



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 6GFE / pdb_00006gfe
Title : High-resolution Structure of a therapeutic full-length anti-NPRA Antibody with exceptional Conformational Diversity
Authors : Hoerer, S.
Deposited on : 2018-04-30
Resolution : 1.80 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

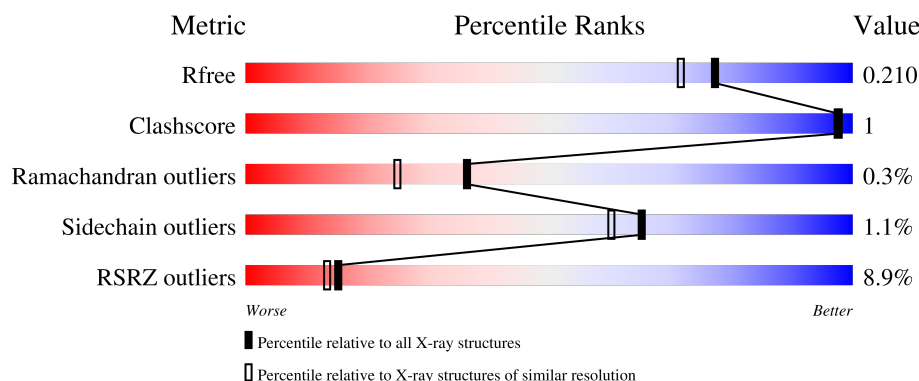
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



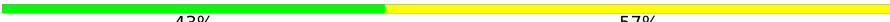
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	H	450	16% 90% 6% 5%
1	K	450	4% 91% • 5%
2	L	215	2% 97% •
2	M	215	9% 96% •
3	A	7	71% 29%

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Mol	Chain	Length	Quality of chain
3	B	7	 A horizontal bar chart showing the quality of chain B. The bar is divided into two segments: a green segment on the left representing 43% and a yellow segment on the right representing 57%. The percentages are written below their respective segments.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11641 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.

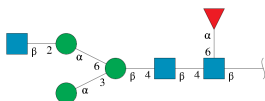
- Molecule 1 is a protein called Immunoglobulin gamma-4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	429	Total	C	N	O	S	6	7	0
			3405	2148	574	666	17			
1	K	426	Total	C	N	O	S	6	10	0
			3400	2143	573	665	19			

- Molecule 2 is a protein called Immunoglobulin gamma-4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	9	0
			1703	1056	293	347	7			
2	M	215	Total	C	N	O	S	6	3	0
			1662	1035	285	335	7			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
3	A	7	Total	C	N	O	0	0	0
			85	48	3	34			
3	B	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

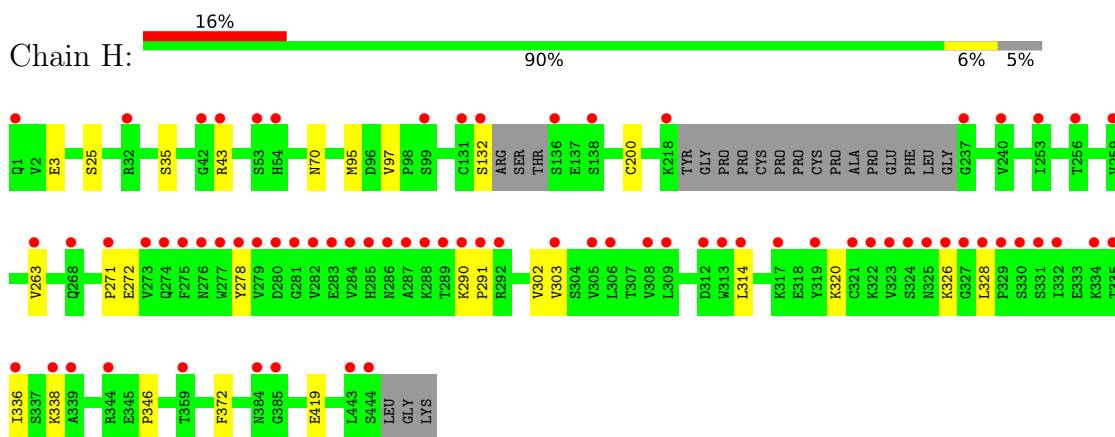
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	372	Total O 372 372	0	1
6	K	493	Total O 494 494	0	2
6	L	249	Total O 249 249	0	0
6	M	172	Total O 172 172	0	0

