



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 PM GMT

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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

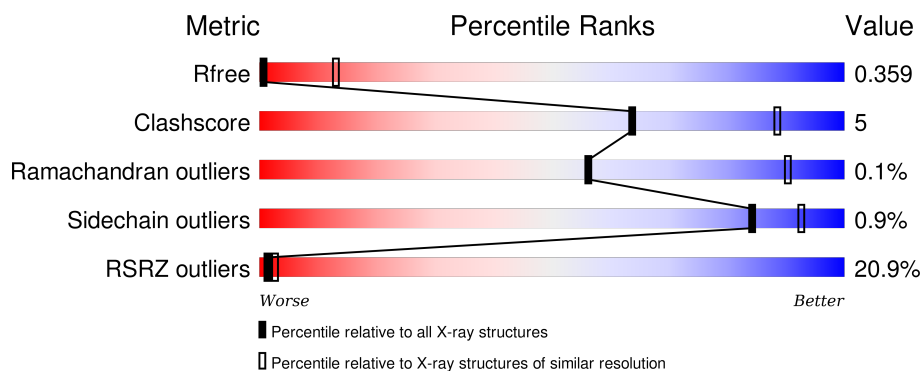
1 Overall quality at a glance ⓘ

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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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>11%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	214	<div> <div>30%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
3	D	229	<div> <div>31%</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	MAN	G	506	-	-	-	X
5	MAN	G	507	-	-	-	X
5	MAN	G	508	-	-	-	X
7	NAG	G	517	-	-	-	X
8	NAG	G	521	-	-	-	X

2 Entry composition [i](#)

There are 9 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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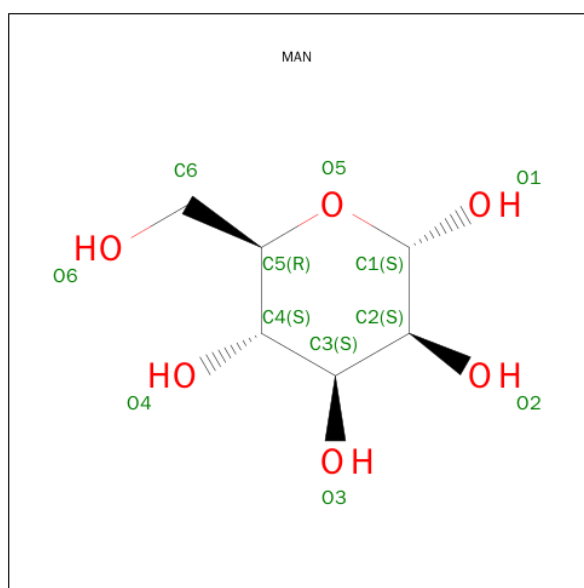
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Chain	Residue	Modelled	Actual	Comment	Reference
G	81	ARG	-	EXPRESSION TAG	UNP P35961
G	82	SER	-	EXPRESSION TAG	UNP P35961
G	128	GLY	-	LINKER	UNP P35961
G	129	ALA	-	LINKER	UNP P35961
G	194	GLY	-	LINKER	UNP P35961
G	298	GLY	-	LINKER	UNP P35961
G	299	ALA	-	LINKER	UNP P35961
G	300	GLY	-	LINKER	UNP P35961

- Molecule 5 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	8	Total	C	N	O	0	0
			94	52	2	40		

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



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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	2	Total	C	N	O	0	0
			28	16	2	10		

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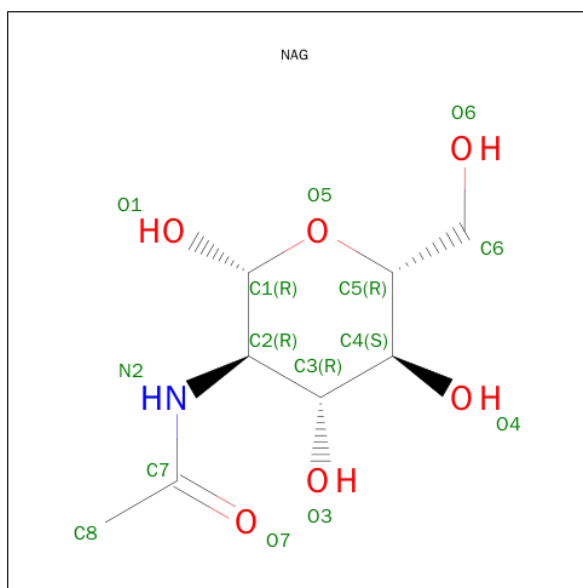
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	3	Total	C	N	O	0	0
			39	22	2	15		
8	G	3	Total	C	N	O	0	0
			39	22	2	15		
8	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

