



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:42 AM UTC

PDB ID : 2NY1 / pdb_00002ny1
Title : HIV-1 gp120 Envelope Glycoprotein (I109C, T257S, S334A, S375W, Q428C)
Complexed with CD4 and Antibody 17b
Authors : Zhou, T.; Xu, L.; Dey, B.; Hessel, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.;
Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski,
J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.
Deposited on : 2006-11-20
Resolution : 1.99 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

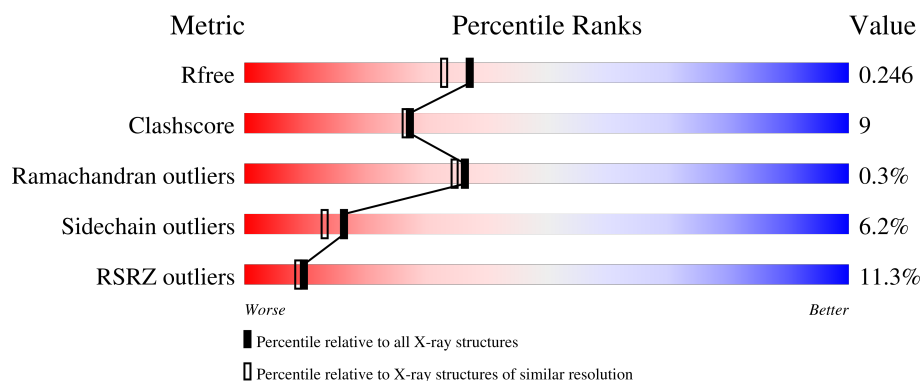
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	317	20% 75% 19% • •
2	B	184	10% 79% 16% • •
3	C	214	5% 85% 15%
4	D	229	6% 82% 14% • •

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Mol	Chain	Length	Quality of chain
5	E	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7852 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 GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2362	1482	411	447	22			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	MET	-	initiating methionine	UNP P01730

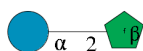
- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

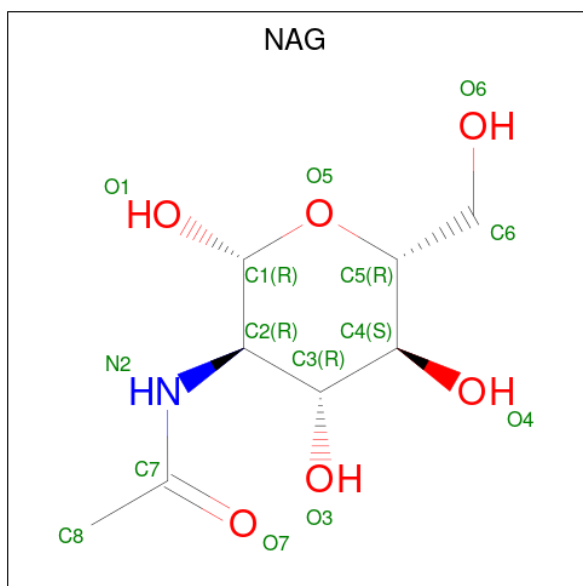
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	223	Total	C	N	O	S	0	0	0
			1681	1064	282	330	5			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			23	12	11			

- 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	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		

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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		

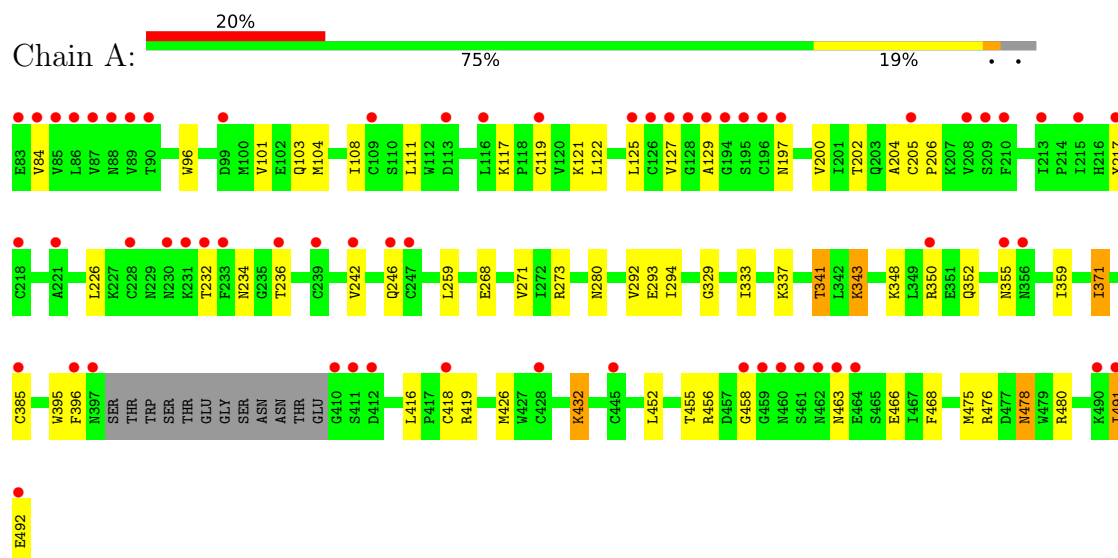
- Molecule 7 is water.

