



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:06 AM UTC

PDB ID : 4NE9 / pdb_00004ne9
Title : PCSK9 in complex with LDLR peptide
Authors : Liu, S.
Deposited on : 2013-10-28
Resolution : 2.60 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

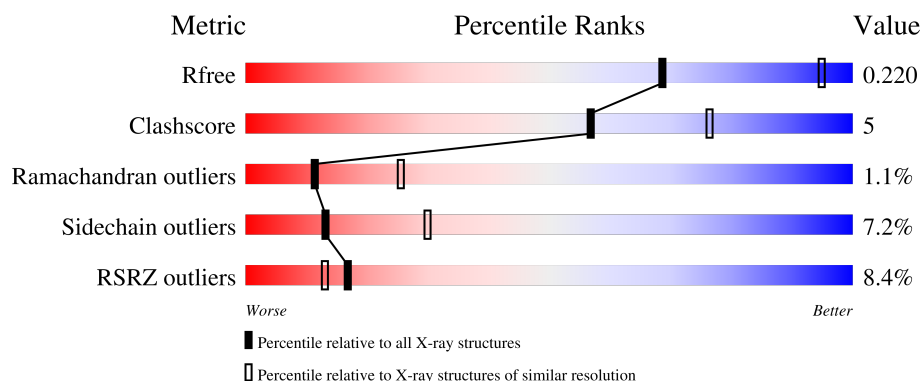
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	540	8% 76% 13% 9%
1	B	540	10% 75% 13% 9%
2	C	152	52% 7% 39%
2	P	152	% 53% 8% 39%
3	D	26	88% 12%

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Mol	Chain	Length	Quality of chain
4	E	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8999 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			3646	2246	676	692	32			
1	B	490	Total	C	N	O	S	0	1	0
			3623	2230	669	692	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ILE	VAL	engineered mutation	UNP Q8NBP7
A	670	GLU	GLY	engineered mutation	UNP Q8NBP7
B	474	ILE	VAL	engineered mutation	UNP Q8NBP7
B	670	GLU	GLY	engineered mutation	UNP Q8NBP7

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			
2	P	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

- Molecule 3 is a protein called Low-density lipoprotein receptor.

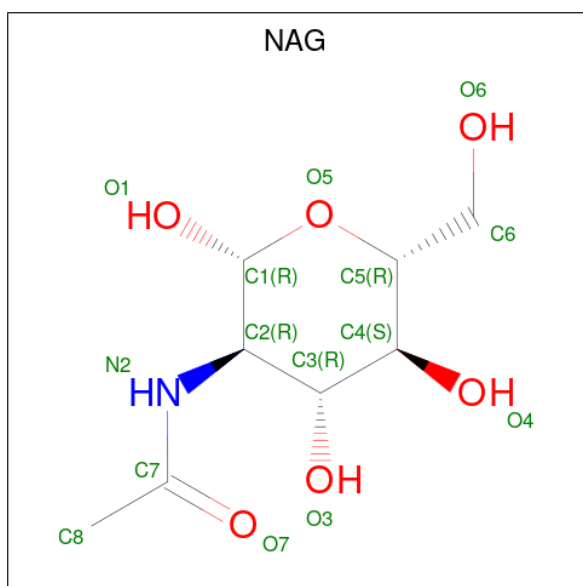
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	26	Total	C	N	O	S	0	0	0
			189	111	33	41	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	5	Total	O	0	0
			5	5		

