



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:46 am GMT

PDB ID : 5LXB  
Title : Crystal structure of a mutant binding protein (5HTBP-AChBP) in complex with palonosetron  
Authors : Ulens, C.  
Deposited on : 2016-09-20  
Resolution : 2.34 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

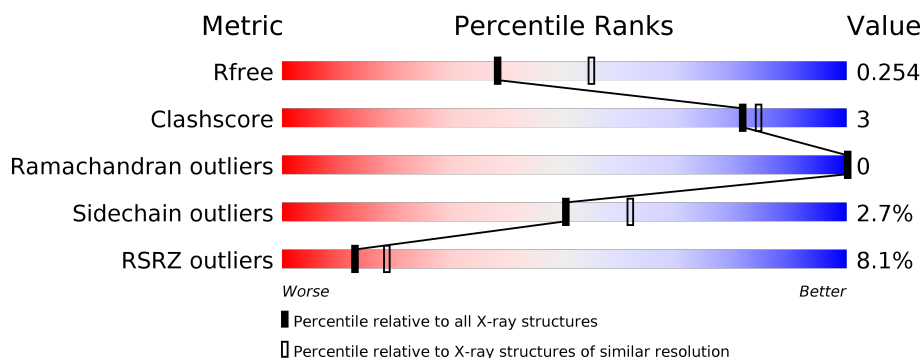
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	242	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>15%</div> </div> </div>
1	B	242	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	C	242	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	D	242	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>6%</div> <div>15%</div> </div> </div>
1	E	242	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>15%</div> </div> </div>
1	F	242	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>15%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	242	<div><div></div><div>9%</div><div>75%</div><div>8%</div><div>15%</div></div>
1	H	242	<div><div></div><div>9%</div><div>76%</div><div>8%</div><div>15%</div></div>
1	I	242	<div><div></div><div>8%</div><div>77%</div><div>6%</div><div>15%</div></div>
1	J	242	<div><div></div><div>6%</div><div>77%</div><div>7%</div><div>15%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16946 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	B	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	C	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	D	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	E	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	F	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	G	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	H	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	I	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	J	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	53	TRP	TYR	conflict	UNP Q8WSF8
A	55	ARG	GLN	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
A	218	HIS	-	expression tag	UNP Q8WSF8
A	219	HIS	-	expression tag	UNP Q8WSF8
A	220	HIS	-	expression tag	UNP Q8WSF8
A	221	HIS	-	expression tag	UNP Q8WSF8
A	222	HIS	-	expression tag	UNP Q8WSF8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	53	TRP	TYR	conflict	UNP Q8WSF8
B	55	ARG	GLN	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
B	218	HIS	-	expression tag	UNP Q8WSF8
B	219	HIS	-	expression tag	UNP Q8WSF8
B	220	HIS	-	expression tag	UNP Q8WSF8
B	221	HIS	-	expression tag	UNP Q8WSF8
B	222	HIS	-	expression tag	UNP Q8WSF8
B	223	HIS	-	expression tag	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	53	TRP	TYR	conflict	UNP Q8WSF8
C	55	ARG	GLN	conflict	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8
C	218	HIS	-	expression tag	UNP Q8WSF8
C	219	HIS	-	expression tag	UNP Q8WSF8
C	220	HIS	-	expression tag	UNP Q8WSF8
C	221	HIS	-	expression tag	UNP Q8WSF8
C	222	HIS	-	expression tag	UNP Q8WSF8
C	223	HIS	-	expression tag	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	53	TRP	TYR	conflict	UNP Q8WSF8
D	55	ARG	GLN	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
D	218	HIS	-	expression tag	UNP Q8WSF8
D	219	HIS	-	expression tag	UNP Q8WSF8
D	220	HIS	-	expression tag	UNP Q8WSF8
D	221	HIS	-	expression tag	UNP Q8WSF8
D	222	HIS	-	expression tag	UNP Q8WSF8
D	223	HIS	-	expression tag	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8
E	53	TRP	TYR	conflict	UNP Q8WSF8
E	55	ARG	GLN	conflict	UNP Q8WSF8
E	136	VAL	ALA	conflict	UNP Q8WSF8
E	218	HIS	-	expression tag	UNP Q8WSF8
E	219	HIS	-	expression tag	UNP Q8WSF8
E	220	HIS	-	expression tag	UNP Q8WSF8
E	221	HIS	-	expression tag	UNP Q8WSF8
E	222	HIS	-	expression tag	UNP Q8WSF8
E	223	HIS	-	expression tag	UNP Q8WSF8
F	41	VAL	ALA	conflict	UNP Q8WSF8

*Continued on next page...*

*Continued from previous page...*

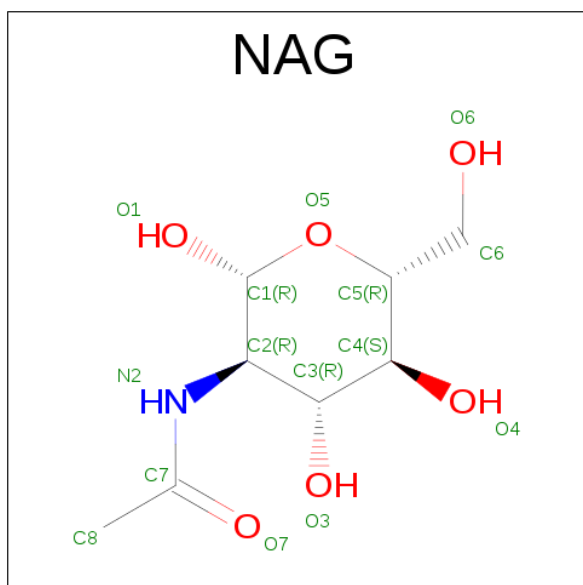
Chain	Residue	Modelled	Actual	Comment	Reference
F	53	TRP	TYR	conflict	UNP Q8WSF8
F	55	ARG	GLN	conflict	UNP Q8WSF8
F	136	VAL	ALA	conflict	UNP Q8WSF8
F	218	HIS	-	expression tag	UNP Q8WSF8
F	219	HIS	-	expression tag	UNP Q8WSF8
F	220	HIS	-	expression tag	UNP Q8WSF8
F	221	HIS	-	expression tag	UNP Q8WSF8
F	222	HIS	-	expression tag	UNP Q8WSF8
F	223	HIS	-	expression tag	UNP Q8WSF8
G	41	VAL	ALA	conflict	UNP Q8WSF8
G	53	TRP	TYR	conflict	UNP Q8WSF8
G	55	ARG	GLN	conflict	UNP Q8WSF8
G	136	VAL	ALA	conflict	UNP Q8WSF8
G	218	HIS	-	expression tag	UNP Q8WSF8
G	219	HIS	-	expression tag	UNP Q8WSF8
G	220	HIS	-	expression tag	UNP Q8WSF8
G	221	HIS	-	expression tag	UNP Q8WSF8
G	222	HIS	-	expression tag	UNP Q8WSF8
G	223	HIS	-	expression tag	UNP Q8WSF8
H	41	VAL	ALA	conflict	UNP Q8WSF8
H	53	TRP	TYR	conflict	UNP Q8WSF8
H	55	ARG	GLN	conflict	UNP Q8WSF8
H	136	VAL	ALA	conflict	UNP Q8WSF8
H	218	HIS	-	expression tag	UNP Q8WSF8
H	219	HIS	-	expression tag	UNP Q8WSF8
H	220	HIS	-	expression tag	UNP Q8WSF8
H	221	HIS	-	expression tag	UNP Q8WSF8
H	222	HIS	-	expression tag	UNP Q8WSF8
H	223	HIS	-	expression tag	UNP Q8WSF8
I	41	VAL	ALA	conflict	UNP Q8WSF8
I	53	TRP	TYR	conflict	UNP Q8WSF8
I	55	ARG	GLN	conflict	UNP Q8WSF8
I	136	VAL	ALA	conflict	UNP Q8WSF8
I	218	HIS	-	expression tag	UNP Q8WSF8
I	219	HIS	-	expression tag	UNP Q8WSF8
I	220	HIS	-	expression tag	UNP Q8WSF8
I	221	HIS	-	expression tag	UNP Q8WSF8
I	222	HIS	-	expression tag	UNP Q8WSF8
I	223	HIS	-	expression tag	UNP Q8WSF8
J	41	VAL	ALA	conflict	UNP Q8WSF8
J	53	TRP	TYR	conflict	UNP Q8WSF8
J	55	ARG	GLN	conflict	UNP Q8WSF8

