



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:27 PM GMT

PDB ID : 3ZDG
Title : Crystal Structure of Ls-AChBP complexed with carbamoylcholine analogue 3-(dimethylamino)butyl dimethylcarbamate (DMABC)
Authors : Ussing, C.A.; Hansen, C.P.; Petersen, J.G.; Jensen, A.A.; Rohde, L.A.H.; Ahring, P.K.; Nielsen, E.O.; Kastrup, J.S.; Gajhede, M.; Frolund, B.; Balle, T.
Deposited on : 2012-11-26
Resolution : 2.48 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

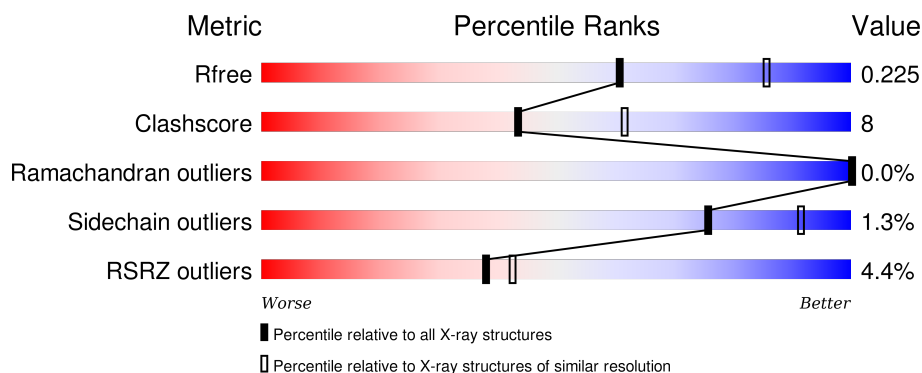
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	B	210	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	210	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>
1	D	210	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	E	210	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XRX	L	301	-	-	-	X
2	XRX	S	301	-	-	-	X
3	SO4	A	1206	-	-	X	-
3	SO4	B	1206	-	-	-	X
3	SO4	C	1205	-	-	-	X
3	SO4	H	1207	-	-	-	X
3	SO4	K	1205	-	-	X	X
3	SO4	L	1206	-	-	-	X
3	SO4	N	1205	-	-	-	X
3	SO4	Q	1206	-	-	-	X
3	SO4	R	1205	-	-	-	X
3	SO4	R	1206	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	M	501	-	-	-	X
6	1PE	R	501	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34575 atoms, of which 10 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.

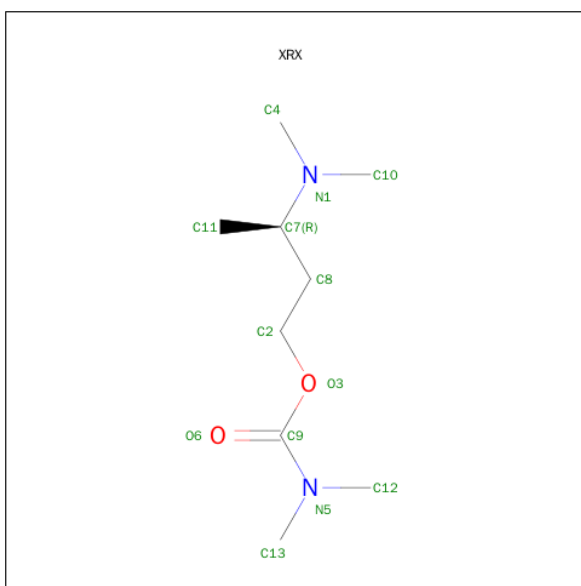
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	1	0
			1604	1007	274	318	5			
1	B	201	Total	C	N	O	S	0	3	0
			1620	1016	275	323	6			
1	C	204	Total	C	N	O	S	0	0	0
			1632	1021	279	327	5			
1	D	199	Total	C	N	O	S	0	2	0
			1603	1007	273	317	6			
1	E	199	Total	C	N	O	S	0	1	0
			1600	1005	273	317	5			
1	F	200	Total	C	N	O	S	0	2	0
			1607	1009	274	318	6			
1	G	200	Total	C	N	O	S	0	2	0
			1607	1009	274	318	6			
1	H	200	Total	C	N	O	S	0	1	0
			1604	1007	274	318	5			
1	I	199	Total	C	N	O	S	0	2	0
			1603	1007	273	317	6			
1	J	200	Total	C	N	O	S	0	1	0
			1604	1007	274	318	5			
1	K	199	Total	C	N	O	S	0	0	0
			1594	1001	273	315	5			
1	L	199	Total	C	N	O	S	0	2	0
			1603	1007	273	317	6			
1	M	199	Total	C	N	O	S	0	1	0
			1597	1003	273	315	6			
1	N	197	Total	C	N	O	S	0	1	0
			1586	998	271	312	5			
1	O	200	Total	C	N	O	S	0	1	0
			1601	1005	274	316	6			
1	P	199	Total	C	N	O	S	0	2	0
			1603	1007	273	317	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	198	Total	C	N	O	S	0	5	0
			1617	1019	279	313	6			
1	R	199	Total	C	N	O	S	0	0	0
			1594	1001	273	315	5			
1	S	199	Total	C	N	O	S	0	2	0
			1599	1005	273	315	6			
1	T	200	Total	C	N	O	S	0	4	0
			1620	1019	277	318	6			

- Molecule 2 is 3-(DIMETHYLAMINO)BUTYL DIMETHYLCARBAMATE (three-letter code: XRX) (formula: C₉H₂₀N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	2	2		
2	B	1	Total	C	N	O	0	0
			13	9	2	2		
2	C	1	Total	C	N	O	0	0
			13	9	2	2		
2	D	1	Total	C	N	O	0	0
			13	9	2	2		
2	E	1	Total	C	N	O	0	0
			13	9	2	2		
2	F	1	Total	C	N	O	0	0
			13	9	2	2		
2	G	1	Total	C	N	O	0	0
			13	9	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			13	9	2	2		
2	I	1	Total	C	N	O	0	0
			13	9	2	2		
2	J	1	Total	C	N	O	0	0
			13	9	2	2		
2	K	1	Total	C	N	O	0	0
			13	9	2	2		
2	L	1	Total	C	N	O	0	0
			13	9	2	2		
2	M	1	Total	C	N	O	0	0
			13	9	2	2		
2	N	1	Total	C	N	O	0	0
			13	9	2	2		
2	O	1	Total	C	N	O	0	0
			13	9	2	2		
2	P	1	Total	C	N	O	0	0
			13	9	2	2		
2	Q	1	Total	C	N	O	0	0
			13	9	2	2		
2	R	1	Total	C	N	O	0	0
			13	9	2	2		
2	S	1	Total	C	N	O	0	0
			13	9	2	2		
2	T	1	Total	C	N	O	0	0
			13	9	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