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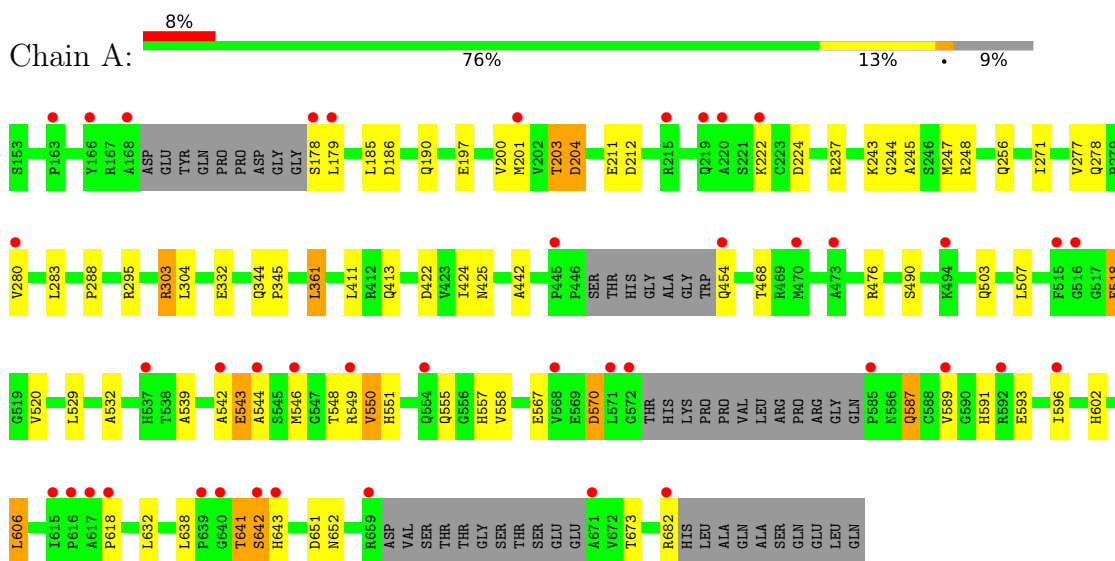
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	4	Total	O	0	0
			4	4		
7	P	4	Total	O	0	0
			4	4		

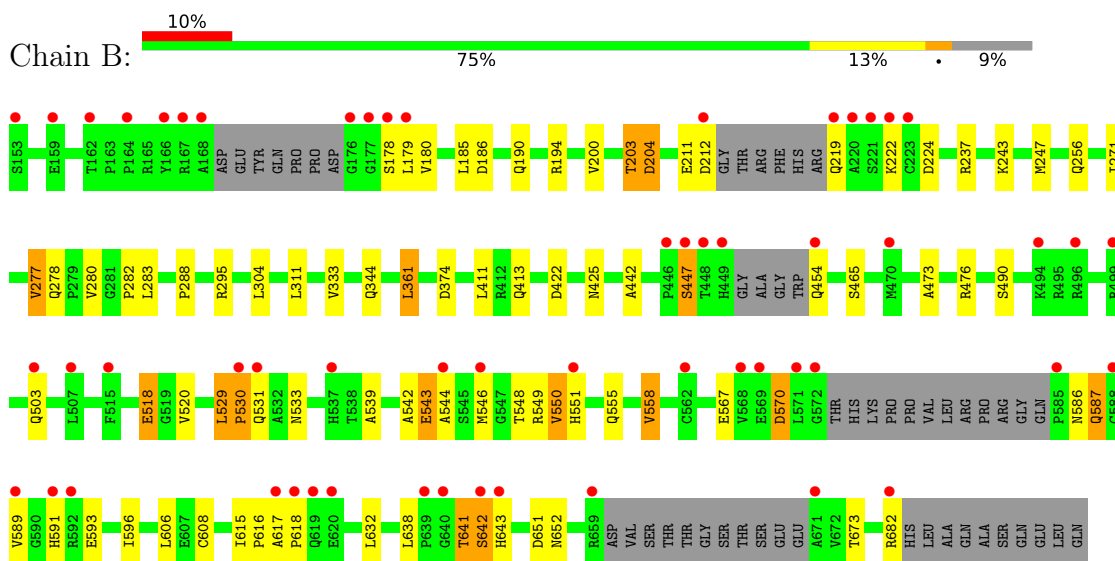
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proprotein convertase subtilisin/kexin type 9

