



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 01:04 am GMT

PDB ID : 5LCV
Title : Structural basis of Zika and Dengue virus potent antibody cross-neutralization
Authors : Barba-Spaeth, G.
Deposited on : 2016-06-22
Resolution : 2.64 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

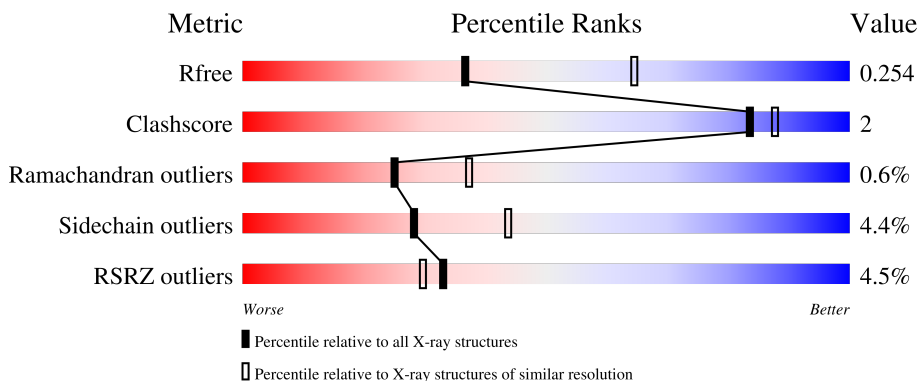
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	447	 82% 8% 9%
1	B	447	 83% 7% 9%
2	H	283	 70% 9% 20%
3	L	216	 88% 9%
4	C	4	 75% 25%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 9620 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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	3100	1939	543	592	26	0	0	0
1	B	405	3102	1938	543	596	25	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP A0A120IIH9
A	410	PRO	-	expression tag	UNP A0A120IIH9
A	411	PHE	-	expression tag	UNP A0A120IIH9
A	412	GLU	-	expression tag	UNP A0A120IIH9
A	413	ASP	-	expression tag	UNP A0A120IIH9
A	414	ASP	-	expression tag	UNP A0A120IIH9
A	415	ASP	-	expression tag	UNP A0A120IIH9
A	416	ASP	-	expression tag	UNP A0A120IIH9
A	417	LYS	-	expression tag	UNP A0A120IIH9
A	418	ALA	-	expression tag	UNP A0A120IIH9
A	419	GLY	-	expression tag	UNP A0A120IIH9
A	420	TRP	-	expression tag	UNP A0A120IIH9
A	421	SER	-	expression tag	UNP A0A120IIH9
A	422	HIS	-	expression tag	UNP A0A120IIH9
A	423	PRO	-	expression tag	UNP A0A120IIH9
A	424	GLN	-	expression tag	UNP A0A120IIH9
A	425	PHE	-	expression tag	UNP A0A120IIH9
A	426	GLU	-	expression tag	UNP A0A120IIH9
A	427	LYS	-	expression tag	UNP A0A120IIH9
A	428	GLY	-	expression tag	UNP A0A120IIH9
A	429	GLY	-	expression tag	UNP A0A120IIH9
A	430	GLY	-	expression tag	UNP A0A120IIH9
A	431	SER	-	expression tag	UNP A0A120IIH9
A	432	GLY	-	expression tag	UNP A0A120IIH9
A	433	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLY	-	expression tag	UNP A0A120IIH9
A	435	SER	-	expression tag	UNP A0A120IIH9
A	436	GLY	-	expression tag	UNP A0A120IIH9
A	437	GLY	-	expression tag	UNP A0A120IIH9
A	438	GLY	-	expression tag	UNP A0A120IIH9
A	439	SER	-	expression tag	UNP A0A120IIH9
A	440	TRP	-	expression tag	UNP A0A120IIH9
A	441	SER	-	expression tag	UNP A0A120IIH9
A	442	HIS	-	expression tag	UNP A0A120IIH9
A	443	PRO	-	expression tag	UNP A0A120IIH9
A	444	GLN	-	expression tag	UNP A0A120IIH9
A	445	PHE	-	expression tag	UNP A0A120IIH9
A	446	GLU	-	expression tag	UNP A0A120IIH9
A	447	LYS	-	expression tag	UNP A0A120IIH9
B	409	GLY	-	expression tag	UNP A0A120IIH9
B	410	PRO	-	expression tag	UNP A0A120IIH9
B	411	PHE	-	expression tag	UNP A0A120IIH9
B	412	GLU	-	expression tag	UNP A0A120IIH9
B	413	ASP	-	expression tag	UNP A0A120IIH9
B	414	ASP	-	expression tag	UNP A0A120IIH9
B	415	ASP	-	expression tag	UNP A0A120IIH9
B	416	ASP	-	expression tag	UNP A0A120IIH9
B	417	LYS	-	expression tag	UNP A0A120IIH9
B	418	ALA	-	expression tag	UNP A0A120IIH9
B	419	GLY	-	expression tag	UNP A0A120IIH9
B	420	TRP	-	expression tag	UNP A0A120IIH9
B	421	SER	-	expression tag	UNP A0A120IIH9
B	422	HIS	-	expression tag	UNP A0A120IIH9
B	423	PRO	-	expression tag	UNP A0A120IIH9
B	424	GLN	-	expression tag	UNP A0A120IIH9
B	425	PHE	-	expression tag	UNP A0A120IIH9
B	426	GLU	-	expression tag	UNP A0A120IIH9
B	427	LYS	-	expression tag	UNP A0A120IIH9
B	428	GLY	-	expression tag	UNP A0A120IIH9
B	429	GLY	-	expression tag	UNP A0A120IIH9
B	430	GLY	-	expression tag	UNP A0A120IIH9
B	431	SER	-	expression tag	UNP A0A120IIH9
B	432	GLY	-	expression tag	UNP A0A120IIH9
B	433	GLY	-	expression tag	UNP A0A120IIH9
B	434	GLY	-	expression tag	UNP A0A120IIH9
B	435	SER	-	expression tag	UNP A0A120IIH9
B	436	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	GLY	-	expression tag	UNP A0A120IIH9
B	438	GLY	-	expression tag	UNP A0A120IIH9
B	439	SER	-	expression tag	UNP A0A120IIH9
B	440	TRP	-	expression tag	UNP A0A120IIH9
B	441	SER	-	expression tag	UNP A0A120IIH9
B	442	HIS	-	expression tag	UNP A0A120IIH9
B	443	PRO	-	expression tag	UNP A0A120IIH9
B	444	GLN	-	expression tag	UNP A0A120IIH9
B	445	PHE	-	expression tag	UNP A0A120IIH9
B	446	GLU	-	expression tag	UNP A0A120IIH9
B	447	LYS	-	expression tag	UNP A0A120IIH9

