



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:17 PM GMT

PDB ID : 1A14  
Title : COMPLEX BETWEEN NC10 ANTI-INFLUENZA VIRUS NEURAMINIDASE SINGLE CHAIN ANTIBODY WITH A 5 RESIDUE LINKER AND INFLUENZA VIRUS NEURAMINIDASE  
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Deposited on : 1997-12-21  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

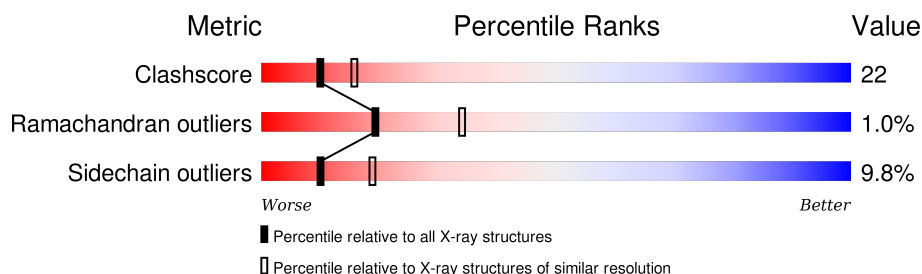
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	
2	H	120	
3	L	104	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5124 atoms, of which 212 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	388	Total	C	N	O	S	8	0	0
			3067	1914	538	592	23			

- Molecule 2 is a protein called NC10 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	120	Total	C	H	N	O	S	22	0	0
			1143	585	212	153	188	5			

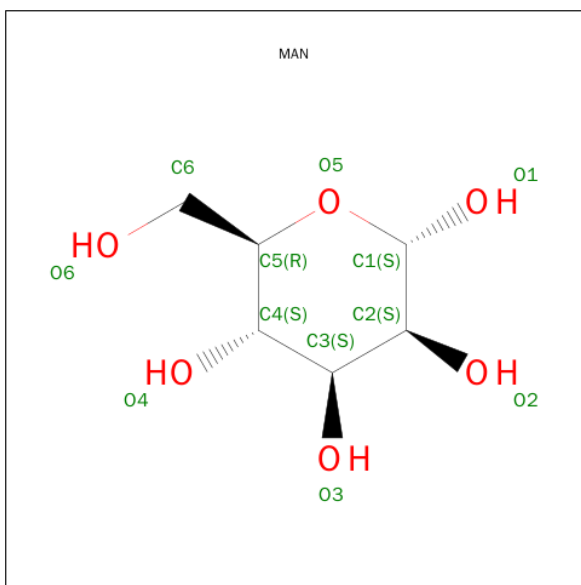
- Molecule 3 is a protein called NC10 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	104	Total	C	N	O	S	0	0	0
			802	499	129	172	2			

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

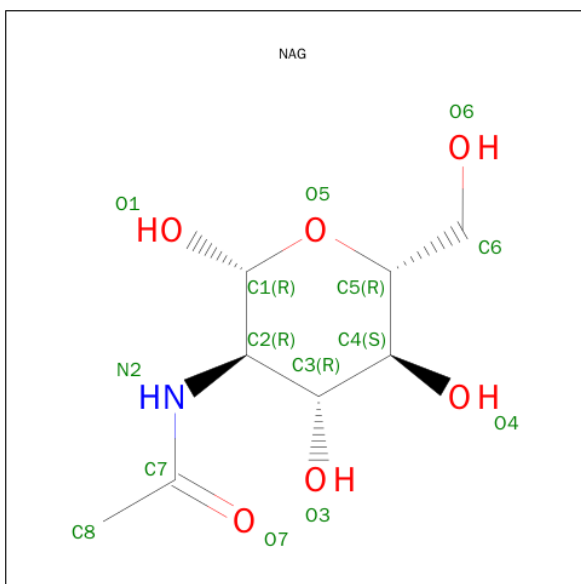
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

