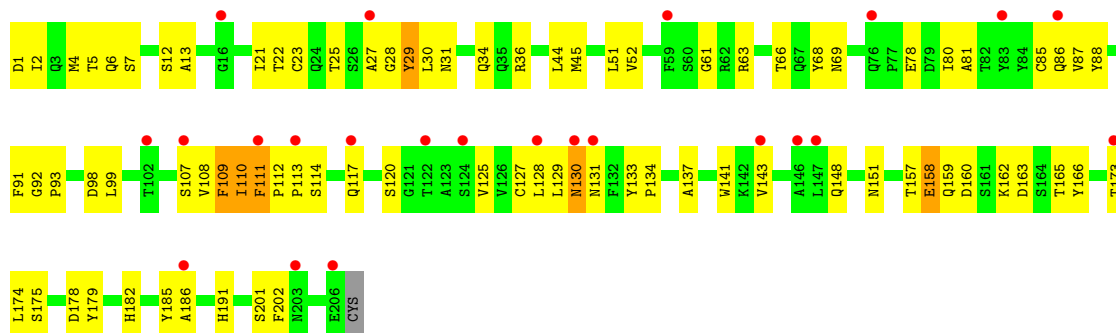




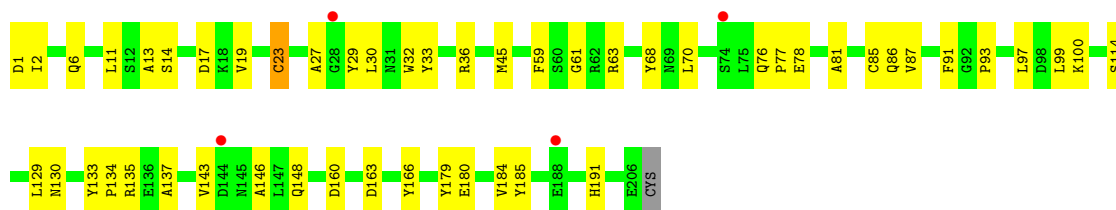
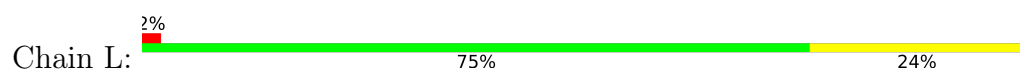
• Molecule 2: 3BNC55 Fab heavy chain



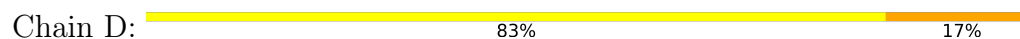
• Molecule 3: 3BNC55 light chain



• Molecule 3: 3BNC55 light chain



• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.85Å 122.85Å 264.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.54 – 3.00 37.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (37.54-3.00) 80.3 (37.54-3.00)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.251 , 0.270 0.256 , 0.271	Depositor DCC
R_{free} test set	2028 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11445	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, PGE, NAG, EDO, MAN

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	0.23	0/2550	0.41	3/3486 (0.1%)
1	G	0.20	0/2587	0.37	0/3532
2	B	0.32	0/1539	0.61	3/2110 (0.1%)
2	H	0.21	0/1676	0.40	0/2292
3	C	0.53	0/1474	0.79	10/2024 (0.5%)
3	L	0.24	0/1595	0.45	2/2178 (0.1%)
All	All	0.29	0/11421	0.50	18/15622 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	SER	N-CA-C	-7.79	98.95	110.48
3	C	29	TYR	N-CA-C	7.01	121.20	111.74
3	C	130	ASN	N-CA-C	6.63	119.97	108.76
1	A	298	ARG	N-CA-C	-6.28	95.74	109.11
3	C	7	SER	C-N-CD	6.18	134.21	120.60
3	L	130	ASN	N-CA-C	5.91	118.53	108.90
3	C	158	GLU	N-CA-C	-5.79	102.19	110.59
2	B	184	VAL	CA-C-N	-5.64	113.74	119.83
2	B	184	VAL	C-N-CA	-5.64	113.74	119.83
3	C	111	PHE	CA-C-N	-5.52	114.69	120.38
3	C	111	PHE	C-N-CA	-5.52	114.69	120.38
1	A	298	ARG	CA-C-N	-5.40	114.40	119.85
1	A	298	ARG	C-N-CA	-5.40	114.40	119.85
3	C	112	PRO	CA-C-N	-5.38	114.38	119.76
3	C	112	PRO	C-N-CA	-5.38	114.38	119.76
3	C	7	SER	CA-C-N	-5.37	114.12	127.00
3	C	7	SER	C-N-CA	-5.37	114.12	127.00
3	L	129	LEU	N-CA-C	-5.13	100.81	109.07