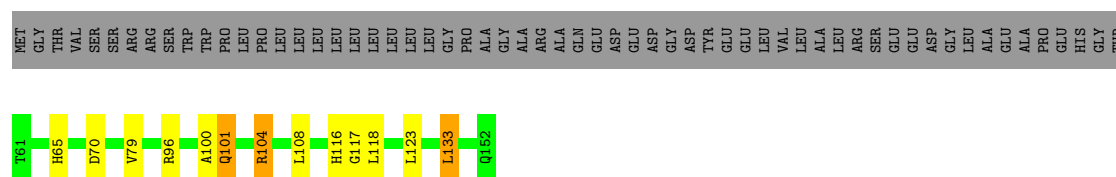


- Molecule 1: Proprotein convertase subtilisin/kexin type 9

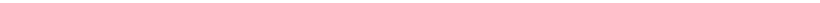


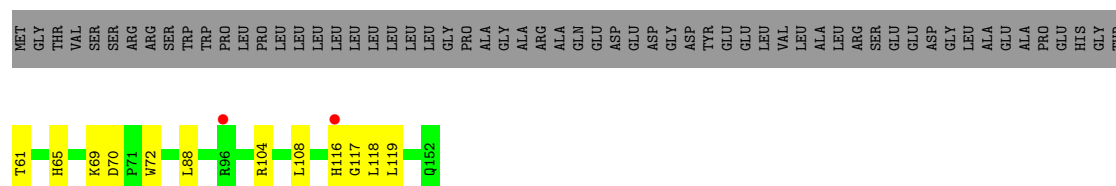
- Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain C:  52% 7% 39%

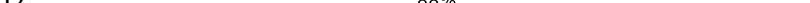


- Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain P:  %

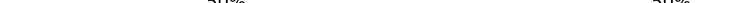


- Molecule 3: Low-density lipoprotein receptor

Chain D:  88% 12%



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

Chain E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.40Å 131.39Å 134.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 2.60 30.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.02-2.60) 95.1 (30.02-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.190 , 0.211 0.198 , 0.220	Depositor DCC
R_{free} test set	3329 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8999	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, CA, 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	0.81	0/3718	1.15	7/5048 (0.1%)
1	B	0.85	1/3693 (0.0%)	1.20	8/5014 (0.2%)
2	C	0.78	0/757	1.25	2/1023 (0.2%)
2	P	0.80	0/757	1.17	1/1023 (0.1%)
3	D	1.21	1/190 (0.5%)	1.30	0/255
All	All	0.83	2/9115 (0.0%)	1.18	18/12363 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	14	HIS	CA-C	10.38	1.57	1.52
1	B	447	SER	CA-C	5.13	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	THR	N-CA-C	7.96	121.05	111.82
1	B	203	THR	N-CA-C	6.50	120.41	112.23
1	A	244	GLY	CA-C-N	6.44	133.84	121.54
1	A	244	GLY	C-N-CA	6.44	133.84	121.54
1	B	224	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	570	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	224	ASP	CA-CB-CG	5.39	117.99	112.60
2	P	116	HIS	CA-CB-CG	5.32	119.12	113.80
1	B	544	ALA	CA-C-N	5.27	129.57	121.19
1	B	544	ALA	C-N-CA	5.27	129.57	121.19
2	C	116	HIS	CA-CB-CG	5.18	118.98	113.80
1	B	570	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	529	LEU	O-C-N	5.10	127.39	121.47
1	A	544	ALA	CA-C-N	5.09	129.28	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ALA	C-N-CA	5.09	129.28	121.19
1	B	533	ASN	CA-CB-CG	5.06	117.66	112.60
2	C	117	GLY	N-CA-C	5.04	125.13	113.18
1	B	586	ASN	CA-CB-CG	5.02	117.62	112.60

