



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2018 – 12:16 PM EST

PDB ID : 6F39
Title : C1r homodimer CUB1-EGF-CUB2
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Deposited on : 2017-11-28
Resolution : 5.80 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

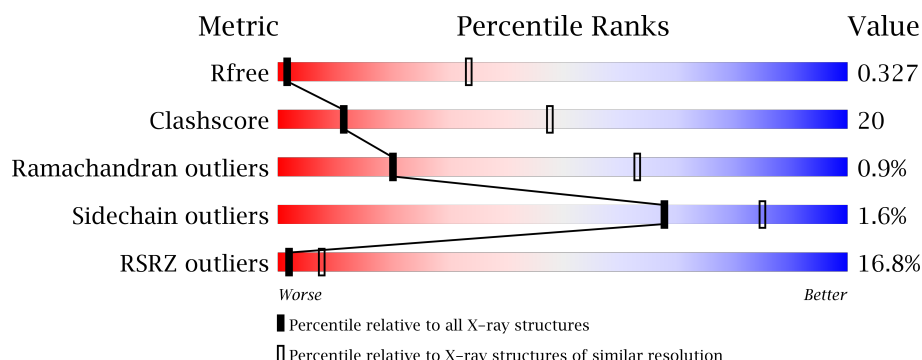
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 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	1077 (7.88-3.70)
Clashscore	112137	1007 (7.80-3.80)
Ramachandran outliers	110173	1106 (7.88-3.70)
Sidechain outliers	110143	1078 (7.88-3.70)
RSRZ outliers	101464	1086 (7.88-3.70)

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	285	<div> <div>14%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
1	B	285	<div> <div>19%</div> <div>59%</div> <div>37%</div> <div>..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4612 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 Complement C1r subcomponent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2206	1397	362	433	14			
1	B	280	Total	C	N	O	S	0	0	0
			2240	1417	368	440	15			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

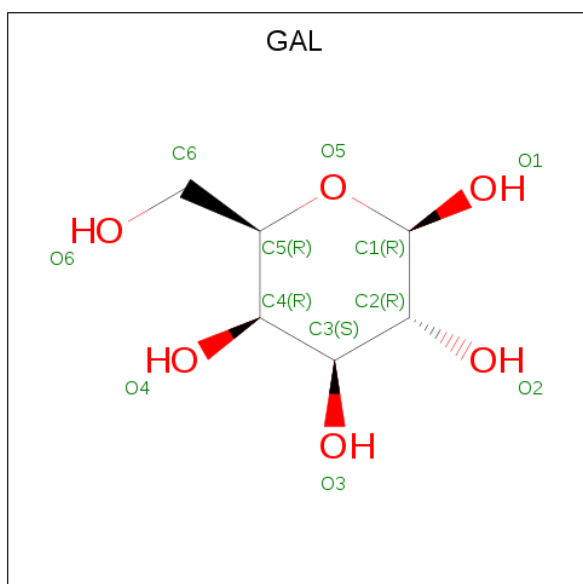
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



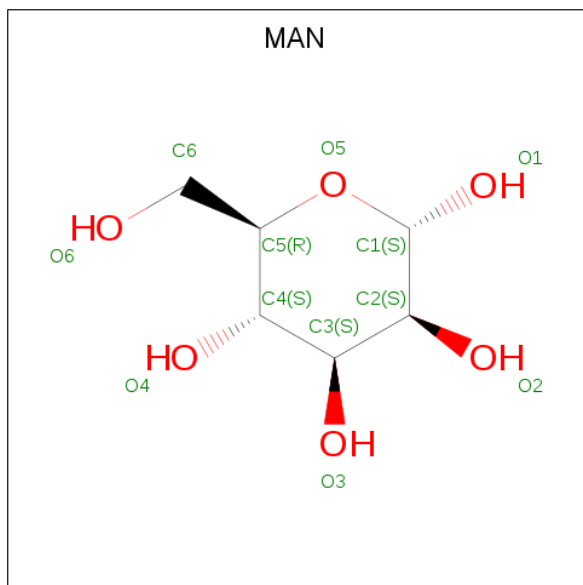
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
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 BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).