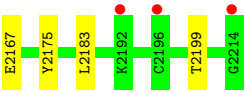
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	154	Total	O	0	0
			154	154		
7	B	86	Total	O	0	0
			86	86		
7	C	131	Total	O	0	0
			131	131		
7	D	161	Total	O	0	0
			161	161		

3 Residue-property plots

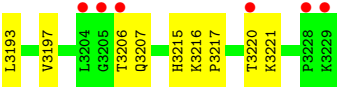
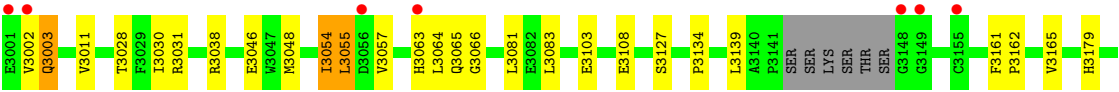
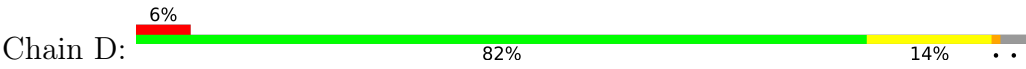
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 GP120





● Molecule 4: ANTIBODY 17B, HEAVY CHAIN



● Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.11Å 88.16Å 197.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.40 – 1.99 42.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	81.0 (42.40-1.99) 81.5 (42.40-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.250 0.209 , 0.246	Depositor DCC
R_{free} test set	3536 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FRU, NAG

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	0.41	0/2410	0.70	0/3267
2	B	0.36	0/1432	0.71	0/1930
3	C	0.41	0/1683	0.74	0/2288
4	D	0.44	0/1720	0.70	0/2343
All	All	0.41	0/7245	0.71	0/9828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2362	0	2294	60	0
2	B	1412	0	1441	19	0
3	C	1646	0	1590	29	0
4	D	1681	0	1647	28	0
5	E	23	0	21	2	0
6	A	196	0	182	6	0
7	A	154	0	0	11	0
7	B	86	0	0	8	0
7	C	131	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	161	0	0	5	0
All	All	7852	0	7175	132	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 9.

