



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 09:03 PM EDT

PDB ID : 6N50  
Title : Metabotropic Glutamate Receptor 5 Extracellular Domain in Complex with Nb43 and L-quisqualic acid  
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Chu, M.; Weis, W.I.; Skiniotis, G.; Mathiesen, J.M.; Kobilka, B.K.  
Deposited on : 2018-11-20  
Resolution : 3.75 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

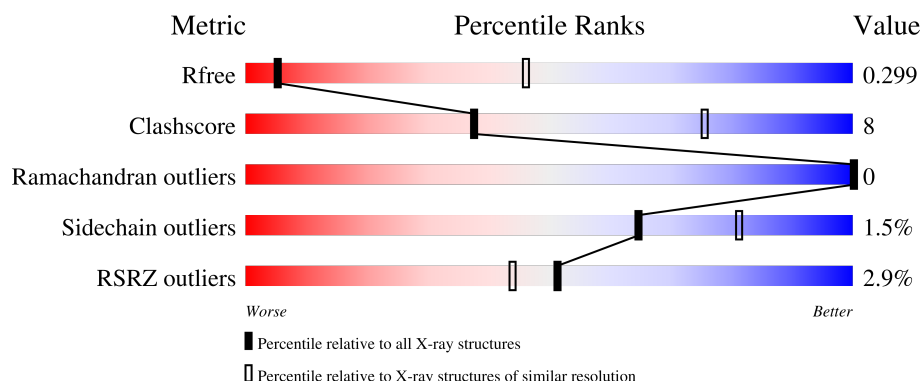
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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  $\geq 3$ , 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	596	<div> <div>0%</div> <div>68%</div> <div>18%</div> <div>13%</div> </div>
1	B	596	<div> <div>2%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	C	596	<div> <div>3%</div> <div>69%</div> <div>16%</div> <div>14%</div> </div>
2	E	123	<div> <div>7%</div> <div>80%</div> <div>20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	QUS	C	603	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12146 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3977	2511	673	755	38			
1	B	444	Total	C	N	O	S	0	0	0
			3262	2063	559	611	29			
1	C	511	Total	C	N	O	S	0	0	0
			3873	2448	652	736	37			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P41594
A	-15	LEU	-	expression tag	UNP P41594
A	-14	LEU	-	expression tag	UNP P41594
A	-13	VAL	-	expression tag	UNP P41594
A	-12	ASN	-	expression tag	UNP P41594
A	-11	GLN	-	expression tag	UNP P41594
A	-10	SER	-	expression tag	UNP P41594
A	-9	HIS	-	expression tag	UNP P41594
A	-8	GLN	-	expression tag	UNP P41594
A	-7	GLY	-	expression tag	UNP P41594
A	-6	PHE	-	expression tag	UNP P41594
A	-5	ASN	-	expression tag	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	GLU	-	expression tag	UNP P41594
A	-2	HIS	-	expression tag	UNP P41594
A	-1	THR	-	expression tag	UNP P41594
A	0	SER	-	expression tag	UNP P41594
A	1	LYS	-	expression tag	UNP P41594
A	2	MET	-	expression tag	UNP P41594
A	3	VAL	-	expression tag	UNP P41594
A	4	SER	-	expression tag	UNP P41594
A	5	ALA	-	expression tag	UNP P41594
A	6	ILE	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	-	expression tag	UNP P41594
A	8	LEU	-	expression tag	UNP P41594
A	9	TYR	-	expression tag	UNP P41594
A	10	VAL	-	expression tag	UNP P41594
A	11	LEU	-	expression tag	UNP P41594
A	12	LEU	-	expression tag	UNP P41594
A	13	ALA	-	expression tag	UNP P41594
A	14	ALA	-	expression tag	UNP P41594
A	15	ALA	-	expression tag	UNP P41594
A	16	ALA	-	expression tag	UNP P41594
A	17	HIS	-	expression tag	UNP P41594
A	18	SER	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594
A	20	PHE	-	expression tag	UNP P41594
A	572	HIS	-	expression tag	UNP P41594
A	573	HIS	-	expression tag	UNP P41594
A	574	HIS	-	expression tag	UNP P41594
A	575	HIS	-	expression tag	UNP P41594
A	576	HIS	-	expression tag	UNP P41594
A	577	HIS	-	expression tag	UNP P41594
A	578	HIS	-	expression tag	UNP P41594
A	579	HIS	-	expression tag	UNP P41594
B	-16	MET	-	initiating methionine	UNP P41594
B	-15	LEU	-	expression tag	UNP P41594
B	-14	LEU	-	expression tag	UNP P41594
B	-13	VAL	-	expression tag	UNP P41594
B	-12	ASN	-	expression tag	UNP P41594
B	-11	GLN	-	expression tag	UNP P41594
