



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2016 – 12:05 PM GMT

PDB ID : 4UM3  
Title : Engineered Ls-AChBP with alpha4-alpha4 interface in complex with NS3920  
Authors : Shahsavar, A.; Kastrup, J.S.; Balle, T.; Gajhede, M.  
Deposited on : 2014-05-14  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

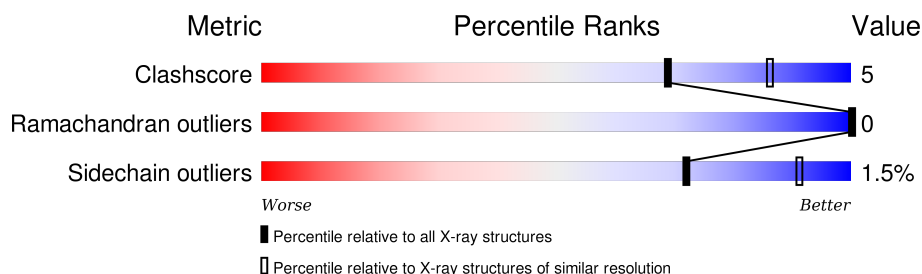
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	229	 71% 15% • 12%
1	B	229	 72% 14% 14%
1	C	229	 74% 14% 12%
1	D	229	 71% 16% 12%
1	E	229	 71% 14% 15%
1	F	229	 72% 14% 14%
1	G	229	 72% 15% 13%

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Mol	Chain	Length	Quality of chain
1	H	229	
1	I	229	
1	J	229	
1	K	229	
1	L	229	
1	M	229	
1	N	229	
1	O	229	
1	Q	229	
1	R	229	
1	T	229	
1	U	229	
1	V	229	
1	W	229	
1	X	229	
1	Y	229	
1	Z	229	
1	a	229	
1	b	229	
1	c	229	
1	d	229	
1	e	229	
1	f	229	
1	g	229	
1	h	229	

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Mol	Chain	Length	Quality of chain
1	i	229	 86% 14%
1	j	229	 85% 14%
1	k	229	 85% 14%
1	l	229	 85% 13%
1	m	229	 86% 12%
1	n	229	 83% 14%
2	P	228	 78% 10% 12%
3	S	229	 78% 10% 12%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 64774 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 ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	2	0
			1619	1015	280	320	4			
1	B	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	C	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			
1	D	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			
1	E	195	Total	C	N	O	S	0	1	0
			1560	983	265	308	4			
1	F	196	Total	C	N	O	S	0	1	0
			1572	989	270	309	4			
1	G	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	H	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	I	200	Total	C	N	O	S	0	1	0
			1603	1005	274	320	4			
1	J	200	Total	C	N	O	S	0	1	0
			1605	1006	277	318	4			
1	K	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	L	195	Total	C	N	O	S	0	1	0
			1565	985	268	308	4			
1	M	198	Total	C	N	O	S	0	1	0
			1590	998	272	316	4			
1	N	196	Total	C	N	O	S	0	1	0
			1564	984	264	312	4			
1	O	196	Total	C	N	O	S	0	0	0
			1563	983	264	312	4			
1	Q	196	Total	C	N	O	S	0	2	0
			1574	991	269	310	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	T	194	Total	C	N	O	S	0	0	0
			1552	978	265	305	4			
1	U	197	Total	C	N	O	S	0	0	0
			1575	990	271	310	4			
1	V	199	Total	C	N	O	S	0	0	0
			1589	997	273	315	4			
1	W	197	Total	C	N	O	S	0	0	0
			1570	987	268	311	4			
1	X	202	Total	C	N	O	S	0	0	0
			1611	1008	276	323	4			
1	Y	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	Z	196	Total	C	N	O	S	0	0	0
			1564	984	267	309	4			
1	a	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	b	198	Total	C	N	O	S	0	1	0
			1590	999	274	313	4			
1	c	200	Total	C	N	O	S	0	2	0
			1604	1005	273	322	4			
1	d	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	e	198	Total	C	N	O	S	0	0	0
			1583	994	272	313	4			
1	f	195	Total	C	N	O	S	0	0	0
			1560	982	266	308	4			
1	g	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	h	199	Total	C	N	O	S	0	1	0
			1596	1001	273	318	4			
1	i	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	j	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	k	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	l	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	m	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	196	Total	C	N	O	S	0	0	0
			1559	981	264	310	4			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
A	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
A	114	THR	MET	ENGINEERED MUTATION	UNP P58154
B	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
B	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
B	114	THR	MET	ENGINEERED MUTATION	UNP P58154
C	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
C	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
C	114	THR	MET	ENGINEERED MUTATION	UNP P58154
D	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
D	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
D	114	THR	MET	ENGINEERED MUTATION	UNP P58154
E	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
E	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
E	114	THR	MET	ENGINEERED MUTATION	UNP P58154
F	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
F	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
F	114	THR	MET	ENGINEERED MUTATION	UNP P58154
G	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
G	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
G	114	THR	MET	ENGINEERED MUTATION	UNP P58154
H	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
H	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
H	114	THR	MET	ENGINEERED MUTATION	UNP P58154
I	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
I	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
I	114	THR	MET	ENGINEERED MUTATION	UNP P58154
J	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
J	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
J	114	THR	MET	ENGINEERED MUTATION	UNP P58154
K	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
K	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
K	114	THR	MET	ENGINEERED MUTATION	UNP P58154
L	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
L	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
L	114	THR	MET	ENGINEERED MUTATION	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
M	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
M	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
M	114	THR	MET	ENGINEERED MUTATION	UNP P58154
N	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
N	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
N	114	THR	MET	ENGINEERED MUTATION	UNP P58154
O	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
O	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
O	114	THR	MET	ENGINEERED MUTATION	UNP P58154
Q	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
Q	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
Q	114	THR	MET	ENGINEERED MUTATION	UNP P58154
R	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
R	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
R	114	THR	MET	ENGINEERED MUTATION	UNP P58154
T	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
T	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
T	114	THR	MET	ENGINEERED MUTATION	UNP P58154
U	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
U	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
U	114	THR	MET	ENGINEERED MUTATION	UNP P58154
V	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
V	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
V	114	THR	MET	ENGINEERED MUTATION	UNP P58154
W	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
W	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
W	114	THR	MET	ENGINEERED MUTATION	UNP P58154
X	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
X	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
X	114	THR	MET	ENGINEERED MUTATION	UNP P58154
Y	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
Y	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
Y	114	THR	MET	ENGINEERED MUTATION	UNP P58154
Z	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
Z	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
Z	114	THR	MET	ENGINEERED MUTATION	UNP P58154
a	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
a	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
a	114	THR	MET	ENGINEERED MUTATION	UNP P58154
b	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
b	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
b	114	THR	MET	ENGINEERED MUTATION	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
c	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
c	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
c	114	THR	MET	ENGINEERED MUTATION	UNP P58154
d	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
d	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
d	114	THR	MET	ENGINEERED MUTATION	UNP P58154
e	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
e	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
e	114	THR	MET	ENGINEERED MUTATION	UNP P58154
f	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
f	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
f	114	THR	MET	ENGINEERED MUTATION	UNP P58154
g	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
g	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
g	114	THR	MET	ENGINEERED MUTATION	UNP P58154
h	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
h	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
h	114	THR	MET	ENGINEERED MUTATION	UNP P58154
i	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
i	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
i	114	THR	MET	ENGINEERED MUTATION	UNP P58154
j	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
j	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
j	114	THR	MET	ENGINEERED MUTATION	UNP P58154
k	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
k	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
k	114	THR	MET	ENGINEERED MUTATION	UNP P58154
l	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
l	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
l	114	THR	MET	ENGINEERED MUTATION	UNP P58154
m	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
m	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
m	114	THR	MET	ENGINEERED MUTATION	UNP P58154
n	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
n	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
n	114	THR	MET	ENGINEERED MUTATION	UNP P58154