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	3646	0	3559	39	0
1	B	3623	0	3531	38	0
2	C	740	0	750	4	0
2	P	740	0	750	6	0
3	D	189	0	168	1	0
4	E	24	0	22	0	0
5	B	14	0	13	0	0
6	D	1	0	0	0	0
7	A	9	0	0	0	0
7	B	5	0	0	0	0
7	C	4	0	0	0	0
7	P	4	0	0	0	0
All	All	8999	0	8793	81	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 5.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:VAL:HG21	1:A:606:LEU:HD13	1.38	1.04
1:A:203:THR:O	1:A:204:ASP:HB2	1.57	1.02
1:B:203:THR:O	1:B:204:ASP:HB2	1.57	1.02
1:A:558:VAL:CG2	1:A:606:LEU:HD13	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:HE22	1:B:425:ASN:H	1.12	0.88
1:A:344:GLN:HE22	1:A:425:ASN:H	1.16	0.87
1:A:201:MET:HE3	1:A:248:ARG:NH1	2.07	0.69
1:A:186:ASP:OD1	1:A:288:PRO:HG2	1.93	0.68
1:A:518:GLU:H	1:A:518:GLU:CD	2.02	0.68
1:B:278:GLN:HE22	2:P:88:LEU:H	1.41	0.67
1:B:518:GLU:H	1:B:518:GLU:CD	2.03	0.67
1:A:548:THR:HG22	1:A:596:ILE:HG22	1.77	0.67
1:A:641:THR:HG22	1:A:643:HIS:CE1	2.30	0.67
1:B:186:ASP:OD1	1:B:288:PRO:HG2	1.95	0.66
1:B:548:THR:HG22	1:B:596:ILE:HG22	1.79	0.65
1:B:641:THR:HG22	1:B:643:HIS:CE1	2.31	0.64
1:A:212:ASP:H	1:A:256:GLN:HE22	1.46	0.62
1:B:212:ASP:H	1:B:256:GLN:HE22	1.46	0.62
1:B:539:ALA:HB2	1:B:550:VAL:HG13	1.83	0.60
1:A:203:THR:O	1:A:204:ASP:CB	2.38	0.59
1:A:543:GLU:HG2	1:A:546:MET:HE2	1.83	0.59
1:A:539:ALA:HB2	1:A:550:VAL:HG13	1.85	0.58
1:B:277:VAL:HG13	2:P:117:GLY:HA2	1.85	0.58
1:B:543:GLU:HG2	1:B:546:MET:HE2	1.84	0.57
2:C:101:GLN:HE21	2:C:133:LEU:HD11	1.72	0.55
1:A:632:LEU:H	1:A:652:ASN:ND2	2.03	0.55
1:A:185:LEU:HD11	1:A:271:ILE:HD11	1.88	0.54
1:B:311:LEU:HB2	1:B:333:VAL:HG12	1.89	0.54
1:B:549:ARG:HG2	1:B:589:VAL:HG22	1.89	0.54
1:A:529:LEU:HG	1:A:532:ALA:HB2	1.89	0.54
1:B:185:LEU:HD11	1:B:271:ILE:HD11	1.89	0.54
1:B:632:LEU:H	1:B:652:ASN:ND2	2.06	0.54
1:A:549:ARG:HG2	1:A:589:VAL:HG22	1.90	0.54
1:A:476:ARG:HH21	1:A:503:GLN:NE2	2.07	0.53
1:A:237:ARG:O	1:A:243:LYS:HD2	2.09	0.52
1:A:200:VAL:HG22	1:A:247:MET:HB2	1.92	0.52
1:A:295:ARG:HH11	2:P:65:HIS:CE1	2.28	0.52
1:B:212:ASP:H	1:B:256:GLN:NE2	2.07	0.51
1:B:638:LEU:HB2	1:B:673:THR:HB	1.93	0.51
1:B:476:ARG:HH21	1:B:503:GLN:NE2	2.09	0.51
1:B:542:ALA:HB1	1:B:546:MET:HE3	1.93	0.50
1:A:542:ALA:HB1	1:A:546:MET:HE3	1.93	0.50