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	2497	0	2286	59	0
1	G	2535	0	2375	41	0
2	B	1497	0	1366	58	0
2	H	1630	0	1556	32	0
3	C	1442	0	1263	97	0
3	L	1560	0	1452	35	0
4	D	72	0	61	5	0
5	E	50	0	43	3	0
6	A	70	0	65	0	0
6	C	14	0	13	0	0
6	G	42	0	39	3	0
6	L	14	0	13	0	0
7	A	8	0	12	0	0
7	G	4	0	6	0	0
8	G	10	0	14	0	0
All	All	11445	0	10564	306	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 (306) 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:273:ARG:NH1	1:A:484:TYR:CE1	1.99	1.27
1:A:273:ARG:NH1	1:A:484:TYR:CD1	2.02	1.26
2:B:138:LEU:O	2:B:181:VAL:HB	1.50	1.10
1:A:212:PRO:HG2	4:D:1:NAG:O7	1.51	1.09
1:A:297:THR:HG23	1:A:444:THR:HG22	1.39	1.04
1:A:248:THR:HG22	1:A:486:TYR:CE2	1.94	1.02
1:A:248:THR:HG22	1:A:486:TYR:CD2	1.97	0.99
3:C:23:CYS:SG	3:C:30:LEU:HD11	2.05	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:CG2	1:A:486:TYR:CD2	2.48	0.95
2:B:126:PRO:HB3	2:B:137:ALA:O	1.68	0.92
1:A:212:PRO:CG	4:D:1:NAG:O7	2.18	0.91
3:C:179:TYR:CE1	3:C:185:TYR:CE1	2.59	0.89
3:C:179:TYR:HE1	3:C:185:TYR:CE1	1.90	0.88
1:A:297:THR:HG23	1:A:444:THR:CG2	2.06	0.85
2:B:19:ARG:NE	2:B:78:ASP:OD1	2.11	0.84
1:A:248:THR:CG2	1:A:486:TYR:CE2	2.60	0.83
1:A:297:THR:CG2	1:A:444:THR:HG22	2.09	0.83
3:C:175:SER:OG	3:C:178:ASP:OD2	1.98	0.81
1:G:430:VAL:CG1	2:H:72(A):THR:HG21	2.12	0.79
1:A:273:ARG:NH2	1:A:287:GLN:OE1	2.16	0.79
3:C:98:ASP:CB	3:C:159:GLN:NE2	2.46	0.77
1:A:248:THR:HG21	1:A:486:TYR:CD2	2.19	0.77
3:L:14:SER:OG	3:L:17:ASP:OD2	2.04	0.76
1:G:280:ASN:ND2	1:G:456:ARG:O	2.18	0.76
1:A:273:ARG:NH1	1:A:484:TYR:CG	2.54	0.75
1:A:212:PRO:CD	4:D:1:NAG:O7	2.37	0.73
3:C:2:ILE:HG13	3:C:27:ALA:CB	2.17	0.73
3:C:128:LEU:C	3:C:129:LEU:HD12	2.15	0.71
1:A:212:PRO:HD2	4:D:1:NAG:O7	1.91	0.71
3:C:148:GLN:HB3	3:C:151:ASN:HD21	1.56	0.70
3:C:131:ASN:HA	3:C:165:THR:HB	1.72	0.70
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.73	0.69
3:C:2:ILE:HG13	3:C:27:ALA:HB3	1.74	0.69
1:G:298:ARG:NH1	1:G:441:GLY:O	2.26	0.68
2:B:153:SER:O	2:B:197:ASN:N	2.19	0.68
1:G:298:ARG:NH2	1:G:439:ILE:O	2.28	0.66
3:C:6:GLN:HG2	3:C:23:CYS:HB3	1.77	0.65
2:B:138:LEU:C	2:B:181:VAL:HB	2.22	0.65
3:C:179:TYR:CD1	3:C:185:TYR:CZ	2.85	0.65
2:B:145:TYR:CE2	2:B:150:VAL:CG2	2.80	0.65
2:B:145:TYR:CE2	2:B:150:VAL:HG23	2.32	0.65
3:C:6:GLN:HG3	3:C:23:CYS:HB2	1.79	0.64
2:H:192:GLN:OE1	2:H:193:THR:N	2.31	0.64
3:C:98:ASP:CB	3:C:159:GLN:HE22	2.10	0.63
1:G:234:ASN:O	1:G:273:ARG:HG2	1.98	0.63
1:G:447:SER:HB3	5:E:1:NAG:HN2	1.63	0.63
3:L:143:VAL:CG2	3:L:148:GLN:HE21	2.12	0.62
1:G:430:VAL:HG11	2:H:72(A):THR:HG21	1.82	0.62
3:L:27:ALA:HB1	3:L:87:VAL:HG21	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:THR:HG22	3:C:66:THR:O	2.00	0.62
3:C:179:TYR:HD1	3:C:185:TYR:OH	1.83	0.62
3:C:22:THR:OG1	3:C:69:ASN:OD1	2.12	0.61
3:C:131:ASN:CA	3:C:165:THR:HB	2.31	0.61
2:H:145:TYR:CE1	2:H:150:VAL:HG23	2.34	0.61
3:C:179:TYR:HD1	3:C:185:TYR:CZ	2.19	0.61
1:A:264:SER:OG	1:A:482:GLU:OE1	2.18	0.61
3:C:29:TYR:HD2	3:C:88:TYR:HH	1.48	0.60
3:C:131:ASN:C	3:C:165:THR:HB	2.27	0.59
1:A:93:PHE:HE2	1:A:487:LYS:CB	2.16	0.59
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.83	0.59
1:G:86:LEU:HB3	1:G:89:VAL:HG11	1.83	0.59
3:C:45:MET:HE1	3:C:61:GLY:HA3	1.84	0.59
3:C:159:GLN:CG	3:C:166:TYR:CZ	2.86	0.59
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.85	0.59
1:A:282:LYS:NZ	2:B:98:ASP:OD1	2.28	0.59
2:H:39:GLN:HB3	2:H:45:LEU:HD23	1.84	0.58
1:A:93:PHE:CE2	1:A:487:LYS:CB	2.85	0.58
1:A:273:ARG:NH1	1:A:484:TYR:CZ	2.49	0.58
2:B:39:GLN:HB3	2:B:45:LEU:HD23	1.85	0.58
1:G:95:MET:HE2	1:G:235:GLY:HA3	1.86	0.58
2:B:163:VAL:HG22	2:B:182:VAL:CB	2.34	0.58
3:C:131:ASN:HA	3:C:165:THR:CB	2.33	0.57
2:B:87:THR:HG23	2:B:110:ILE:HA	1.86	0.57
2:B:122:PHE:O	2:B:141:LEU:HB3	2.04	0.56
3:C:131:ASN:HA	3:C:165:THR:HG1	1.70	0.56
3:C:2:ILE:HG13	3:C:27:ALA:HB2	1.88	0.56
3:C:109:PHE:N	3:C:109:PHE:CD2	2.74	0.55
3:C:179:TYR:HD1	3:C:185:TYR:HH	1.51	0.55
2:B:138:LEU:O	2:B:181:VAL:CB	2.40	0.55
1:A:430:VAL:HG11	2:B:72(A):THR:HG21	1.88	0.55
3:C:4:MET:HE2	3:C:92:GLY:HA2	1.89	0.55
2:B:163:VAL:HA	2:B:182:VAL:CB	2.37	0.54
2:H:142:VAL:HG11	2:H:150:VAL:HG11	1.88	0.54
3:C:107:SER:HB2	3:C:109:PHE:HE2	1.72	0.54
2:B:43:GLN:HG3	2:B:44:GLY:N	2.23	0.53
3:C:159:GLN:NE2	3:C:166:TYR:OH	2.36	0.53
1:A:55:ALA:HA	1:A:75:VAL:O	2.09	0.53
3:C:108:VAL:C	3:C:109:PHE:CD2	2.87	0.53
3:C:159:GLN:HG2	3:C:166:TYR:CE2	2.43	0.53
3:L:27:ALA:CB	3:L:87:VAL:HG21	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLY:O	2:B:80:ARG:CZ	2.57	0.53
2:B:185:PRO:HD2	2:B:188:SER:CB	2.39	0.53
3:C:2:ILE:CG1	3:C:27:ALA:HB3	2.39	0.53
3:C:159:GLN:HG3	3:C:166:TYR:CZ	2.44	0.53
2:H:23:GLN:HG3	2:H:74:MET:HG2	1.90	0.53
2:B:185:PRO:HD2	2:B:188:SER:HB3	1.90	0.52
3:C:159:GLN:HG2	3:C:166:TYR:CZ	2.44	0.52
3:L:63:ARG:HD3	3:L:68:TYR:CE1	2.45	0.52
3:C:129:LEU:CD1	3:C:129:LEU:N	2.72	0.52
2:B:145:TYR:CE2	2:B:150:VAL:HG21	2.45	0.52
3:C:30:LEU:HD23	3:C:31:ASN:N	2.24	0.52
3:C:148:GLN:OE1	3:C:151:ASN:ND2	2.42	0.52
3:C:157:THR:HG22	3:C:158:GLU:O	2.10	0.52
1:A:298:ARG:NH1	1:A:326:ILE:O	2.40	0.52
1:G:430:VAL:HG13	2:H:72(A):THR:HG21	1.91	0.52
3:L:2:ILE:CG1	3:L:27:ALA:HB2	2.39	0.51
2:H:12:LYS:O	2:H:111:VAL:HA	2.10	0.51
2:H:38:ARG:NH2	2:H:85:ASP:O	2.42	0.51
2:B:65:GLY:O	2:B:80:ARG:NH1	2.43	0.51
3:C:4:MET:SD	3:C:87:VAL:HG12	2.51	0.51
3:C:6:GLN:HG2	3:C:23:CYS:CB	2.40	0.51
1:A:390:PHE:CG	1:A:470:PRO:HG3	2.46	0.51
3:C:98:ASP:CB	3:C:159:GLN:HE21	2.24	0.51
1:G:430:VAL:HG21	2:H:30:THR:HG21	1.93	0.51
3:C:111:PHE:N	3:C:111:PHE:CD2	2.79	0.51
3:C:6:GLN:CG	3:C:23:CYS:CB	2.89	0.51
3:C:160:ASP:OD1	3:C:162:LYS:N	2.41	0.51
3:L:76:GLN:HG2	3:L:77:PRO:HD2	1.92	0.51
3:C:129:LEU:HD12	3:C:129:LEU:N	2.23	0.51
2:H:150:VAL:HG22	2:H:200:HIS:HD2	1.74	0.51
3:C:34:GLN:HB2	3:C:44:LEU:HD11	1.92	0.50
3:C:111:PHE:CE2	3:C:128:LEU:HD12	2.45	0.50
1:A:226:LEU:HD22	1:A:242:VAL:CG1	2.42	0.50
1:G:430:VAL:HG11	2:H:72(A):THR:CG2	2.41	0.50
1:A:428:GLN:OE1	1:A:428:GLN:N	2.37	0.50
3:L:143:VAL:HG13	3:L:184:VAL:O	2.12	0.50
2:B:100(A):ASP:N	2:B:100(A):ASP:OD1	2.45	0.49
3:C:179:TYR:CD1	3:C:185:TYR:CE1	2.99	0.49
1:G:258:GLN:NE2	1:G:370:ILE:O	2.46	0.49
2:H:85:ASP:OD1	2:H:85:ASP:N	2.45	0.49
3:L:6:GLN:HB3	3:L:93:PRO:HG2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:TYR:O	3:L:87:VAL:HG23	2.13	0.49
1:A:212:PRO:HG2	4:D:1:NAG:C7	2.36	0.49
3:C:31:ASN:HB2	3:C:86:GLN:HG2	1.95	0.49
2:H:87:THR:HG22	2:H:111:VAL:H	1.77	0.49
2:B:6:GLN:HG2	2:B:22:CYS:SG	2.53	0.49
3:C:4:MET:HE3	3:C:85:CYS:SG	2.52	0.49
3:C:107:SER:CB	3:C:109:PHE:HE2	2.24	0.49
3:L:143:VAL:CG2	3:L:148:GLN:NE2	2.74	0.49
1:G:240:ASN:HD21	6:G:602:NAG:C7	2.24	0.49
2:H:145:TYR:CE1	2:H:150:VAL:CG2	2.96	0.49
2:B:180:SER:O	2:B:181:VAL:HG13	2.13	0.49
3:L:143:VAL:HG23	3:L:148:GLN:HG3	1.94	0.49
3:L:160:ASP:HB3	3:L:163:ASP:OD1	2.13	0.48
3:C:6:GLN:CG	3:C:23:CYS:HB2	2.43	0.48
1:A:297:THR:HG22	1:A:298:ARG:N	2.28	0.48
3:C:179:TYR:HE1	3:C:185:TYR:CD1	2.27	0.48
3:C:107:SER:CB	3:C:109:PHE:CE2	2.97	0.48
3:C:133:TYR:CD1	3:C:134:PRO:HA	2.49	0.48
1:G:104:MET:HE3	1:G:483:LEU:HD11	1.95	0.47
3:C:80:ILE:O	3:C:80:ILE:HG13	2.13	0.47
3:L:143:VAL:O	3:L:146:ALA:HB3	2.13	0.47
1:A:279:ASP:OD2	2:B:95:ARG:NH2	2.45	0.47
3:C:80:ILE:O	3:C:80:ILE:CG1	2.61	0.47
3:C:110:ILE:HD13	3:C:202:PHE:HD2	1.80	0.47
2:H:6:GLN:OE1	2:H:106:GLY:N	2.40	0.47
3:L:143:VAL:HG23	3:L:148:GLN:HE21	1.78	0.47
1:A:86:LEU:HD23	1:A:89:VAL:HG11	1.96	0.47
3:L:13:ALA:O	3:L:100:LYS:N	2.47	0.47
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.97	0.47
1:G:282:LYS:NZ	2:H:98:ASP:OD1	2.46	0.47
2:B:178:LEU:HD12	2:B:179:SER:H	1.78	0.47