B	-10	SER	-	expression tag	UNP P41594
B	-9	HIS	-	expression tag	UNP P41594
B	-8	GLN	-	expression tag	UNP P41594
B	-7	GLY	-	expression tag	UNP P41594
B	-6	PHE	-	expression tag	UNP P41594
B	-5	ASN	-	expression tag	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	GLU	-	expression tag	UNP P41594
B	-2	HIS	-	expression tag	UNP P41594
B	-1	THR	-	expression tag	UNP P41594
B	0	SER	-	expression tag	UNP P41594
B	1	LYS	-	expression tag	UNP P41594
B	2	MET	-	expression tag	UNP P41594
B	3	VAL	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP P41594
B	5	ALA	-	expression tag	UNP P41594
B	6	ILE	-	expression tag	UNP P41594
B	7	VAL	-	expression tag	UNP P41594
B	8	LEU	-	expression tag	UNP P41594
B	9	TYR	-	expression tag	UNP P41594
B	10	VAL	-	expression tag	UNP P41594
B	11	LEU	-	expression tag	UNP P41594
B	12	LEU	-	expression tag	UNP P41594
B	13	ALA	-	expression tag	UNP P41594
B	14	ALA	-	expression tag	UNP P41594
B	15	ALA	-	expression tag	UNP P41594
B	16	ALA	-	expression tag	UNP P41594
B	17	HIS	-	expression tag	UNP P41594
B	18	SER	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	20	PHE	-	expression tag	UNP P41594
B	572	HIS	-	expression tag	UNP P41594
B	573	HIS	-	expression tag	UNP P41594
B	574	HIS	-	expression tag	UNP P41594
B	575	HIS	-	expression tag	UNP P41594
B	576	HIS	-	expression tag	UNP P41594
B	577	HIS	-	expression tag	UNP P41594
B	578	HIS	-	expression tag	UNP P41594
B	579	HIS	-	expression tag	UNP P41594
C	-16	MET	-	initiating methionine	UNP P41594
C	-15	LEU	-	expression tag	UNP P41594
C	-14	LEU	-	expression tag	UNP P41594
C	-13	VAL	-	expression tag	UNP P41594
C	-12	ASN	-	expression tag	UNP P41594
C	-11	GLN	-	expression tag	UNP P41594
C	-10	SER	-	expression tag	UNP P41594
C	-9	HIS	-	expression tag	UNP P41594
C	-8	GLN	-	expression tag	UNP P41594
C	-7	GLY	-	expression tag	UNP P41594
C	-6	PHE	-	expression tag	UNP P41594
C	-5	ASN	-	expression tag	UNP P41594
C	-4	LYS	-	expression tag	UNP P41594
C	-3	GLU	-	expression tag	UNP P41594
C	-2	HIS	-	expression tag	UNP P41594
C	-1	THR	-	expression tag	UNP P41594
C	0	SER	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LYS	-	expression tag	UNP P41594
C	2	MET	-	expression tag	UNP P41594
C	3	VAL	-	expression tag	UNP P41594
C	4	SER	-	expression tag	UNP P41594
C	5	ALA	-	expression tag	UNP P41594
C	6	ILE	-	expression tag	UNP P41594
C	7	VAL	-	expression tag	UNP P41594
C	8	LEU	-	expression tag	UNP P41594
C	9	TYR	-	expression tag	UNP P41594
C	10	VAL	-	expression tag	UNP P41594
C	11	LEU	-	expression tag	UNP P41594
C	12	LEU	-	expression tag	UNP P41594
C	13	ALA	-	expression tag	UNP P41594
C	14	ALA	-	expression tag	UNP P41594
C	15	ALA	-	expression tag	UNP P41594
C	16	ALA	-	expression tag	UNP P41594
C	17	HIS	-	expression tag	UNP P41594
C	18	SER	-	expression tag	UNP P41594
C	19	ALA	-	expression tag	UNP P41594
C	20	PHE	-	expression tag	UNP P41594
C	572	HIS	-	expression tag	UNP P41594
C	573	HIS	-	expression tag	UNP P41594
C	574	HIS	-	expression tag	UNP P41594
C	575	HIS	-	expression tag	UNP P41594
C	576	HIS	-	expression tag	UNP P41594
C	577	HIS	-	expression tag	UNP P41594
C	578	HIS	-	expression tag	UNP P41594
C	579	HIS	-	expression tag	UNP P41594