1:B:203:THR:O	1:B:204:ASP:CB	2.38	0.50
1:B:550:VAL:HG22	1:B:596:ILE:HG23	1.94	0.49
1:A:201:MET:HE3	1:A:248:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLN:NE2	2:P:88:LEU:H	2.09	0.49
1:A:638:LEU:HB2	1:A:673:THR:HB	1.94	0.49
1:A:212:ASP:H	1:A:256:GLN:NE2	2.09	0.48
1:B:374:ASP:OD2	3:D:15:VAL:HG21	2.12	0.48
1:B:490:SER:HB2	1:B:520:VAL:HG12	1.94	0.48
1:A:557:HIS:CE1	1:A:602:HIS:HB2	2.49	0.48
1:B:615:ILE:HG13	1:B:616:PRO:HD2	1.95	0.48
1:B:361:LEU:HD22	1:B:442:ALA:HB2	1.95	0.47
1:B:200:VAL:HG22	1:B:247:MET:HB2	1.97	0.47
1:A:490:SER:HB2	1:A:520:VAL:HG12	1.94	0.47
1:A:361:LEU:HD22	1:A:442:ALA:HB2	1.96	0.47
1:A:550:VAL:HG22	1:A:596:ILE:HG23	1.96	0.47
2:C:79:VAL:HG22	2:C:123:LEU:HD13	1.97	0.46
1:B:551:HIS:HB3	1:B:587:GLN:HB2	1.97	0.46
1:A:551:HIS:HB3	1:A:587:GLN:HB2	1.97	0.46
1:A:303:ARG:HE	1:A:303:ARG:HB2	1.48	0.44
1:A:539:ALA:CB	1:A:550:VAL:HG13	2.48	0.44
1:A:277:VAL:HG12	1:A:278:GLN:HG2	1.99	0.43
2:C:100:ALA:O	2:C:104:ARG:HG2	2.18	0.43
1:B:558:VAL:HG21	1:B:608:CYS:SG	2.58	0.43
1:B:529:LEU:HA	1:B:530:PRO:HD2	1.66	0.43
1:B:237:ARG:O	1:B:243:LYS:HD2	2.18	0.43
1:A:591:HIS:CD2	1:A:593:GLU:H	2.37	0.42
1:B:591:HIS:CD2	1:B:593:GLU:H	2.38	0.42
1:A:632:LEU:H	1:A:652:ASN:HD22	1.67	0.42
1:B:277:VAL:HG13	2:P:117:GLY:CA	2.49	0.42
1:B:465:SER:HB3	1:B:473:ALA:HB2	2.01	0.41
1:B:539:ALA:CB	1:B:550:VAL:HG13	2.48	0.41
2:P:69:LYS:HD3	2:P:72:TRP:CE2	2.56	0.41
1:A:332:GLU:H	1:A:332:GLU:CD	2.28	0.40
1:B:591:HIS:HD2	1:B:593:GLU:H	1.70	0.40
1:A:345:PRO:HD3	1:A:424:ILE:HG23	2.03	0.40
1:A:591:HIS:HD2	1:A:593:GLU:H	1.69	0.40
1:B:180:VAL:HG22	1:B:282:PRO:HG2	2.02	0.40
1:B:295:ARG:HH11	2:C:65:HIS:CE1	2.38	0.40
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/540 (89%)	458 (95%)	18 (4%)	6 (1%)	10	23
1	B	479/540 (89%)	453 (95%)	19 (4%)	7 (2%)	8	18
2	C	90/152 (59%)	86 (96%)	4 (4%)	0	100	100
2	P	90/152 (59%)	87 (97%)	3 (3%)	0	100	100
3	D	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
All	All	1165/1410 (83%)	1107 (95%)	45 (4%)	13 (1%)	11	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
1	B	530	PRO
1	A	543	GLU
1	A	642	SER
1	B	204	ASP
1	B	447	SER
1	B	543	GLU
1	A	204	ASP
1	B	642	SER
1	A	618	PRO
1	B	618	PRO
1	A	280	VAL
1	B	617	ALA