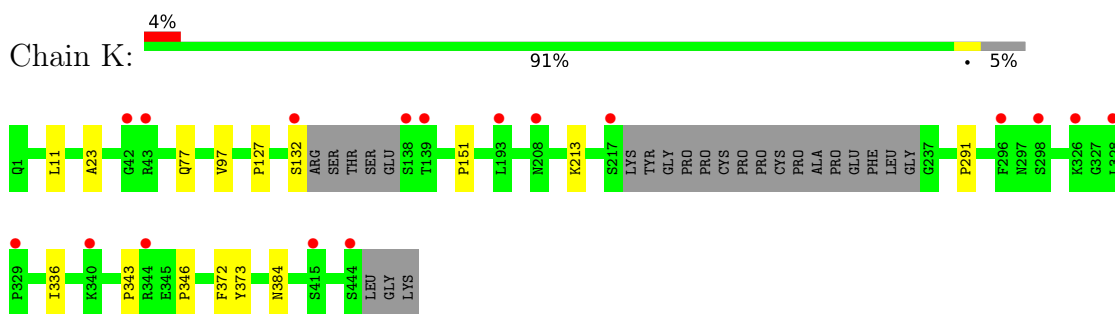
3 Residue-property plots [i](#)

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.

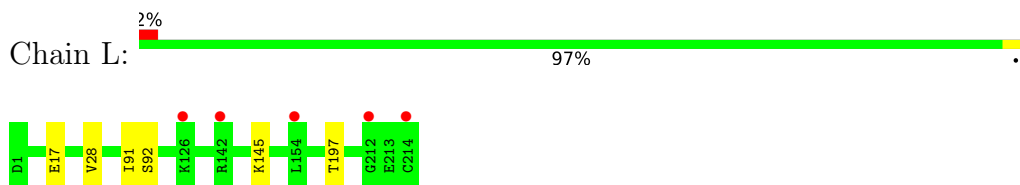
- Molecule 1: Immunoglobulin gamma-4 heavy chain



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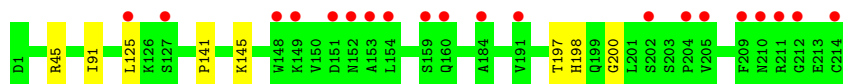


- Molecule 2: Immunoglobulin gamma-4 light chain



- Molecule 2: Immunoglobulin gamma-4 light chain





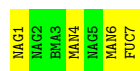
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 71% 29%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 B: 43% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.78Å 160.51Å 87.30Å 90.00° 110.72° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.80) 99.5 (40.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.200 0.189 , 0.210	Depositor DCC
R_{free} test set	7796 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, MAN, BMA, ACT

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	H	0.68	0/3496	0.98	3/4762 (0.1%)
1	K	0.68	0/3488	0.95	2/4754 (0.0%)
2	L	0.68	0/1738	0.96	0/2362
2	M	0.66	0/1701	1.03	3/2311 (0.1%)
All	All	0.68	0/10423	0.97	8/14189 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	45	ARG	CB-CG-CD	5.57	124.11	111.30
2	M	125	LEU	CA-C-N	5.34	127.43	120.28
2	M	125	LEU	C-N-CA	5.34	127.43	120.28
1	H	291	PRO	CA-C-N	5.21	128.50	121.05
1	H	291	PRO	C-N-CA	5.21	128.50	121.05
1	K	291	PRO	CA-C-N	5.19	129.04	121.31
1	K	291	PRO	C-N-CA	5.19	129.04	121.31
1	H	70	ASN	CA-CB-CG	5.03	117.63	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	H	3405	0	3303	7	0
1	K	3400	0	3285	5	0
2	L	1703	0	1648	2	0
2	M	1662	0	1612	3	0
3	A	85	0	73	0	0
3	B	85	0	73	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	K	4	0	3	0	0
5	L	8	0	6	0	0
6	H	372	0	0	0	0
6	K	494	0	0	0	0
6	L	249	0	0	0	0
6	M	172	0	0	0	0
All	All	11641	0	10003	17	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 1.

