



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FUS  
Title : Improved Structure of the Unliganded Simian Immunodeficiency Virus gp120 Core  
Authors : Chen, X.; Poon, B.; Wang, Q.; Ma, J.  
Deposited on : 2009-01-14  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

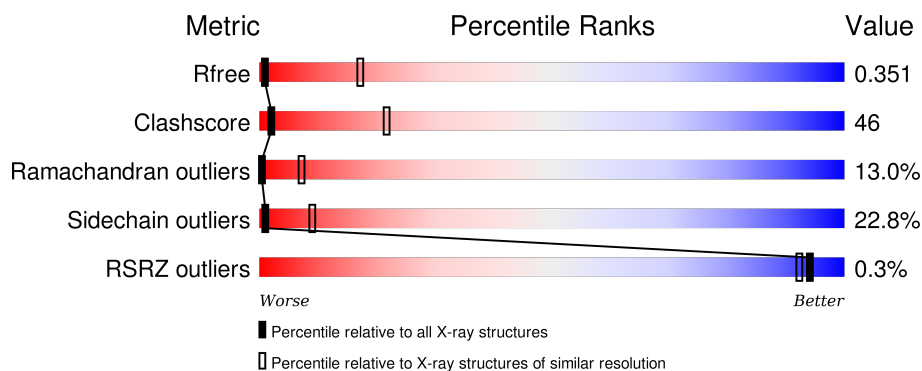
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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  $\geq 3$ , 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	316	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NDG	A	25	X	-	-	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 3140 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.

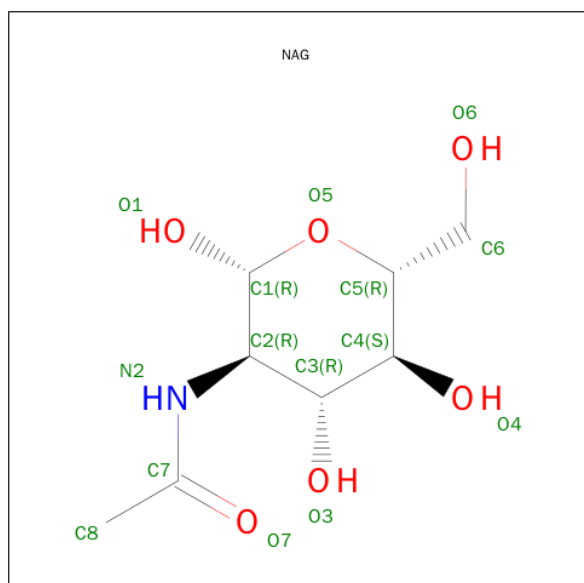
- Molecule 1 is a protein called EXTERIOR MEMBRANE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2470	1556	436	455	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	HIS	-	expression tag	UNP Q07374
A	65	MET	-	expression tag	UNP Q07374
A	110	GLY	-	linker	UNP Q07374
A	207	ALA	-	linker	UNP Q07374
A	208	GLY	-	linker	UNP Q07374
A	312	GLY	-	linker	UNP Q07374
A	313	ALA	-	linker	UNP Q07374
A	341	GLY	-	linker	UNP Q07374

- Molecule 2 is MULTIPLE SUGAR CHAINS (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		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			71	40	2	29		
4	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 10 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	6	Total	C	N	O	0	0
			72	40	2	30		

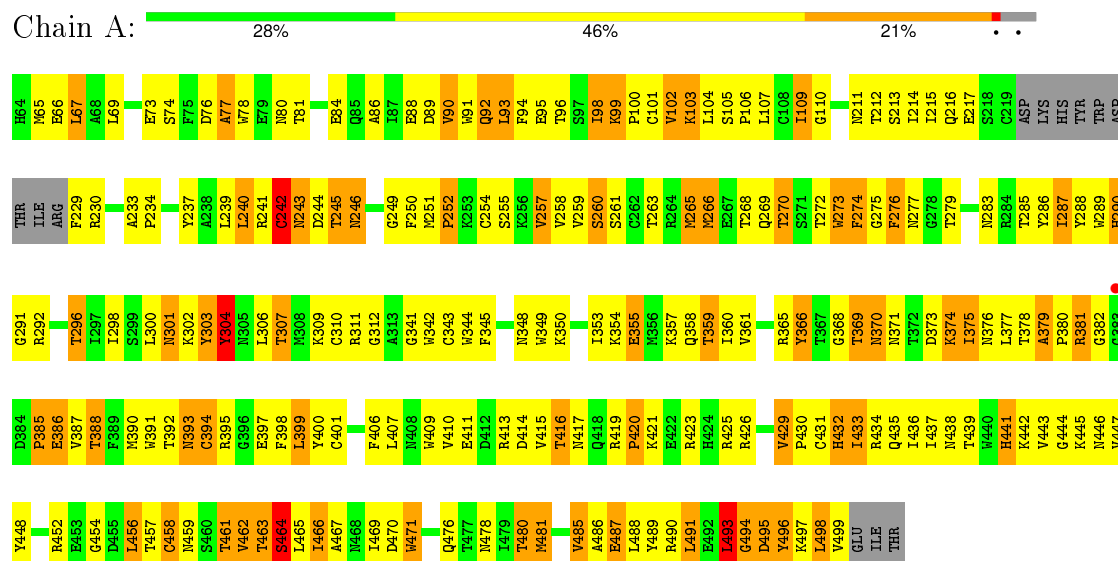
- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	4	Total	C	N	O	0	0
			50	28	2	20		

### 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 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: EXTERIOR MEMBRANE GLYCOPROTEIN GP120



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.05Å 108.05Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.58 – 4.00 25.58 – 4.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.58-4.00) 98.1 (25.58-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.346 , 0.354 0.346 , 0.351	Depositor DCC
$R_{free}$ test set	279 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	174.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 1892.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 6121 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: FUL, BMA, NAG, NDG, 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	0.51	0/2534	0.77	1/3441 (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
9	A	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LYS	N-CA-C	5.51	125.86	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	25	NDG	C1

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2470	0	2349	264	2
2	A	28	0	26	0	0
3	A	60	0	52	1	1
4	A	142	0	122	11	1
5	A	38	0	34	4	0
6	A	49	0	43	4	1
7	A	49	0	43	0	0
8	A	28	0	25	1	0
9	A	71	0	61	1	0
10	A	83	0	70	3	0
11	A	72	0	61	1	0
12	A	50	0	43	0	0
All	All	3140	0	2929	279	4

