



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:50 AM UTC

PDB ID : 3U8K / pdb_00003u8k
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

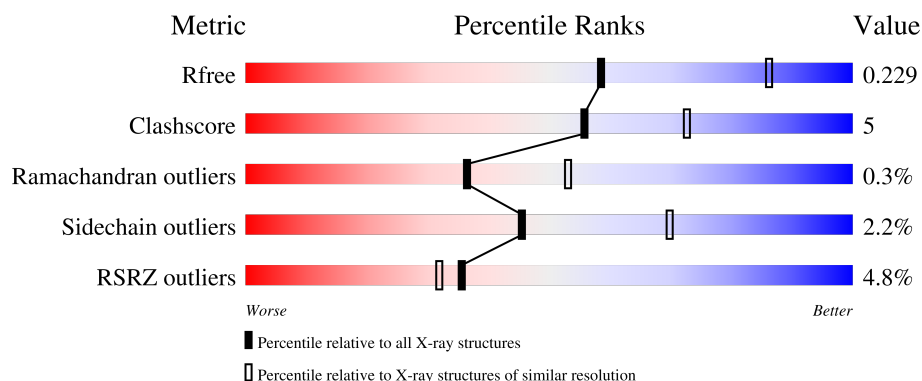
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



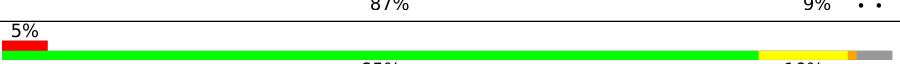
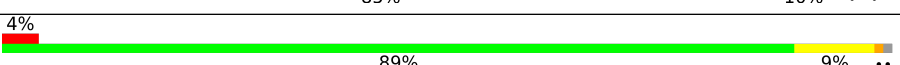
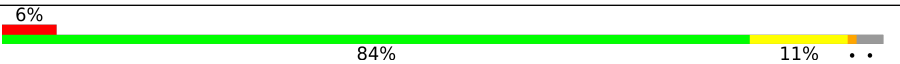
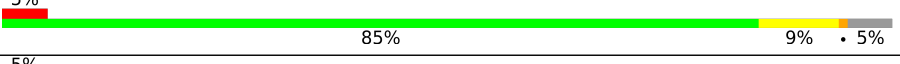
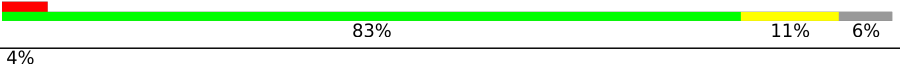
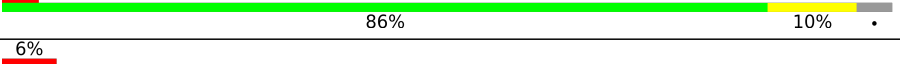
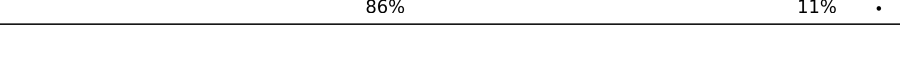
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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 $\leq 5\%$. 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	210	5% 90% 8%
1	B	210	4% 87% 8% 5%
1	C	210	5% 85% 10% • •
1	D	210	2% 84% 12% •
1	E	210	5% 85% 9% • •

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Mol	Chain	Length	Quality of chain
1	F	210	
1	G	210	
1	H	210	
1	I	210	
1	J	210	
1	K	210	
1	L	210	
1	M	210	
1	N	210	
1	O	210	
1	P	210	
1	Q	210	
1	R	210	
1	S	210	
1	T	210	

2 Entry composition

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.