- Molecule 2 is a protein called Nanobody 43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			925	575	159	186	5			

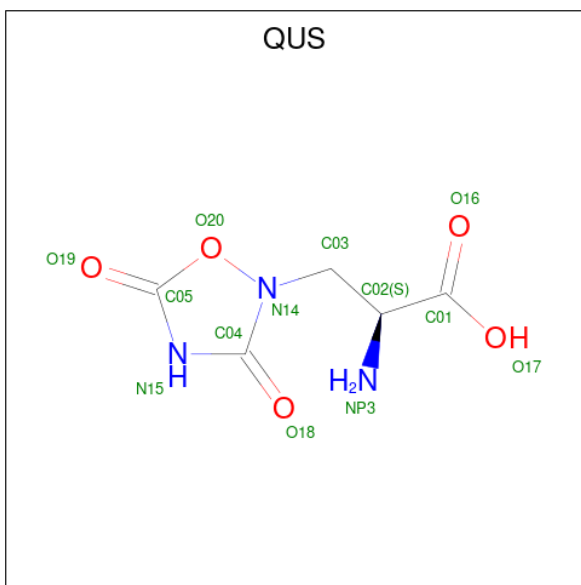
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

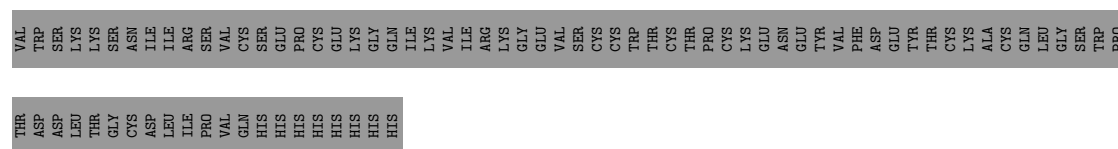
- Molecule 4 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>5</sub>).



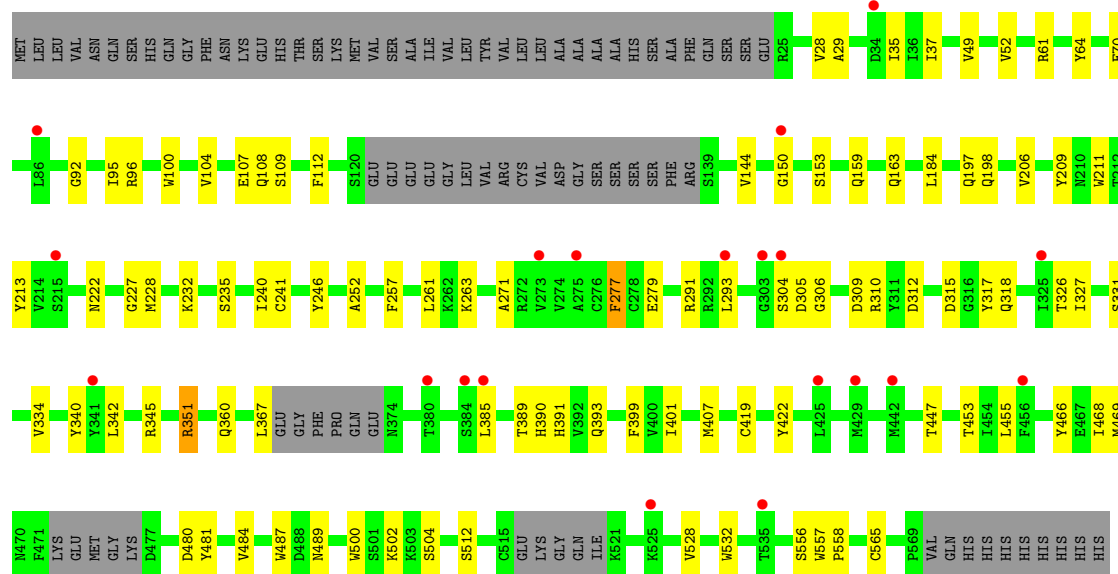


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	5	3	5		
4	B	1	Total	C	N	O	0	0
			13	5	3	5		
4	C	1	Total	C	N	O	0	0
			13	5	3	5		