- Molecule 2 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
P	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
P	114	THR	MET	ENGINEERED MUTATION	UNP P58154
P	.	-	ASP	DELETION	UNP P58154

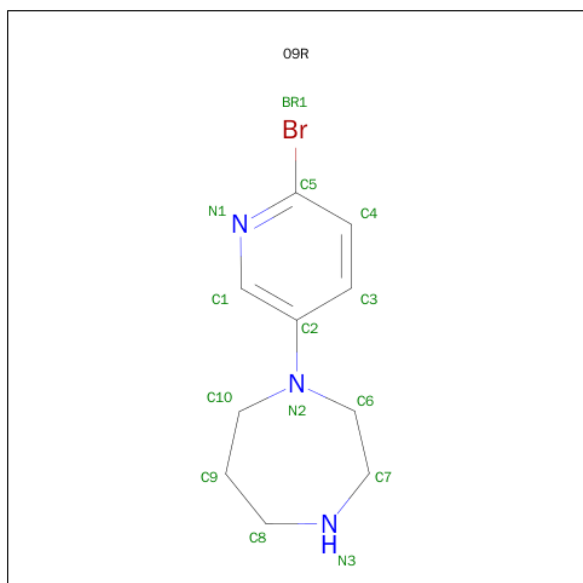
- Molecule 3 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	201	Total	C	N	O	S	0	0	0
			1603	1004	276	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	104	HIS	ARG	ENGINEERED MUTATION	UNP P58154
S	112	GLN	LEU	ENGINEERED MUTATION	UNP P58154
S	114	THR	MET	ENGINEERED MUTATION	UNP P58154
S	131	GLN	GLU	CONFLICT	UNP P58154

- Molecule 4 is 1-(6-BROMOPYRIDIN-3-YL)-1,4-DIAZEPANE (three-letter code: 09R) (formula: C<sub>10</sub>H<sub>14</sub>BrN<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	N	0	0
			14	1	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 14	Br 1	C 10	N 3	0	0
4	C	1	Total 14	Br 1	C 10	N 3	0	0
4	D	1	Total 14	Br 1	C 10	N 3	0	0
4	E	1	Total 14	Br 1	C 10	N 3	0	0
4	F	1	Total 14	Br 1	C 10	N 3	0	0
4	G	1	Total 14	Br 1	C 10	N 3	0	0
4	H	1	Total 14	Br 1	C 10	N 3	0	0
4	I	1	Total 14	Br 1	C 10	N 3	0	0
4	J	1	Total 14	Br 1	C 10	N 3	0	0
4	K	1	Total 14	Br 1	C 10	N 3	0	0
4	L	1	Total 14	Br 1	C 10	N 3	0	0
4	M	1	Total 14	Br 1	C 10	N 3	0	0
4	N	1	Total 14	Br 1	C 10	N 3	0	0
4	O	1	Total 14	Br 1	C 10	N 3	0	0
4	P	1	Total 14	Br 1	C 10	N 3	0	0
4	Q	1	Total 14	Br 1	C 10	N 3	0	0
4	R	1	Total 14	Br 1	C 10	N 3	0	0
4	S	1	Total 14	Br 1	C 10	N 3	0	0
4	T	1	Total 14	Br 1	C 10	N 3	0	0
4	U	1	Total 14	Br 1	C 10	N 3	0	0
4	V	1	Total 14	Br 1	C 10	N 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	W	1	Total	Br	C	N	0	0
			14	1	10	3		
4	X	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Y	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Z	1	Total	Br	C	N	0	0
			14	1	10	3		
4	a	1	Total	Br	C	N	0	0
			14	1	10	3		
4	b	1	Total	Br	C	N	0	0
			14	1	10	3		
4	c	1	Total	Br	C	N	0	0
			14	1	10	3		
4	d	1	Total	Br	C	N	0	0
			14	1	10	3		
4	e	1	Total	Br	C	N	0	0
			14	1	10	3		
4	f	1	Total	Br	C	N	0	0
			14	1	10	3		
4	g	1	Total	Br	C	N	0	0
			14	1	10	3		
4	h	1	Total	Br	C	N	0	0
			14	1	10	3		
4	i	1	Total	Br	C	N	0	0
			14	1	10	3		
4	j	1	Total	Br	C	N	0	0
			14	1	10	3		
4	k	1	Total	Br	C	N	0	0
			14	1	10	3		
4	l	1	Total	Br	C	N	0	0
			14	1	10	3		
4	m	1	Total	Br	C	N	0	0
			14	1	10	3		
4	n	1	Total	Br	C	N	0	0
			14	1	10	3		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	33	Total O 33 33	0	0
7	C	25	Total O 25 25	0	0
7	D	22	Total O 22 22	0	0
7	E	24	Total O 24 24	0	0
7	F	35	Total O 35 35	0	0
7	G	25	Total O 25 25	0	0
7	H	22	Total O 22 22	0	0
7	I	30	Total O 30 30	0	0
7	J	32	Total O 32 32	0	0
7	K	32	Total O 32 32	0	0
7	L	24	Total O 24 24	0	0
7	M	17	Total O 17 17	0	0
7	N	23	Total O 23 23	0	0
7	O	26	Total O 26 26	0	0
7	P	45	Total O 45 45	0	0
7	Q	38	Total O 38 38	0	0
7	R	30	Total O 30 30	0	0
7	S	27	Total O 27 27	0	0
7	T	24	Total O 24 24	0	0
7	U	40	Total O 40 40	0	0

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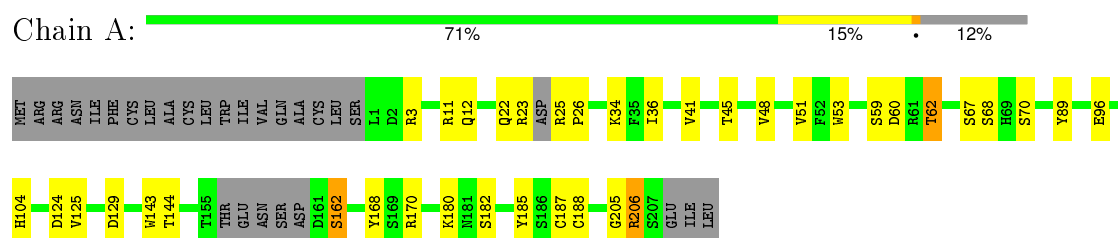
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	39	Total 39	O 39	0	0
7	W	27	Total 27	O 27	0	0
7	X	26	Total 26	O 26	0	0
7	Y	13	Total 13	O 13	0	0
7	Z	29	Total 29	O 29	0	0
7	a	14	Total 14	O 14	0	0
7	b	9	Total 9	O 9	0	0
7	c	5	Total 5	O 5	0	0
7	d	15	Total 15	O 15	0	0
7	e	3	Total 3	O 3	0	0
7	f	2	Total 2	O 2	0	0
7	g	1	Total 1	O 1	0	0
7	h	6	Total 6	O 6	0	0
7	i	3	Total 3	O 3	0	0
7	j	6	Total 6	O 6	0	0
7	k	6	Total 6	O 6	0	0
7	l	5	Total 5	O 5	0	0
7	m	2	Total 2	O 2	0	0
7	n	4	Total 4	O 4	0	0