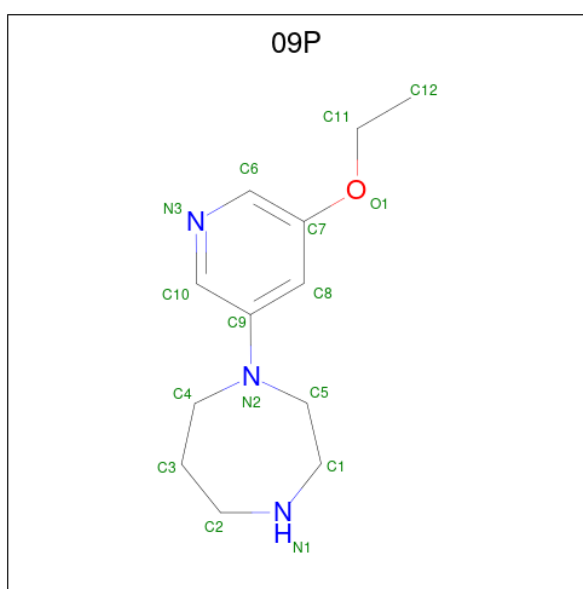
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1670	1043	287	335	5			
1	B	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			
1	C	203	Total	C	N	O	S	0	1	0
			1625	1018	277	324	6			
1	D	203	Total	C	N	O	S	0	2	0
			1630	1021	280	322	7			
1	E	201	Total	C	N	O	S	0	1	0
			1611	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 (CCD ID: 09P) (formula: C₁₂H₁₉N₃O).



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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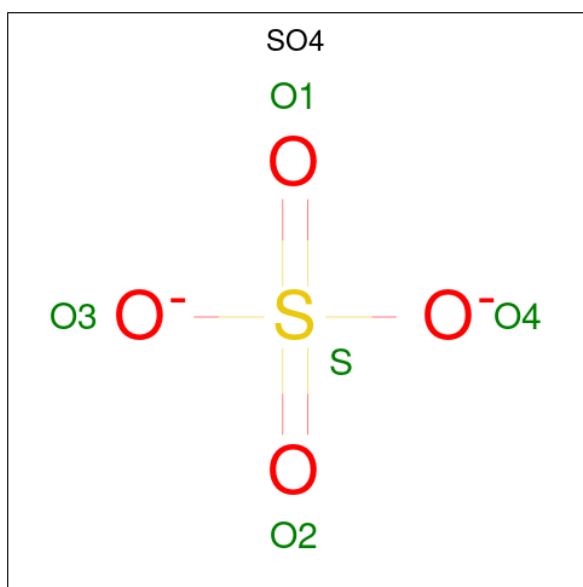
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			16	12	3	1		
2	I	1	Total	C	N	O	0	0
			16	12	3	1		
2	J	1	Total	C	N	O	0	0
			16	12	3	1		
2	K	1	Total	C	N	O	0	0
			16	12	3	1		
2	L	1	Total	C	N	O	0	0
			16	12	3	1		
2	M	1	Total	C	N	O	0	0
			16	12	3	1		
2	N	1	Total	C	N	O	0	0
			16	12	3	1		
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 5 is water.

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

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

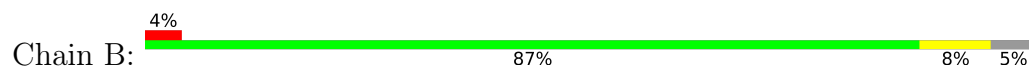
3 Residue-property plots [i](#)

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 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.

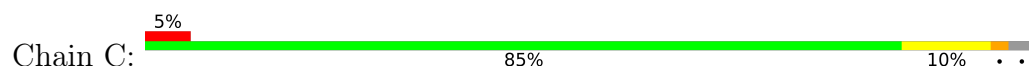
- Molecule 1: Acetylcholine-binding protein



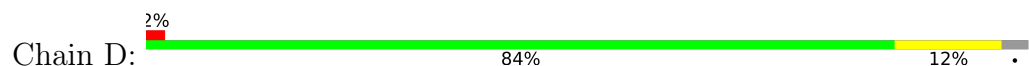
- Molecule 1: Acetylcholine-binding protein



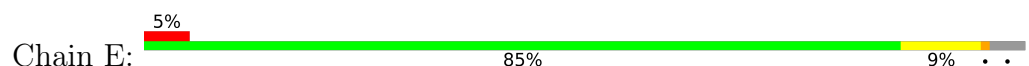
- Molecule 1: Acetylcholine-binding protein



