



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 AM UTC

PDB ID : 7ZWM / pdb_00007zwm
Title : Pfs48/45 central and C-terminal domains bound to Fab fragments of monoclonal antibody 10D8 and 32F3
Authors : Ko, K.T.; Lennartz, F.L.; Higgins, M.K.
Deposited on : 2022-05-19
Resolution : 3.69 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

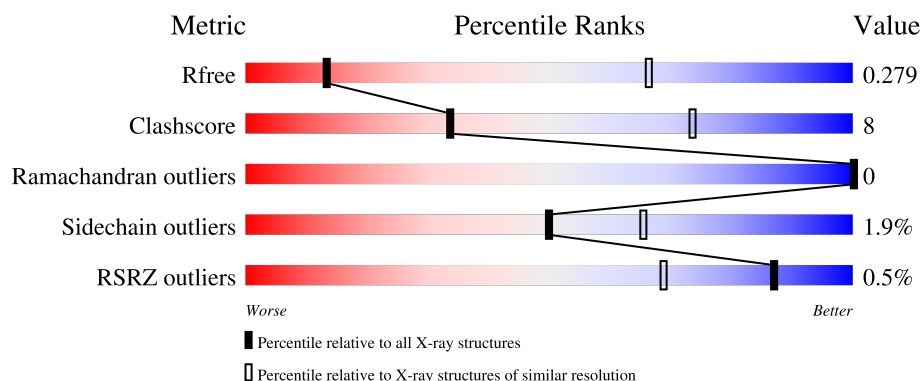
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

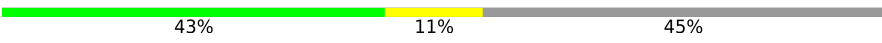
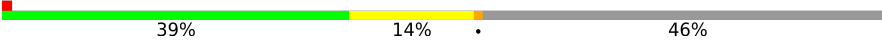
The reported resolution of this entry is 3.69 Å.

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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	428	
1	F	428	
2	B	444	
2	G	444	
3	C	213	

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Mol	Chain	Length	Quality of chain
3	H	213	80%19%
4	D	466	36%9%54%
4	I	466	37%9%54%
5	E	240	69%22%10%
5	J	240	2%69%21%10%
6	K	3	33%67%
7	L	4	50%50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16969 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 Gametocyte surface protein P45/48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1888	1204	301	372	11			
1	F	230	Total	C	N	O	S	0	0	0
			1831	1169	292	359	11			

- Molecule 2 is a protein called 32F3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1627	1036	267	317	7			
2	G	216	Total	C	N	O	S	0	0	0
			1647	1046	271	323	7			

- Molecule 3 is a protein called 32F3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1613	1004	274	329	6			
3	H	211	Total	C	N	O	S	0	0	0
			1613	1004	274	329	6			

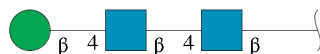
- Molecule 4 is a protein called 10D8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	213	Total	C	N	O	S	0	0	0
			1617	1021	271	315	10			
4	I	215	Total	C	N	O	S	0	0	0
			1631	1028	274	319	10			

- Molecule 5 is a protein called 10D8 light chain.

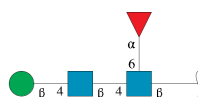
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	217	Total	C	N	O	S	0	0	0
			1690	1061	278	344	7			
5	J	216	Total	C	N	O	S	0	0	0
			1682	1057	277	341	7			

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



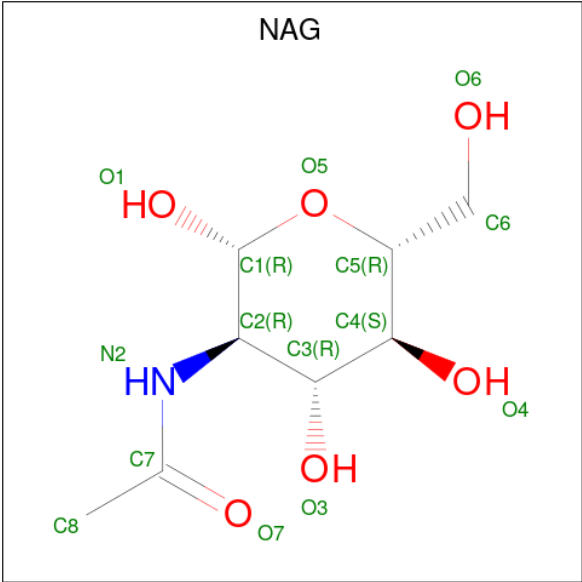
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