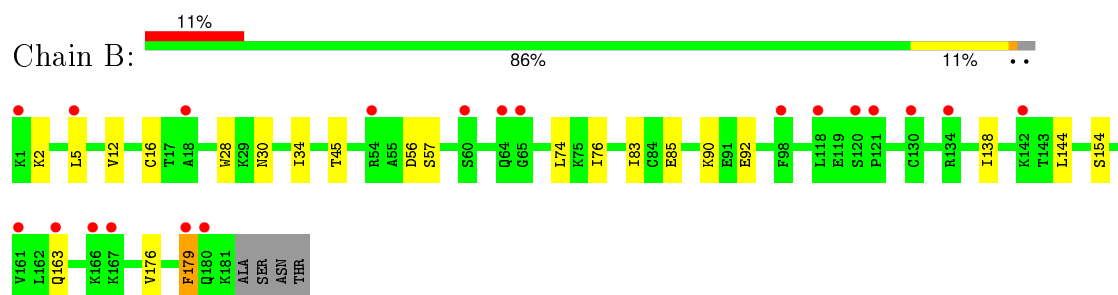


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	N	O	0	0
			14	8	1	5		

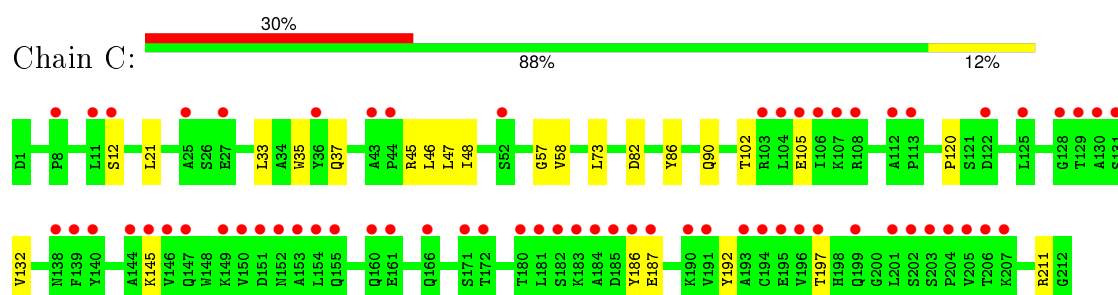
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