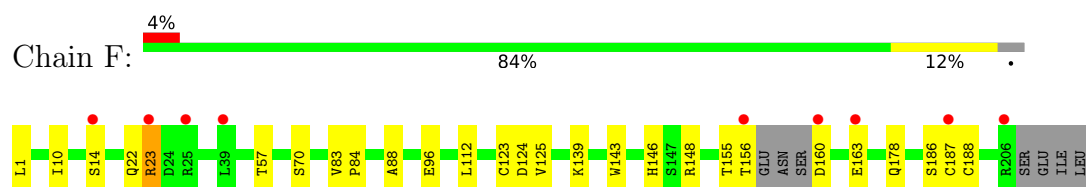
- Molecule 1: Acetylcholine-binding protein



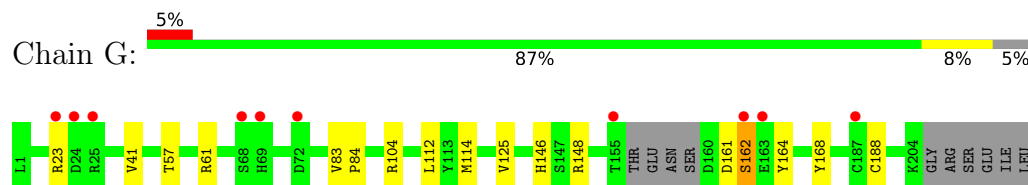
- Molecule 1: Acetylcholine-binding protein



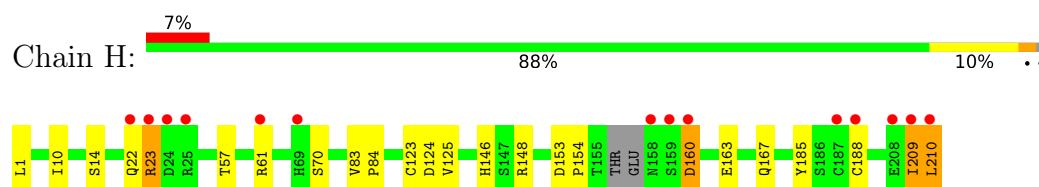
- Molecule 1: Acetylcholine-binding protein



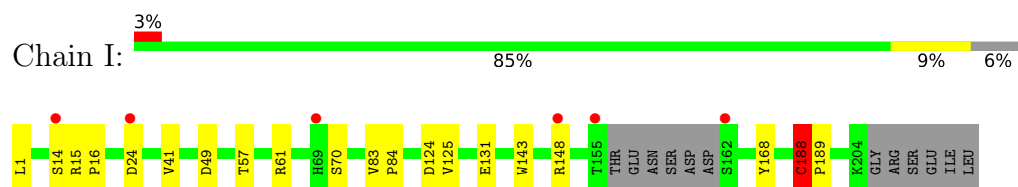
- Molecule 1: Acetylcholine-binding protein



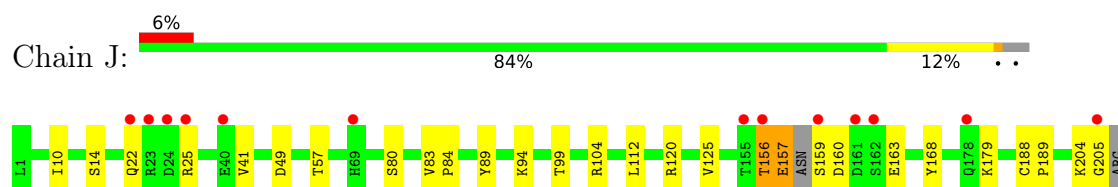
- Molecule 1: Acetylcholine-binding protein



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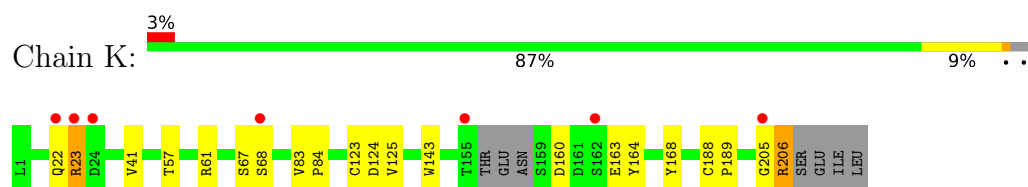


