



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:26 PM GMT

PDB ID : 4TW2
Title : Crystal Structure of SCARB2 in Neural Condition (pH7.5)
Authors : Dang, M.H.; Wang, X.X.; Rao, Z.H.
Deposited on : 2014-06-29
Resolution : 2.89 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

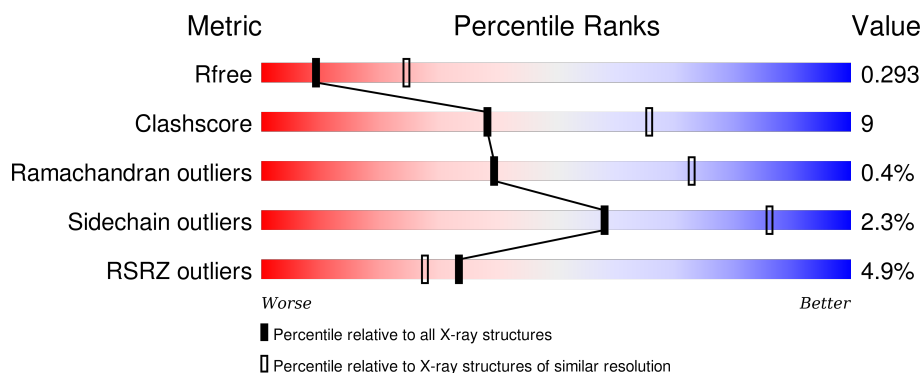
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	394	<div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	394	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition [i](#)

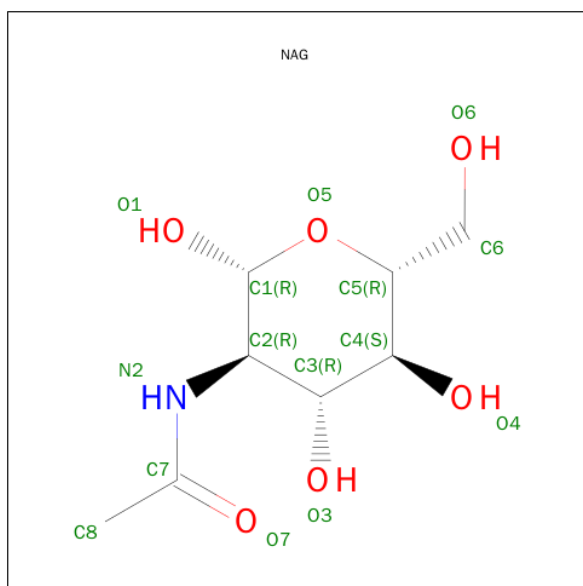
There are 4 unique types of molecules in this entry. The entry contains 6822 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Scavenger receptor class B member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3183	2053	515	603	12			
1	B	394	Total	C	N	O	S	0	0	0
			3185	2056	514	603	12			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



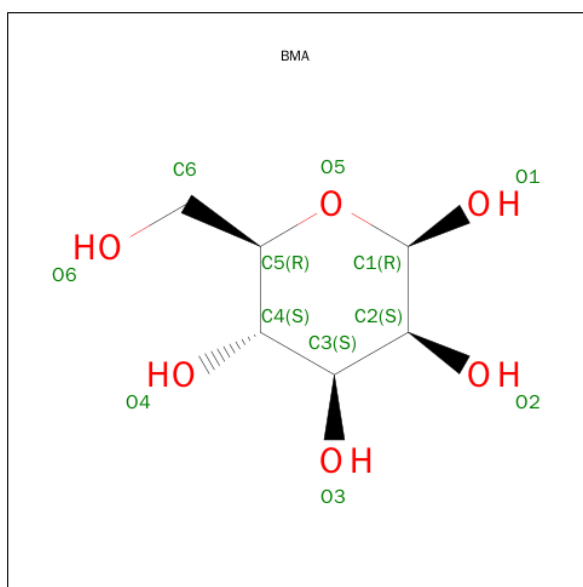
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