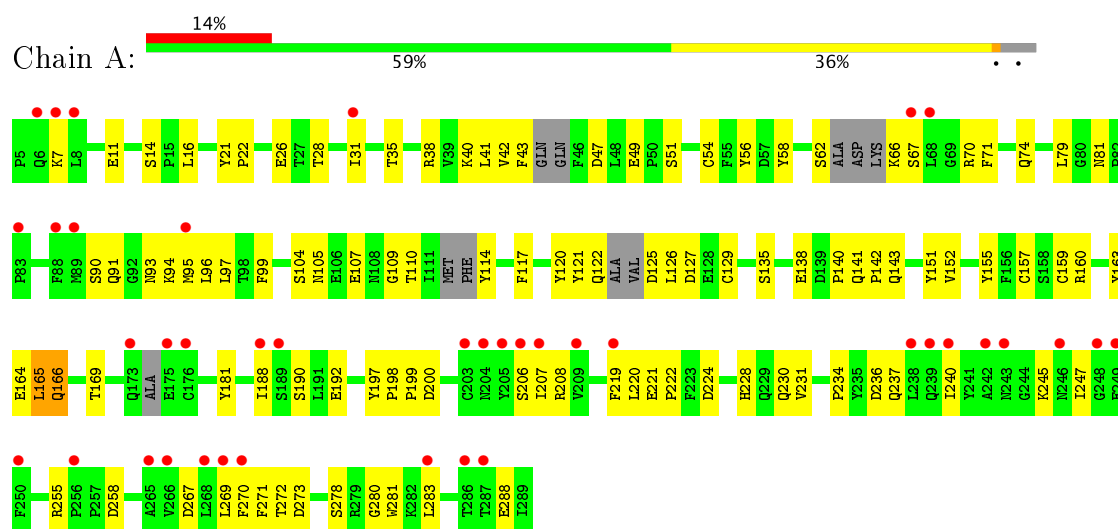


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

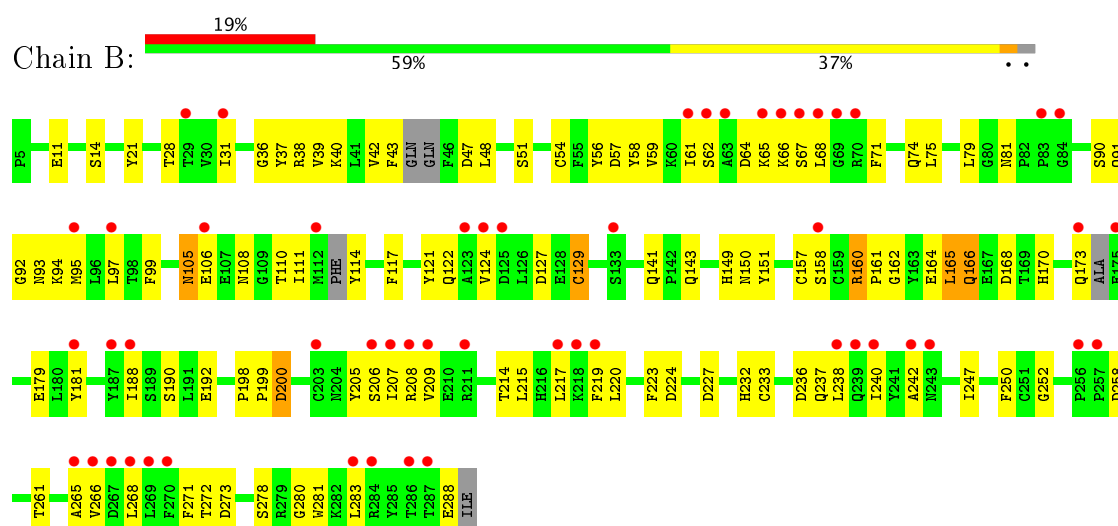
3 Residue-property plots

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: Complement C1r subcomponent



• Molecule 1: Complement C1r subcomponent



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.56 Å 54.62 Å 138.18 Å 90.00° 99.90° 90.00°	Depositor
Resolution (Å)	68.06 – 5.80 68.06 – 5.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (68.06-5.80) 98.9 (68.06-5.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 5.75 Å)	Xtriage
Refinement program	PHENIX dev_2722	Depositor
R, R_{free}	0.308 , 0.338 0.277 , 0.327	Depositor DCC
R_{free} test set	130 reflections (4.40%)	DCC
Wilson B-factor (Å ²)	140.5	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 359.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å ²)	351.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: BMA, NAG, NA, CA, GAL, 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	0.49	0/2264	0.71	0/3060
1	B	0.50	0/2300	0.71	2/3111 (0.1%)
All	All	0.49	0/4564	0.71	2/6171 (0.0%)

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
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	165	LEU	CA-CB-CG	5.30	127.48	115.30
1	B	192	GLU	C-N-CA	5.13	134.52	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	GLN	Peptide
1	B	166	GLN	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	2206	0	2052	90	1
1	B	2240	0	2087	85	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	42	0	37	5	0
4	B	28	0	24	3	0
5	A	11	0	10	0	0
5	B	11	0	10	0	0
6	A	22	0	19	0	0
6	B	22	0	19	0	0
7	A	11	0	8	1	0
7	B	11	0	8	1	0
All	All	4612	0	4274	174	1

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 20.