All (17) 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:H:346:PRO:HB3	1:H:372:PHE:HB3	1.78	0.66
1:H:278:TYR:HB2	1:H:320:LYS:HB3	1.85	0.59
1:K:127:PRO:HD3	1:K:213:LYS:HE2	1.85	0.58
1:H:3:GLU:HG3	1:H:25:SER:HB2	1.87	0.56
1:H:314:LEU:HD23	1:H:338:LYS:HE3	1.89	0.54
2:M:145:LYS:HB3	2:M:197:THR:HB	1.89	0.53
2:M:198[A]:HIS:CD2	2:M:200:GLY:H	2.26	0.53
2:L:145:LYS:HB3	2:L:197:THR:HB	1.90	0.53
1:K:346:PRO:HB3	1:K:372:PHE:HB3	1.94	0.48
1:H:35:SER:HB2	1:H:95:MET:HB3	1.97	0.47
1:K:23:ALA:HA	1:K:77:GLN:HG2	1.97	0.47
1:H:290:LYS:HB2	1:H:303:VAL:HG13	2.00	0.44
2:M:141:PRO:O	2:M:198[A]:HIS:HE1	2.00	0.44
2:L:28:VAL:HG13	2:L:92:SER:HB2	1.99	0.44
1:K:11:LEU:HB2	1:K:151:PRO:HG3	2.01	0.43
1:H:263:VAL:HG12	1:H:302:VAL:HB	2.02	0.41
1:K:343:PRO:HA	1:K:373:TYR:O	2.22	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	H	430/450 (96%)	423 (98%)	4 (1%)	3 (1%)	18	8
1	K	430/450 (96%)	425 (99%)	4 (1%)	1 (0%)	43	31
2	L	222/215 (103%)	217 (98%)	5 (2%)	0	100	100
2	M	216/215 (100%)	211 (98%)	5 (2%)	0	100	100
All	All	1298/1330 (98%)	1276 (98%)	18 (1%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	VAL
1	H	272	GLU
1	K	97	VAL
1	H	271	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	398/408 (98%)	390 (98%)	8 (2%)	48	38
1	K	398/408 (98%)	395 (99%)	3 (1%)	73	70
2	L	195/186 (105%)	193 (99%)	2 (1%)	68	64
2	M	189/186 (102%)	188 (100%)	1 (0%)	81	80
All	All	1180/1188 (99%)	1166 (99%)	14 (1%)	65	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	43	ARG
1	H	132	SER
1	H	200[A]	CYS
1	H	200[B]	CYS
1	H	326	LYS
1	H	328	LEU
1	H	336	ILE
1	H	419	GLU
1	K	132	SER
1	K	336	ILE
1	K	384	ASN
2	L	17	GLU
2	L	91	ILE
2	M	91	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	16	GLN
1	H	82(A)	ASN
1	H	325	ASN
1	H	362	GLN
1	H	433	HIS
1	H	438	GLN
1	K	70	ASN
1	K	82(A)	ASN
1	K	418	GLN
1	K	433	HIS
1	K	438	GLN
2	L	93	ASN
2	M	42	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 ⓘ

14 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
3	NAG	A	1	3,1	14,14,15	0.32	0	17,19,21	0.62	0
3	NAG	A	2	3	14,14,15	0.32	0	17,19,21	0.76	1 (5%)
3	BMA	A	3	3	11,11,12	0.30	0	15,15,17	0.60	0
3	MAN	A	4	3	11,11,12	0.31	0	15,15,17	0.84	1 (6%)
3	NAG	A	5	3	14,14,15	0.31	0	17,19,21	0.46	0
3	MAN	A	6	3	11,11,12	0.24	0	15,15,17	0.66	0
3	FUC	A	7	3	10,10,11	0.53	0	14,14,16	0.62	0
3	NAG	B	1	3,1	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
3	NAG	B	2	3	14,14,15	0.29	0	17,19,21	0.60	0
3	BMA	B	3	3	11,11,12	0.28	0	15,15,17	0.60	0
3	MAN	B	4	3	11,11,12	0.31	0	15,15,17	0.92	1 (6%)
3	NAG	B	5	3	14,14,15	0.29	0	17,19,21	0.43	0
3	MAN	B	6	3	11,11,12	0.39	0	15,15,17	0.77	1 (6%)
3	FUC	B	7	3	10,10,11	0.40	0	14,14,16	0.70	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
3	NAG	A	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	MAN	A	6	3	-	0/2/19/22	0/1/1/1
3	FUC	A	7	3	-	-	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	NAG	B	5	3	-	0/6/23/26	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	FUC	B	7	3	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4	MAN	C1-O5-C5	3.13	116.38	112.19
3	A	4	MAN	C1-O5-C5	3.03	116.24	112.19
3	B	6	MAN	C1-O5-C5	2.23	115.17	112.19
3	B	1	NAG	C1-O5-C5	2.14	115.06	112.19
3	A	2	NAG	O5-C1-C2	-2.14	107.99	111.29
3	B	7	FUC	C1-O5-C5	2.13	118.00	112.97

