wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 05:42 PM EDT

PDB ID	:	4NZB
Title	:	NS9283 bound to Ls-AChBP
Authors	:	Olsen, J.A.; Kastrup, J.S.; Gajhede, M.
Deposited on	:	2013-12-11
Resolution	:	2.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

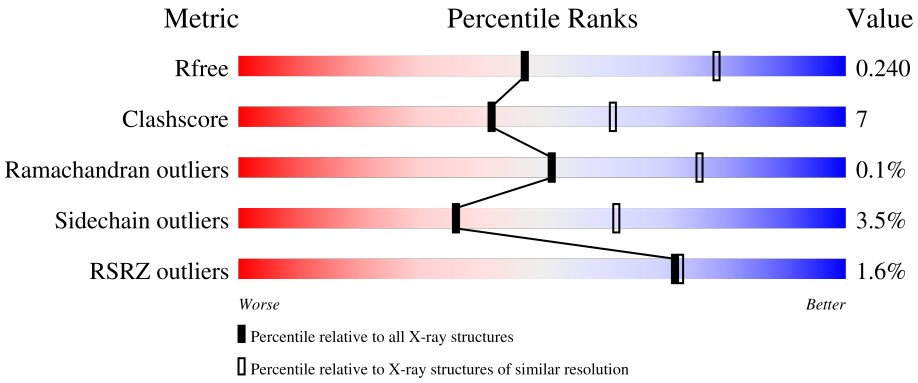
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	77% 15% • 6%
1	B	210	2% 77% 14% • 6%
1	C	210	% 77% 14% • • 6%
1	D	210	80% 11% • 6%
1	E	210	2% 76% 14% • • 6%

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Mol	Chain	Length	Quality of chain
1	F	210	2% 77% 15% 5%
1	G	210	% 75% 16% 6%
1	H	210	% 79% 12% 6%
1	I	210	2% 78% 13% 7%
1	J	210	% 76% 16% 6%
1	K	210	77% 14% 6%
1	L	210	% 79% 13% 6%
1	M	210	3% 80% 11% 8%
1	N	210	3% 78% 12% 6%
1	O	210	% 78% 14% 6%

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
4	SO4	F	302	-	-	-	X

2 Entry composition (i)

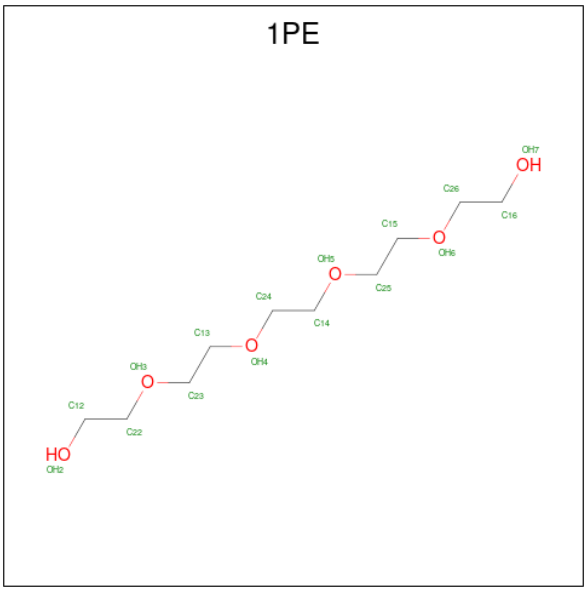
There are 9 unique types of molecules in this entry. The entry contains 24523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

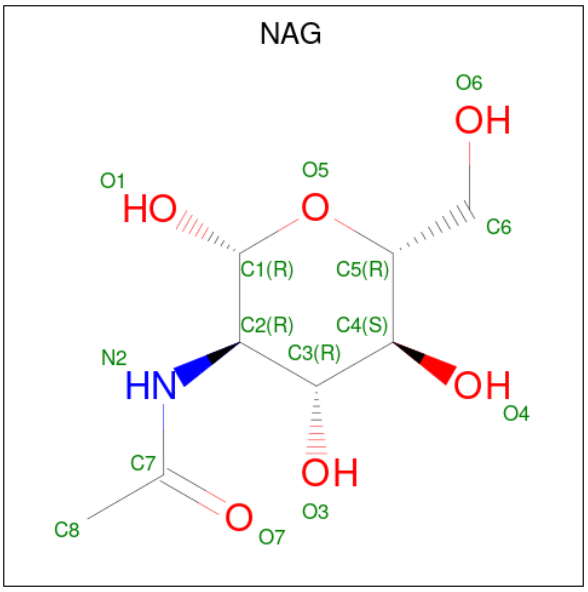
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	198	Total	C	N	O	S	0	1	0
			1591	1002	272	312	5			
1	D	197	Total	C	N	O	S	0	0	0
			1578	991	271	311	5			
1	E	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	A	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	B	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	C	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	F	200	Total	C	N	O	S	0	1	0
			1607	1010	274	318	5			
1	H	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	I	195	Total	C	N	O	S	0	0	0
			1568	988	269	308	3			
1	J	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	K	197	Total	C	N	O	S	0	0	0
			1571	989	268	309	5			
1	L	198	Total	C	N	O	S	0	1	0
			1591	1000	272	314	5			
1	M	194	Total	C	N	O	S	0	1	0
			1566	988	268	307	3			
1	N	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			
1	O	198	Total	C	N	O	S	0	0	0
			1586	997	272	312	5			