- Molecule 1: Acetylcholine-binding protein

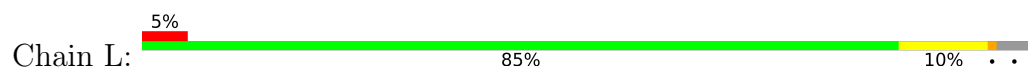


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- Molecule 1: Acetylcholine-binding protein

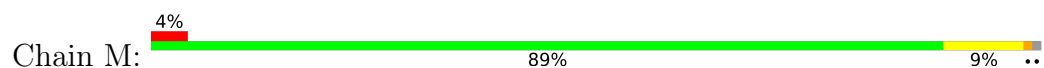


- Molecule 1: Acetylcholine-binding protein

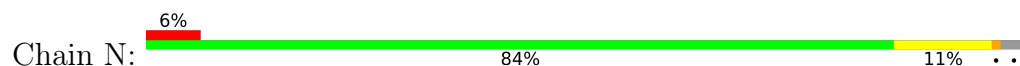




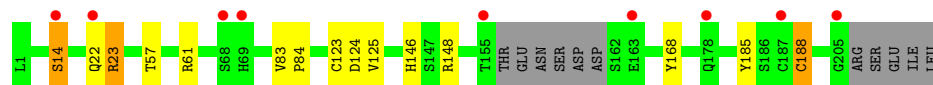
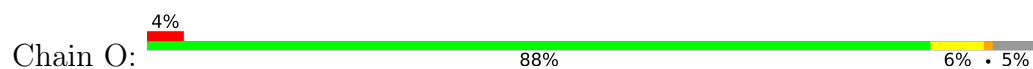
- Molecule 1: Acetylcholine-binding protein



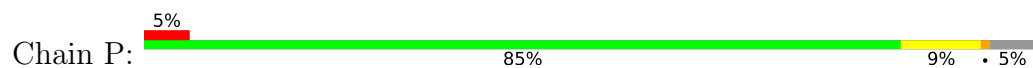
- Molecule 1: Acetylcholine-binding protein



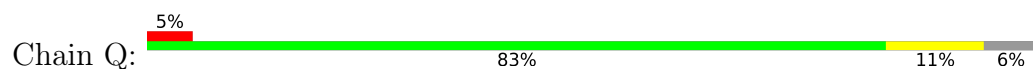
- Molecule 1: Acetylcholine-binding protein



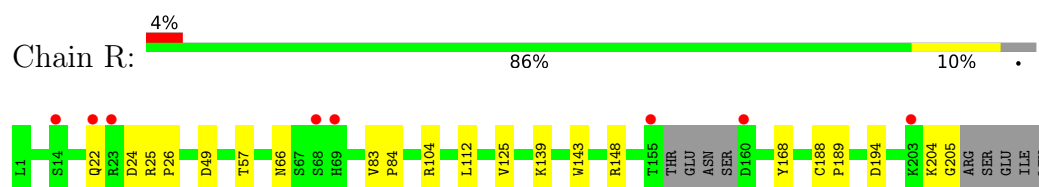
- Molecule 1: Acetylcholine-binding protein



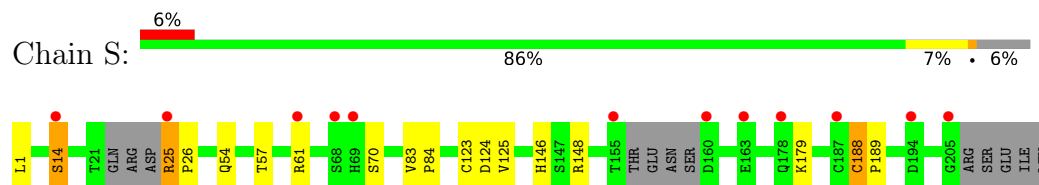
- Molecule 1: Acetylcholine-binding protein



