



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:57 AM UTC

PDB ID : 1DQ5 / pdb_00001dq5
Title : Manganese;Manganese concanavalin A at pH 5.0
Authors : Bouckaert, J.; Dewallef, Y.; Poortmans, F.; Wyns, L.; Loris, R.
Deposited on : 1999-12-30
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

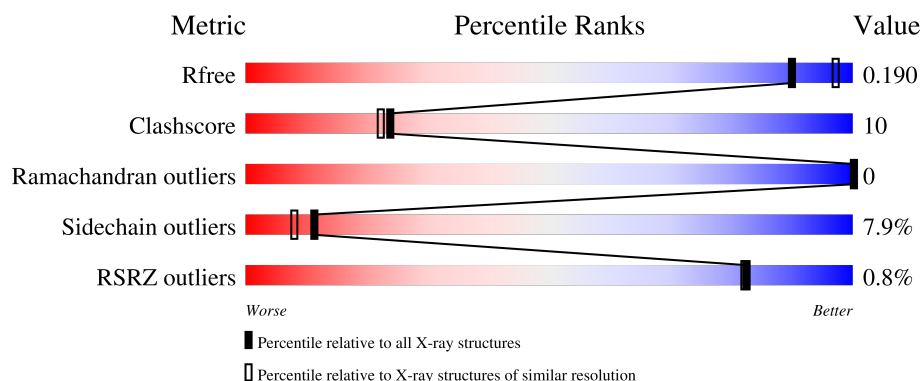
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1917 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 Concanavalin-Br.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ASP	GLY	conflict	UNP P55915
A	70	ALA	GLY	conflict	UNP P55915
A	151	ASP	GLU	conflict	UNP P55915
A	155	GLU	ARG	conflict	UNP P55915

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

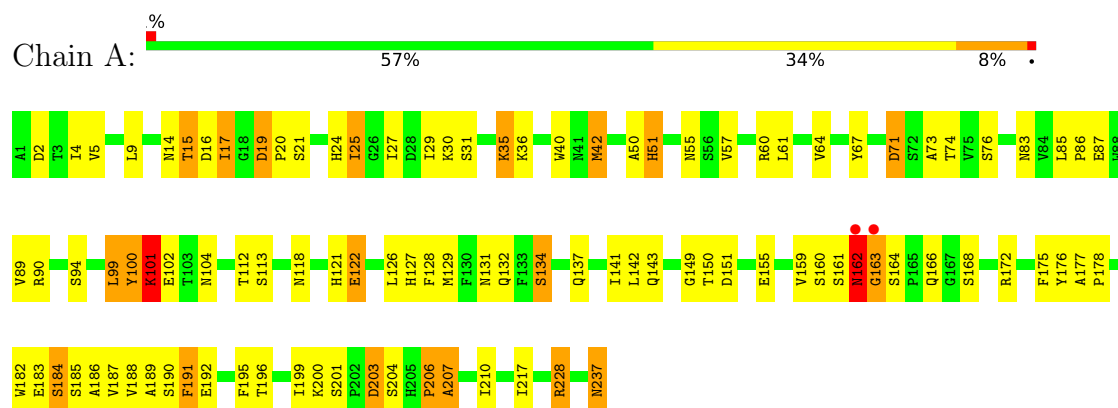
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

3 Residue-property plots

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: Concanavalin-Br



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	63.23Å 87.44Å 89.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (8.00-2.00) 86.0 (8.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.189 , 0.210 0.188 , 0.190	Depositor DCC
R_{free} test set	1491 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1917	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: MN

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	1.03	1/1851 (0.1%)	2.34	95/2522 (3.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ASN	CG-OD1	5.12	1.33	1.23