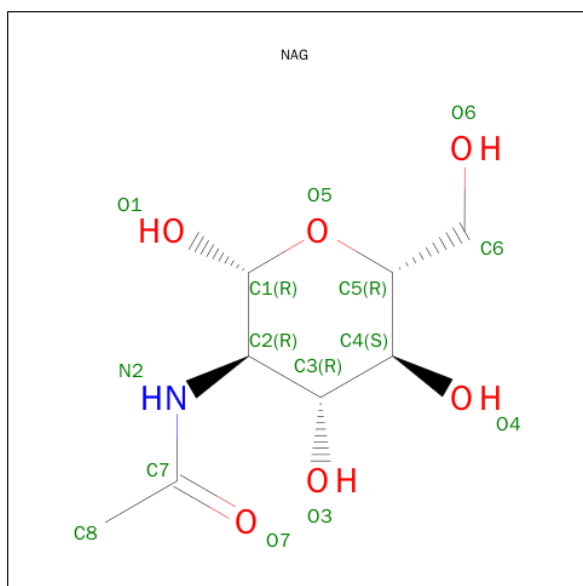
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

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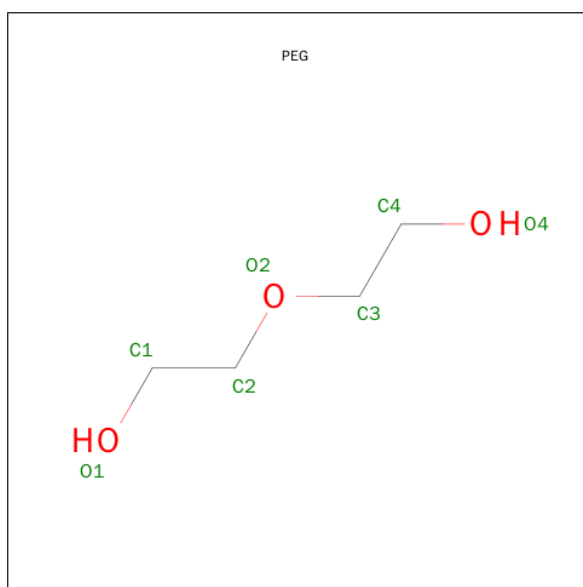
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



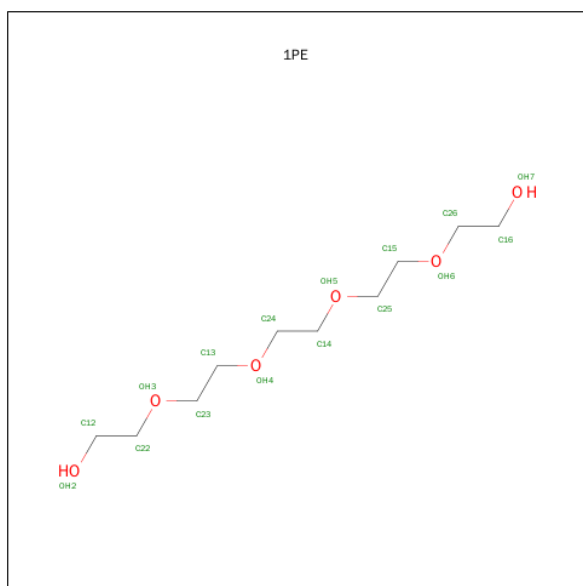
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	C	O	0	0
			16	10	6		

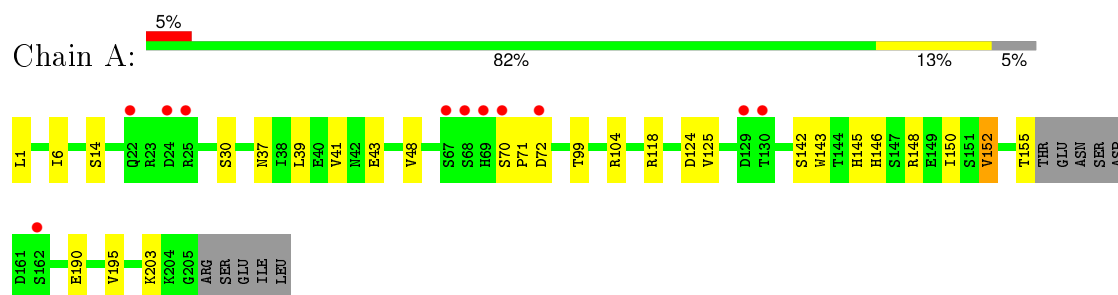
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total 116	O 116	0	0
7	B	109	Total 109	O 109	0	0
7	C	112	Total 112	O 112	0	0
7	D	121	Total 121	O 121	0	0
7	E	91	Total 91	O 91	0	0
7	F	136	Total 136	O 136	0	0
7	G	106	Total 106	O 106	0	0
7	H	125	Total 125	O 125	0	0
7	I	91	Total 91	O 91	0	0
7	J	89	Total 89	O 89	0	0
7	K	72	Total 72	O 72	0	0
7	L	104	Total 104	O 104	0	0
7	M	90	Total 90	O 90	0	0
7	N	97	Total 97	O 97	0	0
7	O	76	Total 76	O 76	0	0
7	P	127	Total 127	O 127	0	0
7	Q	93	Total 93	O 93	0	0
7	R	82	Total 82	O 82	0	0
7	S	100	Total 100	O 100	0	0
7	T	105	Total 105	O 105	0	0

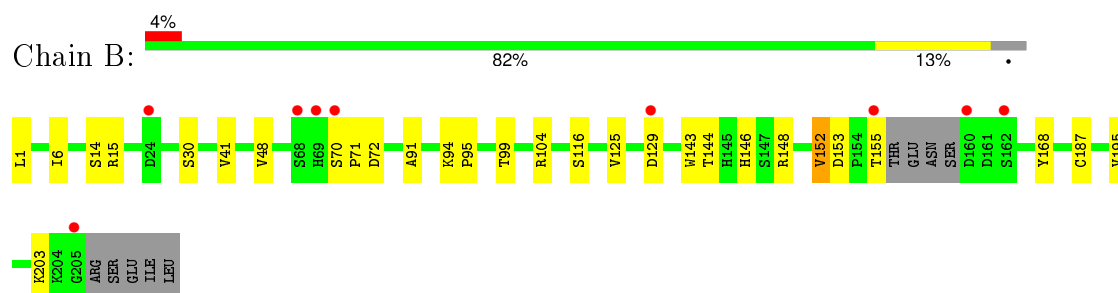
3 Residue-property plots [i](#)

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.