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

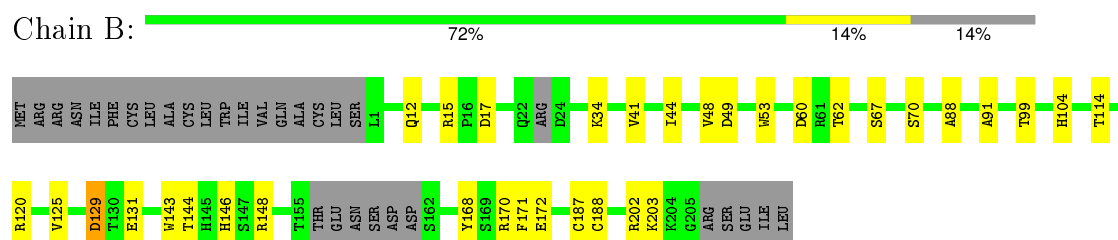
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

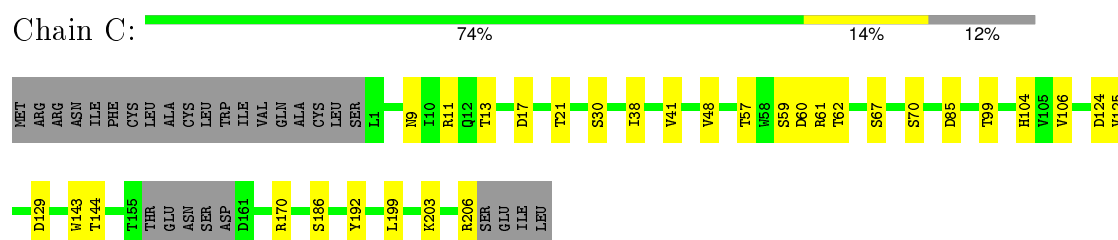
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



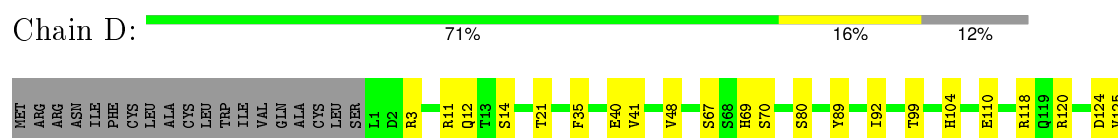
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN

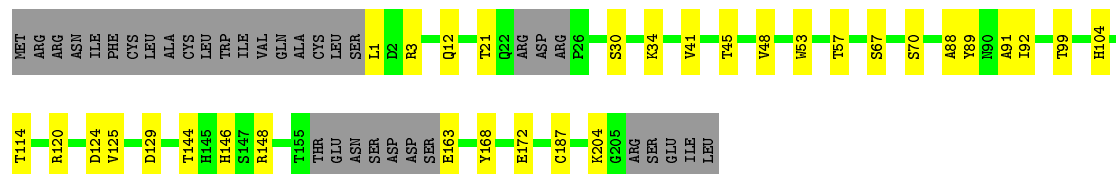






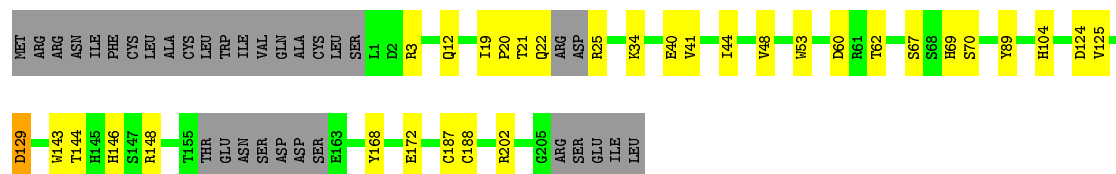
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain E: 71% 14% 15%



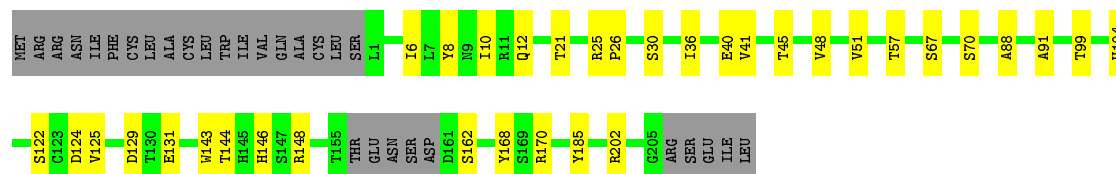
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain F: 72% 14% 14%



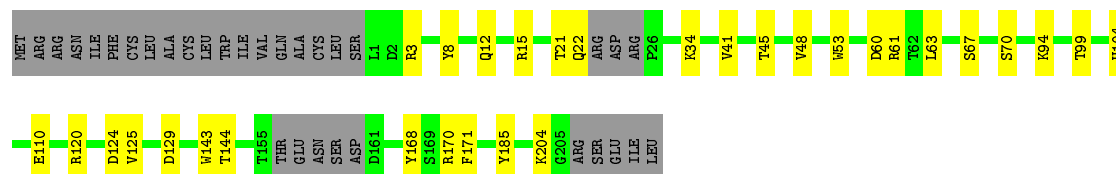
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain G: 72% 15% 13%



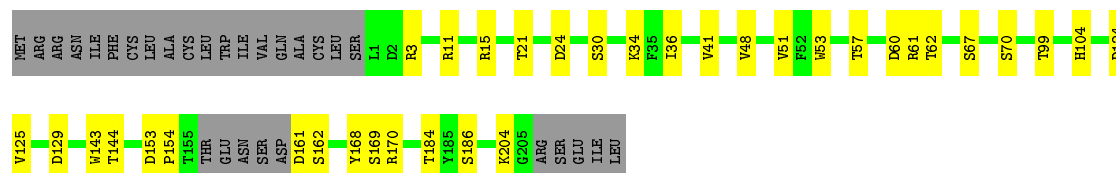
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain H: 72% 14% 14%