3:C:36:ARG:HA	3:C:81:ALA:HB1	1.95	0.47
1:G:197:ASN:OD1	1:G:198:THR:N	2.47	0.47
1:G:230:ASN:ND2	6:G:602:NAG:O7	2.47	0.47
1:A:123:THR:HG23	1:A:198:THR:H	1.80	0.47
3:C:117:GLN:O	3:C:120:SER:HB2	2.15	0.47
3:C:137:ALA:HB2	3:C:191:HIS:HD2	1.79	0.47
1:G:236:LYS:NZ	1:G:275:LYS:O	2.45	0.46
3:C:12:SER:HA	3:C:98:ASP:O	2.15	0.46
3:L:23:CYS:SG	3:L:30:LEU:HD11	2.55	0.46
3:L:135:ARG:HB2	3:L:166:TYR:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:LEU:HD12	3:L:91:PHE:CE2	2.51	0.46
3:C:163:ASP:OD1	3:C:165:THR:HG23	2.16	0.46
2:H:100(A):ASP:OD1	2:H:100(A):ASP:N	2.49	0.46
1:A:248:THR:HG21	1:A:486:TYR:HD2	1.79	0.46
1:G:95:MET:HE1	1:G:234:ASN:O	2.16	0.46
2:B:35:TYR:OH	2:B:95:ARG:NH1	2.49	0.46
2:B:142:VAL:O	2:B:142:VAL:HG23	2.16	0.46
3:L:33:TYR:HE1	3:L:86:GLN:HG2	1.81	0.46
1:A:200:THR:HG21	1:G:202:THR:OG1	2.16	0.46
1:A:258:GLN:NE2	1:A:370:ILE:O	2.49	0.46
1:A:422:GLN:NE2	1:A:435:TYR:O	2.47	0.46
1:G:383:TYR:CE2	1:G:421:LYS:HB2	2.51	0.46
2:B:71:ARG:HH21	2:B:72(A):THR:HG23	1.81	0.46
2:B:154:TRP:CZ2	2:B:181:VAL:HA	2.51	0.46
2:B:165:THR:HG23	2:B:180:SER:HB2	1.98	0.46
1:A:442:GLN:HG2	1:A:444:THR:HG23	1.97	0.45
3:C:5:THR:O	3:C:23:CYS:HA	2.16	0.45
2:H:115:SER:O	2:H:116:THR:OG1	2.26	0.45
1:A:58:ALA:HB1	1:A:71:THR:HG23	1.97	0.45
5:E:1:NAG:H62	5:E:2:NAG:C7	2.46	0.45
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.99	0.45
2:B:185:PRO:HB2	2:B:188:SER:CB	2.47	0.45
3:C:6:GLN:CG	3:C:23:CYS:HB3	2.45	0.45
1:A:69:TRP:CD2	1:A:111:ILE:HG12	2.52	0.45
1:A:107:ASP:OD2	1:A:217:TYR:OH	2.31	0.45
1:A:297:THR:HA	1:A:443:ILE:O	2.17	0.45
2:B:96:HIS:ND1	2:B:101:ASP:OD1	2.41	0.45
3:C:113:PRO:HD3	3:C:125:VAL:HG22	1.99	0.45
1:A:48:ALA:O	1:A:488:VAL:O	2.35	0.45
1:A:271:VAL:CG1	1:A:273:ARG:HE	2.29	0.45
1:A:271:VAL:HG11	1:A:273:ARG:NE	2.32	0.45
1:A:331:CYS:SG	1:A:384:CYS:SG	3.15	0.45
1:G:58:ALA:HB2	1:G:70:ALA:HB3	1.99	0.44
3:L:59:PHE:HD2	3:L:70:LEU:HD11	1.82	0.44
1:G:335:GLY:HA3	1:G:412:ALA:O	2.17	0.44
2:B:43:GLN:HG3	2:B:44:GLY:H	1.82	0.44
1:G:428:GLN:OE1	1:G:428:GLN:N	2.43	0.44
2:H:21:SER:HA	2:H:75:LEU:O	2.18	0.44
3:C:6:GLN:HB2	3:C:93:PRO:HD2	2.00	0.44
2:B:67:LEU:HD11	2:B:77:MET:SD	2.58	0.44
3:C:6:GLN:HB2	3:C:93:PRO:CG	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:TYR:CE1	3:C:185:TYR:CZ	3.01	0.44
3:L:133:TYR:CD1	3:L:134:PRO:HA	2.53	0.44
2:B:30:THR:HG23	2:B:53:LEU:HA	1.99	0.44
3:C:28:GLY:O	3:C:87:VAL:HG21	2.18	0.44
3:L:36:ARG:NH1	3:L:78:GLU:O	2.51	0.44
3:C:1:ASP:C	3:C:2:ILE:HD12	2.43	0.44
1:G:90:THR:HG22	1:G:240:ASN:HA	2.00	0.43
3:C:148:GLN:HB3	3:C:151:ASN:ND2	2.27	0.43
3:L:27:ALA:HB3	3:L:87:VAL:HG11	2.00	0.43
1:G:69:TRP:CD2	1:G:111:ILE:HG12	2.53	0.43
1:A:254:VAL:HG21	1:A:262:ASN:HB2	2.01	0.43
3:C:131:ASN:OD1	3:C:165:THR:OG1	2.35	0.43
2:H:38:ARG:NH2	2:H:86:ASP:HA	2.33	0.43
2:H:72(C):ASP:HB3	2:H:74:MET:HG3	2.00	0.43
3:L:45:MET:HE1	3:L:61:GLY:HA3	1.99	0.43
1:G:255:VAL:HG13	1:G:475:MET:SD	2.58	0.43
3:C:30:LEU:HA	3:C:86:GLN:O	2.18	0.43
3:C:110:ILE:HD13	3:C:202:PHE:CD2	2.54	0.43
3:L:32:TRP:CZ3	3:L:85:CYS:HB3	2.53	0.43
1:G:327:ARG:NH1	1:G:422:GLN:OE1	2.46	0.43
1:G:389:LEU:HD12	1:G:390:PHE:CD1	2.53	0.43
2:B:154:TRP:CH2	2:B:196:CYS:SG	3.12	0.43
2:H:122:PHE:HB3	3:L:114:SER:OG	2.19	0.43
1:G:268:GLU:O	1:G:289:GLN:NE2	2.52	0.43
3:C:173:THR:C	3:C:174:LEU:HD12	2.43	0.43
1:G:462:THR:HG23	1:G:463:ASP:N	2.34	0.43
3:L:1:ASP:C	3:L:2:ILE:HD12	2.44	0.43
3:C:186:ALA:HA	3:C:201:SER:HB3	2.01	0.43
1:A:257:THR:O	1:A:259:LEU:N	2.48	0.42
1:G:389:LEU:CD2	1:G:416:LEU:HD21	2.49	0.42
2:B:65:GLY:O	2:B:80:ARG:NH2	2.51	0.42
3:C:25:THR:O	3:C:25:THR:HG23	2.19	0.42
3:C:157:THR:HG22	3:C:158:GLU:N	2.35	0.42
3:L:11:LEU:HD21	3:L:19:VAL:HG13	2.00	0.42
1:G:331:CYS:SG	1:G:418:CYS:SG	3.17	0.42
3:C:28:GLY:O	3:C:87:VAL:CG2	2.67	0.42
3:L:179:TYR:O	3:L:185:TYR:OH	2.38	0.42
3:C:29:TYR:HD2	3:C:88:TYR:OH	2.02	0.42
3:C:143:VAL:CG1	3:C:182:HIS:CB	2.97	0.42
1:A:95:MET:HE3	1:A:484:TYR:HB3	2.01	0.42
1:A:123:THR:HG22	1:A:199:SER:OG	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:N	6:G:601:NAG:O4	2.53	0.42
2:B:145:TYR:CD2	2:B:150:VAL:CG2	3.03	0.42
3:L:2:ILE:HG13	3:L:27:ALA:HB2	2.01	0.42
2:B:83:ARG:O	2:B:111:VAL:HG11	2.20	0.42
3:L:30:LEU:HA	3:L:86:GLN:O	2.19	0.42
1:A:331:CYS:SG	1:A:418:CYS:SG	3.18	0.42
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.54	0.42
2:H:87:THR:CG2	2:H:111:VAL:H	2.33	0.42
3:L:36:ARG:HG2	3:L:81:ALA:HB2	2.01	0.42
3:C:63:ARG:CB	3:C:68:TYR:CD2	3.03	0.42
2:H:6:GLN:HG2	2:H:22:CYS:SG	2.59	0.42
3:L:137:ALA:HB2	3:L:191:HIS:HD2	1.84	0.42
1:G:277:LEU:HD13	1:G:352:HIS:HB3	2.01	0.42
2:H:119:PRO:HB2	2:H:142:VAL:HG13	2.02	0.42
3:L:99:LEU:HD23	3:L:99:LEU:HA	1.95	0.42
1:G:264:SER:OG	1:G:482:GLU:OE1	2.28	0.41
1:G:270:ILE:HD13	1:G:345:VAL:HG22	2.02	0.41
3:C:13:ALA:O	3:C:99:LEU:HA	2.20	0.41
2:B:55:SER:CB	2:B:71:ARG:HE	2.33	0.41
2:B:152:VAL:HA	2:B:197:ASN:O	2.20	0.41
1:A:120:VAL:HG12	1:A:122:LEU:HD22	2.02	0.41
2:B:150:VAL:HG22	2:B:200:HIS:HD2	1.85	0.41
2:B:166:PHE:O	2:B:178:LEU:HD11	2.20	0.41
1:A:52:LEU:HB3	1:A:218:CYS:O	2.20	0.41
1:G:104:MET:HE2	1:G:217:TYR:CE2	2.56	0.41
2:B:142:VAL:HG23	2:B:178:LEU:HB3	2.03	0.41
2:B:164:HIS:CE1	3:C:130:ASN:OD1	2.74	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.56	0.41
1:A:265:LEU:HD21	1:A:289:GLN:HA	2.02	0.41
1:A:390:PHE:CD1	1:A:470:PRO:HG3	2.55	0.41
3:C:127:CYS:HB2	3:C:141:TRP:CH2	2.55	0.41
1:G:261:LEU:HD13	5:E:1:NAG:H82	2.02	0.41
3:C:51:LEU:HD23	3:C:52:VAL:O	2.21	0.41
2:B:123:PRO:HD2	3:C:114:SER:HB3	2.03	0.41
3:C:6:GLN:OE1	3:C:85:CYS:SG	2.79	0.41
1:A:64:GLU:OE1	1:A:67:ASN:ND2	2.49	0.41
2:B:45:LEU:HD12	3:C:91:PHE:CE2	2.56	0.41
2:B:180:SER:O	2:B:181:VAL:CG1	2.68	0.41
3:C:166:TYR:CD2	3:C:166:TYR:N	2.89	0.41
1:A:300:ASN:OD1	1:A:301:ASN:N	2.54	0.41
1:A:338:TRP:CD1	1:A:394:ILE:HD13	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ALA:O	3:C:111:PHE:HD1	2.04	0.41
3:C:2:ILE:CG1	3:C:27:ALA:CB	2.94	0.41
1:G:260:LEU:HD12	1:G:451:GLY:HA3	2.03	0.40
2:B:185:PRO:O	2:B:188:SER:HB3	2.21	0.40
2:H:145:TYR:CD1	2:H:150:VAL:CG2	3.04	0.40
2:B:45:LEU:HD12	3:C:91:PHE:CD2	2.56	0.40
2:B:145:TYR:CD2	2:B:150:VAL:HG21	2.56	0.40
2:B:55:SER:HB3	2:B:71:ARG:HE	1.87	0.40
2:H:117:LYS:HG2	2:H:144:ASP:O	2.22	0.40
2:B:138:LEU:HB2	2:B:211:VAL:HG11	2.03	0.40
3:C:21:ILE:HG22	3:C:22:THR:N	2.35	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	338/353 (96%)	329 (97%)	9 (3%)	0	100	100
1	G	335/353 (95%)	328 (98%)	7 (2%)	0	100	100
2	B	196/225 (87%)	190 (97%)	5 (3%)	1 (0%)	24	60
2	H	209/225 (93%)	203 (97%)	6 (3%)	0	100	100
3	C	204/207 (99%)	201 (98%)	3 (2%)	0	100	100
3	L	204/207 (99%)	200 (98%)	4 (2%)	0	100	100
All	All	1486/1570 (95%)	1451 (98%)	34 (2%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	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	260/313 (83%)	258 (99%)	2 (1%)	73	86
1	G	271/313 (87%)	267 (98%)	4 (2%)	57	80
2	B	155/195 (80%)	154 (99%)	1 (1%)	78	88
2	H	181/195 (93%)	179 (99%)	2 (1%)	65	83
3	C	142/182 (78%)	139 (98%)	3 (2%)	47	75
3	L	169/182 (93%)	166 (98%)	3 (2%)	51	77
All	All	1178/1380 (85%)	1163 (99%)	15 (1%)	61	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	ASN
1	A	420	ILE
1	G	205	CYS
1	G	385	ASN
1	G	420	ILE
1	G	444	THR
2	B	66	ARG
3	C	78	GLU
3	C	109	PHE
3	C	110	ILE
2	H	192	GLN
2	H	195	ILE
3	L	23	CYS
3	L	97	LEU
3	L	180	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	332	GLN
1	G	373	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	43	GLN
2	B	164	HIS
2	B	200	HIS
3	C	35	GLN
3	C	86	GLN
3	C	159	GLN
3	L	148	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 ⓘ