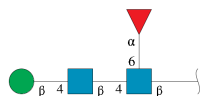
- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	226	1722	1091	292	332	7	0	0	0

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1572	982	263	321	6	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	C	4	49	28	2	19	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



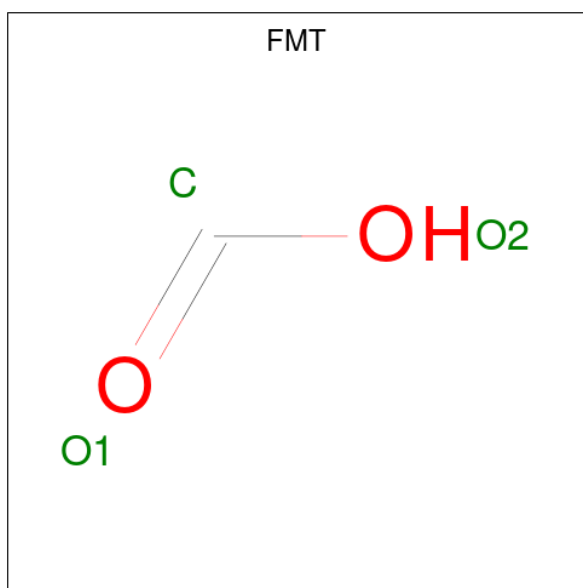
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	A	1	14	8	1	5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
6	A	1	6	3	3	0	0
6	B	1	6	3	3	0	0

