



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 03:05 AM EST

PDB ID : 5OUG
Title : Humanized alpha-AChBP (acetylcholine binding protein) in complex with lobeline and allosteric binder fragment 4.
Authors : Delbart, F.; Gruss, F.; Ulens, C.
Deposited on : 2017-08-23
Resolution : 2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

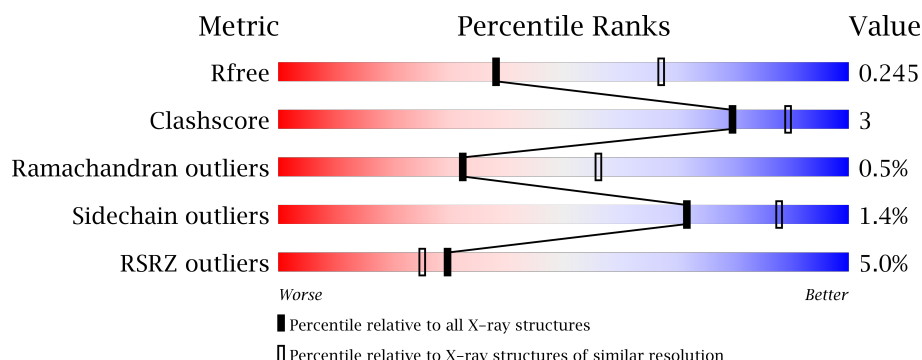
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	100719	2899 (2.60-2.56)
Clashscore	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

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	205	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	205	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	C	205	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	D	205	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	E	205	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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	L0B	A	1101	-	-	-	X
2	L0B	A	1106	-	-	-	X
2	L0B	B	308	-	-	-	X
2	L0B	C	306	-	-	-	X
2	L0B	D	306	-	-	-	X
4	9Z0	A	1104	-	-	-	X
4	9Z0	A	1105	-	-	-	X
4	9Z0	B	306	-	-	-	X
4	9Z0	B	307	-	-	-	X
4	9Z0	C	304	-	-	-	X
4	9Z0	C	305	-	-	-	X
4	9Z0	D	304	-	-	-	X
4	9Z0	D	305	-	-	-	X
4	9Z0	E	301	-	-	-	X
4	9Z0	E	302	-	-	-	X
7	DMS	E	303	-	-	-	X

2 Entry composition [i](#)

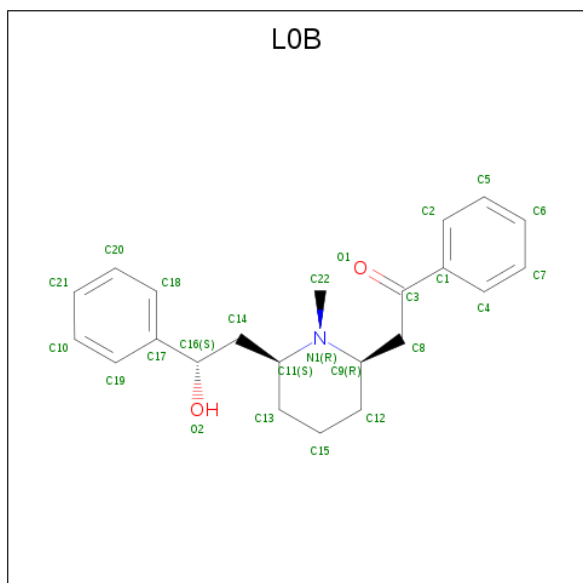
There are 8 unique types of molecules in this entry. The entry contains 8950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Humanized alpha-AChBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1680	1077	282	314	7			
1	B	205	Total	C	N	O	S	0	0	0
			1680	1077	282	314	7			
1	C	205	Total	C	N	O	S	0	0	0
			1680	1077	282	314	7			
1	D	205	Total	C	N	O	S	0	0	0
			1680	1077	282	314	7			
1	E	205	Total	C	N	O	S	0	0	0
			1676	1075	282	312	7			

- Molecule 2 is Alpha-Lobeline (three-letter code: L0B) (formula: C₂₂H₂₇NO₂).