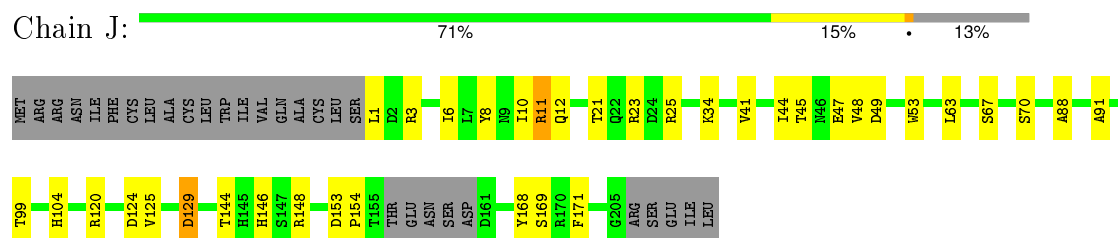


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

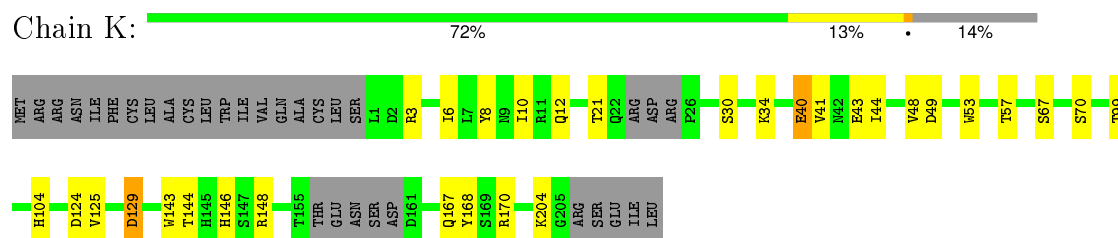
Chain I: 72% 15% 13%



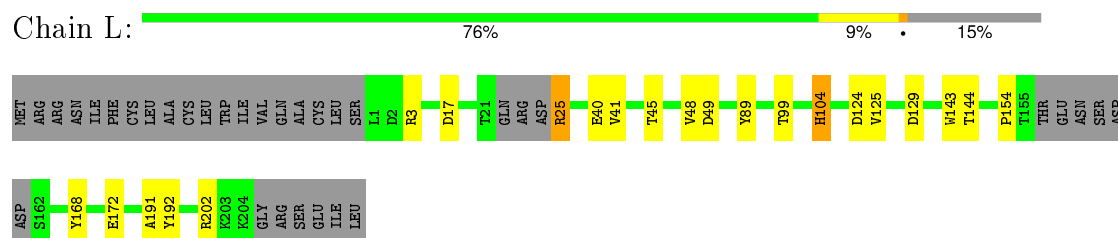
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



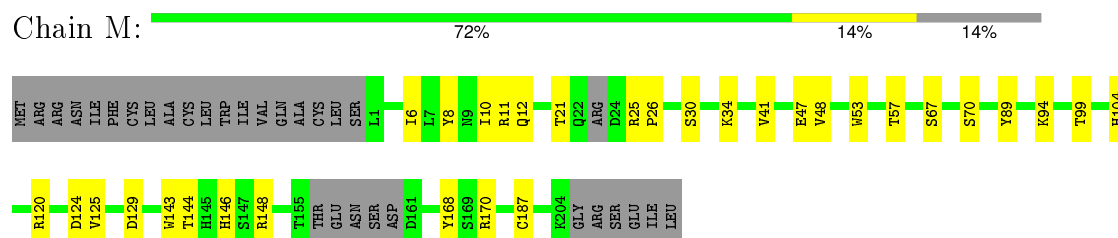
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



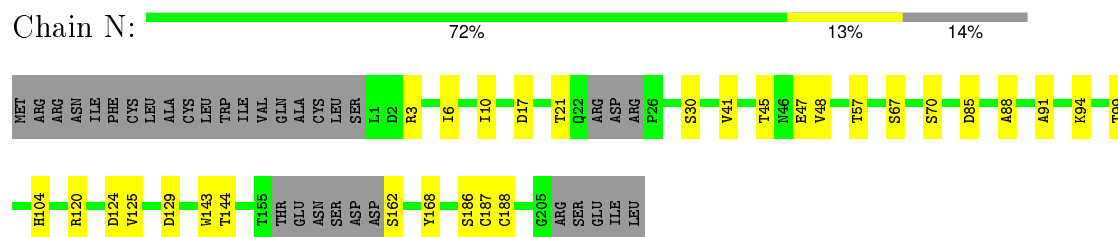
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



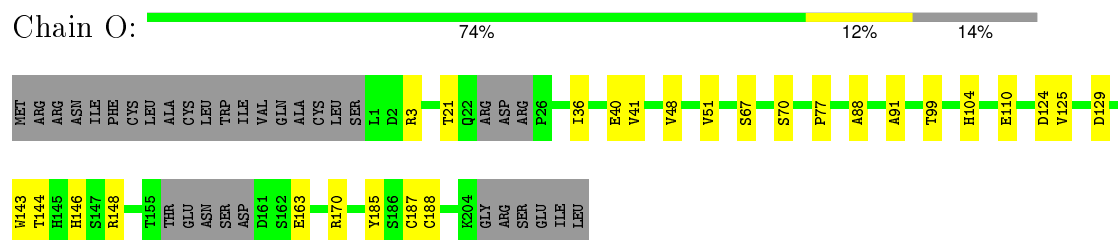
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



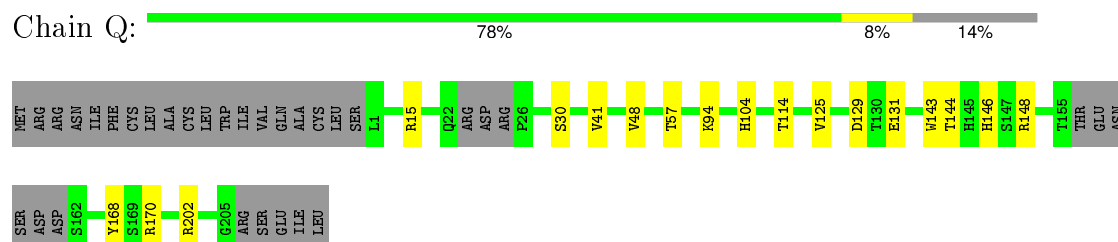
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



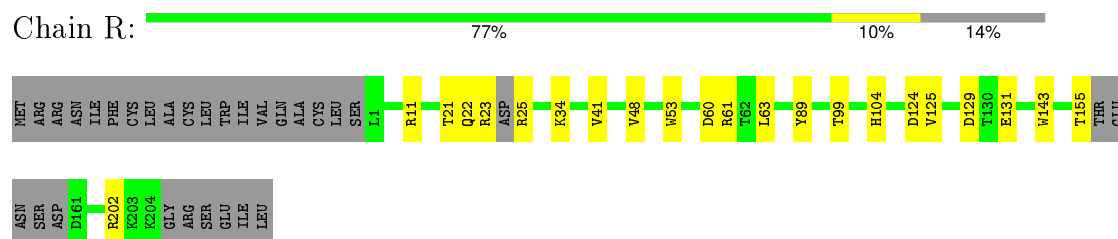
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



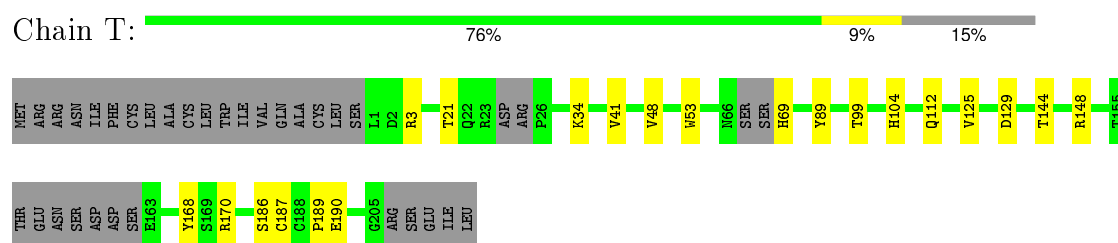
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



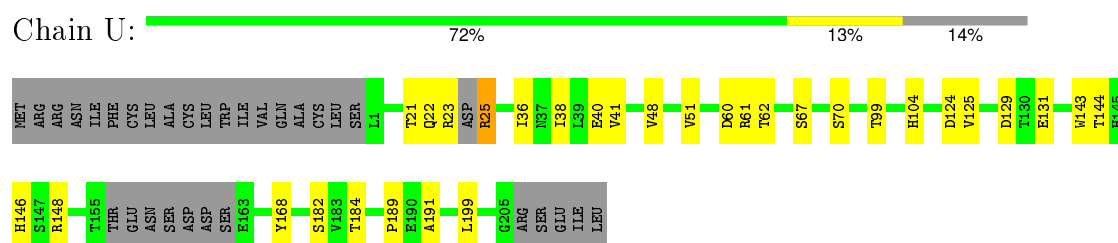
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