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	391/431 (91%)	364 (93%)	27 (7%)	14	32
1	B	389/431 (90%)	359 (92%)	30 (8%)	12	27
2	C	79/127 (62%)	72 (91%)	7 (9%)	9	20
2	P	79/127 (62%)	73 (92%)	6 (8%)	12	27
3	D	22/22 (100%)	21 (96%)	1 (4%)	24	50
All	All	960/1138 (84%)	889 (93%)	71 (7%)	13	29

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	A	179	LEU
1	A	190	GLN
1	A	197	GLU
1	A	211	GLU
1	A	222	LYS
1	A	283	LEU
1	A	303	ARG
1	A	361	LEU
1	A	411	LEU
1	A	413	GLN
1	A	422	ASP
1	A	454	GLN
1	A	468	THR
1	A	507	LEU
1	A	518	GLU
1	A	550	VAL
1	A	555	GLN
1	A	567	GLU
1	A	570	ASP
1	A	587	GLN
1	A	606	LEU
1	A	641	THR
1	A	642	SER
1	A	651[A]	ASP
1	A	651[B]	ASP
1	A	682	ARG
1	B	178	SER
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	190	GLN
1	B	194	ARG
1	B	211	GLU
1	B	219	GLN
1	B	222	LYS
1	B	277	VAL
1	B	280	VAL
1	B	283	LEU
1	B	304	LEU
1	B	361	LEU
1	B	411	LEU
1	B	413	GLN
1	B	422	ASP
1	B	454	GLN
1	B	518	GLU
1	B	531	GLN
1	B	550	VAL
1	B	555	GLN
1	B	558	VAL
1	B	567	GLU
1	B	570	ASP
1	B	587	GLN
1	B	606	LEU
1	B	641	THR
1	B	642	SER
1	B	651[A]	ASP
1	B	651[B]	ASP
1	B	682	ARG
2	C	70	ASP
2	C	96	ARG
2	C	101	GLN
2	C	104	ARG
2	C	108	LEU
2	C	118	LEU
2	C	133	LEU
3	D	2	THR
2	P	61	THR
2	P	70	ASP
2	P	104	ARG
2	P	108	LEU
2	P	118	LEU
2	P	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	298	ASN
1	A	302	GLN
1	A	344	GLN
1	A	413	GLN
1	A	464	HIS
1	A	551	HIS
1	A	553	HIS
1	A	591	HIS
1	A	619	GLN
1	A	643	HIS
1	A	652	ASN
1	B	256	GLN
1	B	278	GLN
1	B	298	ASN
1	B	344	GLN
1	B	413	GLN
1	B	464	HIS
1	B	554	GLN
1	B	557	HIS
1	B	587	GLN
1	B	591	HIS
1	B	619	GLN
1	B	621	GLN
1	B	643	HIS
1	B	652	ASN
2	C	65	HIS
2	C	101	GLN
3	D	9	ASN
2	P	65	HIS
2	P	139	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

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	$\# Z > 2$
4	NAG	E	1	1,4	14,14,15	0.34	0	17,19,21	0.55	0
4	FUC	E	2	4	10,10,11	0.46	0	14,14,16	0.80	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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	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($^{\circ}$)	Ideal($^{\circ}$)
4	E	2	FUC	C1-O5-C5	2.47	118.80	112.97