All (132) 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)
3:C:2144:ARG:NH1	7:C:355:HOH:O	1.79	1.09
1:A:476:ARG:HB3	1:A:480:ARG:HH12	1.28	0.97
2:B:1025:GLN:HG2	7:B:442:HOH:O	1.66	0.95
3:C:2167:GLU:O	7:C:205:HOH:O	1.86	0.93
2:B:1066:ASN:ND2	7:B:74:HOH:O	2.02	0.89
4:D:3215:HIS:HB3	4:D:3220:THR:HG22	1.55	0.88
4:D:3215:HIS:HB3	4:D:3220:THR:CG2	2.06	0.85
4:D:3046:GLU:OE2	4:D:3063:HIS:NE2	2.15	0.79
1:A:491:ILE:O	1:A:492:GLU:HG3	1.82	0.78
4:D:3065:GLN:NE2	7:D:8:HOH:O	2.16	0.77
4:D:3048:MET:HG2	7:D:435:HOH:O	1.81	0.77
7:A:1104:HOH:O	4:D:3108:GLU:HB2	1.83	0.77
1:A:476:ARG:HB3	1:A:480:ARG:NH1	1.99	0.76
1:A:280:ASN:HD22	1:A:458:GLY:HA3	1.51	0.75
1:A:395:TRP:CZ3	6:A:839:NAG:O7	2.40	0.75
1:A:491:ILE:HG13	1:A:492:GLU:H	1.52	0.73
1:A:280:ASN:ND2	1:A:458:GLY:HA3	2.03	0.73
1:A:395:TRP:HZ3	6:A:839:NAG:O7	1.72	0.71
1:A:456:ARG:HB2	7:A:1040:HOH:O	1.92	0.69
1:A:292:VAL:HG21	1:A:341:THR:HG21	1.73	0.69
3:C:2144:ARG:NE	7:C:500:HOH:O	1.97	0.69
2:B:1148:GLN:OE1	7:B:103:HOH:O	2.13	0.67
4:D:3134:PRO:HD2	4:D:3220:THR:HG21	1.74	0.67
1:A:456:ARG:HD3	7:A:1088:HOH:O	1.95	0.67
3:C:2013:VAL:HG11	3:C:2078:LEU:CD1	2.25	0.67
3:C:2013:VAL:HG11	3:C:2078:LEU:HD12	1.76	0.66
3:C:2107:GLU:HG2	3:C:2108:ILE:N	2.13	0.64
2:B:1033:GLN:NE2	7:B:494:HOH:O	2.08	0.64
1:A:104:MET:HE2	1:A:217:TYR:HE1	1.61	0.64
2:B:1164:ASN:O	2:B:1165:GLN:HB2	1.99	0.62
1:A:104:MET:O	1:A:108:ILE:HG12	1.99	0.62
1:A:337:LYS:O	1:A:341:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:CG2	1:A:341:THR:HG21	2.32	0.59
2:B:1066:ASN:HB2	7:B:396:HOH:O	2.03	0.59
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.85	0.58
6:A:588:NAG:O7	6:A:588:NAG:C3	2.51	0.58
4:D:3063:HIS:CE1	5:E:2:FRU:O6	2.57	0.57
1:A:119:CYS:N	1:A:205:CYS:SG	2.76	0.57
3:C:2029:VAL:HG11	3:C:2090:GLN:CG	2.35	0.57
4:D:3002:VAL:C	4:D:3003:GLN:NE2	2.63	0.57
1:A:104:MET:HE2	1:A:217:TYR:CE1	2.40	0.56
3:C:2078:LEU:HD21	3:C:2106:LEU:HD21	1.88	0.56
4:D:3046:GLU:OE2	4:D:3063:HIS:CE1	2.59	0.56
3:C:2029:VAL:HG11	3:C:2090:GLN:HG3	1.87	0.56
4:D:3065:GLN:HG3	7:D:174:HOH:O	2.06	0.56
1:A:329:GLY:C	1:A:418:CYS:HB2	2.31	0.55
1:A:350:ARG:NH2	1:A:355:ASN:O	2.40	0.55
1:A:280:ASN:HD22	1:A:458:GLY:CA	2.19	0.54
1:A:491:ILE:HG13	1:A:492:GLU:N	2.21	0.54
1:A:432:LYS:HE2	7:A:1089:HOH:O	2.07	0.54
3:C:2019:ALA:HB2	3:C:2078:LEU:HD11	1.88	0.54
1:A:350:ARG:HD3	1:A:396:PHE:CD1	2.43	0.54
1:A:350:ARG:HD3	1:A:396:PHE:CE1	2.42	0.54
3:C:2094:TRP:HA	3:C:2095:PRO:C	2.33	0.54
1:A:491:ILE:CG1	1:A:492:GLU:H	2.19	0.53
1:A:121:LYS:HE3	1:A:426:MET:HE1	1.91	0.53
2:B:1157:TRP:HB3	7:B:440:HOH:O	2.09	0.53
4:D:3065:GLN:CG	7:D:174:HOH:O	2.55	0.53
6:A:588:NAG:O7	6:A:588:NAG:O3	2.26	0.53
3:C:2037:GLN:HB2	3:C:2047:LEU:HD11	1.91	0.53
1:A:259:LEU:HD23	1:A:452:LEU:HD22	1.92	0.52
1:A:293:GLU:OE1	6:A:795:NAG:H3	2.08	0.52
2:B:1083:ILE:HG13	2:B:1092:GLU:HG3	1.92	0.52
3:C:2021:LEU:HD22	3:C:2104:THR:HG21	1.91	0.52
4:D:3002:VAL:O	4:D:3003:GLN:NE2	2.44	0.50
3:C:2004:MET:SD	3:C:2090:GLN:HB2	2.52	0.50
3:C:2175:TYR:HA	7:C:205:HOH:O	2.11	0.50
3:C:2013:VAL:CG1	3:C:2078:LEU:CD1	2.90	0.49
1:A:122:LEU:HD21	4:D:3057:VAL:HG21	1.95	0.49
4:D:3193:LEU:C	4:D:3193:LEU:HD12	2.38	0.49
1:A:259:LEU:CD2	1:A:452:LEU:HD22	2.43	0.49
2:B:1141:GLY:C	7:B:493:HOH:O	2.56	0.49
1:A:234:ASN:CG	6:A:734:NAG:N2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HB3	1:A:197:ASN:O	2.13	0.48
1:A:129:ALA:HB3	7:A:1073:HOH:O	2.13	0.48
4:D:3011:VAL:HG21	4:D:3162:PRO:HG3	1.95	0.48