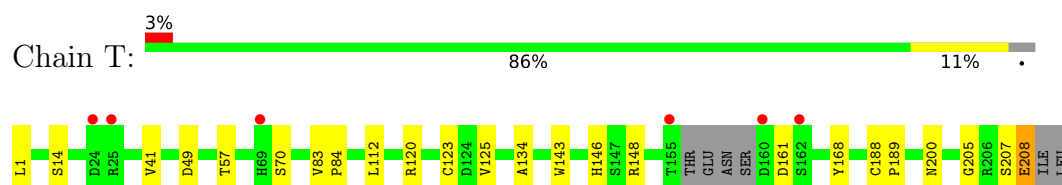
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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 51.51 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.9 (51.51-2.47) 98.9 (51.51-2.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.236 0.185 , 0.229	Depositor DCC
R_{free} test set	8428 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 09P, 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	0.50	0/1706	0.78	0/2327
1	B	0.48	0/1633	0.79	0/2227
1	C	0.49	0/1663	0.78	1/2269 (0.0%)
1	D	0.50	0/1671	0.77	0/2278
1	E	0.49	0/1649	0.78	1/2249 (0.0%)
1	F	0.51	0/1659	0.77	0/2262
1	G	0.49	0/1637	0.79	2/2233 (0.1%)
1	H	0.47	0/1697	0.77	0/2313
1	I	0.49	0/1627	0.81	4/2220 (0.2%)
1	J	0.49	0/1675	0.78	0/2285
1	K	0.49	0/1670	0.78	0/2277
1	L	0.49	0/1650	0.78	0/2252
1	M	0.52	0/1702	0.85	6/2321 (0.3%)
1	N	0.51	0/1665	0.79	0/2269
1	O	0.51	0/1625	0.81	3/2216 (0.1%)
1	P	0.54	0/1645	0.89	5/2244 (0.2%)
1	Q	0.54	0/1625	0.79	1/2216 (0.0%)
1	R	0.55	0/1653	0.79	0/2255
1	S	0.52	0/1624	0.80	1/2215 (0.0%)
1	T	0.54	0/1690	0.79	0/2303
All	All	0.51	0/33166	0.80	24/45231 (0.1%)

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.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	162	SER	N-CA-C	-10.01	99.97	112.88
1	E	23	ARG	N-CA-C	8.31	121.04	110.24
1	P	188[A]	CYS	CA-C-N	8.19	127.83	119.56
1	P	188[A]	CYS	C-N-CA	8.19	127.83	119.56
1	P	188[B]	CYS	CA-C-N	8.19	127.83	119.56

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

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	17	0
1	D	1630	0	1586	20	0
1	E	1611	0	1563	20	0
1	F	1624	0	1576	21	0
1	G	1602	0	1552	12	0
1	H	1662	0	1613	18	0
1	I	1589	0	1550	13	0
1	J	1634	0	1584	22	0
1	K	1629	0	1584	22	0
1	L	1612	0	1565	18	0
1	M	1661	0	1619	15	0
1	N	1627	0	1588	19	0
1	O	1590	0	1548	11	0
1	P	1604	0	1562	12	0
1	Q	1585	0	1544	15	0
1	R	1612	0	1564	14	0
1	S	1584	0	1540	13	0
1	T	1646	0	1603	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	303	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 303 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%)	24 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
1	C	200/210 (95%)	193 (96%)	5 (2%)	2 (1%)	12	22
1	D	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	40
1	E	198/210 (94%)	193 (98%)	3 (2%)	2 (1%)	12	22
1	F	199/210 (95%)	196 (98%)	3 (2%)	0	100	100
1	G	196/210 (93%)	191 (97%)	5 (3%)	0	100	100
1	H	204/210 (97%)	201 (98%)	3 (2%)	0	100	100
1	I	195/210 (93%)	193 (99%)	1 (0%)	1 (0%)	24	40
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%)	12	22
1	M	205/210 (98%)	202 (98%)	3 (2%)	0	100	100
1	N	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	24	40
1	O	195/210 (93%)	191 (98%)	4 (2%)	0	100	100
1	P	198/210 (94%)	194 (98%)	3 (2%)	1 (0%)	24	40
1	Q	194/210 (92%)	188 (97%)	5 (3%)	1 (0%)	24	40
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%)	36	53

