wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 09:49 AM EDT

PDB ID	:	3U8K
Title	:	Crystal structure of the acetylcholine binding protein (AChBP) from Lymnaea stagnalis in complex with NS3573 (1-(5-ethoxypyridin-3-yl)-1,4-diazepane)
Authors	:	Rohde, L.A.H.; Ahring, P.K.; Jensen, M.L.; Nielsen, E.O.; Peters, D.; Helgstrand, C.; Krintel, C.; Harpsoe, K.; Gajhede, M.; Kastrup, J.S.; Balle, T.
Deposited on	:	2011-10-17
Resolution	:	2.47 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

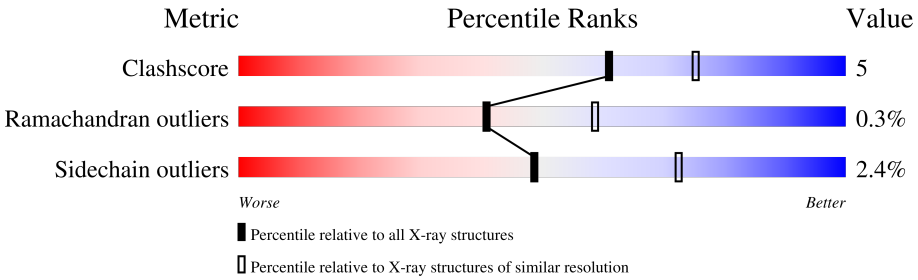
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	210	90% 9%
1	B	210	86% 9% 5%
1	C	210	85% 10% • •
1	D	210	84% 12% •
1	E	210	85% 10% • •
1	F	210	84% 12% •
1	G	210	87% 8% 5%
1	H	210	87% 10% ••

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Mol	Chain	Length	Quality of chain
1	I	210	85% 9% 6%
1	J	210	85% 11%
1	K	210	87% 9%
1	L	210	84% 10%
1	M	210	90% 8%
1	N	210	85% 10%
1	O	210	88% 7% 5%
1	P	210	88% 7% 5%
1	Q	210	83% 11% 6%
1	R	210	85% 10%
1	S	210	86% 8% 6%
1	T	210	85% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34188 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	209	Total	C	N	O	S	0	0	0
			1670	1043	287	335	5			
1	B	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			
1	C	203	Total	C	N	O	S	0	1	0
			1625	1018	277	324	6			
1	D	203	Total	C	N	O	S	0	2	0
			1630	1021	280	322	7			
1	E	201	Total	C	N	O	S	0	1	0
			1611	1010	275	320	6			
1	F	203	Total	C	N	O	S	0	0	0
			1624	1017	280	322	5			
1	G	200	Total	C	N	O	S	0	0	0
			1602	1005	274	318	5			
1	H	208	Total	C	N	O	S	0	0	0
			1662	1040	286	331	5			
1	I	198	Total	C	N	O	S	0	1	0
			1589	999	272	312	6			
1	J	204	Total	C	N	O	S	0	2	0
			1634	1023	278	326	7			
1	K	203	Total	C	N	O	S	0	2	0
			1629	1020	280	322	7			
1	L	201	Total	C	N	O	S	0	1	0
			1612	1011	275	320	6			
1	M	207	Total	C	N	O	S	0	2	0
			1661	1041	284	329	7			
1	N	203	Total	C	N	O	S	0	1	0
			1627	1021	280	320	6			
1	O	199	Total	C	N	O	S	0	0	0
			1590	999	273	313	5			
1	P	200	Total	C	N	O	S	0	2	0
			1604	1007	274	316	7			

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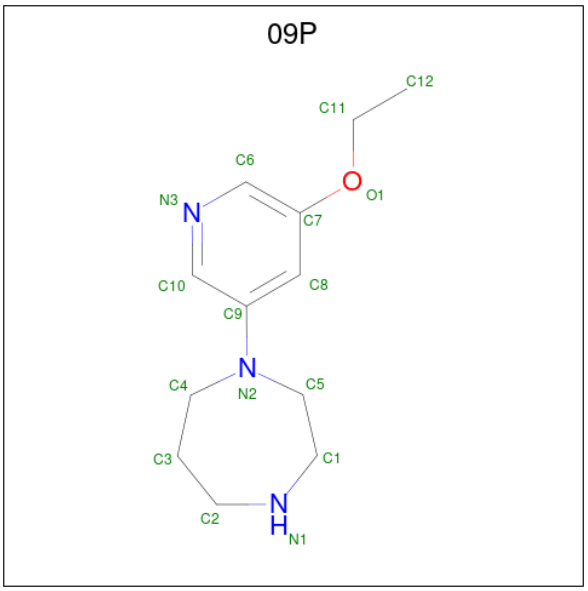
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	198	Total	C	N	O	S	0	2	0
			1585	997	269	312	7			
1	R	201	Total	C	N	O	S	0	2	0
			1612	1011	275	319	7			
1	S	198	Total	C	N	O	S	0	2	0
			1584	996	268	313	7			
1	T	204	Total	C	N	O	S	0	3	0
			1646	1030	284	325	7			