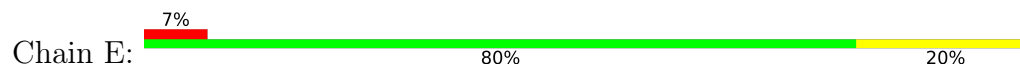




- Molecule 1: Metabotropic glutamate receptor 5



- Molecule 2: Nanobody 43



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.43Å 157.16Å 208.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 3.75 39.29 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.29-3.75) 98.5 (39.29-3.75)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.14 _3211	Depositor
R, $R_{free}$	0.266 , 0.300 0.265 , 0.299	Depositor DCC
$R_{free}$ test set	2003 reflections (7.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	122.2	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 111.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: QUS, 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	0.26	0/4069	0.49	0/5526
1	B	0.25	0/3334	0.45	0/4537
1	C	0.26	0/3961	0.48	0/5385
2	E	0.27	0/947	0.58	0/1284
All	All	0.26	0/12311	0.49	0/16732

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	3977	0	3704	68	0
1	B	3262	0	2975	44	0
1	C	3873	0	3578	55	0
2	E	925	0	852	15	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	26	0	0
4	A	13	0	6	0	0
4	B	13	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	13	0	6	0	0
All	All	12146	0	11192	179	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 (179) 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:C:29:ALA:HB3	1:C:95:ILE:HB	1.55	0.88
1:A:527:GLU:HG2	1:A:528:VAL:HG23	1.63	0.81
1:A:29:ALA:HB3	1:A:95:ILE:HB	1.62	0.80
1:A:360:GLN:HE22	1:A:373:GLU:HA	1.50	0.75
1:C:198:GLN:NE2	1:C:304:SER:OG	2.20	0.75
1:C:340:TYR:OH	1:C:351:ARG:NH2	2.20	0.75
1:B:29:ALA:HB3	1:B:95:ILE:HB	1.67	0.75
1:A:340:TYR:OH	1:A:351:ARG:NH2	2.23	0.72
1:A:350:HIS:HB3	2:E:103:TYR:HB3	1.75	0.69
1:B:37:ILE:HD11	1:B:91:LEU:HD22	1.77	0.67
1:A:109:SER:HA	1:A:112:PHE:HD2	1.60	0.67
1:A:220:GLU:HG2	1:A:249:TYR:CE1	2.30	0.66
1:C:252:ALA:HB3	1:C:257:PHE:HE1	1.60	0.66
1:B:381:CYS:HB2	1:B:385:LEU:HD21	1.76	0.66
2:E:93:THR:HG23	2:E:122:THR:HA	1.78	0.66
1:A:252:ALA:HB3	1:A:257:PHE:HE1	1.61	0.66
1:B:252:ALA:HB3	1:B:257:PHE:HE1	1.62	0.65
1:B:220:GLU:HG2	1:B:249:TYR:CE1	2.32	0.65
1:C:228:MET:HG3	1:C:232:LYS:HE3	1.79	0.64
1:C:109:SER:HA	1:C:112:PHE:HD2	1.64	0.63
1:C:326:THR:HG23	1:C:469:MET:HB2	1.81	0.62
1:C:419:CYS:HB3	1:C:422:TYR:HB2	1.81	0.62
1:B:109:SER:HA	1:B:112:PHE:HD2	1.64	0.62
2:E:26:ALA:O	2:E:79:ASN:ND2	2.35	0.60
1:B:36:ILE:HD13	1:B:141:LYS:HE3	1.83	0.60
1:B:326:THR:HG23	1:B:469:MET:HB2	1.82	0.60
1:B:35:ILE:HG23	1:B:144:VAL:HG21	1.83	0.59
1:A:556:SER:HB3	1:A:565:CYS:HB3	1.83	0.59
1:B:286:LEU:O	1:B:290:MET:HG3	2.03	0.59
1:A:326:THR:HG23	1:A:469:MET:HB2	1.84	0.58
1:C:556:SER:HB3	1:C:565:CYS:HB3	1.85	0.58
1:B:227:GLY:HA3	1:B:277:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG11	1:A:94:GLU:HG3	1.85	0.57
1:A:227:GLY:HA3	1:A:277:PHE:CE2	2.40	0.57
1:A:35:ILE:HG23	1:A:144:VAL:HG21	1.86	0.56
1:A:334:VAL:HG13	1:A:337:PHE:HB3	1.87	0.56
1:B:419:CYS:HB3	1:B:422:TYR:HB3	1.87	0.55
1:A:356:GLN:HE22	1:A:370:PHE:HD2	1.56	0.54
1:C:291:ARG:HD2	1:C:317:TYR:CE2	2.42	0.54
1:B:480:ASP:OD1	1:B:481:TYR:N	2.41	0.54
1:B:246:TYR:HE1	1:B:263:LYS:HE2	1.73	0.54
2:E:107:TRP:CD1	2:E:108:PRO:HA	2.43	0.53
1:A:520:ILE:HG21	1:A:534:CYS:HB3	1.90	0.53
1:C:197:GLN:HB3	1:C:487:TRP:CZ3	2.44	0.53
1:B:28:VAL:HG11	1:B:94:GLU:HG3	1.91	0.53