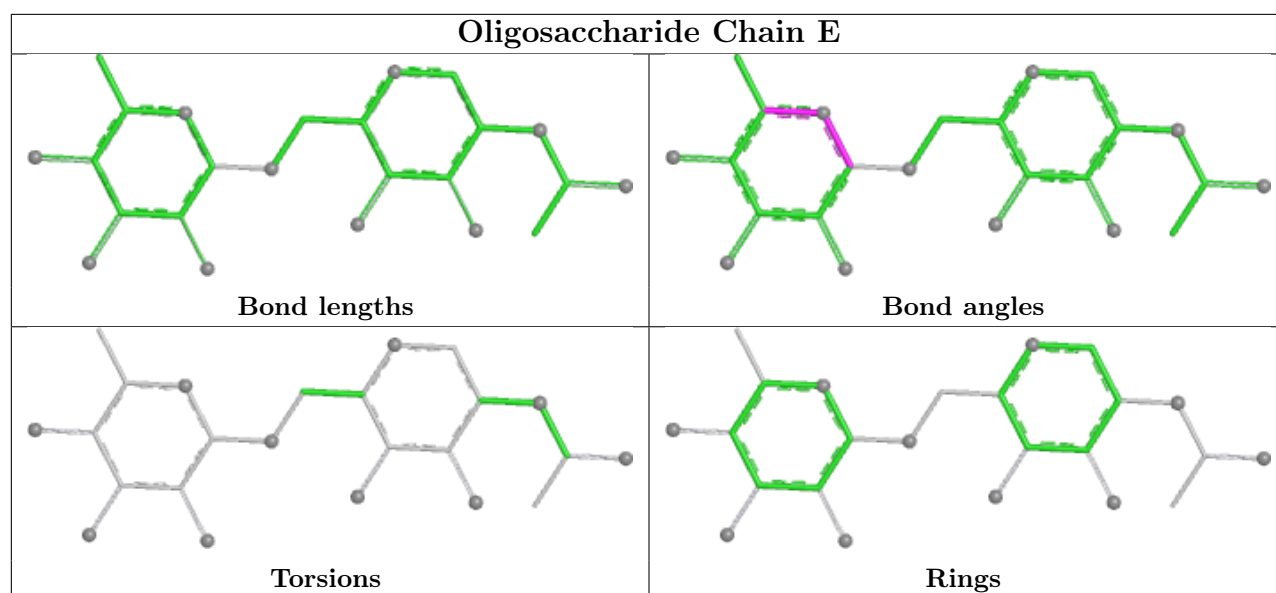
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	901	1	14,14,15	0.34	0	17,19,21	0.75	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
5	NAG	B	901	1	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
5	B	901	NAG	C1-O5-C5	2.72	115.83	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	491/540 (90%)	0.28	42 (8%) 16 12	34, 61, 127, 158	1 (0%)
1	B	490/540 (90%)	0.40	56 (11%) 10 7	36, 65, 139, 189	1 (0%)
2	C	92/152 (60%)	-0.18	0 100 100	41, 60, 87, 105	0
2	P	92/152 (60%)	-0.41	2 (2%) 62 57	35, 47, 70, 87	0
3	D	26/26 (100%)	0.03	0 100 100	50, 61, 79, 92	0
All	All	1191/1410 (84%)	0.24	100 (8%) 17 13	34, 61, 127, 189	2 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	SER	8.3
1	A	178	SER	7.8
1	B	585	PRO	7.4
1	B	168	ALA	7.1
1	A	168	ALA	6.9
1	B	176	GLY	6.8
1	B	177	GLY	6.2
1	B	220	ALA	6.0
1	A	585	PRO	5.9
1	B	572	GLY	5.7
1	B	682	ARG	5.4
1	A	572	GLY	5.2
1	A	682	ARG	5.2
1	B	618	PRO	5.1
1	B	449	HIS	5.0
1	A	179	LEU	4.8
1	B	617	ALA	4.7
1	B	448	THR	4.6
1	A	515	PHE	4.5
1	B	221	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	219	GLN	4.2
1	B	659	ARG	4.1
1	A	544	ALA	4.1
1	B	544	ALA	4.1
1	B	212	ASP	4.1
1	B	537	HIS	4.0
1	B	515	PHE	4.0
1	A	568	VAL	3.9
1	B	640	GLY	3.9
1	B	166	TYR	3.7
1	B	153	SER	3.5
1	A	615	ILE	3.4
1	A	617	ALA	3.4
1	B	671	ALA	3.4
1	B	219	GLN	3.4
1	A	616	PRO	3.3
1	B	588	CYS	3.3
1	B	179	LEU	3.3
1	B	546	MET	3.3
1	B	167	ARG	3.2
1	B	164	PRO	3.2
1	A	537	HIS	3.2
1	B	447	SER	3.2
1	A	516	GLY	3.1
1	A	280	VAL	3.1
1	B	643	HIS	3.0
1	A	659	ARG	3.0
1	B	222	LYS	3.0
1	B	592	ARG	3.0
1	A	201	MET	2.9
1	B	496	ARG	2.8
1	A	640	GLY	2.8
2	P	116	HIS	2.8
1	B	470	MET	2.8
1	A	470	MET	2.7
1	B	551	HIS	2.7
1	A	542	ALA	2.7
1	B	571	LEU	2.7
1	A	546	MET	2.7
1	A	618	PRO	2.7
1	A	554	GLN	2.7
1	A	643	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	223	CYS	2.6
1	A	215	ARG	2.6
1	A	642	SER	2.6
1	B	589	VAL	2.6
1	A	454	GLN	2.5
1	B	454	GLN	2.5
1	B	507	LEU	2.5
1	A	589	VAL	2.5
1	A	445	PRO	2.5
1	A	571	LEU	2.4
1	B	620	GLU	2.4
1	B	531	GLN	2.4
1	B	499	ARG	2.4
1	B	446	PRO	2.4
1	B	639	PRO	2.3
1	A	592	ARG	2.3
2	P	96	ARG	2.3
1	B	591	HIS	2.3
1	A	163	PRO	2.2
1	A	222	LYS	2.2
1	B	568	VAL	2.2
1	B	159	GLU	2.2
1	A	166	TYR	2.2
1	B	619	GLN	2.1
1	A	473	ALA	2.1
1	A	671	ALA	2.1
1	A	639	PRO	2.1
1	B	642	SER	2.1
1	A	494	LYS	2.1
1	B	530	PRO	2.1
1	B	562	CYS	2.1
1	A	549	ARG	2.1
1	B	503	GLN	2.1
1	A	596	ILE	2.1
1	A	220	ALA	2.0
1	B	569	GLU	2.0
1	B	494	LYS	2.0
1	B	162	THR	2.0