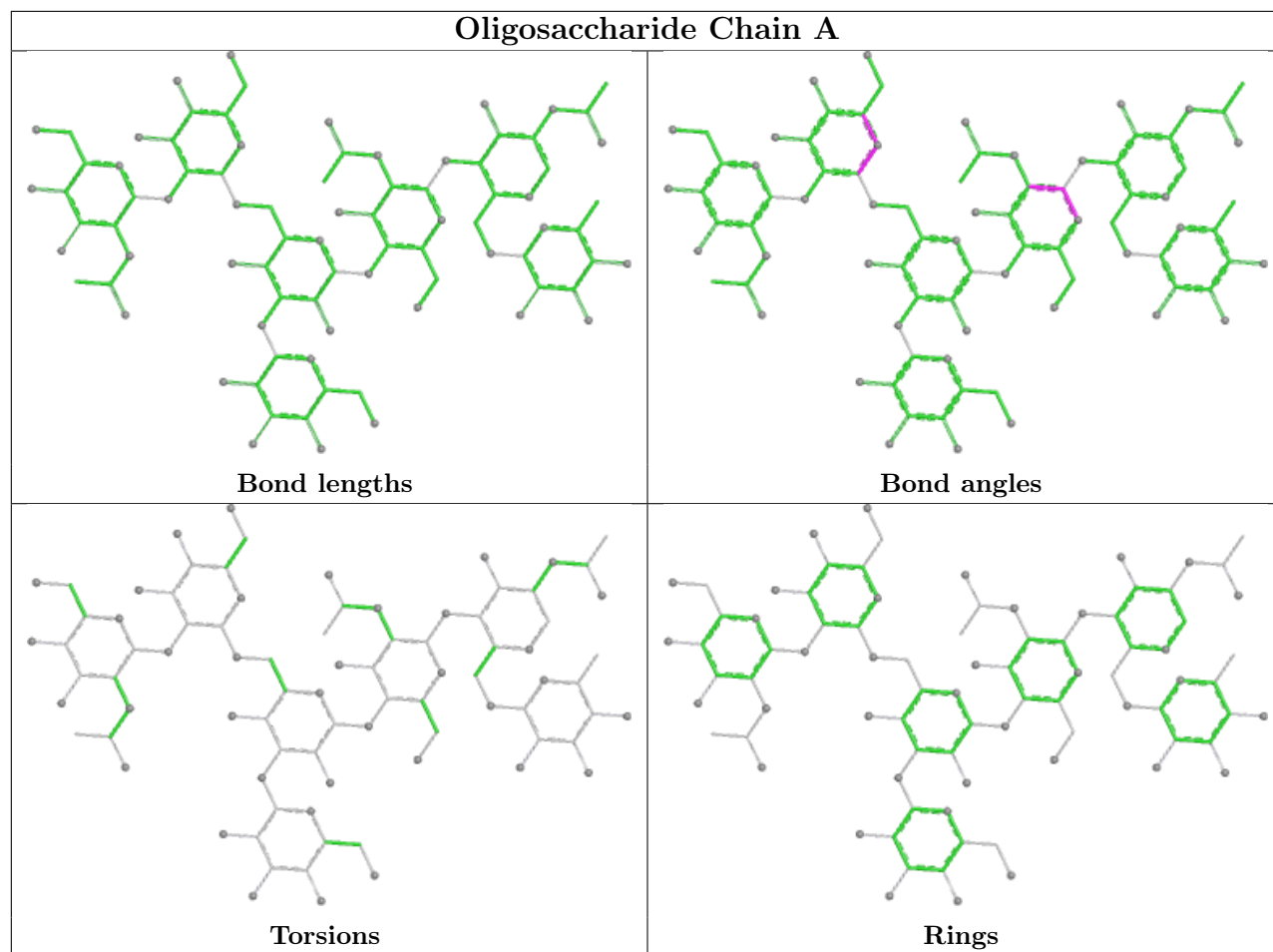
There are no chirality outliers.