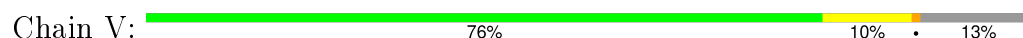
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

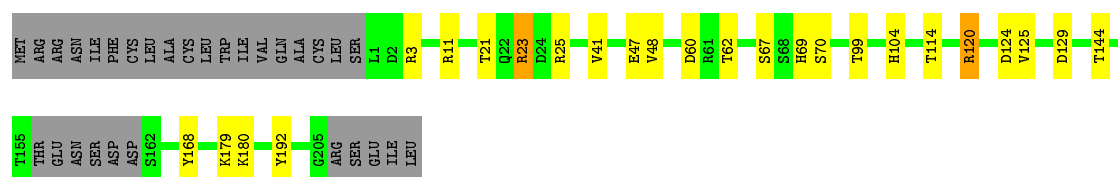


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



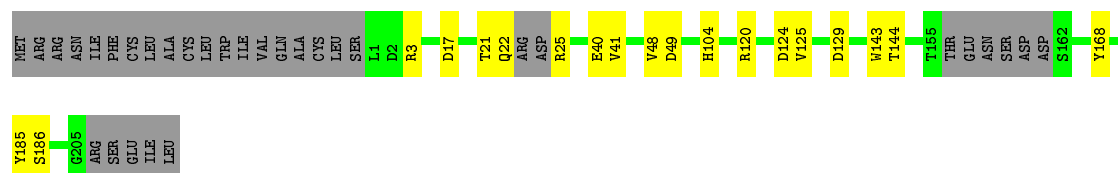
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN





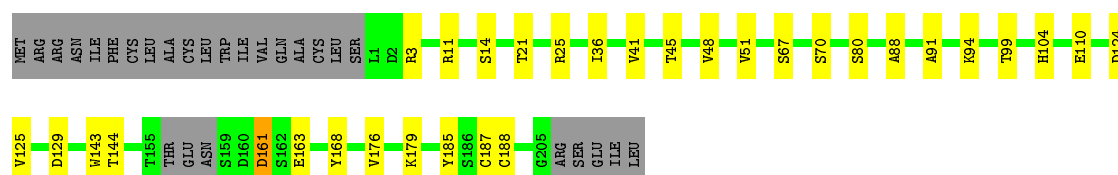
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain W: 78% 8% 14%



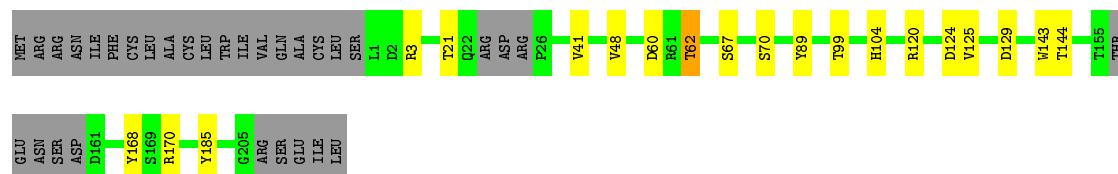
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain X: 74% 14% 12%



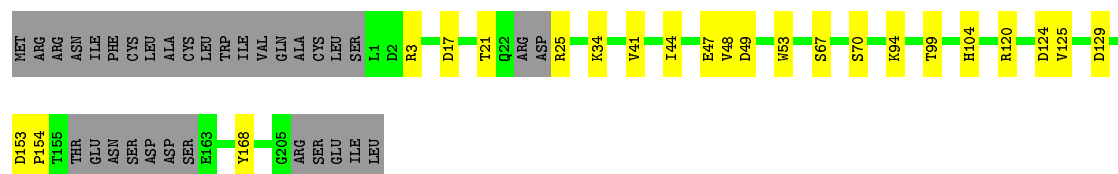
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Y: 77% 8% 14%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Z: 76% 10% 14%


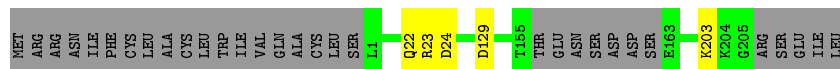


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

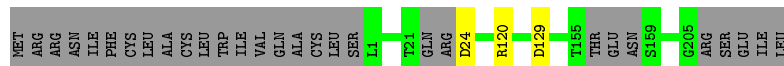
Chain a: 86% 14%




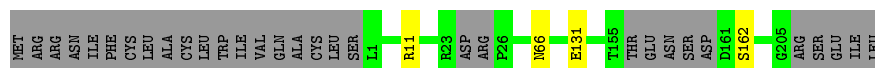
## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain b:  84% 14%


## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain c:  86% 13%


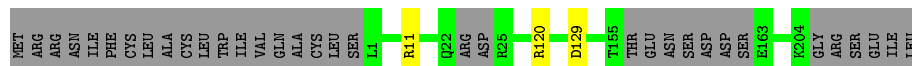
## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain d:  85% 14%


## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain e:  84% 14%


## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain f:  84% 15%


## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain g:  86% 14%

## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

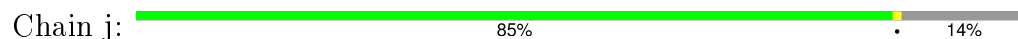
Chain h:  86% 13%

## ● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

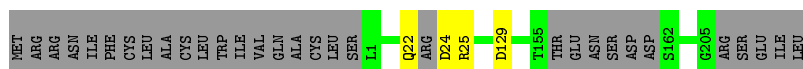
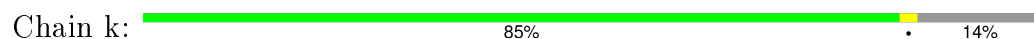
Chain i:  86% 14%



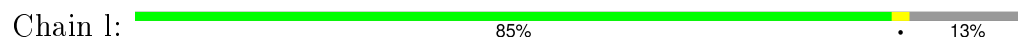
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



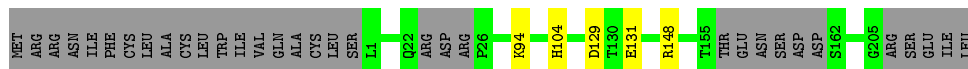
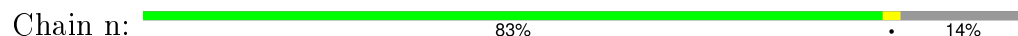
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



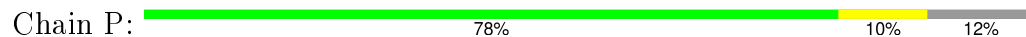
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

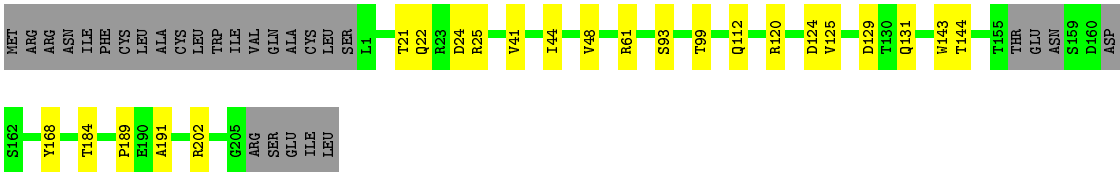


• Molecule 2: ACETYLCHOLINE BINDING PROTEIN



• Molecule 3: ACETYLCHOLINE BINDING PROTEIN





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.49Å 145.42Å 234.91Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	30.07 – 2.70	Depositor
% Data completeness (in resolution range)	99.5 (30.07-2.70)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.198 , 0.244	Depositor
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.622	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	3 of 242674 reflections (0.001%)	Xtriage
Total number of atoms	64774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 09R, NAG, SO4