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 3 1 2	0	0

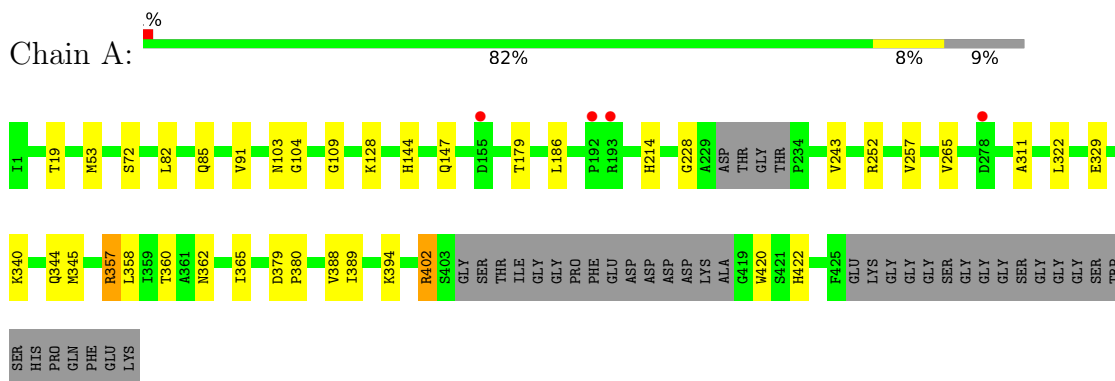
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	16	Total O 16 16	0	0
8	B	15	Total O 15 15	0	0
8	H	8	Total O 8 8	0	0
8	L	1	Total O 1 1	0	0

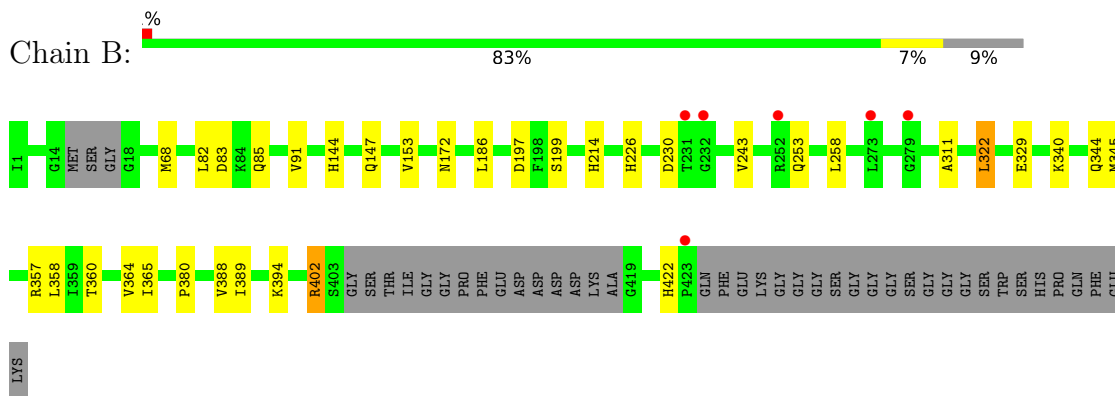
3 Residue-property plots [i](#)

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.