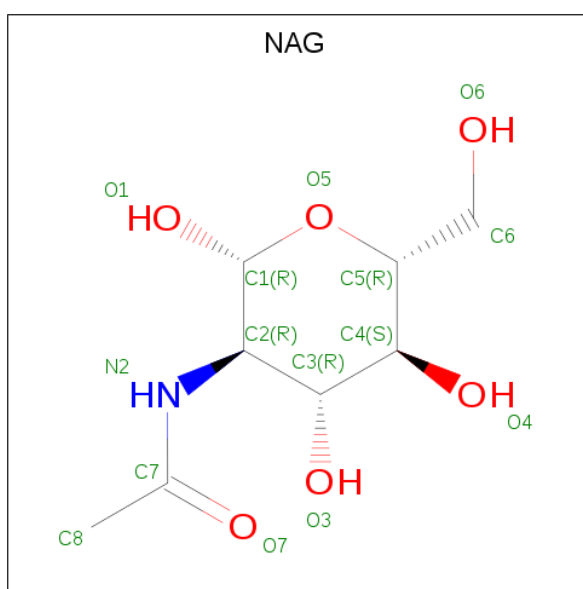
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	22	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	22	1	2		
2	B	1	Total	C	N	O	0	0
			25	22	1	2		
2	C	1	Total	C	N	O	0	0
			25	22	1	2		
2	D	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



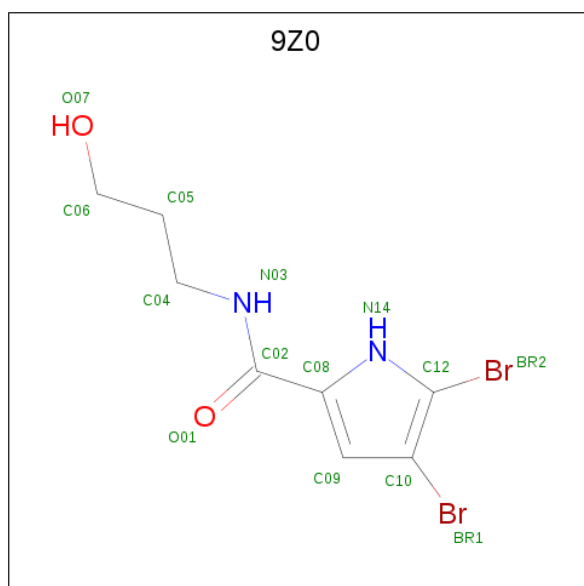
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is 4,5-dibromo-N-(3-hydroxypropyl)-1H-pyrrole-2-carboxamide (three-letter code: 9Z0) (formula: C₈H₁₀Br₂N₂O₂).



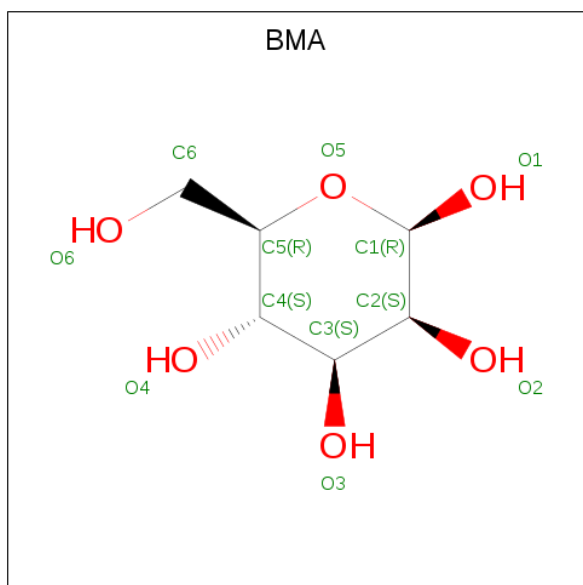
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	A	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	B	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	B	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	C	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	C	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	D	1	Total 14	Br 2	C 8	N 2	O 2	0	0
4	D	1	Total 14	Br 2	C 8	N 2	O 2	0	0