1:A:480:ARG:CZ	7:A:1024:HOH:O	2.62	0.48
3:C:2140:ASN:HD21	4:D:3179:HIS:CE1	2.32	0.47
3:C:2097:ARG:HD2	7:C:460:HOH:O	2.13	0.47
4:D:3066:GLY:HA3	7:D:504:HOH:O	2.14	0.47
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.78	0.47
2:B:1010:ASP:O	2:B:1074:LEU:HD22	2.15	0.47
1:A:456:ARG:HG2	7:A:1088:HOH:O	2.14	0.47
3:C:2147:LYS:HB3	3:C:2199:THR:HB	1.97	0.47
3:C:2001:ASP:OD2	3:C:2001:ASP:N	2.48	0.47
1:A:117:LYS:HD3	7:A:1020:HOH:O	2.14	0.46
1:A:352:GLN:NE2	7:A:976:HOH:O	2.05	0.46
1:A:478:ASN:HD22	1:A:478:ASN:H	1.63	0.46
4:D:3063:HIS:CE1	5:E:2:FRU:HO6	2.34	0.46
3:C:2122:PRO:HD3	3:C:2134:VAL:HG22	1.98	0.46
2:B:1008:LYS:HD2	2:B:1076:ILE:HD11	1.98	0.46
1:A:259:LEU:HD22	1:A:452:LEU:CD2	2.46	0.45
3:C:2013:VAL:CG1	3:C:2078:LEU:HD12	2.45	0.45
3:C:2153:ASP:O	3:C:2154:ASN:CB	2.64	0.45
1:A:419:ARG:NH2	4:D:3103:GLU:OE2	2.36	0.44
1:A:96:TRP:CD1	1:A:236:THR:HG21	2.52	0.44
2:B:1020:GLN:HG2	7:B:130:HOH:O	2.18	0.44
2:B:1081:THR:CG2	2:B:1092:GLU:HG2	2.48	0.44
1:A:232:THR:O	1:A:232:THR:HG22	2.17	0.44
1:A:456:ARG:HB3	1:A:468:PHE:CE2	2.53	0.44
2:B:1166:LYS:N	2:B:1166:LYS:HD2	2.33	0.44
4:D:3028:THR:HB	4:D:3031:ARG:HD2	2.00	0.44
1:A:271:VAL:HG11	1:A:273:ARG:NH1	2.32	0.44
1:A:466:GLU:HB3	7:A:1040:HOH:O	2.18	0.44
4:D:3206:THR:OG1	4:D:3207:GLN:N	2.51	0.44
1:A:121:LYS:HE2	7:A:1093:HOH:O	2.16	0.43
2:B:1021:LYS:HE3	2:B:1064:GLN:HE21	1.84	0.43
3:C:2153:ASP:O	3:C:2154:ASN:HB3	2.18	0.43
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.88	0.43
1:A:121:LYS:HB2	1:A:426:MET:CE	2.48	0.43
3:C:2107:GLU:HG3	3:C:2175:TYR:OH	2.19	0.43
3:C:2144:ARG:NH2	7:C:500:HOH:O	2.51	0.43
1:A:122:LEU:HD22	1:A:200:VAL:HG22	1.99	0.43
1:A:202:THR:HG22	3:C:2095:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3054:ILE:HG23	4:D:3055:LEU:HD13	2.00	0.42
1:A:104:MET:CE	1:A:217:TYR:CE1	3.02	0.42
1:A:268:GLU:HA	1:A:268:GLU:OE1	2.19	0.42
4:D:3030:ILE:HD12	4:D:3030:ILE:C	2.44	0.42
4:D:3003:GLN:N	4:D:3003:GLN:CD	2.79	0.41
1:A:343:LYS:HB3	1:A:343:LYS:HE2	1.76	0.41
2:B:1028:TRP:CE2	2:B:1069:LEU:HB2	2.56	0.41
2:B:1139:GLN:HE21	2:B:1139:GLN:HB2	1.70	0.41
1:A:101:VAL:HG11	1:A:480:ARG:NH1	2.35	0.41
1:A:371:ILE:HG12	2:B:1043:PHE:HB3	2.02	0.41
1:A:96:TRP:HD1	1:A:236:THR:HG21	1.86	0.41
1:A:204:ALA:C	1:A:206:PRO:HD3	2.46	0.41
1:A:259:LEU:CD2	1:A:452:LEU:CD2	2.99	0.41
3:C:2140:ASN:HD21	4:D:3179:HIS:HE1	1.68	0.41
4:D:3127:SER:HB3	4:D:3161:PHE:CZ	2.56	0.41
2:B:1164:ASN:O	2:B:1166:LYS:HD2	2.22	0.40
1:A:478:ASN:HD22	1:A:478:ASN:N	2.19	0.40
3:C:2047:LEU:HA	3:C:2058:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/317 (95%)	283 (94%)	16 (5%)	2 (1%)	18	14
2	B	179/184 (97%)	171 (96%)	7 (4%)	1 (1%)	21	17
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	D	219/229 (96%)	213 (97%)	6 (3%)	0	100	100
All	All	911/944 (96%)	871 (96%)	37 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
2	B	1105	ASP
1	A	491	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	269/280 (96%)	252 (94%)	17 (6%)	16	13
2	B	164/166 (99%)	148 (90%)	16 (10%)	7	5
3	C	184/184 (100%)	178 (97%)	6 (3%)	33	34
4	D	187/193 (97%)	176 (94%)	11 (6%)	18	14
All	All	804/823 (98%)	754 (94%)	50 (6%)	16	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	103	GLN
1	A	111	LEU
1	A	226	LEU
1	A	242	VAL
1	A	246	GLN
1	A	341	THR
1	A	343	LYS
1	A	359	ILE
1	A	371	ILE
1	A	385	CYS
1	A	416	LEU
1	A	432	LYS
1	A	455	THR
1	A	463	ASN
1	A	475	MET
1	A	478	ASN
2	B	1002	LYS
2	B	1037	LEU