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 46.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:O	1:A:395:ARG:HG3	1.44	1.14
1:A:285:THR:HG23	1:A:302:LYS:HB2	1.40	1.03
1:A:106:PRO:HA	1:A:212:THR:HA	1.05	1.03
1:A:489:TYR:O	1:A:493:LEU:HG	1.62	0.99
1:A:91:TRP:O	1:A:448:TYR:OH	1.80	0.98
1:A:290:HIS:HE1	1:A:292:ARG:HG2	1.31	0.96
1:A:437:ILE:O	1:A:445:LYS:HA	1.64	0.95
1:A:65:MET:CE	1:A:240:LEU:HD21	1.97	0.94
1:A:106:PRO:CA	1:A:212:THR:HA	1.98	0.93
1:A:237:TYR:OH	1:A:498:LEU:HB2	1.69	0.92
1:A:375:ILE:HG12	1:A:411:GLU:HB2	1.51	0.92
1:A:470:ASP:HB2	1:A:478:ASN:HB3	1.51	0.92
1:A:65:MET:HE2	1:A:240:LEU:HD21	1.49	0.91
1:A:106:PRO:HA	1:A:212:THR:CA	1.99	0.91
1:A:306:LEU:O	1:A:462:VAL:HG21	1.71	0.90
1:A:80:ASN:HB3	1:A:84:GLU:HG2	1.53	0.90
1:A:244:ASP:O	1:A:245:THR:OG1	1.91	0.88
1:A:287:ILE:HG13	1:A:287:ILE:O	1.73	0.88
1:A:353:ILE:HG22	1:A:357:LYS:HE3	1.55	0.88
1:A:241:ARG:HG2	1:A:242:CYS:H	1.40	0.86
1:A:381:ARG:HH21	1:A:382:GLY:HA2	1.39	0.86
1:A:415:VAL:HG12	1:A:416:THR:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HG2	1:A:385:PRO:HG3	1.57	0.85
1:A:269:GLN:HE21	4:A:7:NAG:C8	1.89	0.85
1:A:269:GLN:HE21	4:A:7:NAG:H83	1.41	0.84
1:A:275:GLY:HA3	1:A:464:SER:HB2	1.60	0.84
1:A:395:ARG:O	1:A:395:ARG:CG	2.25	0.82
1:A:391:TRP:CZ2	1:A:393:ASN:HB2	2.15	0.82
1:A:107:LEU:N	1:A:211:ASN:O	2.12	0.82
1:A:258:VAL:HG12	1:A:259:VAL:H	1.46	0.81
1:A:306:LEU:O	1:A:462:VAL:CG2	2.28	0.80
1:A:269:GLN:HA	1:A:393:ASN:O	1.81	0.80
1:A:105:SER:O	1:A:213:SER:N	2.14	0.80
1:A:290:HIS:CE1	1:A:292:ARG:HG2	2.16	0.79
1:A:496:TYR:C	1:A:496:TYR:HD1	1.85	0.79
1:A:241:ARG:HG2	1:A:242:CYS:N	1.98	0.78
1:A:77:ALA:HA	1:A:80:ASN:HD22	1.48	0.78
1:A:266:MET:SD	1:A:398:PHE:HZ	2.07	0.77
1:A:80:ASN:CB	1:A:84:GLU:HG2	2.15	0.75
1:A:496:TYR:CD1	1:A:496:TYR:C	2.58	0.75
1:A:93:LEU:O	1:A:96:THR:HG22	1.88	0.74
10:A:33:MAN:H4	10:A:34:BMA:C1	2.18	0.74
1:A:274:PHE:CE2	1:A:349:TRP:CH2	2.75	0.73
5:A:13:NDG:H6C2	5:A:14:NAG:N2	2.03	0.73
1:A:289:TRP:NE1	1:A:291:GLY:HA2	2.04	0.73
1:A:94:PHE:CZ	1:A:265:MET:SD	2.82	0.73
1:A:435:GLN:O	1:A:447:VAL:HA	1.89	0.72
1:A:381:ARG:NH2	1:A:382:GLY:HA2	2.04	0.72
1:A:273:TRP:CE3	1:A:481:MET:HG3	2.24	0.72
1:A:89:ASP:HA	1:A:92:GLN:HB3	1.72	0.72
1:A:486:ALA:O	1:A:490:ARG:HB2	1.90	0.72
1:A:283:ASN:HA	1:A:303:TYR:HB3	1.73	0.71
1:A:342:TRP:HA	1:A:429:VAL:O	1.90	0.71
1:A:354:LYS:O	1:A:358:GLN:N	2.23	0.71
1:A:435:GLN:OE1	1:A:435:GLN:N	2.24	0.71
1:A:437:ILE:HB	1:A:446:ASN:HB2	1.72	0.70
1:A:98:ILE:O	1:A:99:LYS:HG3	1.91	0.69
1:A:86:ALA:O	1:A:90:VAL:HB	1.92	0.69
1:A:290:HIS:HE1	1:A:292:ARG:CG	2.05	0.69
1:A:343:CYS:HB2	1:A:429:VAL:CG2	2.24	0.68
1:A:480:THR:O	1:A:481:MET:HB2	1.94	0.68
1:A:421:LYS:NZ	1:A:423:ARG:HH21	1.92	0.67
1:A:400:TYR:OH	1:A:437:ILE:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG12	1:A:416:THR:N	2.08	0.66
1:A:78:TRP:HH2	1:A:381:ARG:NH1	1.93	0.66
1:A:287:ILE:CG1	1:A:287:ILE:O	2.43	0.66
1:A:421:LYS:HZ2	1:A:423:ARG:HH21	1.41	0.66
1:A:65:MET:HE1	1:A:240:LEU:HD21	1.75	0.66
1:A:240:LEU:O	1:A:497:LYS:HB2	1.97	0.65
1:A:273:TRP:HB2	1:A:390:MET:SD	2.37	0.65
1:A:241:ARG:HH11	1:A:494:GLY:HA3	1.61	0.64
1:A:269:GLN:NE2	4:A:7:NAG:H83	2.13	0.64
1:A:349:TRP:CZ2	1:A:353:ILE:HD11	2.33	0.64
1:A:289:TRP:HE1	1:A:291:GLY:HA2	1.63	0.63
1:A:487:GLU:HA	1:A:490:ARG:HB3	1.80	0.63
1:A:245:THR:HG22	1:A:246:ASN:H	1.62	0.63
1:A:268:THR:HG22	1:A:269:GLN:H	1.62	0.63
1:A:241:ARG:NH1	1:A:494:GLY:HA3	2.13	0.63
1:A:471:TRP:HA	1:A:476:GLN:O	1.98	0.63
1:A:275:GLY:CA	1:A:464:SER:HB2	2.29	0.63
4:A:41:NAG:H61	4:A:46:FUL:O2	1.96	0.62
1:A:343:CYS:HB2	1:A:429:VAL:HG21	1.80	0.62
1:A:471:TRP:CE2	6:A:16:NAG:H81	2.34	0.62
1:A:289:TRP:HE1	1:A:296:THR:HG21	1.65	0.62
1:A:268:THR:HG22	1:A:269:GLN:N	2.14	0.62
1:A:302:LYS:HZ2	1:A:304:TYR:H	1.48	0.62
1:A:394:CYS:O	1:A:395:ARG:HB3	2.00	0.62
1:A:307:THR:O	1:A:345:PHE:HA	1.99	0.62
1:A:273:TRP:HD1	1:A:274:PHE:CZ	2.18	0.62
1:A:307:THR:OG1	10:A:30:NAG:H83	2.00	0.62
1:A:273:TRP:CZ3	1:A:481:MET:HG3	2.35	0.61