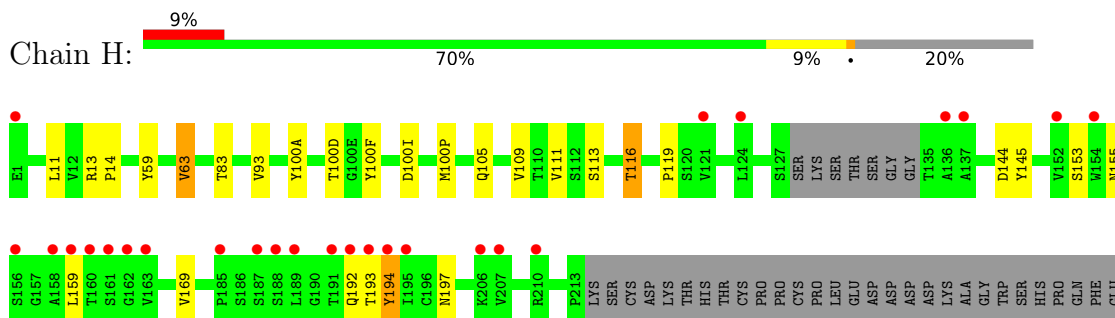
- Molecule 1: Polyprotein



- Molecule 1: Polyprotein




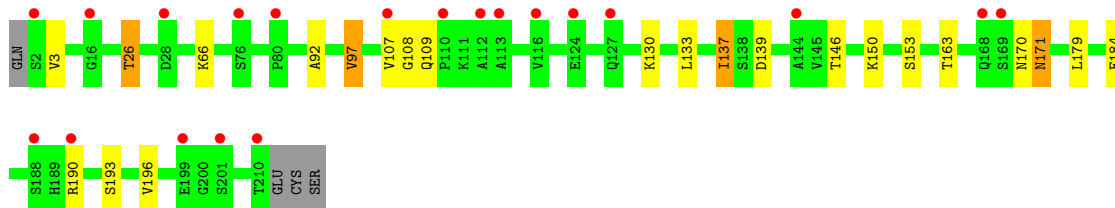
- Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11



LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11

Chain L:  9% 88% 9%



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

Chain C:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	204.29Å 207.32Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.64 39.93 – 2.64	Depositor EDS
% Data completeness (in resolution range)	61.9 (40.00-2.64) 61.9 (39.93-2.64)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.65Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.237 0.242 , 0.254	Depositor DCC
R_{free} test set	2436 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: GOL, FUC, NAG, BMA, FMT

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	0.35	0/3167	0.60	0/4289
1	B	0.36	0/3169	0.59	0/4294
2	H	0.37	0/1768	0.61	0/2412
3	L	0.36	0/1608	0.61	0/2196
All	All	0.36	0/9712	0.60	0/13191

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	3100	0	3017	15	0
1	B	3102	0	3020	11	0
2	H	1722	0	1646	16	0
3	L	1572	0	1539	9	0
4	C	49	0	43	0	0
5	A	14	0	13	0	0
6	A	12	0	16	0	0
6	B	6	0	8	0	0
7	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	16	0	0	0	0
8	B	15	0	0	0	0
8	H	8	0	0	0	0
8	L	1	0	0	0	0
All	All	9620	0	9303	45	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 2.