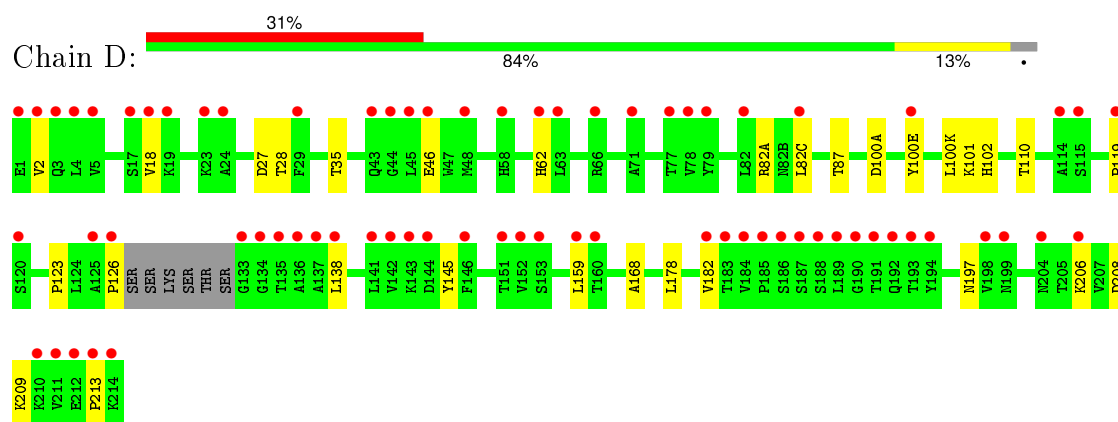
- Molecule 1: 2-domain CD4



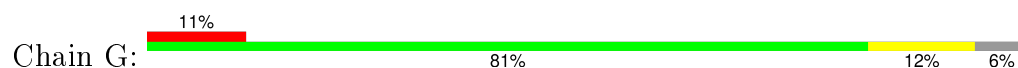
- Molecule 2: 17b Fab Light Chain

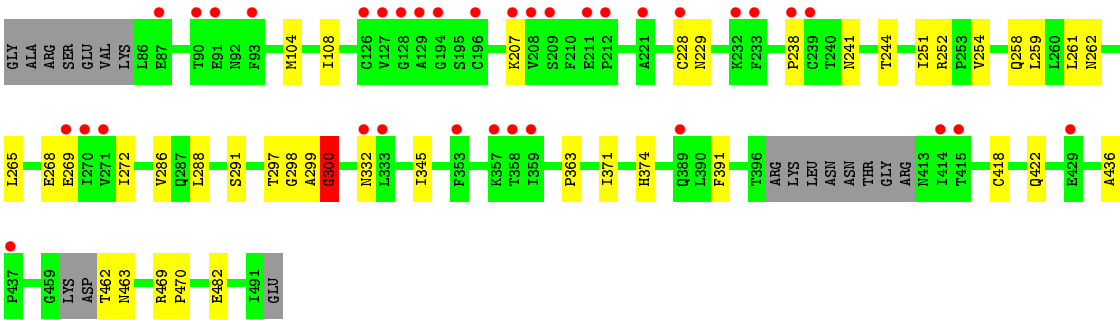


- Molecule 3: 17b Fab Heavy Chain



- 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 0.328 , 0.359	Depositor DCC
R_{free} test set	667 reflections (5.28%)	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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 13299 reflections	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	94	0	78	6	0
6	G	11	0	10	3	0
7	G	112	0	100	3	0
8	G	117	0	102	1	0
9	G	14	0	13	0	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)
5:G:504:MAN:C6	6:G:509:MAN:C1	2.46	0.93
5:G:504:MAN:O6	6:G:509:MAN:C2	2.22	0.87
4:G:297:THR:HG22	4:G:298:GLY:H	1.40	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
5:G:504:MAN:O6	6: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	7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:502:NAG:C8	7:G:519:NAG:H81	2.37	0.55
3:D:35:THR:HB	3:D:100(K):LEU:HD21	1.89	0.54
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
4:G:252:ARG:HD2	4:G:262:ASN:HB3	1.92	0.50
2:C:145:LYS:HB3	2:C:197:THR:HB	1.93	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:HD12	1:B:76:ILE:H	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
4:G:238:PRO:HD2	8:G:521:NAG:H61	1.97	0.46
2:C:46:LEU:HD22	3:D:101:LYS:HA	1.97	0.46
2:C:82:ASP:O	2:C:86:TYR:OH	2.26	0.46
1:B:56:ASP:OD1	1:B:57:SER:N	2.40	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
4:G:258:GLN:NE2	4:G:371:ILE:O	2.50	0.45
2:C:12:SER:OG	2:C:105:GLU:OE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:197:ASN:ND2	3:D:208:ASP:OD2	2.49	0.41
1:B:16:CYS:HB2	1:B:28:TRP:HZ2	1.85	0.41
4:G:251:ILE:HG23	4:G:482:GLU:HG3	2.02	0.41
2:C:187:GLU:O	2:C:211:ARG:NH2	2.53	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
4:G:259:LEU:HD12	4:G:374:HIS:CD2	2.57	0.40
1:B:45:THR:HG22	4:G:371:ILE:HD13	2.03	0.40
4:G:332:ASN:HD22	7:G:517:NAG:C7	2.32	0.40
3:D:18:VAL:HG12	3:D:82(C):LEU:HD21	2.04	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%)	46	83
All	All	899/941 (96%)	875 (97%)	23 (3%)	1 (0%)	56	90

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%)	78	90
2	C	184/184 (100%)	182 (99%)	2 (1%)	80	90
3	D	187/193 (97%)	186 (100%)	1 (0%)	92	96
4	G	261/276 (95%)	259 (99%)	2 (1%)	86	93
All	All	796/820 (97%)	789 (99%)	7 (1%)	84	92