1:A:406:PHE:O	1:A:409:TRP:NE1	2.33	0.61
1:A:266:MET:SD	1:A:398:PHE:CZ	2.91	0.61
1:A:439:THR:HB	1:A:442:LYS:O	2.01	0.60
1:A:355:GLU:O	1:A:359:THR:N	2.33	0.60
1:A:496:TYR:O	1:A:496:TYR:HD1	1.84	0.60
1:A:290:HIS:ND1	1:A:290:HIS:C	2.54	0.60
1:A:285:THR:OG1	1:A:302:LYS:HD3	2.01	0.60
1:A:488:LEU:O	1:A:491:LEU:HB2	2.02	0.59
1:A:269:GLN:NE2	4:A:7:NAG:C8	2.63	0.59
1:A:400:TYR:O	1:A:431:CYS:HB3	2.02	0.59
1:A:381:ARG:NH2	1:A:382:GLY:CA	2.65	0.59
1:A:268:THR:HG22	1:A:269:GLN:HG2	1.85	0.58
1:A:241:ARG:O	1:A:257:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TRP:CD1	1:A:430:PRO:HA	2.39	0.57
1:A:243:ASN:CG	1:A:244:ASP:H	2.08	0.57
1:A:234:PRO:HG3	1:A:263:THR:N	2.19	0.57
1:A:269:GLN:CA	1:A:393:ASN:O	2.50	0.57
1:A:241:ARG:CG	1:A:242:CYS:H	2.15	0.56
1:A:290:HIS:HD1	1:A:290:HIS:C	2.08	0.56
1:A:498:LEU:O	1:A:499:VAL:HB	2.05	0.56
1:A:385:PRO:O	1:A:386:GLU:HB2	2.04	0.56
1:A:302:LYS:NZ	1:A:304:TYR:H	2.04	0.56
1:A:401:CYS:HA	1:A:431:CYS:HA	1.87	0.56
1:A:486:ALA:HB1	1:A:490:ARG:HH21	1.70	0.56
1:A:303:TYR:O	1:A:304:TYR:O	2.24	0.55
1:A:437:ILE:HD12	1:A:446:ASN:HB2	1.87	0.55
1:A:237:TYR:CZ	1:A:498:LEU:HB2	2.41	0.55
1:A:244:ASP:C	1:A:245:THR:OG1	2.45	0.55
1:A:417:ASN:HA	1:A:420:PRO:HG2	1.86	0.55
1:A:309:LYS:O	1:A:344:TRP:HD1	1.90	0.55
1:A:286:TYR:O	1:A:300:LEU:HA	2.06	0.55
1:A:498:LEU:O	1:A:499:VAL:CB	2.54	0.55
1:A:270:THR:N	1:A:393:ASN:O	2.39	0.54
1:A:259:VAL:O	1:A:260:SER:HB2	2.07	0.54
1:A:437:ILE:HB	1:A:446:ASN:CB	2.37	0.54
1:A:269:GLN:HE21	4:A:7:NAG:H82	1.69	0.54
1:A:421:LYS:HD2	1:A:423:ARG:HE	1.72	0.54
1:A:241:ARG:CG	1:A:242:CYS:N	2.71	0.53
1:A:237:TYR:OH	1:A:498:LEU:CB	2.51	0.53
1:A:102:VAL:HG22	1:A:103:LYS:N	2.23	0.53
1:A:380:PRO:HG2	1:A:385:PRO:CG	2.34	0.53
3:A:4:NAG:H61	3:A:5:BMA:H2	1.91	0.53
1:A:102:VAL:HG22	1:A:103:LYS:H	1.73	0.53
1:A:498:LEU:O	1:A:499:VAL:HG23	2.09	0.53
1:A:391:TRP:CG	1:A:392:THR:N	2.77	0.52
1:A:286:TYR:CD2	1:A:288:TYR:CE1	2.96	0.52
1:A:306:LEU:C	1:A:462:VAL:HG21	2.30	0.52
1:A:234:PRO:HG3	1:A:263:THR:H	1.73	0.52
1:A:306:LEU:HD23	1:A:462:VAL:HG11	1.91	0.52
1:A:273:TRP:CE3	1:A:481:MET:CG	2.93	0.52
1:A:415:VAL:CG1	1:A:416:THR:H	2.16	0.52
1:A:215:ILE:HG22	1:A:216:GLN:N	2.25	0.52
1:A:306:LEU:O	1:A:462:VAL:HG23	2.09	0.51
1:A:365:ARG:O	1:A:366:TYR:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:13:NDG:H6C2	5:A:14:NAG:C7	2.41	0.51
1:A:357:LYS:O	1:A:361:VAL:HG23	2.11	0.51
1:A:309:LYS:HG3	1:A:459:ASN:HA	1.92	0.51
4:A:41:NAG:C6	4:A:46:FUL:O2	2.59	0.51
1:A:354:LYS:O	1:A:358:GLN:HG3	2.11	0.51
1:A:437:ILE:CD1	1:A:446:ASN:HB2	2.40	0.50
1:A:273:TRP:CZ3	1:A:481:MET:CG	2.95	0.50
1:A:77:ALA:HA	1:A:80:ASN:ND2	2.23	0.50
1:A:104:LEU:HB3	1:A:214:ILE:HG12	1.93	0.50
1:A:274:PHE:CE2	1:A:349:TRP:HH2	2.28	0.50
1:A:447:VAL:O	1:A:448:TYR:CG	2.64	0.50
1:A:311:ARG:HB2	1:A:344:TRP:HE1	1.77	0.50
1:A:395:ARG:HE	1:A:452:ARG:HA	1.76	0.50
1:A:109:ILE:O	1:A:499:VAL:HG22	2.11	0.50
1:A:273:TRP:CD1	1:A:274:PHE:CZ	2.99	0.50
1:A:357:LYS:HE2	1:A:411:GLU:OE2	2.12	0.50
1:A:432:HIS:O	1:A:434:ARG:HG2	2.11	0.50
1:A:388:THR:HB	1:A:407:LEU:HD13	1.93	0.50
1:A:463:THR:HG22	1:A:464:SER:N	2.27	0.50
1:A:311:ARG:HG3	1:A:344:TRP:NE1	2.27	0.50
1:A:490:ARG:HG3	1:A:495:ASP:HA	1.92	0.50
1:A:310:CYS:N	1:A:458:CYS:O	2.45	0.50
1:A:381:ARG:HH21	1:A:382:GLY:CA	2.16	0.50
6:A:17:NAG:O3	6:A:52:MAN:H5	2.11	0.50
1:A:239:LEU:O	1:A:260:SER:HB3	2.12	0.49
1:A:78:TRP:HH2	1:A:381:ARG:HH11	1.60	0.49
1:A:391:TRP:CD1	1:A:392:THR:N	2.80	0.49
1:A:243:ASN:OD1	1:A:244:ASP:N	2.39	0.49
1:A:90:VAL:O	1:A:94:PHE:CD1	2.66	0.49
1:A:437:ILE:N	1:A:446:ASN:O	2.30	0.49
4:A:42:NAG:O3	4:A:43:BMA:H62	2.13	0.49
1:A:487:GLU:HA	1:A:490:ARG:CB	2.43	0.49
1:A:395:ARG:HG2	1:A:456:LEU:HD13	1.95	0.48
1:A:397:GLU:O	1:A:399:LEU:HG	2.12	0.48
1:A:376:ASN:OD1	1:A:410:VAL:HG12	2.13	0.48
5:A:13:NDG:H6C2	5:A:14:NAG:HN2	1.74	0.48
1:A:496:TYR:CD1	1:A:496:TYR:O	2.64	0.48
1:A:258:VAL:HG12	1:A:259:VAL:N	2.22	0.48
6:A:17:NAG:O6	6:A:52:MAN:H2	2.14	0.48
1:A:466:ILE:HD13	1:A:481:MET:SD	2.54	0.48