All (45) 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)
2:H:11:LEU:HD23	2:H:116:THR:OG1	1.58	1.01
2:H:83:THR:C	2:H:111:VAL:HG11	2.10	0.72
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.73	0.70
2:H:169:VAL:HB	3:L:163:THR:HG22	1.75	0.68
2:H:11:LEU:CD2	2:H:116:THR:OG1	2.41	0.67
3:L:150:LYS:HB2	3:L:193:SER:HB3	1.76	0.66
1:B:214:HIS:H	1:B:422:HIS:HE1	1.45	0.64
3:L:3:VAL:HB	3:L:26:THR:HG23	1.85	0.58
2:H:93:VAL:HG11	2:H:100(P):MET:HB3	1.89	0.55
1:A:82:LEU:H	1:A:85:GLN:HE21	1.55	0.53
2:H:155:ASN:HD21	2:H:194:TYR:HB3	1.73	0.53
2:H:153:SER:HB3	2:H:197:ASN:HB2	1.90	0.53
1:A:357:ARG:HD2	1:A:379:ASP:HB3	1.91	0.52
1:B:82:LEU:H	1:B:85:GLN:HE21	1.56	0.52
1:A:214:HIS:H	1:A:422:HIS:HE1	1.58	0.52
1:A:340:LYS:HE2	1:A:362:ASN:HD21	1.75	0.52
3:L:137:ILE:HD12	3:L:196:VAL:HG21	1.92	0.51
2:H:59:TYR:HB3	2:H:63:VAL:HG13	1.95	0.49
3:L:133:LEU:HD13	3:L:179:LEU:HD23	1.94	0.49
3:L:92:ALA:HB2	3:L:97:VAL:HG22	1.97	0.47
2:H:83:THR:CA	2:H:111:VAL:HG11	2.45	0.47
1:A:72:SER:O	2:H:100(I):ASP:HA	2.15	0.46
2:H:14:PRO:HD3	2:H:113:SER:HA	1.97	0.46
1:B:380:PRO:HG2	1:B:402:ARG:HG3	1.98	0.46
1:B:153:VAL:HG11	2:H:100(D):THR:HG22	1.98	0.45
1:A:380:PRO:HG2	1:A:402:ARG:HG3	1.98	0.45
1:A:311:ALA:HB2	1:A:394:LYS:HD2	1.99	0.45
1:B:226:HIS:HD2	1:B:230:ASP:HB3	1.82	0.44
1:A:109:GLY:HA2	1:B:322:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG11	1:A:243:VAL:HG21	2.00	0.44
3:L:133:LEU:HB2	3:L:179:LEU:HB3	2.00	0.44
1:B:311:ALA:HB2	1:B:394:LYS:HD2	2.00	0.43
1:A:144:HIS:HB3	1:A:360:THR:HG23	2.00	0.43
1:B:344:GLN:HG3	1:B:388:VAL:HG13	2.00	0.43
2:H:111:VAL:O	2:H:111:VAL:HG12	2.19	0.43
1:A:344:GLN:HG3	1:A:388:VAL:HG13	2.00	0.42
1:B:340:LYS:HA	1:B:364:VAL:HG12	2.02	0.42
1:B:91:VAL:HG11	1:B:243:VAL:HG21	2.02	0.42
1:A:104:GLY:HA2	2:H:100(A):TYR:C	2.40	0.42
3:L:109:GLN:HE22	3:L:171:ASN:HB3	1.85	0.42
1:A:252:ARG:HG2	2:H:100(F):TYR:CZ	2.56	0.41
1:A:265:VAL:HG22	1:A:420:TRP:HH2	1.84	0.41
1:B:144:HIS:HB3	1:B:360:THR:HG23	2.02	0.40
1:A:53:MET:HB3	1:A:128:LYS:HB3	2.03	0.40
3:L:107:VAL:HG12	3:L:108:GLY:N	2.36	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	400/447 (90%)	384 (96%)	14 (4%)	2 (0%)	29	43
1	B	399/447 (89%)	382 (96%)	15 (4%)	2 (0%)	29	43
2	H	222/283 (78%)	210 (95%)	10 (4%)	2 (1%)	17	26
3	L	210/216 (97%)	202 (96%)	6 (3%)	2 (1%)	15	22
All	All	1231/1393 (88%)	1178 (96%)	45 (4%)	8 (1%)	25	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	B	147	GLN
2	H	144	ASP
3	L	153	SER
2	H	116	THR
3	L	139	ASP
1	B	197	ASP
1	A	228	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/367 (92%)	324 (96%)	13 (4%)	32	48
1	B	339/367 (92%)	324 (96%)	15 (4%)	28	44
2	H	189/236 (80%)	181 (96%)	8 (4%)	30	45
3	L	178/183 (97%)	168 (94%)	10 (6%)	21	32
All	All	1043/1153 (90%)	997 (96%)	46 (4%)	28	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	103	ASN
1	A	179	THR
1	A	186	LEU
1	A	257	VAL
1	A	322	LEU
1	A	329	GLU
1	A	345	MET
1	A	357	ARG
1	A	358	LEU
1	A	365	ILE
1	A	389	ILE
1	A	402	ARG
1	B	68	MET

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Mol	Chain	Res	Type
1	B	83	ASP
1	B	172	ASN
1	B	186	LEU
1	B	199	SER
1	B	253	GLN
1	B	258	LEU
1	B	322	LEU
1	B	329	GLU
1	B	345	MET
1	B	357	ARG
1	B	358	LEU
1	B	365	ILE
1	B	389	ILE
1	B	402	ARG
2	H	13	ARG
2	H	63	VAL
2	H	105	GLN
2	H	109	VAL
2	H	159	LEU
2	H	192	GLN
2	H	193	THR
2	H	194	TYR
3	L	26	THR
3	L	66	LYS
3	L	97	VAL
3	L	130	LYS
3	L	137	ILE
3	L	146	THR
3	L	170	ASN
3	L	171	ASN
3	L	184	GLU
3	L	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	85	GLN
1	A	103	ASN
1	A	144	HIS
1	A	266	HIS
1	A	362	ASN