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	0.68	0/1661	0.64	0/2264
1	B	0.55	0/1613	0.58	0/2201
1	C	0.56	0/1644	0.67	2/2243 (0.1%)
1	D	0.60	0/1640	0.61	0/2237
1	E	0.59	0/1599	0.60	0/2182
1	F	0.63	0/1610	0.62	0/2196
1	G	0.56	0/1633	0.59	0/2229
1	H	0.53	0/1602	0.57	0/2186
1	I	0.61	0/1642	0.62	0/2241
1	J	0.55	0/1644	0.61	0/2243
1	K	0.47	0/1613	0.55	0/2200
1	L	0.50	0/1603	0.58	1/2187 (0.0%)
1	M	0.47	0/1628	0.54	0/2221
1	N	0.53	0/1602	0.59	1/2187 (0.0%)
1	O	0.58	0/1598	0.58	0/2181
1	Q	0.51	0/1616	0.57	0/2204
1	R	0.57	0/1620	0.62	0/2210
1	T	0.59	0/1586	0.60	0/2162
1	U	0.65	0/1610	0.61	0/2196
1	V	0.61	0/1625	0.61	0/2218
1	W	0.54	0/1605	0.59	0/2190
1	X	0.56	0/1647	0.57	0/2248
1	Y	0.51	0/1602	0.58	0/2186
1	Z	0.52	0/1599	0.56	0/2182
1	a	0.53	0/1613	0.56	0/2201
1	b	0.55	0/1630	0.59	0/2225
1	c	0.50	0/1645	0.56	0/2245
1	d	0.52	0/1613	0.58	0/2200
1	e	0.49	0/1619	0.56	0/2210
1	f	0.46	0/1595	0.57	0/2177
1	g	0.50	0/1621	0.54	0/2213
1	h	0.47	0/1634	0.55	0/2229

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	i	0.51	0/1602	0.57	0/2186
1	j	0.46	0/1621	0.53	0/2213
1	k	0.45	0/1613	0.54	0/2201
1	l	0.47	0/1633	0.57	0/2229
1	m	0.43	0/1640	0.53	0/2237
1	n	0.45	0/1594	0.54	0/2175
2	P	0.63	0/1644	0.63	0/2243
3	S	0.60	0/1638	0.57	0/2234
All	All	0.54	0/64797	0.58	4/88412 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	ASP	CB-CG-OD2	-9.30	109.93	118.30
1	C	85	ASP	CB-CG-OD1	7.45	125.00	118.30
1	L	25	ARG	C-N-CD	5.93	140.85	128.40
1	N	85	ASP	CB-CG-OD2	5.29	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1619	0	1565	43	0
1	B	1578	0	1523	30	0
1	C	1608	0	1554	32	0
1	D	1605	0	1544	49	2
1	E	1560	0	1509	32	0
1	F	1572	0	1527	36	0
1	G	1597	0	1541	27	0
1	H	1567	0	1511	38	0
1	I	1603	0	1547	26	1
1	J	1605	0	1554	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1575	0	1524	34	0
1	L	1565	0	1521	20	0
1	M	1590	0	1537	23	0
1	N	1564	0	1511	24	0
1	O	1563	0	1507	20	0
1	Q	1574	0	1527	19	0
1	R	1585	0	1533	22	0
1	T	1552	0	1504	24	0
1	U	1575	0	1527	27	0
1	V	1589	0	1537	27	1
1	W	1570	0	1519	15	0
1	X	1611	0	1550	23	0
1	Y	1567	0	1511	15	0
1	Z	1564	0	1514	17	0
1	a	1575	0	1523	0	0
1	b	1590	0	1539	0	0
1	c	1604	0	1545	0	0
1	d	1578	0	1522	0	1
1	e	1583	0	1532	0	0
1	f	1560	0	1511	0	0
1	g	1585	0	1534	0	0
1	h	1596	0	1542	0	0
1	i	1567	0	1511	0	0
1	j	1585	0	1536	0	0
1	k	1578	0	1523	0	1
1	l	1597	0	1541	0	0
1	m	1605	0	1544	0	0
1	n	1559	0	1507	0	0
2	P	1608	0	1554	19	0
3	S	1603	0	1547	18	0
4	A	14	0	14	3	0
4	B	14	0	14	3	0
4	C	14	0	14	3	0
4	D	14	0	14	4	0
4	E	14	0	14	2	0
4	F	14	0	14	2	0
4	G	14	0	14	3	0
4	H	14	0	14	2	0
4	I	14	0	14	0	0
4	J	14	0	14	2	0
4	K	14	0	14	0	0
4	L	14	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	14	0	14	2	0
4	N	14	0	14	1	0
4	O	14	0	14	2	0
4	P	14	0	14	5	0
4	Q	14	0	14	0	0
4	R	14	0	14	2	0
4	S	14	0	14	3	0
4	T	14	0	14	2	0
4	U	14	0	14	2	0
4	V	14	0	14	1	0
4	W	14	0	14	2	0
4	X	14	0	14	3	0
4	Y	14	0	14	2	0
4	Z	14	0	14	1	0
4	a	14	0	14	0	0
4	b	14	0	14	0	0
4	c	14	0	14	0	0
4	d	14	0	14	0	0
4	e	14	0	14	0	0
4	f	14	0	14	0	0
4	g	14	0	14	0	0
4	h	14	0	14	0	0
4	i	14	0	14	0	0
4	j	14	0	14	0	0
4	k	14	0	14	0	0
4	l	14	0	14	0	0
4	m	14	0	14	0	0
4	n	14	0	14	0	0
5	A	14	0	13	0	0
5	O	14	0	13	0	0
5	d	14	0	13	0	0
6	R	5	0	0	0	0
7	A	47	0	0	2	0
7	B	33	0	0	0	0
7	C	25	0	0	0	0
7	D	22	0	0	1	0
7	E	24	0	0	0	0
7	F	35	0	0	1	0
7	G	25	0	0	0	0
7	H	22	0	0	0	0
7	I	30	0	0	0	0
7	J	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	32	0	0	0	0
7	L	24	0	0	1	0
7	M	17	0	0	0	0
7	N	23	0	0	1	0
7	O	26	0	0	0	0
7	P	45	0	0	1	0
7	Q	38	0	0	1	0
7	R	30	0	0	2	0
7	S	27	0	0	0	0
7	T	24	0	0	1	0
7	U	40	0	0	0	0
7	V	39	0	0	0	0
7	W	27	0	0	0	0
7	X	26	0	0	0	0
7	Y	13	0	0	1	0
7	Z	29	0	0	0	0
7	a	14	0	0	0	0
7	b	9	0	0	0	0
7	c	5	0	0	0	0
7	d	15	0	0	0	0
7	e	3	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	h	6	0	0	0	0
7	i	3	0	0	0	0
7	j	6	0	0	0	0
7	k	6	0	0	0	0
7	l	5	0	0	0	0
7	m	2	0	0	0	0
7	n	4	0	0	0	0
All	All	64774	0	61807	516	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 516 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:U:41:VAL:HG13	1:U:125:VAL:HG11	1.44	0.99
1:J:6:ILE:O	1:J:10:ILE:HG13	2.58	0.94
1:V:60:ASP:OD1	1:V:62:THR:HB	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:VAL:HG13	1:E:125:VAL:HG11	1.53	0.91
1:Y:60:ASP:OD1	1:Y:62:THR:HB	1.69	0.91