*Continued on next page...*

Continued from previous page...

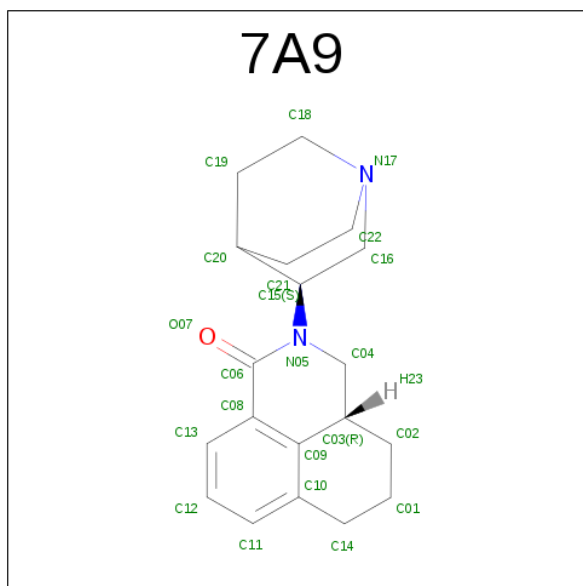
Chain	Residue	Modelled	Actual	Comment	Reference
J	136	VAL	ALA	conflict	UNP Q8WSF8
J	218	HIS	-	expression tag	UNP Q8WSF8
J	219	HIS	-	expression tag	UNP Q8WSF8
J	220	HIS	-	expression tag	UNP Q8WSF8
J	221	HIS	-	expression tag	UNP Q8WSF8
J	222	HIS	-	expression tag	UNP Q8WSF8
J	223	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is palonosetron (three-letter code: 7A9) (formula:  $C_{19}H_{24}N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	19	2	1		
3	C	1	Total	C	N	O	0	0
			22	19	2	1		
3	D	1	Total	C	N	O	0	0
			22	19	2	1		
3	E	1	Total	C	N	O	0	0
			22	19	2	1		
3	G	1	Total	C	N	O	0	0
			22	19	2	1		
3	H	1	Total	C	N	O	0	0
			22	19	2	1		
3	J	1	Total	C	N	O	0	0
			22	19	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	27	Total	O	0	0
			27	27		
4	C	11	Total	O	0	0
			11	11		
4	D	34	Total	O	0	0
			34	34		

*Continued on next page...*



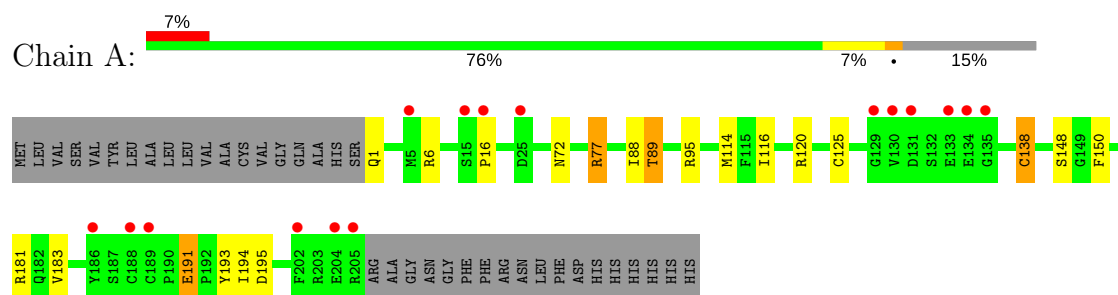
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	54	Total 54	O 54	0	0
4	F	46	Total 46	O 46	0	0
4	G	20	Total 20	O 20	0	0
4	H	14	Total 14	O 14	0	0
4	I	20	Total 20	O 20	0	0
4	J	25	Total 25	O 25	0	0

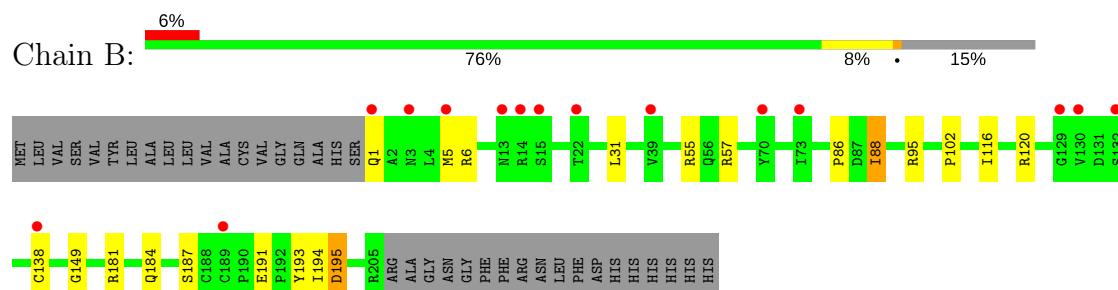
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