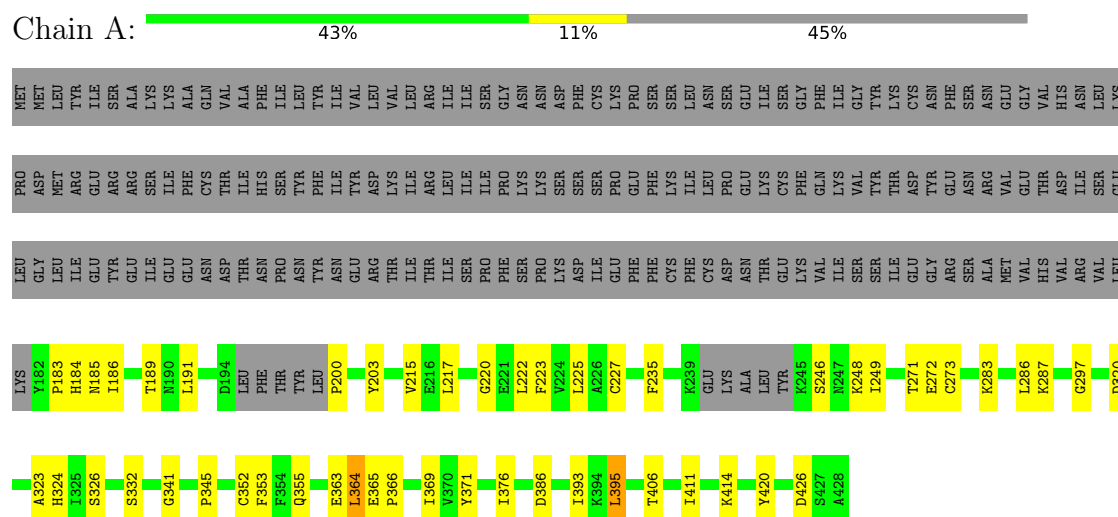


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

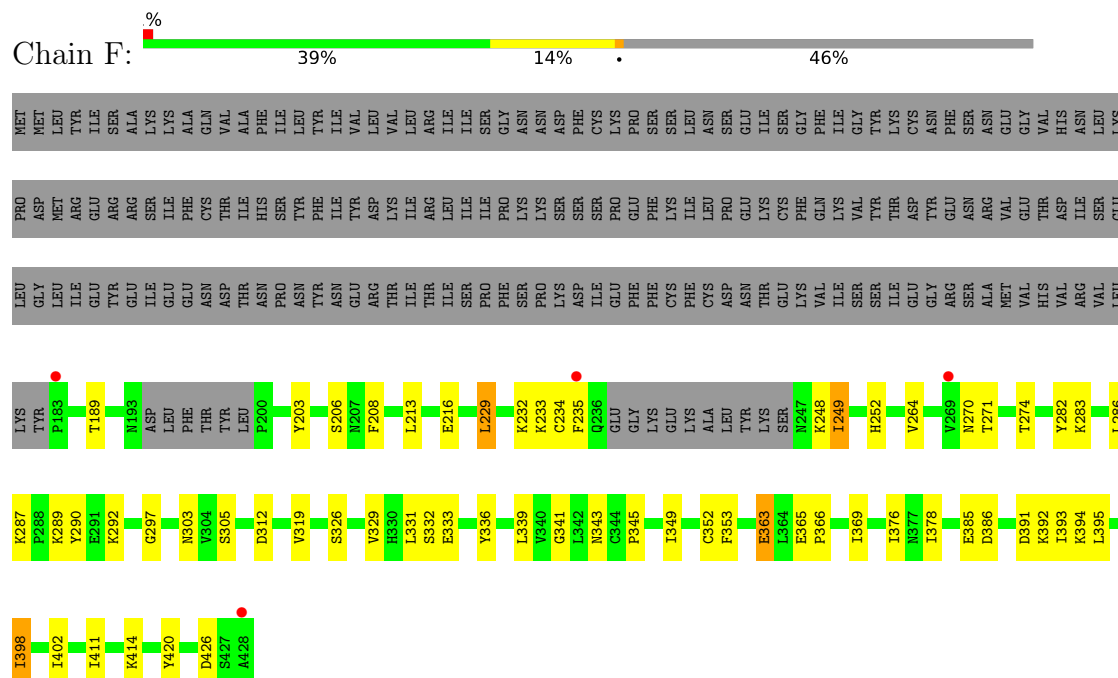
3 Residue-property plots

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: Gametocyte surface protein P45/48