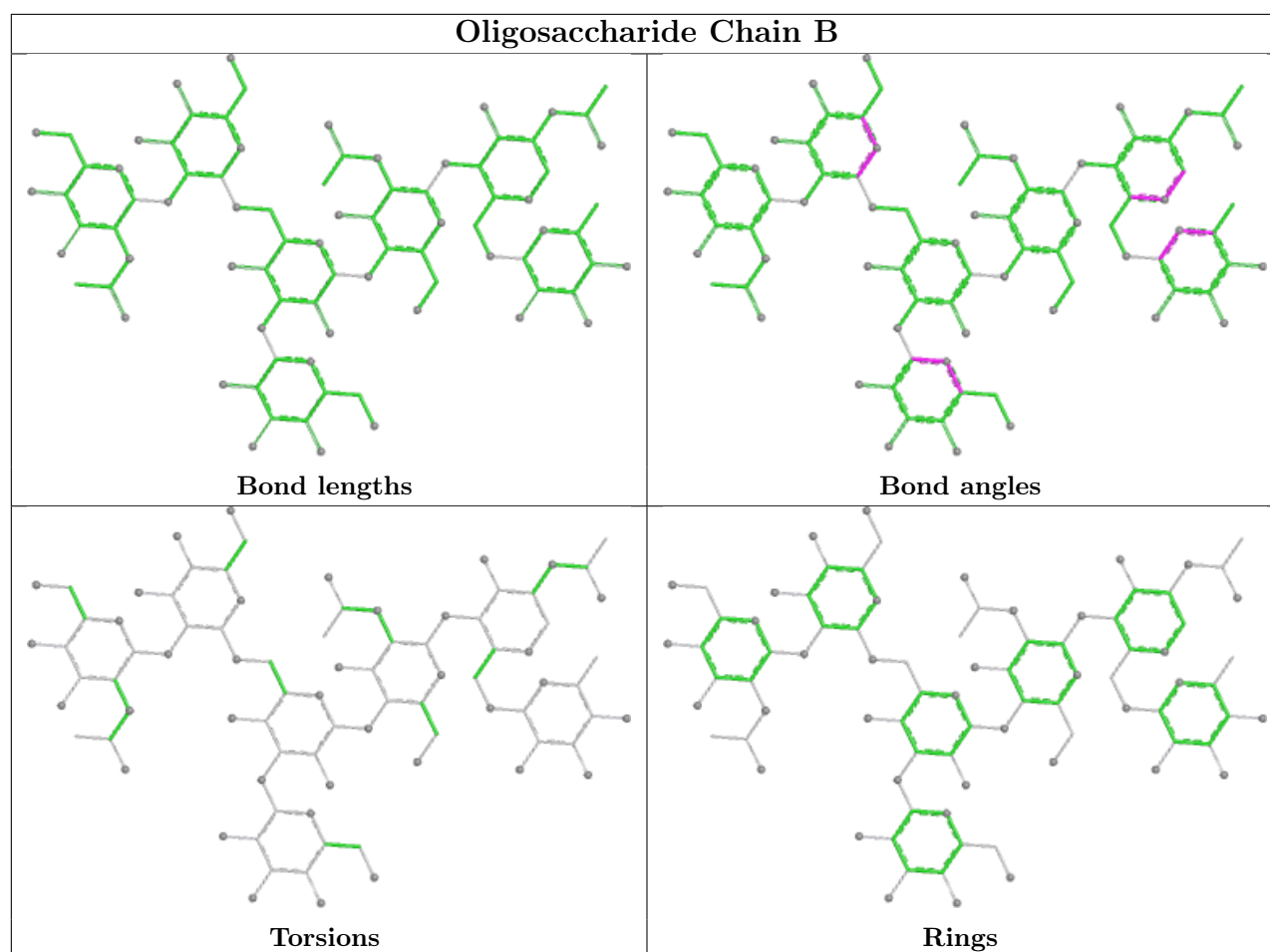
There are no torsion outliers.