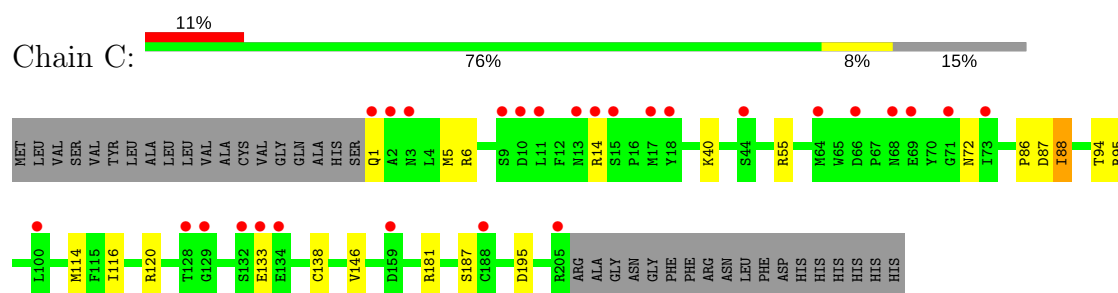
#### • Molecule 1: Soluble acetylcholine receptor



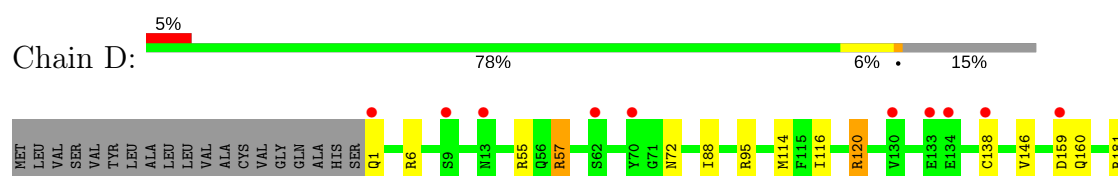
#### • Molecule 1: Soluble acetylcholine receptor



#### • Molecule 1: Soluble acetylcholine receptor

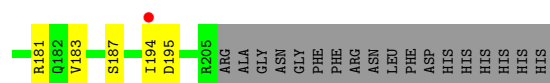
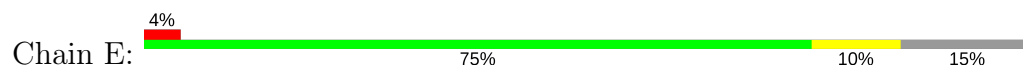


#### • Molecule 1: Soluble acetylcholine receptor

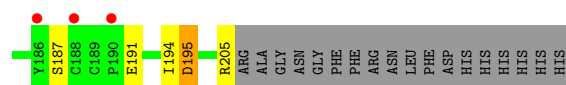
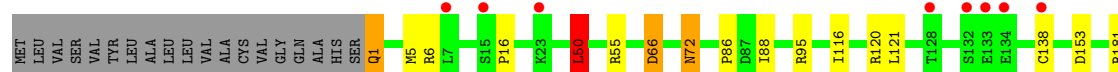
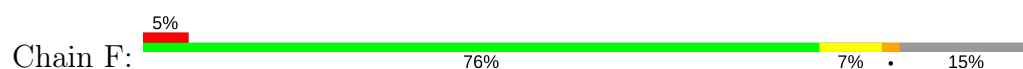




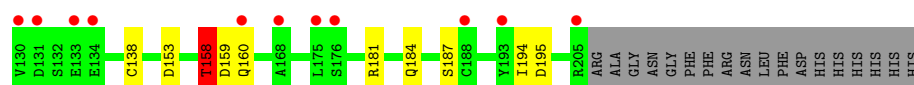
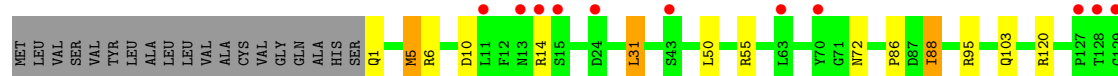
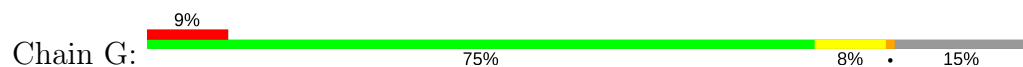
• Molecule 1: Soluble acetylcholine receptor



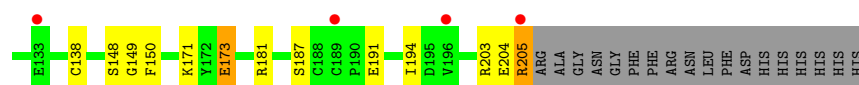
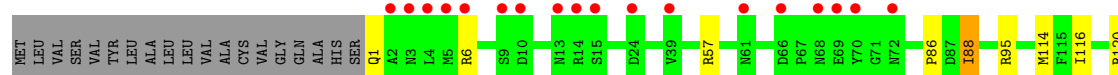
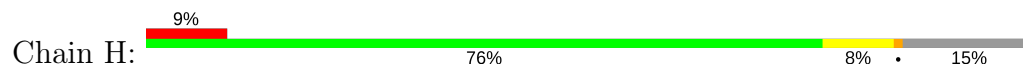
• Molecule 1: Soluble acetylcholine receptor



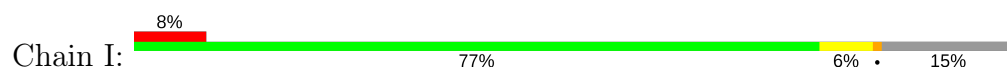
• Molecule 1: Soluble acetylcholine receptor

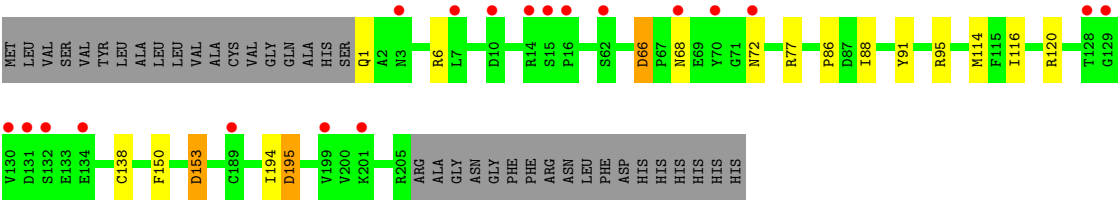


• Molecule 1: Soluble acetylcholine receptor

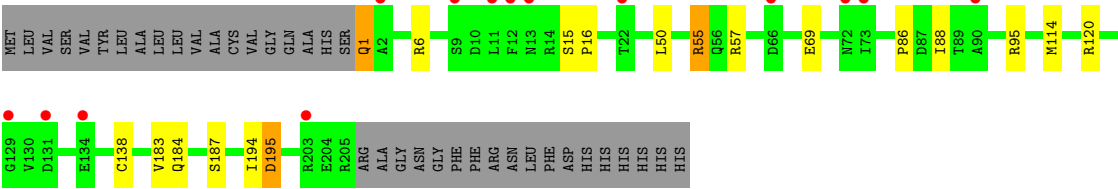
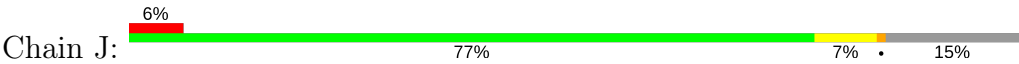