- Molecule 2 is 1-(5-ethoxypyridin-3-yl)-1,4-diazepane (three-letter code: 09P) (formula: $C_{12}H_{19}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	12	3	1		
2	B	1	Total	C	N	O	0	0
			16	12	3	1		
2	C	1	Total	C	N	O	0	0
			16	12	3	1		
2	D	1	Total	C	N	O	0	0
			16	12	3	1		
2	E	1	Total	C	N	O	0	0
			16	12	3	1		
2	F	1	Total	C	N	O	0	0
			16	12	3	1		
2	G	1	Total	C	N	O	0	0
			16	12	3	1		

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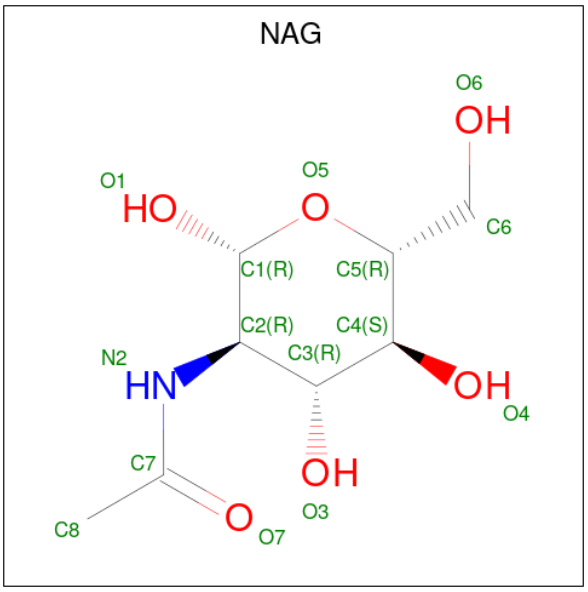
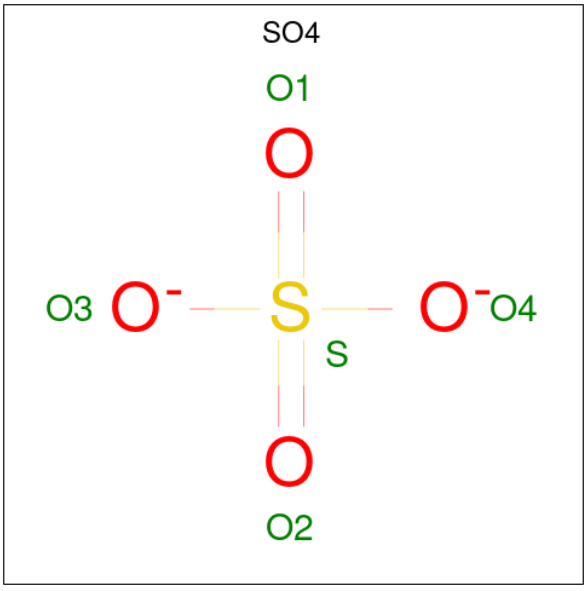
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			16	12	3	1		
2	I	1	Total	C	N	O	0	0
			16	12	3	1		
2	J	1	Total	C	N	O	0	0
			16	12	3	1		
2	K	1	Total	C	N	O	0	0
			16	12	3	1		
2	L	1	Total	C	N	O	0	0
			16	12	3	1		
2	M	1	Total	C	N	O	0	0
			16	12	3	1		
2	N	1	Total	C	N	O	0	0
			16	12	3	1		
2	O	1	Total	C	N	O	0	0
			16	12	3	1		
2	P	1	Total	C	N	O	0	0
			16	12	3	1		
2	Q	1	Total	C	N	O	0	0
			16	12	3	1		
2	R	1	Total	C	N	O	0	0
			16	12	3	1		
2	S	1	Total	C	N	O	0	0
			16	12	3	1		
2	T	1	Total	C	N	O	0	0
			16	12	3	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	P	1	Total O S 5 4 1	0	0
4	T	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	69	Total O 69 69	0	0
5	C	80	Total O 80 80	0	0
5	D	80	Total O 80 80	0	0
5	E	61	Total O 61 61	0	0
5	F	81	Total O 81 81	0	0
5	G	54	Total O 54 54	0	0
5	H	50	Total O 50 50	0	0
5	I	52	Total O 52 52	0	0
5	J	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	62	Total O 62 62	0	0
5	L	63	Total O 63 63	0	0
5	M	83	Total O 83 83	0	0
5	N	73	Total O 73 73	0	0
5	O	59	Total O 59 59	0	0
5	P	73	Total O 73 73	0	0
5	Q	66	Total O 66 66	0	0
5	R	85	Total O 85 85	0	0
5	S	79	Total O 79 79	0	0
5	T	80	Total O 80 80	0	0