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ASN	OD1-CG-ND2	-12.11	110.49	122.60
1	A	207	ALA	O-C-N	-11.15	110.73	123.33
1	A	16	ASP	CA-CB-CG	10.97	123.57	112.60
1	A	137	GLN	CA-C-O	-9.69	111.23	122.37
1	A	61	LEU	CA-C-O	-9.04	110.31	120.43
1	A	137	GLN	OE1-CD-NE2	-8.95	113.65	122.60
1	A	60	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	A	17	ILE	CA-C-O	8.39	129.98	120.42
1	A	76	SER	CA-C-O	-8.26	111.77	121.44
1	A	206	PRO	CB-CA-C	8.04	121.70	110.60
1	A	186	ALA	CA-C-O	-8.01	111.60	120.81
1	A	176	TYR	O-C-N	-8.00	113.83	122.07
1	A	131	ASN	CB-CG-ND2	7.96	128.35	116.40
1	A	161	SER	N-CA-C	7.91	120.81	111.71
1	A	195	PHE	CA-CB-CG	7.72	121.52	113.80
1	A	4	ILE	CB-CG1-CD1	7.70	129.97	113.80
1	A	176	TYR	N-CA-CB	-7.49	99.16	110.01
1	A	196	THR	CA-C-O	7.41	128.70	120.70
1	A	131	ASN	N-CA-CB	7.34	121.44	110.65
1	A	64	VAL	CA-C-O	-7.25	112.68	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ASN	N-CA-C	-7.24	104.31	113.72
1	A	185	SER	CA-C-O	-7.21	110.73	119.59
1	A	100	TYR	CA-C-N	-7.16	110.73	122.11
1	A	100	TYR	C-N-CA	-7.16	110.73	122.11
1	A	142	LEU	CA-C-O	-6.96	112.80	120.38
1	A	188	VAL	O-C-N	-6.90	115.62	123.07
1	A	55	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	15	THR	CA-C-N	6.74	131.98	120.72
1	A	15	THR	C-N-CA	6.74	131.98	120.72
1	A	237	ASN	CA-CB-CG	-6.73	105.87	112.60
1	A	192	GLU	CB-CG-CD	-6.68	101.24	112.60
1	A	40	TRP	CA-C-O	6.63	127.40	120.30
1	A	149	GLY	CA-C-O	-6.57	112.25	119.27
1	A	162	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	71	ASP	N-CA-C	-6.39	101.48	110.50
1	A	168	SER	CA-C-O	-6.37	113.70	121.28
1	A	87	GLU	CA-CB-CG	-6.20	101.70	114.10
1	A	176	TYR	N-CA-C	6.20	117.70	111.07
1	A	89	VAL	N-CA-CB	-6.14	105.26	112.32
1	A	101	LYS	N-CA-C	6.10	117.16	108.74
1	A	94	SER	CA-C-O	-6.06	114.56	121.40
1	A	102	GLU	CA-C-O	-5.95	114.92	121.28
1	A	143	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	A	175	PHE	O-C-N	-5.86	115.73	122.93
1	A	86	PRO	O-C-N	-5.82	115.64	122.86
1	A	50	ALA	O-C-N	-5.79	116.45	123.29
1	A	228	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	73	ALA	CA-C-O	-5.77	114.64	121.16
1	A	191	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	161	SER	CA-C-O	5.68	126.52	120.10
1	A	85	LEU	CB-CA-C	-5.65	100.26	108.91
1	A	199	ILE	CA-C-O	5.60	126.53	120.53
1	A	132	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	A	51	HIS	N-CA-CB	5.58	120.05	110.68
1	A	189	ALA	O-C-N	-5.55	116.82	123.31
1	A	163	GLY	O-C-N	5.52	128.91	122.45
1	A	86	PRO	CA-C-N	5.52	127.68	120.28
1	A	86	PRO	C-N-CA	5.52	127.68	120.28
1	A	19	ASP	CA-C-O	-5.51	114.69	120.70
1	A	128	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	4	ILE	CA-C-N	5.48	130.39	123.10
1	A	4	ILE	C-N-CA	5.48	130.39	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ILE	CA-C-O	-5.45	114.50	120.72
1	A	42	MET	CA-C-O	-5.45	115.20	121.19
1	A	134	SER	CA-C-O	-5.45	114.81	121.78
1	A	126	LEU	N-CA-CB	5.43	120.20	110.80
1	A	118	ASN	N-CA-C	-5.42	106.67	113.28
1	A	35	LYS	N-CA-C	-5.33	105.51	112.23
1	A	102	GLU	CB-CG-CD	5.33	121.65	112.60
1	A	155	GLU	CA-C-O	-5.33	115.00	120.54
1	A	172	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	29	ILE	O-C-N	-5.32	115.91	122.88
1	A	113	SER	CA-CB-OG	-5.30	100.50	111.10
1	A	87	GLU	CA-C-N	5.29	130.31	123.00
1	A	87	GLU	C-N-CA	5.29	130.31	123.00
1	A	57	VAL	N-CA-C	-5.29	105.69	110.82
1	A	100	TYR	O-C-N	5.28	128.86	122.94
1	A	90	ARG	CA-C-O	-5.21	115.07	120.70
1	A	141	ILE	N-CA-C	-5.20	100.40	107.99
1	A	134	SER	CB-CA-C	5.20	119.61	110.36
1	A	2	ASP	CA-C-O	5.18	127.04	121.55
1	A	14	ASN	N-CA-C	-5.18	99.55	108.56
1	A	5	VAL	CA-C-O	-5.17	115.01	120.39
1	A	21	SER	N-CA-CB	-5.17	103.07	110.57
1	A	86	PRO	CA-C-O	5.12	129.53	122.31
1	A	196	THR	O-C-N	-5.08	116.62	123.23
1	A	83	ASN	CA-C-N	-5.07	117.75	122.66
1	A	83	ASN	C-N-CA	-5.07	117.75	122.66
1	A	67	TYR	N-CA-C	-5.06	100.27	108.82
1	A	188	VAL	CA-C-O	5.06	125.94	120.43
1	A	29	ILE	CA-C-O	5.04	126.55	120.66
1	A	9	LEU	N-CA-C	-5.02	96.64	107.49
1	A	190	SER	CA-CB-OG	-5.02	101.05	111.10
1	A	94	SER	O-C-N	5.02	129.25	123.17
1	A	203	ASP	CA-C-O	5.00	127.62	121.72

