



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2017 – 05:30 AM EDT

PDB ID : 4RQS
Title : Crystal structure of fully glycosylated HIV-1 gp120 core bound to CD4 and 17b Fab
Authors : Kong, L.; Wilson, I.A.; Kwong, P.D.
Deposited on : 2014-11-05
Resolution : 4.49 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-20029077
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-20029077

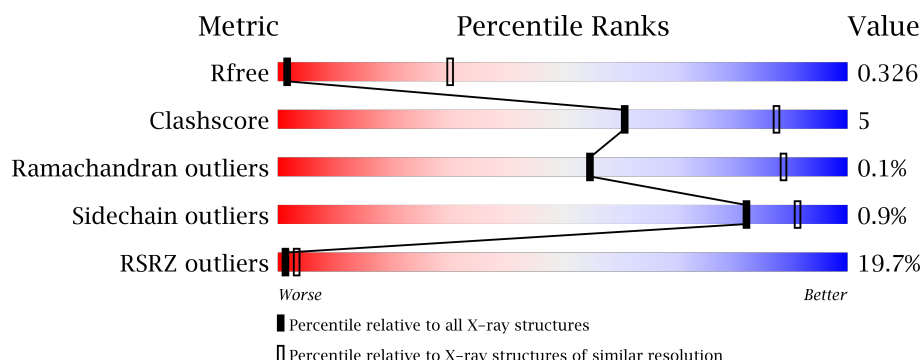
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.49 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	1007 (5.30-3.64)
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1015 (5.30-3.64)

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	B	185	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	214	<div> <div>28%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
3	D	229	<div> <div>30%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
4	G	313	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	502	-	-	-	X
5	NAG	G	517	-	-	-	X
5	NAG	G	521	-	-	-	X
7	MAN	G	506	-	-	-	X
7	MAN	G	507	-	-	-	X
7	MAN	G	508	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7379 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 2-domain CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ASN	-	EXPRESSION TAG	UNP P01730
B	185	THR	-	EXPRESSION TAG	UNP P01730

- Molecule 2 is a protein called 17b Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 3 is a protein called 17b Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	223	Total	C	N	O	S	0	0	0
			1681	1064	282	330	5			

- Molecule 4 is a protein called HIV-1 YU2 gp120 core chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	295	Total	C	N	O	S	0	0	0
			2292	1441	396	435	20			

There are 10 discrepancies between the modelled and reference sequences:

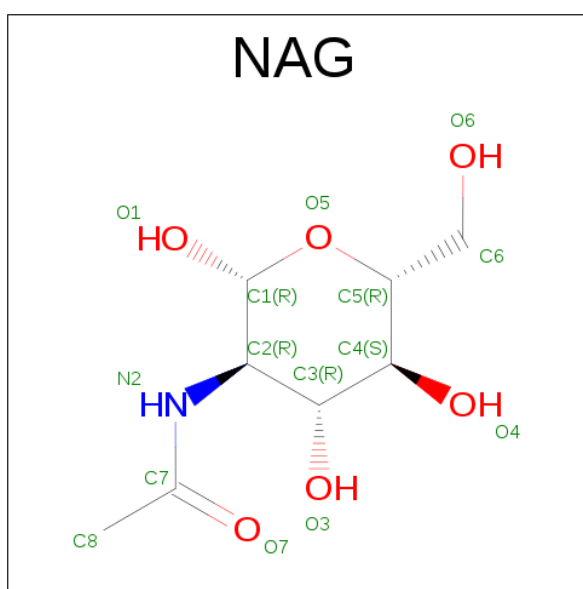
Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	EXPRESSION TAG	UNP P35961
G	80	ALA	-	EXPRESSION TAG	UNP P35961

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Chain	Residue	Modelled	Actual	Comment	Reference
G	81	ARG	-	EXPRESSION TAG	UNP P35961
G	82	SER	-	EXPRESSION TAG	UNP P35961
G	128	GLY	-	LINKER	UNP P35961
G	129	ALA	-	LINKER	UNP P35961
G	194	GLY	-	LINKER	UNP P35961
G	298	GLY	-	LINKER	UNP P35961
G	299	ALA	-	LINKER	UNP P35961
G	300	GLY	-	LINKER	UNP P35961