All (174) 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:208:ARG:NH1	1:B:266:VAL:O	2.11	0.82
1:B:190:SER:HB3	1:B:281:TRP:CE2	2.17	0.79
1:B:93:ASN:HD21	1:B:94:LYS:HE3	1.48	0.77
1:A:237:GLN:HB2	1:A:271:PHE:HB3	1.64	0.77
1:B:38:ARG:NE	1:B:90:SER:O	2.14	0.74
1:A:206:SER:OG	1:A:208:ARG:NH1	2.20	0.73
1:B:31:ILE:HB	1:B:95:MET:HB3	1.68	0.73
1:A:38:ARG:HD2	1:A:126:LEU:HB2	1.71	0.72
1:A:31:ILE:HB	1:A:95:MET:HB3	1.72	0.72
1:B:158:SER:HA	1:B:165:LEU:HD21	1.72	0.72
1:A:188:ILE:HB	1:A:283:LEU:HD11	1.71	0.72
1:A:206:SER:OG	1:A:267:ASP:OD1	2.03	0.71
1:B:129:CYS:HB3	1:B:150:ASN:ND2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASN:HD21	1:A:94:LYS:HE3	1.56	0.69
1:A:236:ASP:OD1	1:A:273:ASP:N	2.25	0.69
7:A:308:BMA:O2	4:A:309:NAG:O3	2.06	0.68
1:B:143:GLN:HG3	1:B:157:CYS:SG	2.34	0.68
1:B:71:PHE:CD1	1:B:81:ASN:HB3	2.28	0.68
1:A:221:GLU:HB3	1:A:222:PRO:HA	1.76	0.68
1:A:181:TYR:HB2	1:A:207:ILE:HG12	1.76	0.67
1:A:51:SER:HB3	1:A:56:TYR:HD2	1.59	0.66
1:A:208:ARG:NH2	4:A:310:NAG:O6	2.29	0.66
1:A:135:SER:HB2	1:A:138:GLU:HG2	1.76	0.66
1:A:142:PRO:HB2	1:A:155:TYR:CE2	2.31	0.64
1:A:224:ASP:HB3	1:A:280:GLY:H	1.61	0.64
1:A:26:GLU:HA	1:A:99:PHE:O	1.98	0.64
1:B:160:ARG:O	1:B:162:GLY:N	2.30	0.64
1:A:51:SER:HB3	1:A:56:TYR:CD2	2.33	0.64
1:A:54:CYS:HB3	1:A:58:TYR:HB3	1.80	0.63
1:B:129:CYS:HB3	1:B:150:ASN:HD21	1.63	0.63
1:B:62:SER:HA	1:B:68:LEU:HG	1.80	0.63
1:B:47:ASP:O	1:B:114:TYR:HB3	1.99	0.62
1:A:142:PRO:HB2	1:A:155:TYR:HE2	1.65	0.61
1:B:237:GLN:HB2	1:B:271:PHE:HB2	1.83	0.60
1:B:64:ASP:HB3	1:B:65:LYS:HG2	1.82	0.60
1:A:208:ARG:HH21	4:A:309:NAG:C7	2.15	0.59
1:A:51:SER:OG	1:A:54:CYS:HA	2.03	0.59
1:B:208:ARG:HG3	1:B:265:ALA:HB1	1.85	0.58
1:B:214:THR:HG23	1:B:288:GLU:HB3	1.85	0.58
1:A:14:SER:HB3	1:A:117:PHE:CD1	2.39	0.57
1:A:58:TYR:HB2	1:A:70:ARG:HG3	1.86	0.57
1:A:122:GLN:HE22	1:B:150:ASN:N	2.03	0.57
1:A:66:LYS:HE2	1:A:67:SER:H	1.69	0.57
1:B:39:VAL:HG21	1:B:95:MET:HB2	1.88	0.55
1:B:93:ASN:ND2	1:B:94:LYS:HE3	2.18	0.55
1:B:206:SER:HB2	1:B:208:ARG:NH1	2.22	0.55
1:A:109:GLY:O	1:A:110:THR:OG1	2.25	0.54
1:B:108:ASN:O	1:B:110:THR:HG23	2.08	0.54
1:B:215:LEU:HB2	1:B:261:THR:HG21	1.90	0.53
1:B:28:THR:HG23	1:B:97:LEU:O	2.08	0.53
1:A:219:PHE:O	1:A:220:LEU:HD13	2.09	0.53
1:A:71:PHE:CD1	1:A:81:ASN:HB3	2.43	0.53
4:A:309:NAG:N2	4:A:310:NAG:O6	2.39	0.53
1:A:228:HIS:NE2	1:A:230:GLN:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:CG	1:A:152:VAL:N	2.78	0.52
1:A:197:TYR:HE2	1:A:278:SER:HB2	1.74	0.52
1:B:106:GLU:HG2	1:B:111:ILE:HG23	1.91	0.52