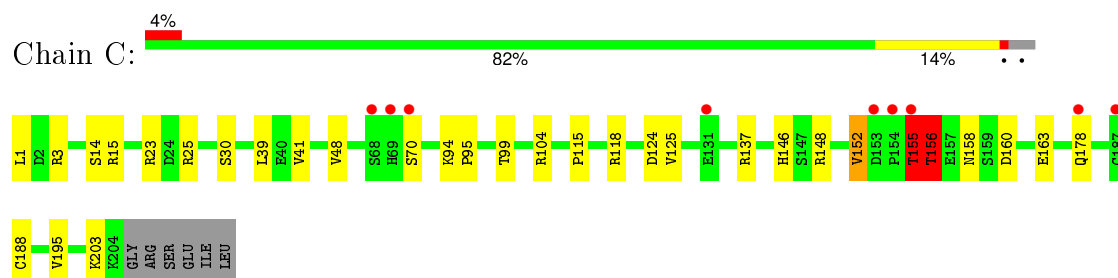
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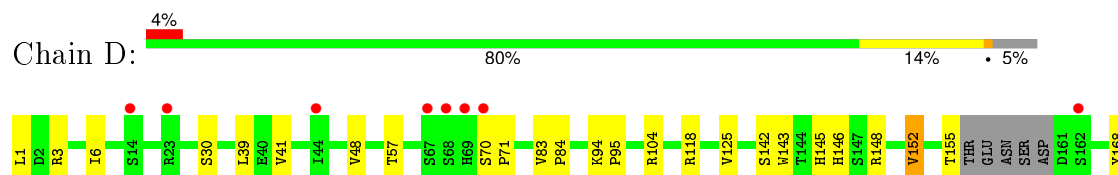
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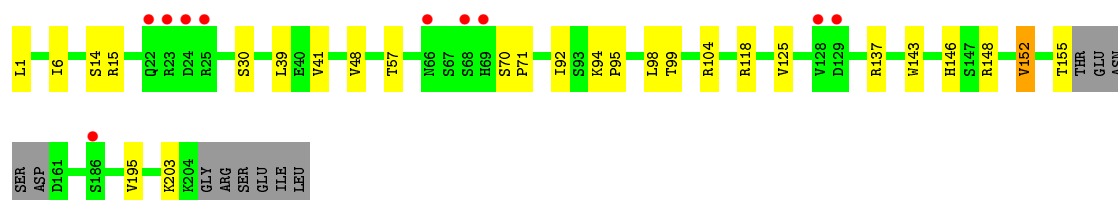
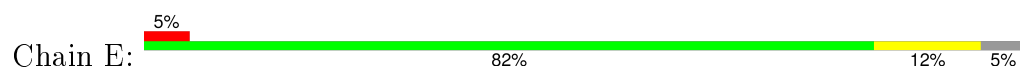


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

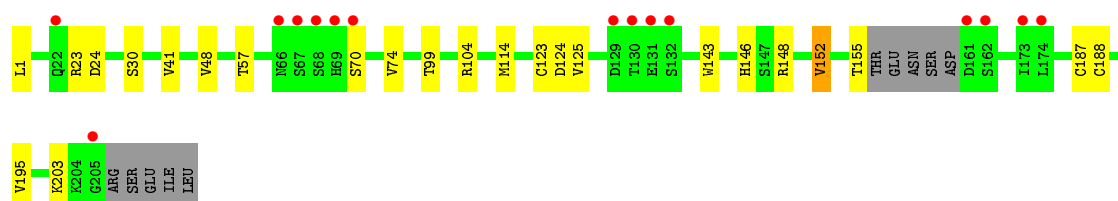
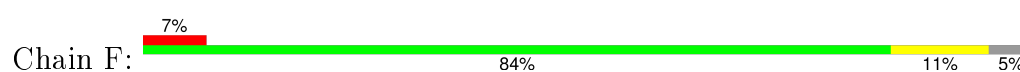




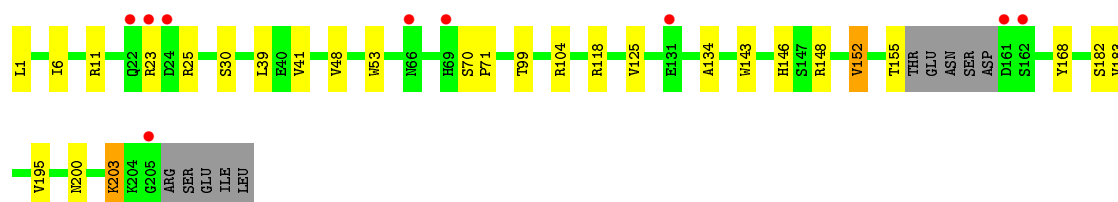
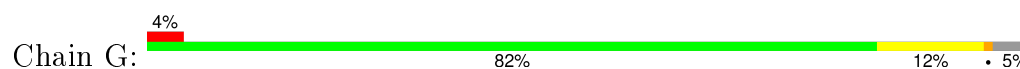
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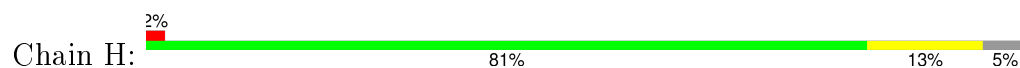
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