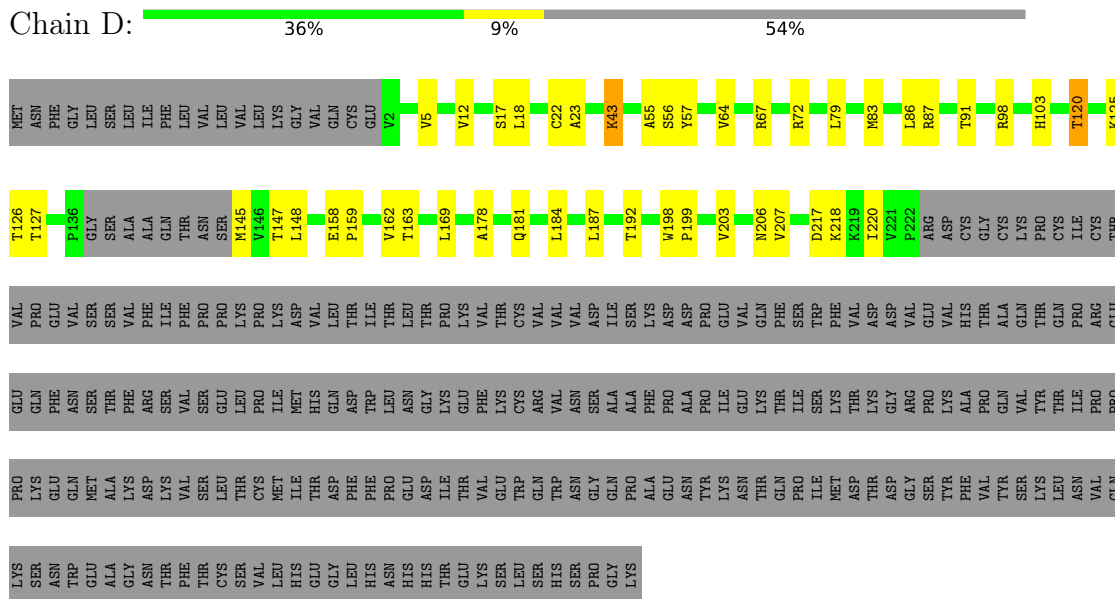


• Molecule 1: Gametocyte surface protein P45/48

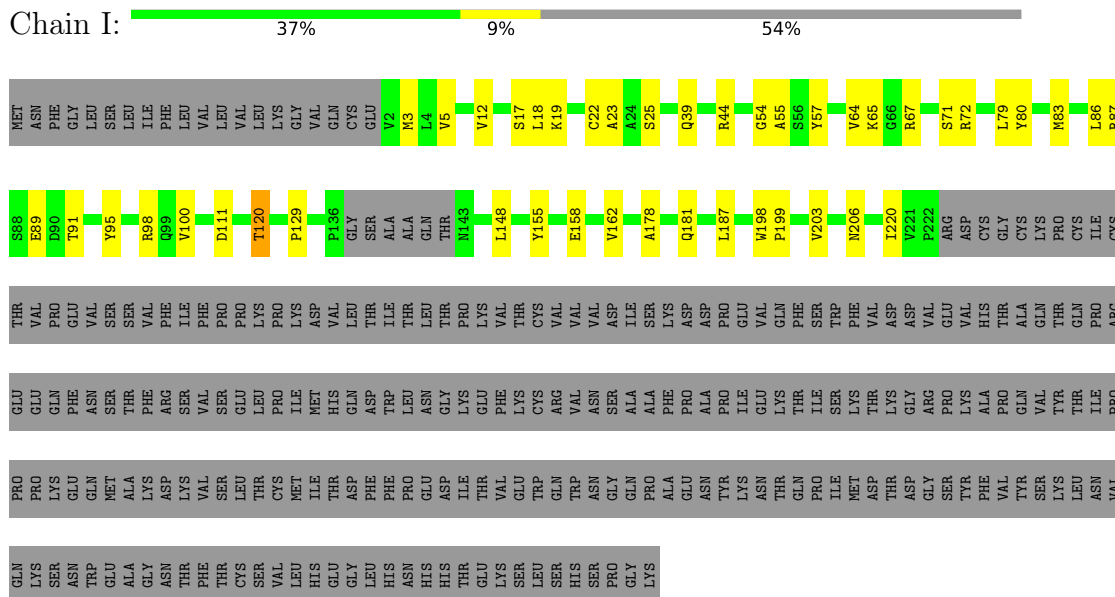




- Molecule 4: 10D8 heavy chain

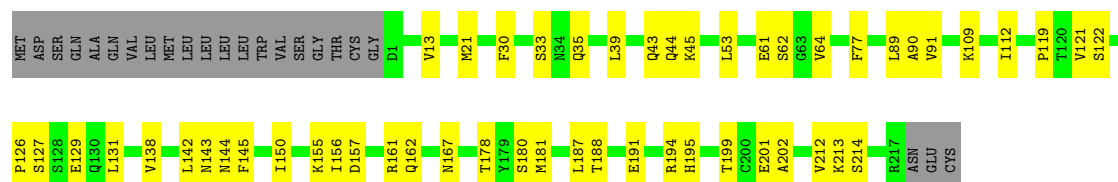


- Molecule 4: 10D8 heavy chain

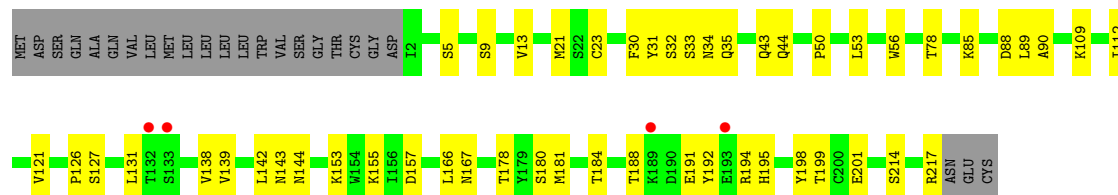


- Molecule 5: 10D8 light chain





- Molecule 5: 10D8 light chain



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.58Å 158.45Å 186.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.79 – 3.69 93.79 – 3.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (93.79-3.69) 99.9 (93.79-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.67Å)	Xtriage
Refinement program	BUSTER 1.19_4092, PHENIX 1.19_4092	Depositor
R, R_{free}	0.255 , 0.280 0.252 , 0.279	Depositor DCC
R_{free} test set	1806 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	138.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16969	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/1927	0.37	0/2605
1	F	0.18	0/1869	0.39	0/2528
2	B	0.15	0/1669	0.37	0/2278
2	G	0.16	0/1689	0.40	0/2305
3	C	0.15	0/1652	0.34	0/2248
3	H	0.16	0/1652	0.35	0/2248
4	D	0.19	0/1659	0.40	0/2266
4	I	0.17	0/1673	0.37	0/2285
5	E	0.17	0/1731	0.37	0/2350
5	J	0.15	0/1723	0.36	0/2339
All	All	0.17	0/17244	0.37	0/23452

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

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	1888	0	1838	36	0
1	F	1831	0	1785	47	0
2	B	1627	0	1600	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1647	0	1613	19	0
3	C	1613	0	1552	22	0
3	H	1613	0	1552	23	0
4	D	1617	0	1582	28	0
4	I	1631	0	1593	28	0
5	E	1690	0	1623	32	0
5	J	1682	0	1616	31	0
6	K	39	0	34	1	0
7	L	49	0	43	0	0
8	A	14	0	13	0	0
8	F	28	0	26	0	0
All	All	16969	0	16470	257	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 8.