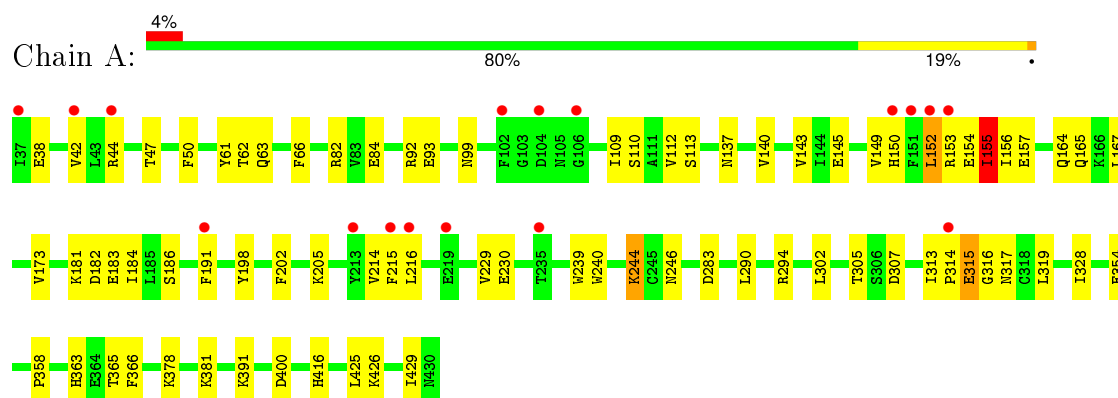


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

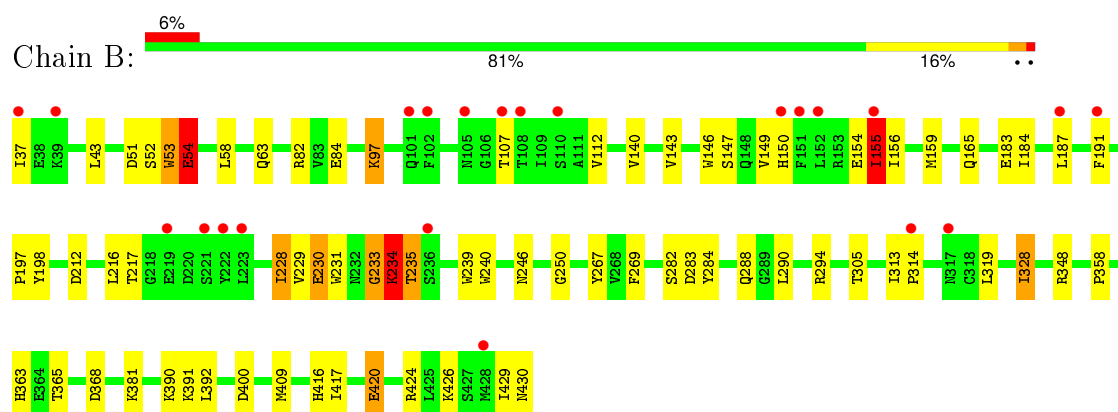
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Scavenger receptor class B member 2



- Molecule 1: Scavenger receptor class B member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.80Å 100.32Å 105.17Å 90.00° 98.69° 90.00°	Depositor
Resolution (Å)	47.15 – 2.89 47.15 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.15-2.89) 95.1 (47.15-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.244 , 0.293 0.243 , 0.293	Depositor DCC
R_{free} test set	1297 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25404 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6822	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 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.32	0/3266	0.62	4/4442 (0.1%)
1	B	0.45	2/3268 (0.1%)	0.69	8/4443 (0.2%)
All	All	0.39	2/6534 (0.0%)	0.65	12/8885 (0.1%)