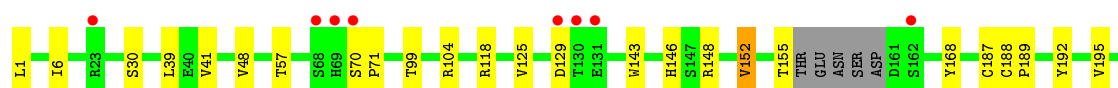
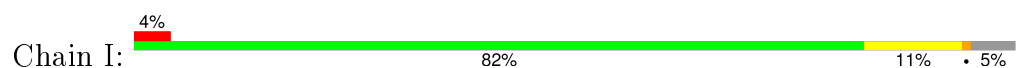
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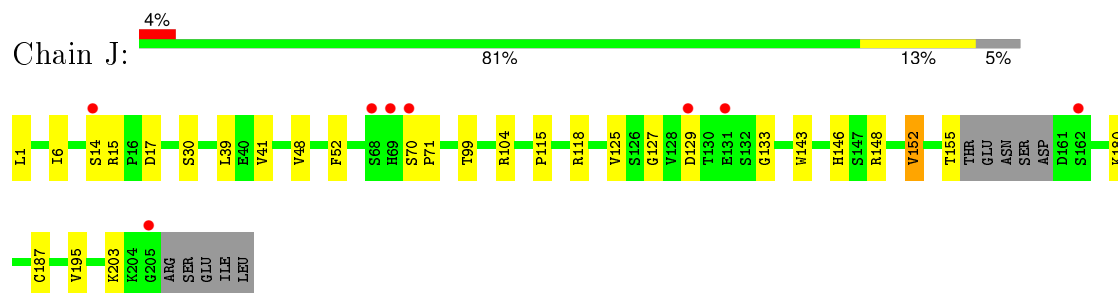


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

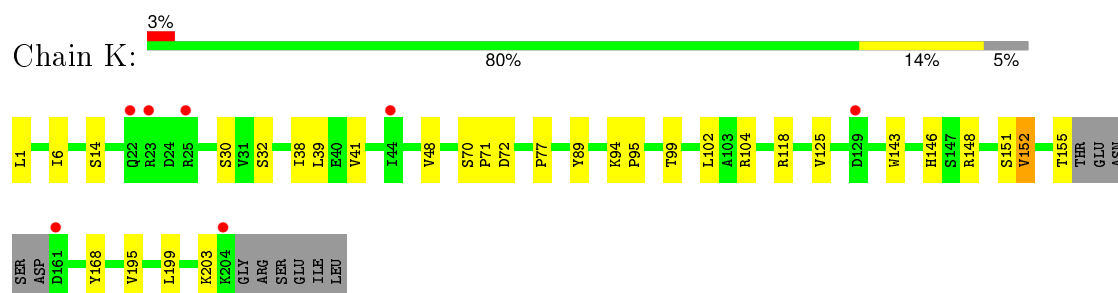




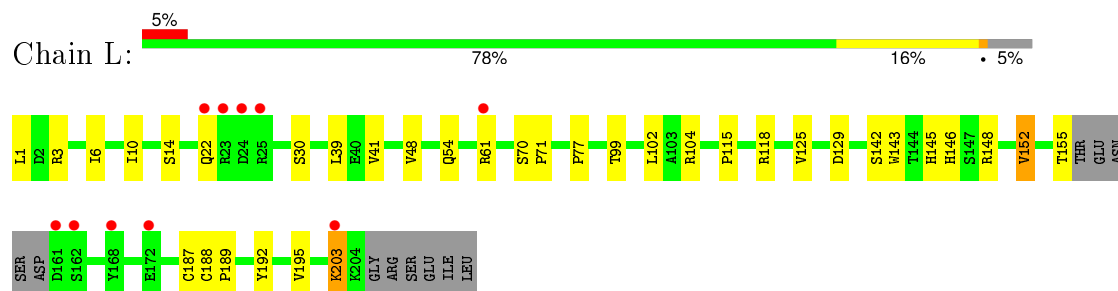
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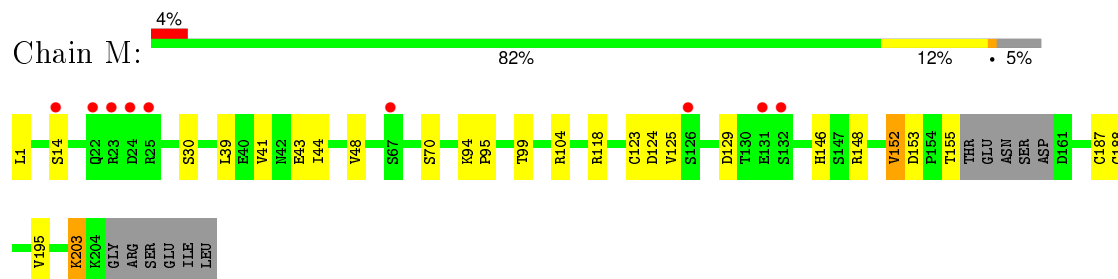
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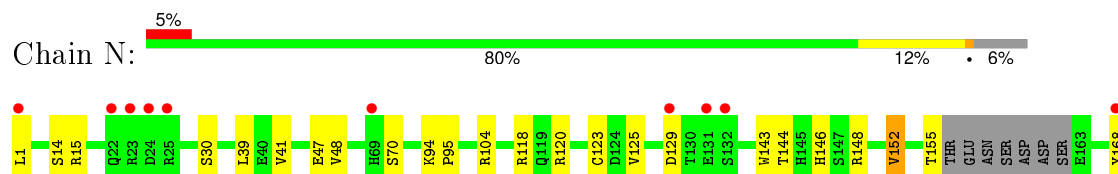
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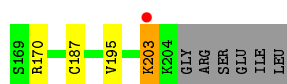


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

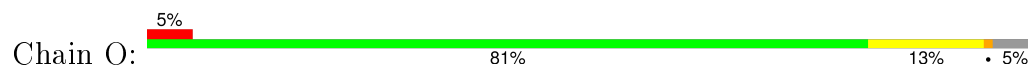


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

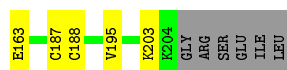
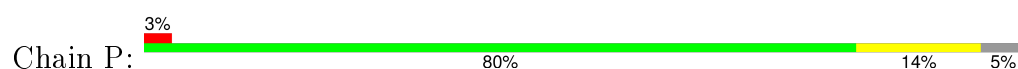




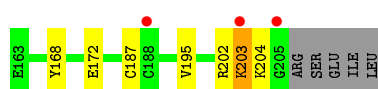
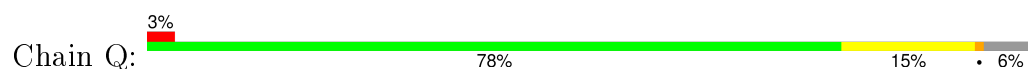
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