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



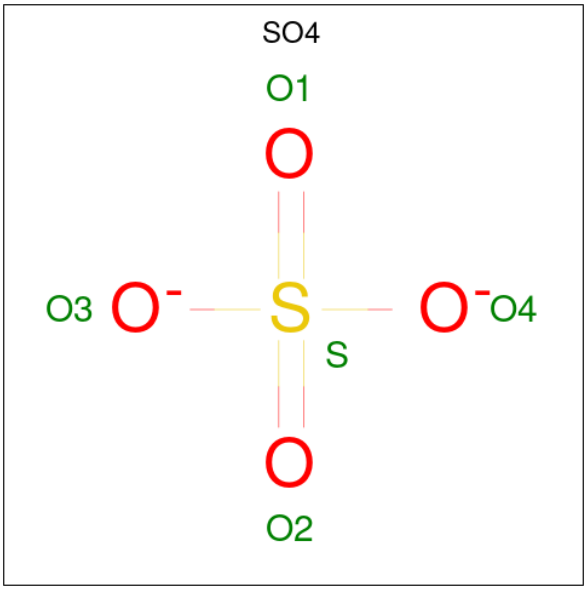
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 16 10 6	0	0
2	D	1	Total C O 16 10 6	0	0
2	E	1	Total C O 16 10 6	0	0
2	A	1	Total C O 16 10 6	0	0
2	B	1	Total C O 16 10 6	0	0
2	C	1	Total C O 16 10 6	0	0
2	H	1	Total C O 16 10 6	0	0
2	I	1	Total C O 16 10 6	0	0

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



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

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



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

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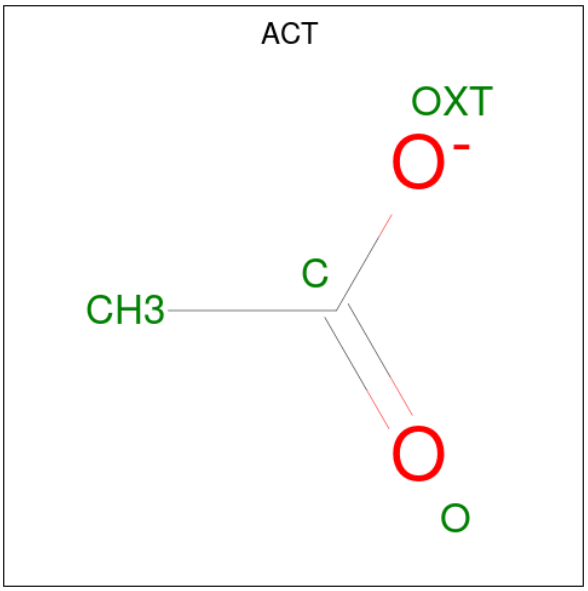
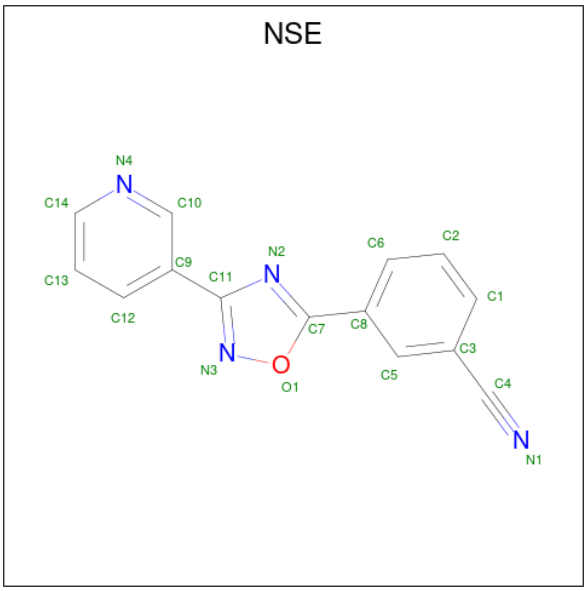
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0

- Molecule 6 is 3-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]benzonitrile (three-letter code: NSE) (formula: $C_{14}H_8N_4O$).

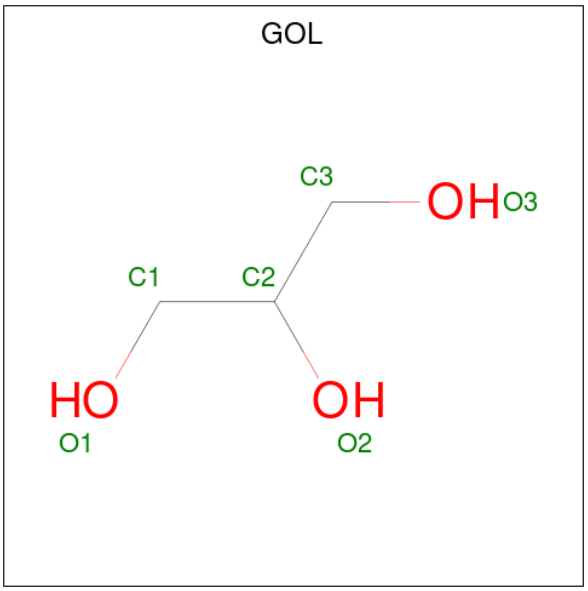


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 19 14 4 1	0	0
6	A	1	Total C N O 19 14 4 1	0	0
6	B	1	Total C N O 19 14 4 1	0	0
6	I	1	Total C N O 19 14 4 1	0	0
6	K	1	Total C N O 19 14 4 1	0	0
6	M	1	Total C N O 19 14 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	K	1	Total Cl 1 1	0	0
7	L	1	Total Cl 1 1	0	0
7	N	1	Total Cl 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	28	Total O 28 28	0	0
9	D	27	Total O 27 27	0	0
9	E	23	Total O 23 23	0	0
9	A	28	Total O 28 28	0	0
9	B	19	Total O 19 19	0	0
9	C	22	Total O 22 22	0	0
9	F	31	Total O 31 31	0	0
9	H	26	Total O 26 26	0	0
9	I	21	Total O 21 21	0	0
9	J	21	Total O 21 21	0	0
9	K	26	Total O 26 26	0	0

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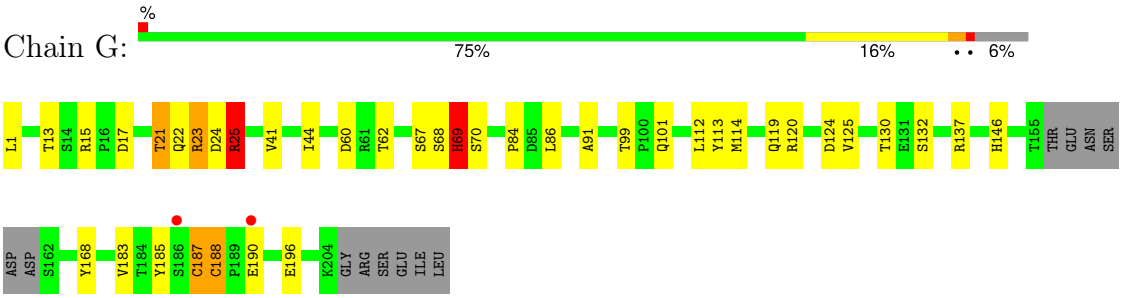
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	24	Total O 24 24	0	0
9	M	21	Total O 21 21	0	0
9	N	5	Total O 5 5	0	0
9	O	13	Total O 13 13	0	0

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.