• Molecule 1: Soluble acetylcholine receptor





● Molecule 1: Soluble acetylcholine receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.22Å 137.05Å 131.25Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	130.96 – 2.34 47.34 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.8 (130.96-2.34) 98.8 (47.34-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.218 , 0.245 0.226 , 0.254	Depositor DCC
$R_{free}$ test set	5294 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 7A9

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	0.86	2/1681 (0.1%)	0.98	11/2294 (0.5%)
1	B	0.80	2/1681 (0.1%)	0.94	6/2294 (0.3%)
1	C	0.76	1/1681 (0.1%)	0.92	7/2294 (0.3%)
1	D	0.80	0/1681	1.02	8/2294 (0.3%)
1	E	0.96	2/1681 (0.1%)	0.98	8/2294 (0.3%)
1	F	0.85	1/1681 (0.1%)	1.06	13/2294 (0.6%)
1	G	0.82	1/1681 (0.1%)	1.00	11/2294 (0.5%)
1	H	0.80	1/1681 (0.1%)	0.97	10/2294 (0.4%)
1	I	0.75	0/1681	0.97	12/2294 (0.5%)
1	J	0.81	0/1681	0.94	6/2294 (0.3%)
All	All	0.82	10/16810 (0.1%)	0.98	92/22940 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLU	CD-OE1	-9.19	1.15	1.25
1	G	158	THR	CB-CG2	-8.64	1.23	1.52
1	E	187	SER	CB-OG	-7.33	1.32	1.42
1	H	150	PHE	CG-CD2	6.52	1.48	1.38
1	A	89	THR	CB-CG2	-6.32	1.31	1.52
1	F	191	GLU	CD-OE1	-6.18	1.18	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	SER	CB-OG	-5.59	1.34	1.42
1	E	14	ARG	C-O	-5.52	1.12	1.23
1	B	191	GLU	CG-CD	5.43	1.60	1.51
1	B	193	TYR	CG-CD2	5.03	1.45	1.39

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	ARG	NE-CZ-NH2	16.05	128.32	120.30
1	D	6	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	F	6	ARG	NE-CZ-NH2	14.27	127.43	120.30
1	D	181	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	B	6	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	6	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	C	6	ARG	NE-CZ-NH2	9.59	125.09	120.30
1	J	6	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	I	6	ARG	NE-CZ-NH2	9.31	124.96	120.30
1	H	6	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	H	181	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	E	95	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	F	55	ARG	NE-CZ-NH2	8.43	124.51	120.30
1	I	66	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	G	6	ARG	NH1-CZ-NH2	-8.36	110.20	119.40
1	F	50	LEU	CB-CG-CD1	-8.36	96.79	111.00
1	D	6	ARG	NH1-CZ-NH2	-8.32	110.25	119.40
1	E	95	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	E	6	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	F	6	ARG	NH1-CZ-NH2	-8.08	110.52	119.40
1	E	181	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	F	66	ASP	CB-CG-OD2	7.62	125.15	118.30
1	H	95	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	F	66	ASP	CB-CG-OD1	-7.42	111.63	118.30
1	I	150	PHE	CB-CG-CD2	-7.40	115.62	120.80
1	F	95	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	I	150	PHE	CB-CG-CD1	7.16	125.81	120.80
1	A	77	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	55	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	95	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	57	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	I	77	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	95	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	120	ARG	NE-CZ-NH1	6.79	123.70	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	195	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	150	PHE	CB-CG-CD2	-6.71	116.10	120.80
1	B	31	LEU	CA-CB-CG	6.69	130.69	115.30
1	E	6	ARG	CG-CD-NE	-6.46	98.24	111.80
1	C	181	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	95	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	F	95	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	H	120	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	31	LEU	CA-CB-CG	6.10	129.34	115.30
1	G	31	LEU	CA-CB-CG	6.10	129.34	115.30
1	J	55	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	H	120	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	I	195	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	193	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	138	CYS	CA-CB-SG	-5.87	103.43	114.00
1	F	120	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	95	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	J	95	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	95	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	J	95	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	181	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	I	153	ASP	CB-CG-OD1	5.66	123.39	118.30
1	I	95	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	I	120	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	5	MET	CG-SD-CE	5.61	109.18	100.20
1	H	173	GLU	CA-CB-CG	5.60	125.71	113.40
1	G	181	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	95	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	120	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	95	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	120	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	I	95	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	F	181	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	120	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	H	205	ARG	CA-CB-CG	5.45	125.40	113.40
1	J	114	MET	CG-SD-CE	5.42	108.87	100.20
1	E	12	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	C	95	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	89	THR	CA-CB-CG2	-5.34	104.93	112.40
1	G	95	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	H	95	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	55	ARG	CB-CG-CD	5.31	125.40	111.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	120	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	I	66	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	95	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	I	91	TYR	CB-CG-CD1	5.26	124.16	121.00
1	A	6	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	G	88	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	B	120	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	203	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	G	184	GLN	CA-CB-CG	5.13	124.69	113.40
1	H	88	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	B	181	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	103	GLN	CA-CB-CG	-5.04	102.31	113.40
1	A	120	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	114	MET	CG-SD-CE	-5.03	92.16	100.20
1	G	5	MET	CG-SD-CE	5.03	108.24	100.20
1	J	120	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	15	SER	Peptide
1	F	72	ASN	Sidechain

## 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	1640	0	1580	17	0
1	B	1640	0	1578	12	0
1	C	1640	0	1578	7	0
1	D	1640	0	1578	9	0
1	E	1640	0	1578	10	0
1	F	1640	0	1578	12	0
1	G	1640	0	1578	11	0
1	H	1640	0	1578	13	0
1	I	1640	0	1578	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1640	0	1578	7	0
2	A	14	0	13	3	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
2	E	14	0	13	1	0
2	F	14	0	13	2	0
2	G	14	0	13	1	0
2	I	14	0	13	3	0
2	J	14	0	13	0	0
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
3	E	22	0	0	0	0
3	G	22	0	0	0	0
3	H	22	0	0	0	0
3	J	22	0	0	0	0
4	A	29	0	0	0	0
4	B	27	0	0	0	0
4	C	11	0	0	0	0
4	D	34	0	0	0	0
4	E	54	0	0	1	0
4	F	46	0	0	0	0
4	G	20	0	0	0	0
4	H	14	0	0	0	0
4	I	20	0	0	0	0
4	J	25	0	0	0	0
All	All	16946	0	15886	97	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 3.