1:B:51:SER:HB3	1:B:56:TYR:CD2	2.45	0.52
1:A:125:ASP:O	1:A:126:LEU:HD12	2.09	0.52
1:A:71:PHE:HD1	1:A:81:ASN:HB3	1.74	0.52
1:B:48:LEU:HD21	1:B:99:PHE:HE1	1.75	0.52
1:A:11:GLU:HG3	1:A:120:TYR:CE1	2.45	0.52
1:A:221:GLU:HG3	1:A:255:ARG:HD3	1.92	0.52
1:A:35:THR:HA	1:A:93:ASN:HB2	1.91	0.52
1:B:14:SER:HB3	1:B:117:PHE:CD1	2.45	0.51
1:B:57:ASP:OD2	1:B:105:ASN:ND2	2.42	0.51
1:A:151:TYR:CE1	1:B:122:GLN:HB3	2.45	0.51
1:B:188:ILE:O	1:B:283:LEU:HG	2.10	0.51
1:A:240:ILE:O	1:A:247:ILE:HG12	2.10	0.51
1:B:143:GLN:OE1	1:B:157:CYS:HB2	2.11	0.51
1:A:197:TYR:HE1	1:A:272:THR:HG1	1.60	0.50
1:B:215:LEU:O	1:B:261:THR:HG23	2.11	0.50
1:A:104:SER:HB2	1:A:107:GLU:OE1	2.10	0.50
1:A:159:CYS:SG	1:A:165:LEU:HD13	2.51	0.50
1:B:59:VAL:HG22	1:B:99:PHE:CD1	2.46	0.50
1:A:127:ASP:OD1	1:A:155:TYR:HB3	2.11	0.50
1:A:40:LYS:O	1:A:121:TYR:HA	2.12	0.49
1:B:188:ILE:HB	1:B:283:LEU:HD11	1.94	0.49
1:B:62:SER:HB2	1:B:66:LYS:O	2.12	0.49
1:A:160:ARG:HH21	1:A:192:GLU:HG3	1.76	0.49
1:A:38:ARG:NE	1:A:90:SER:O	2.44	0.49
1:B:127:ASP:HB3	1:B:150:ASN:OD1	2.11	0.49
1:A:11:GLU:HG3	1:A:120:TYR:CD1	2.48	0.49
1:A:151:TYR:CE1	1:A:152:VAL:HG22	2.48	0.49
1:B:61:ILE:HD12	1:B:68:LEU:HB2	1.94	0.49
1:A:47:ASP:O	1:A:114:TYR:HB3	2.13	0.49
1:A:56:TYR:HB3	1:A:107:GLU:OE2	2.13	0.48
1:B:208:ARG:NH2	4:B:305:NAG:O6	2.45	0.48
1:B:215:LEU:HB2	1:B:261:THR:CG2	2.43	0.48
1:A:14:SER:HB3	1:A:117:PHE:CE1	2.48	0.48
1:B:224:ASP:CG	1:B:278:SER:HB3	2.34	0.48
1:A:7:LYS:HD3	1:A:121:TYR:OH	2.13	0.48
1:A:270:PHE:CE2	1:A:272:THR:HB	2.49	0.48
1:B:21:TYR:CE2	1:B:114:TYR:HB2	2.48	0.48
1:B:224:ASP:HB3	1:B:280:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH1	1:A:126:LEU:HD22	2.29	0.48
1:B:36:GLY:C	1:B:37:TYR:CD1	2.87	0.48
1:B:190:SER:HB3	1:B:281:TRP:NE1	2.28	0.47
1:A:157:CYS:HB2	1:A:169:THR:O	2.15	0.47
1:A:62:SER:OG	1:A:96:LEU:HB2	2.13	0.47
1:A:224:ASP:N	1:A:280:GLY:O	2.47	0.47
1:B:59:VAL:HG22	1:B:99:PHE:HD1	1.80	0.47
1:A:221:GLU:CB	1:A:222:PRO:HA	2.45	0.47
1:B:227:ASP:CG	1:B:252:GLY:HA2	2.35	0.47
1:B:141:GLN:HB2	1:B:170:HIS:NE2	2.30	0.46
1:B:205:TYR:O	1:B:268:LEU:HB2	2.15	0.46
1:A:190:SER:HB3	1:A:281:TRP:CE2	2.49	0.46
1:B:66:LYS:HE2	1:B:67:SER:H	1.81	0.46
1:A:127:ASP:OD2	1:A:151:TYR:N	2.48	0.46
1:A:160:ARG:HE	1:A:192:GLU:HG3	1.80	0.46
1:A:41:LEU:HD11	1:A:95:MET:HG2	1.98	0.46
1:B:223:PHE:CE1	1:B:281:TRP:HB3	2.51	0.46
1:A:164:GLU:HG2	1:A:164:GLU:O	2.16	0.45
4:B:306:NAG:O3	7:B:307:BMA:O2	2.15	0.45
1:A:21:TYR:CE2	1:A:114:TYR:HB2	2.51	0.45
1:B:209:VAL:HG11	1:B:215:LEU:HD21	1.98	0.45
1:A:198:PRO:HA	1:A:199:PRO:HD3	1.77	0.45