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 ⓘ

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%)	188 (96%)	7 (4%)	31	55
1	B	186/196 (95%)	182 (98%)	4 (2%)	45	70
1	C	190/196 (97%)	184 (97%)	6 (3%)	34	58
1	D	191/196 (97%)	189 (99%)	2 (1%)	68	84
1	E	189/196 (96%)	184 (97%)	5 (3%)	40	65
1	F	189/196 (96%)	186 (98%)	3 (2%)	55	77
1	G	187/196 (95%)	182 (97%)	5 (3%)	39	64
1	H	194/196 (99%)	188 (97%)	6 (3%)	35	60
1	I	186/196 (95%)	179 (96%)	7 (4%)	29	53
1	J	192/196 (98%)	188 (98%)	4 (2%)	47	71
1	K	191/196 (97%)	188 (98%)	3 (2%)	55	77
1	L	189/196 (96%)	185 (98%)	4 (2%)	47	71
1	M	195/196 (100%)	191 (98%)	4 (2%)	47	71
1	N	190/196 (97%)	184 (97%)	6 (3%)	34	58
1	O	185/196 (94%)	181 (98%)	4 (2%)	45	70
1	P	188/196 (96%)	184 (98%)	4 (2%)	47	71
1	Q	186/196 (95%)	184 (99%)	2 (1%)	65	83
1	R	189/196 (96%)	185 (98%)	4 (2%)	47	71
1	S	186/196 (95%)	182 (98%)	4 (2%)	45	70
1	T	193/196 (98%)	190 (98%)	3 (2%)	55	77
All	All	3791/3920 (97%)	3704 (98%)	87 (2%)	45	69

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	49	ASP
1	P	24	ASP
1	M	156	THR
1	N	208	GLU
1	Q	162	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	55	GLN
1	M	54	GLN
1	S	54	GLN
1	K	22	GLN
1	M	55	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 oligosaccharides 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	-	16,17,17	1.08	0	16,21,21	1.23	1 (6%)
4	SO4	T	212	-	4,4,4	0.25	0	6,6,6	0.09	0
2	09P	L	211	-	16,17,17	0.96	0	16,21,21	1.17	1 (6%)
2	09P	H	211	-	16,17,17	1.12	2 (12%)	16,21,21	1.43	2 (12%)
2	09P	T	211	-	16,17,17	1.09	1 (6%)	16,21,21	1.34	1 (6%)
4	SO4	H	212	-	4,4,4	0.24	0	6,6,6	0.14	0
2	09P	G	211	-	16,17,17	1.22	3 (18%)	16,21,21	1.39	1 (6%)
2	09P	O	211	-	16,17,17	1.13	1 (6%)	16,21,21	1.68	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	212	1	14,14,15	0.51	0	17,19,21	1.28	1 (5%)
2	09P	R	211	-	16,17,17	1.17	1 (6%)	16,21,21	1.88	4 (25%)
2	09P	B	211	-	16,17,17	1.31	3 (18%)	16,21,21	1.73	3 (18%)
4	SO4	D	212	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	C	212	-	4,4,4	0.23	0	6,6,6	0.12	0
2	09P	D	211	-	16,17,17	1.34	3 (18%)	16,21,21	1.12	1 (6%)
3	NAG	R	214	1	14,14,15	0.48	0	17,19,21	1.36	3 (17%)
4	SO4	K	212	-	4,4,4	0.25	0	6,6,6	0.20	0
4	SO4	I	212	-	4,4,4	0.20	0	6,6,6	0.21	0
4	SO4	N	212	-	4,4,4	0.22	0	6,6,6	0.18	0
3	NAG	G	213	1	14,14,15	0.51	0	17,19,21	1.24	2 (11%)
4	SO4	P	212	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	M	212	-	4,4,4	0.22	0	6,6,6	0.13	0
2	09P	C	211	-	16,17,17	1.30	2 (12%)	16,21,21	1.19	2 (12%)
2	09P	F	211	-	16,17,17	1.12	1 (6%)	16,21,21	1.20	2 (12%)
2	09P	I	211	-	16,17,17	1.22	2 (12%)	16,21,21	1.43	2 (12%)
2	09P	P	211	-	16,17,17	1.13	2 (12%)	16,21,21	1.47	2 (12%)
2	09P	E	211	-	16,17,17	1.06	1 (6%)	16,21,21	0.98	1 (6%)
4	SO4	O	212	-	4,4,4	0.24	0	6,6,6	0.09	0
2	09P	K	211	-	16,17,17	1.15	2 (12%)	16,21,21	1.68	2 (12%)
2	09P	M	211	-	16,17,17	1.18	1 (6%)	16,21,21	1.61	3 (18%)
2	09P	Q	211	-	16,17,17	1.02	1 (6%)	16,21,21	1.56	1 (6%)
2	09P	N	211	-	16,17,17	1.24	2 (12%)	16,21,21	1.36	2 (12%)
2	09P	A	211	-	16,17,17	1.16	1 (6%)	16,21,21	1.35	2 (12%)
2	09P	S	211	-	16,17,17	1.18	2 (12%)	16,21,21	1.72	3 (18%)