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



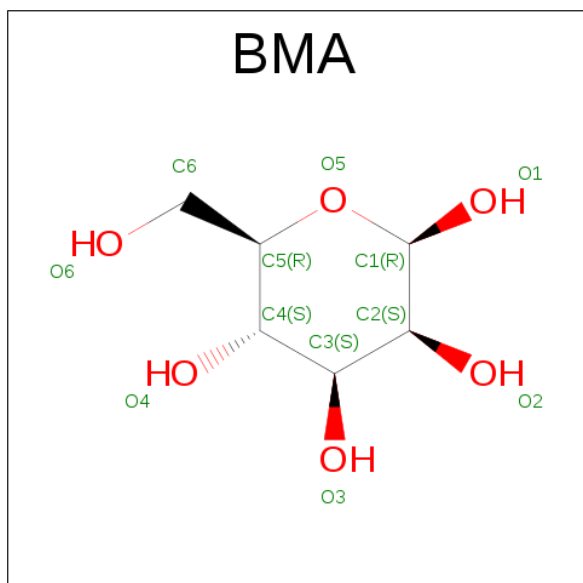
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

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

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



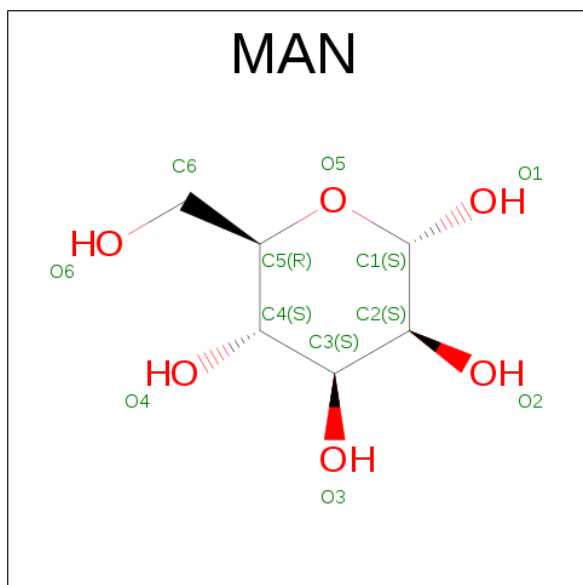
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

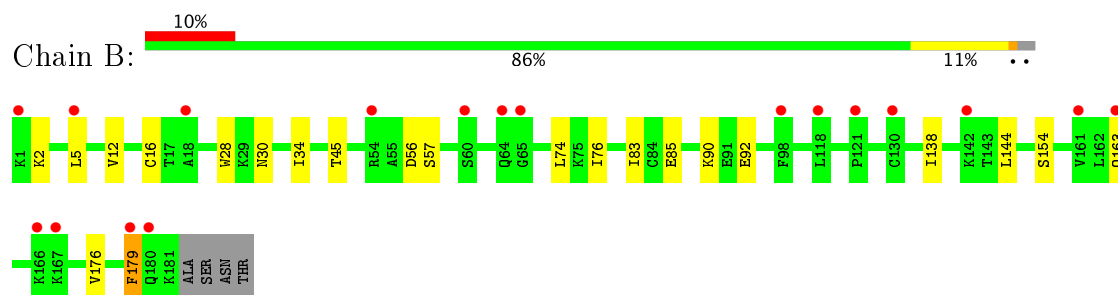


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		

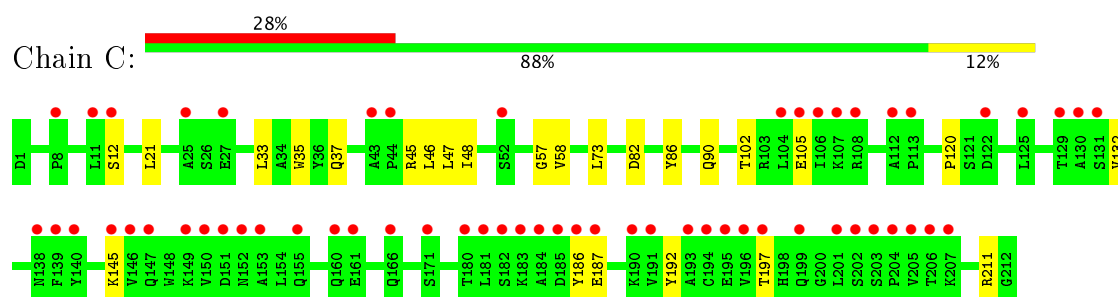
3 Residue-property plots [i](#)