All (257) 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)
4:I:91:THR:HG23	4:I:120:THR:HA	1.57	0.84
4:D:91:THR:HG23	4:D:120:THR:HA	1.59	0.84
4:I:19:LYS:HD3	4:I:80:TYR:HB3	1.59	0.83
1:A:186:ILE:HG22	1:A:222:LEU:HB3	1.64	0.79
5:J:155:LYS:HB2	5:J:199:THR:HB	1.69	0.74
1:A:191:LEU:HB2	1:A:227:CYS:HB3	1.70	0.73
2:G:91:THR:HG23	2:G:117:THR:HA	1.71	0.72
3:C:194:GLU:HG2	3:C:205:VAL:HG22	1.72	0.70
1:F:234:CYS:SG	1:F:235:PHE:N	2.65	0.69
5:E:155:LYS:HB2	5:E:199:THR:HB	1.74	0.69
2:B:91:THR:HG23	2:B:117:THR:HA	1.76	0.67
5:E:191:GLU:HA	5:E:194:ARG:HD3	1.76	0.67
4:I:5:VAL:HG23	4:I:23:ALA:HB3	1.76	0.67
5:J:85:LYS:HB2	5:J:88:ASP:OD1	1.96	0.65
1:A:369:ILE:HD11	2:B:104:LEU:HD21	1.78	0.65
4:I:3:MET:HB2	4:I:25:SER:HB3	1.77	0.65
5:E:167:ASN:HB3	5:E:181:MET:HE3	1.79	0.64
3:H:34:TRP:HB2	3:H:47:ILE:HB	1.79	0.63
1:F:235:PHE:CD1	1:F:271:THR:HB	2.34	0.62
3:H:192:THR:HG23	3:H:207:SER:HB2	1.80	0.62
3:C:65:GLY:HA3	3:C:70:TYR:HA	1.81	0.61
5:J:191:GLU:HA	5:J:194:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:178:ALA:HB2	4:I:187:LEU:HD23	1.82	0.61
5:E:91:VAL:HG22	5:E:109:LYS:HG2	1.83	0.61
3:H:119:PRO:HD3	3:H:131:VAL:HG22	1.83	0.61
1:F:289:LYS:HD3	4:I:54:GLY:HA3	1.84	0.60
1:A:363:GLU:HG3	1:A:365:GLU:HG2	1.83	0.59
1:F:332:SER:HA	1:F:426:ASP:OD1	2.01	0.59
1:F:369:ILE:HD11	2:G:104:LEU:HD21	1.84	0.59
3:C:34:TRP:HB2	3:C:47:ILE:HB	1.84	0.59
1:F:287:LYS:HG2	4:I:57:TYR:CZ	2.38	0.59
1:F:363:GLU:CD	1:F:363:GLU:H	2.10	0.59
1:F:385:GLU:HB3	1:F:394:LYS:HZ3	1.68	0.58
5:E:201:GLU:HB3	5:E:212:VAL:HG12	1.84	0.58
4:I:148:LEU:HD22	4:I:220:ILE:HG21	1.86	0.58
1:A:189:THR:HA	1:A:203:TYR:O	2.03	0.58
1:A:376:ILE:HG22	1:A:406:THR:HG21	1.85	0.58
2:B:155:GLU:HG3	2:B:156:PRO:HA	1.85	0.58
3:C:119:PRO:HD3	3:C:131:VAL:HG22	1.86	0.57
1:F:312:ASP:OD2	1:F:329:VAL:HG22	2.04	0.57
1:F:270:ASN:HB3	1:F:287:LYS:HE2	1.84	0.57
2:G:175:ALA:HB2	2:G:184:LEU:HD23	1.85	0.57
5:E:89:LEU:HD13	5:E:112:ILE:HD11	1.87	0.56
1:A:235:PHE:CD2	1:A:246:SER:HB3	2.40	0.56
5:E:143:ASN:HA	5:E:180:SER:HA	1.88	0.56
1:F:363:GLU:HG2	1:F:365:GLU:HG2	1.87	0.56
2:G:155:GLU:HG2	2:G:156:PRO:HA	1.87	0.56
1:F:216:GLU:HB3	1:F:289:LYS:HE2	1.87	0.56
3:H:107:ARG:HG3	3:H:170:SER:HB2	1.88	0.56
1:A:366:PRO:HB3	3:C:90:TRP:CD2	2.40	0.56
5:J:43:GLN:HB2	5:J:53:LEU:HD11	1.88	0.56
1:F:290:TYR:CZ	1:F:292:LYS:HE3	2.40	0.56
5:J:167:ASN:HB3	5:J:181:MET:HE3	1.88	0.56
3:H:1:GLN:HA	3:H:94:PRO:HD2	1.88	0.55
4:D:158:GLU:HG3	4:D:159:PRO:HA	1.89	0.55
3:H:65:GLY:HA3	3:H:70:TYR:HA	1.88	0.55
1:F:366:PRO:HB3	3:H:90:TRP:CD2	2.42	0.55
4:I:67:ARG:NH2	4:I:87:ARG:HG3	2.22	0.55
1:F:189:THR:HG22	1:F:203:TYR:HB2	1.88	0.55
4:I:181:GLN:HG3	5:J:166:LEU:HD21	1.89	0.55
4:D:12:VAL:HG21	4:D:86:LEU:HD13	1.89	0.54
5:J:144:ASN:HA	5:J:178:THR:HB	1.89	0.54
4:D:64:VAL:HA	4:D:67:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:ASN:HB3	3:C:196:THR:HB	1.89	0.54
5:J:89:LEU:HD11	5:J:112:ILE:HD11	1.90	0.54
1:A:248:LYS:HE2	1:F:248:LYS:HA	1.89	0.54
1:A:189:THR:HG22	1:A:191:LEU:HG	1.91	0.53
4:D:55:ALA:HB2	4:D:72:ARG:HG2	1.91	0.53
5:E:188:THR:HG23	5:E:191:GLU:H	1.73	0.53
3:C:7:SER:OG	3:C:24:ARG:NH1	2.43	0.52
5:E:144:ASN:HA	5:E:178:THR:HB	1.90	0.52
5:E:199:THR:HA	5:E:214:SER:HB3	1.91	0.52
5:J:44:GLN:HG3	5:J:50:PRO:HG3	1.91	0.52
4:D:206:ASN:ND2	4:D:217:ASP:OD1	2.42	0.52
5:J:32:SER:O	5:J:35:GLN:HG3	2.10	0.52
3:C:146:LYS:HB2	3:C:194:GLU:HB2	1.91	0.52
4:I:22:CYS:HB3	4:I:79:LEU:HB3	1.92	0.52
1:A:341:GLY:HA3	1:A:395:LEU:HB3	1.92	0.52
3:C:18:LYS:HG2	3:C:75:SER:O	2.10	0.52
5:E:122:SER:HA	5:E:213:LYS:NZ	2.25	0.52
5:E:150:ILE:HD11	5:E:202:ALA:HB1	1.92	0.51
1:F:303:ASN:OD1	1:F:305:SER:N	2.42	0.51
3:C:10:ILE:HG23	3:C:104:GLU:HG3	1.92	0.51
1:F:292:LYS:HE2	1:F:292:LYS:HA	1.92	0.51
4:D:67:ARG:NH2	4:D:87:ARG:HG3	2.26	0.51
5:E:43:GLN:HB2	5:E:53:LEU:HD11	1.93	0.51
1:F:398:ILE:HD11	1:F:402:ILE:HD11	1.92	0.51
4:I:55:ALA:HB2	4:I:72:ARG:HG2	1.91	0.51
4:D:145:MET:HG2	4:D:192:THR:HG22	1.92	0.51
1:A:235:PHE:HA	1:A:271:THR:HG23	1.93	0.51
5:E:121:VAL:HA	5:E:142:LEU:HD23	1.92	0.51
1:A:248:LYS:NZ	1:F:249:ILE:H	2.08	0.51
2:B:175:ALA:HB2	2:B:184:LEU:HD23	1.94	0.51
5:J:153:LYS:HB2	5:J:201:GLU:HG3	1.92	0.51
1:F:235:PHE:CD2	1:F:249:ILE:HG12	2.46	0.50
1:F:339:LEU:HD22	1:F:395:LEU:HD13	1.92	0.50
1:A:364:LEU:HD23	2:B:59:TYR:HB3	1.93	0.50
4:D:148:LEU:HD22	4:D:220:ILE:HG21	1.93	0.50