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 ⓘ

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

5.5 Carbohydrates ⓘ

25 carbohydrates 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	0.56	0	15,19,21	0.67	0
5	NAG	G	502	5	14,14,15	0.54	0	15,19,21	0.88	0
5	BMA	G	503	5	11,11,12	0.64	0	14,15,17	0.79	1 (7%)
5	MAN	G	504	5,6	11,11,12	0.64	0	14,15,17	1.02	2 (14%)
5	MAN	G	505	5	11,11,12	0.59	0	14,15,17	0.59	0
5	MAN	G	506	5	11,11,12	0.58	0	14,15,17	0.68	0
5	MAN	G	507	5	11,11,12	0.52	0	14,15,17	0.72	0
5	MAN	G	508	5	11,11,12	0.61	0	14,15,17	0.62	0
7	NAG	G	510	4,7	14,14,15	0.50	0	15,19,21	0.76	0
7	NAG	G	511	7	14,14,15	0.51	0	15,19,21	0.60	0
8	NAG	G	512	8,4	14,14,15	0.52	0	15,19,21	0.75	0
8	NAG	G	513	8	14,14,15	0.48	0	15,19,21	0.69	0
8	BMA	G	514	8	11,11,12	0.59	0	14,15,17	0.64	0
7	NAG	G	515	4,7	14,14,15	0.50	0	15,19,21	0.70	0
7	NAG	G	516	7	14,14,15	0.47	0	15,19,21	0.70	0
7	NAG	G	517	4,7	14,14,15	0.49	0	15,19,21	0.61	0
7	NAG	G	518	7	14,14,15	0.52	0	15,19,21	0.64	0
7	NAG	G	519	4,7	14,14,15	0.52	0	15,19,21	0.66	0
7	NAG	G	520	7	14,14,15	0.51	0	15,19,21	0.67	0
8	NAG	G	521	8,4	14,14,15	0.52	0	15,19,21	0.68	0
8	NAG	G	522	8	14,14,15	0.55	0	15,19,21	0.85	0
8	BMA	G	523	8	11,11,12	0.65	0	14,15,17	0.70	0
8	NAG	G	525	8,4	14,14,15	0.51	0	15,19,21	0.70	0
8	NAG	G	526	8	14,14,15	0.52	0	15,19,21	0.66	0
8	BMA	G	527	8	11,11,12	0.61	0	14,15,17	0.60	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	-	0/6/23/26	0/1/1/1
5	BMA	G	503	5	-	0/2/19/22	0/1/1/1
5	MAN	G	504	5,6	-	0/2/19/22	0/1/1/1
5	MAN	G	505	5	-	0/2/19/22	0/1/1/1
5	MAN	G	506	5	-	0/2/19/22	0/1/1/1
5	MAN	G	507	5	-	0/2/19/22	0/1/1/1
5	MAN	G	508	5	-	0/2/19/22	0/1/1/1
7	NAG	G	510	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	511	7	-	0/6/23/26	0/1/1/1
8	NAG	G	512	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	513	8	-	0/6/23/26	0/1/1/1
8	BMA	G	514	8	-	0/2/19/22	0/1/1/1
7	NAG	G	515	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	516	7	-	0/6/23/26	0/1/1/1
7	NAG	G	517	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	518	7	-	0/6/23/26	0/1/1/1
7	NAG	G	519	4,7	-	0/6/23/26	0/1/1/1
7	NAG	G	520	7	-	0/6/23/26	0/1/1/1
8	NAG	G	521	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	522	8	-	0/6/23/26	0/1/1/1
8	BMA	G	523	8	-	0/2/19/22	0/1/1/1
8	NAG	G	525	8,4	-	0/6/23/26	0/1/1/1
8	NAG	G	526	8	-	0/6/23/26	0/1/1/1
8	BMA	G	527	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	504	MAN	C1-O5-C5	-2.20	109.46	112.25
5	G	504	MAN	C1-C2-C3	2.03	111.94	109.54
5	G	503	BMA	C1-C2-C3	2.04	111.95	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 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
5	G	504	MAN	3	0
7	G	517	NAG	1	0
7	G	519	NAG	2	0
8	G	521	NAG	1	0