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ACT	K	509	-	3,3,3	1.16	0	3,3,3	0.63	0
5	ACT	L	302	-	3,3,3	1.10	0	3,3,3	0.81	0
5	ACT	L	301	-	3,3,3	0.87	0	3,3,3	1.31	0

There are no bond length outliers.

There are no bond angle outliers.

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	H	429/450 (95%)	0.68	73 (17%) 4 3	9, 34, 87, 103	7 (1%)
1	K	426/450 (94%)	0.01	17 (3%) 42 41	10, 26, 54, 102	12 (2%)
2	L	215/215 (100%)	-0.04	5 (2%) 61 61	10, 27, 51, 71	9 (4%)
2	M	215/215 (100%)	0.43	20 (9%) 14 12	18, 31, 70, 79	3 (1%)
All	All	1285/1330 (96%)	0.29	115 (8%) 15 13	9, 29, 68, 103	31 (2%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	282	VAL	6.4
1	H	277	TRP	6.1
1	K	217	SER	6.0
1	H	279	VAL	5.6
1	H	284	VAL	5.4
1	H	328	LEU	5.3
1	H	332	ILE	5.2
1	H	273	VAL	5.2
1	H	281	GLY	5.0
1	H	323	VAL	5.0
1	H	132	SER	4.9
1	K	444	SER	4.9
1	H	275	PHE	4.7
1	H	278	TYR	4.3
1	H	329	PRO	4.3
1	H	289	THR	4.0
1	K	132	SER	4.0
1	H	287	ALA	3.9
1	H	444	SER	3.9
2	M	154	LEU	3.9
1	H	319	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	218	LYS	3.8
1	H	321	CYS	3.6
1	H	324	SER	3.6
1	H	330	SER	3.6
1	H	336	ILE	3.5
2	L	214	CYS	3.5
1	H	331	SER	3.4
1	H	285	HIS	3.3
1	K	296	PHE	3.3
1	H	53	SER	3.3
1	K	326	LYS	3.2
1	K	329	PRO	3.2
2	M	153	ALA	3.2
1	H	283	GLU	3.2
1	H	253	ILE	3.1
1	H	308	VAL	3.1
1	H	385	GLY	3.1
1	H	276	ASN	3.1
1	K	42	GLY	3.1
2	M	212	GLY	3.1
1	H	309	LEU	3.0
1	H	303	VAL	3.0
1	H	327	GLY	3.0
2	M	160	GLN	3.0
1	K	328	LEU	3.0
1	H	259	VAL	3.0
1	K	138	SER	2.9
1	H	138	SER	2.9
2	M	202	SER	2.9
1	H	291	PRO	2.9
2	L	126	LYS	2.9
1	H	314	LEU	2.8
2	L	142[A]	ARG	2.8
1	H	322	LYS	2.8
2	M	214	CYS	2.8
1	H	286	ASN	2.8
2	M	152	ASN	2.8
1	H	317	LYS	2.8
1	H	271	PRO	2.8
2	M	184	ALA	2.7
1	H	54	HIS	2.7
1	H	280	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	325	ASN	2.7
1	H	240	VAL	2.7
1	H	263	VAL	2.6
2	L	212	GLY	2.6
2	M	210	ASN	2.6
1	H	42	GLY	2.6
1	K	340	LYS	2.6
1	H	326	LYS	2.5
2	M	149	LYS	2.5
1	H	131	CYS	2.5
1	K	43	ARG	2.5
2	M	211	ARG	2.5
1	H	1	GLN	2.5
1	H	334	LYS	2.5
1	H	288	LYS	2.4
2	M	205	VAL	2.4
1	H	99	SER	2.4
1	K	415[A]	SER	2.4
2	M	159	SER	2.4
2	M	151	ASP	2.4
1	K	139	THR	2.4
1	H	274	GLN	2.4
2	M	204	PRO	2.4
1	H	306	LEU	2.3
1	H	43	ARG	2.3
2	M	125	LEU	2.3
1	K	193	LEU	2.3
2	M	148	TRP	2.3
1	H	290	LYS	2.3
1	H	237	GLY	2.3
1	H	384	ASN	2.2
1	H	256	THR	2.2
1	H	305	VAL	2.2
1	H	338	LYS	2.2
1	H	344	ARG	2.2
2	M	191	VAL	2.2
1	H	292	ARG	2.2
1	K	208	ASN	2.1
2	M	209	PHE	2.1
1	H	268	GLN	2.1
1	H	335	THR	2.1
1	H	359	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	313	TRP	2.1
1	H	32	ARG	2.1
2	L	154	LEU	2.1
1	H	312	ASP	2.1
1	H	136	SER	2.1
1	K	298	SER	2.0
2	M	127	SER	2.0
1	H	443	LEU	2.0
1	H	339	ALA	2.0
1	K	344	ARG	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](#)