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Mol	Chain	Res	Type
2	B	1049	SER
2	B	1059	ARG
2	B	1064	GLN
2	B	1066	ASN
2	B	1069	LEU
2	B	1074	LEU
2	B	1096	LEU
2	B	1137	ASN
2	B	1139	GLN
2	B	1142	LYS
2	B	1143	THR
2	B	1149	LEU
2	B	1162	LEU
2	B	1168	VAL
3	C	2001	ASP
3	C	2073	LEU
3	C	2076	SER
3	C	2127	LEU
3	C	2131	THR
3	C	2183	LEU
4	D	3003	GLN
4	D	3038	ARG
4	D	3054	ILE
4	D	3055	LEU
4	D	3064	LEU
4	D	3081	LEU
4	D	3083	LEU
4	D	3139	LEU
4	D	3165	VAL
4	D	3197	VAL
4	D	3221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	332	ASN
1	A	355	ASN
1	A	442	GLN
1	A	478	ASN
2	B	1064	GLN
2	B	1148	GLN

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Mol	Chain	Res	Type
3	C	2038	GLN
3	C	2140	ASN
3	C	2149	GLN
4	D	3003	GLN
4	D	3039	GLN
4	D	3112	ASN
4	D	3207	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 ⓘ

2 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	$\# Z > 2$
5	GLC	E	1	5	11,11,12	0.60	0	15,15,17	0.54	0
5	FRU	E	2	5	11,12,12	0.46	0	10,18,18	0.67	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	GLC	E	1	5	–	0/2/19/22	0/1/1/1
5	FRU	E	2	5	–	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

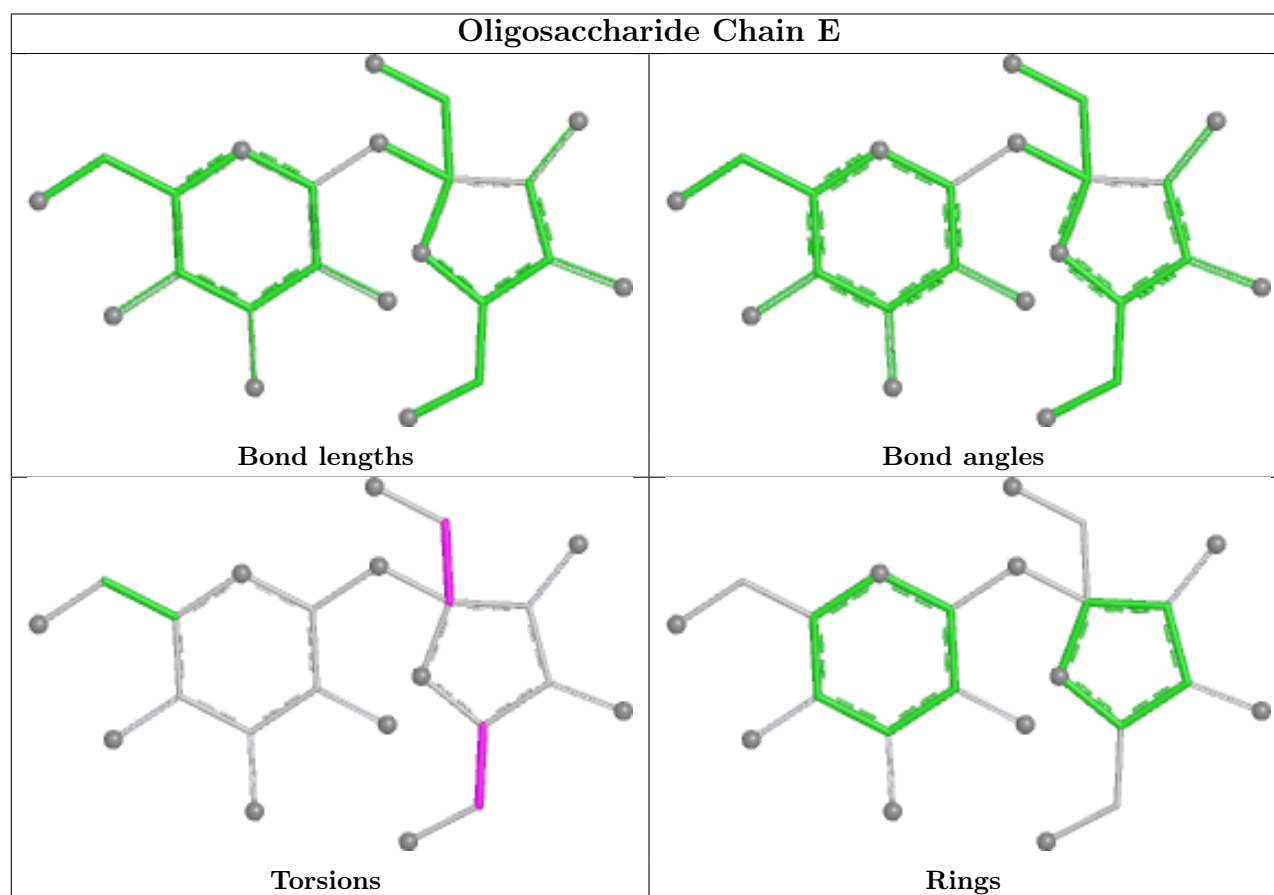
Mol	Chain	Res	Type	Atoms
5	E	2	FRU	O1-C1-C2-C3
5	E	2	FRU	O1-C1-C2-O2
5	E	2	FRU	O1-C1-C2-O5
5	E	2	FRU	C4-C5-C6-O6
5	E	2	FRU	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	FRU	2	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