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

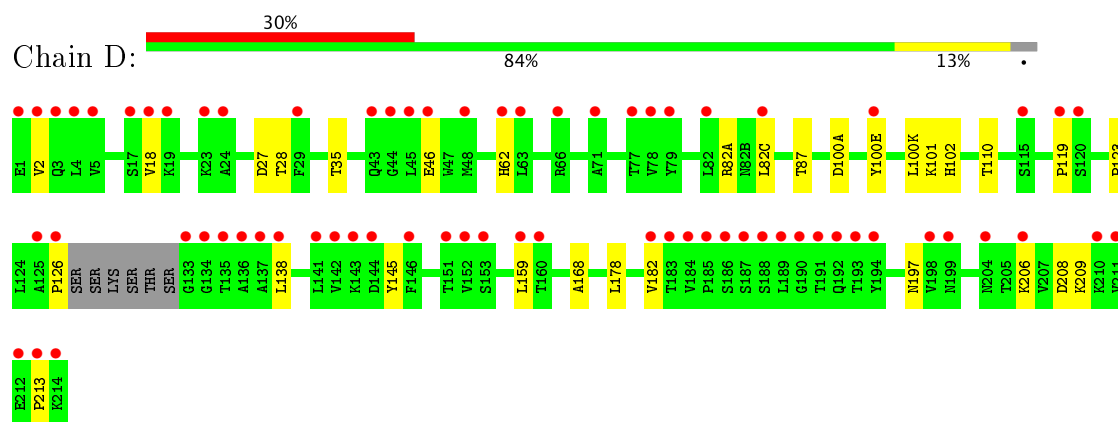
- Molecule 1: 2-domain CD4



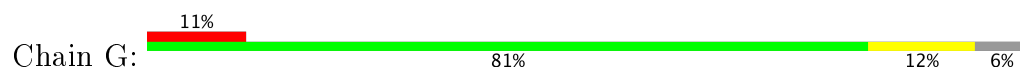
- Molecule 2: 17b Fab Light Chain

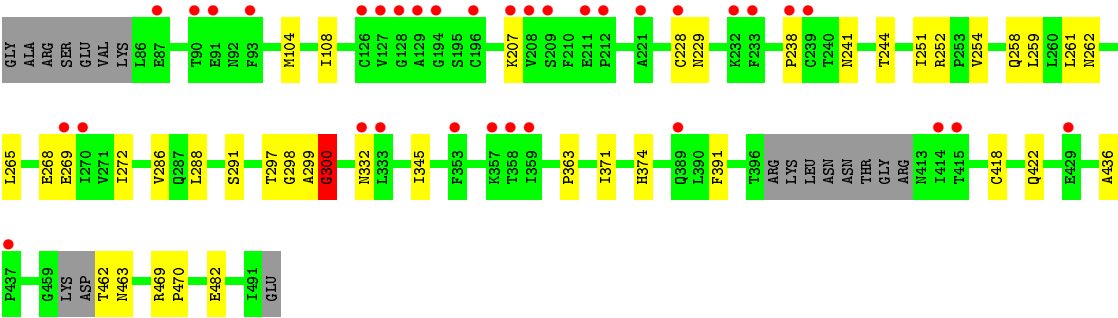


- Molecule 3: 17b Fab Heavy Chain



- Molecule 4: HIV-1 YU2 gp120 core chimeric protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.32Å 171.32Å 151.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 4.49 47.52 – 4.49	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.50-4.49) 95.1 (47.52-4.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.276 , 0.322 0.276 , 0.326	Depositor DCC
R_{free} test set	665 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	248.9	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 213.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 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	B	0.21	0/1432	0.38	0/1930
2	C	0.21	0/1683	0.38	0/2288
3	D	0.20	0/1720	0.37	0/2343
4	G	0.21	0/2337	0.40	1/3169 (0.0%)
All	All	0.21	0/7172	0.38	1/9730 (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
4	G	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	300	GLY	CA-C-N	-6.96	101.89	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	300	GLY	Mainchain,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	B	1412	0	1444	13	0
2	C	1646	0	1593	13	0
3	D	1681	0	1650	17	0
4	G	2292	0	2246	29	0
5	G	238	0	209	5	0
6	G	44	0	38	0	0
7	G	66	0	56	3	0
All	All	7379	0	7236	75	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 5.