1:B:236:ASP:OD1	1:B:273:ASP:N	2.42	0.45
1:A:152:VAL:HG13	1:B:124:VAL:HG13	1.99	0.45
1:A:228:HIS:CD2	1:A:230:GLN:HB2	2.52	0.45
1:B:242:ALA:HB2	1:B:247:ILE:HD13	1.99	0.45
1:B:232:HIS:HB3	1:B:233:CYS:SG	2.57	0.45
1:B:179:GLU:HB2	1:B:205:TYR:CE1	2.52	0.44
1:A:38:ARG:HD3	1:A:126:LEU:HD13	2.00	0.44
1:A:122:GLN:NE2	1:B:149:HIS:HB3	2.32	0.44
1:B:160:ARG:O	1:B:160:ARG:HG3	2.17	0.44
1:B:42:VAL:HG23	1:B:43:PHE:O	2.18	0.44
1:A:62:SER:OG	1:A:62:SER:O	2.36	0.43
1:B:238:LEU:HB3	1:B:250:PHE:O	2.18	0.43
1:A:16:LEU:HD13	1:A:22:PRO:HD3	2.00	0.43
1:A:31:ILE:HD12	1:A:95:MET:HB3	2.00	0.43
1:B:90:SER:OG	1:B:92:GLY:O	2.28	0.43
1:A:197:TYR:OH	1:A:236:ASP:OD2	2.28	0.43
1:A:28:THR:HG23	1:A:97:LEU:O	2.19	0.43
1:B:160:ARG:NH2	1:B:173:GLN:HB2	2.34	0.43
1:B:198:PRO:HA	1:B:199:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:HD21	1:A:114:TYR:N	2.17	0.43
1:A:231:VAL:O	1:A:234:PRO:HD3	2.19	0.42
1:A:140:PRO:O	1:A:142:PRO:HD3	2.19	0.42
1:A:269:LEU:HD21	4:A:310:NAG:O7	2.20	0.42
1:B:181:TYR:O	1:B:207:ILE:HG12	2.20	0.42
1:B:71:PHE:HD1	1:B:81:ASN:HB3	1.82	0.42
1:A:142:PRO:HD2	1:A:143:GLN:HG2	2.00	0.42
1:B:240:ILE:O	1:B:247:ILE:HG12	2.19	0.42
1:A:49:GLU:OE2	1:A:107:GLU:HB2	2.19	0.42
1:B:66:LYS:HE2	1:B:67:SER:N	2.34	0.42
1:A:35:THR:HA	1:A:93:ASN:CB	2.48	0.42
1:A:38:ARG:HH21	1:A:91:GLN:HA	1.85	0.42
1:A:42:VAL:HG23	1:A:43:PHE:O	2.19	0.42
1:B:40:LYS:O	1:B:121:TYR:HA	2.20	0.42
1:B:79:LEU:HA	1:B:79:LEU:HD23	1.85	0.42
1:A:258:ASP:OD1	1:A:258:ASP:N	2.53	0.42
1:A:47:ASP:OD1	1:A:74:GLN:HG3	2.19	0.42
1:A:219:PHE:C	1:A:220:LEU:HD22	2.41	0.41
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.95	0.41
1:A:165:LEU:HD12	1:A:169:THR:HA	2.02	0.41
1:B:160:ARG:C	1:B:162:GLY:H	2.23	0.41
1:B:91:GLN:N	1:B:91:GLN:OE1	2.53	0.41
1:B:31:ILE:HD12	1:B:95:MET:HG2	2.03	0.41
1:B:219:PHE:O	1:B:220:LEU:HD13	2.20	0.41
1:A:163:TYR:HD2	1:A:165:LEU:H	1.69	0.41
1:B:168:ASP:HB2	1:B:170:HIS:ND1	2.36	0.41
1:B:199:PRO:HA	1:B:272:THR:HB	2.01	0.41
1:B:217:LEU:HD11	1:B:261:THR:HG22	2.02	0.41
1:A:38:ARG:HH11	1:A:126:LEU:HD22	1.84	0.41
1:B:164:GLU:C	1:B:165:LEU:HD23	2.41	0.41
1:B:200:ASP:N	1:B:273:ASP:O	2.45	0.40
1:A:41:LEU:HD23	1:A:120:TYR:O	2.20	0.40
1:B:208:ARG:HH21	4:B:306:NAG:C7	2.34	0.40
1:B:74:GLN:HG2	1:B:75:LEU:H	1.86	0.40
1:B:64:ASP:OD2	1:B:92:GLY:HA3	2.21	0.40
1:B:179:GLU:HB2	1:B:205:TYR:CD1	2.55	0.40
1:B:258:ASP:OD1	1:B:258:ASP:N	2.54	0.40
1:B:54:CYS:HB3	1:B:58:TYR:HB3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:NZ	1:A:288:GLU:OE1[4_646]	2.19	0.01