1:B:197:GLN:HB3	1:B:487:TRP:CZ3	2.45	0.52
1:C:163:GLN:NE2	1:C:184:LEU:O	2.42	0.52
1:C:159:GLN:OE1	1:C:163:GLN:HG2	2.08	0.52
1:C:241:CYS:HB3	1:C:528:VAL:HG11	1.92	0.52
1:B:159:GLN:OE1	1:B:163:GLN:HB3	2.10	0.52
2:E:22:LEU:O	2:E:82:TYR:HA	2.10	0.52
1:C:252:ALA:HB3	1:C:257:PHE:CE1	2.44	0.52
1:A:506:ILE:H	1:A:506:ILE:HD12	1.75	0.51
1:A:246:TYR:HE1	1:A:263:LYS:HE2	1.76	0.51
1:A:265:THR:HG21	1:A:295:LEU:HD13	1.92	0.51
1:A:527:GLU:N	1:A:527:GLU:OE1	2.44	0.51
1:C:246:TYR:HE1	1:C:263:LYS:HE2	1.76	0.51
1:B:246:TYR:CE1	1:B:263:LYS:HE2	2.46	0.51
1:B:217:VAL:O	1:B:276:CYS:HA	2.10	0.50
1:C:502:LYS:HD3	1:C:504:SER:H	1.77	0.50
1:C:35:ILE:HG23	1:C:144:VAL:HG21	1.92	0.50
1:C:227:GLY:HA3	1:C:277:PHE:CE2	2.47	0.50
1:A:198:GLN:HB2	1:A:466:TYR:CE2	2.47	0.50
1:A:360:GLN:HE21	1:A:367:LEU:H	1.59	0.50
1:A:261:LEU:HD23	1:A:295:LEU:HD12	1.94	0.50
1:A:197:GLN:HB3	1:A:487:TRP:CZ3	2.47	0.49
1:A:265:THR:HG22	1:A:268:LEU:HD12	1.93	0.49
1:C:104:VAL:O	1:C:107:GLU:HG2	2.12	0.49
1:C:198:GLN:HB2	1:C:466:TYR:CE2	2.47	0.49
1:C:480:ASP:OD1	1:C:481:TYR:N	2.43	0.49
1:A:252:ALA:HB3	1:A:257:PHE:CE1	2.45	0.49
1:A:480:ASP:OD1	1:A:481:TYR:N	2.44	0.49
1:A:522:VAL:HG13	1:A:532:TRP:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:SER:HB2	1:B:399:PHE:CE2	2.48	0.49
1:C:246:TYR:CE1	1:C:263:LYS:HE2	2.47	0.49
1:C:331:SER:HB2	1:C:399:PHE:CE2	2.48	0.49
1:A:310:ARG:HB3	1:A:312:ASP:OD1	2.13	0.49
1:A:371:PRO:HG2	2:E:104:GLY:H	1.78	0.49
1:A:246:TYR:CE1	1:A:263:LYS:HE2	2.48	0.49
1:A:283:VAL:O	1:A:287:LEU:HG	2.13	0.49
1:C:345:ARG:NH2	1:C:385:LEU:O	2.43	0.49
1:A:331:SER:HB2	1:A:399:PHE:CE2	2.48	0.48
1:A:557:TRP:CG	1:A:558:PRO:HD2	2.48	0.48
1:A:235:SER:HB2	1:A:240:ILE:HB	1.94	0.48
1:C:70:GLU:HB3	1:C:340:TYR:HE2	1.78	0.48
1:A:371:PRO:HG2	2:E:104:GLY:N	2.29	0.48
1:B:310:ARG:HB3	1:B:312:ASP:OD1	2.14	0.48
1:C:557:TRP:CG	1:C:558:PRO:HD2	2.48	0.47
1:C:235:SER:HB2	1:C:240:ILE:HB	1.97	0.47
1:C:261:LEU:HD23	1:C:293:LEU:HD22	1.95	0.47
1:A:520:ILE:CG2	1:A:534:CYS:HB3	2.44	0.47
1:B:198:GLN:HB2	1:B:466:TYR:CE2	2.49	0.47
1:C:310:ARG:HB3	1:C:312:ASP:OD1	2.14	0.47
1:A:305:ASP:HA	1:A:327:ILE:O	2.15	0.47
1:C:315:ASP:HA	1:C:318:GLN:NE2	2.30	0.47
2:E:102:MET:HG2	2:E:103:TYR:CD1	2.50	0.47
1:B:474:MET:HB2	1:B:478:TYR:CD2	2.50	0.46
1:A:527:GLU:HG2	1:A:528:VAL:N	2.29	0.46
1:B:235:SER:HB2	1:B:240:ILE:HB	1.97	0.46
1:B:279:GLU:HA	1:B:306:GLY:HA3	1.97	0.46
1:B:309:ASP:N	1:B:309:ASP:OD1	2.48	0.46
1:C:512:SER:HB3	1:C:532:TRP:CH2	2.50	0.46
1:C:159:GLN:O	1:C:163:GLN:HG3	2.16	0.46
1:A:104:VAL:O	1:A:107:GLU:HG2	2.15	0.46
1:B:104:VAL:O	1:B:107:GLU:HG2	2.15	0.46
1:A:43:VAL:HB	1:A:97:ASP:OD1	2.16	0.46
1:A:109:SER:HA	1:A:112:PHE:CD2	2.47	0.46
1:A:213:TYR:CD2	1:A:271:ALA:HB2	2.51	0.46
1:C:153:SER:OG	1:C:222:ASN:N	2.38	0.46
1:B:180:SER:OG	1:B:190:ARG:NH2	2.49	0.46
2:E:36:MET:HG3	2:E:81:VAL:HG11	1.96	0.46
1:A:345:ARG:NH2	1:A:385:LEU:O	2.46	0.45
1:A:394:ASP:HB3	1:A:397:MET:HB2	1.98	0.45
1:C:228:MET:O	1:C:232:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:OE1	1:A:163:GLN:HB3	2.17	0.45
1:A:188:PHE:HE2	1:A:190:ARG:HD2	1.81	0.45
1:C:96:ARG:HD3	1:C:108:GLN:HB3	1.98	0.45
1:C:206:VAL:HG13	1:C:211:TRP:HB2	1.98	0.45
1:C:309:ASP:N	1:C:309:ASP:OD1	2.49	0.45
1:C:334:VAL:HG21	1:C:401:ILE:HD12	1.98	0.45
1:A:318:GLN:HB3	1:A:479:PHE:CD2	2.51	0.45