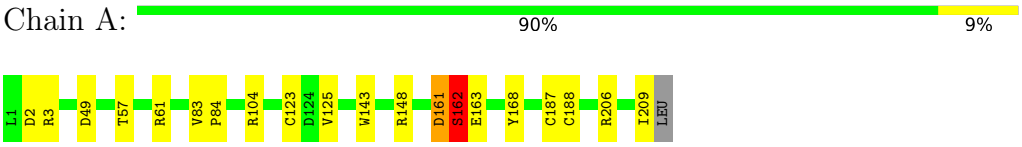
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

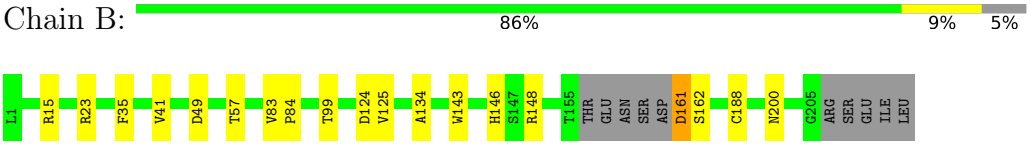
- Molecule 1: Acetylcholine-binding protein

Chain A:



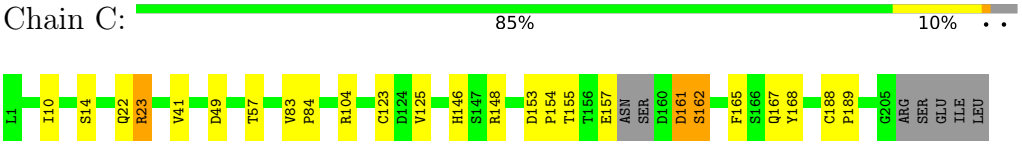
- Molecule 1: Acetylcholine-binding protein

Chain B:



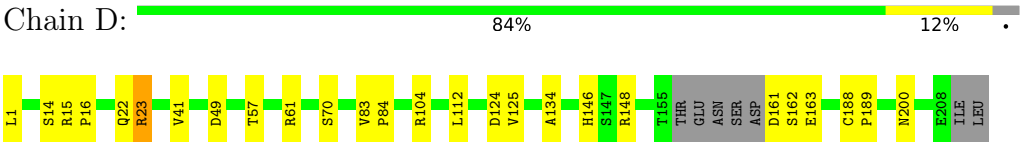
- Molecule 1: Acetylcholine-binding protein

Chain C:



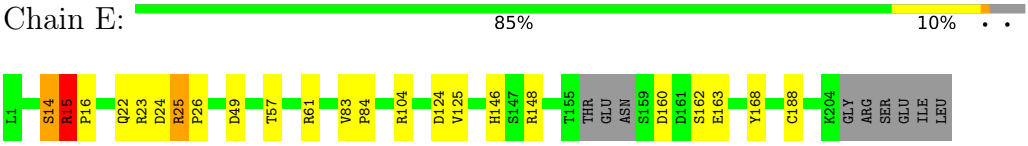
- Molecule 1: Acetylcholine-binding protein

Chain D:



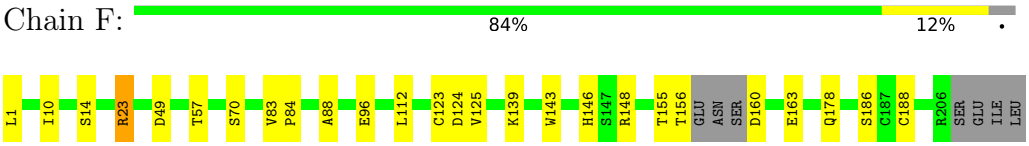
- Molecule 1: Acetylcholine-binding protein

Chain E:



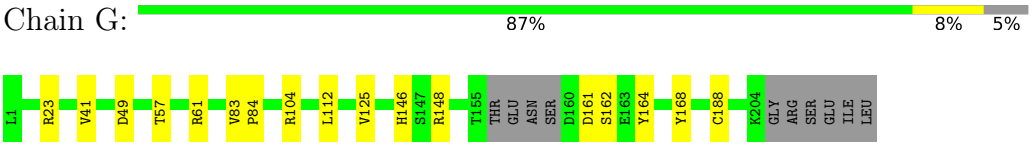
- Molecule 1: Acetylcholine-binding protein