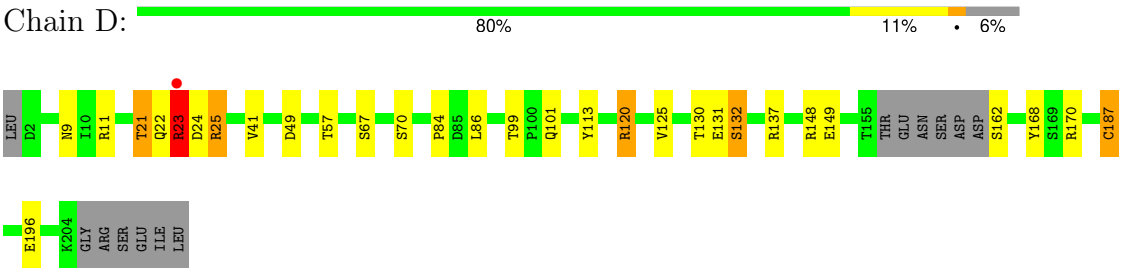
• Molecule 1: Acetylcholine-binding protein

Chain G:



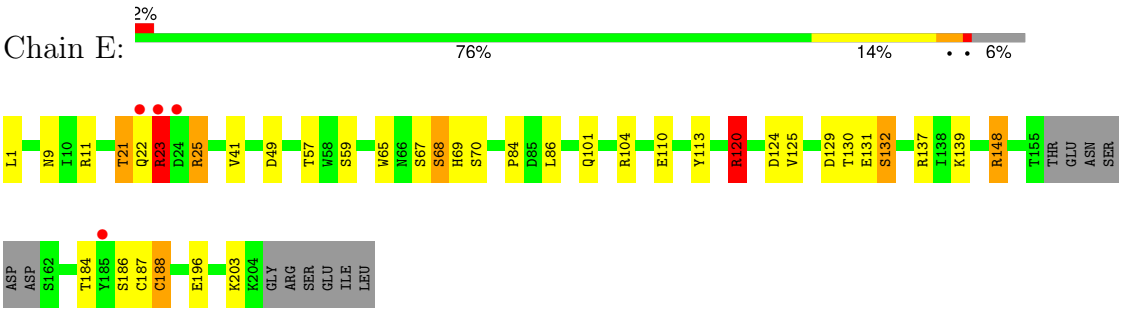
• Molecule 1: Acetylcholine-binding protein

Chain D:



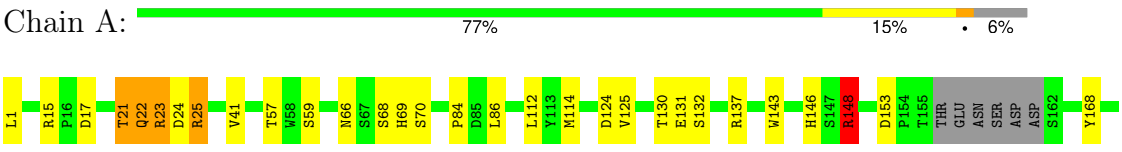
• Molecule 1: Acetylcholine-binding protein

Chain E:



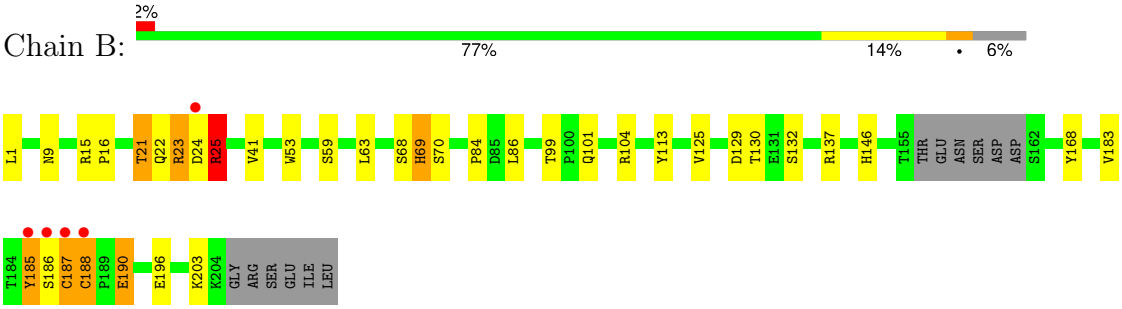
• Molecule 1: Acetylcholine-binding protein

Chain A:



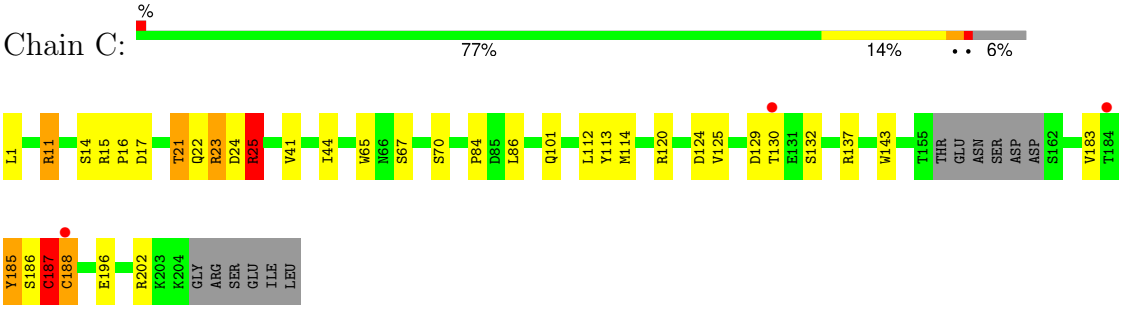
• Molecule 1: Acetylcholine-binding protein