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	2
1	B	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	GLU	CG-CD	-12.11	1.33	1.51
1	B	53	TRP	CB-CG	7.58	1.63	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LEU	CA-CB-CG	9.96	138.21	115.30
1	B	54	GLU	N-CA-C	9.60	136.91	111.00
1	A	155	ILE	CB-CA-C	-8.74	94.11	111.60
1	A	155	ILE	N-CA-C	7.17	130.37	111.00
1	B	233	GLY	N-CA-C	6.60	129.60	113.10
1	B	54	GLU	CA-CB-CG	-6.40	99.31	113.40
1	B	97	LYS	CD-CE-NZ	-6.28	97.26	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	GLU	N-CA-C	5.54	125.95	111.00
1	A	152	LEU	N-CA-C	-5.45	96.28	111.00
1	B	54	GLU	CB-CA-C	-5.34	99.71	110.40
1	B	230	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	B	230	GLU	C-N-CA	5.29	134.92	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	THR	Peptide
1	A	38	GLU	Peptide
1	B	234	LYS	Peptide
1	B	305	THR	Peptide
1	B	54	GLU	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	3183	0	3075	55	0
1	B	3185	0	3087	67	0
2	A	182	0	159	5	0
2	B	140	0	124	5	0
3	A	44	0	36	0	0
3	B	22	0	18	0	0
4	A	44	0	40	0	0
4	B	22	0	20	0	0
All	All	6822	0	6559	122	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 9.