All (97) 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:F:72:ASN:HD21	2:F:301:NAG:C1	1.75	0.99
1:A:125:CYS:SG	1:A:138:CYS:HB3	2.16	0.85
1:A:89:THR:HG21	1:B:102:PRO:HD3	1.67	0.76
1:F:72:ASN:ND2	2:F:301:NAG:C1	2.50	0.74
1:E:1:GLN:N	1:E:1:GLN:OE1	2.22	0.73
1:D:159:ASP:OD1	1:D:160:GLN:NE2	2.22	0.73
1:G:1:GLN:OE1	1:G:1:GLN:N	2.23	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASN:OD1	2:D:301:NAG:C1	2.38	0.71
1:H:1:GLN:OE1	1:H:1:GLN:N	2.23	0.71
1:C:1:GLN:N	1:C:1:GLN:OE1	2.23	0.71
1:A:1:GLN:N	1:A:1:GLN:OE1	2.24	0.71
1:B:149:GLY:CA	1:B:194:ILE:CD1	2.69	0.71
1:F:1:GLN:N	1:F:1:GLN:OE1	2.23	0.70
1:H:149:GLY:CA	1:H:194:ILE:CD1	2.69	0.70
1:B:149:GLY:HA2	1:B:194:ILE:CD1	2.22	0.70
1:H:149:GLY:HA2	1:H:194:ILE:CD1	2.22	0.69
1:J:1:GLN:N	1:J:1:GLN:OE1	2.25	0.69
1:G:158:THR:HG23	1:G:160:GLN:H	1.59	0.67
1:B:1:GLN:N	1:B:1:GLN:OE1	2.22	0.67
1:H:149:GLY:HA2	1:H:194:ILE:HD13	1.78	0.66
1:I:1:GLN:N	1:I:1:GLN:OE1	2.23	0.65
1:E:90:ALA:O	4:E:401:HOH:O	2.13	0.65
1:A:72:ASN:HD21	2:A:301:NAG:C1	2.10	0.64
1:B:149:GLY:HA2	1:B:194:ILE:HD13	1.79	0.64
1:B:149:GLY:HA3	1:B:194:ILE:HD11	1.80	0.64
1:F:5:MET:CE	1:J:16:PRO:HD2	2.29	0.62
1:H:173:GLU:HG3	1:H:205:ARG:C	2.21	0.61
1:H:149:GLY:HA3	1:H:194:ILE:HD11	1.83	0.60
1:C:86:PRO:HB2	1:C:88:ILE:HD13	1.83	0.60
1:B:86:PRO:HB2	1:B:88:ILE:HD13	1.85	0.58
1:D:1:GLN:N	1:D:1:GLN:OE1	2.34	0.58
1:F:16:PRO:HD2	1:G:5:MET:HE3	1.84	0.58
1:J:184:GLN:HG3	1:J:195:ASP:OD2	2.03	0.58
1:H:149:GLY:HA3	1:H:194:ILE:CD1	2.33	0.57
1:H:86:PRO:HB2	1:H:88:ILE:HD13	1.86	0.57
1:B:149:GLY:HA3	1:B:194:ILE:CD1	2.33	0.57
1:G:153:ASP:OD1	1:G:194:ILE:HD13	2.04	0.56
1:H:204:GLU:O	1:H:205:ARG:HG3	2.05	0.56
1:G:158:THR:CG2	1:G:160:GLN:H	2.19	0.55
1:F:153:ASP:OD1	1:F:194:ILE:HD13	2.06	0.55
1:H:148:SER:HB3	1:H:191:GLU:HG3	1.88	0.55
1:E:72:ASN:OD1	2:E:301:NAG:C1	2.56	0.54
1:I:153:ASP:OD1	1:I:194:ILE:HD13	2.08	0.53
1:A:16:PRO:HD2	1:B:5:MET:CE	2.39	0.53
1:F:86:PRO:HB2	1:F:88:ILE:HD13	1.90	0.53
1:A:114:MET:HG3	1:A:116:ILE:HD11	1.89	0.53
1:I:72:ASN:HD21	2:I:301:NAG:C1	2.21	0.52
1:D:114:MET:HG3	1:D:116:ILE:HD11	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:MET:HG3	1:H:116:ILE:HD11	1.93	0.51
1:G:86:PRO:HB2	1:G:88:ILE:HD13	1.91	0.51
1:A:148:SER:HB3	1:A:191:GLU:HG3	1.93	0.51
1:I:86:PRO:HB2	1:I:88:ILE:HD13	1.93	0.50
1:I:72:ASN:ND2	2:I:301:NAG:C1	2.75	0.50
1:A:183:VAL:HG22	1:A:194:ILE:HD12	1.93	0.50
1:G:72:ASN:HD21	2:G:301:NAG:C1	2.25	0.50
1:A:125:CYS:SG	1:A:138:CYS:CB	2.94	0.49
1:A:72:ASN:HD21	2:A:301:NAG:C2	2.24	0.49
1:A:16:PRO:HG2	1:B:5:MET:HE2	1.94	0.48
1:B:184:GLN:HG3	1:B:195:ASP:OD2	2.14	0.48
1:I:114:MET:HG3	1:I:116:ILE:HD11	1.96	0.48
1:J:86:PRO:HB2	1:J:88:ILE:HD13	1.95	0.47
1:A:72:ASN:HD21	2:A:301:NAG:H2	1.79	0.47
1:E:133:GLU:N	1:E:133:GLU:OE1	2.48	0.47
1:C:72:ASN:OD1	2:C:301:NAG:C7	2.63	0.47
1:A:77:ARG:HD3	1:E:147:TYR:CE1	2.50	0.46
1:C:55:ARG:HG2	1:C:116:ILE:HD13	1.97	0.46
1:B:55:ARG:HG2	1:B:116:ILE:HD13	1.97	0.46
1:F:50:LEU:HD11	1:F:121:LEU:HD23	1.99	0.45
1:I:72:ASN:OD1	2:I:301:NAG:C7	2.66	0.44
1:F:1:GLN:N	1:F:1:GLN:CD	2.72	0.44
1:A:148:SER:CB	1:A:191:GLU:HG3	2.48	0.43
1:F:16:PRO:HD2	1:G:5:MET:CE	2.47	0.43
1:H:116:ILE:N	1:H:116:ILE:HD12	2.33	0.43
1:E:116:ILE:HD12	1:E:116:ILE:N	2.33	0.43
1:I:116:ILE:HD12	1:I:116:ILE:N	2.34	0.43
1:I:66:ASP:CG	1:I:68:ASN:OD1	2.56	0.43
1:D:146:VAL:HG23	1:E:77:ARG:HG2	1.99	0.43
1:F:116:ILE:N	1:F:116:ILE:HD12	2.34	0.43
1:J:183:VAL:HG22	1:J:194:ILE:HD12	2.01	0.43
1:G:1:GLN:CD	1:G:1:GLN:N	2.72	0.43
1:D:116:ILE:N	1:D:116:ILE:HD12	2.34	0.43
1:D:1:GLN:N	1:D:1:GLN:CD	2.73	0.42
1:C:1:GLN:N	1:C:1:GLN:CD	2.73	0.42
1:J:1:GLN:N	1:J:1:GLN:CD	2.72	0.42
1:A:116:ILE:HD12	1:A:116:ILE:N	2.33	0.42
1:H:1:GLN:CD	1:H:1:GLN:N	2.73	0.42
1:I:1:GLN:N	1:I:1:GLN:CD	2.73	0.42
1:G:10:ASP:HA	1:G:14:ARG:HD3	2.02	0.42
1:G:158:THR:HG23	1:G:159:ASP:N	2.35	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:VAL:HG22	1:E:194:ILE:HD12	2.02	0.41
1:A:1:GLN:CD	1:A:1:GLN:N	2.73	0.41
1:A:77:ARG:HG2	1:E:146:VAL:HG23	2.03	0.41
1:C:94:THR:O	1:D:120:ARG:HD2	2.21	0.41
1:E:87:ASP:OD2	1:E:146:VAL:HG22	2.21	0.41
1:D:159:ASP:OD1	1:D:159:ASP:C	2.58	0.40
1:C:87:ASP:OD2	1:C:146:VAL:HG22	2.22	0.40
1:F:5:MET:HE1	1:J:16:PRO:HD2	1.99	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	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	B	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	C	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	D	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	E	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	F	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	G	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	H	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	I	203/242 (84%)	199 (98%)	4 (2%)	0	100	100
1	J	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
All	All	2030/2420 (84%)	2003 (99%)	27 (1%)	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	188/218 (86%)	186 (99%)	2 (1%)	78	87
1	B	188/218 (86%)	183 (97%)	5 (3%)	50	62
1	C	188/218 (86%)	182 (97%)	6 (3%)	44	54
1	D	188/218 (86%)	183 (97%)	5 (3%)	50	62
1	E	188/218 (86%)	184 (98%)	4 (2%)	59	71
1	F	188/218 (86%)	181 (96%)	7 (4%)	39	49
1	G	188/218 (86%)	181 (96%)	7 (4%)	39	49
1	H	188/218 (86%)	184 (98%)	4 (2%)	59	71
1	I	188/218 (86%)	186 (99%)	2 (1%)	78	87
1	J	188/218 (86%)	179 (95%)	9 (5%)	30	37
All	All	1880/2180 (86%)	1829 (97%)	51 (3%)	50	62

