



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:45 AM BST

PDB ID : 3U8J
Title : Crystal structure of the acetylcholine binding protein (AChBP) from *Lymnaea stagnalis* in complex with NS3531 (1-(pyridin-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 : 2.35 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

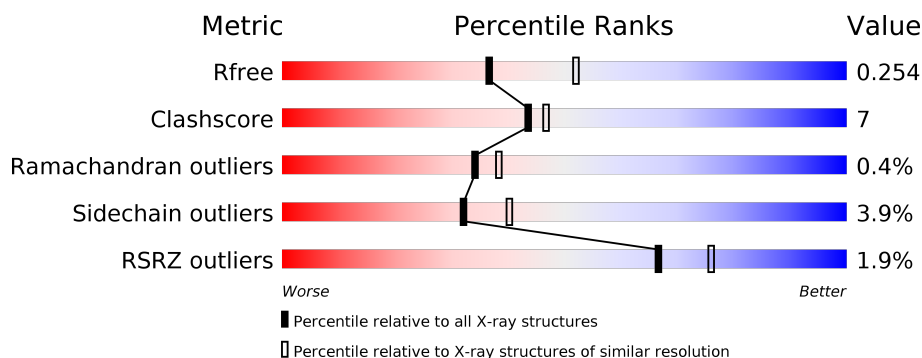
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	
1	B	210	
1	C	210	
1	D	210	
1	E	210	
1	F	210	

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Mol	Chain	Length	Quality of chain
1	G	210	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>85%</div><div>10%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	210	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>83%</div><div>9%</div><div></div><div>5%</div></div><div><div></div><div></div><div></div></div></div>
1	I	210	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>79%</div><div>15%</div><div></div><div>5%</div></div><div><div></div><div></div><div></div></div></div>
1	J	210	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>82%</div><div>11%</div><div></div><div>5%</div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition

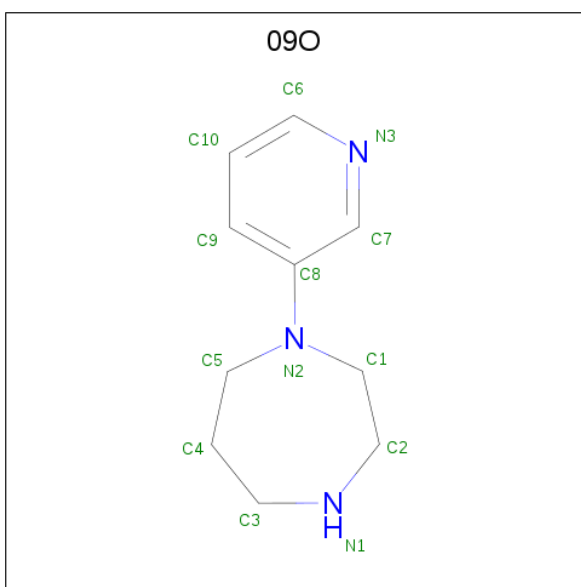
There are 5 unique types of molecules in this entry. The entry contains 16887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	B	210	Total	C	N	O	S	0	0	0
			1678	1049	288	336	5			
1	A	206	Total	C	N	O	S	0	0	0
			1647	1029	284	329	5			
1	C	204	Total	C	N	O	S	0	0	0
			1632	1021	279	327	5			
1	D	204	Total	C	N	O	S	0	1	0
			1640	1026	282	327	5			
1	E	198	Total	C	N	O	S	0	1	0
			1594	1002	275	312	5			
1	F	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	G	203	Total	C	N	O	S	0	0	0
			1617	1013	275	324	5			
1	J	199	Total	C	N	O	S	0	0	0
			1594	1001	273	315	5			
1	I	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			
1	H	200	Total	C	N	O	S	0	0	0
			1602	1005	274	318	5			