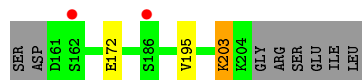
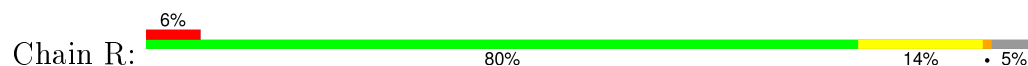
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



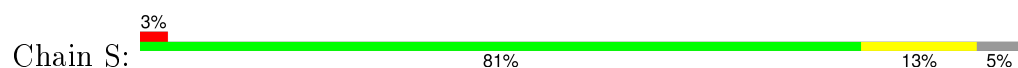
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

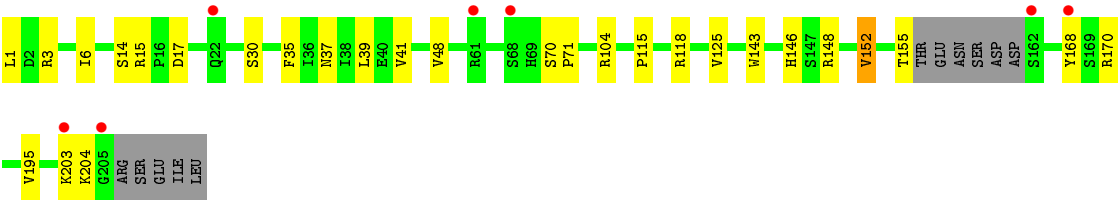


● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

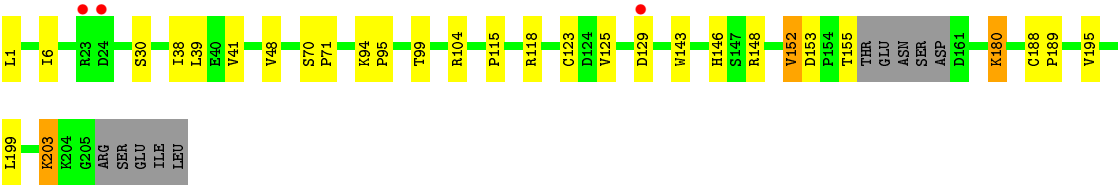
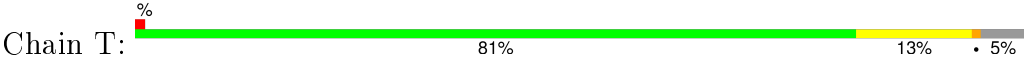


● Molecule 1: ACETYLCHOLINE BINDING PROTEIN





● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.73 Å 144.88 Å 139.03 Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	37.34 – 2.48 37.34 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.34-2.48) 99.6 (37.34-2.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.48 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.173 , 0.221 0.184 , 0.225	Depositor DCC
R_{free} test set	8252 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 164161 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34575	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.15% 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, 0.375 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: SO4, PEG, XRX, NAG, 1PE

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	0.64	0/1642	0.64	0/2239
1	B	0.63	0/1664	0.66	0/2269
1	C	0.66	0/1668	0.68	1/2277 (0.0%)
1	D	0.66	0/1644	0.65	0/2242
1	E	0.64	0/1638	0.65	0/2234
1	F	0.67	0/1648	0.67	0/2247
1	G	0.67	0/1648	0.65	0/2247
1	H	0.66	0/1642	0.66	0/2239
1	I	0.65	0/1644	0.65	0/2242
1	J	1.05	4/1642 (0.2%)	0.77	6/2239 (0.3%)
1	K	0.59	0/1629	0.61	0/2222
1	L	0.63	0/1644	0.62	0/2242
1	M	0.64	0/1635	0.65	0/2230
1	N	0.64	0/1624	0.63	0/2215
1	O	0.64	0/1639	0.64	0/2235
1	P	0.65	0/1644	0.65	0/2242
1	Q	0.63	0/1668	0.66	0/2273
1	R	0.62	0/1629	0.64	0/2222
1	S	0.64	0/1640	0.68	2/2236 (0.1%)
1	T	0.63	0/1668	0.64	0/2273
All	All	0.67	4/32900 (0.0%)	0.66	9/44865 (0.0%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	52	PHE	CE1-CZ	-18.56	1.02	1.37
1	J	52	PHE	CE2-CZ	-18.32	1.02	1.37
1	J	52	PHE	CG-CD1	-15.12	1.16	1.38
1	J	52	PHE	CG-CD2	-14.98	1.16	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	52	PHE	CD1-CG-CD2	-9.86	105.48	118.30
1	J	52	PHE	CB-CG-CD2	9.76	127.63	120.80
1	J	52	PHE	CB-CG-CD1	8.70	126.89	120.80
1	C	155	THR	N-CA-C	-7.54	90.64	111.00
1	J	52	PHE	CD1-CE1-CZ	7.54	129.15	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	155	THR	Mainchain

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	1604	0	1558	27	0
1	B	1620	0	1571	25	0
1	C	1632	0	1578	48	0
1	D	1603	0	1560	24	0
1	E	1600	0	1555	20	0
1	F	1607	0	1563	23	0
1	G	1607	0	1563	44	0
1	H	1604	0	1558	25	0
1	I	1603	0	1560	24	0
1	J	1604	0	1558	28	0
1	K	1594	0	1549	30	0
1	L	1603	0	1560	28	0
1	M	1597	0	1553	23	0
1	N	1586	0	1546	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1601	0	1556	40	0
1	P	1603	0	1559	26	0
1	Q	1617	0	1589	31	0
1	R	1594	0	1549	28	0
1	S	1599	0	1559	24	0
1	T	1620	0	1583	27	0
2	A	13	0	20	1	0
2	B	13	0	20	3	0
2	C	13	0	20	2	0
2	D	13	0	20	2	0
2	E	13	0	20	2	0
2	F	13	0	20	2	0
2	G	13	0	20	2	0
2	H	13	0	20	3	0
2	I	13	0	20	3	0
2	J	13	0	20	3	0
2	K	13	0	20	5	0
2	L	13	0	20	3	0
2	M	13	0	20	2	0
2	N	13	0	20	4	0
2	O	13	0	20	3	0
2	P	13	0	20	3	0
2	Q	13	0	20	2	0
2	R	13	0	20	2	0
2	S	13	0	20	2	0
2	T	13	0	20	1	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
3	C	10	0	0	1	0
3	E	10	0	0	1	0
3	F	10	0	0	0	0
3	H	10	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	3	0
3	L	10	0	0	1	0
3	N	10	0	0	0	0
3	O	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	10	0	0	1	0
4	M	14	0	13	0	0
4	O	14	0	13	1	0
4	P	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	7	10	10	0	0
6	R	16	0	22	7	0
7	A	116	0	0	4	0
7	B	109	0	0	7	0
7	C	112	0	0	1	0
7	D	121	0	0	2	0
7	E	91	0	0	1	1
7	F	136	0	0	8	0
7	G	106	0	0	4	0
7	H	125	0	0	3	0
7	I	91	0	0	1	0
7	J	89	0	0	7	0
7	K	72	0	0	3	0
7	L	104	0	0	4	0
7	M	90	0	0	4	0
7	N	97	0	0	5	0
7	O	76	0	0	4	1
7	P	127	0	0	7	0
7	Q	93	0	0	4	0
7	R	82	0	0	3	0
7	S	100	0	0	5	0
7	T	105	0	0	1	0
All	All	34565	10	31698	521	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 521 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH2	1:G:23:ARG:HE	1.24	1.30
1:C:23:ARG:HH21	1:G:23:ARG:NE	1.32	1.26
1:C:155:THR:O	1:G:182:SER:O	1.65	1.13
1:C:25:ARG:HH21	1:G:25:ARG:NH2	1.56	1.03
1:I:152:VAL:HG13	1:I:195:VAL:HG23	1.42	1.01