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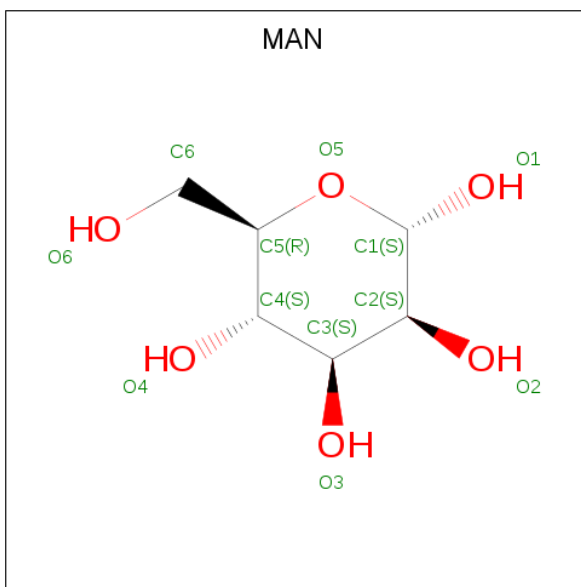
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	Br	C	N	O	0	0
			14	2	8	2	2		
4	E	1	Total	Br	C	N	O	0	0
			14	2	8	2	2		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



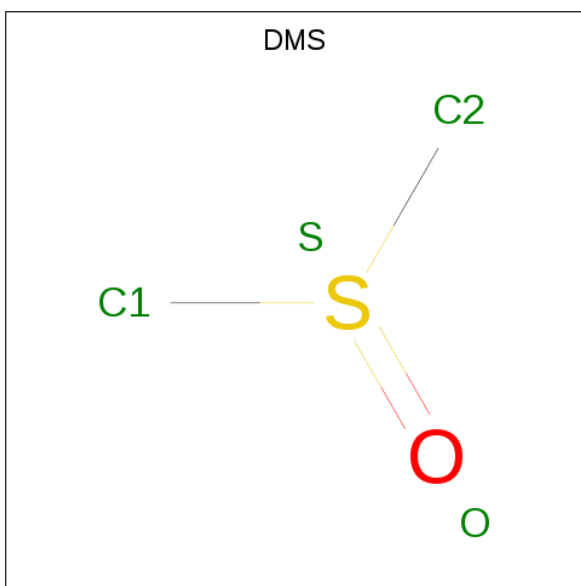
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total 17	O 17	0	0
8	B	26	Total 26	O 26	0	0
8	C	19	Total 19	O 19	0	0
8	D	18	Total 18	O 18	0	0
8	E	10	Total 10	O 10	0	0

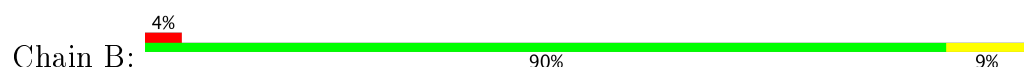
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

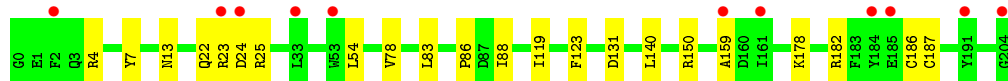
- Molecule 1: Humanized alpha-AChBP



- Molecule 1: Humanized alpha-AChBP



- Molecule 1: Humanized alpha-AChBP



- Molecule 1: Humanized alpha-AChBP



- Molecule 1: Humanized alpha-AChBP



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.67Å 119.81Å 84.54Å 90.00° 107.29° 90.00°	Depositor
Resolution (Å)	80.72 – 2.57 66.94 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.72-2.57) 99.7 (66.94-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.214 , 0.240 0.222 , 0.245	Depositor DCC
R_{free} test set	2106 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8950	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 9Z0, BMA, NAG, DMS, L0B, MAN

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	0/1724	0.82	4/2344 (0.2%)
1	B	0.64	0/1724	0.86	5/2344 (0.2%)
1	C	0.61	0/1724	0.82	2/2344 (0.1%)
1	D	0.64	0/1724	0.83	3/2344 (0.1%)
1	E	0.64	0/1720	0.84	4/2339 (0.2%)
All	All	0.63	0/8616	0.83	18/11715 (0.2%)