- Molecule 2 is 1-(pyridin-3-yl)-1,4-diazepane (three-letter code: 09O) (formula: C₁₀H₁₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	N	0	0
			13	10	3		
2	A	1	Total	C	N	0	0
			13	10	3		
2	C	1	Total	C	N	0	0
			13	10	3		
2	D	1	Total	C	N	0	0
			13	10	3		
2	E	1	Total	C	N	0	0
			13	10	3		
2	F	1	Total	C	N	0	0
			13	10	3		
2	G	1	Total	C	N	0	0
			13	10	3		
2	J	1	Total	C	N	0	0
			13	10	3		
2	I	1	Total	C	N	0	0
			13	10	3		
2	H	1	Total	C	N	0	0
			13	10	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

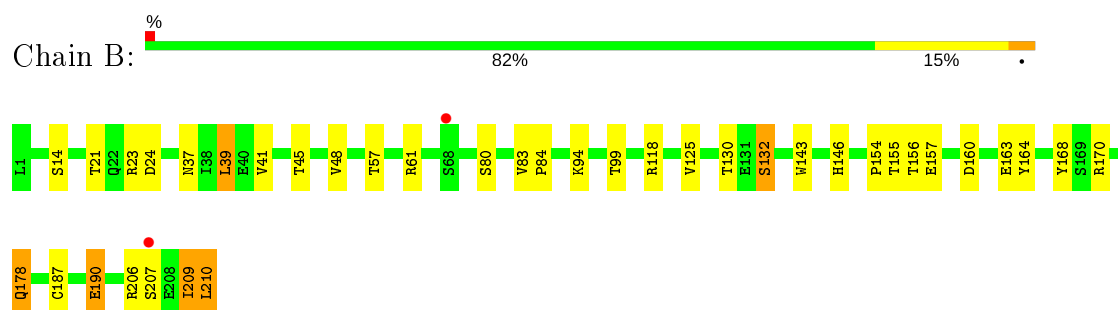
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	63	Total	O	0	0
			63	63		
5	A	71	Total	O	0	0
			71	71		
5	C	63	Total	O	0	0
			63	63		
5	D	56	Total	O	0	0
			56	56		
5	E	51	Total	O	0	0
			51	51		
5	F	50	Total	O	0	0
			50	50		
5	G	31	Total	O	0	0
			31	31		
5	J	46	Total	O	0	0
			46	46		
5	I	52	Total	O	0	0
			52	52		
5	H	42	Total	O	0	0
			42	42		

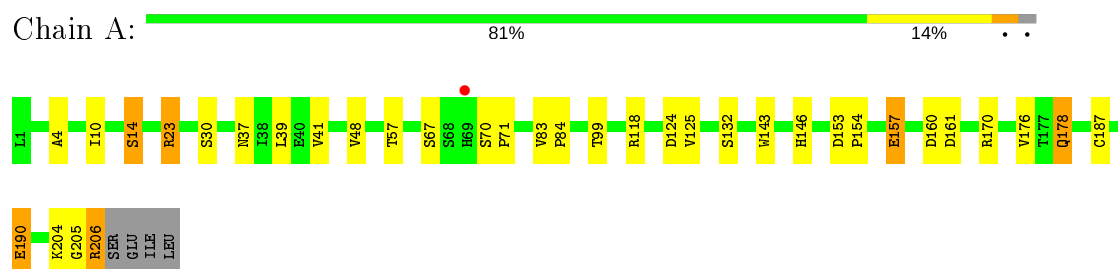
3 Residue-property plots [i](#)

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.