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	1809	0	1755	36	0
2	A	2	0	0	0	0
3	A	106	0	0	7	0
All	All	1917	0	1755	36	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 10.

All (36) 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:183:GLU:HG3	3:A:332:HOH:O	1.48	1.11
1:A:160:SER:OG	1:A:162:ASN:ND2	1.91	1.03
1:A:162:ASN:ND2	1:A:162:ASN:H	1.72	0.86
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.59	0.85
1:A:160:SER:HG	1:A:162:ASN:ND2	1.77	0.83
1:A:159:VAL:CG1	1:A:163:GLY:HA2	2.13	0.78
1:A:150:THR:O	1:A:151:ASP:HB2	1.94	0.66
1:A:134:SER:HB3	3:A:351:HOH:O	1.97	0.65
1:A:159:VAL:HG13	1:A:163:GLY:C	2.25	0.61
1:A:99:LEU:N	1:A:99:LEU:HD23	2.17	0.59
1:A:164:SER:O	1:A:166:GLN:NE2	2.35	0.59
1:A:71:ASP:O	3:A:360:HOH:O	2.18	0.57
1:A:162:ASN:ND2	1:A:162:ASN:N	2.41	0.55
1:A:121:HIS:CE1	3:A:356:HOH:O	2.58	0.54
1:A:150:THR:O	1:A:150:THR:HG22	2.08	0.53
1:A:182:TRP:CG	1:A:183:GLU:N	2.77	0.53
1:A:15:THR:HG22	1:A:19:ASP:O	2.09	0.51
1:A:127:HIS:HE2	1:A:129:MET:HE3	1.75	0.50
1:A:35:LYS:HE2	3:A:339:HOH:O	2.12	0.49
1:A:182:TRP:CZ2	1:A:184:SER:HA	2.48	0.47
1:A:51:HIS:CD2	3:A:348:HOH:O	2.68	0.47
1:A:159:VAL:HG13	1:A:163:GLY:HA2	1.94	0.46
1:A:100:TYR:HB2	1:A:207:ALA:HB3	1.97	0.46
1:A:159:VAL:HG13	1:A:163:GLY:CA	2.47	0.45
1:A:35:LYS:HA	1:A:35:LYS:HD3	1.75	0.45
1:A:122:GLU:N	3:A:358:HOH:O	2.35	0.44
1:A:159:VAL:CG1	1:A:163:GLY:CA	2.93	0.44
1:A:237:ASN:HD22	1:A:237:ASN:HA	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:NZ	1:A:203:ASP:OD2	2.50	0.44
1:A:127:HIS:NE2	1:A:129:MET:HE3	2.33	0.43
1:A:177:ALA:HA	1:A:178:PRO:HD3	1.74	0.43
1:A:112:THR:O	1:A:191:PHE:HA	2.19	0.42
1:A:182:TRP:CH2	1:A:184:SER:HA	2.54	0.42
1:A:201:SER:CB	1:A:206:PRO:HB3	2.50	0.41
1:A:104:ASN:HD22	1:A:210:ILE:CG1	2.33	0.40
1:A:20:PRO:HD2	1:A:24:HIS:CE1	2.56	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	235/237 (99%)	224 (95%)	11 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	203/203 (100%)	187 (92%)	16 (8%)	11	8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	27	ILE
1	A	30	LYS
1	A	31	SER
1	A	36	LYS
1	A	42	MET
1	A	74	THR
1	A	99	LEU
1	A	101	LYS
1	A	122	GLU
1	A	162	ASN
1	A	184	SER
1	A	187	VAL
1	A	200	LYS
1	A	204	SER
1	A	217	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	HIS
1	A	69	ASN
1	A	121	HIS
1	A	131	ASN
1	A	162	ASN
1	A	237	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	237/237 (100%)	-0.58	2 (0%) 82 82	10, 20, 37, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	2.8
1	A	163	GLY	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	301	1/1	0.95	0.03	28,28,28,28	0
2	MN	A	302	1/1	0.99	0.03	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.