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE
1	A	195	ASP
1	B	57	ARG
1	B	88	ILE
1	B	138	CYS
1	B	187	SER
1	B	195	ASP
1	C	14	ARG
1	C	40	LYS
1	C	88	ILE
1	C	133	GLU
1	C	138	CYS
1	C	195	ASP
1	D	57	ARG
1	D	88	ILE
1	D	138	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	187	SER
1	D	195	ASP
1	E	57	ARG
1	E	88	ILE
1	E	138	CYS
1	E	195	ASP
1	F	1	GLN
1	F	50	LEU
1	F	66	ASP
1	F	138	CYS
1	F	187	SER
1	F	195	ASP
1	F	205	ARG
1	G	31	LEU
1	G	50	LEU
1	G	55	ARG
1	G	138	CYS
1	G	158	THR
1	G	187	SER
1	G	195	ASP
1	H	57	ARG
1	H	138	CYS
1	H	171	LYS
1	H	187	SER
1	I	138	CYS
1	I	195	ASP
1	J	1	GLN
1	J	15	SER
1	J	50	LEU
1	J	55	ARG
1	J	57	ARG
1	J	69	GLU
1	J	138	CYS
1	J	187	SER
1	J	195	ASP

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

Mol	Chain	Res	Type
1	A	72	ASN
1	A	182	GLN
1	A	184	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	103	GLN
1	B	182	GLN
1	C	103	GLN
1	C	182	GLN
1	D	103	GLN
1	D	182	GLN
1	E	182	GLN
1	F	72	ASN
1	F	182	GLN
1	G	182	GLN
1	H	182	GLN
1	I	72	ASN
1	I	182	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
2	NAG	A	301	-	14,14,15	0.64	0	15,19,21	1.88	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	7A9	B	301	-	26,26,26	0.83	1 (3%)	29,39,39	1.35	4 (13%)
2	NAG	C	301	-	14,14,15	0.60	0	15,19,21	1.40	3 (20%)
3	7A9	C	302	-	26,26,26	1.20	4 (15%)	29,39,39	1.48	3 (10%)
2	NAG	D	301	-	14,14,15	0.70	0	15,19,21	2.48	6 (40%)
3	7A9	D	302	-	26,26,26	1.06	3 (11%)	29,39,39	1.01	2 (6%)
2	NAG	E	301	-	14,14,15	0.71	0	15,19,21	1.88	4 (26%)
3	7A9	E	302	-	26,26,26	0.76	1 (3%)	29,39,39	1.16	4 (13%)
2	NAG	F	301	-	14,14,15	0.81	0	15,19,21	3.48	7 (46%)
2	NAG	G	301	-	14,14,15	0.42	0	15,19,21	1.04	1 (6%)
3	7A9	G	302	-	26,26,26	0.76	0	29,39,39	1.01	1 (3%)
3	7A9	H	301	-	26,26,26	0.96	2 (7%)	29,39,39	0.95	0
2	NAG	I	301	-	14,14,15	0.73	0	15,19,21	1.83	4 (26%)
2	NAG	J	301	-	14,14,15	0.59	0	15,19,21	0.91	1 (6%)
3	7A9	J	302	-	26,26,26	0.97	1 (3%)	29,39,39	1.15	1 (3%)