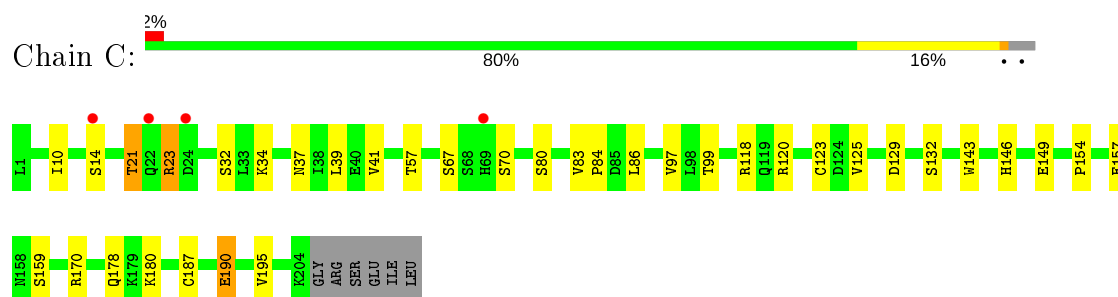
- Molecule 1: Acetylcholine-binding protein



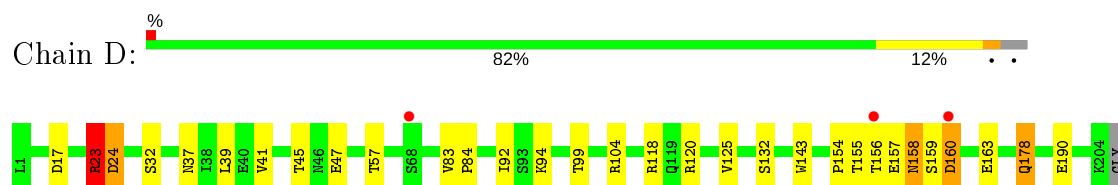
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein




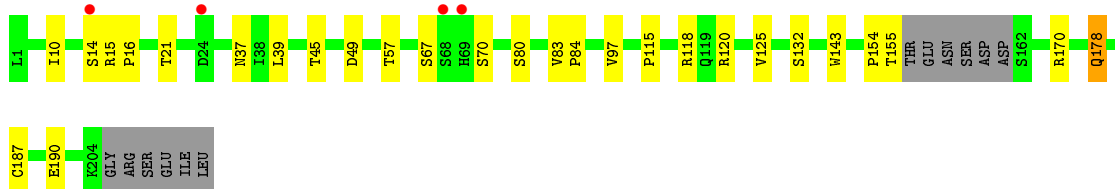
- Molecule 1: Acetylcholine-binding protein




ARG
SER
GLU
ILE
LEU

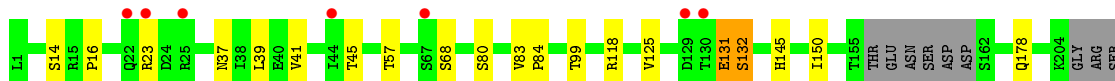
• Molecule 1: Acetylcholine-binding protein

Chain E: 




• Molecule 1: Acetylcholine-binding protein

Chain F: 




GLU
ILE
LEU

• Molecule 1: Acetylcholine-binding protein

Chain G: 




• Molecule 1: Acetylcholine-binding protein

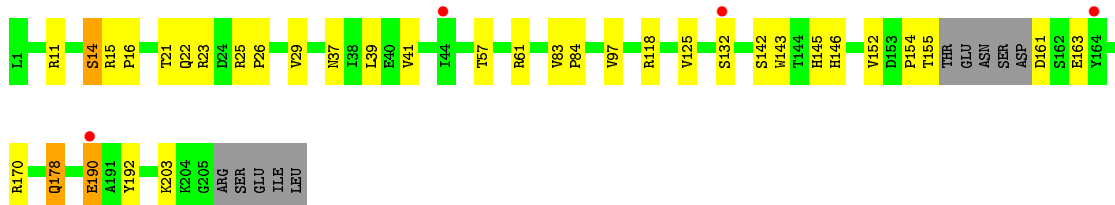
Chain J: 