1:B:48:THR:O	1:B:52:VAL:HG13	2.17	0.45
1:B:334:VAL:HG21	1:B:401:ILE:HD12	1.99	0.45
1:C:305:ASP:HA	1:C:327:ILE:O	2.16	0.45
1:A:288:MET:HG2	1:A:317:TYR:CZ	2.53	0.44
1:C:279:GLU:HA	1:C:306:GLY:HA3	1.99	0.44
1:B:220:GLU:OE1	1:B:247:LYS:HD2	2.17	0.44
1:B:48:THR:HG23	1:B:51:LYS:H	1.82	0.44
1:B:43:VAL:HB	1:B:97:ASP:OD1	2.17	0.44
1:A:366:ARG:HG2	1:A:379:LYS:O	2.17	0.44
1:B:66:ILE:HG13	1:B:358:PHE:CG	2.53	0.44
1:B:307:TRP:HE1	1:B:314:THR:HG23	1.82	0.44
2:E:14:VAL:HG11	2:E:88:LEU:HD13	1.99	0.44
1:A:206:VAL:HG13	1:A:211:TRP:HB2	2.00	0.43
1:A:485:GLY:HA3	1:A:494:MET:SD	2.58	0.43
1:C:468:ILE:HG22	1:C:484:VAL:HG23	2.00	0.43
1:C:61:ARG:HE	1:C:64:TYR:HB2	1.82	0.43
1:C:342:LEU:HD21	1:C:391:HIS:CG	2.53	0.43
1:B:252:ALA:HB3	1:B:257:PHE:CE1	2.47	0.43
1:A:36:ILE:HD12	1:A:141:LYS:HB2	2.00	0.43
1:B:109:SER:O	1:B:113:ILE:HG12	2.19	0.43
1:A:374:ASN:HD22	1:A:375:SER:N	2.17	0.43
1:C:37:ILE:HG22	1:C:92:GLY:O	2.18	0.43
1:C:360:GLN:HE21	1:C:367:LEU:H	1.67	0.42
1:C:28:VAL:HG12	1:C:96:ARG:HG2	2.01	0.42
2:E:7:VAL:O	2:E:24:CYS:HA	2.20	0.42
1:C:37:ILE:HD12	1:C:407:MET:HG2	2.00	0.42
1:A:468:ILE:HG22	1:A:484:VAL:HG23	2.01	0.42
1:A:70:GLU:HB3	1:A:340:TYR:HE2	1.84	0.42
1:A:221:GLY:O	1:A:225:GLU:HB2	2.19	0.42
1:B:156:ILE:HD11	1:B:222:ASN:OD1	2.19	0.42
1:A:307:TRP:HE1	1:A:314:THR:HG23	1.85	0.41
1:C:213:TYR:CD2	1:C:271:ALA:HB2	2.56	0.41
1:A:273:VAL:HG12	1:A:509:SER:OG	2.20	0.41
1:A:334:VAL:HG11	1:A:401:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HD3	1:A:108:GLN:HB3	2.03	0.41
1:B:205:ILE:HD11	1:B:468:ILE:HG12	2.03	0.41
1:C:512:SER:HB3	1:C:532:TRP:CZ2	2.56	0.41
1:B:290:MET:HB2	1:B:320:GLU:HG2	2.03	0.41
1:C:100:TRP:CZ3	1:C:150:GLY:HA3	2.56	0.41
1:C:389:THR:HG22	1:C:390:HIS:ND1	2.36	0.41
2:E:113:ASP:OD1	2:E:113:ASP:N	2.52	0.41
1:A:370:PHE:N	1:A:370:PHE:CD1	2.89	0.41
2:E:31:PHE:HE2	2:E:76:ASN:HA	1.85	0.41
2:E:100:ALA:HB3	2:E:114:TYR:HB2	2.03	0.41
1:C:209:TYR:HE2	1:C:500:TRP:HE1	1.69	0.40
1:A:156:ILE:HD11	1:A:222:ASN:OD1	2.20	0.40
1:A:360:GLN:HG2	1:A:365:CYS:O	2.21	0.40
1:B:72:MET:HA	1:B:404:ILE:HD13	2.03	0.40
1:A:109:SER:O	1:A:113:ILE:HG12	2.22	0.40
1:A:153:SER:HG	1:A:222:ASN:H	1.67	0.40
1:A:265:THR:CG2	1:A:295:LEU:HD13	2.51	0.40
1:B:315:ASP:HA	1:B:318:GLN:NE2	2.37	0.40
1:B:96:ARG:HD3	1:B:108:GLN:HB3	2.03	0.40
1:C:447:THR:HA	1:C:453:THR:HA	2.04	0.40
1:A:72:MET:HA	1:A:404:ILE:HD13	2.04	0.40
1:B:214:VAL:HG12	1:B:273:VAL:HG23	2.03	0.40
1:C:49:VAL:HA	1:C:52:VAL:HG23	2.03	0.40
2:E:39:PHE:HB3	2:E:49:SER:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/596 (86%)	478 (93%)	34 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/596 (74%)	424 (97%)	14 (3%)	0	100	100
1	C	501/596 (84%)	472 (94%)	29 (6%)	0	100	100
2	E	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
All	All	1572/1911 (82%)	1488 (95%)	84 (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	418/520 (80%)	409 (98%)	9 (2%)	52	73
1	B	321/520 (62%)	317 (99%)	4 (1%)	71	84
1	C	404/520 (78%)	399 (99%)	5 (1%)	71	84
2	E	94/97 (97%)	94 (100%)	0	100	100
All	All	1237/1657 (75%)	1219 (98%)	18 (2%)	65	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	233	ASP
1	A	262	LYS
1	A	277	PHE
1	A	351	ARG
1	A	374	ASN
1	A	393	GLN
1	A	415	GLN
1	A	560	ASP
1	B	190	ARG
1	B	222	ASN
1	B	393	GLN
1	B	489	ASN