All (122) 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:B:54:GLU:HG2	1:B:97:LYS:HG2	1.29	1.11
1:A:155:ILE:HD13	1:A:156:ILE:HG12	1.34	1.08
1:B:230:GLU:CG	1:B:231:TRP:H	1.81	0.92
1:B:230:GLU:HG3	1:B:231:TRP:H	1.38	0.88
1:B:239:TRP:HB3	1:B:328:ILE:HD12	1.55	0.87
1:B:230:GLU:OE2	1:B:234:LYS:N	2.06	0.86
1:A:315:GLU:O	1:A:317:ASN:N	2.09	0.85
1:A:150:HIS:HB3	1:A:153:ARG:HA	1.57	0.84
1:B:230:GLU:CG	1:B:231:TRP:N	2.42	0.81
1:B:54:GLU:CG	1:B:97:LYS:HG2	2.12	0.78
1:B:290:LEU:HD21	1:B:426:LYS:HB2	1.64	0.77
1:B:230:GLU:HG2	1:B:231:TRP:N	2.01	0.75
1:A:165:GLN:HE21	1:A:184:ILE:HG12	1.51	0.75
1:B:51:ASP:OD1	1:B:52:SER:N	2.21	0.73
1:A:63:GLN:NE2	2:A:518:NAG:O7	2.20	0.71
1:B:230:GLU:OE1	1:B:235:THR:HA	1.91	0.70
1:B:53:TRP:CD2	1:B:54:GLU:OE1	2.45	0.69
1:B:391:LYS:HD2	1:B:400:ASP:HA	1.72	0.69
1:A:165:GLN:NE2	1:A:183:GLU:OE1	2.28	0.67
1:A:154:GLU:O	1:A:155:ILE:HG13	1.94	0.67
1:B:54:GLU:OE1	1:B:54:GLU:N	2.28	0.67
1:B:154:GLU:O	1:B:155:ILE:HB	1.93	0.66
1:B:319:LEU:HD21	2:B:509:NAG:H81	1.79	0.64
1:B:63:GLN:NE2	2:B:511:NAG:O7	2.26	0.64
1:B:230:GLU:HG2	1:B:231:TRP:H	1.57	0.64
1:B:43:LEU:H	1:B:217:THR:HG1	1.44	0.64
1:B:233:GLY:O	1:B:234:LYS:HD2	1.98	0.64
1:B:54:GLU:OE2	1:B:97:LYS:HD3	1.96	0.64
1:A:365:THR:HG23	1:A:381:LYS:HA	1.80	0.64
1:A:290:LEU:HD21	1:A:426:LYS:HB2	1.81	0.63
1:B:390:LYS:HE2	1:B:392:LEU:HD21	1.82	0.61
1:B:240:TRP:O	1:B:246:ASN:ND2	2.31	0.61
1:B:165:GLN:HE21	1:B:184:ILE:HG12	1.65	0.61
1:B:165:GLN:HE22	1:B:183:GLU:HB3	1.66	0.60
1:B:156:ILE:HD12	1:B:191:PHE:HE2	1.65	0.60
1:A:62:THR:OG1	1:A:93:GLU:OE2	2.17	0.60
1:A:84:GLU:OE2	1:B:82:ARG:NH2	2.35	0.60
1:B:288:GLN:HE21	1:B:416:HIS:HE1	1.50	0.59
1:A:391:LYS:HD2	1:A:400:ASP:HA	1.84	0.59
1:B:53:TRP:CG	1:B:54:GLU:OE1	2.55	0.59
1:A:244:LYS:NZ	1:A:307:ASP:HB3	2.18	0.59
1:A:82:ARG:NH2	1:B:84:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:VAL:O	1:B:230:GLU:HB2	2.03	0.58
1:A:47:THR:HG23	1:A:50:PHE:H	1.70	0.57
1:B:319:LEU:O	1:B:348:ARG:NH2	2.38	0.56
1:A:315:GLU:O	1:A:317:ASN:HB2	2.07	0.55
1:B:426:LYS:O	1:B:429:ILE:HG22	2.07	0.54
1:B:365:THR:HG23	1:B:381:LYS:HA	1.90	0.53
1:A:239:TRP:HB3	1:A:328:ILE:HG21	1.90	0.53
1:A:140:VAL:HA	1:A:143:VAL:HG22	1.90	0.53
1:A:214:VAL:HG13	1:A:229:VAL:HG23	1.90	0.53
1:A:109:ILE:O	1:A:215:PHE:N	2.39	0.52
1:B:283:ASP:CG	1:B:284:TYR:H	2.13	0.52
1:A:99:ASN:HB2	1:A:112:VAL:HG22	1.91	0.52
1:B:143:VAL:HA	1:B:146:TRP:HB2	1.91	0.52
1:A:165:GLN:HE22	1:A:183:GLU:HB3	1.76	0.51
1:B:358:PRO:HA	1:B:363:HIS:ND1	2.25	0.51
1:A:240:TRP:O	1:A:246:ASN:ND2	2.41	0.51
1:A:181:LYS:HE3	1:A:186:SER:OG	2.10	0.51
1:B:53:TRP:C	1:B:54:GLU:OE1	2.49	0.51
1:A:202:PHE:O	1:A:205:LYS:HB2	2.10	0.51
1:A:358:PRO:HA	1:A:363:HIS:ND1	2.25	0.51
1:B:358:PRO:HA	1:B:363:HIS:CE1	2.46	0.51