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
2	NAG	A	301	-	-	0/6/23/26	0/1/1/1
3	7A9	B	301	-	-	0/4/44/44	0/3/5/5
2	NAG	C	301	-	-	0/6/23/26	0/1/1/1
3	7A9	C	302	-	-	0/4/44/44	0/3/5/5
2	NAG	D	301	-	-	0/6/23/26	0/1/1/1
3	7A9	D	302	-	-	0/4/44/44	0/3/5/5
2	NAG	E	301	-	-	0/6/23/26	0/1/1/1
3	7A9	E	302	-	-	0/4/44/44	0/3/5/5
2	NAG	F	301	-	-	0/6/23/26	0/1/1/1
2	NAG	G	301	-	-	0/6/23/26	0/1/1/1
3	7A9	G	302	-	-	0/4/44/44	0/3/5/5
3	7A9	H	301	-	-	0/4/44/44	0/3/5/5
2	NAG	I	301	-	-	0/6/23/26	0/1/1/1
2	NAG	J	301	-	-	0/6/23/26	0/1/1/1
3	7A9	J	302	-	-	0/4/44/44	0/3/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	7A9	C06-N05	-2.67	1.32	1.35
3	C	302	7A9	C09-C03	-2.62	1.47	1.51
3	D	302	7A9	C09-C03	-2.26	1.47	1.51
3	C	302	7A9	C04-C03	-2.02	1.51	1.53
3	E	302	7A9	C16-C15	2.10	1.55	1.52
3	D	302	7A9	C16-C15	2.11	1.55	1.52
3	C	302	7A9	C16-N17	2.26	1.50	1.46
3	H	301	7A9	C08-C06	2.28	1.52	1.47
3	H	301	7A9	C16-C15	2.58	1.56	1.52
3	B	301	7A9	C16-C15	2.62	1.56	1.52
3	J	302	7A9	C16-C15	2.75	1.56	1.52
3	C	302	7A9	C16-C15	3.10	1.57	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAG	O5-C1-C2	-8.04	100.28	111.47
2	F	301	NAG	C1-O5-C5	-5.27	104.91	112.17
2	A	301	NAG	C4-C3-C2	-3.85	105.38	111.02
2	E	301	NAG	C1-O5-C5	-3.81	106.92	112.17
3	B	301	7A9	C19-C20-C21	-3.18	104.02	109.43
2	F	301	NAG	O7-C7-N2	-2.96	116.21	121.92
3	C	302	7A9	O07-C06-C08	-2.79	115.13	122.86
2	F	301	NAG	C4-C3-C2	-2.66	107.11	111.02
2	I	301	NAG	C3-C4-C5	-2.66	105.53	110.22
3	J	302	7A9	C19-C20-C21	-2.61	104.99	109.43
3	E	302	7A9	C19-C20-C21	-2.23	105.64	109.43
3	B	301	7A9	O07-C06-C08	-2.07	117.13	122.86
3	E	302	7A9	C21-C20-C15	-2.02	105.31	110.03
2	E	301	NAG	O7-C7-N2	2.01	125.78	121.92
2	C	301	NAG	C2-N2-C7	2.03	125.91	122.94
3	D	302	7A9	O07-C06-N05	2.04	123.56	122.02
3	D	302	7A9	C03-C04-N05	2.13	115.18	110.86
2	C	301	NAG	C3-C4-C5	2.19	114.08	110.22
2	D	301	NAG	O7-C7-N2	2.27	126.30	121.92
3	E	302	7A9	C03-C04-N05	2.29	115.50	110.86
2	I	301	NAG	C6-C5-C4	2.33	118.45	113.00
2	E	301	NAG	O3-C3-C2	2.40	114.52	109.39
3	B	301	7A9	C08-C06-N05	2.41	118.91	116.22
2	J	301	NAG	C4-C3-C2	2.44	114.59	111.02
3	G	302	7A9	C03-C04-N05	2.44	115.81	110.86
3	E	302	7A9	O07-C06-N05	2.52	123.92	122.02
3	B	301	7A9	O07-C06-N05	2.55	123.94	122.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAG	C8-C7-N2	2.83	121.22	116.11
2	I	301	NAG	C1-O5-C5	2.88	116.13	112.17
3	C	302	7A9	C08-C06-N05	2.95	119.51	116.22
2	D	301	NAG	C1-C2-N2	3.08	115.75	110.49
2	G	301	NAG	C1-O5-C5	3.23	116.61	112.17
2	D	301	NAG	C4-C3-C2	3.29	115.84	111.02
2	E	301	NAG	C2-N2-C7	3.39	127.89	122.94
2	F	301	NAG	C1-C2-N2	3.42	116.33	110.49
2	C	301	NAG	C1-O5-C5	3.51	117.00	112.17
2	D	301	NAG	O5-C1-C2	3.77	116.72	111.47
2	I	301	NAG	O4-C4-C5	3.94	119.20	109.28
2	A	301	NAG	C1-O5-C5	4.28	118.07	112.17
2	D	301	NAG	C1-O5-C5	4.34	118.15	112.17
3	C	302	7A9	O07-C06-N05	4.35	125.30	122.02
2	D	301	NAG	C2-N2-C7	4.78	129.91	122.94
2	F	301	NAG	C2-N2-C7	6.93	133.06	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAG	3	0
2	C	301	NAG	1	0
2	D	301	NAG	1	0
2	E	301	NAG	1	0
2	F	301	NAG	2	0
2	G	301	NAG	1	0
2	I	301	NAG	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	205/242 (84%)	0.76	16 (7%) 14 20	35, 51, 76, 96	0
1	B	205/242 (84%)	0.85	15 (7%) 16 23	38, 52, 80, 99	0
1	C	205/242 (84%)	0.91	27 (13%) 4 6	37, 55, 78, 113	0
1	D	205/242 (84%)	0.68	11 (5%) 26 37	35, 50, 72, 104	0
1	E	205/242 (84%)	0.78	10 (4%) 30 42	32, 46, 68, 94	0
1	F	205/242 (84%)	0.70	11 (5%) 26 37	36, 51, 80, 94	0
1	G	205/242 (84%)	0.96	22 (10%) 7 10	40, 59, 88, 108	0
1	H	205/242 (84%)	0.99	22 (10%) 7 10	41, 58, 83, 102	0
1	I	205/242 (84%)	0.86	19 (9%) 9 15	40, 56, 84, 105	0
1	J	205/242 (84%)	0.84	14 (6%) 18 26	36, 52, 79, 99	0
All	All	2050/2420 (84%)	0.83	167 (8%) 13 18	32, 53, 80, 113	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	134	GLU	5.1
1	H	68	ASN	5.1
1	G	14	ARG	5.0
1	F	133	GLU	4.8
1	H	133	GLU	4.8
1	H	72	ASN	4.6
1	I	68	ASN	4.6
1	I	14	ARG	4.6
1	F	134	GLU	4.5
1	C	15	SER	4.4
1	C	128	THR	4.4
1	C	11	LEU	4.3
1	A	134	GLU	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	69	GLU	4.2
1	C	68	ASN	4.1
1	G	129	GLY	4.1
1	G	205	ARG	4.0
1	G	133	GLU	4.0
1	C	18	TYR	4.0
1	B	14	ARG	4.0
1	B	15	SER	3.9
1	E	133	GLU	3.8
1	G	131	ASP	3.7
1	G	130	VAL	3.7
1	I	132	SER	3.6
1	C	188	CYS	3.6
1	I	131	ASP	3.6
1	G	15	SER	3.5
1	H	15	SER	3.5
1	H	70	TYR	3.5
1	H	5	MET	3.5
1	J	11	LEU	3.5
1	I	10	ASP	3.4
1	G	13	ASN	3.4
1	C	14	ARG	3.4
1	I	16	PRO	3.4
1	H	66	ASP	3.4
1	A	133	GLU	3.4
1	C	134	GLU	3.4
1	I	128	THR	3.4
1	A	131	ASP	3.4
1	I	130	VAL	3.3
1	C	73	ILE	3.3
1	E	130	VAL	3.3
1	C	3	ASN	3.3
1	C	69	GLU	3.2
1	C	1	GLN	3.2
1	G	70	TYR	3.1
1	C	9	SER	3.1
1	C	64	MET	3.1
1	I	129	GLY	3.1
1	J	9	SER	3.0
1	B	5	MET	3.0
1	C	2	ALA	3.0
1	F	188	CYS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	3.0
1	B	1	GLN	3.0
1	G	168	ALA	3.0
1	A	188	CYS	3.0
1	B	13	ASN	3.0
1	F	132	SER	3.0
1	H	196	VAL	3.0
1	J	73	ILE	2.9
1	B	22	THR	2.9
1	G	176	SER	2.9
1	D	13	ASN	2.9
1	I	201	LYS	2.9
1	H	3	ASN	2.8
1	B	3	ASN	2.8
1	C	13	ASN	2.8
1	D	130	VAL	2.8
1	A	5	MET	2.8
1	H	24	ASP	2.8
1	I	3	ASN	2.8
1	D	133	GLU	2.8
1	J	13	ASN	2.7
1	B	73	ILE	2.7
1	F	23	LYS	2.7
1	A	186	TYR	2.7
1	A	202	PHE	2.7
1	G	43	SER	2.7
1	I	199	VAL	2.7
1	H	9	SER	2.6
1	J	203	ARG	2.6
1	C	71	GLY	2.6
1	E	129	GLY	2.6
1	H	10	ASP	2.6
1	B	130	VAL	2.6
1	G	127	PRO	2.6
1	B	138	CYS	2.6
1	E	132	SER	2.6
1	G	188	CYS	2.6
1	A	130	VAL	2.6
1	F	128	THR	2.5
1	H	205	ARG	2.5
1	C	10	ASP	2.5
1	D	159	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	132	SER	2.5
1	D	1	GLN	2.5
1	E	194	ILE	2.5
1	I	15	SER	2.5
1	A	25	ASP	2.5
1	J	131	ASP	2.5
1	J	134	GLU	2.5
1	C	17	MET	2.5
1	G	175	LEU	2.5
1	H	4	LEU	2.5
1	A	16	PRO	2.4
1	J	22	THR	2.4
1	A	15	SER	2.4
1	D	9	SER	2.4
1	A	129	GLY	2.4
1	A	204	GLU	2.4
1	C	133	GLU	2.4
1	C	44	SER	2.4
1	H	13	ASN	2.4
1	E	134	GLU	2.3
1	I	7	LEU	2.3
1	H	6	ARG	2.3
1	B	129	GLY	2.3
1	J	12	PHE	2.3
1	B	39	VAL	2.3
1	I	72	ASN	2.3
1	B	189	CYS	2.3
1	F	138	CYS	2.3
1	I	189	CYS	2.3
1	D	138	CYS	2.2
1	H	39	VAL	2.2
1	E	5	MET	2.2
1	G	160	GLN	2.2
1	G	128	THR	2.2
1	J	90	ALA	2.2
1	C	205	ARG	2.2
1	C	100	LEU	2.2
1	G	63	LEU	2.2
1	D	70	TYR	2.2
1	H	61	ASN	2.2
1	F	15	SER	2.2
1	F	7	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	11	LEU	2.1
1	J	129	GLY	2.1
1	G	193	TYR	2.1
1	J	66	ASP	2.1
1	I	134	GLU	2.1
1	A	189	CYS	2.1
1	C	66	ASP	2.1
1	I	70	TYR	2.1
1	F	190	PRO	2.1
1	E	128	THR	2.1
1	E	138	CYS	2.1
1	B	70	TYR	2.1
1	C	132	SER	2.1
1	F	186	TYR	2.1
1	D	205	ARG	2.1
1	J	72	ASN	2.1
1	H	2	ALA	2.1
1	C	129	GLY	2.1
1	H	189	CYS	2.1
1	I	62	SER	2.1
1	J	2	ALA	2.0
1	D	62	SER	2.0
1	C	159	ASP	2.0
1	G	24	ASP	2.0
1	D	134	GLU	2.0
1	A	135	GLY	2.0
1	H	14	ARG	2.0
1	E	90	ALA	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](#)