1:F:331:LEU:HB3	1:F:336:TYR:HE2	1.75	0.50
5:J:199:THR:HA	5:J:214:SER:HB3	1.93	0.50
5:E:33:SER:HB2	6:K:1:NAG:H83	1.94	0.50
1:A:386:ASP:HB3	1:A:393:ILE:HG23	1.94	0.50
5:J:192:TYR:O	5:J:198:TYR:OH	2.30	0.50
5:E:191:GLU:HG2	5:E:195:HIS:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:GLN:N	4:D:184:LEU:O	2.40	0.49
4:I:12:VAL:HG21	4:I:86:LEU:HD13	1.94	0.49
5:J:166:LEU:HB2	5:J:184:THR:HB	1.94	0.49
2:G:142:MET:HE2	2:G:191:PRO:HG3	1.95	0.49
1:A:223:PHE:HE1	1:A:225:LEU:HD23	1.78	0.49
1:F:208:PHE:CE2	1:F:213:LEU:HB2	2.48	0.49
4:I:64:VAL:HA	4:I:67:ARG:HD3	1.95	0.49
1:A:287:LYS:HB2	4:D:57:TYR:OH	2.12	0.48
1:A:217:LEU:HD11	1:A:286:LEU:HD22	1.96	0.48
1:A:287:LYS:HE2	4:D:56:SER:HB3	1.95	0.48
1:F:345:PRO:HG2	1:F:414:LYS:HD2	1.95	0.48
1:F:235:PHE:HD2	1:F:249:ILE:HG12	1.78	0.48
1:F:376:ILE:HG13	1:F:378:ILE:HG12	1.94	0.48
3:H:37:GLN:HA	3:H:44:LYS:HZ3	1.78	0.48
5:J:195:HIS:O	5:J:217:ARG:NH2	2.47	0.48
1:F:392:LYS:HB3	1:F:394:LYS:HE2	1.95	0.48
4:D:198:TRP:CG	4:D:199:PRO:HA	2.48	0.48
5:J:5:SER:O	5:J:23:CYS:HA	2.14	0.48
1:A:326:SER:HB3	1:A:420:TYR:CZ	2.49	0.48
5:E:61:GLU:HG3	5:E:62:SER:N	2.28	0.48
2:G:201:THR:OG1	2:G:216:LYS:HG2	2.14	0.48
4:D:22:CYS:HB3	4:D:79:LEU:HB3	1.96	0.48
1:F:206:SER:OG	5:J:34:ASN:ND2	2.44	0.47
5:E:45:LYS:HD2	5:E:90:ALA:HB2	1.95	0.47
2:G:193:SER:HB2	2:G:194:PRO:HD3	1.94	0.47
2:B:51:ILE:HG13	2:B:58:THR:HG22	1.95	0.47
4:I:198:TRP:CG	4:I:199:PRO:HA	2.50	0.47
2:G:51:ILE:HG13	2:G:58:THR:HG22	1.97	0.47
5:J:126:PRO:HD3	5:J:138:VAL:HG22	1.96	0.47
5:E:199:THR:HG23	5:E:214:SER:HB3	1.97	0.47
1:F:274:THR:HG22	1:F:283:LYS:HG2	1.96	0.47
3:H:89:GLN:O	3:H:95:LEU:HG	2.15	0.46
5:J:21:MET:O	5:J:78:THR:HA	2.15	0.46
2:G:64:VAL:HG12	2:G:67:ARG:HH21	1.80	0.46
3:C:165:GLN:HG2	3:C:170:SER:HA	1.96	0.46
3:H:148:LYS:HB2	3:H:192:THR:HB	1.97	0.46
2:G:153:PHE:HA	2:G:154:PRO:HA	1.67	0.46
1:F:352:CYS:HA	1:F:353:PHE:HA	1.49	0.46
1:A:297:GLY:HA3	1:A:341:GLY:O	2.16	0.46
4:I:71:SER:OG	4:I:80:TYR:HB2	2.15	0.46
5:J:157:ASP:CG	5:J:195:HIS:HB3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:14:SER:HB3	3:H:106:LYS:HD2	1.98	0.46
1:F:341:GLY:HA2	1:F:353:PHE:CE1	2.51	0.46
2:G:11:LEU:HB2	2:G:154:PRO:HG3	1.98	0.46
2:G:103:ASN:HB2	3:H:48:GLN:NE2	2.32	0.45
2:G:143:VAL:HG21	2:G:195:TRP:CD1	2.51	0.45
4:I:12:VAL:HG11	4:I:18:LEU:HB2	1.98	0.45
1:A:320:ASP:HB2	1:A:323:ALA:HB2	1.98	0.45
1:A:332:SER:HA	1:A:426:ASP:HB2	1.98	0.45
3:C:149:ILE:HD11	3:C:178:LEU:HD21	1.99	0.45
5:E:126:PRO:HD3	5:E:138:VAL:HG22	1.98	0.45
1:F:386:ASP:HB3	1:F:393:ILE:HB	1.98	0.45
1:A:411:ILE:HD13	2:B:102:GLY:O	2.17	0.45
4:D:5:VAL:HG23	4:D:23:ALA:HB3	1.98	0.45
3:C:139:TYR:CD1	3:C:140:PRO:HA	2.51	0.45
2:G:142:MET:HA	2:G:191:PRO:HA	1.99	0.45
3:C:145:VAL:HA	3:C:194:GLU:O	2.17	0.45
2:G:191:PRO:O	2:G:194:PRO:HD2	2.16	0.45
3:H:48:GLN:N	3:H:52:SER:O	2.43	0.45
5:J:192:TYR:O	5:J:217:ARG:NH2	2.50	0.45
5:J:143:ASN:HA	5:J:180:SER:HA	2.00	0.44
2:G:2:VAL:HG13	2:G:27:PHE:CD1	2.52	0.44
3:H:112:PRO:HB3	3:H:138:PHE:HB3	2.00	0.44
2:B:83:MET:HE3	2:B:83:MET:HB2	1.90	0.44
5:E:162:GLN:CD	5:E:162:GLN:H	2.25	0.44
4:D:148:LEU:HD13	4:D:203:VAL:HG21	1.99	0.44
1:F:326:SER:HB3	1:F:420:TYR:CZ	2.53	0.44
5:J:56:TRP:CE3	5:J:56:TRP:HA	2.51	0.44
2:B:19:LYS:HE2	2:B:80:ASN:HB3	2.00	0.44
4:I:178:ALA:HA	4:I:187:LEU:HB3	1.99	0.44
3:H:149:ILE:HD11	3:H:178:LEU:HD21	1.99	0.44
1:A:366:PRO:HB3	3:C:90:TRP:CE2	2.53	0.44
5:E:39:LEU:HD13	5:E:77:PHE:CG	2.52	0.44
5:E:156:ILE:HD12	5:E:161:ARG:HD3	2.00	0.43
1:F:349:ILE:HB	1:F:411:ILE:HB	1.99	0.43
1:A:183:PRO:HD2	1:A:200:PRO:HD3	1.99	0.43
3:C:209:ASN:C	3:C:211:ASN:H	2.25	0.43
1:F:297:GLY:HA2	1:F:329:VAL:HG21	1.98	0.43
1:A:345:PRO:HG2	1:A:414:LYS:HD2	1.99	0.43
3:C:82:ALA:HA	3:C:103:LEU:HD22	2.01	0.43
3:C:203:PRO:O	3:C:205:VAL:HG23	2.18	0.43
1:F:235:PHE:CG	1:F:271:THR:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PHE:HE1	1:F:286:LEU:HD13	1.82	0.43
4:I:162:VAL:HA	4:I:206:ASN:O	2.19	0.43
5:J:31:TYR:CZ	5:J:33:SER:HB2	2.54	0.43
1:F:297:GLY:HA3	1:F:341:GLY:O	2.18	0.43
2:G:108:ASP:HA	3:H:45:PRO:HG3	2.01	0.43
4:I:148:LEU:HD13	4:I:203:VAL:HG21	2.00	0.43
5:J:30:PHE:CZ	5:J:35:GLN:HA	2.54	0.43
5:J:188:THR:HG23	5:J:191:GLU:H	1.83	0.43
1:F:233:LYS:HG2	1:F:234:CYS:N	2.34	0.43
1:A:324:HIS:CD2	2:B:103:ASN:HB3	2.53	0.43
5:E:21:MET:HE3	5:E:21:MET:HB2	1.93	0.43
5:E:44:GLN:O	5:E:90:ALA:HB1	2.19	0.43