Chain F:



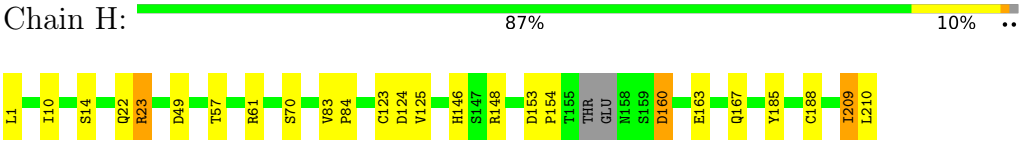
• Molecule 1: Acetylcholine-binding protein

Chain G:



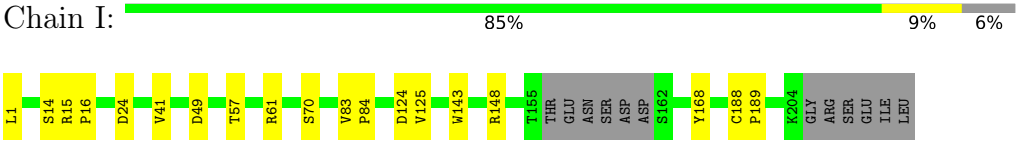
• Molecule 1: Acetylcholine-binding protein

Chain H:



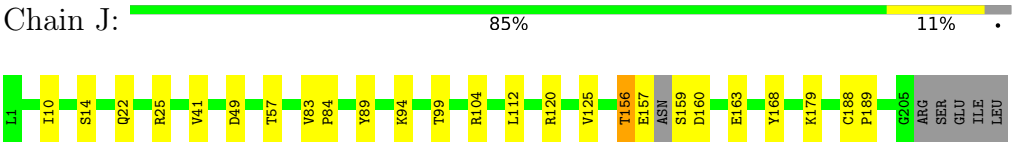
• Molecule 1: Acetylcholine-binding protein

Chain I:



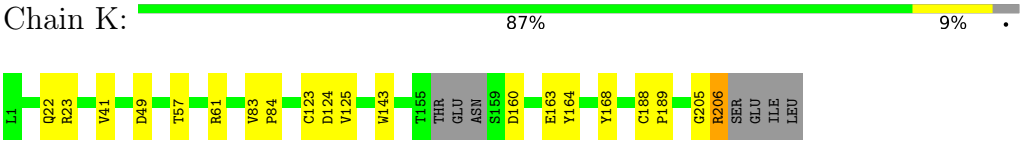
• Molecule 1: Acetylcholine-binding protein

Chain J:



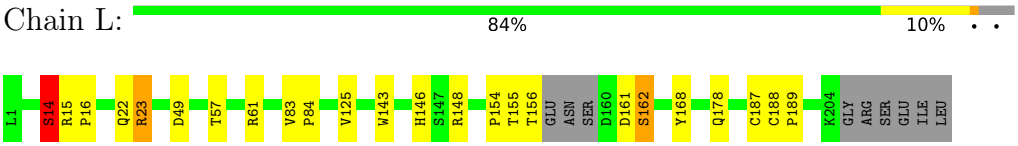
• Molecule 1: Acetylcholine-binding protein

Chain K:



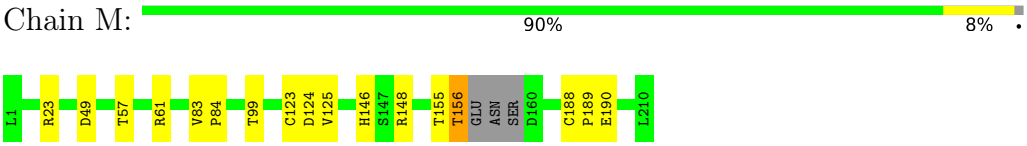
• Molecule 1: Acetylcholine-binding protein

Chain L:



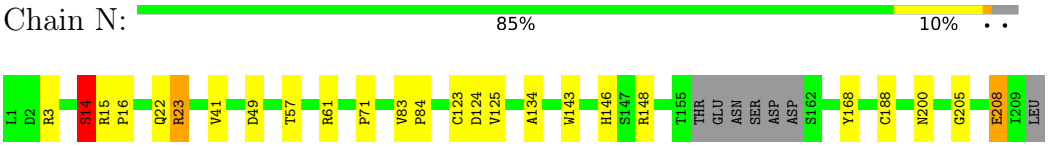
• Molecule 1: Acetylcholine-binding protein

Chain M:



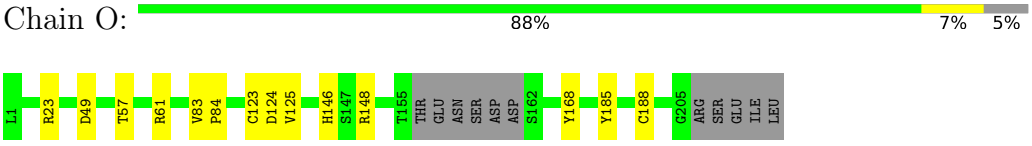
• Molecule 1: Acetylcholine-binding protein

Chain N:



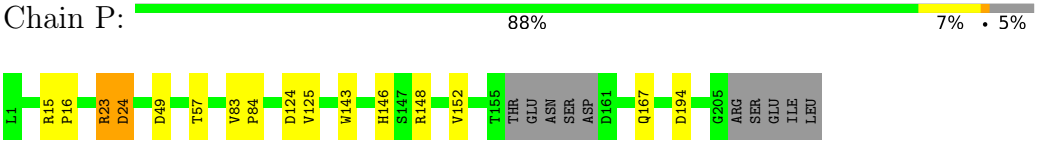
• Molecule 1: Acetylcholine-binding protein

Chain O:



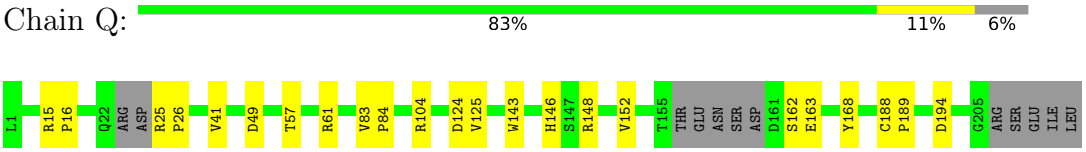
• Molecule 1: Acetylcholine-binding protein

Chain P:



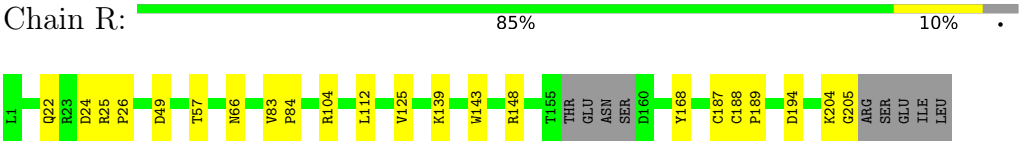
• Molecule 1: Acetylcholine-binding protein

Chain Q:



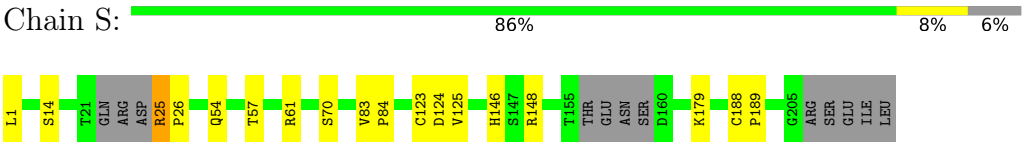
• Molecule 1: Acetylcholine-binding protein

Chain R:



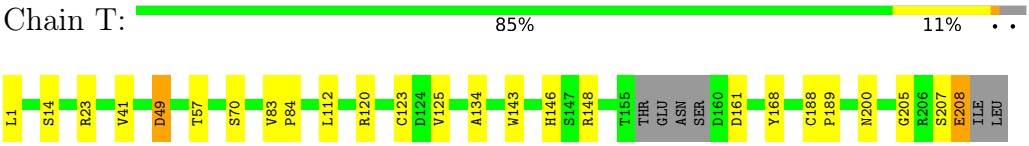
• Molecule 1: Acetylcholine-binding protein

Chain S:



• Molecule 1: Acetylcholine-binding protein

Chain T:


85%
11%
L1
S14
R23
V41
D49
T57
S70
V83
P84
L112
R120
C123
D124
V125
A134
W143
H146
S147
R148
T155
THR
GLU
ASN
SER
D160
D161
Y168
C188
P189
N200
G205
R206
S207
E208
ILE
LEU

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	235.41Å 273.16Å 73.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.51 – 2.47	Depositor
% Data completeness (in resolution range)	98.9 (51.51-2.47)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.236	Depositor
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.413	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34188	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, 09P