Chain B:



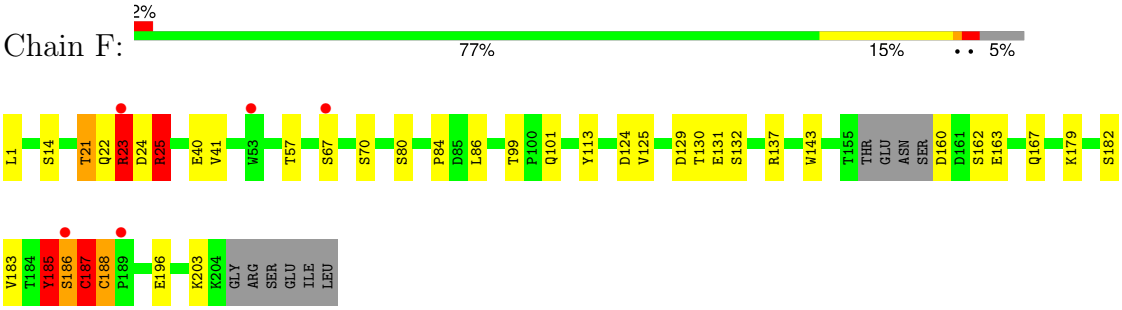
• Molecule 1: Acetylcholine-binding protein

Chain C:



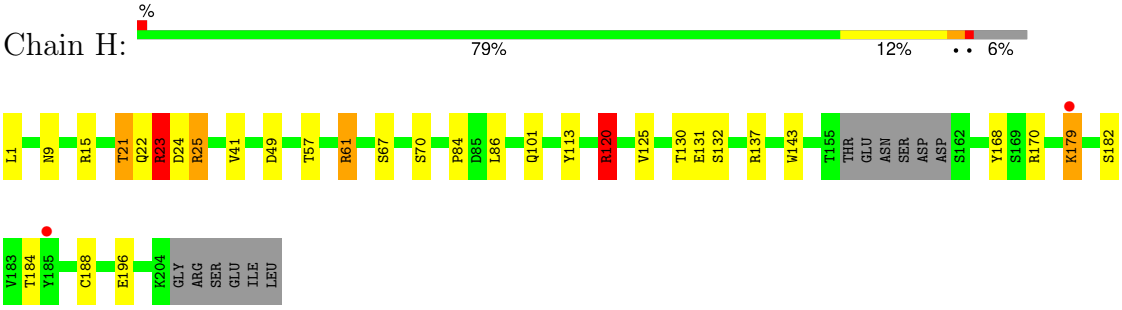
• Molecule 1: Acetylcholine-binding protein

Chain F:



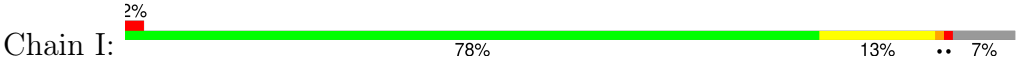
• Molecule 1: Acetylcholine-binding protein

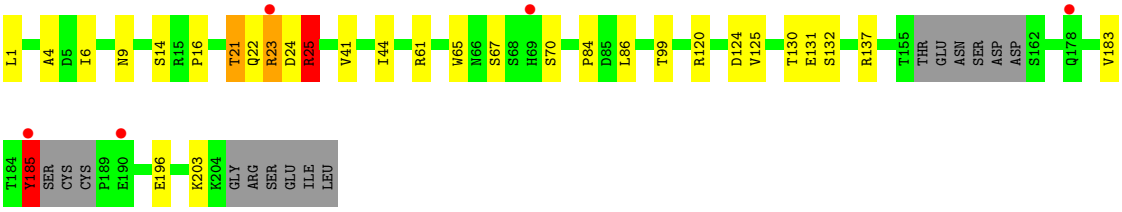
Chain H:



• Molecule 1: Acetylcholine-binding protein

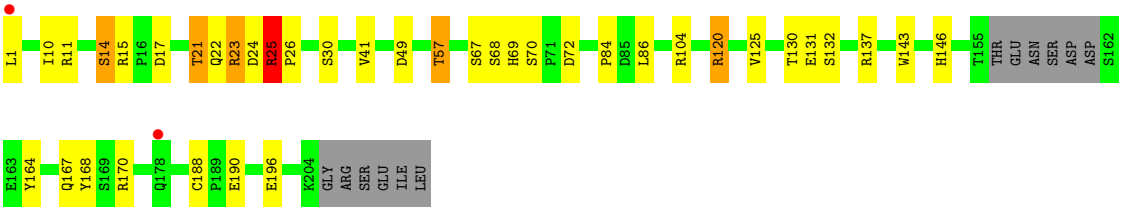
Chain I:





• Molecule 1: Acetylcholine-binding protein

Chain J:

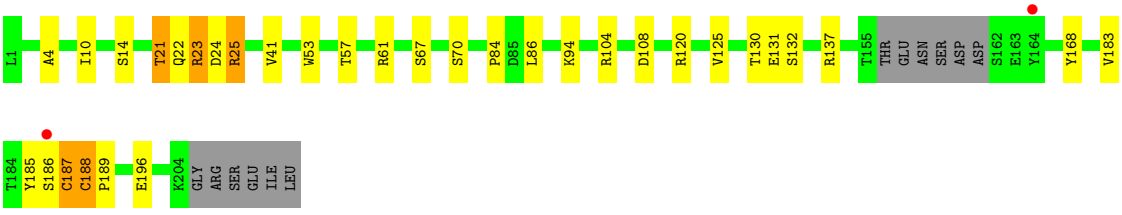


• Molecule 1: Acetylcholine-binding protein

Chain K:

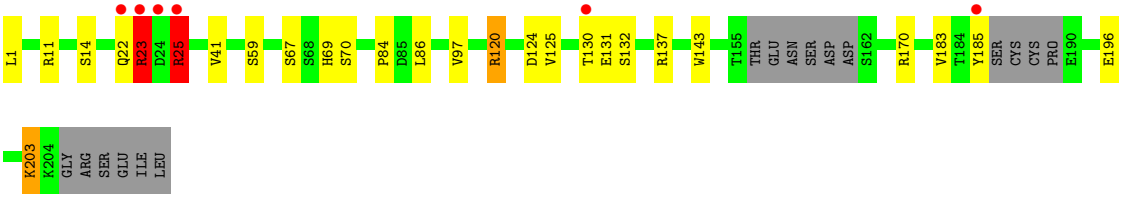
• Molecule 1: Acetylcholine-binding protein

Chain L:



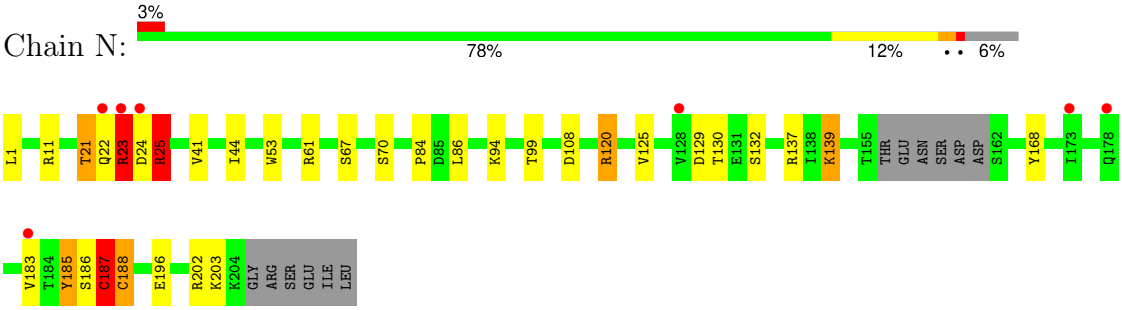
• Molecule 1: Acetylcholine-binding protein

Chain M:



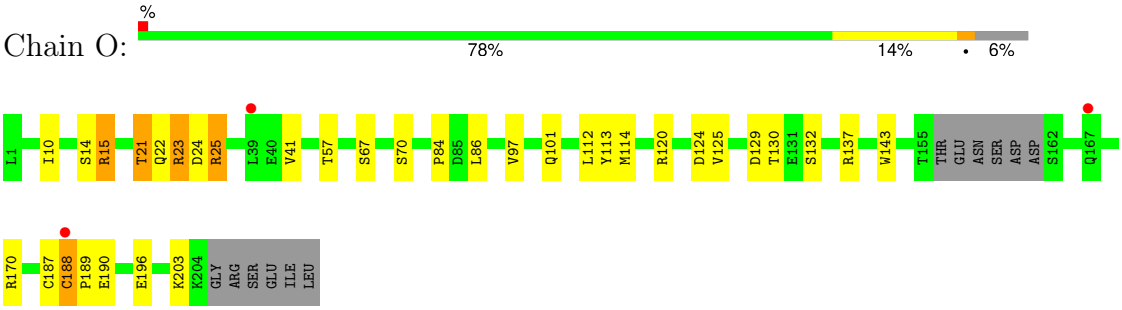
• Molecule 1: Acetylcholine-binding protein

Chain N:



• Molecule 1: Acetylcholine-binding protein

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.73Å 140.38Å 119.55Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	28.24 – 2.68 28.24 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.24-2.68) 98.1 (28.24-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.240 0.208 , 0.240	Depositor DCC
R_{free} test set	5278 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.069 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.064 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.075 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.064 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.104 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24523	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, 1PE, CL, NSE, 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	0.64	4/1621 (0.2%)	0.91	10/2211 (0.5%)
1	B	0.64	3/1621 (0.2%)	0.83	8/2211 (0.4%)
1	C	0.60	4/1621 (0.2%)	0.81	10/2211 (0.5%)
1	D	0.84	8/1613 (0.5%)	1.45	16/2200 (0.7%)
1	E	0.68	5/1621 (0.3%)	0.85	7/2211 (0.3%)
1	F	0.76	7/1645 (0.4%)	0.94	8/2244 (0.4%)
1	G	0.72	4/1629 (0.2%)	1.01	4/2222 (0.2%)
1	H	0.81	8/1621 (0.5%)	0.93	15/2211 (0.7%)
1	I	0.70	6/1602 (0.4%)	0.79	10/2183 (0.5%)
1	J	0.67	7/1621 (0.4%)	0.84	9/2211 (0.4%)
1	K	0.55	3/1605 (0.2%)	0.81	7/2188 (0.3%)
1	L	0.76	2/1629 (0.1%)	0.81	9/2222 (0.4%)
1	M	0.80	7/1602 (0.4%)	0.85	10/2183 (0.5%)
1	N	0.77	6/1621 (0.4%)	1.17	13/2211 (0.6%)
1	O	0.59	3/1621 (0.2%)	0.79	7/2211 (0.3%)
All	All	0.71	77/24293 (0.3%)	0.93	143/33130 (0.4%)

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	A	0	1
1	D	0	1
1	F	0	4
1	G	0	2
1	M	0	1
1	N	0	2
1	O	0	1
All	All	0	12

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	131	GLU	CD-OE1	-18.59	1.05	1.25
1	H	131	GLU	CD-OE1	-16.84	1.07	1.25
1	N	25	ARG	CZ-NH1	-16.34	1.11	1.33
1	G	23	ARG	CZ-NH1	-14.01	1.14	1.33
1	D	131	GLU	CD-OE1	-13.45	1.10	1.25

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	23	ARG	NE-CZ-NH2	32.15	136.38	120.30
1	N	25	ARG	NE-CZ-NH2	28.76	134.68	120.30
1	D	11	ARG	NE-CZ-NH2	26.92	133.76	120.30
1	G	23	ARG	NE-CZ-NH2	24.77	132.69	120.30
1	D	11	ARG	NE-CZ-NH1	-23.80	108.40	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	D	23	ARG	Sidechain
1	F	23	ARG	Sidechain
1	G	25	ARG	Sidechain
1	G	69	HIS	Sidechain