3:H:150:ASP:OD1	3:H:190:SER:N	2.51	0.43
3:H:183:ASP:O	3:H:187:ARG:HG3	2.19	0.43
5:E:157:ASP:CG	5:E:195:HIS:HB3	2.43	0.43
3:H:121:SER:HA	3:H:124:LEU:HD12	2.01	0.43
4:I:39:GLN:HB2	4:I:95:TYR:HE2	1.84	0.43
5:J:9:SER:O	5:J:109:LYS:HD2	2.19	0.43
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.53	0.42
1:F:233:LYS:HG2	1:F:234:CYS:H	1.84	0.42
2:B:68:PHE:HB3	2:B:81:LEU:HD11	2.00	0.42
4:D:162:VAL:HG12	4:D:207:VAL:HG13	2.00	0.42
1:A:184:HIS:O	1:A:185:ASN:HB3	2.18	0.42
1:A:246:SER:HB2	1:A:249:ILE:HG23	2.01	0.42
5:E:119:PRO:HB3	5:E:145:PHE:HB3	2.01	0.42
2:B:108:ASP:HA	3:C:45:PRO:HG3	2.02	0.42
5:E:30:PHE:CZ	5:E:35:GLN:HA	2.54	0.42
5:J:127:SER:O	5:J:131:LEU:HG	2.20	0.42
1:A:272:GLU:HB3	1:A:283:LYS:HD2	2.02	0.42
4:D:178:ALA:HB2	4:D:187:LEU:HD23	2.01	0.42
4:D:218:LYS:NZ	5:E:129:GLU:OE1	2.45	0.42
3:H:209:ASN:C	3:H:211:ASN:H	2.27	0.42
1:A:341:GLY:HA2	1:A:353:PHE:CE2	2.55	0.42
4:D:125:LYS:O	4:D:127:THR:HG23	2.19	0.42
1:F:385:GLU:HB3	1:F:394:LYS:NZ	2.32	0.42
5:J:44:GLN:O	5:J:90:ALA:HB1	2.20	0.42
1:A:220:GLY:O	1:F:252:HIS:HE1	2.02	0.42
4:D:158:GLU:HG3	4:D:159:PRO:CA	2.49	0.42
4:I:65:LYS:HE3	4:I:65:LYS:HB2	1.82	0.42
4:D:17:SER:HA	4:D:83:MET:O	2.20	0.41
4:D:163:THR:OG1	4:D:206:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:SER:O	5:E:131:LEU:HG	2.20	0.41
3:C:11:LEU:HD21	3:C:19:VAL:HB	2.01	0.41
3:H:147:TRP:O	3:H:153:GLU:HA	2.20	0.41
1:F:343:ASN:OD1	1:F:391:ASP:HB3	2.20	0.41
2:G:103:ASN:HB2	3:H:48:GLN:HE22	1.85	0.41
1:A:352:CYS:HA	1:A:353:PHE:HA	1.52	0.41
3:C:183:ASP:O	3:C:187:ARG:HG3	2.21	0.41
4:D:147:THR:HA	4:D:192:THR:HA	2.02	0.41
4:D:178:ALA:HA	4:D:187:LEU:HB3	2.03	0.41
1:F:235:PHE:CE1	1:F:286:LEU:HD13	2.56	0.41
4:I:100:VAL:HG22	4:I:111:ASP:OD1	2.21	0.41
4:D:12:VAL:HG11	4:D:18:LEU:HB2	2.03	0.41
4:I:89:GLU:H	4:I:89:GLU:CD	2.29	0.41
5:J:139:VAL:HG22	5:J:184:THR:HG23	2.03	0.41
4:D:43:LYS:HB3	4:D:43:LYS:HE3	1.61	0.41
4:D:125:LYS:NZ	4:D:126:THR:OG1	2.50	0.41
4:I:89:GLU:OE1	4:I:89:GLU:N	2.46	0.41
5:E:119:PRO:HB3	5:E:145:PHE:CD2	2.57	0.40
2:G:39:GLN:HA	2:G:44:ARG:O	2.21	0.40
1:A:355:GLN:HG2	1:A:371:TYR:HE1	1.87	0.40
1:F:208:PHE:CE2	1:F:282:TYR:HB3	2.56	0.40
3:H:114:VAL:O	3:H:206:LYS:NZ	2.45	0.40
1:F:229:LEU:HB3	1:F:232:LYS:HA	2.03	0.40
4:I:129:PRO:HB3	4:I:155:TYR:HB3	2.03	0.40
5:J:121:VAL:HG12	5:J:142:LEU:HD23	2.02	0.40
3:C:160:ASN:HB3	3:C:174:MET:HE3	2.03	0.40
5:E:61:GLU:HB3	5:E:64:VAL:CG2	2.52	0.40
4:I:17:SER:HA	4:I:83:MET:O	2.21	0.40
4:I:39:GLN:HA	4:I:44:ARG:O	2.21	0.40
1:A:355:GLN:HG2	1:A:371:TYR:CE1	2.56	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	231/428 (54%)	209 (90%)	22 (10%)	0	100	100
1	F	224/428 (52%)	203 (91%)	21 (9%)	0	100	100
2	B	209/444 (47%)	204 (98%)	5 (2%)	0	100	100
2	G	212/444 (48%)	203 (96%)	9 (4%)	0	100	100
3	C	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
3	H	209/213 (98%)	201 (96%)	8 (4%)	0	100	100
4	D	209/466 (45%)	197 (94%)	12 (6%)	0	100	100
4	I	211/466 (45%)	201 (95%)	10 (5%)	0	100	100
5	E	215/240 (90%)	206 (96%)	9 (4%)	0	100	100
5	J	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
All	All	2143/3582 (60%)	2034 (95%)	109 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	222/402 (55%)	218 (98%)	4 (2%)	51	67
1	F	216/402 (54%)	209 (97%)	7 (3%)	34	56
2	B	186/398 (47%)	181 (97%)	5 (3%)	39	59
2	G	188/398 (47%)	184 (98%)	4 (2%)	47	64
3	C	184/186 (99%)	181 (98%)	3 (2%)	55	68
3	H	184/186 (99%)	182 (99%)	2 (1%)	65	73
4	D	185/417 (44%)	180 (97%)	5 (3%)	39	59
4	I	187/417 (45%)	184 (98%)	3 (2%)	55	68
5	E	194/214 (91%)	192 (99%)	2 (1%)	68	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	193/214 (90%)	192 (100%)	1 (0%)	81	80
All	All	1939/3234 (60%)	1903 (98%)	36 (2%)	50	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
1	A	273	CYS
1	A	364	LEU
1	A	395	LEU
2	B	104	LEU
2	B	150	LYS
2	B	157	VAL
2	B	166	LEU
2	B	213	VAL
3	C	135	LEU
3	C	198	LYS
3	C	210	ARG
4	D	43	LYS
4	D	98	ARG
4	D	103	HIS
4	D	120	THR
4	D	169	LEU
5	E	13	VAL
5	E	187	LEU
1	F	229	LEU
1	F	249	ILE
1	F	264	VAL
1	F	319	VAL
1	F	333	GLU
1	F	363	GLU
1	F	398	ILE
2	G	43	LYS
2	G	104	LEU
2	G	157	VAL
2	G	213	VAL
3	H	77	VAL
3	H	135	LEU
4	I	98	ARG
4	I	120	THR
4	I	158	GLU
5	J	13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	GLN
3	C	136	ASN
4	D	77	ASN
4	D	206	ASN
5	E	48	GLN
1	F	328	ASN
1	F	337	ASN
2	G	80	ASN
4	I	82	GLN
4	I	103	HIS