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	0.42	0/1706	0.53	0/2327
1	B	0.40	0/1633	0.52	0/2227
1	C	0.41	0/1663	0.52	0/2269
1	D	0.42	0/1671	0.52	0/2278
1	E	0.42	0/1649	0.53	0/2249
1	F	0.43	0/1659	0.52	0/2262
1	G	0.41	0/1637	0.55	0/2233
1	H	0.38	0/1697	0.53	0/2313
1	I	0.41	0/1627	0.53	0/2220
1	J	0.41	0/1675	0.54	0/2285
1	K	0.42	0/1670	0.55	0/2277
1	L	0.41	0/1650	0.54	0/2252
1	M	0.44	0/1702	0.55	0/2321
1	N	0.43	0/1665	0.54	0/2269
1	O	0.42	0/1625	0.53	0/2216
1	P	0.46	0/1645	0.56	0/2244
1	Q	0.45	0/1625	0.54	0/2216
1	R	0.46	0/1653	0.55	0/2255
1	S	0.44	0/1624	0.53	0/2215
1	T	0.44	0/1690	0.54	0/2303
All	All	0.42	0/33166	0.54	0/45231

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	22	GLN	Peptide

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	1670	0	1617	14	0
1	B	1598	0	1552	12	0
1	C	1625	0	1574	18	0
1	D	1630	0	1586	19	0
1	E	1611	0	1563	20	0
1	F	1624	0	1576	19	0
1	G	1602	0	1552	11	0
1	H	1662	0	1613	18	0
1	I	1589	0	1550	13	0
1	J	1634	0	1584	20	0
1	K	1629	0	1584	20	0
1	L	1612	0	1565	18	0
1	M	1661	0	1619	14	0
1	N	1627	0	1588	18	0
1	O	1590	0	1548	10	0
1	P	1604	0	1562	9	0
1	Q	1585	0	1544	13	0
1	R	1612	0	1564	14	0
1	S	1584	0	1540	13	0
1	T	1646	0	1603	19	0
2	A	16	0	19	0	0
2	B	16	0	19	2	0
2	C	16	0	19	2	0
2	D	16	0	19	1	0
2	E	16	0	19	1	0
2	F	16	0	19	3	0
2	G	16	0	19	1	0
2	H	16	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	16	0	19	4	0
2	J	16	0	19	2	0
2	K	16	0	19	1	0
2	L	16	0	19	1	0
2	M	16	0	19	0	0
2	N	16	0	19	2	0
2	O	16	0	19	1	0
2	P	16	0	19	2	0
2	Q	16	0	19	5	0
2	R	16	0	19	3	0
2	S	16	0	19	3	0
2	T	16	0	19	1	0
3	A	14	0	13	0	0
3	G	14	0	13	0	0
3	R	14	0	13	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	0	0
4	P	5	0	0	0	0
4	T	5	0	0	0	0
5	A	69	0	0	2	0
5	B	69	0	0	1	0
5	C	80	0	0	2	0
5	D	80	0	0	3	0
5	E	61	0	0	1	0
5	F	81	0	0	2	0
5	G	54	0	0	0	0
5	H	50	0	0	2	0
5	I	52	0	0	0	0
5	J	62	0	0	1	0
5	K	62	0	0	2	0
5	L	63	0	0	0	0
5	M	83	0	0	1	0
5	N	73	0	0	1	0
5	O	59	0	0	1	0
5	P	73	0	0	1	0
5	Q	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	85	0	0	1	0
5	S	79	0	0	3	0
5	T	80	0	0	2	0
All	All	34188	0	31903	292	0

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

The worst 5 of 292 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:T:49:ASP:OD1	1:T:120[B]:ARG:HG2	1.41	1.17
1:L:14:SER:HB3	1:L:16:PRO:HD3	1.48	0.96
1:K:206:ARG:HH11	1:K:206:ARG:CG	1.86	0.88
2:S:211:09P:H16	1:T:112:LEU:HD23	1.56	0.87
1:T:49:ASP:OD1	1:T:120[B]:ARG:CG	2.21	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	207/210 (99%)	204 (99%)	2 (1%)	1 (0%)	29 46
1	B	196/210 (93%)	195 (100%)	1 (0%)	0	100 100
1	C	200/210 (95%)	193 (96%)	5 (2%)	2 (1%)	15 26
1	D	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29 46
1	E	198/210 (94%)	193 (98%)	3 (2%)	2 (1%)	15 26
1	F	199/210 (95%)	196 (98%)	3 (2%)	0	100 100
1	G	196/210 (93%)	191 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	204/210 (97%)	201 (98%)	3 (2%)	0	100 100
1	I	195/210 (93%)	193 (99%)	1 (0%)	1 (0%)	29 46
1	J	202/210 (96%)	198 (98%)	4 (2%)	0	100 100
1	K	201/210 (96%)	196 (98%)	5 (2%)	0	100 100
1	L	198/210 (94%)	194 (98%)	2 (1%)	2 (1%)	15 26
1	M	205/210 (98%)	202 (98%)	3 (2%)	0	100 100
1	N	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	29 46
1	O	195/210 (93%)	191 (98%)	4 (2%)	0	100 100
1	P	198/210 (94%)	194 (98%)	3 (2%)	1 (0%)	29 46
1	Q	194/210 (92%)	188 (97%)	5 (3%)	1 (0%)	29 46
1	R	199/210 (95%)	195 (98%)	4 (2%)	0	100 100
1	S	194/210 (92%)	192 (99%)	2 (1%)	0	100 100
1	T	203/210 (97%)	200 (98%)	3 (2%)	0	100 100
All	All	3985/4200 (95%)	3908 (98%)	65 (2%)	12 (0%)	41 59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	E	14	SER
1	L	14	SER
1	L	162	SER
1	N	14	SER