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Mol	Chain	Res	Type
1	B	85	GLN
1	B	144	HIS
1	B	214	HIS
1	B	226	HIS
1	B	249	HIS
1	B	362	ASN
1	B	422	HIS
2	H	155	ASN
3	L	109	GLN
3	L	170	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	C	1	4,1	14,14,15	0.34	0	17,19,21	0.65	0
4	NAG	C	2	4	14,14,15	0.32	0	17,19,21	0.61	0
4	BMA	C	3	4	11,11,12	0.50	0	15,15,17	1.68	1 (6%)
4	FUC	C	4	4	10,10,11	0.41	0	14,14,16	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	1/1/1/1
4	FUC	C	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	C1-O5-C5	6.06	120.40	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

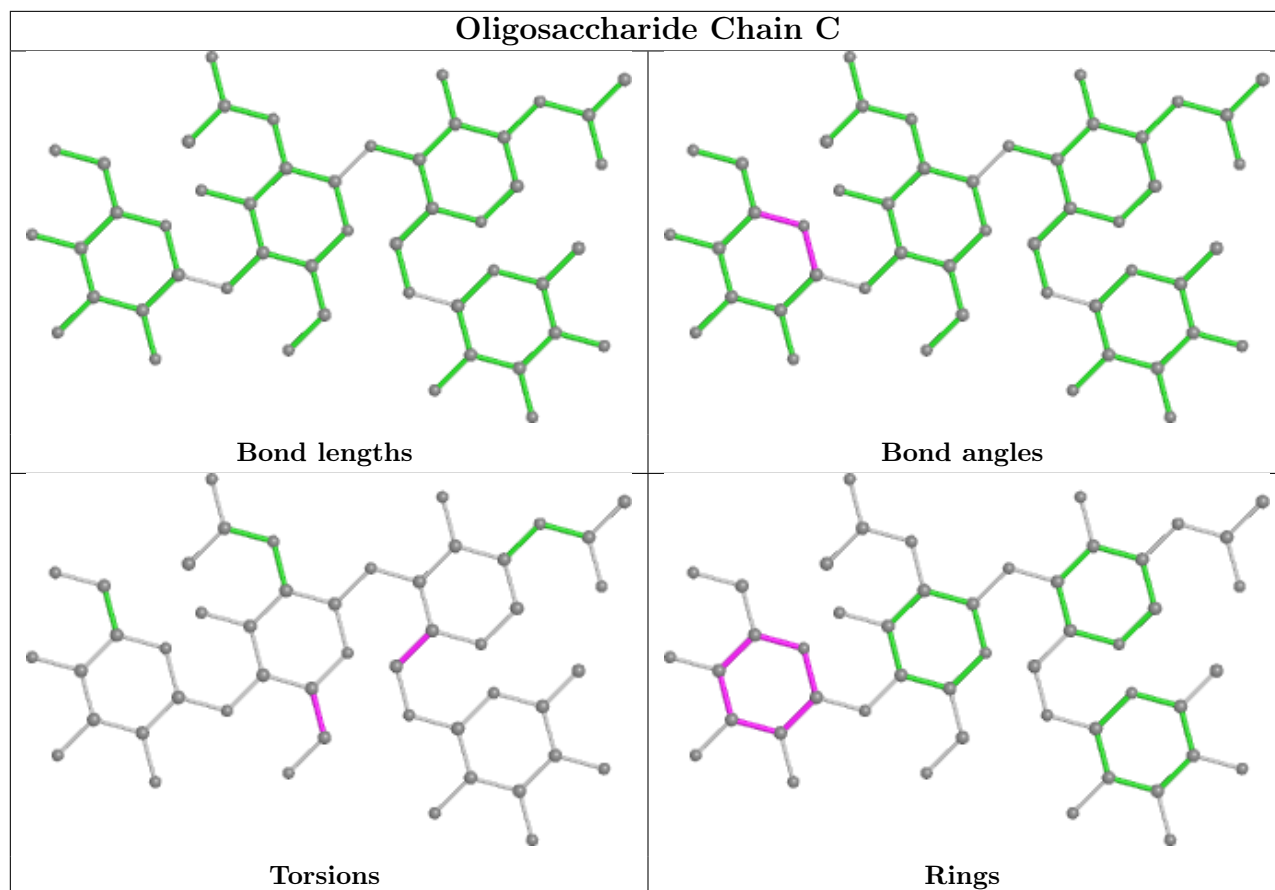
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