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 ⓘ

7 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	$\# Z > 2$
6	NAG	K	1	6,1	14,14,15	0.41	0	17,19,21	0.48	0
6	NAG	K	2	6	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
6	BMA	K	3	6	11,11,12	0.72	0	15,15,17	0.67	0
7	NAG	L	1	7,1	14,14,15	0.25	0	17,19,21	0.61	0
7	NAG	L	2	7	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
7	BMA	L	3	7	11,11,12	0.87	0	15,15,17	0.71	0
7	FUC	L	4	7	10,10,11	0.82	0	14,14,16	0.97	1 (7%)

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	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
7	NAG	L	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	0/2/19/22	0/1/1/1
7	FUC	L	4	7	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	2	NAG	C1-O5-C5	3.32	116.64	112.19
6	K	2	NAG	C1-O5-C5	3.24	116.53	112.19
7	L	4	FUC	C1-O5-C5	2.15	118.04	112.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

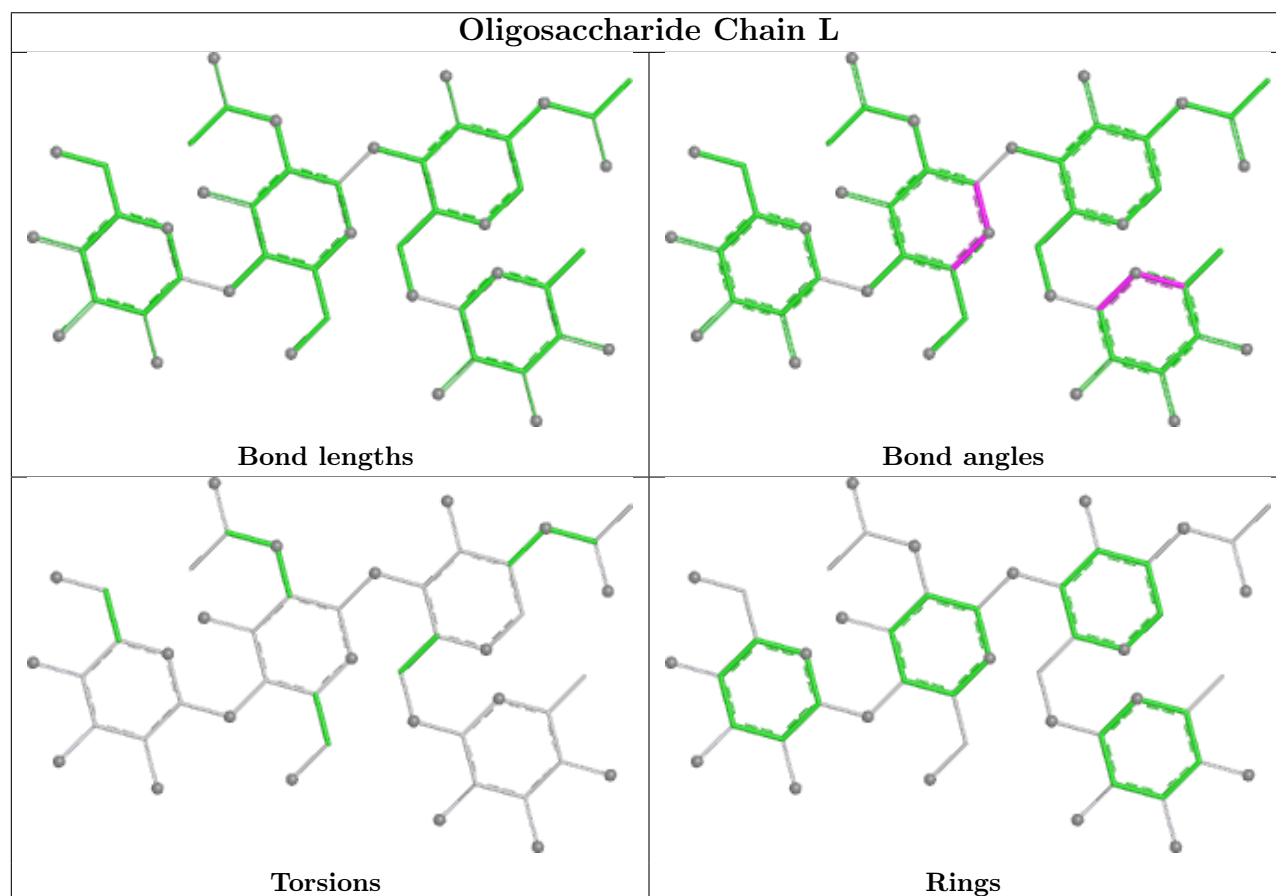
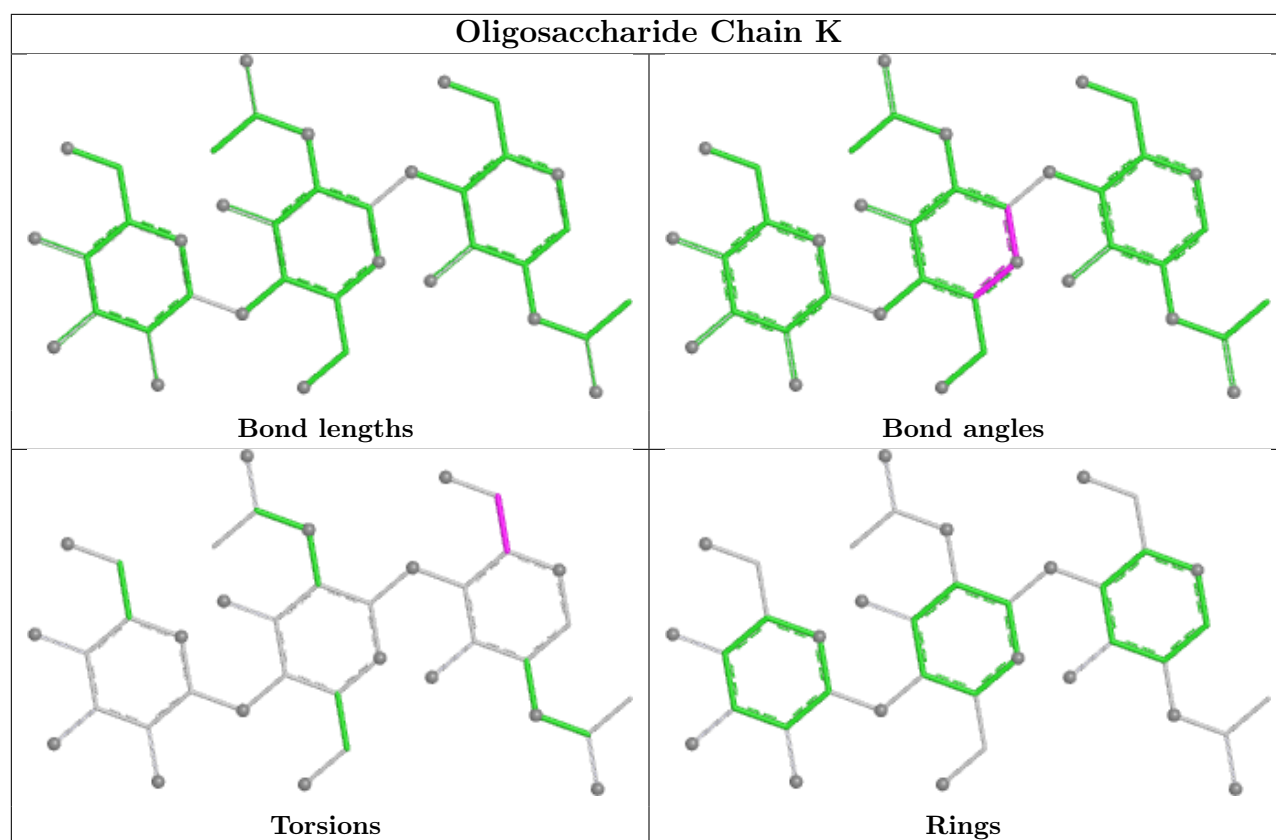
Mol	Chain	Res	Type	Atoms
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	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

3 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
8	NAG	F	902	1	14,14,15	0.60	1 (7%)	17,19,21	0.68	1 (5%)
8	NAG	A	501	1	14,14,15	0.57	0	17,19,21	0.58	0
8	NAG	F	901	1	14,14,15	0.35	0	17,19,21	0.55	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
8	NAG	F	902	1	-	1/6/23/26	0/1/1/1
8	NAG	A	501	1	-	2/6/23/26	0/1/1/1
8	NAG	F	901	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	902	NAG	O5-C1	2.14	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	902	NAG	C1-O5-C5	2.18	115.10	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	901	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	501	NAG	C4-C5-C6-O6
8	A	501	NAG	O5-C5-C6-O6
8	F	902	NAG	O5-C5-C6-O6
8	F	901	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	237/428 (55%)	-0.22	0 100 100	98, 146, 208, 234	0
1	F	230/428 (53%)	-0.24	4 (1%) 69 43	108, 157, 189, 214	0
2	B	213/444 (47%)	-0.40	0 100 100	103, 146, 191, 207	0
2	G	216/444 (48%)	-0.37	2 (0%) 81 58	111, 142, 193, 257	0
3	C	211/213 (99%)	-0.51	0 100 100	94, 154, 200, 222	0
3	H	211/213 (99%)	-0.52	0 100 100	103, 134, 165, 182	0
4	D	213/466 (45%)	-0.51	0 100 100	106, 157, 204, 238	0
4	I	215/466 (46%)	-0.26	0 100 100	117, 180, 277, 310	0
5	E	217/240 (90%)	-0.47	0 100 100	105, 158, 204, 222	0
5	J	216/240 (90%)	-0.13	4 (1%) 66 42	123, 222, 287, 297	0
All	All	2179/3582 (60%)	-0.36	10 (0%) 87 69	94, 153, 239, 310	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	132	THR	4.2
2	G	134	GLY	3.8
1	F	183	PRO	3.6
1	F	235	PHE	3.1
5	J	189	LYS	3.1
5	J	133	SER	2.5
2	G	133	PRO	2.4
5	J	193	GLU	2.0
1	F	428	ALA	2.0
1	F	269	VAL	2.0