There are no carbohydrates in this entry.

## 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. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	7A9	H	301	22/22	0.83	0.17	-0.06	51,60,69,72	0
3	7A9	E	302	22/22	0.86	0.16	-0.26	33,47,52,57	0
3	7A9	G	302	22/22	0.86	0.18	-0.35	46,57,61,66	0
3	7A9	J	302	22/22	0.86	0.17	-0.39	47,58,78,88	0
2	NAG	I	301	14/15	0.74	0.18	-0.72	52,58,69,80	0
3	7A9	C	302	22/22	0.93	0.14	-0.77	30,41,52,53	0
3	7A9	D	302	22/22	0.88	0.16	-1.07	26,39,48,50	0
3	7A9	B	301	22/22	0.86	0.18	-1.14	52,65,81,85	0
2	NAG	D	301	14/15	0.67	0.29	-	66,95,114,127	0
2	NAG	C	301	14/15	0.42	0.55	-	74,128,148,158	0
2	NAG	G	301	14/15	0.49	0.48	-	84,122,135,135	0
2	NAG	F	301	14/15	0.81	0.23	-	46,61,68,85	0
2	NAG	E	301	14/15	0.61	0.48	-	65,94,104,106	0
2	NAG	J	301	14/15	0.60	0.59	-	91,132,161,163	0
2	NAG	A	301	14/15	0.69	0.45	-	73,112,132,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.