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	263/285 (92%)	227 (86%)	34 (13%)	2 (1%)	22	66
1	B	272/285 (95%)	233 (86%)	36 (13%)	3 (1%)	17	59
All	All	535/570 (94%)	460 (86%)	70 (13%)	5 (1%)	20	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	166	GLN
1	B	161	PRO
1	B	160	ARG
1	A	141	GLN

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	248/255 (97%)	245 (99%)	3 (1%)	75	88
1	B	251/255 (98%)	246 (98%)	5 (2%)	60	82
All	All	499/510 (98%)	491 (98%)	8 (2%)	68	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	CYS
1	A	165	LEU
1	A	200	ASP
1	B	11	GLU
1	B	105	ASN
1	B	129	CYS
1	B	151	TYR
1	B	200	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	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 ⓘ

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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
4	NAG	A	305	1	14,14,15	1.30	2 (14%)	15,19,21	1.41	1 (6%)
5	GAL	A	306	6	11,11,12	1.15	2 (18%)	13,15,17	1.25	1 (7%)
6	MAN	A	307	5,7	11,11,12	1.56	3 (27%)	13,15,17	1.97	2 (15%)
7	BMA	A	308	4,6	11,11,12	1.62	3 (27%)	13,15,17	1.13	2 (15%)
4	NAG	A	309	4,7	14,14,15	0.35	0	15,19,21	0.60	0
4	NAG	A	310	1,4	14,14,15	0.41	0	15,19,21	0.97	1 (6%)
6	MAN	A	311	7	11,11,12	0.82	1 (9%)	13,15,17	1.03	1 (7%)
4	NAG	B	305	1,4	14,14,15	0.20	0	15,19,21	0.88	1 (6%)
4	NAG	B	306	4,7	14,14,15	0.47	0	15,19,21	0.72	0
7	BMA	B	307	4,6	11,11,12	1.28	2 (18%)	13,15,17	1.00	0
6	MAN	B	308	5,7	11,11,12	1.81	4 (36%)	13,15,17	1.83	1 (7%)
5	GAL	B	309	6	11,11,12	1.30	3 (27%)	13,15,17	1.45	3 (23%)
6	MAN	B	310	7	11,11,12	0.76	0	13,15,17	1.25	1 (7%)