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

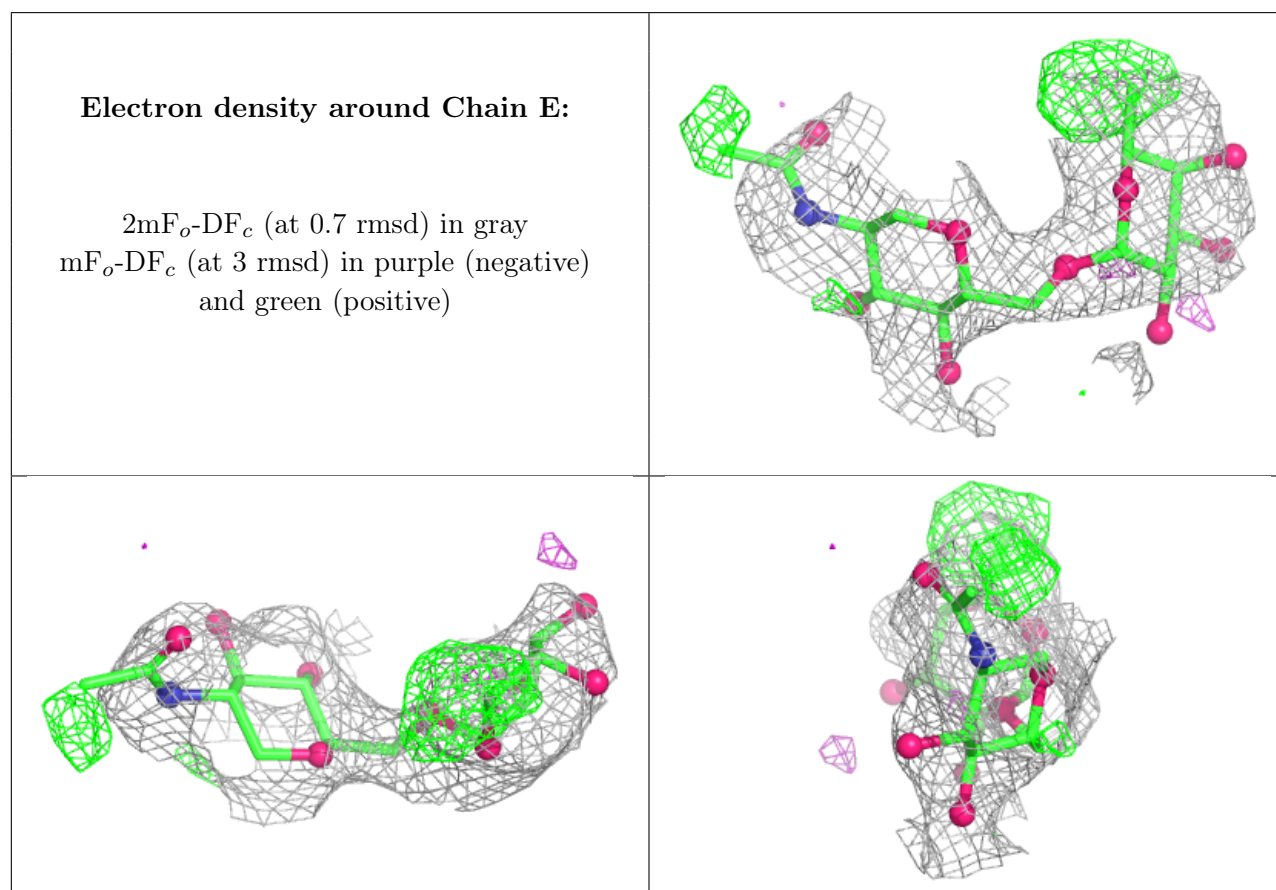
There are no non-standard protein/DNA/RNA residues in this entry.

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	E	1	14/15	-	-	116,133,142,144	0
4	FUC	E	2	10/11	-	-	139,146,149,151	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($\text{\AA}^2$)	Q<0.9
5	NAG	B	901	14/15	0.59	0.19	123,134,138,141	0
6	CA	D	101	1/1	0.99	0.03	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.