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:HIS:NE2	1:k:22:GLN:NE2[2_454]	1.66	0.54
1:D:184:THR:OG1	1:l:184:THR:OG1[2_454]	1.81	0.39
1:V:25:ARG:NH2	1:d:66:ASN:OD1[1_455]	2.19	0.01

## 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	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	B	192/229 (84%)	192 (100%)	0	0	100	100
1	C	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	D	195/229 (85%)	195 (100%)	0	0	100	100
1	E	190/229 (83%)	190 (100%)	0	0	100	100
1	F	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	G	196/229 (86%)	194 (99%)	2 (1%)	0	100	100
1	H	191/229 (83%)	188 (98%)	3 (2%)	0	100	100
1	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	J	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	K	192/229 (84%)	189 (98%)	3 (2%)	0	100	100
1	L	190/229 (83%)	189 (100%)	1 (0%)	0	100	100
1	M	193/229 (84%)	190 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	O	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	Q	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	R	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	T	186/229 (81%)	186 (100%)	0	0	100	100
1	U	191/229 (83%)	191 (100%)	0	0	100	100
1	V	195/229 (85%)	195 (100%)	0	0	100	100
1	W	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	X	198/229 (86%)	197 (100%)	1 (0%)	0	100	100
1	Y	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	Z	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	a	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	b	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	c	196/229 (86%)	193 (98%)	3 (2%)	0	100	100
1	d	192/229 (84%)	190 (99%)	2 (1%)	0	100	100
1	e	194/229 (85%)	193 (100%)	1 (0%)	0	100	100
1	f	189/229 (82%)	187 (99%)	2 (1%)	0	100	100
1	g	194/229 (85%)	193 (100%)	1 (0%)	0	100	100
1	h	194/229 (85%)	190 (98%)	4 (2%)	0	100	100
1	i	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	j	194/229 (85%)	192 (99%)	2 (1%)	0	100	100
1	k	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	l	196/229 (86%)	195 (100%)	1 (0%)	0	100	100
1	m	195/229 (85%)	192 (98%)	3 (2%)	0	100	100
1	n	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
2	P	197/228 (86%)	194 (98%)	3 (2%)	0	100	100
3	S	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
All	All	7721/9159 (84%)	7657 (99%)	64 (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	189/213 (89%)	184 (97%)	5 (3%)	54	83
1	B	184/213 (86%)	183 (100%)	1 (0%)	92	98
1	C	187/213 (88%)	186 (100%)	1 (0%)	92	98
1	D	187/213 (88%)	184 (98%)	3 (2%)	70	91
1	E	182/213 (85%)	181 (100%)	1 (0%)	92	98
1	F	183/213 (86%)	180 (98%)	3 (2%)	70	91
1	G	186/213 (87%)	182 (98%)	4 (2%)	60	86
1	H	183/213 (86%)	180 (98%)	3 (2%)	70	91
1	I	187/213 (88%)	182 (97%)	5 (3%)	52	82
1	J	187/213 (88%)	185 (99%)	2 (1%)	80	94
1	K	184/213 (86%)	182 (99%)	2 (1%)	80	94
1	L	183/213 (86%)	181 (99%)	2 (1%)	80	94
1	M	186/213 (87%)	184 (99%)	2 (1%)	80	94
1	N	183/213 (86%)	182 (100%)	1 (0%)	92	98
1	O	183/213 (86%)	180 (98%)	3 (2%)	70	91
1	Q	184/213 (86%)	183 (100%)	1 (0%)	92	98
1	R	185/213 (87%)	184 (100%)	1 (0%)	92	98
1	T	180/213 (84%)	179 (99%)	1 (1%)	90	97
1	U	183/213 (86%)	179 (98%)	4 (2%)	60	86
1	V	185/213 (87%)	182 (98%)	3 (2%)	70	91
1	W	183/213 (86%)	180 (98%)	3 (2%)	70	91
1	X	188/213 (88%)	183 (97%)	5 (3%)	52	82
1	Y	183/213 (86%)	180 (98%)	3 (2%)	70	91
1	Z	182/213 (85%)	180 (99%)	2 (1%)	80	94
1	a	184/213 (86%)	183 (100%)	1 (0%)	92	98
1	b	185/213 (87%)	180 (97%)	5 (3%)	52	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	188/213 (88%)	184 (98%)	4 (2%)	61	87
1	d	184/213 (86%)	181 (98%)	3 (2%)	70	91
1	e	184/213 (86%)	178 (97%)	6 (3%)	45	76
1	f	182/213 (85%)	179 (98%)	3 (2%)	70	91
1	g	185/213 (87%)	183 (99%)	2 (1%)	80	94
1	h	187/213 (88%)	186 (100%)	1 (0%)	92	98
1	i	183/213 (86%)	182 (100%)	1 (0%)	92	98
1	j	185/213 (87%)	182 (98%)	3 (2%)	70	91
1	k	184/213 (86%)	181 (98%)	3 (2%)	70	91
1	l	186/213 (87%)	181 (97%)	5 (3%)	52	82
1	m	187/213 (88%)	183 (98%)	4 (2%)	61	87
1	n	182/213 (85%)	177 (97%)	5 (3%)	52	82
2	P	187/212 (88%)	182 (97%)	5 (3%)	52	82
3	S	187/213 (88%)	184 (98%)	3 (2%)	70	91
All	All	7387/8519 (87%)	7272 (98%)	115 (2%)	72	91

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	129	ASP
1	Y	62	THR
1	m	25	ARG
1	V	23	ARG
1	W	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	104	HIS
1	T	104	HIS
1	j	104	HIS
1	R	22	GLN
3	S	104	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