5 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	GOL	A	503	-	5,5,5	0.04	0	5,5,5	0.14	0
6	GOL	B	505	-	5,5,5	0.05	0	5,5,5	0.15	0
6	GOL	A	502	-	5,5,5	0.06	0	5,5,5	0.23	0
5	NAG	A	501	1	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
7	FMT	A	504	-	2,2,2	1.13	0	1,1,1	1.12	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	GOL	A	503	-	-	0/4/4/4	-
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	GOL	A	502	-	-	0/4/4/4	-
6	GOL	B	505	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C1-O5-C5	2.95	116.19	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	505	GOL	C1-C2-C3-O3

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	406/447 (90%)	0.01	4 (0%) 82 81	23, 46, 71, 100	0
1	B	405/447 (90%)	0.05	6 (1%) 73 71	23, 50, 77, 90	0
2	H	226/283 (79%)	0.63	26 (11%) 4 3	26, 64, 111, 136	0
3	L	212/216 (98%)	0.65	20 (9%) 8 6	31, 75, 100, 142	0
All	All	1249/1393 (89%)	0.24	56 (4%) 33 30	23, 53, 99, 142	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ARG	6.4
2	H	137	ALA	5.6
2	H	159	LEU	5.2
3	L	169	SER	4.8
2	H	162	GLY	4.7
2	H	185	PRO	4.6
2	H	163	VAL	4.5
2	H	193	THR	4.4
3	L	2	SER	4.4
3	L	190	ARG	4.1
2	H	207	VAL	4.1
2	H	161	SER	4.0
2	H	195	ILE	4.0
2	H	158	ALA	3.9
2	H	192	GLN	3.7
2	H	136	ALA	3.6
3	L	113	ALA	3.5
2	H	156	SER	3.4
3	L	199	GLU	3.4
3	L	210	THR	3.4
1	A	192	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	194	TYR	3.3
2	H	191	THR	3.2
3	L	168	GLN	3.1
2	H	121	VAL	3.1
1	A	155	ASP	2.8
2	H	187	SER	2.8
2	H	210	ARG	2.8
3	L	201	SER	2.8
1	B	279	GLY	2.8
2	H	154	TRP	2.8
3	L	124	GLU	2.7
3	L	127	GLN	2.7
1	B	232	GLY	2.6
3	L	112	ALA	2.6
2	H	188	SER	2.5
3	L	80	PRO	2.5
1	A	278	ASP	2.5
1	B	252	ARG	2.5
3	L	144	ALA	2.5
3	L	110	PRO	2.5
3	L	76	SER	2.5
2	H	124	LEU	2.4
2	H	160	THR	2.3
3	L	16	GLY	2.2
1	B	423	PRO	2.2
2	H	206	LYS	2.2
3	L	116	VAL	2.2
2	H	189	LEU	2.2
3	L	107	VAL	2.2
3	L	188	SER	2.2
1	B	231	THR	2.1
2	H	1	GLU	2.0
1	B	273	LEU	2.0
2	H	152	VAL	2.0
3	L	28	ASP	2.0