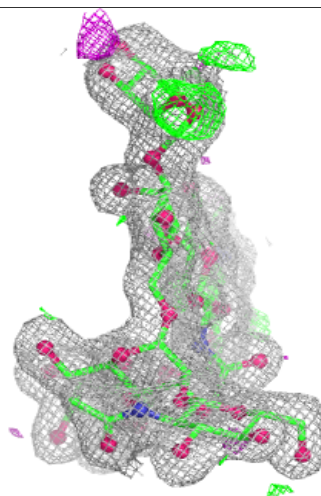
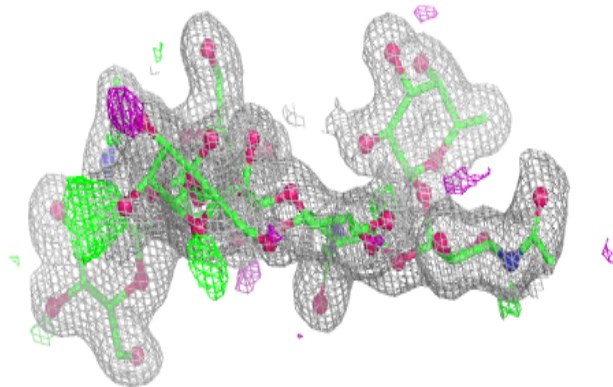
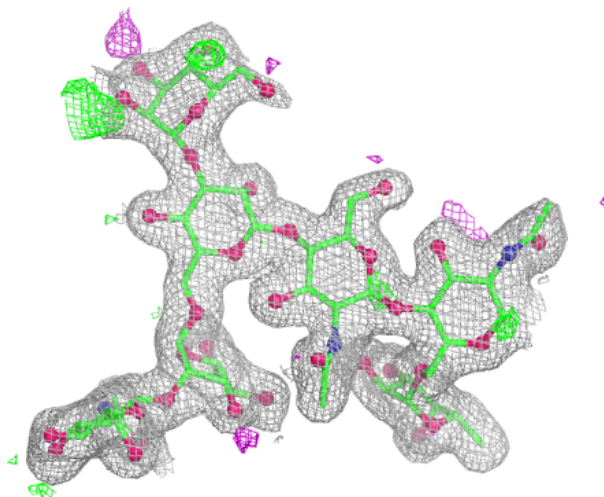
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