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	1586	0	1545	26	0
1	B	1586	0	1545	28	0
1	C	1586	0	1545	22	0
1	D	1578	0	1530	18	0
1	E	1586	0	1545	35	0
1	F	1607	0	1564	34	0
1	G	1591	0	1557	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1586	0	1545	21	0
1	I	1568	0	1532	26	0
1	J	1586	0	1545	25	0
1	K	1571	0	1530	20	0
1	L	1591	0	1549	21	0
1	M	1566	0	1535	30	0
1	N	1586	0	1545	21	0
1	O	1586	0	1545	20	0
2	A	16	0	22	0	0
2	B	16	0	22	2	0
2	C	16	0	22	1	0
2	D	16	0	22	3	0
2	E	16	0	22	2	0
2	G	16	0	22	1	0
2	H	16	0	22	3	0
2	I	16	0	22	5	0
3	D	14	0	13	0	0
3	G	14	0	12	0	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	E	25	0	0	1	0
4	F	10	0	0	0	0
4	G	15	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	1	0
4	M	5	0	0	0	0
5	A	8	0	6	0	0
5	D	4	0	3	0	0
5	F	16	0	12	1	0
5	G	12	0	9	0	0
5	J	4	0	3	0	0
5	O	4	0	3	0	0
6	A	19	0	8	2	0
6	B	19	0	8	0	0
6	E	19	0	8	1	0
6	I	19	0	8	1	0
6	K	19	0	8	2	0
6	M	19	0	8	2	0
7	A	1	0	0	0	0
7	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	1	0	0	0	0
7	N	1	0	0	0	0
8	J	6	0	8	0	0
9	A	28	0	0	1	0
9	B	19	0	0	0	0
9	C	22	0	0	1	0
9	D	27	0	0	2	0
9	E	23	0	0	1	0
9	F	31	0	0	0	0
9	G	28	0	0	0	0
9	H	26	0	0	1	0
9	I	21	0	0	0	0
9	J	21	0	0	1	0
9	K	26	0	0	2	0
9	L	24	0	0	0	0
9	M	21	0	0	1	0
9	N	5	0	0	0	0
9	O	13	0	0	0	0
All	All	24523	0	23450	332	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 332 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:E:148:ARG:CZ	1:M:25:ARG:HH22	1.57	1.18
1:E:148:ARG:CZ	1:M:25:ARG:NH2	2.21	1.02
1:A:153:ASP:OD1	1:F:179:LYS:NZ	1.93	1.01
1:E:65:TRP:HB3	2:E:302:1PE:H261	1.43	0.98
1:D:23:ARG:O	1:D:23:ARG:HG3	1.67	0.93

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	194/210 (92%)	187 (96%)	7 (4%)	0	100	100
1	B	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
1	C	194/210 (92%)	185 (95%)	9 (5%)	0	100	100
1	D	193/210 (92%)	186 (96%)	6 (3%)	1 (0%)	29	52
1	E	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
1	F	197/210 (94%)	186 (94%)	11 (6%)	0	100	100
1	G	195/210 (93%)	189 (97%)	6 (3%)	0	100	100
1	H	194/210 (92%)	187 (96%)	7 (4%)	0	100	100
1	I	189/210 (90%)	185 (98%)	4 (2%)	0	100	100
1	J	194/210 (92%)	186 (96%)	8 (4%)	0	100	100
1	K	191/210 (91%)	186 (97%)	5 (3%)	0	100	100
1	L	195/210 (93%)	189 (97%)	6 (3%)	0	100	100
1	M	189/210 (90%)	184 (97%)	5 (3%)	0	100	100
1	N	194/210 (92%)	186 (96%)	7 (4%)	1 (0%)	29	52
1	O	194/210 (92%)	185 (95%)	7 (4%)	2 (1%)	15	34
All	All	2901/3150 (92%)	2799 (96%)	98 (3%)	4 (0%)	51	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	CYS
1	O	189	PRO
1	N	187	CYS
1	O	190	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/196 (94%)	179 (97%)	6 (3%)	39	65
1	B	185/196 (94%)	177 (96%)	8 (4%)	29	54
1	C	185/196 (94%)	178 (96%)	7 (4%)	33	59
1	D	184/196 (94%)	179 (97%)	5 (3%)	44	71
1	E	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	F	188/196 (96%)	182 (97%)	6 (3%)	39	65
1	G	186/196 (95%)	180 (97%)	6 (3%)	39	65
1	H	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	I	182/196 (93%)	178 (98%)	4 (2%)	52	77
1	J	185/196 (94%)	180 (97%)	5 (3%)	44	71
1	K	183/196 (93%)	175 (96%)	8 (4%)	28	53
1	L	186/196 (95%)	181 (97%)	5 (3%)	44	71
1	M	182/196 (93%)	177 (97%)	5 (3%)	44	71
1	N	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	O	185/196 (94%)	181 (98%)	4 (2%)	52	77
All	All	2771/2940 (94%)	2675 (96%)	96 (4%)	36	62

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	25	ARG
1	K	186	SER
1	I	185	TYR
1	K	11	ARG
1	L	186	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	119	GLN
1	D	167	GLN
1	E	9	ASN
1	C	9	ASN
1	I	9	ASN

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

Of 53 ligands modelled in this entry, 4 are monoatomic - leaving 49 for Mogul analysis.