All (75) 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)
7:G:504:MAN:C6	7:G:509:MAN:C1	2.46	0.93
4:G:297:THR:HG22	4:G:298:GLY:H	1.40	0.87
7:G:504:MAN:O6	7:G:509:MAN:C2	2.22	0.87
5:G:501:NAG:H61	5:G:502:NAG:H82	1.66	0.76
4:G:297:THR:HG22	4:G:298:GLY:N	2.03	0.72
1:B:5:LEU:HD21	1:B:163:GLN:HB3	1.74	0.69
4:G:300:GLY:CA	4:G:418:CYS:HB2	2.26	0.66
3:D:100(E):TYR:O	4:G:422:GLN:NE2	2.29	0.65
4:G:268:GLU:HG3	4:G:269:GLU:HG2	1.80	0.64
4:G:297:THR:CG2	4:G:298:GLY:H	2.15	0.59
4:G:207:LYS:HE2	4:G:436:ALA:HB3	1.85	0.58
3:D:126:PRO:HG3	3:D:138:LEU:HB3	1.85	0.58
7:G:504:MAN:O6	7:G:509:MAN:H2	2.03	0.58
3:D:197:ASN:HB3	3:D:206:LYS:HE2	1.87	0.57
5:G:502:NAG:H82	5:G:519:NAG:H81	1.87	0.56
1:B:85:GLU:HG2	1:B:90:LYS:HG2	1.88	0.56
4:G:298:GLY:O	4:G:299:ALA:HB3	2.06	0.55
4:G:300:GLY:HA2	4:G:418:CYS:HB2	1.89	0.55
5:G:502:NAG:C8	5:G:519:NAG:H81	2.37	0.55
3:D:35:THR:HB	3:D:100(K):LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:PRO:HD2	3:D:213:PRO:HA	1.89	0.54
3:D:159:LEU:HD21	3:D:182:VAL:HG21	1.90	0.53
4:G:265:LEU:HD11	4:G:291:SER:HB3	1.90	0.53
3:D:123:PRO:HD3	3:D:209:LYS:HE2	1.91	0.52
4:G:229:ASN:HB2	4:G:241:ASN:HD22	1.74	0.52
1:B:154:SER:HB2	1:B:176:VAL:HB	1.92	0.52
1:B:83:ILE:HG13	1:B:92:GLU:HG3	1.92	0.52
2:C:21:LEU:HD22	2:C:102:THR:HG21	1.92	0.51
2:C:45:ARG:NH2	2:C:57:GLY:O	2.43	0.51
4:G:363:PRO:O	4:G:469:ARG:NH1	2.39	0.50
3:D:87:THR:HG23	3:D:110:THR:HA	1.92	0.50
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.93	0.50
2:C:145:LYS:HB3	2:C:197:THR:HB	1.93	0.50
4:G:252:ARG:HD2	4:G:262:ASN:HB3	1.92	0.50
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.94	0.50
1:B:138:ILE:HG22	1:B:144:LEU:HD11	1.94	0.49
1:B:76:ILE:H	1:B:76:ILE:HD12	1.77	0.49
4:G:254:VAL:HG11	4:G:261:LEU:HB2	1.95	0.48
1:B:30:ASN:HD21	1:B:34:ILE:HB	1.78	0.48
2:C:120:PRO:HD3	2:C:132:VAL:HG22	1.97	0.47
2:C:46:LEU:HD22	3:D:101:LYS:HA	1.97	0.46