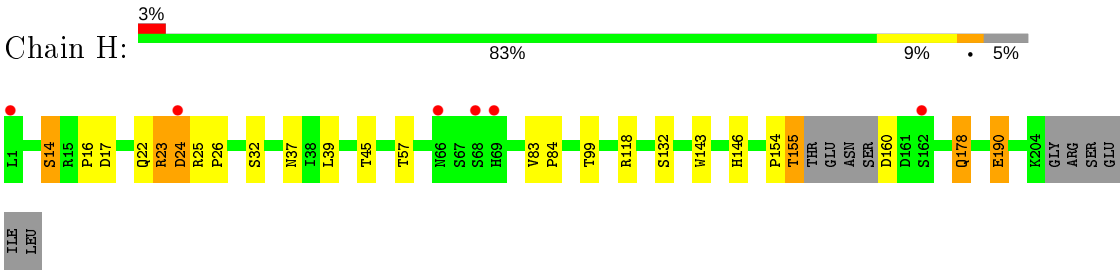
ARG
SER
GLU
ILE
LEU

• Molecule 1: Acetylcholine-binding protein

Chain I: 



● Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.35Å 114.43Å 247.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.88 – 2.35 44.88 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.88-2.35) 96.5 (44.88-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.205 , 0.258 0.202 , 0.254	Depositor DCC
R_{free} test set	1646 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16887	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 09O, SO4, NAG

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	0.41	0/1683	0.56	0/2296
1	B	0.41	0/1714	0.57	0/2338
1	C	0.42	0/1668	0.91	4/2277 (0.2%)
1	D	0.39	0/1679	0.52	0/2291
1	E	0.41	0/1632	0.52	0/2225
1	F	0.38	0/1621	0.53	0/2211
1	G	0.39	0/1652	0.54	0/2254
1	H	0.37	0/1637	0.54	0/2233
1	I	0.38	0/1633	0.51	0/2227
1	J	0.39	0/1629	0.55	0/2222
All	All	0.39	0/16548	0.59	4/22574 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	ARG	NE-CZ-NH1	-23.99	108.31	120.30
1	C	120	ARG	NE-CZ-NH2	22.65	131.62	120.30
1	C	120	ARG	CD-NE-CZ	11.53	139.74	123.60
1	C	120	ARG	CG-CD-NE	-5.27	100.72	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1647	0	1594	33	0
1	B	1678	0	1627	30	0
1	C	1632	0	1578	26	0
1	D	1640	0	1591	21	0
1	E	1594	0	1558	24	0
1	F	1586	0	1545	13	0
1	G	1617	0	1561	17	0
1	H	1602	0	1553	21	0
1	I	1598	0	1552	30	0
1	J	1594	0	1549	22	0
2	A	13	0	15	2	0
2	B	13	0	15	2	0
2	C	13	0	15	1	0
2	D	13	0	15	1	0
2	E	13	0	15	1	0
2	F	13	0	15	0	0
2	G	13	0	15	1	0
2	H	13	0	15	2	0
2	I	13	0	15	3	0
2	J	13	0	15	3	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	G	14	0	13	1	0
5	A	71	0	0	2	0
5	B	63	0	0	4	0
5	C	63	0	0	3	0
5	D	56	0	0	1	0
5	E	51	0	0	3	0
5	F	50	0	0	0	0
5	G	31	0	0	0	0
5	H	42	0	0	0	0
5	I	52	0	0	2	0
5	J	46	0	0	2	0
All	All	16887	0	15871	216	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 7.

The worst 5 of 216 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:A:206:ARG:HG2	1:A:206:ARG:HH11	1.15	1.08
1:I:154:PRO:HB3	1:I:178:GLN:HE21	1.20	1.02
1:H:32:SER:HB2	1:H:155:THR:HB	1.47	0.97
1:B:155:THR:HG22	1:B:156:THR:H	1.32	0.94
1:B:132:SER:HB2	5:B:669:HOH:O	1.75	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	204/210 (97%)	202 (99%)	2 (1%)	0	100	100
1	B	208/210 (99%)	204 (98%)	4 (2%)	0	100	100
1	C	202/210 (96%)	198 (98%)	3 (2%)	1 (0%)	29	32
1	D	203/210 (97%)	197 (97%)	4 (2%)	2 (1%)	15	15
1	E	195/210 (93%)	194 (100%)	1 (0%)	0	100	100
1	F	194/210 (92%)	192 (99%)	2 (1%)	0	100	100
1	G	199/210 (95%)	196 (98%)	2 (1%)	1 (0%)	29	32
1	H	196/210 (93%)	188 (96%)	5 (3%)	3 (2%)	10	8
1	I	196/210 (93%)	194 (99%)	2 (1%)	0	100	100
1	J	195/210 (93%)	192 (98%)	3 (2%)	0	100	100
All	All	1992/2100 (95%)	1957 (98%)	28 (1%)	7 (0%)	34	38