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	B	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ASP	N-CA-CB	8.34	125.61	110.60
1	D	131	ASP	N-CA-CB	8.33	125.59	110.60
1	E	122	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	B	122	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	120	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	120	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	120	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	E	150	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	182	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	120	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	120	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	120	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	150	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	150	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	4	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	4	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	179	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	CYS	Peptide
1	B	186	CYS	Peptide
1	E	186	CYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1680	0	1651	10	0
1	B	1680	0	1651	11	0
1	C	1680	0	1651	13	0
1	D	1680	0	1651	12	0
1	E	1676	0	1647	10	0
2	A	50	0	54	6	0
2	B	25	0	27	0	0
2	C	25	0	27	1	0
2	D	25	0	27	2	0
3	A	28	0	25	0	0
3	B	28	0	24	1	0
3	C	28	0	24	0	0
3	D	28	0	24	0	0
3	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	20	4	0
4	B	28	0	20	4	0
4	C	28	0	20	4	0
4	D	28	0	20	4	0
4	E	28	0	20	3	0
5	B	11	0	8	0	0
5	C	11	0	10	0	0
5	D	11	0	10	0	0
6	B	22	0	20	0	0
7	E	4	0	6	0	0
8	A	17	0	0	0	0
8	B	26	0	0	0	0
8	C	19	0	0	1	0
8	D	18	0	0	0	0
8	E	10	0	0	0	0
All	All	8950	0	8662	56	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 3.

All (56) 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:D:182:ARG:NH1	1:D:193:ASP:OD2	2.16	0.77
1:C:78:VAL:CG1	1:C:83:LEU:HD11	2.25	0.66
1:C:78:VAL:HG12	1:C:83:LEU:HD11	1.80	0.64
1:D:7:TYR:HA	4:D:305:9Z0:BR2	2.52	0.63
2:C:306:L0B:C5	1:D:116:LEU:HD13	2.30	0.62
1:E:103:GLN:NE2	1:E:115:TYR:OH	2.35	0.59
1:D:103:GLN:NE2	1:D:115:TYR:OH	2.34	0.59
1:C:83:LEU:N	1:C:83:LEU:HD12	2.18	0.59
1:B:7:TYR:HA	4:B:307:9Z0:BR2	2.59	0.58
1:C:159:ALA:HB2	8:C:1104:HOH:O	2.03	0.58
1:C:119:ILE:HD12	4:C:304:9Z0:BR2	2.60	0.56
1:B:119:ILE:HD12	4:B:306:9Z0:BR2	2.61	0.56
1:C:119:ILE:CD1	4:C:304:9Z0:BR2	3.10	0.55
1:C:54:LEU:CD1	4:C:304:9Z0:BR1	3.10	0.54
1:E:7:TYR:HA	4:E:302:9Z0:BR2	2.64	0.52
1:E:25:ARG:HE	1:E:26:PRO:HD2	1.74	0.52
1:D:119:ILE:HD12	4:D:304:9Z0:BR2	2.65	0.52
1:B:186:CYS:SG	1:B:187:CYS:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:CD1	4:A:1104:9Z0:BR2	3.14	0.51
1:A:186:CYS:SG	1:A:187:CYS:N	2.85	0.50
1:A:22:GLN:HG2	1:A:23:ARG:HG3	1.92	0.50
1:C:186:CYS:SG	1:C:187:CYS:N	2.84	0.50
1:E:186:CYS:SG	1:E:187:CYS:N	2.85	0.50
2:A:1106:L0B:C7	1:B:116:LEU:HD13	2.42	0.50
1:D:186:CYS:SG	1:D:187:CYS:N	2.84	0.50
1:C:7:TYR:HA	4:C:305:9Z0:BR2	2.66	0.50
1:B:119:ILE:CD1	4:B:306:9Z0:BR2	3.15	0.50
2:D:306:L0B:C4	1:E:106:LEU:HD12	2.42	0.49
1:A:106:LEU:HD12	2:A:1101:L0B:C2	2.42	0.49
1:E:119:ILE:CD1	4:E:301:9Z0:BR2	3.16	0.49
1:D:121:GLN:OE1	4:D:304:9Z0:BR2	2.86	0.48
1:D:46:GLN:OE1	1:D:126:ASP:HA	2.13	0.48
1:A:86:PRO:HB2	1:A:88:ILE:HG12	1.96	0.47
1:A:7:TYR:HA	4:A:1105:9Z0:BR2	2.69	0.47
1:D:119:ILE:CD1	4:D:304:9Z0:BR2	3.19	0.45
1:B:86:PRO:HB2	1:B:88:ILE:HG12	1.98	0.45
1:C:13:ASN:O	1:D:4:ARG:NH2	2.50	0.45
1:E:119:ILE:HD12	4:E:301:9Z0:BR2	2.72	0.45
1:D:115:TYR:C	1:D:116:LEU:HD12	2.38	0.44
1:C:22:GLN:HE21	1:C:23:ARG:HE	1.66	0.44
1:D:13:ASN:O	1:E:4:ARG:NH2	2.51	0.44
1:B:115:TYR:C	1:B:116:LEU:HD12	2.38	0.44
1:E:86:PRO:HB2	1:E:88:ILE:HG12	1.99	0.44
1:B:109:SER:OG	3:B:301:NAG:H82	2.18	0.43
1:C:86:PRO:HB2	1:C:88:ILE:HG13	1.99	0.43
2:D:306:L0B:H221	2:D:306:L0B:H82C	1.85	0.43
1:B:54:LEU:CD1	4:B:306:9Z0:BR1	3.21	0.43
1:A:106:LEU:HD12	2:A:1101:L0B:H2	2.01	0.42
2:A:1106:L0B:H221	2:A:1106:L0B:H82C	1.85	0.42
1:A:107:VAL:HG11	4:A:1105:9Z0:BR1	2.74	0.42
2:A:1106:L0B:C4	1:B:106:LEU:HD12	2.50	0.41
2:A:1101:L0B:H81C	1:E:145:TRP:O	2.20	0.41
1:C:123:PHE:CZ	1:C:140:LEU:HD11	2.56	0.41
1:A:103:GLN:OE1	1:A:115:TYR:OH	2.39	0.40
1:B:60:ASP:HB3	1:B:63:LEU:HD12	2.03	0.40
1:A:119:ILE:HD12	4:A:1104:9Z0:BR2	2.77	0.40