4:G:238:PRO:HD2	5:G:521:NAG:H61	1.97	0.46
1:B:56:ASP:OD1	1:B:57:SER:N	2.40	0.46
2:C:82:ASP:O	2:C:86:TYR:OH	2.26	0.46
4:G:272:ILE:HG22	4:G:286:VAL:HG22	1.97	0.46
3:D:46:GLU:OE2	3:D:62:HIS:NE2	2.48	0.46
4:G:462:THR:HA	4:G:463:ASN:HA	1.50	0.45
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.51	0.45
2:C:186:TYR:O	2:C:192:TYR:OH	2.34	0.45
2:C:12:SER:OG	2:C:105:GLU:OE1	2.27	0.45
4:G:258:GLN:NE2	4:G:371:ILE:O	2.50	0.45
4:G:288:LEU:HD21	4:G:345:ILE:HD11	1.99	0.44
3:D:27:ASP:OD2	3:D:28:THR:N	2.41	0.44
3:D:2:VAL:HG11	3:D:102:HIS:CD2	2.53	0.44
4:G:297:THR:CG2	4:G:298:GLY:N	2.73	0.44
1:B:12:VAL:HG12	1:B:74:LEU:HD11	2.00	0.43
4:G:300:GLY:HA3	4:G:418:CYS:O	2.18	0.43
4:G:229:ASN:HB2	4:G:241:ASN:ND2	2.34	0.43
2:C:21:LEU:HD12	2:C:73:LEU:HD23	2.01	0.43
2:C:35:TRP:HB2	2:C:48:ILE:HB	2.00	0.42
4:G:104:MET:O	4:G:108:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:168:ALA:HB2	3:D:178:LEU:HD23	2.02	0.42
1:B:179:PHE:HA	1:B:179:PHE:HD1	1.69	0.42
1:B:16:CYS:HB2	1:B:28:TRP:CZ2	2.55	0.42
1:B:16:CYS:HB2	1:B:28:TRP:HZ2	1.85	0.41
3:D:197:ASN:ND2	3:D:208:ASP:OD2	2.49	0.41
2:C:187:GLU:O	2:C:211:ARG:NH2	2.53	0.41
4:G:251:ILE:HG23	4:G:482:GLU:HG3	2.02	0.41
2:C:47:LEU:HA	2:C:58:VAL:HG21	2.03	0.41
4:G:391:PHE:CZ	4:G:470:PRO:HB3	2.55	0.41
3:D:100(A):ASP:OD1	3:D:100(A):ASP:N	2.55	0.40
3:D:18:VAL:HG12	3:D:82(C):LEU:HD21	2.04	0.40
1:B:45:THR:HG22	4:G:371:ILE:HD13	2.03	0.40
4:G:259:LEU:HD12	4:G:374:HIS:CD2	2.57	0.40
4:G:332:ASN:HD22	5:G:517:NAG:C7	2.32	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	B	179/185 (97%)	174 (97%)	5 (3%)	0	100	100
2	C	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	D	219/229 (96%)	216 (99%)	3 (1%)	0	100	100
4	G	289/313 (92%)	280 (97%)	8 (3%)	1 (0%)	44	81
All	All	899/941 (96%)	875 (97%)	23 (3%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	300	GLY