10 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	D	1	1,4	14,14,15	1.48	2 (14%)	17,19,21	0.89	0
4	NAG	D	2	4	14,14,15	1.36	2 (14%)	17,19,21	1.03	0
4	BMA	D	3	4	11,11,12	1.41	2 (18%)	15,15,17	1.26	1 (6%)
4	MAN	D	4	4	11,11,12	1.50	2 (18%)	15,15,17	0.94	1 (6%)
4	MAN	D	5	4	11,11,12	1.33	2 (18%)	15,15,17	1.35	1 (6%)
4	MAN	D	6	4	11,11,12	1.40	2 (18%)	15,15,17	0.91	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.65	0	17,19,21	0.53	0
5	NAG	E	2	5	14,14,15	0.32	0	17,19,21	0.43	0
5	BMA	E	3	5	11,11,12	0.66	0	15,15,17	0.85	0
5	MAN	E	4	5	11,11,12	0.66	0	15,15,17	1.12	2 (13%)

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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	MAN	O5-C1	3.42	1.49	1.43
4	D	6	MAN	C2-C3	-3.09	1.47	1.52
4	D	3	BMA	O5-C1	2.94	1.48	1.43
4	D	4	MAN	C2-C3	-2.75	1.48	1.52
4	D	3	BMA	C2-C3	-2.72	1.48	1.52
4	D	5	MAN	O5-C1	2.69	1.48	1.43
4	D	2	NAG	C7-N2	2.56	1.42	1.34
4	D	1	NAG	C7-N2	2.54	1.42	1.34
4	D	6	MAN	O5-C1	2.51	1.47	1.43
4	D	5	MAN	C2-C3	-2.35	1.48	1.52
4	D	1	NAG	O7-C7	2.23	1.28	1.23
4	D	2	NAG	O7-C7	2.06	1.27	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	MAN	C1-C2-C3	4.00	115.47	109.64
5	E	4	MAN	C1-O5-C5	3.29	116.60	112.19
4	D	3	BMA	C1-O5-C5	-3.14	107.97	112.19
4	D	4	MAN	C1-O5-C5	2.25	115.20	112.19
5	E	4	MAN	O2-C2-C3	-2.20	105.59	110.15
4	D	6	MAN	O3-C3-C2	-2.07	105.84	110.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
4	D	5	MAN	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6