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	203/205 (99%)	199 (98%)	3 (2%)	1 (0%)	32	56
1	B	203/205 (99%)	198 (98%)	4 (2%)	1 (0%)	32	56
1	C	203/205 (99%)	199 (98%)	3 (2%)	1 (0%)	32	56
1	D	203/205 (99%)	198 (98%)	4 (2%)	1 (0%)	32	56
1	E	203/205 (99%)	199 (98%)	3 (2%)	1 (0%)	32	56
All	All	1015/1025 (99%)	993 (98%)	17 (2%)	5 (0%)	32	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	B	24	ASP
1	C	24	ASP
1	E	24	ASP
1	D	24	ASP

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	192/192 (100%)	189 (98%)	3 (2%)	68	86
1	B	192/192 (100%)	189 (98%)	3 (2%)	68	86
1	C	192/192 (100%)	188 (98%)	4 (2%)	59	81
1	D	192/192 (100%)	190 (99%)	2 (1%)	80	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	191/192 (100%)	190 (100%)	1 (0%)	91	97
All	All	959/960 (100%)	946 (99%)	13 (1%)	71	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	131	ASP
1	A	133	GLU
1	B	25	ARG
1	B	131	ASP
1	B	133	GLU
1	C	25	ARG
1	C	131	ASP
1	C	178	LYS
1	C	182	ARG
1	D	23	ARG
1	D	131	ASP
1	E	131	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	B	37	GLN
1	B	61	HIS
1	C	3	GLN
1	C	22	GLN
1	C	37	GLN
1	C	61	HIS
1	C	177	GLN
1	D	37	GLN
1	D	103	GLN
1	D	121	GLN
1	D	177	GLN
1	E	37	GLN
1	E	61	HIS
1	E	103	GLN
1	E	157	GLN
1	E	177	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	L0B	A	1101	-	27,27,27	0.49	0	33,36,36	1.25	3 (9%)
3	NAG	A	1102	1,3	14,14,15	0.42	0	15,19,21	1.21	2 (13%)
3	NAG	A	1103	3	14,14,15	0.53	0	15,19,21	1.42	2 (13%)
4	9Z0	A	1104	-	12,14,14	0.95	1 (8%)	11,18,18	0.81	0
4	9Z0	A	1105	-	12,14,14	0.91	1 (8%)	11,18,18	0.95	0
2	L0B	A	1106	-	27,27,27	0.54	0	33,36,36	1.18	1 (3%)
3	NAG	B	301	1,3	14,14,15	0.47	0	15,19,21	1.05	0
3	NAG	B	302	3,5	14,14,15	0.43	0	15,19,21	0.80	0
5	BMA	B	303	3,6	11,11,12	0.47	0	13,15,17	1.30	2 (15%)
6	MAN	B	304	5	11,11,12	0.32	0	13,15,17	1.10	1 (7%)
6	MAN	B	305	5	11,11,12	0.52	0	13,15,17	1.02	1 (7%)
4	9Z0	B	306	-	12,14,14	1.02	1 (8%)	11,18,18	0.90	0
4	9Z0	B	307	-	12,14,14	0.91	1 (8%)	11,18,18	0.96	0
2	L0B	B	308	-	27,27,27	0.46	0	33,36,36	1.16	2 (6%)
3	NAG	C	301	1,3	14,14,15	0.39	0	15,19,21	1.48	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	302	3,5	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
5	BMA	C	303	3	11,11,12	0.63	0	13,15,17	0.99	1 (7%)
4	9Z0	C	304	-	12,14,14	1.06	1 (8%)	11,18,18	0.93	0
4	9Z0	C	305	-	12,14,14	0.91	1 (8%)	11,18,18	1.30	2 (18%)
2	L0B	C	306	-	27,27,27	0.48	0	33,36,36	1.16	2 (6%)
3	NAG	D	301	1,3	14,14,15	0.51	0	15,19,21	1.45	1 (6%)
3	NAG	D	302	3,5	14,14,15	0.66	0	15,19,21	1.33	3 (20%)
5	BMA	D	303	3	11,11,12	0.67	0	13,15,17	1.48	2 (15%)
4	9Z0	D	304	-	12,14,14	1.11	1 (8%)	11,18,18	0.89	1 (9%)
4	9Z0	D	305	-	12,14,14	0.84	1 (8%)	11,18,18	0.96	0
2	L0B	D	306	-	27,27,27	0.50	0	33,36,36	1.23	1 (3%)
4	9Z0	E	301	-	12,14,14	1.05	1 (8%)	11,18,18	0.97	0
4	9Z0	E	302	-	12,14,14	0.96	1 (8%)	11,18,18	0.87	0
7	DMS	E	303	-	3,3,3	0.53	0	3,3,3	0.73	0
3	NAG	E	304	1,3	14,14,15	0.48	0	15,19,21	1.46	2 (13%)
3	NAG	E	305	3	14,14,15	0.35	0	15,19,21	1.05	1 (6%)