1:A:273:TRP:CZ2	1:A:481:MET:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TRP:HZ2	1:A:393:ASN:OD1	1.98	0.47
1:A:234:PRO:HD3	1:A:263:THR:H	1.79	0.47
1:A:306:LEU:HD22	1:A:349:TRP:CZ3	2.50	0.47
1:A:243:ASN:OD1	4:A:41:NAG:O5	2.33	0.47
1:A:353:ILE:HD13	1:A:353:ILE:HA	1.82	0.47
1:A:78:TRP:CH2	1:A:381:ARG:NH1	2.80	0.47
5:A:14:NAG:HN2	5:A:15:FUL:C1	2.28	0.47
1:A:399:LEU:HA	1:A:433:ILE:HG23	1.97	0.47
1:A:489:TYR:C	1:A:491:LEU:H	2.18	0.47
1:A:242:CYS:O	1:A:243:ASN:HB2	2.15	0.46
1:A:360:ILE:HD11	1:A:469:ILE:CD1	2.45	0.46
1:A:77:ALA:O	1:A:80:ASN:HB2	2.15	0.46
1:A:289:TRP:NE1	1:A:296:THR:HG21	2.30	0.46
1:A:251:MET:N	1:A:252:PRO:HD3	2.31	0.46
1:A:406:PHE:HD2	1:A:407:LEU:HG	1.80	0.46
1:A:277:ASN:HA	1:A:461:THR:OG1	2.15	0.46
1:A:416:THR:O	1:A:420:PRO:HG2	2.15	0.46
1:A:249:GLY:O	1:A:250:PHE:HD1	1.99	0.46
1:A:73:GLU:HB2	1:A:292:ARG:NH1	2.31	0.46
1:A:269:GLN:HA	1:A:393:ASN:C	2.36	0.45
1:A:395:ARG:CB	1:A:456:LEU:HD13	2.46	0.45
1:A:349:TRP:CE2	1:A:406:PHE:CZ	3.05	0.45
1:A:311:ARG:HE	1:A:344:TRP:HZ2	1.62	0.45
1:A:273:TRP:HD1	1:A:274:PHE:CE2	2.35	0.45
1:A:343:CYS:HB2	1:A:429:VAL:HG23	1.97	0.45
1:A:290:HIS:CE1	1:A:292:ARG:CG	2.90	0.45
1:A:493:LEU:CD1	1:A:496:TYR:HA	2.47	0.45
1:A:349:TRP:NE1	1:A:353:ILE:HG13	2.32	0.45
1:A:413:ARG:HG2	1:A:414:ASP:OD2	2.16	0.45
1:A:419:ARG:N	1:A:420:PRO:CD	2.79	0.45
1:A:463:THR:O	1:A:465:LEU:N	2.51	0.44
1:A:374:LYS:HE2	9:A:26:NAG:H81	1.99	0.44
1:A:393:ASN:HD22	1:A:394:CYS:N	2.15	0.44
1:A:486:ALA:HB1	1:A:496:TYR:CD2	2.52	0.44
1:A:469:ILE:HA	1:A:478:ASN:O	2.17	0.44
1:A:378:THR:HG22	1:A:379:ALA:N	2.32	0.44
1:A:274:PHE:HE2	1:A:349:TRP:CH2	2.35	0.44
1:A:426:ARG:HB3	1:A:426:ARG:HH11	1.83	0.44
1:A:471:TRP:NE1	6:A:16:NAG:O7	2.50	0.44
4:A:9:BMA:O4	4:A:11:MAN:H2	2.18	0.44
1:A:485:VAL:O	1:A:488:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HH11	1:A:438:ASN:ND2	2.15	0.44
1:A:285:THR:CG2	1:A:302:LYS:HB2	2.29	0.44
1:A:105:SER:HB3	1:A:106:PRO:HD2	1.99	0.44
1:A:244:ASP:HA	4:A:41:NAG:O6	2.18	0.44
1:A:109:ILE:HB	1:A:499:VAL:HG22	2.00	0.44
1:A:273:TRP:HB3	1:A:274:PHE:CE2	2.53	0.44
1:A:80:ASN:CG	1:A:81:THR:H	2.18	0.44
1:A:88:GLU:HA	1:A:91:TRP:CZ2	2.53	0.43
1:A:391:TRP:HE1	1:A:398:PHE:HA	1.82	0.43
1:A:98:ILE:O	1:A:99:LYS:CG	2.63	0.43
1:A:302:LYS:HG3	1:A:304:TYR:H	1.83	0.43
1:A:498:LEU:O	1:A:499:VAL:CG2	2.66	0.43
1:A:369:THR:O	1:A:371:ASN:ND2	2.52	0.43
1:A:273:TRP:CE2	1:A:481:MET:HG2	2.53	0.43
1:A:80:ASN:HB3	1:A:84:GLU:CG	2.36	0.43
1:A:353:ILE:HG22	1:A:357:LYS:CE	2.38	0.43
1:A:107:LEU:O	1:A:211:ASN:O	2.37	0.43
1:A:462:VAL:O	1:A:463:THR:CB	2.66	0.43
1:A:105:SER:HB3	1:A:106:PRO:CD	2.49	0.42
1:A:349:TRP:NE1	1:A:353:ILE:CG1	2.82	0.42
1:A:342:TRP:CD1	1:A:429:VAL:O	2.72	0.42
8:A:23:NDG:H2	8:A:23:NDG:H8C1	1.77	0.42
1:A:493:LEU:HB2	1:A:494:GLY:H	1.50	0.42
11:A:39:MAN:O3	11:A:53:MAN:C1	2.67	0.42
1:A:275:GLY:N	1:A:464:SER:O	2.48	0.42
1:A:470:ASP:N	1:A:478:ASN:O	2.47	0.42
1:A:302:LYS:HG3	1:A:304:TYR:N	2.34	0.42
1:A:215:ILE:HG22	1:A:216:GLN:H	1.85	0.42
1:A:489:TYR:C	1:A:491:LEU:N	2.73	0.42
1:A:290:HIS:ND1	1:A:290:HIS:O	2.53	0.42
10:A:33:MAN:C4	10:A:34:BMA:C1	2.87	0.42
1:A:437:ILE:HG21	1:A:446:ASN:HD22	1.85	0.41
1:A:273:TRP:HB3	1:A:274:PHE:CD2	2.55	0.41
1:A:466:ILE:HG12	1:A:467:ALA:N	2.34	0.41
1:A:90:VAL:HG22	1:A:94:PHE:CE1	2.56	0.41
1:A:241:ARG:HD3	1:A:493:LEU:CB	2.49	0.41
1:A:304:TYR:CE1	1:A:348:ASN:HB2	2.56	0.41
1:A:273:TRP:CH2	1:A:481:MET:HG2	2.55	0.41
1:A:417:ASN:HA	1:A:420:PRO:CG	2.51	0.41
1:A:496:TYR:O	1:A:497:LYS:HG3	2.21	0.41
1:A:441:HIS:CD2	1:A:441:HIS:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:HA	1:A:360:ILE:HG22	2.03	0.41
1:A:439:THR:HB	1:A:444:GLY:H	1.86	0.41
1:A:309:LYS:HG2	1:A:458:CYS:O	2.22	0.40
1:A:369:THR:HG22	1:A:370:ASN:H	1.86	0.40
1:A:276:PHE:HB3	1:A:461:THR:HG23	2.03	0.40
1:A:277:ASN:CG	1:A:461:THR:HG21	2.42	0.40
1:A:98:ILE:O	1:A:99:LYS:CB	2.69	0.40
1:A:276:PHE:CD2	1:A:461:THR:O	2.74	0.40
1:A:301:ASN:HD22	1:A:463:THR:CG2	2.34	0.40
1:A:309:LYS:O	1:A:344:TRP:CD1	2.72	0.40
1:A:376:ASN:OD1	1:A:410:VAL:HA	2.22	0.40