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
4	NAG	A	305	1	-	0/6/23/26	0/1/1/1
5	GAL	A	306	6	-	0/2/19/22	0/1/1/1
6	MAN	A	307	5,7	-	0/2/19/22	1/1/1/1
7	BMA	A	308	4,6	-	0/2/19/22	0/1/1/1
4	NAG	A	309	4,7	-	0/6/23/26	0/1/1/1
4	NAG	A	310	1,4	-	0/6/23/26	0/1/1/1
6	MAN	A	311	7	-	0/2/19/22	0/1/1/1
4	NAG	B	305	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	306	4,7	-	0/6/23/26	0/1/1/1
7	BMA	B	307	4,6	-	0/2/19/22	0/1/1/1
6	MAN	B	308	5,7	-	0/2/19/22	0/1/1/1
5	GAL	B	309	6	-	0/2/19/22	0/1/1/1
6	MAN	B	310	7	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	311	MAN	O5-C1	-2.03	1.40	1.43
5	B	309	GAL	O5-C5	2.03	1.47	1.43
5	A	306	GAL	C1-C2	2.05	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	309	GAL	C2-C3	2.07	1.55	1.52
6	B	308	MAN	C4-C3	2.09	1.57	1.52
6	B	308	MAN	O5-C5	2.12	1.47	1.43
5	A	306	GAL	C2-C3	2.20	1.55	1.52
7	B	307	BMA	C4-C5	2.27	1.57	1.53
6	A	307	MAN	C2-C3	2.37	1.55	1.52
7	B	307	BMA	C1-C2	2.39	1.57	1.52
6	B	308	MAN	C2-C3	2.40	1.55	1.52
7	A	308	BMA	C4-C5	2.40	1.58	1.53
6	A	307	MAN	O4-C4	2.47	1.48	1.43
5	B	309	GAL	C1-C2	2.50	1.58	1.52
7	A	308	BMA	O3-C3	2.59	1.48	1.43
4	A	305	NAG	C1-C2	2.71	1.56	1.52
6	A	307	MAN	O5-C5	2.73	1.49	1.43
7	A	308	BMA	C4-C3	2.90	1.59	1.52
4	A	305	NAG	O5-C1	3.99	1.50	1.43
6	B	308	MAN	O4-C4	4.09	1.52	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	308	BMA	O2-C2-C3	-2.87	104.54	110.17
6	A	311	MAN	O2-C2-C3	-2.54	105.19	110.17
5	B	309	GAL	O5-C1-C2	-2.43	106.98	110.79
5	A	306	GAL	O5-C1-C2	-2.05	107.58	110.79
6	A	307	MAN	O2-C2-C3	-2.03	106.19	110.17
7	A	308	BMA	C3-C4-C5	2.13	113.97	110.22
5	B	309	GAL	O2-C2-C1	2.22	113.68	109.18
5	B	309	GAL	C1-O5-C5	2.53	115.66	112.17
4	B	305	NAG	C1-O5-C5	2.58	115.72	112.17
4	A	310	NAG	C1-O5-C5	3.24	116.64	112.17
6	B	310	MAN	C1-O5-C5	3.27	116.68	112.17
4	A	305	NAG	C1-O5-C5	5.07	119.16	112.17
6	B	308	MAN	C1-O5-C5	5.12	119.22	112.17
6	A	307	MAN	C1-O5-C5	5.93	120.34	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	307	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	308	BMA	1	0
4	A	309	NAG	3	0
4	A	310	NAG	3	0
4	B	305	NAG	1	0
4	B	306	NAG	2	0
7	B	307	BMA	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	275/285 (96%)	0.65	40 (14%) 3 9	289, 347, 395, 429	0
1	B	280/285 (98%)	0.91	53 (18%) 1 7	316, 354, 400, 430	0
All	All	555/570 (97%)	0.78	93 (16%) 2 8	289, 352, 399, 430	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	ILE	12.6
1	A	265	ALA	9.9
1	B	265	ALA	9.4
1	A	207	ILE	9.2
1	A	239	GLN	7.9
1	B	266	VAL	7.5
1	A	266	VAL	6.9
1	B	209	VAL	6.5
1	B	206	SER	6.3
1	A	238	LEU	5.9
1	B	239	GLN	5.2