1:A:110:SER:HA	1:A:214:VAL:HA	1.92	0.50
1:B:58:LEU:HD21	1:B:417:ILE:HG13	1.93	0.50
1:A:358:PRO:HA	1:A:363:HIS:CE1	2.47	0.50
1:B:53:TRP:CE3	1:B:54:GLU:OE1	2.65	0.50
2:A:509:NAG:H5	2:A:510:NAG:HN2	1.77	0.50
1:B:313:ILE:HG23	1:B:314:PRO:HA	1.94	0.49
1:B:112:VAL:HG12	1:B:212:ASP:HA	1.95	0.49
1:B:149:VAL:HG11	2:B:510:NAG:H2	1.95	0.49
1:A:61:TYR:CE2	1:A:92:ARG:HB2	2.49	0.48
1:B:230:GLU:HG3	1:B:231:TRP:N	2.13	0.47
1:B:426:LYS:HG3	1:B:426:LYS:O	2.14	0.47
1:B:228:ILE:HD11	1:B:269:PHE:HB3	1.95	0.47
1:B:147:SER:O	1:B:154:GLU:HB2	2.15	0.47
1:B:267:TYR:CZ	2:B:508:NAG:H62	2.50	0.47
1:B:420:GLU:O	1:B:424:ARG:HB3	2.16	0.46
1:B:240:TRP:CH2	1:B:328:ILE:HD11	2.50	0.46
1:A:216:LEU:HB2	1:A:229:VAL:HG13	1.96	0.46
1:A:44:ARG:O	1:A:47:THR:HG22	2.15	0.46
1:A:425:LEU:O	1:A:429:ILE:HG12	2.16	0.46
1:B:282:SER:HB3	1:B:294:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.80	0.46
1:A:244:LYS:HD2	2:A:509:NAG:O3	2.15	0.46
1:A:378:LYS:HD3	1:A:416:HIS:CD2	2.50	0.45
1:A:137:ASN:N	1:A:167:LEU:O	2.45	0.45
1:B:140:VAL:HA	1:B:143:VAL:HG22	1.97	0.45
1:A:315:GLU:O	1:A:315:GLU:HG2	2.15	0.45
1:B:216:LEU:HB2	1:B:229:VAL:HG13	1.99	0.44
1:A:165:GLN:NE2	1:A:184:ILE:HG12	2.27	0.44
1:A:164:GLN:H	1:A:164:GLN:CD	2.21	0.44
1:B:429:ILE:HG23	1:B:430:ASN:ND2	2.32	0.44
1:A:214:VAL:HG12	1:A:230:GLU:HB2	2.00	0.44
1:A:294:ARG:HD2	1:A:366:PHE:HB2	1.99	0.44
1:A:319:LEU:HD21	2:A:514:NAG:H81	1.98	0.44
1:B:107:THR:O	1:B:217:THR:HG22	2.18	0.44
2:A:509:NAG:H5	2:A:510:NAG:N2	2.32	0.44
1:B:149:VAL:HG12	2:B:510:NAG:H4	2.01	0.43
1:A:47:THR:CG2	1:A:50:PHE:H	2.31	0.43
1:B:159:MET:SD	1:B:187:LEU:HB3	2.58	0.43
1:A:244:LYS:HB3	1:A:244:LYS:HE3	1.52	0.43
1:B:197:PRO:HG2	1:B:198:TYR:CD2	2.53	0.42
1:A:191:PHE:N	1:A:191:PHE:CD1	2.87	0.42
1:A:182:ASP:O	1:A:186:SER:OG	2.15	0.42
1:B:43:LEU:N	1:B:217:THR:OG1	2.37	0.42
1:A:214:VAL:CG1	1:A:230:GLU:HB2	2.50	0.42
1:A:145:GLU:O	1:A:149:VAL:HG22	2.20	0.41
1:B:58:LEU:HD22	1:B:417:ILE:HA	2.01	0.41
1:B:228:ILE:HG12	1:B:250:GLY:O	2.20	0.41
1:A:154:GLU:HG3	1:A:157:GLU:OE1	2.20	0.41
1:B:191:PHE:CD1	1:B:191:PHE:N	2.89	0.41
1:B:283:ASP:CG	1:B:284:TYR:N	2.73	0.41
1:B:165:GLN:NE2	1:B:183:GLU:HB3	2.34	0.41
1:A:313:ILE:HG23	1:A:314:PRO:HA	2.02	0.41
1:A:82:ARG:NH2	1:A:354:GLU:HG2	2.35	0.41
1:B:212:ASP:O	1:B:231:TRP:HA	2.21	0.41
1:A:66:PHE:CE1	1:A:173:VAL:HG13	2.56	0.41
1:B:294:ARG:NE	1:B:368:ASP:OD1	2.40	0.41
1:A:150:HIS:CD2	1:A:150:HIS:N	2.89	0.40
1:A:181:LYS:HB2	1:A:198:TYR:CE1	2.56	0.40
1:A:154:GLU:C	1:A:155:ILE:CG1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/394 (100%)	379 (97%)	11 (3%)	2 (0%)	34	69
1	B	392/394 (100%)	376 (96%)	15 (4%)	1 (0%)	46	78
All	All	784/788 (100%)	755 (96%)	26 (3%)	3 (0%)	39	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	A	316	GLY
1	B	155	ILE