5.3.2 Protein sidechains (i)

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	195/196 (100%)	187 (96%)	8 (4%)	30 53
1	B	186/196 (95%)	180 (97%)	6 (3%)	39 63
1	C	190/196 (97%)	187 (98%)	3 (2%)	62 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	191/196 (97%)	188 (98%)	3 (2%)	62 82
1	E	189/196 (96%)	183 (97%)	6 (3%)	39 63
1	F	189/196 (96%)	185 (98%)	4 (2%)	53 76
1	G	187/196 (95%)	181 (97%)	6 (3%)	39 63
1	H	194/196 (99%)	188 (97%)	6 (3%)	40 64
1	I	186/196 (95%)	182 (98%)	4 (2%)	52 75
1	J	192/196 (98%)	189 (98%)	3 (2%)	62 82
1	K	191/196 (97%)	187 (98%)	4 (2%)	53 76
1	L	189/196 (96%)	184 (97%)	5 (3%)	46 70
1	M	195/196 (100%)	191 (98%)	4 (2%)	53 76
1	N	190/196 (97%)	184 (97%)	6 (3%)	39 63
1	O	185/196 (94%)	181 (98%)	4 (2%)	52 75
1	P	188/196 (96%)	184 (98%)	4 (2%)	53 76
1	Q	186/196 (95%)	183 (98%)	3 (2%)	62 82
1	R	189/196 (96%)	183 (97%)	6 (3%)	39 63
1	S	186/196 (95%)	184 (99%)	2 (1%)	73 88
1	T	193/196 (98%)	188 (97%)	5 (3%)	46 70
All	All	3791/3920 (97%)	3699 (98%)	92 (2%)	49 72

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	187	CYS
1	O	188	CYS
1	M	49	ASP
1	N	57	THR
1	P	57	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	22	GLN
1	S	54	GLN
1	T	22	GLN
1	K	22	GLN

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Mol	Chain	Res	Type
1	K	167	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

33 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	09P	J	211	-	15,17,17	1.08	0	17,21,21	1.26	1 (5%)
2	09P	K	211	-	15,17,17	1.16	1 (6%)	17,21,21	1.73	2 (11%)
2	09P	C	211	-	15,17,17	1.31	2 (13%)	17,21,21	1.19	2 (11%)
2	09P	L	211	-	15,17,17	0.95	0	17,21,21	1.20	1 (5%)
2	09P	P	211	-	15,17,17	1.13	2 (13%)	17,21,21	1.48	2 (11%)
2	09P	T	211	-	15,17,17	1.09	1 (6%)	17,21,21	1.35	1 (5%)
4	SO4	M	212	-	4,4,4	0.11	0	6,6,6	0.11	0
3	NAG	A	212	1	14,14,15	0.50	0	17,19,21	1.31	1 (5%)
4	SO4	I	212	-	4,4,4	0.15	0	6,6,6	0.21	0
4	SO4	P	212	-	4,4,4	0.15	0	6,6,6	0.14	0
2	09P	S	211	-	15,17,17	1.17	1 (6%)	17,21,21	1.72	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	09P	I	211	-	15,17,17	1.20	1 (6%)	17,21,21	1.42	1 (5%)
2	09P	H	211	-	15,17,17	1.12	1 (6%)	17,21,21	1.45	2 (11%)
2	09P	O	211	-	15,17,17	1.14	1 (6%)	17,21,21	1.67	2 (11%)
4	SO4	K	212	-	4,4,4	0.14	0	6,6,6	0.24	0
4	SO4	T	212	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	O	212	-	4,4,4	0.14	0	6,6,6	0.12	0
2	09P	F	211	-	15,17,17	1.12	1 (6%)	17,21,21	1.26	2 (11%)
4	SO4	D	212	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	N	212	-	4,4,4	0.12	0	6,6,6	0.16	0
4	SO4	H	212	-	4,4,4	0.14	0	6,6,6	0.14	0
2	09P	D	211	-	15,17,17	1.35	3 (20%)	17,21,21	1.16	2 (11%)
3	NAG	R	214	1	14,14,15	0.46	0	17,19,21	1.41	4 (23%)
2	09P	Q	211	-	15,17,17	1.03	0	17,21,21	1.60	1 (5%)
2	09P	N	211	-	15,17,17	1.23	1 (6%)	17,21,21	1.41	2 (11%)
2	09P	E	211	-	15,17,17	1.07	1 (6%)	17,21,21	0.96	1 (5%)
4	SO4	C	212	-	4,4,4	0.14	0	6,6,6	0.14	0
2	09P	G	211	-	15,17,17	1.23	2 (13%)	17,21,21	1.41	1 (5%)
3	NAG	G	213	1	14,14,15	0.49	0	17,19,21	1.28	3 (17%)
2	09P	B	211	-	15,17,17	1.29	3 (20%)	17,21,21	1.80	2 (11%)
2	09P	R	211	-	15,17,17	1.17	1 (6%)	17,21,21	1.92	4 (23%)
2	09P	M	211	-	15,17,17	1.17	1 (6%)	17,21,21	1.59	4 (23%)
2	09P	A	211	-	15,17,17	1.15	0	17,21,21	1.36	2 (11%)