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	741	1	14,14,15	0.59	0	17,19,21	0.88	1 (5%)
6	NAG	A	789	1	14,14,15	0.56	0	17,19,21	0.77	0
6	NAG	A	886	1	14,14,15	0.74	0	17,19,21	0.82	0
6	NAG	A	697	1	14,14,15	0.48	0	17,19,21	1.17	2 (11%)
6	NAG	A	776	1	14,14,15	0.54	0	17,19,21	0.87	0
6	NAG	A	948	1	14,14,15	0.50	0	17,19,21	0.78	0
6	NAG	A	588	1	14,14,15	0.43	0	17,19,21	0.80	0
6	NAG	A	795	1	14,14,15	0.53	0	17,19,21	1.11	0
6	NAG	A	734	1	14,14,15	0.44	0	17,19,21	2.72	6 (35%)
6	NAG	A	963	1	14,14,15	0.59	0	17,19,21	1.13	2 (11%)
6	NAG	A	892	1	14,14,15	0.48	0	17,19,21	0.80	0
6	NAG	A	839	1	14,14,15	0.67	0	17,19,21	1.17	1 (5%)
6	NAG	A	730	1	14,14,15	0.58	0	17,19,21	0.89	0
6	NAG	A	762	1	14,14,15	0.54	0	17,19,21	1.09	1 (5%)