5.6 Ligand geometry

2 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	$\# Z > 2$
6	MAN	G	509	5	11,11,12	0.64	0	14,15,17	0.75	1 (7%)
9	NAG	G	524	4	14,14,15	0.48	0	15,19,21	0.85	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
6	MAN	G	509	5	-	0/2/19/22	0/1/1/1
9	NAG	G	524	4	-	0/6/23/26	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(°)
6	G	509	MAN	O5-C1-C2	-2.12	107.42	110.86
9	G	524	NAG	C1-O5-C5	2.04	114.84	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	509	MAN	3	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%)	0.84	20 (11%) 7 7	109, 175, 233, 284	0
2	C	214/214 (100%)	1.51	65 (30%) 1 2	134, 237, 326, 438	0
3	D	223/229 (97%)	1.76	71 (31%) 1 2	124, 223, 326, 448	0
4	G	295/313 (94%)	0.86	35 (11%) 6 6	103, 164, 241, 304	0
All	All	913/941 (97%)	1.23	191 (20%) 1 3	103, 196, 311, 448	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	190	GLY	13.9
3	D	185	PRO	10.6
2	C	206	THR	10.5
2	C	146	VAL	10.2
3	D	191	THR	9.0
3	D	194	TYR	9.0
3	D	184	VAL	8.9
3	D	45	LEU	8.7
2	C	205	VAL	7.5
3	D	189	LEU	7.5
4	G	126	CYS	7.3
2	C	196	VAL	7.2
3	D	126	PRO	7.1
2	C	108	ARG	7.0
3	D	44	GLY	6.7
2	C	113	PRO	6.3
2	C	187	GLU	6.3
3	D	187	SER	6.2
3	D	188	SER	6.2
2	C	182	SER	6.1
3	D	211	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
2	C	131	SER	6.0
3	D	138	LEU	6.0
2	C	152	ASN	5.9
2	C	129	THR	5.9
3	D	183	THR	5.8
4	G	194	GLY	5.8
3	D	120	SER	5.7
2	C	43	ALA	5.7
4	G	232	LYS	5.5
1	B	167	LYS	5.5
3	D	186	SER	5.5
4	G	270	ILE	5.4
2	C	104	LEU	5.3
2	C	145	LYS	5.2
4	G	209	SER	5.2
2	C	112	ALA	5.1
3	D	2	VAL	5.1
3	D	29	PHE	5.0
3	D	142	VAL	5.0
2	C	122	ASP	5.0
3	D	18	VAL	5.0
3	D	160	THR	4.9
2	C	194	CYS	4.9
2	C	203	SER	4.8
2	C	195	GLU	4.8
2	C	204	PRO	4.7
2	C	183	LYS	4.7
4	G	128	GLY	4.6
3	D	119	PRO	4.6
1	B	5	LEU	4.5
2	C	130	ALA	4.5
3	D	152	VAL	4.4
3	D	82	LEU	4.3
3	D	143	LYS	4.3
3	D	144	ASP	4.3
4	G	238	PRO	4.2
2	C	171	SER	4.2
2	C	184	ALA	4.2
4	G	359	ILE	4.2
3	D	199	ASN	4.1
3	D	198	VAL	4.0
3	D	136	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	54	ARG	4.0
3	D	212	GLU	4.0
3	D	3	GLN	3.9
3	D	213	PRO	3.9
2	C	181	LEU	3.9
1	B	130	CYS	3.9
4	G	269	GLU	3.8
2	C	147	GLN	3.8
2	C	149	LYS	3.8
1	B	166	LYS	3.8
2	C	166	GLN	3.7
3	D	192	GLN	3.7
2	C	107	LYS	3.6
4	G	228	CYS	3.6
4	G	90	THR	3.6
3	D	62	HIS	3.5
2	C	106	ILE	3.5
4	G	389	GLN	3.5
1	B	1	LYS	3.4
3	D	63	LEU	3.4
4	G	196	CYS	3.4
2	C	138	ASN	3.4
3	D	17	SER	3.4
4	G	211	GLU	3.4
2	C	180	THR	3.4
3	D	159	LEU	3.4
4	G	127	VAL	3.4
2	C	207	LYS	3.4
3	D	210	LYS	3.3
2	C	11	LEU	3.3
4	G	207	LYS	3.2
3	D	77	THR	3.2
1	B	161	VAL	3.2
1	B	98	PHE	3.2
3	D	115	SER	3.2
3	D	137	ALA	3.2
3	D	206	LYS	3.1
2	C	140	TYR	3.1
2	C	185	ASP	3.1
4	G	415	THR	3.1
3	D	82(C)	LEU	3.1
3	D	193	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	4	LEU	3.1
3	D	78	VAL	3.0
2	C	150	VAL	3.0
4	G	93	PHE	3.0
1	B	60	SER	3.0
2	C	151	ASP	3.0
3	D	46	GLU	3.0
3	D	48	MET	3.0
2	C	27	GLU	3.0
3	D	1	GLU	3.0
4	G	239	CYS	3.0
3	D	66	ARG	3.0
3	D	125	ALA	2.9
4	G	333	LEU	2.9
2	C	25	ALA	2.9
4	G	208	VAL	2.9
3	D	146	PHE	2.9
3	D	134	GLY	2.9
1	B	180	GLN	2.8
4	G	233	PHE	2.8
2	C	190	LYS	2.8
1	B	163	GLN	2.8
2	C	193	ALA	2.8
4	G	87	GLU	2.8
2	C	202	SER	2.8
2	C	161	GLU	2.7
1	B	142	LYS	2.7
3	D	204	ASN	2.7
2	C	105	GLU	2.7
2	C	201	LEU	2.7
2	C	160	GLN	2.7
2	C	52	SER	2.7
4	G	414	ILE	2.7
2	C	155	GLN	2.7
4	G	91	GLU	2.6
1	B	18	ALA	2.6
3	D	214	LYS	2.6
3	D	135	THR	2.6
3	D	141	LEU	2.6
3	D	71	ALA	2.6
2	C	197	THR	2.5
2	C	8	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	G	212	PRO	2.5
3	D	5	VAL	2.5
3	D	100(E)	TYR	2.5
2	C	186	TYR	2.5
4	G	129	ALA	2.5
1	B	179	PHE	2.5
2	C	44	PRO	2.4
2	C	199	GLN	2.4
1	B	118	LEU	2.4
4	G	429	GLU	2.4
2	C	139	PHE	2.4
3	D	23	LYS	2.4
4	G	332	ASN	2.4
2	C	125	LEU	2.4
3	D	43	GLN	2.4
3	D	151	THR	2.4
4	G	353	PHE	2.4
3	D	24	ALA	2.3
4	G	221	ALA	2.3
3	D	133	GLY	2.3
1	B	65	GLY	2.3
3	D	19	LYS	2.3
2	C	153	ALA	2.3
4	G	358	THR	2.3
3	D	79	TYR	2.3
2	C	191	VAL	2.2
4	G	357	LYS	2.2
3	D	114	ALA	2.2
2	C	12	SER	2.2
1	B	64	GLN	2.2
2	C	172	THR	2.2
3	D	182	VAL	2.1
1	B	121	PRO	2.1
4	G	437	PRO	2.1
2	C	128	GLY	2.1
3	D	153	SER	2.1
2	C	144	ALA	2.1
4	G	271	VAL	2.1
1	B	134	ARG	2.1
3	D	58	HIS	2.1
1	B	120	SER	2.1
2	C	36	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	103	ARG	2.0
2	C	154	LEU	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](#)