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	$\#\|Z\| > 2$
6	NSE	B	301	-	17,21,21	0.85	0	23,28,28	1.28	3 (13%)
5	ACT	F	305	-	3,3,3	0.74	0	3,3,3	0.98	0
2	1PE	I	302	-	15,15,15	0.88	0	14,14,14	1.10	2 (14%)
2	1PE	A	302	-	15,15,15	0.77	0	14,14,14	1.15	2 (14%)
4	SO4	B	303	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	E	304	-	4,4,4	0.30	0	6,6,6	0.31	0
2	1PE	H	301	-	15,15,15	0.82	0	14,14,14	1.29	2 (14%)
5	ACT	A	307	-	3,3,3	0.82	0	3,3,3	0.83	0
5	ACT	J	302	-	3,3,3	1.08	0	3,3,3	0.72	0
6	NSE	I	301	-	17,21,21	0.88	0	23,28,28	1.69	4 (17%)
6	NSE	M	301	-	17,21,21	0.78	0	23,28,28	1.12	2 (8%)
5	ACT	F	304	-	3,3,3	0.83	0	3,3,3	0.78	0
4	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.27	0
4	SO4	B	304	-	4,4,4	0.31	0	6,6,6	0.24	0
2	1PE	B	302	-	15,15,15	0.76	0	14,14,14	1.92	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	E	306	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	A	304	-	4,4,4	0.30	0	6,6,6	0.08	0
6	NSE	E	301	-	17,21,21	0.90	1 (5%)	23,28,28	1.17	1 (4%)
5	ACT	F	306	-	3,3,3	0.78	0	3,3,3	0.85	0
4	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	J	301	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.27	0
5	ACT	O	301	-	3,3,3	0.84	0	3,3,3	0.70	0
5	ACT	G	308	-	3,3,3	0.76	0	3,3,3	1.08	0
4	SO4	G	303	-	4,4,4	0.30	0	6,6,6	0.16	0
4	SO4	D	303	-	4,4,4	0.38	0	6,6,6	0.26	0
5	ACT	G	306	-	3,3,3	0.89	0	3,3,3	0.65	0
2	1PE	C	301	-	15,15,15	1.03	0	14,14,14	1.36	3 (21%)
4	SO4	E	305	-	4,4,4	0.29	0	6,6,6	0.09	0
4	SO4	I	303	-	4,4,4	0.27	0	6,6,6	0.05	0
4	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.11	0
5	ACT	D	304	-	3,3,3	0.79	0	3,3,3	0.78	0
2	1PE	G	301	-	15,15,15	0.60	0	14,14,14	1.35	2 (14%)
4	SO4	E	307	-	4,4,4	0.29	0	6,6,6	0.22	0
4	SO4	F	302	-	4,4,4	0.26	0	6,6,6	0.32	0
5	ACT	A	305	-	3,3,3	0.82	0	3,3,3	1.01	0
2	1PE	D	301	-	15,15,15	0.84	0	14,14,14	1.14	1 (7%)
6	NSE	A	301	-	17,21,21	0.76	0	23,28,28	1.99	7 (30%)
6	NSE	K	301	-	17,21,21	0.80	0	23,28,28	1.98	8 (34%)
3	NAG	D	302	1	14,14,15	2.18	2 (14%)	17,19,21	2.06	5 (29%)
8	GOL	J	303	-	5,5,5	0.35	0	5,5,5	0.47	0
2	1PE	E	302	-	15,15,15	0.73	0	14,14,14	1.98	3 (21%)
5	ACT	G	307	-	3,3,3	0.79	0	3,3,3	1.04	0
4	SO4	D	305	-	4,4,4	0.24	0	6,6,6	0.15	0
5	ACT	F	303	-	3,3,3	0.73	0	3,3,3	0.96	0
3	NAG	G	302	1	14,14,15	4.33	7 (50%)	17,19,21	3.93	12 (70%)
4	SO4	G	305	-	4,4,4	0.32	0	6,6,6	0.26	0
4	SO4	M	302	-	4,4,4	0.25	0	6,6,6	0.14	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
6	NSE	M	301	-	-	0/8/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	D	301	-	-	1/13/13/13	-
6	NSE	B	301	-	-	1/8/10/10	0/3/3/3
6	NSE	K	301	-	-	1/8/10/10	0/3/3/3
3	NAG	D	302	1	-	2/6/23/26	0/1/1/1
2	1PE	I	302	-	-	3/13/13/13	-
2	1PE	A	302	-	-	3/13/13/13	-
2	1PE	B	302	-	-	5/13/13/13	-
2	1PE	E	302	-	-	4/13/13/13	-
2	1PE	C	301	-	-	5/13/13/13	-
6	NSE	E	301	-	-	1/8/10/10	0/3/3/3
8	GOL	J	303	-	-	3/4/4/4	-
2	1PE	H	301	-	-	3/13/13/13	-
6	NSE	A	301	-	-	2/8/10/10	0/3/3/3
3	NAG	G	302	1	-	2/6/23/26	0/1/1/1
2	1PE	G	301	-	-	1/13/13/13	-
6	NSE	I	301	-	-	2/8/10/10	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	NAG	C1-C2	-10.96	1.37	1.52
3	G	302	NAG	C8-C7	8.20	1.67	1.50
3	G	302	NAG	O7-C7	-5.96	1.09	1.23
3	D	302	NAG	C1-C2	5.76	1.60	1.52
3	D	302	NAG	C2-N2	5.02	1.54	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	302	NAG	C1-O5-C5	7.38	122.08	112.19
3	G	302	NAG	C2-N2-C7	7.08	132.39	122.90
3	G	302	NAG	O7-C7-N2	-6.43	110.61	121.98
6	A	301	NSE	C9-C11-N3	6.25	127.25	119.12
3	D	302	NAG	O5-C1-C2	-5.60	102.63	111.29

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NSE	N3-C11-C9-C12
3	G	302	NAG	O7-C7-N2-C2
3	G	302	NAG	O5-C5-C6-O6
3	D	302	NAG	O5-C5-C6-O6
2	E	302	1PE	C14-C24-OH4-C13

There are no ring outliers.