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ARG

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Mol	Chain	Res	Type
1	D	158	ASN
1	G	162	SER
1	H	22	GLN
1	H	23	ARG

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	192/196 (98%)	184 (96%)	8 (4%)	30	36
1	B	196/196 (100%)	184 (94%)	12 (6%)	18	20
1	C	191/196 (97%)	184 (96%)	7 (4%)	34	42
1	D	192/196 (98%)	184 (96%)	8 (4%)	30	36
1	E	186/196 (95%)	181 (97%)	5 (3%)	44	55
1	F	185/196 (94%)	179 (97%)	6 (3%)	39	47
1	G	189/196 (96%)	182 (96%)	7 (4%)	34	42
1	H	187/196 (95%)	180 (96%)	7 (4%)	34	42
1	I	186/196 (95%)	180 (97%)	6 (3%)	39	47
1	J	186/196 (95%)	178 (96%)	8 (4%)	29	35
All	All	1890/1960 (96%)	1816 (96%)	74 (4%)	32	40

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	178	GLN
1	F	57	THR
1	H	57	THR
1	D	190	GLU
1	E	132	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	178	GLN
1	E	178	GLN
1	I	22	GLN
1	D	158	ASN
1	J	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	212	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	G	212	-	4,4,4	0.13	0	6,6,6	0.20	0
2	09O	F	211	-	12,14,14	1.12	1 (8%)	13,17,17	0.68	0
4	NAG	G	213	1	14,14,15	0.52	0	17,19,21	1.53	3 (17%)
2	09O	D	211	-	12,14,14	1.12	1 (8%)	13,17,17	0.85	0
2	09O	J	211	-	12,14,14	1.01	1 (8%)	13,17,17	0.81	0
3	SO4	H	212	-	4,4,4	0.17	0	6,6,6	0.22	0
2	09O	I	211	-	12,14,14	1.06	1 (8%)	13,17,17	0.75	0
3	SO4	A	213	-	4,4,4	0.15	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	09O	B	211	-	12,14,14	1.25	1 (8%)	13,17,17	1.11	1 (7%)
2	09O	C	211	-	12,14,14	1.15	0	13,17,17	0.80	1 (7%)
2	09O	A	211	-	12,14,14	1.16	1 (8%)	13,17,17	0.83	0
2	09O	G	211	-	12,14,14	1.12	1 (8%)	13,17,17	0.70	0
3	SO4	E	212	-	4,4,4	0.16	0	6,6,6	0.16	0
2	09O	E	211	-	12,14,14	1.04	1 (8%)	13,17,17	1.00	1 (7%)
3	SO4	B	212	-	4,4,4	0.12	0	6,6,6	0.18	0
2	09O	H	211	-	12,14,14	1.05	0	13,17,17	0.70	0