All (1) 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)
7:E:2011:HOH:O	7:O:2076:HOH:O[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	B	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
1	C	202/210 (96%)	198 (98%)	3 (2%)	1 (0%)	34	53
1	D	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	E	196/210 (93%)	194 (99%)	2 (1%)	0	100	100
1	F	198/210 (94%)	195 (98%)	3 (2%)	0	100	100
1	G	198/210 (94%)	194 (98%)	4 (2%)	0	100	100
1	H	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	I	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	J	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	K	195/210 (93%)	191 (98%)	4 (2%)	0	100	100
1	L	197/210 (94%)	194 (98%)	3 (2%)	0	100	100
1	M	196/210 (93%)	193 (98%)	3 (2%)	0	100	100
1	N	194/210 (92%)	192 (99%)	2 (1%)	0	100	100
1	O	197/210 (94%)	194 (98%)	3 (2%)	0	100	100
1	P	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	Q	199/210 (95%)	197 (99%)	2 (1%)	0	100	100
1	R	195/210 (93%)	192 (98%)	3 (2%)	0	100	100
1	S	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	T	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
All	All	3946/4200 (94%)	3888 (98%)	57 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	156	THR

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	187/196 (95%)	185 (99%)	2 (1%)	80	93
1	B	190/196 (97%)	189 (100%)	1 (0%)	92	97
1	C	191/196 (97%)	187 (98%)	4 (2%)	61	84
1	D	188/196 (96%)	185 (98%)	3 (2%)	70	89
1	E	187/196 (95%)	185 (99%)	2 (1%)	80	93
1	F	188/196 (96%)	186 (99%)	2 (1%)	80	93
1	G	188/196 (96%)	186 (99%)	2 (1%)	80	93
1	H	187/196 (95%)	185 (99%)	2 (1%)	80	93
1	I	188/196 (96%)	184 (98%)	4 (2%)	61	84
1	J	187/196 (95%)	186 (100%)	1 (0%)	92	97
1	K	186/196 (95%)	184 (99%)	2 (1%)	80	93
1	L	188/196 (96%)	184 (98%)	4 (2%)	61	84
1	M	187/196 (95%)	185 (99%)	2 (1%)	80	93
1	N	185/196 (94%)	183 (99%)	2 (1%)	80	93
1	O	187/196 (95%)	182 (97%)	5 (3%)	52	78
1	P	188/196 (96%)	184 (98%)	4 (2%)	61	84
1	Q	189/196 (96%)	185 (98%)	4 (2%)	61	84
1	R	186/196 (95%)	184 (99%)	2 (1%)	80	93
1	S	187/196 (95%)	185 (99%)	2 (1%)	80	93
1	T	190/196 (97%)	186 (98%)	4 (2%)	61	84
All	All	3754/3920 (96%)	3700 (99%)	54 (1%)	76	90

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	203	LYS
1	M	203	LYS
1	S	203	LYS
1	L	152	VAL
1	L	187[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	178	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