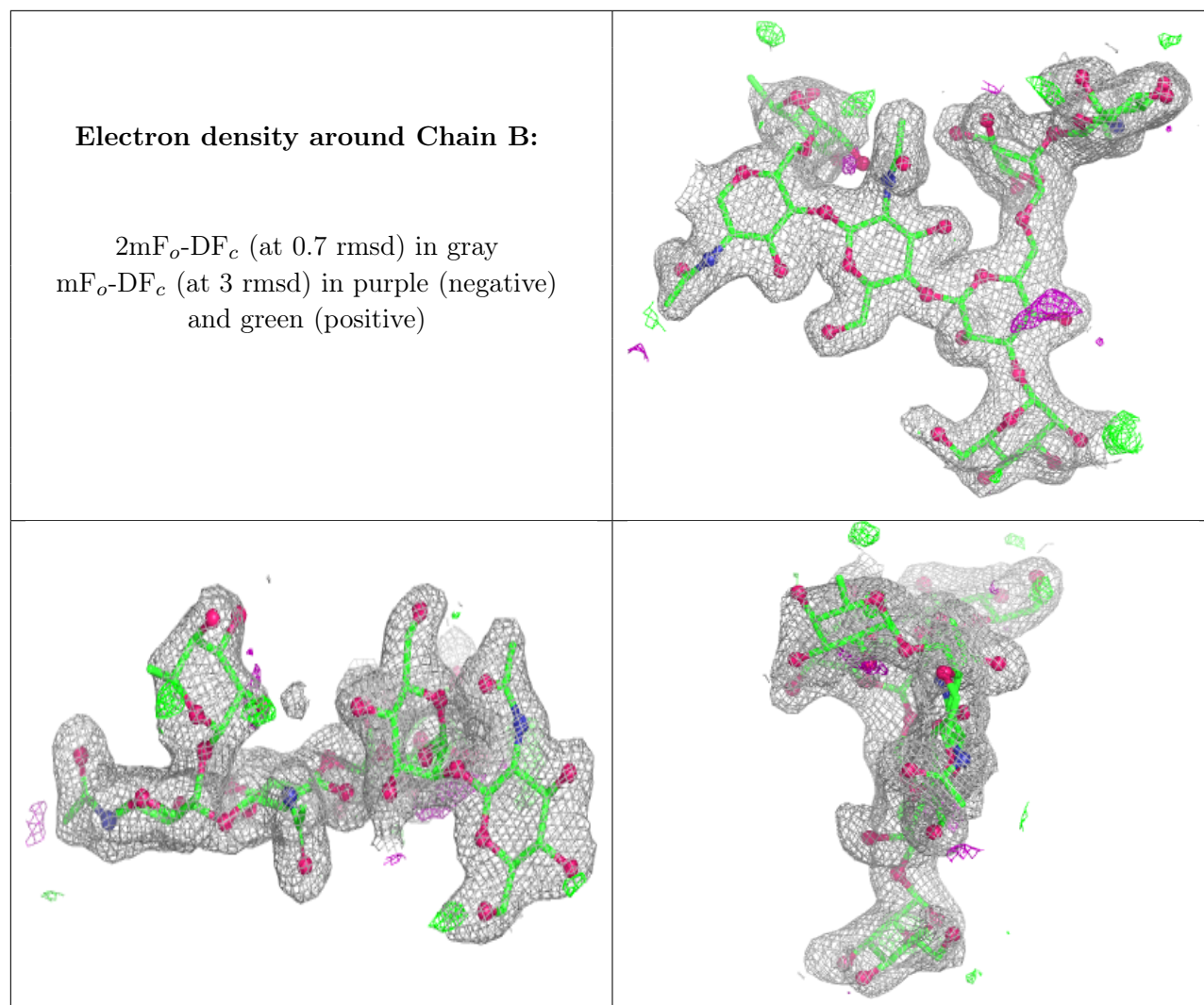
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1	14/15	-	-	26,32,40,40	0
3	NAG	A	2	14/15	-	-	25,31,38,42	0
3	BMA	A	3	11/12	-	-	25,28,31,34	0
3	MAN	A	4	11/12	-	-	29,30,32,33	0
3	NAG	A	5	14/15	-	-	35,38,40,42	0
3	MAN	A	6	11/12	-	-	40,45,49,51	0
3	FUC	A	7	10/11	-	-	23,24,25,27	0
3	NAG	B	1	14/15	-	-	31,37,46,55	0
3	NAG	B	2	14/15	-	-	27,31,34,36	0
3	BMA	B	3	11/12	-	-	28,33,37,40	0
3	MAN	B	4	11/12	-	-	38,40,45,46	0
3	NAG	B	5	14/15	-	-	39,42,44,44	0
3	MAN	B	6	11/12	-	-	40,43,50,53	0
3	FUC	B	7	10/11	-	-	62,68,69,70	0

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

Electron density around Chain A:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	K	509	4/4	0.74	0.19	39,40,43,48	0
5	ACT	L	301	4/4	0.88	0.15	44,49,50,51	0
5	ACT	L	302	4/4	0.88	0.17	40,46,47,47	0
4	CA	H	508	1/1	0.92	0.09	75,75,75,75	0
4	CA	K	508	1/1	0.99	0.10	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.