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	B	164/167 (98%)	162 (99%)	2 (1%)	75	88
2	C	184/184 (100%)	182 (99%)	2 (1%)	78	89
3	D	187/193 (97%)	186 (100%)	1 (0%)	91	95
4	G	261/276 (95%)	259 (99%)	2 (1%)	85	92
All	All	796/820 (97%)	789 (99%)	7 (1%)	82	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
1	B	179	PHE
2	C	33	LEU
2	C	90	GLN
3	D	82(A)	ARG
4	G	228	CYS
4	G	244	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	90	GLN
3	D	171	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

27 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	$\# Z > 2$
5	NAG	G	501	5,4	14,14,15	0.58	0	15,19,21	0.73	0
5	NAG	G	502	5,6	14,14,15	0.56	0	15,19,21	0.90	0
6	BMA	G	503	5,7	11,11,12	0.65	0	13,15,17	0.69	0
7	MAN	G	504	7,6	11,11,12	0.65	0	13,15,17	0.82	0
7	MAN	G	505	7	11,11,12	0.61	0	13,15,17	0.55	0
7	MAN	G	506	7,6	11,11,12	0.59	0	13,15,17	0.62	0
7	MAN	G	507	7	11,11,12	0.53	0	13,15,17	0.68	0
7	MAN	G	508	7	11,11,12	0.62	0	13,15,17	0.61	0
7	MAN	G	509	7	11,11,12	0.65	0	13,15,17	0.76	1 (7%)
5	NAG	G	510	5,4	14,14,15	0.51	0	15,19,21	0.79	0
5	NAG	G	511	5	14,14,15	0.53	0	15,19,21	0.52	0
5	NAG	G	512	5,4	14,14,15	0.54	0	15,19,21	0.77	0
5	NAG	G	513	5,6	14,14,15	0.49	0	15,19,21	0.69	0
6	BMA	G	514	5	11,11,12	0.60	0	13,15,17	0.54	0
5	NAG	G	515	5,4	14,14,15	0.52	0	15,19,21	0.82	0
5	NAG	G	516	5	14,14,15	0.49	0	15,19,21	0.58	0
5	NAG	G	517	5,4	14,14,15	0.50	0	15,19,21	0.55	0
5	NAG	G	518	5	14,14,15	0.54	0	15,19,21	0.57	0
5	NAG	G	519	5,4	14,14,15	0.53	0	15,19,21	0.70	0
5	NAG	G	520	5	14,14,15	0.52	0	15,19,21	0.59	0
5	NAG	G	521	5,4	14,14,15	0.54	0	15,19,21	0.74	0
5	NAG	G	522	5,6	14,14,15	0.57	0	15,19,21	1.02	1 (6%)
6	BMA	G	523	5	11,11,12	0.66	0	13,15,17	0.60	0
5	NAG	G	524	4	14,14,15	0.49	0	15,19,21	0.81	0
5	NAG	G	525	5,4	14,14,15	0.52	0	15,19,21	0.75	0
5	NAG	G	526	5,6	14,14,15	0.54	0	15,19,21	0.64	0
6	BMA	G	527	5	11,11,12	0.62	0	13,15,17	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	501	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	502	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	503	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	504	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	505	7	-	0/2/19/22	0/1/1/1
7	MAN	G	506	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	507	7	-	0/2/19/22	0/1/1/1
7	MAN	G	508	7	-	0/2/19/22	0/1/1/1
7	MAN	G	509	7	-	0/2/19/22	0/1/1/1
5	NAG	G	510	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	511	5	-	0/6/23/26	0/1/1/1
5	NAG	G	512	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	513	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	514	5	-	0/2/19/22	0/1/1/1
5	NAG	G	515	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	516	5	-	0/6/23/26	0/1/1/1
5	NAG	G	517	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	518	5	-	0/6/23/26	0/1/1/1
5	NAG	G	519	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	520	5	-	0/6/23/26	0/1/1/1
5	NAG	G	521	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	522	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	523	5	-	0/2/19/22	0/1/1/1
5	NAG	G	524	4	-	0/6/23/26	0/1/1/1
5	NAG	G	525	5,4	-	0/6/23/26	0/1/1/1
5	NAG	G	526	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	527	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	522	NAG	O5-C1-C2	-2.27	108.32	111.47
7	G	509	MAN	O5-C1-C2	-2.15	107.42	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	NAG	1	0
5	G	502	NAG	3	0
7	G	504	MAN	3	0
7	G	509	MAN	3	0
5	G	517	NAG	1	0
5	G	519	NAG	2	0
5	G	521	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	B	181/185 (97%)	0.77	18 (9%) 8 9	109, 175, 233, 284	0
2	C	214/214 (100%)	1.41	59 (27%) 1 2	134, 237, 326, 438	0
3	D	223/229 (97%)	1.64	69 (30%) 0 2	124, 223, 326, 448	0
4	G	295/313 (94%)	0.78	34 (11%) 5 7	103, 164, 241, 304	0
All	All	913/941 (97%)	1.13	180 (19%) 1 3	103, 196, 311, 448	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	190	GLY	13.2
3	D	185	PRO	10.3
2	C	206	THR	9.9
2	C	146	VAL	9.6
3	D	184	VAL	8.4
3	D	191	THR	8.4
3	D	194	TYR	8.2
3	D	45	LEU	8.1
4	G	126	CYS	7.2
2	C	205	VAL	7.1
3	D	189	LEU	7.0
3	D	126	PRO	7.0
2	C	196	VAL	6.8
2	C	108	ARG	6.7
3	D	44	GLY	6.4
2	C	113	PRO	6.2
2	C	187	GLU	6.0
3	D	187	SER	6.0
3	D	188	SER	6.0
2	C	182	SER	5.9
2	C	131	SER	5.8