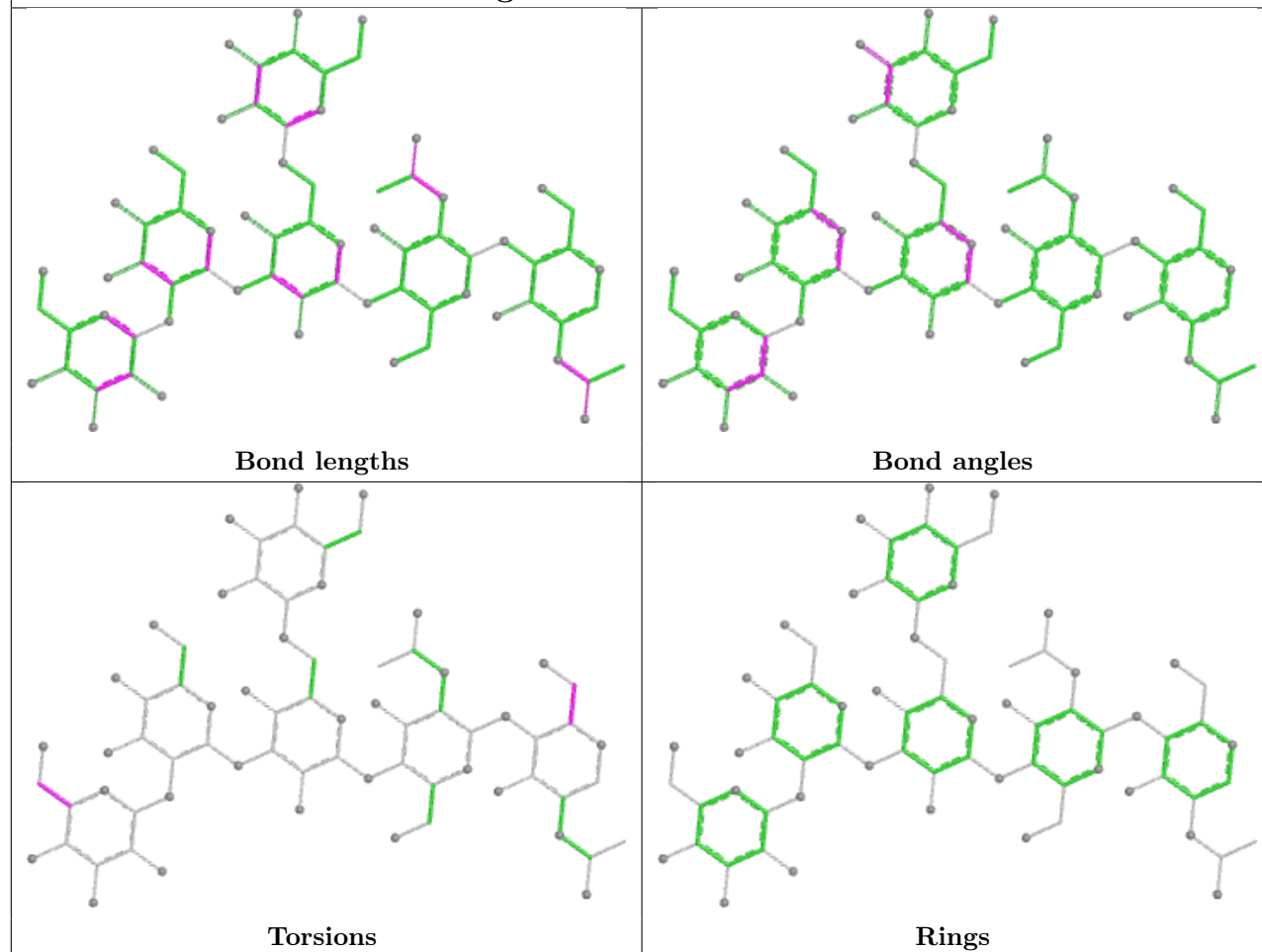
There are no ring outliers.