1	B	123	ALA	5.1
1	B	125	ASP	5.1
1	B	124	VAL	4.9
1	A	205	TYR	4.8
1	B	238	LEU	4.8
1	B	83	PRO	4.7
1	A	270	PHE	4.6
1	B	286	THR	4.4
1	B	175	GLU	4.4
1	A	246	ASN	4.3
1	B	63	ALA	4.1
1	B	188	ILE	3.9
1	B	208	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	69	GLY	3.6
1	A	256	PRO	3.6
1	B	158	SER	3.6
1	B	181	TYR	3.6
1	B	218	LYS	3.6
1	A	286	THR	3.6
1	A	209	VAL	3.5
1	A	173	GLN	3.5
1	A	203	CYS	3.4
1	B	287	THR	3.4
1	A	219	PHE	3.3
1	A	269	LEU	3.3
1	B	270	PHE	3.2
1	B	256	PRO	3.2
1	B	203	CYS	3.2
1	B	268	LEU	3.2
1	B	243	ASN	3.2
1	A	7	LYS	3.1
1	B	173	GLN	3.1
1	B	112	MET	3.0
1	A	89	MET	3.0
1	B	187	TYR	3.0
1	A	31	ILE	3.0
1	A	243	ASN	3.0
1	A	287	THR	2.9
1	A	176	CYS	2.9
1	A	175	GLU	2.9
1	A	188	ILE	2.9
1	A	249	GLU	2.9
1	B	269	LEU	2.8
1	A	67	SER	2.8
1	A	268	LEU	2.8
1	B	283	LEU	2.7
1	B	62	SER	2.7
1	B	219	PHE	2.7
1	B	240	ILE	2.7
1	A	250	PHE	2.6
1	B	84	GLY	2.6
1	A	206	SER	2.6
1	A	248	GLY	2.6
1	B	95	MET	2.6
1	A	68	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	83	PRO	2.5
1	B	106	GLU	2.5
1	B	133	SER	2.4
1	B	267	ASP	2.4
1	B	70	ARG	2.4
1	A	240	ILE	2.4
1	B	68	LEU	2.3
1	A	88	PHE	2.3
1	B	217	LEU	2.3
1	B	65	LYS	2.3
1	B	242	ALA	2.2
1	B	61	ILE	2.2
1	A	8	LEU	2.2
1	B	257	PRO	2.2
1	B	211	ARG	2.2
1	A	204	ASN	2.2
1	A	242	ALA	2.2
1	B	67	SER	2.2
1	B	31	ILE	2.1
1	B	97	LEU	2.1
1	B	29	THR	2.1
1	A	95	MET	2.1
1	B	66	LYS	2.1
1	A	283	LEU	2.1
1	A	6	GLN	2.0
1	A	189	SER	2.0
1	B	284	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
3	NA	A	304	1/1	0.97	0.33	-0.32	374,374,374,374	0
3	NA	B	304	1/1	0.96	0.37	-0.47	315,315,315,315	0
2	CA	A	303	1/1	0.89	0.13	-1.00	376,376,376,376	0
2	CA	B	302	1/1	0.99	0.22	-1.17	254,254,254,254	0
2	CA	B	301	1/1	0.90	0.13	-1.30	359,359,359,359	0
2	CA	A	302	1/1	0.97	0.16	-1.43	276,276,276,276	0
2	CA	A	301	1/1	0.85	0.13	-1.47	303,303,303,303	0
2	CA	B	303	1/1	0.91	0.09	-1.55	350,350,350,350	0
5	GAL	B	309	11/12	0.47	0.70	-	421,421,421,421	0
4	NAG	A	305	14/15	0.66	0.46	-	320,320,320,320	0
7	BMA	A	308	11/12	0.69	0.20	-	427,427,427,427	0
6	MAN	A	307	11/12	0.82	0.28	-	431,431,431,431	0
7	BMA	B	307	11/12	0.82	0.31	-	406,406,406,406	0
5	GAL	A	306	11/12	0.51	0.46	-	422,422,422,422	0
4	NAG	B	306	14/15	0.78	0.25	-	383,383,383,383	0
4	NAG	A	310	14/15	0.84	0.30	-	383,383,383,383	0
4	NAG	A	309	14/15	0.88	0.16	-	393,393,393,393	0
4	NAG	B	305	14/15	0.80	0.27	-	362,362,362,362	0
6	MAN	B	310	11/12	0.75	0.79	-	376,376,376,376	0
6	MAN	B	308	11/12	0.74	0.32	-	398,398,398,398	0
6	MAN	A	311	11/12	0.39	0.66	-	403,403,403,403	0

6.5 Other polymers [i](#)

There are no such residues in this entry.