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Mol	Chain	Res	Type	RSRZ
3	D	211	VAL	5.7
2	C	152	ASN	5.7
3	D	138	LEU	5.6
4	G	194	GLY	5.5
3	D	120	SER	5.5
2	C	129	THR	5.5
3	D	183	THR	5.5
4	G	232	LYS	5.4
1	B	167	LYS	5.4
3	D	186	SER	5.3
2	C	43	ALA	5.2
2	C	145	LYS	5.1
4	G	270	ILE	5.0
4	G	209	SER	5.0
2	C	104	LEU	4.9
2	C	194	CYS	4.8
3	D	2	VAL	4.8
2	C	122	ASP	4.7
3	D	142	VAL	4.7
3	D	29	PHE	4.7
3	D	18	VAL	4.7
2	C	112	ALA	4.7
2	C	183	LYS	4.6
2	C	203	SER	4.6
3	D	160	THR	4.6
2	C	204	PRO	4.6
2	C	195	GLU	4.6
3	D	119	PRO	4.5
4	G	128	GLY	4.4
3	D	143	LYS	4.2
1	B	5	LEU	4.2
3	D	152	VAL	4.2
4	G	238	PRO	4.1
2	C	130	ALA	4.1
3	D	144	ASP	4.1
2	C	171	SER	4.0
3	D	82	LEU	4.0
3	D	199	ASN	4.0
4	G	359	ILE	3.9
2	C	184	ALA	3.8
1	B	54	ARG	3.8
3	D	213	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	130	CYS	3.8
3	D	212	GLU	3.8
3	D	3	GLN	3.8
3	D	198	VAL	3.8
2	C	149	LYS	3.7
1	B	166	LYS	3.7
4	G	269	GLU	3.7
2	C	147	GLN	3.6
2	C	181	LEU	3.6
3	D	136	ALA	3.6
2	C	166	GLN	3.6
2	C	107	LYS	3.6
4	G	228	CYS	3.5
3	D	192	GLN	3.5
1	B	1	LYS	3.4
4	G	196	CYS	3.4
4	G	90	THR	3.3
4	G	389	GLN	3.3
3	D	62	HIS	3.3
2	C	138	ASN	3.3
2	C	207	LYS	3.3
3	D	17	SER	3.3
4	G	211	GLU	3.3
3	D	210	LYS	3.3
2	C	106	ILE	3.2
2	C	180	THR	3.2
3	D	63	LEU	3.2
4	G	207	LYS	3.2
4	G	127	VAL	3.2
3	D	159	LEU	3.1
3	D	206	LYS	3.1
3	D	115	SER	3.1
2	C	11	LEU	3.1
1	B	161	VAL	3.0
1	B	98	PHE	3.0
3	D	77	THR	3.0
2	C	185	ASP	2.9
4	G	239	CYS	2.9
1	B	60	SER	2.9
4	G	415	THR	2.9
3	D	137	ALA	2.9
3	D	46	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	193	THR	2.9
3	D	78	VAL	2.9
2	C	150	VAL	2.8
2	C	151	ASP	2.8
3	D	66	ARG	2.8
3	D	82(C)	LEU	2.8
4	G	93	PHE	2.8
2	C	27	GLU	2.8
3	D	1	GLU	2.8
3	D	4	LEU	2.8
3	D	48	MET	2.8
2	C	140	TYR	2.8
2	C	190	LYS	2.7
4	G	208	VAL	2.7
1	B	180	GLN	2.7
3	D	134	GLY	2.7
3	D	146	PHE	2.7
4	G	333	LEU	2.7
1	B	142	LYS	2.7
1	B	163	GLN	2.7
3	D	125	ALA	2.7
4	G	233	PHE	2.7
2	C	25	ALA	2.6
2	C	202	SER	2.6
3	D	204	ASN	2.6
4	G	87	GLU	2.6
2	C	161	GLU	2.6
2	C	105	GLU	2.6
2	C	160	GLN	2.6
2	C	52	SER	2.6
3	D	214	LYS	2.6
2	C	155	GLN	2.5
2	C	193	ALA	2.5
2	C	201	LEU	2.5
4	G	91	GLU	2.5
4	G	414	ILE	2.5
2	C	8	PRO	2.4