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	741	1	-	2/6/23/26	0/1/1/1
6	NAG	A	789	1	-	2/6/23/26	0/1/1/1
6	NAG	A	886	1	-	4/6/23/26	0/1/1/1
6	NAG	A	697	1	-	3/6/23/26	0/1/1/1
6	NAG	A	776	1	-	0/6/23/26	0/1/1/1
6	NAG	A	948	1	-	2/6/23/26	0/1/1/1
6	NAG	A	588	1	-	3/6/23/26	0/1/1/1
6	NAG	A	795	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	734	1	-	5/6/23/26	0/1/1/1
6	NAG	A	963	1	-	5/6/23/26	0/1/1/1
6	NAG	A	892	1	-	2/6/23/26	0/1/1/1
6	NAG	A	839	1	-	2/6/23/26	0/1/1/1
6	NAG	A	730	1	-	2/6/23/26	0/1/1/1
6	NAG	A	762	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	734	NAG	O5-C5-C6	-5.65	96.67	107.66
6	A	734	NAG	C6-C5-C4	-5.27	100.09	113.02
6	A	734	NAG	C1-O5-C5	4.64	118.41	112.19
6	A	734	NAG	O5-C1-C2	3.44	116.61	111.29
6	A	839	NAG	C4-C3-C2	3.43	116.05	111.02
6	A	734	NAG	C4-C3-C2	-3.11	106.46	111.02
6	A	697	NAG	O5-C1-C2	-3.08	106.52	111.29
6	A	734	NAG	O6-C6-C5	3.08	121.82	111.33
6	A	963	NAG	C1-O5-C5	2.71	115.81	112.19
6	A	762	NAG	O5-C1-C2	-2.50	107.42	111.29
6	A	963	NAG	O5-C1-C2	2.48	115.12	111.29
6	A	741	NAG	C4-C3-C2	2.20	114.25	111.02
6	A	697	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	588	NAG	C3-C2-N2-C7
6	A	730	NAG	C8-C7-N2-C2
6	A	730	NAG	O7-C7-N2-C2
6	A	734	NAG	C3-C2-N2-C7
6	A	734	NAG	C8-C7-N2-C2
6	A	734	NAG	O7-C7-N2-C2
6	A	741	NAG	C8-C7-N2-C2
6	A	741	NAG	O7-C7-N2-C2
6	A	789	NAG	C8-C7-N2-C2
6	A	789	NAG	O7-C7-N2-C2
6	A	839	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	839	NAG	O7-C7-N2-C2
6	A	886	NAG	C1-C2-N2-C7
6	A	886	NAG	C8-C7-N2-C2
6	A	886	NAG	O7-C7-N2-C2
6	A	892	NAG	C8-C7-N2-C2
6	A	892	NAG	O7-C7-N2-C2
6	A	963	NAG	C1-C2-N2-C7
6	A	963	NAG	C8-C7-N2-C2
6	A	963	NAG	O7-C7-N2-C2
6	A	963	NAG	O5-C5-C6-O6
6	A	588	NAG	C8-C7-N2-C2
6	A	588	NAG	O7-C7-N2-C2
6	A	963	NAG	C4-C5-C6-O6
6	A	697	NAG	C8-C7-N2-C2
6	A	795	NAG	C8-C7-N2-C2
6	A	795	NAG	O7-C7-N2-C2
6	A	697	NAG	O7-C7-N2-C2
6	A	734	NAG	C4-C5-C6-O6
6	A	734	NAG	O5-C5-C6-O6
6	A	948	NAG	C4-C5-C6-O6
6	A	948	NAG	O5-C5-C6-O6
6	A	886	NAG	C3-C2-N2-C7
6	A	697	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	588	NAG	2	0
6	A	795	NAG	1	0
6	A	734	NAG	1	0
6	A	839	NAG	2	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	305/317 (96%)	0.98	63 (20%) 2 2	14, 31, 70, 95	0
2	B	181/184 (98%)	0.75	18 (9%) 13 11	17, 35, 62, 76	0
3	C	214/214 (100%)	0.40	10 (4%) 36 35	12, 28, 61, 74	0
4	D	223/229 (97%)	0.27	13 (5%) 29 27	11, 23, 61, 89	0
All	All	923/944 (97%)	0.63	104 (11%) 10 9	11, 30, 65, 95	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1106	THR	7.0
1	A	205	CYS	6.6
1	A	210	PHE	6.4
1	A	129	ALA	6.0
1	A	492	GLU	5.7
4	D	3148	GLY	5.2
1	A	127	VAL	5.0
1	A	491	ILE	4.9
1	A	428	CYS	4.7
3	C	2196	CYS	4.7
1	A	84	VAL	4.6
1	A	228	CYS	4.5
1	A	385	CYS	4.5
1	A	87	VAL	4.5
1	A	458	GLY	4.4
2	B	1141	GLY	4.3
1	A	85	VAL	4.2
2	B	1103	ASN	4.2
1	A	445	CYS	4.1
1	A	410	GLY	4.1
1	A	126	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	128	GLY	3.9
4	D	3206	THR	3.9
3	C	2001	ASP	3.7
1	A	197	ASN	3.7
1	A	247	CYS	3.6
1	A	231	LYS	3.6
4	D	3001	GLU	3.5
4	D	3063	HIS	3.5
4	D	3228	PRO	3.5
2	B	1104	SER	3.5
1	A	89	VAL	3.5
1	A	218	CYS	3.4
1	A	86	LEU	3.2
1	A	213	ILE	3.2
1	A	125	LEU	3.2
1	A	490	LYS	3.2
1	A	418	CYS	3.2
1	A	462	ASN	3.1
1	A	116	LEU	3.1
1	A	208	VAL	3.1
1	A	356	ASN	3.0
1	A	411	SER	3.0
1	A	236	THR	3.0
4	D	3220	THR	3.0
1	A	195	SER	3.0
3	C	2214	GLY	2.9
1	A	221	ALA	2.9
4	D	3155	CYS	2.9
2	B	1139	GLN	2.9
2	B	1107	HIS	2.9
1	A	233	PHE	2.8
4	D	3205	GLY	2.8
1	A	196	CYS	2.8
1	A	230	ASN	2.8
4	D	3002	VAL	2.8
2	B	1105	ASP	2.8
1	A	461	SER	2.8
2	B	1181	LYS	2.8
4	D	3149	GLY	2.8
1	A	232	THR	2.8
1	A	464	GLU	2.8
1	A	412	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1130	CYS	2.7
1	A	397	ASN	2.7
4	D	3229	LYS	2.6
3	C	2076	SER	2.6
1	A	217	TYR	2.6
1	A	239	CYS	2.6
4	D	3204	LEU	2.6
1	A	119	CYS	2.5
1	A	88	ASN	2.5
1	A	460	ASN	2.5
1	A	113	ASP	2.5
1	A	350	ARG	2.4
2	B	1001	LYS	2.4
1	A	463	ASN	2.4
2	B	1166	LYS	2.4
3	C	2192	LYS	2.4
3	C	2023	CYS	2.4
1	A	215	ILE	2.3
2	B	1088	ASP	2.3
2	B	1019	SER	2.2
1	A	242	VAL	2.2
3	C	2152	VAL	2.2
1	A	83	GLU	2.2
1	A	109	CYS	2.2
1	A	194	GLY	2.2
3	C	2128	LYS	2.2
1	A	209	SER	2.2
1	A	459	GLY	2.2
3	C	2156	LEU	2.2
1	A	246	GLN	2.1
1	A	90	THR	2.1
2	B	1086	VAL	2.1
2	B	1091	GLU	2.1
2	B	1137	ASN	2.1
1	A	396	PHE	2.1
1	A	99	ASP	2.1
2	B	1123	GLY	2.1
1	A	355	ASN	2.1
4	D	3056	ASP	2.1
3	C	2154	ASN	2.0
2	B	1125	SER	2.0