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	353/355 (99%)	346 (98%)	7 (2%)	63	88
1	B	354/355 (100%)	345 (98%)	9 (2%)	55	84
All	All	707/710 (100%)	691 (98%)	16 (2%)	58	86

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

Mol	Chain	Res	Type
1	A	42	VAL
1	A	113	SER
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	155	ILE
1	A	244	LYS
1	A	283	ASP
1	A	315	GLU
1	B	37	ILE
1	B	150	HIS
1	B	155	ILE
1	B	228	ILE
1	B	234	LYS
1	B	235	THR
1	B	328	ILE
1	B	409	MET
1	B	420	GLU

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

Mol	Chain	Res	Type
1	A	165	GLN
1	A	288	GLN
1	B	165	GLN
1	B	416	HIS
1	B	430	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

35 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	NAG	A	501	1,2	14,14,15	0.53	0	15,19,21	0.38	0
2	NAG	A	502	3,2	14,14,15	0.43	0	15,19,21	0.36	0
3	BMA	A	503	2,4	11,11,12	0.78	1 (9%)	15,15,17	0.70	0
4	MAN	A	504	3	11,11,12	0.80	0	15,15,17	2.01	2 (13%)
4	MAN	A	505	3	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
2	NAG	A	506	1,2	14,14,15	0.36	0	15,19,21	0.32	0
2	NAG	A	507	2	14,14,15	0.37	0	15,19,21	0.27	0
2	NAG	A	508	1	14,14,15	0.69	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	A	509	1,2	14,14,15	0.68	1 (7%)	15,19,21	1.15	1 (6%)
2	NAG	A	510	3,2	14,14,15	0.39	0	15,19,21	0.95	1 (6%)
3	BMA	A	511	2	11,11,12	1.27	3 (27%)	15,15,17	1.54	2 (13%)
2	NAG	A	512	1,2	14,14,15	0.35	0	15,19,21	0.66	0
2	NAG	A	513	2	14,14,15	0.30	0	15,19,21	0.27	0
2	NAG	A	514	1,2	14,14,15	0.34	0	15,19,21	0.46	0
2	NAG	A	515	3,2	14,14,15	0.67	1 (7%)	15,19,21	0.95	1 (6%)
3	BMA	A	516	2,4	11,11,12	0.71	0	15,15,17	0.83	0
4	MAN	A	517	3	11,11,12	0.78	0	15,15,17	1.18	2 (13%)
2	NAG	A	518	1,2	14,14,15	0.44	0	15,19,21	0.92	1 (6%)
2	NAG	A	519	3,2	14,14,15	0.44	0	15,19,21	0.32	0
3	BMA	A	520	2,4	11,11,12	0.93	1 (9%)	15,15,17	0.95	0
4	MAN	A	521	3	11,11,12	1.01	1 (9%)	15,15,17	1.26	3 (20%)
2	NAG	B	501	1,2	14,14,15	0.74	1 (7%)	15,19,21	0.51	0
2	NAG	B	502	3,2	14,14,15	0.55	0	15,19,21	0.34	0
3	BMA	B	503	2,4	11,11,12	0.92	1 (9%)	15,15,17	0.83	0
4	MAN	B	504	3	11,11,12	0.79	0	15,15,17	1.33	2 (13%)
2	NAG	B	505	1,2	14,14,15	0.31	0	15,19,21	0.32	0
2	NAG	B	506	2	14,14,15	0.39	0	15,19,21	0.33	0
2	NAG	B	507	1	14,14,15	0.58	0	15,19,21	0.72	1 (6%)
2	NAG	B	508	1	14,14,15	0.79	1 (7%)	15,19,21	1.06	1 (6%)
2	NAG	B	509	1,2	14,14,15	0.37	0	15,19,21	0.36	0
2	NAG	B	510	2	14,14,15	0.66	1 (7%)	15,19,21	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	511	1,2	14,14,15	0.23	0	15,19,21	0.86	1 (6%)
2	NAG	B	512	3,2	14,14,15	0.31	0	15,19,21	0.27	0
3	BMA	B	513	2,4	11,11,12	0.56	0	15,15,17	0.73	0
4	MAN	B	514	3	11,11,12	0.85	1 (9%)	15,15,17	0.87	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	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3	-	0/2/19/22	0/1/1/1
4	MAN	A	505	3	-	0/2/19/22	0/1/1/1