4	G	212	PRO	2.4
3	D	135	THR	2.4
3	D	141	LEU	2.4
2	C	44	PRO	2.4
2	C	197	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	18	ALA	2.4
3	D	5	VAL	2.3
3	D	71	ALA	2.3
2	C	199	GLN	2.3
3	D	23	LYS	2.3
4	G	429	GLU	2.3
4	G	332	ASN	2.3
1	B	179	PHE	2.3
3	D	43	GLN	2.3
2	C	139	PHE	2.2
1	B	118	LEU	2.2
3	D	19	LYS	2.2
3	D	100(E)	TYR	2.2
2	C	186	TYR	2.2
4	G	129	ALA	2.2
4	G	353	PHE	2.2
3	D	151	THR	2.2
2	C	125	LEU	2.2
4	G	357	LYS	2.2
3	D	133	GLY	2.2
1	B	65	GLY	2.1
4	G	358	THR	2.1
3	D	24	ALA	2.1
4	G	221	ALA	2.1
2	C	191	VAL	2.1
2	C	12	SER	2.1
1	B	121	PRO	2.1
4	G	437	PRO	2.1
1	B	64	GLN	2.1
2	C	153	ALA	2.0
3	D	79	TYR	2.0
3	D	153	SER	2.0
3	D	182	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
7	MAN	G	508	11/12	0.52	0.96	2.30	159,185,226,233	0
5	NAG	G	517	14/15	0.64	0.92	2.22	160,255,279,296	0
7	MAN	G	507	11/12	0.65	0.61	0.91	114,141,172,191	0
5	NAG	G	521	14/15	0.73	0.50	0.10	211,276,295,296	0
5	NAG	G	502	14/15	0.63	0.46	-0.22	140,146,182,206	0
7	MAN	G	506	11/12	0.92	0.53	-0.67	128,144,175,206	0
5	NAG	G	501	14/15	0.91	0.33	-0.85	145,163,174,185	0
5	NAG	G	516	14/15	0.54	1.30	-	204,260,301,301	0
7	MAN	G	504	11/12	0.78	0.36	-	151,169,196,224	0
7	MAN	G	505	11/12	0.44	0.53	-	199,231,247,267	0
5	NAG	G	511	14/15	0.76	0.80	-	222,266,292,304	0
5	NAG	G	522	14/15	0.51	0.56	-	209,257,284,288	0
6	BMA	G	514	11/12	0.80	0.31	-	154,225,274,276	0
5	NAG	G	518	14/15	0.50	0.65	-	211,249,289,306	0
7	MAN	G	509	11/12	0.76	0.68	-	144,179,230,238	0
5	NAG	G	526	14/15	0.76	0.36	-	175,202,236,260	0
6	BMA	G	503	11/12	0.88	0.42	-	125,139,159,175	0
6	BMA	G	527	11/12	0.59	0.55	-	213,248,269,276	0
5	NAG	G	525	14/15	0.93	0.27	-	176,198,209,210	0
5	NAG	G	520	14/15	0.80	0.29	-	211,255,270,271	0
5	NAG	G	510	14/15	0.60	0.39	-	178,207,235,247	0
5	NAG	G	524	14/15	0.44	0.53	-	139,180,209,209	0
5	NAG	G	519	14/15	0.74	0.38	-	203,252,278,283	0
5	NAG	G	515	14/15	0.53	0.46	-	153,262,303,303	0
6	BMA	G	523	11/12	0.57	0.72	-	173,255,278,283	0
5	NAG	G	512	14/15	0.86	0.59	-	166,251,277,288	0
5	NAG	G	513	14/15	0.86	0.47	-	214,248,300,315	0

6.5 Other polymers ⓘ

There are no such residues in this entry.