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Mol	Chain	Res	Type
1	C	277	PHE
1	C	351	ARG
1	C	393	GLN
1	C	455	LEU
1	C	489	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	360	GLN
1	A	374	ASN
1	A	415	GLN
1	B	489	ASN
1	C	44	HIS
1	C	198	GLN
1	C	489	ASN
2	E	79	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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
3	NAG	A	602	1	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.54	0
4	QUS	B	602	-	6,13,13	0.92	0	4,18,18	1.36	0
4	QUS	C	603	-	6,13,13	0.93	0	4,18,18	1.30	0
3	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	C	602	1	14,14,15	0.28	0	17,19,21	0.31	0
4	QUS	A	603	-	6,13,13	0.94	0	4,18,18	1.33	0
3	NAG	C	601	1	14,14,15	0.32	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
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	QUS	B	602	-	-	1/6/8/8	0/1/1/1
4	QUS	C	603	-	-	2/6/8/8	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
3	NAG	C	602	1	-	2/6/23/26	0/1/1/1
4	QUS	A	603	-	-	2/6/8/8	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
4	A	603	QUS	C01-C02-C03-N14
4	B	602	QUS	C01-C02-C03-N14
4	C	603	QUS	C01-C02-C03-N14
4	A	603	QUS	NP3-C02-C03-N14