45 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1206	-	4,4,4	0.37	0	6,6,6	0.44	0
2	XRX	A	301	-	12,12,12	1.65	1 (8%)	13,15,15	1.08	1 (7%)
3	SO4	B	1206	-	4,4,4	0.46	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XRX	B	301	-	12,12,12	1.45	1 (8%)	13,15,15	1.43	3 (23%)
3	SO4	C	1205	-	4,4,4	0.30	0	6,6,6	0.28	0
3	SO4	C	1206	-	4,4,4	0.33	0	6,6,6	0.41	0
2	XRX	C	301	-	12,12,12	1.71	1 (8%)	13,15,15	0.82	0
2	XRX	D	301	-	12,12,12	1.26	2 (16%)	13,15,15	1.14	0
3	SO4	E	1205	-	4,4,4	0.46	0	6,6,6	0.37	0
3	SO4	E	1206	-	4,4,4	0.35	0	6,6,6	0.24	0
2	XRX	E	301	-	12,12,12	1.42	1 (8%)	13,15,15	1.13	1 (7%)
3	SO4	F	1206	-	4,4,4	0.53	0	6,6,6	0.31	0
3	SO4	F	1207	-	4,4,4	0.37	0	6,6,6	0.17	0
2	XRX	F	301	-	12,12,12	1.43	1 (8%)	13,15,15	1.40	2 (15%)
2	XRX	G	301	-	12,12,12	1.51	1 (8%)	13,15,15	1.11	1 (7%)
3	SO4	H	1206	-	4,4,4	0.39	0	6,6,6	0.27	0
3	SO4	H	1207	-	4,4,4	0.35	0	6,6,6	0.12	0
2	XRX	H	301	-	12,12,12	1.86	2 (16%)	13,15,15	1.27	2 (15%)
2	XRX	I	301	-	12,12,12	1.62	1 (8%)	13,15,15	1.15	2 (15%)
3	SO4	J	1206	-	4,4,4	0.14	0	6,6,6	0.27	0
2	XRX	J	301	-	12,12,12	1.62	2 (16%)	13,15,15	1.06	1 (7%)
3	SO4	K	1205	-	4,4,4	0.25	0	6,6,6	0.18	0
2	XRX	K	301	-	12,12,12	1.31	1 (8%)	13,15,15	1.63	2 (15%)
3	SO4	L	1205	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	L	1206	-	4,4,4	0.26	0	6,6,6	0.31	0
2	XRX	L	301	-	12,12,12	1.32	2 (16%)	13,15,15	0.98	0
2	XRX	M	301	-	12,12,12	1.40	1 (8%)	13,15,15	1.27	2 (15%)
4	NAG	M	401	1	14,14,15	0.92	0	15,19,21	1.84	2 (13%)
5	PEG	M	501	-	6,6,6	0.69	0	5,5,5	0.66	0
3	SO4	N	1205	-	4,4,4	0.38	0	6,6,6	0.30	0
3	SO4	N	1206	-	4,4,4	0.21	0	6,6,6	0.16	0
2	XRX	N	301	-	12,12,12	1.41	1 (8%)	13,15,15	1.11	1 (7%)
3	SO4	O	1206	-	4,4,4	0.12	0	6,6,6	0.27	0
2	XRX	O	301	-	12,12,12	1.51	1 (8%)	13,15,15	1.22	1 (7%)
4	NAG	O	401	1	14,14,15	0.77	0	15,19,21	1.71	2 (13%)
2	XRX	P	301	-	12,12,12	1.89	3 (25%)	13,15,15	1.22	1 (7%)
4	NAG	P	401	1	14,14,15	0.64	0	15,19,21	2.00	3 (20%)
3	SO4	Q	1206	-	4,4,4	0.42	0	6,6,6	0.20	0
2	XRX	Q	301	-	12,12,12	1.59	2 (16%)	13,15,15	1.40	2 (15%)
3	SO4	R	1205	-	4,4,4	0.44	0	6,6,6	0.35	0
3	SO4	R	1206	-	4,4,4	0.45	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XRX	R	301	-	12,12,12	1.72	3 (25%)	13,15,15	1.31	3 (23%)
6	1PE	R	501	-	15,15,15	0.97	0	14,14,14	1.96	6 (42%)
2	XRX	S	301	-	12,12,12	1.55	1 (8%)	13,15,15	1.15	1 (7%)
2	XRX	T	301	-	12,12,12	1.15	1 (8%)	13,15,15	0.95	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	A	301	-	-	0/14/14/14	0/0/0/0
3	SO4	B	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	B	301	-	-	0/14/14/14	0/0/0/0
3	SO4	C	1205	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	C	301	-	-	0/14/14/14	0/0/0/0
2	XRX	D	301	-	-	0/14/14/14	0/0/0/0
3	SO4	E	1205	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	E	301	-	-	0/14/14/14	0/0/0/0
3	SO4	F	1206	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1207	-	-	0/0/0/0	0/0/0/0
2	XRX	F	301	-	-	0/14/14/14	0/0/0/0
2	XRX	G	301	-	-	0/14/14/14	0/0/0/0
3	SO4	H	1206	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1207	-	-	0/0/0/0	0/0/0/0
2	XRX	H	301	-	-	0/14/14/14	0/0/0/0
2	XRX	I	301	-	-	0/14/14/14	0/0/0/0
3	SO4	J	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	J	301	-	-	0/14/14/14	0/0/0/0
3	SO4	K	1205	-	-	0/0/0/0	0/0/0/0
2	XRX	K	301	-	-	0/14/14/14	0/0/0/0
3	SO4	L	1205	-	-	0/0/0/0	0/0/0/0
3	SO4	L	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	L	301	-	-	0/14/14/14	0/0/0/0
2	XRX	M	301	-	-	0/14/14/14	0/0/0/0
4	NAG	M	401	1	-	0/6/23/26	0/1/1/1
5	PEG	M	501	-	-	0/4/4/4	0/0/0/0
3	SO4	N	1205	-	-	0/0/0/0	0/0/0/0
3	SO4	N	1206	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XRX	N	301	-	-	0/14/14/14	0/0/0/0
3	SO4	O	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	O	301	-	-	0/14/14/14	0/0/0/0
4	NAG	O	401	1	-	0/6/23/26	0/1/1/1
2	XRX	P	301	-	-	0/14/14/14	0/0/0/0
4	NAG	P	401	1	-	0/6/23/26	0/1/1/1
3	SO4	Q	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	Q	301	-	-	0/14/14/14	0/0/0/0
3	SO4	R	1205	-	-	0/0/0/0	0/0/0/0
3	SO4	R	1206	-	-	0/0/0/0	0/0/0/0
2	XRX	R	301	-	-	0/14/14/14	0/0/0/0
6	1PE	R	501	-	-	0/13/13/13	0/0/0/0
2	XRX	S	301	-	-	0/14/14/14	0/0/0/0
2	XRX	T	301	-	-	0/14/14/14	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	XRX	C7-N1	2.08	1.51	1.48
2	H	301	XRX	O3-C9	2.10	1.38	1.34
2	J	301	XRX	O6-C9	2.15	1.24	1.21
2	R	301	XRX	O6-C9	2.17	1.24	1.21
2	L	301	XRX	C7-N1	2.28	1.51	1.48