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	L0B	A	1101	-	-	0/16/30/30	0/3/3/3
3	NAG	A	1102	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1103	3	-	0/6/23/26	0/1/1/1
4	9Z0	A	1104	-	-	0/6/9/9	0/1/1/1
4	9Z0	A	1105	-	-	0/6/9/9	0/1/1/1
2	L0B	A	1106	-	-	0/16/30/30	0/3/3/3
3	NAG	B	301	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	302	3,5	-	0/6/23/26	0/1/1/1
5	BMA	B	303	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	304	5	-	0/2/19/22	0/1/1/1
6	MAN	B	305	5	-	0/2/19/22	0/1/1/1
4	9Z0	B	306	-	-	0/6/9/9	0/1/1/1
4	9Z0	B	307	-	-	0/6/9/9	0/1/1/1
2	L0B	B	308	-	-	0/16/30/30	0/3/3/3
3	NAG	C	301	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	302	3,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	C	303	3	-	0/2/19/22	0/1/1/1
4	9Z0	C	304	-	-	0/6/9/9	0/1/1/1
4	9Z0	C	305	-	-	0/6/9/9	0/1/1/1
2	L0B	C	306	-	-	0/16/30/30	0/3/3/3
3	NAG	D	301	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	302	3,5	-	0/6/23/26	0/1/1/1
5	BMA	D	303	3	-	0/2/19/22	0/1/1/1
4	9Z0	D	304	-	-	0/6/9/9	0/1/1/1
4	9Z0	D	305	-	-	0/6/9/9	0/1/1/1
2	L0B	D	306	-	-	0/16/30/30	0/3/3/3
4	9Z0	E	301	-	-	0/6/9/9	0/1/1/1
4	9Z0	E	302	-	-	0/6/9/9	0/1/1/1
7	DMS	E	303	-	-	0/0/0/0	0/0/0/0
3	NAG	E	304	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	305	3	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	9Z0	BR2-C12	-2.99	1.85	1.90
4	E	301	9Z0	BR2-C12	-2.95	1.85	1.90
4	B	306	9Z0	BR2-C12	-2.85	1.86	1.90
4	A	1104	9Z0	BR2-C12	-2.78	1.86	1.90
4	D	304	9Z0	BR2-C12	-2.71	1.86	1.90
4	C	305	9Z0	BR2-C12	-2.46	1.86	1.90
4	E	302	9Z0	BR2-C12	-2.33	1.86	1.90
4	B	307	9Z0	BR2-C12	-2.33	1.86	1.90
4	D	305	9Z0	BR2-C12	-2.28	1.86	1.90
4	A	1105	9Z0	BR2-C12	-2.21	1.86	1.90