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
5	MAN	G	508	11/12	0.52	0.96	2.30	159,185,226,233	0
7	NAG	G	517	14/15	0.64	0.92	2.22	160,255,279,296	0
5	MAN	G	507	11/12	0.65	0.61	0.91	114,141,172,191	0
8	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
5	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	MAN	G	504	11/12	0.78	0.36	-	151,169,196,224	0
5	MAN	G	505	11/12	0.44	0.53	-	199,231,247,267	0
7	NAG	G	511	14/15	0.76	0.80	-	222,266,292,304	0
8	NAG	G	522	14/15	0.51	0.56	-	209,257,284,288	0
8	BMA	G	514	11/12	0.80	0.31	-	154,225,274,276	0
7	NAG	G	518	14/15	0.50	0.65	-	211,249,289,306	0
8	NAG	G	526	14/15	0.76	0.36	-	175,202,236,260	0
5	BMA	G	503	11/12	0.88	0.42	-	125,139,159,175	0
8	BMA	G	527	11/12	0.59	0.55	-	213,248,269,276	0
8	NAG	G	525	14/15	0.93	0.27	-	176,198,209,210	0
7	NAG	G	520	14/15	0.80	0.29	-	211,255,270,271	0
7	NAG	G	510	14/15	0.60	0.39	-	178,207,235,247	0
8	BMA	G	523	11/12	0.57	0.72	-	173,255,278,283	0
7	NAG	G	519	14/15	0.74	0.38	-	203,252,278,283	0
7	NAG	G	515	14/15	0.53	0.46	-	153,262,303,303	0
7	NAG	G	516	14/15	0.54	1.30	-	204,260,301,301	0
8	NAG	G	512	14/15	0.86	0.59	-	166,251,277,288	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	G	513	14/15	0.86	0.47	-	214,248,300,315	0

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(\AA^2)	Q<0.9
9	NAG	G	524	14/15	0.44	0.53	-	139,180,209,209	0
6	MAN	G	509	11/12	0.76	0.68	-	144,179,230,238	0

6.5 Other polymers [i](#)

There are no such residues in this entry.