2	NAG	A	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	2	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	510	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	511	2	-	0/2/19/22	0/1/1/1
2	NAG	A	512	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	513	2	-	0/6/23/26	0/1/1/1
2	NAG	A	514	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	515	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	516	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	517	3	-	0/2/19/22	0/1/1/1
2	NAG	A	518	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	519	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	520	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	521	3	-	0/2/19/22	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3	-	0/2/19/22	0/1/1/1
2	NAG	B	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	506	2	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	510	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	511	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	512	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	513	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	514	3	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	O5-C1	-2.69	1.39	1.43
3	B	503	BMA	O5-C1	-2.51	1.39	1.43
4	B	514	MAN	O5-C1	-2.39	1.39	1.43
4	A	521	MAN	O5-C1	-2.33	1.39	1.43
3	A	520	BMA	O5-C1	-2.26	1.40	1.43
3	A	503	BMA	O5-C1	-2.12	1.40	1.43
3	A	511	BMA	O5-C1	-2.10	1.40	1.43
2	A	508	NAG	O5-C1	2.18	1.47	1.43
2	B	510	NAG	O5-C1	2.31	1.47	1.43
3	A	511	BMA	C4-C5	2.31	1.58	1.53
2	A	515	NAG	O5-C1	2.36	1.47	1.43
2	A	509	NAG	O5-C1	2.44	1.47	1.43
3	A	511	BMA	C4-C3	2.51	1.59	1.52
2	B	508	NAG	O5-C1	2.82	1.48	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	BMA	C1-C2-C3	-3.74	105.02	109.55
4	A	521	MAN	C1-C2-C3	-3.20	105.67	109.55
4	A	505	MAN	O2-C2-C3	-2.48	105.19	110.19
4	B	504	MAN	O2-C2-C3	-2.36	105.43	110.19
4	B	514	MAN	O2-C2-C3	-2.19	105.77	110.19
4	A	517	MAN	O2-C2-C3	-2.18	105.79	110.19
4	A	521	MAN	O2-C2-C3	-2.18	105.80	110.19
4	A	517	MAN	C1-O5-C5	2.07	115.19	112.14
4	A	521	MAN	C1-O5-C5	2.15	115.30	112.14
2	B	511	NAG	C1-O5-C5	2.24	115.44	112.14
2	A	518	NAG	C2-N2-C7	2.42	126.25	123.11
2	A	510	NAG	C1-O5-C5	2.49	115.81	112.14
2	B	507	NAG	C1-O5-C5	2.62	115.99	112.14
4	A	504	MAN	O5-C1-C2	2.68	115.18	110.89
2	A	508	NAG	C1-O5-C5	2.85	116.33	112.14
4	A	505	MAN	C1-O5-C5	2.95	116.48	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	BMA	C3-C4-C5	3.19	115.92	110.23
2	A	515	NAG	C1-O5-C5	3.47	117.24	112.14
2	B	510	NAG	C1-O5-C5	3.60	117.43	112.14
4	B	504	MAN	C1-O5-C5	3.74	117.65	112.14
2	B	508	NAG	C1-O5-C5	3.86	117.81	112.14
2	A	509	NAG	C1-O5-C5	4.15	118.24	112.14
4	A	504	MAN	C1-O5-C5	6.23	121.30	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	509	NAG	3	0
2	A	510	NAG	2	0