All (4) 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:67:LEU:O	1:A:436:ILE:CD1[4_455]	1.88	0.32
1:A:66:GLU:OE1	1:A:445:LYS:CB[4_455]	2.02	0.18
3:A:6:FUL:O3	3:A:6:FUL:O3[8_555]	2.14	0.06
4:A:10:MAN:O3	6:A:18:FUL:O3[6_555]	2.17	0.03

## 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	300/316 (95%)	204 (68%)	57 (19%)	39 (13%)	<b>0</b> <b>7</b>

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	100	PRO

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Mol	Chain	Res	Type
1	A	233	ALA
1	A	304	TYR
1	A	386	GLU
1	A	463	THR
1	A	481	MET
1	A	76	ASP
1	A	77	ALA
1	A	101	CYS
1	A	260	SER
1	A	265	MET
1	A	276	PHE
1	A	312	GLY
1	A	341	GLY
1	A	366	TYR
1	A	385	PRO
1	A	454	GLY
1	A	493	LEU
1	A	217	GLU
1	A	242	CYS
1	A	243	ASN
1	A	246	ASN
1	A	252	PRO
1	A	485	VAL
1	A	261	SER
1	A	279	THR
1	A	368	GLY
1	A	379	ALA
1	A	464	SER
1	A	74	SER
1	A	98	ILE
1	A	102	VAL
1	A	109	ILE
1	A	255	SER
1	A	420	PRO
1	A	443	VAL
1	A	110	GLY
1	A	494	GLY

### 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	272/284 (96%)	210 (77%)	62 (23%)	<b>1</b> <b>9</b>

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	69	LEU
1	A	90	VAL
1	A	92	GLN
1	A	93	LEU
1	A	95	GLU
1	A	229	PHE
1	A	230	ARG
1	A	240	LEU
1	A	242	CYS
1	A	245	THR
1	A	254	CYS
1	A	257	VAL
1	A	266	MET
1	A	270	THR
1	A	272	THR
1	A	273	TRP
1	A	274	PHE
1	A	287	ILE
1	A	290	HIS
1	A	296	THR
1	A	298	ILE
1	A	301	ASN
1	A	303	TYR
1	A	304	TYR
1	A	307	THR
1	A	350	LYS
1	A	355	GLU
1	A	359	THR
1	A	369	THR
1	A	370	ASN
1	A	373	ASP
1	A	374	LYS
1	A	375	ILE

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Mol	Chain	Res	Type
1	A	377	LEU
1	A	381	ARG
1	A	387	VAL
1	A	388	THR
1	A	393	ASN
1	A	394	CYS
1	A	399	LEU
1	A	416	THR
1	A	425	ARG
1	A	429	VAL
1	A	432	HIS
1	A	433	ILE
1	A	441	HIS
1	A	456	LEU
1	A	457	THR
1	A	458	CYS
1	A	461	THR
1	A	462	VAL
1	A	464	SER
1	A	466	ILE
1	A	471	TRP
1	A	480	THR
1	A	487	GLU
1	A	491	LEU
1	A	493	LEU
1	A	495	ASP
1	A	496	TYR
1	A	498	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	209	HIS
1	A	269	GLN
1	A	290	HIS
1	A	363	HIS
1	A	393	ASN
1	A	417	ASN
1	A	438	ASN
1	A	441	HIS
1	A	446	ASN

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Mol	Chain	Res	Type
1	A	468	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

53 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	$\# Z  > 2$
4	MAN	A	10	4	11,11,12	0.49	0	14,15,17	1.68	3 (21%)
4	MAN	A	11	4	11,11,12	0.55	0	14,15,17	1.50	3 (21%)
4	FUL	A	12	4	10,10,11	0.51	0	14,14,16	1.71	4 (28%)
5	NDG	A	13	1,5	14,14,15	0.46	0	15,19,21	1.43	2 (13%)
5	NAG	A	14	5	14,14,15	0.46	0	15,19,21	1.38	2 (13%)
5	FUL	A	15	5	10,10,11	0.50	0	14,14,16	1.76	4 (28%)
6	NAG	A	16	1,6	14,14,15	0.50	0	15,19,21	2.08	4 (26%)
6	NAG	A	17	6	14,14,15	0.67	0	15,19,21	1.41	3 (20%)
6	FUL	A	18	6	10,10,11	0.38	0	14,14,16	1.25	1 (7%)
7	NAG	A	19	1,7	14,14,15	0.54	0	15,19,21	1.63	3 (20%)
7	NAG	A	20	7	14,14,15	0.41	0	15,19,21	1.15	2 (13%)
7	BMA	A	21	7	11,11,12	0.34	0	14,15,17	1.43	3 (21%)
7	FUL	A	22	7	10,10,11	0.55	0	14,14,16	1.45	3 (21%)
8	NDG	A	23	1,8	14,14,15	0.30	0	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	A	24	8	14,14,15	0.68	0	15,19,21	1.03	1 (6%)
9	NDG	A	25	9,1	14,14,15	0.32	0	15,19,21	1.83	2 (13%)
9	NAG	A	26	9	14,14,15	0.54	0	15,19,21	1.51	2 (13%)
9	BMA	A	27	9	11,11,12	0.58	0	14,15,17	1.48	3 (21%)
9	FUL	A	28	9	10,10,11	0.47	0	14,14,16	1.97	5 (35%)
10	NAG	A	29	1,10	14,14,15	0.49	0	15,19,21	1.02	1 (6%)
3	NDG	A	3	1,3	14,14,15	0.54	0	15,19,21	0.92	0
10	NAG	A	30	10	14,14,15	0.45	0	15,19,21	2.67	4 (26%)
10	BMA	A	31	10	11,11,12	0.64	0	14,15,17	2.79	5 (35%)
10	BMA	A	32	10	11,11,12	0.60	0	14,15,17	2.05	3 (21%)
10	MAN	A	33	10	11,11,12	0.68	0	14,15,17	1.67	3 (21%)
10	BMA	A	34	10	11,11,12	0.73	0	14,15,17	1.15	1 (7%)
10	MAN	A	35	10	11,11,12	0.58	0	14,15,17	2.03	4 (28%)
11	NAG	A	36	1,11	14,14,15	0.53	0	15,19,21	1.57	2 (13%)
11	NAG	A	37	11	14,14,15	0.70	0	15,19,21	1.55	3 (20%)
11	BMA	A	38	11	11,11,12	0.73	0	14,15,17	1.67	2 (14%)
11	MAN	A	39	11	11,11,12	0.69	0	14,15,17	1.10	2 (14%)
3	NAG	A	4	3	14,14,15	0.71	0	15,19,21	1.24	2 (13%)
11	MAN	A	40	11	11,11,12	0.53	0	14,15,17	1.32	1 (7%)
4	NAG	A	41	1,4	14,14,15	0.45	0	15,19,21	1.30	1 (6%)
4	NAG	A	42	4	14,14,15	0.41	0	15,19,21	1.51	2 (13%)
4	BMA	A	43	4	11,11,12	0.64	0	14,15,17	1.96	3 (21%)
4	MAN	A	44	4	11,11,12	0.63	0	14,15,17	1.64	3 (21%)
4	MAN	A	45	4	11,11,12	0.59	0	14,15,17	1.84	2 (14%)
4	FUL	A	46	4	10,10,11	0.53	0	14,14,16	1.75	5 (35%)
12	NAG	A	47	1,12	14,14,15	0.53	0	15,19,21	1.18	1 (6%)
12	NAG	A	48	12	14,14,15	0.42	0	15,19,21	0.98	0
12	BMA	A	49	12	11,11,12	0.44	0	14,15,17	1.22	1 (7%)
3	BMA	A	5	3	11,11,12	0.45	0	14,15,17	1.27	2 (14%)
12	MAN	A	50	12	11,11,12	0.57	0	14,15,17	1.38	2 (14%)
3	BMA	A	51	3	11,11,12	0.68	0	14,15,17	0.94	1 (7%)
6	MAN	A	52	6	11,11,12	0.48	0	14,15,17	1.70	3 (21%)
11	MAN	A	53	11	11,11,12	0.56	0	14,15,17	2.49	3 (21%)
9	BMA	A	55	9	11,11,12	0.66	0	14,15,17	1.66	3 (21%)
9	MAN	A	56	9	11,11,12	0.53	0	14,15,17	1.71	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUL	A	6	3	10,10,11	0.47	0	14,14,16	1.31	2 (14%)
4	NAG	A	7	1,4	14,14,15	0.73	1 (7%)	15,19,21	1.95	3 (20%)
4	NAG	A	8	4	14,14,15	0.73	0	15,19,21	1.42	2 (13%)
4	BMA	A	9	4	11,11,12	0.56	0	14,15,17	2.41	4 (28%)