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

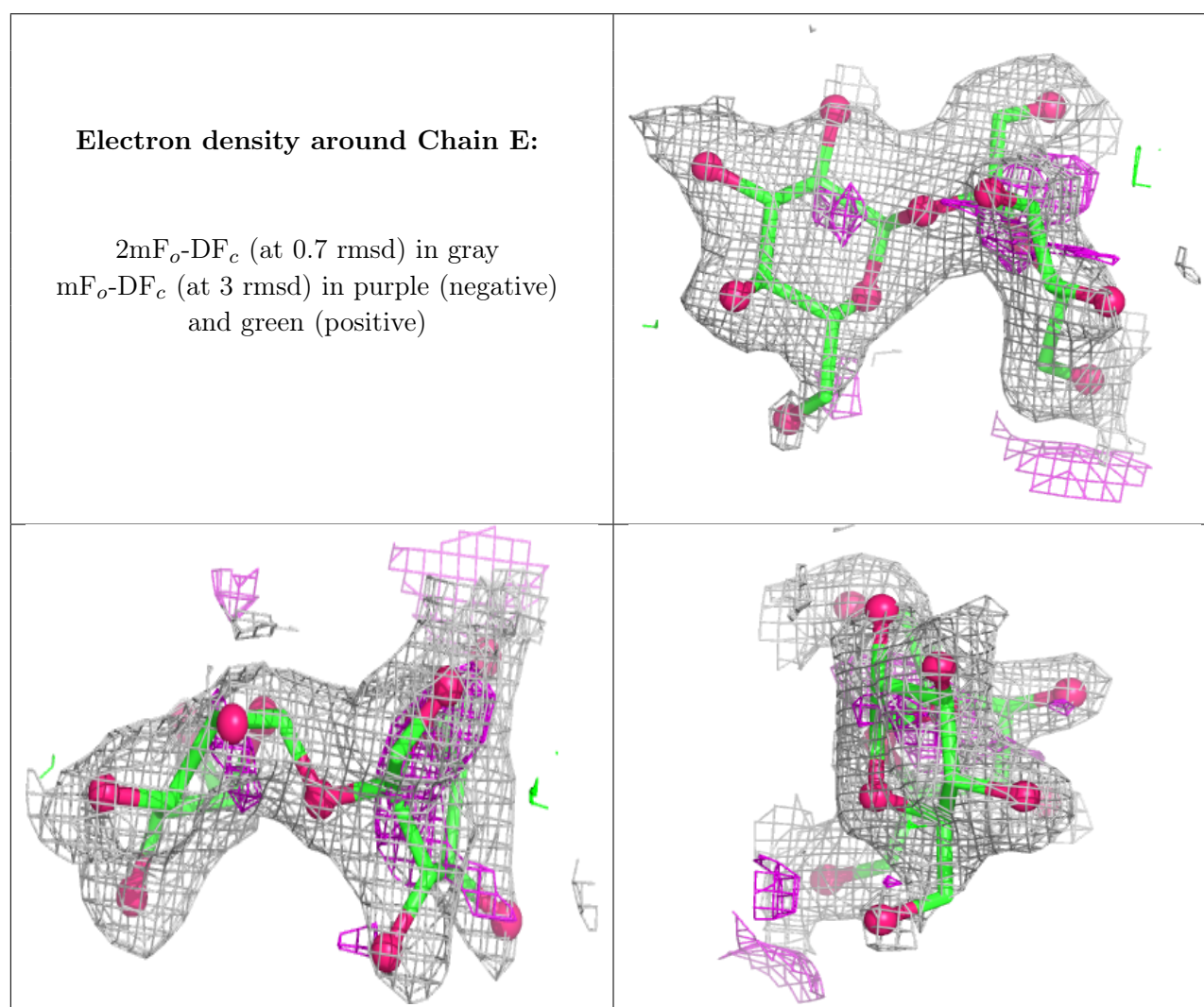
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	FRU	E	2	12/12	0.75	0.15	46,47,48,48	0
5	GLC	E	1	11/12	0.83	0.12	47,48,48,48	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(Å ²)	Q<0.9
6	NAG	A	588	14/15	0.15	0.22	62,63,64,64	0
6	NAG	A	963	14/15	0.23	0.21	60,62,62,62	0
6	NAG	A	839	14/15	0.33	0.21	47,49,51,51	0
6	NAG	A	730	14/15	0.42	0.19	55,57,57,58	0
6	NAG	A	697	14/15	0.46	0.17	52,54,54,55	0
6	NAG	A	892	14/15	0.51	0.17	44,46,48,48	0
6	NAG	A	734	14/15	0.53	0.18	49,51,51,52	0
6	NAG	A	741	14/15	0.60	0.15	50,52,53,54	0
6	NAG	A	948	14/15	0.76	0.13	39,40,42,42	0
6	NAG	A	886	14/15	0.77	0.14	39,41,41,42	0
6	NAG	A	776	14/15	0.80	0.12	38,40,41,41	0
6	NAG	A	762	14/15	0.86	0.11	30,33,34,36	0
6	NAG	A	795	14/15	0.88	0.12	28,29,30,31	0
6	NAG	A	789	14/15	0.89	0.09	35,37,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.