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	304	NAG	O5-C1-C2	-4.08	105.79	111.47
3	C	301	NAG	O5-C1-C2	-3.97	105.94	111.47
3	D	301	NAG	O5-C1-C2	-3.80	106.19	111.47
3	A	1102	NAG	O5-C1-C2	-2.78	107.61	111.47
4	C	305	9Z0	BR1-C10-C12	-2.40	125.02	127.63
4	D	304	9Z0	BR1-C10-C12	-2.25	125.18	127.63
3	D	302	NAG	C3-C4-C5	-2.21	106.33	110.22
2	B	308	L0B	C8-C9-N1	-2.06	110.79	114.59
3	E	305	NAG	O5-C1-C2	-2.02	108.66	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	NAG	O4-C4-C5	2.01	114.35	109.28
3	D	302	NAG	C4-C3-C2	2.02	113.98	111.02
3	A	1102	NAG	C1-C2-N2	2.07	114.03	110.49
3	C	302	NAG	C2-N2-C7	2.10	126.00	122.94
2	A	1101	L0B	C8-C3-C1	2.13	121.01	118.69
3	C	301	NAG	C1-C2-N2	2.22	114.27	110.49
3	C	301	NAG	C1-O5-C5	2.25	115.27	112.17
5	C	303	BMA	C1-C2-C3	2.32	112.59	109.65
6	B	305	MAN	C1-O5-C5	2.33	115.38	112.17
2	A	1101	L0B	C22-N1-C9	2.37	115.23	113.22
3	E	304	NAG	C1-O5-C5	2.42	115.50	112.17
5	B	303	BMA	C1-C2-C3	2.47	112.78	109.65
4	C	305	9Z0	C08-C02-N03	2.64	119.13	115.52
3	A	1103	NAG	C3-C4-C5	2.65	114.89	110.22
6	B	304	MAN	C1-O5-C5	2.75	115.96	112.17
2	C	306	L0B	C22-N1-C9	2.89	115.68	113.22
5	D	303	BMA	C1-O5-C5	3.10	116.43	112.17
3	A	1103	NAG	C4-C3-C2	3.11	115.58	111.02
5	B	303	BMA	C1-O5-C5	3.16	116.52	112.17
5	D	303	BMA	C3-C4-C5	3.29	116.02	110.22
2	C	306	L0B	C22-N1-C11	3.69	116.36	113.22
2	A	1101	L0B	C22-N1-C11	4.01	116.63	113.22
2	B	308	L0B	C22-N1-C11	4.10	116.71	113.22
2	D	306	L0B	C22-N1-C11	4.43	116.99	113.22
2	A	1106	L0B	C22-N1-C11	4.57	117.11	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	L0B	3	0
4	A	1104	9Z0	2	0
4	A	1105	9Z0	2	0
2	A	1106	L0B	3	0
3	B	301	NAG	1	0
4	B	306	9Z0	3	0
4	B	307	9Z0	1	0
4	C	304	9Z0	3	0
4	C	305	9Z0	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	306	L0B	1	0
4	D	304	9Z0	3	0
4	D	305	9Z0	1	0
2	D	306	L0B	2	0
4	E	301	9Z0	2	0
4	E	302	9Z0	1	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	205/205 (100%)	0.43	9 (4%) 35 30	42, 68, 111, 131	0
1	B	205/205 (100%)	0.47	9 (4%) 35 30	44, 65, 115, 133	0
1	C	205/205 (100%)	0.56	11 (5%) 26 22	43, 71, 121, 146	0
1	D	205/205 (100%)	0.51	12 (5%) 23 19	46, 72, 122, 134	0
1	E	205/205 (100%)	0.49	10 (4%) 30 26	46, 68, 114, 126	0
All	All	1025/1025 (100%)	0.49	51 (4%) 30 25	42, 69, 117, 146	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	6.4
1	C	204	GLY	5.7
1	D	68	SER	4.8
1	E	11	VAL	4.7
1	C	159	ALA	4.2
1	C	184	TYR	4.1
1	A	11	VAL	4.1
1	C	2	PHE	3.9
1	B	204	GLY	3.8
1	D	11	VAL	3.7
1	C	161	ILE	3.6
1	B	184	TYR	3.6
1	D	2	PHE	3.6
1	B	23	ARG	3.6
1	B	11	VAL	3.4
1	D	0	GLY	3.2
1	A	2	PHE	3.2
1	C	185	GLU	3.1
1	B	163	GLY	3.1
1	E	159	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	23	ARG	3.0
1	E	204	GLY	2.9
1	A	24	ASP	2.9
1	D	3	GLN	2.8
1	B	35	LEU	2.7
1	C	33	LEU	2.7
1	D	159	ALA	2.6
1	E	74	LYS	2.5
1	C	24	ASP	2.5
1	B	158	GLU	2.5
1	E	0	GLY	2.4
1	E	23	ARG	2.4
1	A	161	ILE	2.3
1	A	159	ALA	2.3
1	E	12	LYS	2.3
1	C	53	TRP	2.3
1	A	12	LYS	2.3
1	D	53	TRP	2.2
1	A	76	VAL	2.2
1	E	161	ILE	2.2
1	B	36	LEU	2.1
1	D	150	ARG	2.1
1	D	170	PHE	2.1
1	D	158	GLU	2.1
1	A	4	ARG	2.1
1	D	24	ASP	2.1
1	C	191	TYR	2.0
1	E	5	LYS	2.0
1	A	186	CYS	2.0
1	B	159	ALA	2.0
1	E	13	ASN	2.0