2	A	514	NAG	1	0
2	A	518	NAG	1	0
2	B	508	NAG	1	0
2	B	509	NAG	1	0
2	B	510	NAG	2	0
2	B	511	NAG	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	394/394 (100%)	0.28	17 (4%)	39 33	20, 45, 90, 116	0
1	B	394/394 (100%)	0.35	22 (5%)	28 22	21, 54, 98, 127	0
All	All	788/788 (100%)	0.31	39 (4%)	33 28	20, 49, 93, 127	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	PHE	6.1
1	A	152	LEU	6.0
1	B	37	ILE	4.9
1	B	107	THR	4.5
1	A	151	PHE	4.0
1	A	215	PHE	3.9
1	A	314	PRO	3.7
1	A	106	GLY	3.3
1	B	105	ASN	3.2
1	B	317	ASN	3.2
1	B	221	SER	3.1
1	B	152	LEU	3.1
1	B	314	PRO	3.1
1	B	187	LEU	3.0
1	B	222	TYR	2.8
1	A	150	HIS	2.7
1	B	191	PHE	2.6
1	A	219	GLU	2.6
1	B	101	GLN	2.6
1	A	37	ILE	2.5
1	B	223	LEU	2.5
1	A	104	ASP	2.5
1	A	191	PHE	2.3
1	B	108	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	2.3
1	A	216	LEU	2.3
1	B	39	LYS	2.2
1	A	213	TYR	2.2
1	B	155	ILE	2.2
1	B	150	HIS	2.2
1	A	42	VAL	2.1
1	B	219	GLU	2.1
1	B	110	SER	2.1
1	A	44	ARG	2.1
1	A	102	PHE	2.1
1	B	236	SER	2.1
1	A	235	THR	2.1
1	B	428	MET	2.1
1	A	153	ARG	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	509	14/15	0.87	0.23	0.95	47,51,54,56	0
2	NAG	B	508	14/15	0.86	0.22	0.46	54,58,59,59	0
2	NAG	A	508	14/15	0.61	0.29	0.43	75,79,81,83	0
2	NAG	A	501	14/15	0.93	0.20	0.30	23,28,30,33	0
2	NAG	A	518	14/15	0.86	0.21	-0.08	41,45,58,71	0
2	NAG	B	511	14/15	0.91	0.19	-0.23	34,39,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	509	14/15	0.90	0.21	-0.28	41,45,49,53	0
2	NAG	A	506	14/15	0.88	0.18	-0.40	41,51,57,60	0
2	NAG	A	515	14/15	0.90	0.19	-0.43	50,54,60,63	0
2	NAG	B	505	14/15	0.91	0.19	-0.48	42,46,50,56	0
2	NAG	B	501	14/15	0.96	0.17	-0.63	15,20,29,35	0
2	NAG	A	514	14/15	0.94	0.15	-0.97	36,40,43,48	0
2	NAG	B	507	14/15	0.87	0.20	-1.05	56,63,64,65	0
2	NAG	A	519	14/15	0.93	0.23	-	25,39,43,50	0
2	NAG	B	510	14/15	0.87	0.22	-	57,60,62,63	0
3	BMA	A	516	11/12	0.79	0.24	-	66,67,75,77	0
2	NAG	A	513	14/15	0.56	0.48	-	92,94,98,99	0
2	NAG	A	507	14/15	0.75	0.29	-	69,74,77,77	0
4	MAN	A	505	11/12	0.39	0.60	-	85,88,90,90	0
2	NAG	B	512	14/15	0.95	0.20	-	31,38,43,52	0
2	NAG	A	502	14/15	0.94	0.17	-	36,38,44,53	0
4	MAN	A	504	11/12	0.86	0.34	-	71,73,74,75	0
4	MAN	A	521	11/12	0.77	0.27	-	69,71,77,77	0
3	BMA	A	520	11/12	0.92	0.30	-	55,58,60,64	0
4	MAN	A	517	11/12	0.85	0.21	-	66,69,69,69	0
3	BMA	B	513	11/12	0.91	0.21	-	58,64,68,68	0
2	NAG	A	512	14/15	0.75	0.17	-	68,71,81,86	0
3	BMA	A	511	11/12	-0.03	0.68	-	86,90,124,124	0
4	MAN	B	514	11/12	0.80	0.26	-	70,71,72,72	0
2	NAG	B	502	14/15	0.93	0.18	-	32,35,41,49	0
2	NAG	A	510	14/15	0.83	0.25	-	61,65,71,81	0
3	BMA	B	503	11/12	0.86	0.15	-	57,60,72,73	0
4	MAN	B	504	11/12	0.84	0.28	-	78,81,84,84	0
3	BMA	A	503	11/12	0.85	0.13	-	62,68,75,80	0
2	NAG	B	506	14/15	0.83	0.24	-	63,68,73,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.