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	MAN	A	10	4	-	0/2/19/22	0/1/1/1
4	MAN	A	11	4	-	0/2/19/22	0/1/1/1
4	FUL	A	12	4	-	0/0/17/20	0/1/1/1
5	NDG	A	13	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	14	5	-	0/6/23/26	0/1/1/1
5	FUL	A	15	5	-	0/0/17/20	0/1/1/1
6	NAG	A	16	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	17	6	-	0/6/23/26	0/1/1/1
6	FUL	A	18	6	-	0/0/17/20	0/1/1/1
7	NAG	A	19	1,7	-	1/6/23/26	0/1/1/1
7	NAG	A	20	7	-	0/6/23/26	0/1/1/1
7	BMA	A	21	7	-	0/2/19/22	0/1/1/1
7	FUL	A	22	7	-	0/0/17/20	0/1/1/1
8	NDG	A	23	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	24	8	-	0/6/23/26	0/1/1/1
9	NDG	A	25	9,1	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	A	26	9	-	0/6/23/26	0/1/1/1
9	BMA	A	27	9	-	0/2/19/22	0/1/1/1
9	FUL	A	28	9	-	0/0/17/20	0/1/1/1
10	NAG	A	29	1,10	-	0/6/23/26	0/1/1/1
3	NDG	A	3	1,3	-	0/6/23/26	0/1/1/1
10	NAG	A	30	10	-	0/6/23/26	0/1/1/1
10	BMA	A	31	10	-	0/2/19/22	0/1/1/1
10	BMA	A	32	10	-	0/2/19/22	0/1/1/1
10	MAN	A	33	10	-	0/2/19/22	0/1/1/1
10	BMA	A	34	10	-	0/2/19/22	0/1/1/1
10	MAN	A	35	10	-	0/2/19/22	0/1/1/1
11	NAG	A	36	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	37	11	-	0/6/23/26	0/1/1/1
11	BMA	A	38	11	-	0/2/19/22	0/1/1/1
11	MAN	A	39	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	4	3	-	0/6/23/26	0/1/1/1
11	MAN	A	40	11	-	0/2/19/22	0/1/1/1
4	NAG	A	41	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	42	4	-	0/6/23/26	0/1/1/1
4	BMA	A	43	4	-	0/2/19/22	0/1/1/1
4	MAN	A	44	4	-	0/2/19/22	0/1/1/1
4	MAN	A	45	4	-	0/2/19/22	0/1/1/1
4	FUL	A	46	4	-	0/0/17/20	0/1/1/1
12	NAG	A	47	1,12	-	0/6/23/26	0/1/1/1
12	NAG	A	48	12	-	0/6/23/26	0/1/1/1
12	BMA	A	49	12	-	0/2/19/22	0/1/1/1
3	BMA	A	5	3	-	0/2/19/22	0/1/1/1
12	MAN	A	50	12	-	0/2/19/22	0/1/1/1
3	BMA	A	51	3	-	0/2/19/22	0/1/1/1
6	MAN	A	52	6	-	0/2/19/22	0/1/1/1
11	MAN	A	53	11	-	0/2/19/22	0/1/1/1
9	BMA	A	55	9	-	0/2/19/22	0/1/1/1
9	MAN	A	56	9	-	0/2/19/22	0/1/1/1
3	FUL	A	6	3	-	0/0/17/20	0/1/1/1
4	NAG	A	7	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	8	4	-	0/6/23/26	0/1/1/1
4	BMA	A	9	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7	NAG	O5-C1	-2.14	1.40	1.43