3 monomers are involved in 8 short contacts:

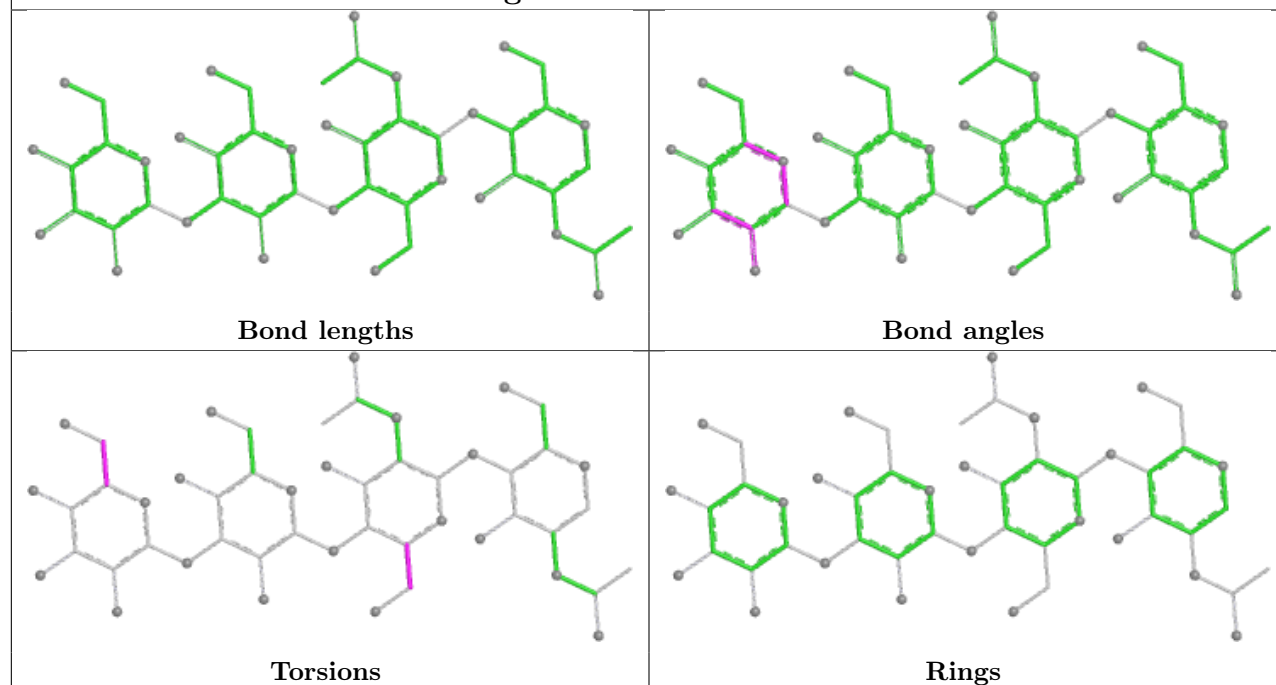
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	3	0
4	D	1	NAG	5	0
5	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry

14 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$
6	NAG	A	604	1	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
6	NAG	G	603	1	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	C	301	3	14,14,15	0.39	0	17,19,21	0.50	0
7	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.32	0
6	NAG	A	603	1	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
7	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.03	0
6	NAG	A	605	1	14,14,15	0.32	0	17,19,21	0.56	0
7	EDO	G	605	-	3,3,3	0.50	0	2,2,2	0.26	0
6	NAG	G	602	1	14,14,15	0.71	1 (7%)	17,19,21	0.81	1 (5%)
8	PGE	G	604	-	9,9,9	0.32	0	8,8,8	0.28	0
6	NAG	L	301	3	14,14,15	0.18	0	17,19,21	0.49	0
6	NAG	A	601	1	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	A	602	1	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
6	NAG	G	601	1	14,14,15	0.52	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	NAG	G	603	1	-	0/6/23/26	0/1/1/1
6	NAG	C	301	3	-	1/6/23/26	0/1/1/1
7	EDO	A	606	-	-	0/1/1/1	-
6	NAG	A	603	1	-	2/6/23/26	0/1/1/1
7	EDO	A	607	-	-	0/1/1/1	-
6	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	EDO	G	605	-	-	1/1/1/1	-
6	NAG	G	602	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	G	604	-	-	4/7/7/7	-
6	NAG	L	301	3	-	1/6/23/26	0/1/1/1
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	A	602	1	-	0/6/23/26	0/1/1/1
6	NAG	G	601	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	602	NAG	C1-C2	2.50	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	602	NAG	C1-O5-C5	2.39	115.39	112.19
6	A	602	NAG	C1-O5-C5	2.25	115.20	112.19
6	A	603	NAG	C1-O5-C5	2.13	115.04	112.19
6	A	604	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	604	NAG	O5-C5-C6-O6
6	A	604	NAG	C4-C5-C6-O6
8	G	604	PGE	O3-C5-C6-O4
6	A	605	NAG	O5-C5-C6-O6
6	A	603	NAG	O5-C5-C6-O6
6	G	602	NAG	C3-C2-N2-C7
6	A	605	NAG	C4-C5-C6-O6
6	G	602	NAG	C1-C2-N2-C7
8	G	604	PGE	C1-C2-O2-C3
8	G	604	PGE	C3-C4-O3-C5
6	L	301	NAG	O5-C5-C6-O6
6	G	601	NAG	C4-C5-C6-O6
6	C	301	NAG	C1-C2-N2-C7
7	G	605	EDO	O1-C1-C2-O2
6	A	603	NAG	C4-C5-C6-O6
8	G	604	PGE	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	602	NAG	2	0
6	G	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	340/353 (96%)	0.55	14 (4%) 41 23	45, 67, 112, 143	0
1	G	339/353 (96%)	0.42	7 (2%) 63 40	41, 63, 90, 122	0
2	B	202/225 (89%)	0.91	22 (10%) 10 6	54, 78, 120, 137	0
2	H	213/225 (94%)	0.36	4 (1%) 66 43	37, 56, 76, 409	0
3	C	206/207 (99%)	1.10	23 (11%) 10 6	57, 85, 116, 128	0
3	L	206/207 (99%)	0.56	4 (1%) 66 43	42, 67, 102, 116	0
All	All	1506/1570 (95%)	0.62	74 (4%) 35 18	37, 68, 111, 409	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	77	MET	5.7
3	C	128	LEU	4.6
3	L	28	GLY	4.4
2	B	182	VAL	3.9
2	B	207	VAL	3.9
3	C	27	ALA	3.6
2	H	140	CYS	3.5
2	H	127	SER	3.4
2	B	212	GLU	3.4
2	B	208	ASP	3.3
3	L	188	GLU	3.3
2	H	115	SER	3.1
1	G	301	ASN	3.1
2	B	114	ALA	3.1
1	A	80	ASN	3.0
1	A	301	ASN	2.9
1	G	447	SER	2.8
3	L	144	ASP	2.8
2	B	115	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	43	GLN	2.8
3	C	107	SER	2.8
2	B	119	PRO	2.7
2	B	209	LYS	2.7
3	C	131	ASN	2.7
3	C	111	PHE	2.6
3	C	203	ASN	2.6
1	A	465	THR	2.6
2	B	45	LEU	2.6
3	C	130	ASN	2.6
3	C	147	LEU	2.6
3	C	124	SER	2.5
3	L	74	SER	2.5
2	B	206	LYS	2.5
2	B	137	ALA	2.5
2	B	116	THR	2.5
2	B	183	THR	2.5
3	C	117	GLN	2.5
2	B	159	LEU	2.5
3	C	186	ALA	2.5
1	G	324	GLY	2.5
2	B	195	ILE	2.4
1	A	47	GLU	2.4
3	C	86	GLN	2.4
1	A	45	TRP	2.4
3	C	113	PRO	2.4
1	A	82	GLN	2.3
2	B	189	LEU	2.3
1	A	306	SER	2.3
1	A	357	ASN	2.3
2	B	44	GLY	2.3
1	A	228	CYS	2.3
1	A	463	ASP	2.3
1	A	229	ASN	2.3
1	G	78	ASP	2.3
3	C	146	ALA	2.2
1	A	50	THR	2.2
1	G	45	TRP	2.2
2	B	205	THR	2.2
3	C	122	THR	2.2
1	A	246	GLN	2.2
2	B	186	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	138	LEU	2.2
2	B	166	PHE	2.2
3	C	173	THR	2.1
3	C	59	PHE	2.1
3	C	102	THR	2.1
1	G	87	GLU	2.1
3	C	16	GLY	2.1
1	A	52	LEU	2.1
3	C	83	TYR	2.1
1	G	458	GLY	2.1
3	C	206	GLU	2.0
3	C	143	VAL	2.0
3	C	76	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