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

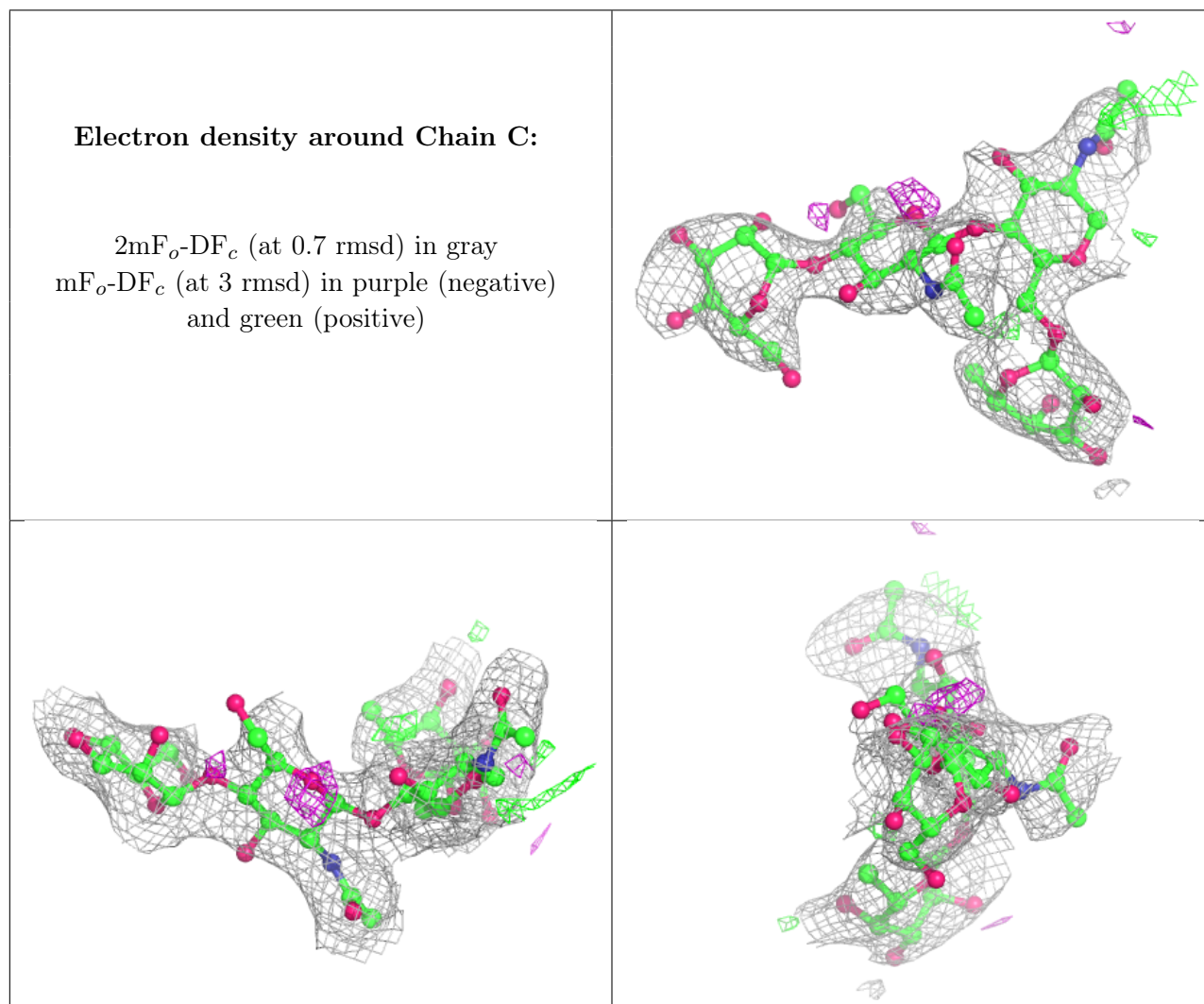
There are no non-standard protein/DNA/RNA residues in this entry.

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	C	2	14/15	0.77	0.32	89,92,94,95	0
4	BMA	C	3	11/12	0.85	0.31	97,99,100,102	0
4	FUC	C	4	10/11	0.86	0.23	79,80,82,82	0
4	NAG	C	1	14/15	0.90	0.19	71,77,81,85	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
5	NAG	A	501	14/15	0.74	0.22	66,70,71,72	0
6	GOL	B	505	6/6	0.76	0.25	76,76,77,77	0
6	GOL	A	502	6/6	0.90	0.22	43,44,44,45	0
6	GOL	A	503	6/6	0.91	0.22	44,45,45,46	0
7	FMT	A	504	3/3	0.97	0.28	45,45,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.