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	30	NAG	C4-C3-C2	-7.36	99.79	111.23
10	A	32	BMA	C1-C2-C3	-5.60	102.92	109.54
6	A	16	NAG	C3-C2-N2	-3.48	102.22	110.56
4	A	7	NAG	C2-N2-C7	-3.11	119.04	123.04
7	A	21	BMA	O5-C1-C2	-2.75	106.39	110.86
4	A	46	FUL	C1-C2-C3	-2.49	106.59	109.54
9	A	25	NDG	C3-C2-N2	-2.48	104.62	110.56
3	A	5	BMA	C3-C4-C5	-2.41	106.00	110.20
4	A	42	NAG	C4-C3-C2	-2.29	107.68	111.23
8	A	23	NDG	C3-C2-N2	-2.21	105.26	110.56
5	A	13	NDG	C4-C3-C2	-2.20	107.82	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	10	MAN	C1-C2-C3	-2.15	107.00	109.54
11	A	36	NAG	C3-C4-C5	-2.14	106.46	110.20
4	A	46	FUL	O2-C2-C3	-2.07	105.96	110.12
7	A	22	FUL	O5-C1-C2	-2.05	107.52	110.86
6	A	16	NAG	C3-C4-C5	-2.02	106.67	110.20
11	A	37	NAG	C3-C4-C5	-2.02	106.68	110.20
11	A	37	NAG	O7-C7-C8	-2.00	118.39	122.06
3	A	51	BMA	C1-C2-C3	2.00	111.91	109.54
4	A	9	BMA	C2-C3-C4	2.04	114.50	111.04
9	A	27	BMA	C1-O5-C5	2.05	114.84	112.25
6	A	17	NAG	C3-C4-C5	2.06	113.78	110.20
4	A	12	FUL	O5-C5-C6	2.06	109.53	106.13
9	A	28	FUL	C1-C2-C3	2.07	111.98	109.54
4	A	9	BMA	O5-C1-C2	2.10	114.26	110.86
4	A	46	FUL	O2-C2-C1	2.10	113.42	109.21
9	A	56	MAN	O5-C1-C2	2.11	114.27	110.86
9	A	55	BMA	O3-C3-C4	2.11	115.08	110.34
7	A	21	BMA	C1-O5-C5	2.12	114.94	112.25
5	A	15	FUL	C3-C4-C5	2.12	113.30	109.72
11	A	39	MAN	O3-C3-C2	2.13	113.85	110.00
4	A	46	FUL	O5-C5-C4	2.16	113.27	109.53
9	A	28	FUL	O5-C1-C2	2.17	114.38	110.86
4	A	11	MAN	O5-C1-C2	2.17	114.38	110.86
4	A	12	FUL	C1-C2-C3	2.20	112.14	109.54
5	A	14	NAG	C3-C4-C5	2.23	114.09	110.20
11	A	39	MAN	O2-C2-C3	2.30	114.75	110.12
5	A	13	NDG	O3-C3-C2	2.32	113.71	109.11
10	A	33	MAN	O4-C4-C5	2.33	115.41	109.24
4	A	10	MAN	C3-C4-C5	2.39	114.37	110.20
4	A	43	BMA	O5-C5-C6	2.40	112.54	107.35
4	A	8	NAG	C2-N2-C7	2.41	126.13	123.04
3	A	6	FUL	O5-C5-C4	2.43	113.74	109.53
4	A	44	MAN	O5-C1-C2	2.44	114.81	110.86
7	A	20	NAG	C1-O5-C5	2.45	115.35	112.25
6	A	52	MAN	C1-O5-C5	2.45	115.35	112.25
6	A	17	NAG	C2-N2-C7	2.45	126.18	123.04
10	A	32	BMA	C1-O5-C5	2.48	115.40	112.25
10	A	32	BMA	O2-C2-C3	2.53	115.22	110.12
6	A	52	MAN	O5-C1-C2	2.56	115.01	110.86
3	A	5	BMA	O5-C5-C6	2.65	113.09	107.35
10	A	34	BMA	C3-C4-C5	2.70	114.90	110.20
10	A	33	MAN	O5-C1-C2	2.70	115.24	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	31	BMA	O5-C1-C2	2.71	115.26	110.86
7	A	19	NAG	C4-C3-C2	2.74	115.48	111.23
4	A	11	MAN	C1-O5-C5	2.74	115.72	112.25
10	A	29	NAG	C1-O5-C5	2.75	115.73	112.25
7	A	22	FUL	C3-C4-C5	2.76	114.36	109.72
4	A	7	NAG	C4-C3-C2	2.77	115.54	111.23
7	A	22	FUL	O5-C5-C4	2.78	114.35	109.53
11	A	38	BMA	O5-C5-C6	2.79	113.39	107.35
9	A	28	FUL	O5-C5-C4	2.79	114.36	109.53
5	A	15	FUL	C1-O5-C5	2.80	116.71	112.38
7	A	19	NAG	C1-O5-C5	2.83	115.84	112.25
3	A	4	NAG	C4-C3-C2	2.83	115.63	111.23
10	A	35	MAN	C1-C2-C3	2.87	112.93	109.54
10	A	30	NAG	O4-C4-C3	2.87	116.80	110.34
12	A	50	MAN	C1-C2-C3	2.87	112.94	109.54
7	A	20	NAG	C2-N2-C7	2.90	126.76	123.04
9	A	26	NAG	C3-C4-C5	2.95	115.35	110.20
9	A	27	BMA	O5-C5-C6	2.96	113.76	107.35
10	A	31	BMA	O3-C3-C2	2.99	115.39	110.00
6	A	16	NAG	O5-C5-C6	3.00	113.85	107.35
10	A	35	MAN	C2-C3-C4	3.00	116.14	111.04
9	A	27	BMA	C1-C2-C3	3.07	113.17	109.54
4	A	44	MAN	C1-O5-C5	3.07	116.14	112.25
3	A	4	NAG	C1-O5-C5	3.10	116.18	112.25
7	A	21	BMA	C3-C4-C5	3.13	115.65	110.20
5	A	15	FUL	C1-C2-C3	3.18	113.31	109.54
12	A	49	BMA	C1-O5-C5	3.21	116.33	112.25
6	A	18	FUL	C1-O5-C5	3.24	117.38	112.38
8	A	24	NAG	C4-C3-C2	3.29	116.34	111.23
6	A	17	NAG	C4-C3-C2	3.29	116.35	111.23
4	A	41	NAG	C1-O5-C5	3.31	116.45	112.25
11	A	37	NAG	C2-N2-C7	3.34	127.33	123.04
3	A	6	FUL	C1-O5-C5	3.39	117.61	112.38
4	A	12	FUL	C2-C3-C4	3.41	116.83	111.04
10	A	31	BMA	C3-C4-C5	3.45	116.21	110.20
4	A	12	FUL	C3-C4-C5	3.46	115.55	109.72
5	A	15	FUL	O5-C5-C6	3.47	111.87	106.13
12	A	47	NAG	C1-O5-C5	3.58	116.80	112.25
9	A	28	FUL	O5-C5-C6	3.59	112.07	106.13
10	A	30	NAG	O4-C4-C5	3.60	118.79	109.24
5	A	14	NAG	C2-N2-C7	3.61	127.67	123.04
9	A	55	BMA	O3-C3-C2	3.65	116.59	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	55	BMA	C1-O5-C5	3.74	116.99	112.25
4	A	8	NAG	C4-C3-C2	3.74	117.04	111.23
4	A	11	MAN	C1-C2-C3	3.76	113.99	109.54
12	A	50	MAN	C1-O5-C5	3.78	117.05	112.25
4	A	45	MAN	C3-C4-C5	3.81	116.84	110.20
9	A	56	MAN	C1-O5-C5	3.82	117.10	112.25
4	A	43	BMA	C1-C2-C3	3.88	114.14	109.54
4	A	46	FUL	C3-C4-C5	3.92	116.33	109.72
4	A	9	BMA	C1-O5-C5	4.05	117.39	112.25
4	A	44	MAN	C1-C2-C3	4.06	114.35	109.54
10	A	35	MAN	C1-O5-C5	4.09	117.43	112.25
10	A	33	MAN	C1-O5-C5	4.09	117.43	112.25
7	A	19	NAG	C3-C4-C5	4.17	117.47	110.20
10	A	30	NAG	C1-O5-C5	4.24	117.63	112.25
9	A	56	MAN	C1-C2-C3	4.27	114.60	109.54
9	A	26	NAG	C4-C3-C2	4.28	117.88	111.23
11	A	40	MAN	C1-O5-C5	4.28	117.68	112.25
4	A	7	NAG	C3-C4-C5	4.46	117.98	110.20
10	A	35	MAN	C3-C4-C5	4.47	117.98	110.20
4	A	42	NAG	C1-O5-C5	4.50	117.96	112.25
11	A	38	BMA	C1-C2-C3	4.61	114.99	109.54
4	A	43	BMA	C1-O5-C5	4.61	118.10	112.25
6	A	52	MAN	C1-C2-C3	4.63	115.02	109.54
9	A	28	FUL	C1-O5-C5	4.67	119.58	112.38
4	A	10	MAN	C1-O5-C5	4.74	118.26	112.25
11	A	53	MAN	O5-C1-C2	4.83	118.69	110.86
6	A	16	NAG	C2-N2-C7	4.84	129.26	123.04
4	A	45	MAN	C1-O5-C5	4.92	118.50	112.25
11	A	53	MAN	C1-O5-C5	4.96	118.55	112.25
11	A	36	NAG	C1-O5-C5	5.22	118.87	112.25
10	A	31	BMA	C1-C2-C3	5.24	115.74	109.54
9	A	25	NDG	C1-O-C5	5.49	119.21	112.25
11	A	53	MAN	C1-C2-C3	5.66	116.23	109.54
10	A	31	BMA	C1-O5-C5	6.61	120.64	112.25
4	A	9	BMA	C1-C2-C3	7.13	117.97	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	25	NDG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	19	NAG	O7-C7-N2-C2