44 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$
5	NAG	A	1207	1	14,14,15	0.68	0	15,19,21	3.41	9 (60%)
4	09R	A	311	-	13,15,15	3.66	4 (30%)	11,19,19	2.35	3 (27%)
4	09R	B	211	-	13,15,15	3.98	4 (30%)	11,19,19	1.82	4 (36%)
4	09R	C	711	-	13,15,15	4.04	4 (30%)	11,19,19	1.47	2 (18%)
4	09R	D	712	-	13,15,15	3.64	4 (30%)	11,19,19	2.39	4 (36%)
4	09R	E	713	-	13,15,15	4.04	4 (30%)	11,19,19	2.17	5 (45%)
4	09R	F	714	-	13,15,15	4.09	4 (30%)	11,19,19	1.90	3 (27%)
4	09R	G	715	-	13,15,15	3.44	4 (30%)	11,19,19	2.65	3 (27%)
4	09R	H	716	-	13,15,15	3.79	4 (30%)	11,19,19	2.70	4 (36%)
4	09R	I	717	-	13,15,15	4.57	3 (23%)	11,19,19	3.02	5 (45%)
4	09R	J	718	-	13,15,15	4.08	4 (30%)	11,19,19	2.08	4 (36%)
4	09R	K	719	-	13,15,15	4.03	4 (30%)	11,19,19	1.98	4 (36%)
4	09R	L	720	-	13,15,15	3.79	4 (30%)	11,19,19	3.17	4 (36%)
4	09R	M	721	-	13,15,15	3.96	4 (30%)	11,19,19	2.03	4 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	09R	N	722	-	13,15,15	4.32	4 (30%)	11,19,19	1.75	2 (18%)
5	NAG	O	1207	1	14,14,15	1.48	2 (14%)	15,19,21	3.42	7 (46%)
4	09R	O	723	-	13,15,15	3.79	3 (23%)	11,19,19	1.90	3 (27%)
4	09R	P	724	-	13,15,15	3.95	4 (30%)	11,19,19	2.17	4 (36%)
4	09R	Q	625	-	13,15,15	4.14	5 (38%)	11,19,19	1.05	1 (9%)
6	SO4	R	1205	-	4,4,4	0.12	0	6,6,6	0.33	0
4	09R	R	726	-	13,15,15	4.03	3 (23%)	11,19,19	1.26	2 (18%)
4	09R	S	311	-	13,15,15	3.97	4 (30%)	11,19,19	1.93	3 (27%)
4	09R	T	311	-	13,15,15	4.13	4 (30%)	11,19,19	1.42	3 (27%)
4	09R	U	211	-	13,15,15	3.96	4 (30%)	11,19,19	2.01	3 (27%)
4	09R	V	311	-	13,15,15	4.14	4 (30%)	11,19,19	2.03	3 (27%)
4	09R	W	311	-	13,15,15	3.85	4 (30%)	11,19,19	2.77	4 (36%)
4	09R	X	311	-	13,15,15	3.91	3 (23%)	11,19,19	2.77	4 (36%)
4	09R	Y	311	-	13,15,15	3.81	4 (30%)	11,19,19	2.79	4 (36%)
4	09R	Z	311	-	13,15,15	3.93	4 (30%)	11,19,19	1.86	2 (18%)
4	09R	a	311	-	13,15,15	3.86	4 (30%)	11,19,19	2.93	4 (36%)
4	09R	b	311	-	13,15,15	3.77	5 (38%)	11,19,19	2.78	4 (36%)
4	09R	c	211	-	13,15,15	3.99	4 (30%)	11,19,19	2.11	4 (36%)
5	NAG	d	1207	1	14,14,15	0.68	0	15,19,21	3.41	9 (60%)
4	09R	d	311	-	13,15,15	4.25	4 (30%)	11,19,19	2.60	6 (54%)
4	09R	e	311	-	13,15,15	3.70	3 (23%)	11,19,19	3.55	6 (54%)
4	09R	f	311	-	13,15,15	4.16	5 (38%)	11,19,19	2.17	4 (36%)
4	09R	g	311	-	13,15,15	3.98	4 (30%)	11,19,19	1.90	3 (27%)
4	09R	h	311	-	13,15,15	3.89	3 (23%)	11,19,19	2.60	4 (36%)
4	09R	i	311	-	13,15,15	4.21	4 (30%)	11,19,19	1.97	4 (36%)
4	09R	j	311	-	13,15,15	4.11	3 (23%)	11,19,19	2.42	4 (36%)
4	09R	k	311	-	13,15,15	3.99	4 (30%)	11,19,19	2.65	4 (36%)
4	09R	l	211	-	13,15,15	3.97	4 (30%)	11,19,19	2.53	4 (36%)
4	09R	m	311	-	13,15,15	4.44	3 (23%)	11,19,19	2.48	6 (54%)
4	09R	n	311	-	13,15,15	4.15	5 (38%)	11,19,19	2.37	4 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
4	09R	A	311	-	-	0/4/13/13	0/1/2/2
4	09R	B	211	-	-	0/4/13/13	0/1/2/2
4	09R	C	711	-	-	0/4/13/13	0/1/2/2
4	09R	D	712	-	-	0/4/13/13	0/1/2/2
4	09R	E	713	-	-	0/4/13/13	0/1/2/2
4	09R	F	714	-	-	0/4/13/13	0/1/2/2
4	09R	G	715	-	-	0/4/13/13	0/1/2/2
4	09R	H	716	-	-	0/4/13/13	0/1/2/2
4	09R	I	717	-	-	0/4/13/13	0/1/2/2
4	09R	J	718	-	-	0/4/13/13	0/1/2/2
4	09R	K	719	-	-	0/4/13/13	0/1/2/2
4	09R	L	720	-	-	0/4/13/13	0/1/2/2
4	09R	M	721	-	-	0/4/13/13	0/1/2/2
4	09R	N	722	-	-	0/4/13/13	0/1/2/2
5	NAG	O	1207	1	-	0/6/23/26	0/1/1/1
4	09R	O	723	-	-	0/4/13/13	0/1/2/2
4	09R	P	724	-	-	0/4/13/13	0/1/2/2
4	09R	Q	625	-	-	0/4/13/13	0/1/2/2
6	SO4	R	1205	-	-	0/0/0/0	0/0/0/0
4	09R	R	726	-	-	0/4/13/13	0/1/2/2
4	09R	S	311	-	-	0/4/13/13	0/1/2/2
4	09R	T	311	-	-	0/4/13/13	0/1/2/2
4	09R	U	211	-	-	0/4/13/13	0/1/2/2
4	09R	V	311	-	-	0/4/13/13	0/1/2/2
4	09R	W	311	-	-	0/4/13/13	0/1/2/2
4	09R	X	311	-	-	0/4/13/13	0/1/2/2
4	09R	Y	311	-	-	0/4/13/13	0/1/2/2
4	09R	Z	311	-	-	0/4/13/13	0/1/2/2
4	09R	a	311	-	-	0/4/13/13	0/1/2/2
4	09R	b	311	-	-	0/4/13/13	0/1/2/2
4	09R	c	211	-	-	0/4/13/13	0/1/2/2
5	NAG	d	1207	1	-	0/6/23/26	0/1/1/1
4	09R	d	311	-	-	0/4/13/13	0/1/2/2
4	09R	e	311	-	-	0/4/13/13	0/1/2/2
4	09R	f	311	-	-	0/4/13/13	0/1/2/2
4	09R	g	311	-	-	0/4/13/13	0/1/2/2
4	09R	h	311	-	-	0/4/13/13	0/1/2/2
4	09R	i	311	-	-	0/4/13/13	0/1/2/2
4	09R	j	311	-	-	0/4/13/13	0/1/2/2
4	09R	k	311	-	-	0/4/13/13	0/1/2/2
4	09R	l	211	-	-	0/4/13/13	0/1/2/2
4	09R	m	311	-	-	0/4/13/13	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	09R	n	311	-	-	0/4/13/13	0/1/2/2

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	717	09R	BR1-C5	-15.70	1.71	1.91
4	m	311	09R	BR1-C5	-15.05	1.71	1.91
4	N	722	09R	BR1-C5	-14.34	1.72	1.91
4	d	311	09R	BR1-C5	-14.19	1.72	1.91
4	i	311	09R	BR1-C5	-14.12	1.73	1.91

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	715	09R	C4-C5-N1	-6.28	119.96	125.64
4	e	311	09R	C4-C5-N1	-6.11	120.11	125.64
4	I	717	09R	C4-C5-N1	-5.55	120.62	125.64
4	L	720	09R	C4-C5-N1	-5.30	120.85	125.64
4	A	311	09R	C4-C5-N1	-5.29	120.85	125.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	311	09R	3	0
4	B	211	09R	3	0
4	C	711	09R	3	0
4	D	712	09R	4	0
4	E	713	09R	2	0
4	F	714	09R	2	0
4	G	715	09R	3	0
4	H	716	09R	2	0
4	J	718	09R	2	0
4	L	720	09R	2	0
4	M	721	09R	2	0
4	N	722	09R	1	0
4	O	723	09R	2	0
4	P	724	09R	5	0
4	R	726	09R	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	311	09R	3	0
4	T	311	09R	2	0
4	U	211	09R	2	0
4	V	311	09R	1	0
4	W	311	09R	2	0
4	X	311	09R	3	0
4	Y	311	09R	2	0
4	Z	311	09R	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.