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	L	211	-	-	1/7/16/16	0/2/2/2
2	09P	H	211	-	-	1/7/16/16	0/2/2/2
2	09P	T	211	-	-	0/7/16/16	0/2/2/2
2	09P	G	211	-	-	1/7/16/16	0/2/2/2
2	09P	O	211	-	-	0/7/16/16	0/2/2/2
3	NAG	A	212	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	09P	R	211	-	-	1/7/16/16	0/2/2/2
2	09P	B	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
3	NAG	G	213	1	-	0/6/23/26	0/1/1/1
2	09P	C	211	-	-	1/7/16/16	0/2/2/2
2	09P	F	211	-	-	0/7/16/16	0/2/2/2
2	09P	I	211	-	-	2/7/16/16	0/2/2/2
2	09P	P	211	-	-	1/7/16/16	0/2/2/2
2	09P	E	211	-	-	0/7/16/16	0/2/2/2
2	09P	K	211	-	-	1/7/16/16	0/2/2/2
2	09P	M	211	-	-	3/7/16/16	0/2/2/2
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	A	211	-	-	1/7/16/16	0/2/2/2
2	09P	S	211	-	-	3/7/16/16	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	211	09P	C6-C7	2.65	1.42	1.38
2	D	211	09P	C10-C9	2.49	1.43	1.38
2	T	211	09P	C10-C9	2.45	1.43	1.38
2	E	211	09P	C6-C7	2.43	1.41	1.38
2	G	211	09P	C6-C7	2.40	1.41	1.38

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	211	09P	C8-C9-C10	-5.15	115.14	119.67
2	B	211	09P	C8-C9-C10	-4.84	115.42	119.67
2	K	211	09P	C8-C9-C10	-4.77	115.48	119.67
2	S	211	09P	C8-C9-C10	-4.75	115.50	119.67
2	Q	211	09P	C8-C9-C10	-4.59	115.64	119.67