There are no ring outliers.

25 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	10	MAN	0	1
4	A	11	MAN	1	0
5	A	13	NDG	3	0
5	A	14	NAG	4	0
5	A	15	FUL	1	0
6	A	16	NAG	2	0
6	A	17	NAG	2	0
6	A	18	FUL	0	1
8	A	23	NDG	1	0
9	A	26	NAG	1	0
10	A	30	NAG	1	0
10	A	33	MAN	2	0
10	A	34	BMA	2	0
11	A	39	MAN	1	0
3	A	4	NAG	1	0
4	A	41	NAG	4	0
4	A	42	NAG	1	0
4	A	43	BMA	1	0
4	A	46	FUL	2	0
3	A	5	BMA	1	0
6	A	52	MAN	2	0
11	A	53	MAN	1	0
3	A	6	FUL	0	1
4	A	7	NAG	5	0
4	A	9	BMA	1	0

## 5.6 Ligand geometry [i](#)

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
2	NAG	A	1	1	14,14,15	0.54	0	15,19,21	0.89	1 (6%)
2	NAG	A	2	1	14,14,15	0.54	0	15,19,21	0.91	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
2	NAG	A	1	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	2	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C4-C3-C2	2.03	114.38	111.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	304/316 (96%)	-0.34	1 (0%) 94 92	104, 124, 167, 245	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	GLY	2.5

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

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

### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	NAG	A	47	14/15	0.93	0.16	-0.46	124,127,132,133	0
10	MAN	A	35	11/12	0.93	0.18	-0.84	120,124,127,128	0
4	NAG	A	41	14/15	0.89	0.17	-0.85	113,114,117,118	0
10	NAG	A	30	14/15	0.81	0.28	-1.05	120,124,129,130	0
9	BMA	A	27	11/12	0.88	0.31	-	163,169,172,174	0
11	NAG	A	36	14/15	0.89	0.21	-	150,153,156,157	0
12	NAG	A	48	14/15	0.92	0.16	-	140,143,147,148	0
4	NAG	A	7	14/15	0.91	0.14	-	111,114,116,117	0
9	NAG	A	26	14/15	0.81	0.21	-	144,148,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	FUL	A	22	10/11	0.85	0.18	-	125,128,131,132	0
8	NDG	A	23	14/15	0.95	0.17	-	179,187,196,201	0
6	MAN	A	52	11/12	0.94	0.20	-	159,163,171,171	0
6	NAG	A	16	14/15	0.90	0.17	-	133,140,146,148	0
3	FUL	A	6	10/11	0.91	0.23	-	118,120,123,123	0
9	MAN	A	56	11/12	0.90	0.18	-	185,191,200,202	0
7	NAG	A	20	14/15	0.93	0.13	-	127,133,137,138	0
7	BMA	A	21	11/12	0.93	0.10	-	147,150,156,156	0
3	BMA	A	5	11/12	0.82	0.27	-	139,141,145,146	0
8	NAG	A	24	14/15	0.95	0.15	-	186,194,202,204	0
5	NDG	A	13	14/15	0.91	0.12	-	117,121,122,122	0
4	FUL	A	46	10/11	0.95	0.27	-	120,123,126,127	0
9	NDG	A	25	14/15	0.81	0.23	-	133,135,139,141	0
10	NAG	A	29	14/15	0.87	0.55	-	119,124,129,130	0
11	MAN	A	40	11/12	0.82	0.22	-	157,163,165,166	0
10	BMA	A	32	11/12	0.85	0.38	-	138,142,148,148	0
4	BMA	A	9	11/12	0.85	0.18	-	129,133,136,137	0
4	NAG	A	42	14/15	0.91	0.21	-	113,116,117,118	0
4	BMA	A	43	11/12	0.92	0.20	-	118,119,121,122	0
10	BMA	A	34	11/12	0.94	0.12	-	151,152,157,160	0
7	NAG	A	19	14/15	0.91	0.18	-	120,123,126,127	0
11	NAG	A	37	14/15	0.61	0.33	-	162,163,173,174	0
4	MAN	A	10	11/12	0.92	0.11	-	142,145,149,149	0
3	NAG	A	4	14/15	0.68	0.35	-	123,128,132,134	0
9	BMA	A	55	11/12	0.93	0.22	-	185,189,199,199	0
11	BMA	A	38	11/12	0.81	0.24	-	175,178,185,189	0
11	MAN	A	53	11/12	0.82	0.14	-	209,217,221,225	0
12	BMA	A	49	11/12	0.77	0.30	-	155,158,165,166	0
11	MAN	A	39	11/12	0.93	0.09	-	194,198,206,209	0
6	NAG	A	17	14/15	0.93	0.09	-	153,157,165,167	0
5	NAG	A	14	14/15	0.81	0.21	-	128,131,136,136	0
3	NDG	A	3	14/15	0.91	0.23	-	116,119,122,122	0
10	BMA	A	31	11/12	0.84	0.22	-	125,129,132,132	0
4	MAN	A	11	11/12	0.94	0.21	-	134,136,141,142	0
4	MAN	A	45	11/12	0.87	0.19	-	125,129,131,132	0
5	FUL	A	15	10/11	0.94	0.13	-	118,122,124,126	0
6	FUL	A	18	10/11	0.91	0.16	-	141,147,153,154	0
4	FUL	A	12	10/11	0.89	0.14	-	116,118,120,122	0
3	BMA	A	51	11/12	0.87	0.40	-	137,140,143,147	0
9	FUL	A	28	10/11	0.94	0.12	-	131,133,135,135	0
4	NAG	A	8	14/15	0.74	0.43	-	118,121,125,126	0
12	MAN	A	50	11/12	0.65	0.26	-	168,173,176,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	A	44	11/12	0.90	0.12	-	126,128,132,133	0
10	MAN	A	33	11/12	0.91	0.14	-	141,142,144,147	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1	14/15	0.89	0.16	-	149,152,154,158	0
2	NAG	A	2	14/15	0.83	0.23	-	158,161,164,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.