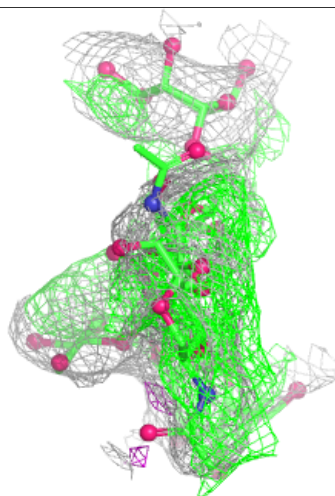
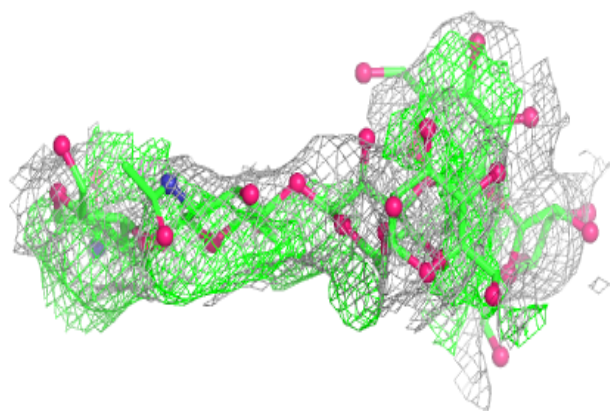
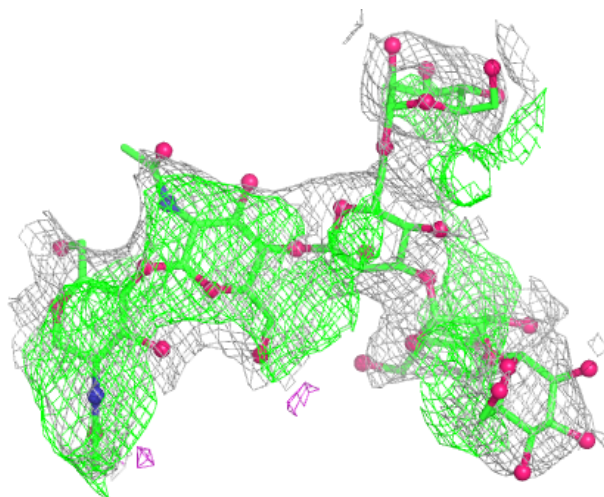
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

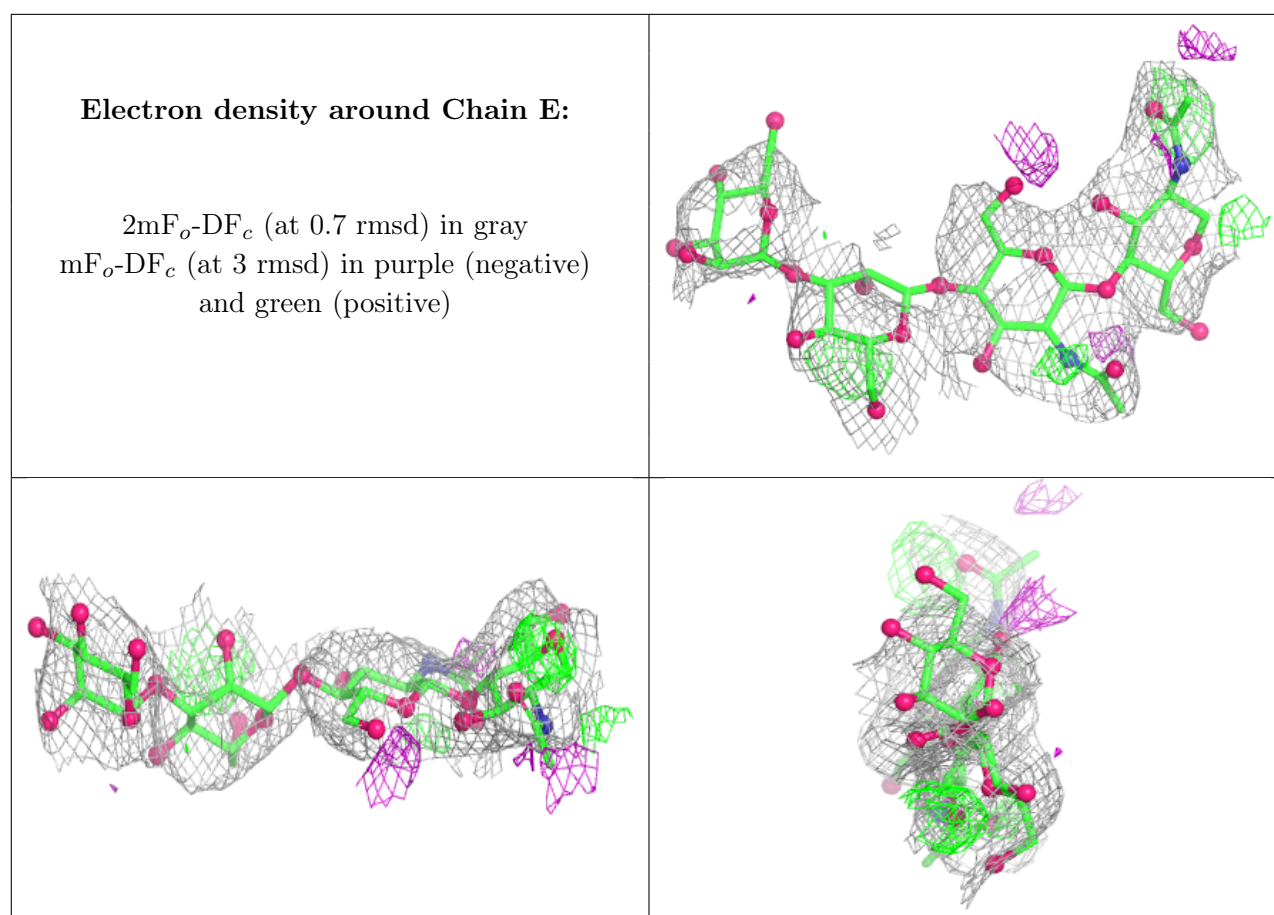
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	1	14/15	-	-	44,56,59,65	14
4	NAG	D	2	14/15	-	-	48,52,61,62	14
4	BMA	D	3	11/12	-	-	53,60,62,68	11
4	MAN	D	4	11/12	-	-	55,57,61,70	11
4	MAN	D	5	11/12	-	-	58,61,66,68	11
4	MAN	D	6	11/12	-	-	57,61,67,68	11
5	NAG	E	1	14/15	-	-	67,74,84,91	0
5	NAG	E	2	14/15	-	-	87,93,110,120	0
5	BMA	E	3	11/12	-	-	117,122,132,140	0
5	MAN	E	4	11/12	-	-	122,134,139,139	0

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

Electron density around Chain D:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	NAG	G	603	14/15	0.37	0.20	81,103,107,108	14
6	NAG	A	602	14/15	0.42	0.16	131,147,153,153	0
6	NAG	A	605	14/15	0.50	0.20	99,119,127,128	14
7	EDO	G	605	4/4	0.51	0.51	67,69,77,120	0
6	NAG	A	603	14/15	0.53	0.17	102,109,114,114	0
6	NAG	G	602	14/15	0.54	0.19	76,90,104,105	14
6	NAG	A	601	14/15	0.57	0.17	104,114,126,134	0
6	NAG	C	301	14/15	0.66	0.16	90,104,107,111	0
8	PGE	G	604	10/10	0.70	0.19	66,74,77,78	0
6	NAG	G	601	14/15	0.75	0.23	74,81,97,103	0
7	EDO	A	606	4/4	0.75	0.23	46,54,57,59	0
6	NAG	L	301	14/15	0.78	0.24	60,82,162,177	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	604	14/15	0.81	0.16	50,61,73,73	0
7	EDO	A	607	4/4	0.89	0.18	50,52,55,58	4

6.5 Other polymers [i](#)

There are no such residues in this entry.