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Mol	Chain	Res	Type	Atoms
4	C	603	QUS	NP3-C02-C03-N14
3	C	602	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	518/596 (86%)	0.01	4 (0%) 86 84	90, 123, 169, 193	0
1	B	444/596 (74%)	0.09	14 (3%) 47 40	122, 160, 197, 221	0
1	C	511/596 (85%)	0.26	20 (3%) 39 34	122, 167, 204, 239	0
2	E	123/123 (100%)	0.44	8 (6%) 18 15	114, 138, 164, 180	0
All	All	1596/1911 (83%)	0.15	46 (2%) 51 44	90, 152, 194, 239	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	12	GLY	6.3
1	C	303	GLY	5.0
2	E	11	GLY	4.5
1	A	518	GLY	3.9
1	B	380	THR	3.5
1	C	150	GLY	3.4
2	E	85	MET	3.3
1	C	425	LEU	3.0
1	A	519	GLN	3.0
1	C	442	MET	3.0
1	C	325	ILE	2.8
1	C	304	SER	2.6
1	B	349	ASN	2.5
1	B	424	GLY	2.5
1	B	346	PRO	2.5
1	B	367	LEU	2.4
1	B	211	TRP	2.4
1	B	425	LEU	2.4
1	B	474	MET	2.4
1	C	525	LYS	2.4
1	C	535	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	517	LYS	2.3
2	E	124	SER	2.3
1	C	34	ASP	2.3
1	B	423	ALA	2.2
1	C	273	VAL	2.2
1	B	27	VAL	2.2
1	C	275	ALA	2.2
2	E	119	THR	2.2
2	E	91	GLU	2.2
2	E	72	ILE	2.2
1	C	215	SER	2.2
1	A	550	LYS	2.2
1	C	429	MET	2.2
1	C	293	LEU	2.1
1	C	385	LEU	2.1
1	C	384	SER	2.1
1	B	359	TRP	2.1
1	B	299	PHE	2.1
1	B	378	ASN	2.1
1	C	456	PHE	2.1
1	C	341	TYR	2.1
1	B	287	LEU	2.1
2	E	15	GLN	2.1
1	C	86	LEU	2.0
1	C	380	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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
3	NAG	C	601	14/15	0.67	0.31	235,237,238,238	0
3	NAG	A	602	14/15	0.72	0.18	177,179,180,180	0
3	NAG	C	602	14/15	0.75	0.34	209,214,219,220	0
3	NAG	B	601	14/15	0.78	0.28	186,187,188,189	0
4	QUS	C	603	13/13	0.79	0.43	149,156,161,162	0
3	NAG	A	601	14/15	0.80	0.33	160,161,164,165	0
4	QUS	B	602	13/13	0.84	0.27	145,152,157,158	0
4	QUS	A	603	13/13	0.91	0.29	100,106,111,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.