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	09O	F	211	-	-	0/4/13/13	0/2/2/2
4	NAG	G	213	1	-	0/6/23/26	0/1/1/1
2	09O	D	211	-	-	0/4/13/13	0/2/2/2
2	09O	J	211	-	-	0/4/13/13	0/2/2/2
2	09O	I	211	-	-	0/4/13/13	0/2/2/2
2	09O	B	211	-	-	0/4/13/13	0/2/2/2
2	09O	C	211	-	-	0/4/13/13	0/2/2/2
2	09O	A	211	-	-	0/4/13/13	0/2/2/2
2	09O	G	211	-	-	0/4/13/13	0/2/2/2
2	09O	E	211	-	-	0/4/13/13	0/2/2/2
2	09O	H	211	-	-	0/4/13/13	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	09O	C7-C8	2.55	1.43	1.38
2	G	211	09O	C7-C8	2.34	1.43	1.38
2	A	211	09O	C7-C8	2.19	1.42	1.38
2	I	211	09O	C7-C8	2.18	1.42	1.38
2	D	211	09O	C7-C8	2.17	1.42	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	213	NAG	C1-O5-C5	-4.25	106.43	112.19
2	E	211	09O	C2-C1-N2	2.76	118.18	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	213	NAG	C4-C3-C2	-2.65	107.13	111.02
2	B	211	09O	C8-C7-N3	2.43	125.62	122.92
2	C	211	09O	C2-C1-N2	2.13	117.02	113.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	213	NAG	1	0
2	D	211	09O	1	0
2	J	211	09O	3	0
2	I	211	09O	3	0
3	A	213	SO4	1	0
2	B	211	09O	2	0
2	C	211	09O	1	0
2	A	211	09O	2	0
2	G	211	09O	1	0
2	E	211	09O	1	0
2	H	211	09O	2	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	206/210 (98%)	-0.20	1 (0%) 91 95	8, 19, 46, 73	0
1	B	210/210 (100%)	-0.23	2 (0%) 82 88	8, 21, 48, 76	0
1	C	204/210 (97%)	-0.21	4 (1%) 65 75	10, 21, 52, 72	0
1	D	204/210 (97%)	-0.17	3 (1%) 73 81	10, 21, 51, 80	0
1	E	198/210 (94%)	-0.16	4 (2%) 65 75	10, 20, 49, 71	0
1	F	198/210 (94%)	-0.14	7 (3%) 44 56	10, 23, 49, 68	0
1	G	203/210 (96%)	-0.09	4 (1%) 65 75	11, 23, 51, 75	0
1	H	200/210 (95%)	0.09	6 (3%) 50 61	19, 32, 64, 89	0
1	I	200/210 (95%)	0.07	4 (2%) 65 75	15, 30, 60, 81	0
1	J	199/210 (94%)	-0.20	3 (1%) 73 81	10, 21, 48, 82	0
All	All	2022/2100 (96%)	-0.13	38 (1%) 66 76	8, 23, 53, 89	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	SER	4.0
1	E	69	HIS	3.8
1	E	68	SER	3.5
1	F	22	GLN	3.4
1	J	25	ARG	3.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	SO4	E	212	5/5	0.87	0.23	59,89,99,102	0
3	SO4	H	212	5/5	0.88	0.18	65,68,85,96	0
4	NAG	G	213	14/15	0.88	0.18	53,78,93,97	0
3	SO4	G	212	5/5	0.91	0.19	61,72,99,102	0
3	SO4	B	212	5/5	0.91	0.14	60,76,86,93	0
3	SO4	A	212	5/5	0.95	0.19	83,86,90,91	0
2	09O	I	211	13/13	0.96	0.14	22,28,40,50	0
2	09O	B	211	13/13	0.96	0.15	6,23,31,37	0
2	09O	H	211	13/13	0.96	0.15	13,20,41,47	0
2	09O	A	211	13/13	0.97	0.14	8,22,33,36	0
2	09O	D	211	13/13	0.97	0.13	4,17,30,34	0
2	09O	E	211	13/13	0.97	0.13	5,18,36,43	0
3	SO4	A	213	5/5	0.97	0.14	43,66,72,86	0
2	09O	F	211	13/13	0.97	0.14	8,20,31,34	0
2	09O	J	211	13/13	0.98	0.14	16,24,32,34	0
2	09O	G	211	13/13	0.98	0.11	6,16,36,41	0
2	09O	C	211	13/13	0.98	0.13	9,16,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.