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 ⓘ

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
4	9Z0	E	302	14/14	0.57	0.83	25.59	115,161,214,246	14
4	9Z0	D	304	14/14	0.62	0.52	13.48	69,94,106,125	14
4	9Z0	B	307	14/14	0.69	0.55	12.75	92,112,136,174	14
4	9Z0	A	1104	14/14	0.49	0.50	12.29	72,93,125,130	14
2	L0B	A	1106	25/25	0.71	0.57	9.47	84,104,114,119	0
2	L0B	A	1101	25/25	0.75	0.40	8.34	77,98,116,118	0
4	9Z0	C	304	14/14	0.73	0.42	7.78	70,87,101,117	14
4	9Z0	E	301	14/14	0.71	0.39	6.99	60,95,115,115	14
2	L0B	D	306	25/25	0.69	0.48	6.97	92,110,118,120	0
4	9Z0	B	306	14/14	0.69	0.42	6.61	64,91,107,118	14
4	9Z0	D	305	14/14	0.51	0.43	6.24	92,103,159,160	14
2	L0B	C	306	25/25	0.74	0.59	6.18	82,102,111,120	0
2	L0B	B	308	25/25	0.66	0.51	5.34	82,108,123,126	0
7	DMS	E	303	4/4	0.91	0.53	5.31	110,112,113,123	0
4	9Z0	A	1105	14/14	0.77	0.38	4.43	81,94,117,125	14
4	9Z0	C	305	14/14	0.82	0.33	3.01	72,79,105,121	14
6	MAN	B	305	11/12	0.90	0.21	1.11	77,88,94,96	0
3	NAG	D	301	14/15	0.94	0.12	-	68,77,86,92	0
3	NAG	B	302	14/15	0.93	0.15	-	64,78,84,87	0
3	NAG	D	302	14/15	0.83	0.24	-	87,108,118,120	0
3	NAG	B	301	14/15	0.93	0.14	-	58,63,71,76	0
3	NAG	E	304	14/15	0.92	0.10	-	73,82,88,97	0
3	NAG	E	305	14/15	0.87	0.18	-	94,120,129,130	0
3	NAG	A	1103	14/15	0.75	0.28	-	70,110,116,118	0
3	NAG	C	302	14/15	0.84	0.31	-	96,111,115,116	0
5	BMA	C	303	11/12	0.78	0.19	-	90,104,111,114	0
5	BMA	B	303	11/12	0.92	0.12	-	81,89,90,91	0
6	MAN	B	304	11/12	0.91	0.21	-	86,87,92,93	0
5	BMA	D	303	11/12	0.42	0.36	-	104,122,125,126	0
3	NAG	C	301	14/15	0.85	0.15	-	73,86,98,106	0
3	NAG	A	1102	14/15	0.94	0.09	-	62,74,83,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.