17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	302	1PE	5	0
4	B	303	SO4	1	0
2	H	301	1PE	3	0
6	I	301	NSE	1	0
6	M	301	NSE	2	0
2	B	302	1PE	2	0
6	E	301	NSE	1	0
5	F	306	ACT	1	0
4	A	303	SO4	1	0
4	J	301	SO4	1	0
2	C	301	1PE	1	0
2	G	301	1PE	1	0
4	E	307	SO4	1	0
2	D	301	1PE	3	0
6	A	301	NSE	2	0
6	K	301	NSE	2	0
2	E	302	1PE	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, 95^{th} 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	198/210 (94%)	-0.12	0	100	100	28, 45, 79, 97	0
1	B	198/210 (94%)	-0.07	5 (2%)	57	57	33, 51, 87, 102	0
1	C	198/210 (94%)	0.03	3 (1%)	73	74	34, 51, 82, 101	0
1	D	197/210 (93%)	-0.06	1 (0%)	91	92	30, 47, 76, 99	0
1	E	198/210 (94%)	-0.05	4 (2%)	65	65	29, 47, 81, 99	0
1	F	200/210 (95%)	0.00	5 (2%)	57	57	26, 42, 78, 95	0
1	G	198/210 (94%)	-0.04	2 (1%)	82	82	27, 46, 79, 102	0
1	H	198/210 (94%)	0.01	2 (1%)	82	82	29, 50, 82, 103	0
1	I	195/210 (92%)	0.15	5 (2%)	56	55	37, 56, 84, 106	0
1	J	198/210 (94%)	0.05	2 (1%)	82	82	32, 50, 74, 96	0
1	K	197/210 (93%)	0.09	1 (0%)	91	92	31, 54, 78, 88	0
1	L	198/210 (94%)	-0.03	2 (1%)	82	82	32, 48, 77, 99	0
1	M	194/210 (92%)	0.11	6 (3%)	49	48	33, 57, 80, 107	0
1	N	198/210 (94%)	0.27	7 (3%)	44	43	38, 64, 89, 112	0
1	O	198/210 (94%)	0.14	3 (1%)	73	74	41, 58, 83, 98	0
All	All	2963/3150 (94%)	0.03	48 (1%)	72	73	26, 51, 83, 112	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	185	TYR	5.6
1	O	39	LEU	5.1
1	N	23	ARG	5.1
1	J	1	LEU	4.6
1	B	186	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 monosaccharides 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, 95^{th} 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
8	GOL	J	303	6/6	0.66	0.25	64,75,83,86	0
4	SO4	J	301	5/5	0.68	0.23	88,90,97,112	0
3	NAG	G	302	14/15	0.70	0.34	93,103,106,109	0
3	NAG	D	302	14/15	0.77	0.19	80,85,91,92	0
6	NSE	I	301	19/19	0.78	0.33	60,70,78,80	0
5	ACT	G	306	4/4	0.78	0.23	48,52,60,62	0
4	SO4	F	302	5/5	0.79	0.42	64,69,75,106	0
5	ACT	F	305	4/4	0.82	0.22	51,60,67,69	0
4	SO4	C	302	5/5	0.83	0.25	84,85,107,110	0
4	SO4	A	304	5/5	0.83	0.29	78,80,93,104	0
5	ACT	A	307	4/4	0.83	0.15	43,66,70,71	0
4	SO4	M	302	5/5	0.84	0.43	80,82,96,100	0
6	NSE	B	301	19/19	0.85	0.33	54,67,78,78	0
4	SO4	D	305	5/5	0.85	0.34	75,85,105,110	0
5	ACT	J	302	4/4	0.85	0.20	34,35,41,55	0
4	SO4	D	303	5/5	0.86	0.39	56,61,72,92	0
4	SO4	G	304	5/5	0.86	0.20	87,91,106,110	0
6	NSE	M	301	19/19	0.86	0.42	61,74,79,80	0
4	SO4	E	304	5/5	0.86	0.23	64,67,85,94	0
4	SO4	E	306	5/5	0.87	0.24	82,85,104,121	0
2	1PE	E	302	16/16	0.87	0.31	46,55,63,64	0
6	NSE	E	301	19/19	0.88	0.25	45,57,74,75	0
5	ACT	A	305	4/4	0.88	0.20	47,60,61,61	0
2	1PE	I	302	16/16	0.88	0.22	46,59,67,69	0
2	1PE	B	302	16/16	0.88	0.31	47,57,64,69	0
5	ACT	G	308	4/4	0.88	0.23	44,44,58,59	0
6	NSE	A	301	19/19	0.89	0.34	50,58,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	F	304	4/4	0.89	0.22	36,51,56,68	0
4	SO4	E	307	5/5	0.89	0.18	76,82,96,96	0
6	NSE	K	301	19/19	0.89	0.32	51,58,68,68	0
2	1PE	D	301	16/16	0.89	0.23	47,55,67,70	0
5	ACT	F	303	4/4	0.89	0.13	59,62,64,69	0
5	ACT	D	304	4/4	0.90	0.14	62,63,63,72	0
4	SO4	B	303	5/5	0.91	0.12	86,87,91,101	0
7	CL	A	306	1/1	0.92	0.18	86,86,86,86	0
7	CL	L	301	1/1	0.92	0.20	60,60,60,60	0
5	ACT	G	307	4/4	0.92	0.13	58,61,70,73	0
4	SO4	B	304	5/5	0.93	0.30	54,61,89,90	0
2	1PE	C	301	16/16	0.93	0.16	49,57,61,63	0
2	1PE	A	302	16/16	0.94	0.18	36,48,56,62	0
4	SO4	F	301	5/5	0.94	0.18	67,71,76,78	0
4	SO4	A	303	5/5	0.94	0.13	71,75,77,79	0
2	1PE	H	301	16/16	0.94	0.24	38,46,58,62	0
2	1PE	G	301	16/16	0.94	0.22	33,34,35,35	16
4	SO4	G	305	5/5	0.94	0.37	64,81,87,93	0
5	ACT	F	306	4/4	0.95	0.11	45,52,57,58	0
4	SO4	I	303	5/5	0.95	0.08	95,97,105,111	0
7	CL	K	302	1/1	0.95	0.08	69,69,69,69	0
5	ACT	O	301	4/4	0.95	0.20	37,43,45,49	0
4	SO4	G	303	5/5	0.95	0.14	63,64,79,83	0
7	CL	N	301	1/1	0.97	0.10	54,54,54,54	0
4	SO4	E	305	5/5	0.97	0.11	79,79,90,94	0
4	SO4	E	303	5/5	0.98	0.08	58,60,66,74	0

6.5 Other polymers (i)

There are no such residues in this entry.