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

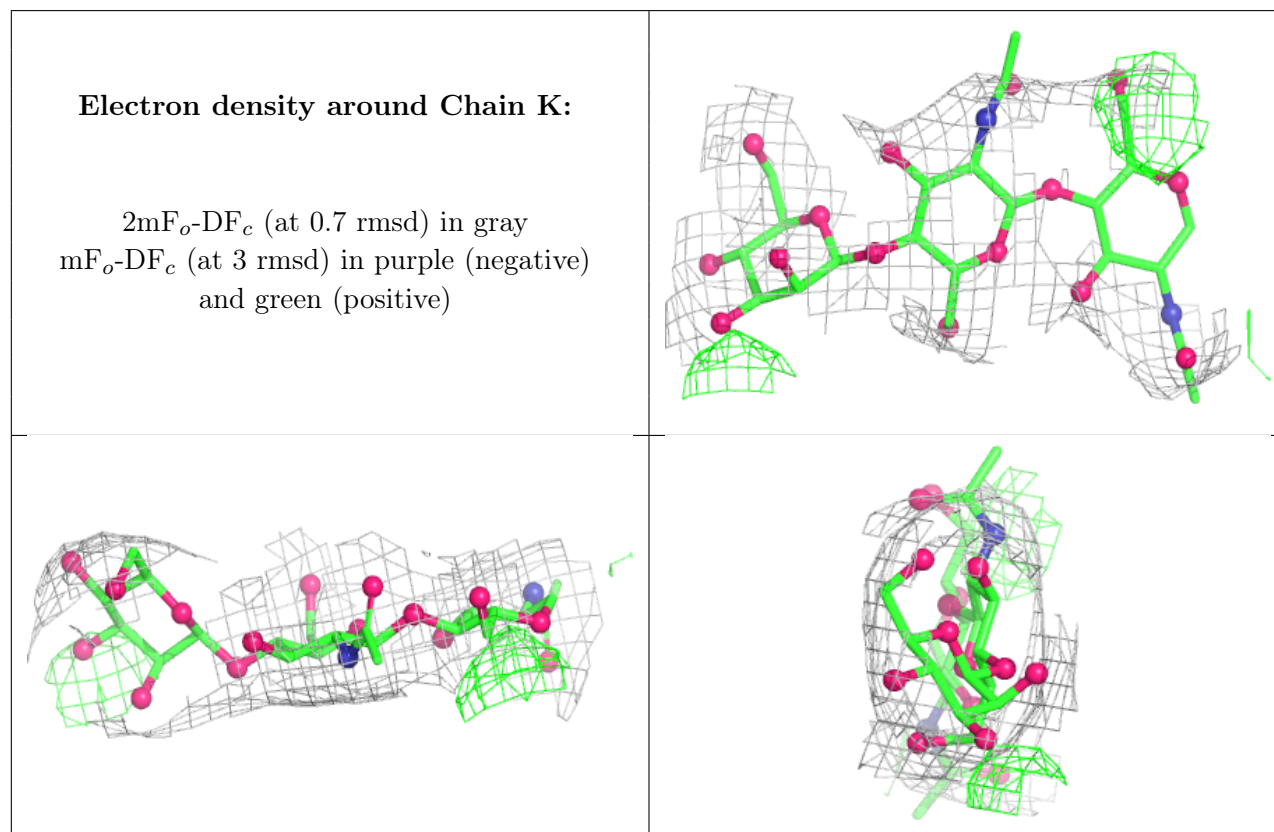
There are no non-standard protein/DNA/RNA residues in this entry.

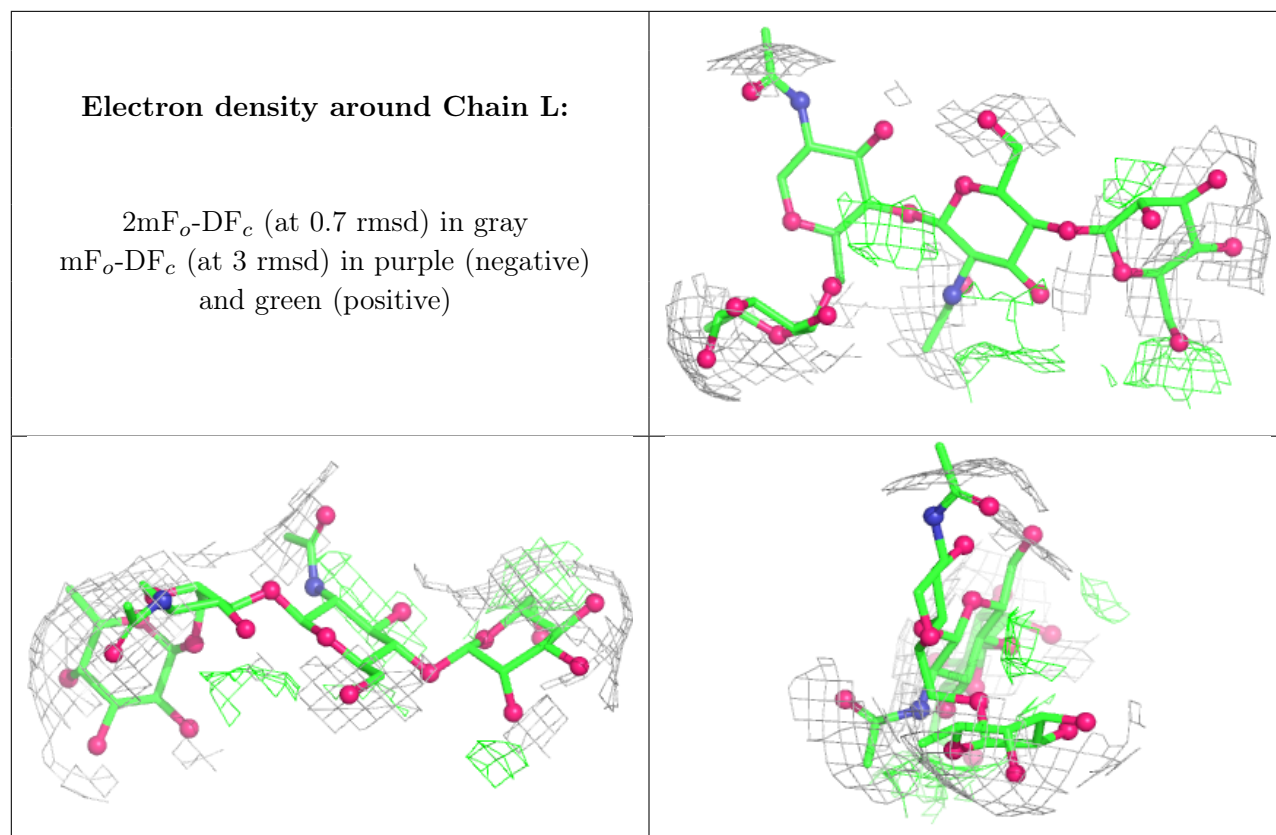
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
7	BMA	L	3	11/12	0.28	0.11	195,195,195,195	0
6	BMA	K	3	11/12	0.60	0.10	167,181,217,233	0
6	NAG	K	1	14/15	0.61	0.13	165,193,237,242	0
7	NAG	L	2	14/15	0.67	0.11	197,197,197,197	0
7	FUC	L	4	10/11	0.72	0.09	188,188,188,188	0
7	NAG	L	1	14/15	0.85	0.07	188,188,188,188	0
6	NAG	K	2	14/15	0.87	0.09	183,208,232,234	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
8	NAG	F	901	14/15	-0.02	0.13	246,253,259,259	0
8	NAG	F	902	14/15	0.66	0.09	198,198,198,198	0
8	NAG	A	501	14/15	0.71	0.11	200,200,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.