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	XRX	C11-C7-N1	-4.85	105.12	114.26
4	P	401	NAG	C2-N2-C7	-4.31	117.50	123.04
4	O	401	NAG	C1-O5-C5	-3.90	107.30	112.25
6	R	501	1PE	OH4-C24-C14	-3.39	95.28	110.36
2	F	301	XRX	O3-C9-O6	-3.37	119.07	124.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1206	SO4	2	0
2	A	301	XRX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1206	SO4	1	0
2	B	301	XRX	3	0
3	C	1206	SO4	1	0
2	C	301	XRX	2	0
2	D	301	XRX	2	0
3	E	1205	SO4	1	0
2	E	301	XRX	2	0
2	F	301	XRX	2	0
2	G	301	XRX	2	0
2	H	301	XRX	3	0
2	I	301	XRX	3	0
2	J	301	XRX	3	0
3	K	1205	SO4	3	0
2	K	301	XRX	5	0
3	L	1206	SO4	1	0
2	L	301	XRX	3	0
2	M	301	XRX	2	0
2	N	301	XRX	4	0
2	O	301	XRX	3	0
4	O	401	NAG	1	0
2	P	301	XRX	3	0
4	P	401	NAG	1	0
3	Q	1206	SO4	1	0
2	Q	301	XRX	2	0
3	R	1205	SO4	1	0
2	R	301	XRX	2	0
6	R	501	1PE	7	0
2	S	301	XRX	2	0
2	T	301	XRX	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	200/210 (95%)	0.07	11 (5%) 29 32	13, 23, 49, 73	0
1	B	201/210 (95%)	0.11	9 (4%) 37 41	11, 22, 48, 81	0
1	C	204/210 (97%)	0.19	9 (4%) 38 42	14, 22, 44, 78	0
1	D	199/210 (94%)	-0.01	8 (4%) 42 46	10, 21, 45, 63	0
1	E	199/210 (94%)	0.09	10 (5%) 32 36	12, 22, 43, 84	0
1	F	200/210 (95%)	0.18	15 (7%) 17 18	10, 20, 47, 81	0
1	G	200/210 (95%)	0.02	9 (4%) 37 41	10, 20, 44, 83	0
1	H	200/210 (95%)	-0.06	5 (2%) 61 64	11, 19, 42, 65	0
1	I	199/210 (94%)	0.07	9 (4%) 37 41	11, 23, 43, 85	0
1	J	200/210 (95%)	0.03	8 (4%) 42 46	14, 24, 45, 82	0
1	K	199/210 (94%)	0.12	7 (3%) 48 52	15, 28, 53, 78	0
1	L	199/210 (94%)	0.08	10 (5%) 32 36	11, 23, 48, 84	0
1	M	199/210 (94%)	0.03	9 (4%) 37 41	12, 23, 42, 72	0
1	N	197/210 (93%)	0.15	11 (5%) 28 31	13, 24, 52, 79	0
1	O	200/210 (95%)	0.01	11 (5%) 29 32	15, 26, 50, 69	0
1	P	199/210 (94%)	-0.02	6 (3%) 54 58	12, 23, 45, 64	0
1	Q	198/210 (94%)	-0.02	6 (3%) 54 58	13, 24, 48, 70	0
1	R	199/210 (94%)	0.16	12 (6%) 25 28	13, 24, 47, 79	0
1	S	199/210 (94%)	0.14	7 (3%) 48 52	13, 24, 51, 65	0
1	T	200/210 (95%)	-0.04	3 (1%) 76 79	10, 22, 46, 82	0
All	All	3991/4200 (95%)	0.06	175 (4%) 38 42	10, 23, 48, 85	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	205	GLY	5.2
1	S	162	SER	5.0
1	H	67	SER	5.0
1	L	23	ARG	4.9
1	B	68	SER	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
5	PEG	M	501	7/7	0.78	0.26	6.81	29,40,61,73	0
3	SO4	L	1206	5/5	0.87	0.43	5.66	48,52,74,76	0
3	SO4	B	1206	5/5	0.80	0.52	5.08	51,57,65,79	0
2	XRX	S	301	13/13	0.97	0.20	4.18	15,20,23,27	0
3	SO4	C	1205	5/5	0.92	0.38	4.13	57,59,74,81	0
3	SO4	Q	1206	5/5	0.90	0.27	3.73	52,60,64,74	0
6	1PE	R	501	16/16	0.89	0.26	3.22	26,34,46,59	0
3	SO4	R	1206	5/5	0.81	0.30	2.89	47,58,69,94	0
3	SO4	N	1205	5/5	0.93	0.29	2.77	44,44,45,51	0
3	SO4	R	1205	5/5	0.92	0.22	2.68	40,43,61,65	0
3	SO4	H	1207	5/5	0.85	0.27	2.58	55,55,68,82	0
2	XRX	L	301	13/13	0.98	0.18	2.40	12,14,17,20	0
3	SO4	K	1205	5/5	0.92	0.23	2.26	54,60,73,80	0
2	XRX	N	301	13/13	0.97	0.15	1.93	14,18,21,22	0
2	XRX	F	301	13/13	0.98	0.17	1.76	8,11,16,16	0
3	SO4	E	1206	5/5	0.84	0.28	1.76	52,53,61,78	0
2	XRX	H	301	13/13	0.98	0.15	1.75	13,17,19,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	XRX	K	301	13/13	0.97	0.19	1.46	20,22,27,27	0
3	SO4	A	1206	5/5	0.84	0.30	1.23	52,55,64,77	0
3	SO4	F	1207	5/5	0.90	0.26	1.18	45,53,61,71	0
2	XRX	O	301	13/13	0.98	0.15	1.11	17,22,28,29	0
2	XRX	M	301	13/13	0.97	0.16	0.95	13,19,24,26	0
2	XRX	T	301	13/13	0.97	0.15	0.91	11,13,18,22	0
2	XRX	D	301	13/13	0.97	0.14	0.90	12,16,18,20	0
2	XRX	E	301	13/13	0.98	0.15	0.47	12,17,20,21	0
2	XRX	C	301	13/13	0.97	0.15	0.27	14,18,20,21	0
2	XRX	B	301	13/13	0.98	0.14	0.20	13,16,18,19	0
2	XRX	G	301	13/13	0.98	0.13	0.14	12,15,19,20	0
4	NAG	M	401	14/15	0.82	0.22	0.14	38,46,56,57	0
2	XRX	I	301	13/13	0.98	0.14	0.10	16,19,23,23	0
2	XRX	J	301	13/13	0.97	0.14	0.06	14,18,22,23	0
2	XRX	Q	301	13/13	0.96	0.14	-0.15	15,20,25,29	0
4	NAG	O	401	14/15	0.79	0.24	-0.21	49,62,68,69	0
4	NAG	P	401	14/15	0.74	0.21	-0.24	51,63,74,75	0
2	XRX	P	301	13/13	0.97	0.13	-0.27	13,17,20,21	0
2	XRX	R	301	13/13	0.97	0.13	-0.40	12,16,20,22	0
3	SO4	L	1205	5/5	0.94	0.14	-0.46	47,47,60,61	0
2	XRX	A	301	13/13	0.98	0.12	-0.70	13,18,21,24	0
3	SO4	E	1205	5/5	0.86	0.28	-	40,50,63,79	0
3	SO4	O	1206	5/5	0.91	0.15	-	71,72,83,95	0
3	SO4	F	1206	5/5	0.91	0.15	-	50,54,62,77	0
3	SO4	H	1206	5/5	0.92	0.18	-	52,55,63,76	0
3	SO4	N	1206	5/5	0.78	0.35	-	60,64,90,94	0
3	SO4	C	1206	5/5	0.81	0.26	-	51,58,68,88	0
3	SO4	J	1206	5/5	0.85	0.29	-	56,71,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.