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/210 (99%)	-0.09	11 (5%) 32 28	12, 27, 70, 129	0
1	B	200/210 (95%)	-0.20	9 (4%) 38 34	12, 25, 70, 109	0
1	C	203/210 (96%)	-0.12	10 (4%) 35 31	13, 27, 73, 123	1 (0%)
1	D	203/210 (96%)	-0.11	5 (2%) 58 55	11, 27, 61, 112	2 (0%)
1	E	201/210 (95%)	-0.03	11 (5%) 30 27	13, 28, 69, 116	1 (0%)
1	F	203/210 (96%)	-0.09	9 (4%) 39 35	13, 26, 64, 100	0
1	G	200/210 (95%)	-0.02	10 (5%) 34 30	13, 31, 75, 108	0
1	H	208/210 (99%)	0.03	14 (6%) 24 21	14, 31, 88, 127	0
1	I	198/210 (94%)	-0.09	6 (3%) 52 49	15, 29, 61, 91	1 (0%)
1	J	204/210 (97%)	-0.04	13 (6%) 25 22	11, 26, 80, 145	2 (0%)
1	K	203/210 (96%)	-0.12	7 (3%) 48 44	11, 26, 70, 114	2 (0%)
1	L	201/210 (95%)	-0.10	11 (5%) 30 27	14, 26, 69, 111	1 (0%)
1	M	207/210 (98%)	-0.17	9 (4%) 40 36	10, 24, 59, 111	2 (0%)
1	N	203/210 (96%)	-0.08	13 (6%) 25 22	11, 25, 62, 109	1 (0%)
1	O	199/210 (94%)	-0.10	9 (4%) 38 34	10, 26, 64, 158	0
1	P	200/210 (95%)	-0.15	11 (5%) 30 27	9, 22, 64, 108	2 (1%)
1	Q	198/210 (94%)	-0.17	11 (5%) 30 26	10, 22, 62, 92	2 (1%)
1	R	201/210 (95%)	-0.19	8 (3%) 42 38	9, 22, 59, 93	2 (0%)
1	S	198/210 (94%)	-0.17	12 (6%) 27 23	9, 25, 58, 107	2 (1%)
1	T	204/210 (97%)	-0.23	6 (2%) 53 50	8, 22, 64, 96	3 (1%)
All	All	4043/4200 (96%)	-0.11	195 (4%) 35 32	8, 26, 68, 158	24 (0%)

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	155	THR	6.9
1	D	155	THR	6.2
1	A	161	ASP	6.1
1	L	187	CYS	5.4
1	N	68	SER	4.5

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	R	214	14/15	0.47	0.22	102,102,102,102	0
3	NAG	G	213	14/15	0.67	0.17	80,80,80,80	0
4	SO4	H	212	5/5	0.74	0.17	114,114,114,114	0
4	SO4	P	212	5/5	0.77	0.16	91,91,91,91	0
4	SO4	D	212	5/5	0.79	0.14	93,93,93,93	0
4	SO4	M	212	5/5	0.80	0.17	107,107,107,107	0
3	NAG	A	212	14/15	0.81	0.13	55,55,55,55	0
4	SO4	O	212	5/5	0.82	0.19	107,107,107,107	0
4	SO4	N	212	5/5	0.82	0.15	93,93,93,93	0
4	SO4	T	212	5/5	0.82	0.15	109,109,109,109	0
4	SO4	K	212	5/5	0.83	0.17	99,99,99,99	0
4	SO4	C	212	5/5	0.84	0.13	90,90,90,90	0
2	09P	P	211	16/16	0.93	0.09	18,18,18,18	0
2	09P	I	211	16/16	0.94	0.08	21,21,21,21	0
2	09P	M	211	16/16	0.94	0.08	16,16,16,16	0
2	09P	C	211	16/16	0.94	0.08	20,20,20,20	0
2	09P	D	211	16/16	0.94	0.08	25,25,25,25	0
2	09P	G	211	16/16	0.94	0.09	25,25,25,25	0
2	09P	K	211	16/16	0.95	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	09P	L	211	16/16	0.95	0.07	19,19,19,19	0
2	09P	B	211	16/16	0.95	0.07	20,20,20,20	0
2	09P	E	211	16/16	0.95	0.08	21,21,21,21	0
2	09P	Q	211	16/16	0.95	0.07	14,14,14,14	0
2	09P	T	211	16/16	0.95	0.07	13,13,13,13	0
2	09P	S	211	16/16	0.96	0.07	21,21,21,21	0
2	09P	J	211	16/16	0.96	0.06	22,22,22,22	0
2	09P	N	211	16/16	0.96	0.07	21,21,21,21	0
2	09P	O	211	16/16	0.96	0.06	16,16,16,16	0
2	09P	A	211	16/16	0.96	0.06	21,21,21,21	0
2	09P	F	211	16/16	0.96	0.06	19,19,19,19	0
2	09P	R	211	16/16	0.96	0.06	17,17,17,17	0
2	09P	H	211	16/16	0.97	0.06	25,25,25,25	0
4	SO4	I	212	5/5	0.97	0.07	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.