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	09P	J	211	-	-	1/7/16/16	0/2/2/2
2	09P	K	211	-	-	1/7/16/16	0/2/2/2
2	09P	C	211	-	-	1/7/16/16	0/2/2/2
2	09P	L	211	-	-	1/7/16/16	0/2/2/2
2	09P	P	211	-	-	1/7/16/16	0/2/2/2
2	09P	T	211	-	-	0/7/16/16	0/2/2/2
3	NAG	A	212	1	-	0/6/23/26	0/1/1/1
2	09P	S	211	-	-	3/7/16/16	0/2/2/2
2	09P	I	211	-	-	2/7/16/16	0/2/2/2
2	09P	H	211	-	-	1/7/16/16	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	09P	O	211	-	-	0/7/16/16	0/2/2/2
2	09P	F	211	-	-	0/7/16/16	0/2/2/2
2	09P	D	211	-	-	1/7/16/16	0/2/2/2
3	NAG	R	214	1	-	0/6/23/26	0/1/1/1
2	09P	Q	211	-	-	1/7/16/16	0/2/2/2
2	09P	N	211	-	-	1/7/16/16	0/2/2/2
2	09P	E	211	-	-	0/7/16/16	0/2/2/2
2	09P	G	211	-	-	1/7/16/16	0/2/2/2
3	NAG	G	213	1	-	0/6/23/26	0/1/1/1
2	09P	B	211	-	-	0/7/16/16	0/2/2/2
2	09P	R	211	-	-	1/7/16/16	0/2/2/2
2	09P	M	211	-	-	3/7/16/16	0/2/2/2
2	09P	A	211	-	-	1/7/16/16	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	211	09P	C6-C7	2.64	1.42	1.38
2	E	211	09P	C6-C7	2.42	1.41	1.38
2	G	211	09P	C6-C7	2.39	1.41	1.38
2	B	211	09P	C6-C7	2.35	1.41	1.38
2	K	211	09P	C6-C7	2.31	1.41	1.38

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	211	09P	C8-C9-C10	-5.47	115.14	119.48
2	B	211	09P	C8-C9-C10	-5.12	115.42	119.48
2	K	211	09P	C8-C9-C10	-5.05	115.48	119.48
2	S	211	09P	C8-C9-C10	-5.02	115.50	119.48
2	Q	211	09P	C8-C9-C10	-4.85	115.64	119.48

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	211	09P	C12-C11-O1-C7
2	M	211	09P	C12-C11-O1-C7
2	H	211	09P	C12-C11-O1-C7
2	G	211	09P	C12-C11-O1-C7
2	Q	211	09P	C12-C11-O1-C7

There are no ring outliers.

19 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	211	09P	2	0
2	K	211	09P	1	0
2	C	211	09P	2	0
2	L	211	09P	1	0
2	P	211	09P	2	0
2	T	211	09P	1	0
2	S	211	09P	3	0
2	I	211	09P	4	0
2	H	211	09P	2	0
2	O	211	09P	1	0
2	F	211	09P	3	0
2	D	211	09P	1	0
3	R	214	NAG	1	0
2	Q	211	09P	5	0
2	N	211	09P	2	0
2	E	211	09P	1	0
2	G	211	09P	1	0
2	B	211	09P	2	0
2	R	211	09P	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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.