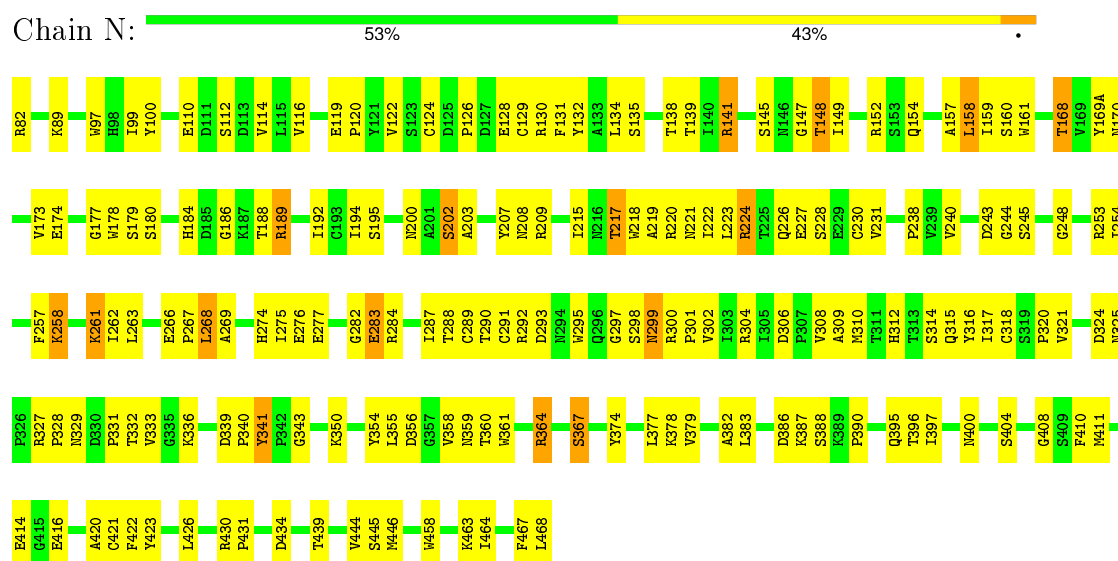
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots

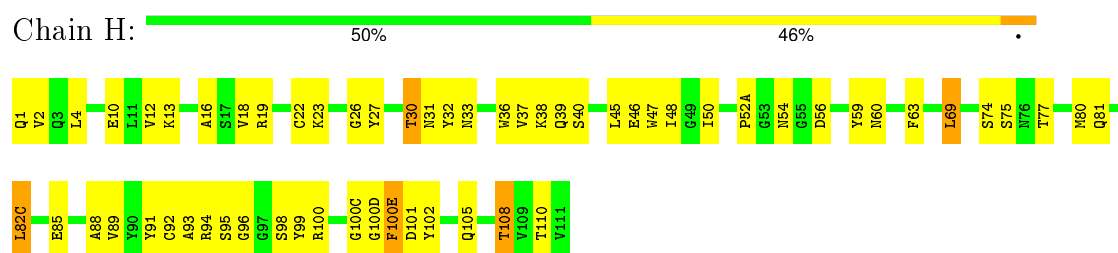
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

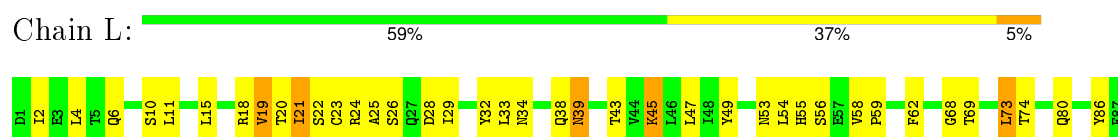
#### • Molecule 1: NEURAMINIDASE



#### • Molecule 2: NC10 FV (HEAVY CHAIN)



#### • Molecule 3: NC10 FV (LIGHT CHAIN)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.30 Å   165.30 Å   182.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	80.0 (7.00-2.50)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.200 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	N	0.73	0/3150	0.93	5/4290 (0.1%)
2	H	0.51	0/954	0.74	0/1290
3	L	0.58	0/818	0.70	0/1113
All	All	0.67	0/4922	0.86	5/6693 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	189	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	N	189	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	299	ASN	N-CA-C	-5.95	94.94	111.00
1	N	226	GLN	N-CA-C	5.34	125.43	111.00
1	N	439	THR	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	341	TYR	Sidechain
1	N	374	TYR	Sidechain

## 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	N	3067	0	2892	133	0
2	H	931	212	870	42	0
3	L	802	0	748	34	0
4	N	72	0	60	2	0
5	N	11	0	9	3	0
6	N	14	0	13	0	0
7	N	14	0	13	0	0
8	N	1	0	0	0	0
All	All	4912	212	4605	208	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 22.

All (208) 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)
3:L:39:ASN:HD21	3:L:45:LYS:HD3	1.40	0.86
1:N:283:GLU:HG2	1:N:284:ARG:HG3	1.56	0.85
1:N:168:THR:HG22	1:N:170:ASN:H	1.41	0.84
1:N:141:ARG:NH2	1:N:467:PHE:HA	1.91	0.83
1:N:159:ILE:HG22	1:N:173:VAL:HA	1.60	0.81
1:N:315:GLN:HG2	1:N:316:TYR:N	1.99	0.77
1:N:356:ASP:HB3	1:N:359:ASN:HB3	1.70	0.74
2:H:93:ALA:HB1	2:H:100(E):PHE:HB3	1.68	0.74
2:H:32:TYR:CD2	2:H:98:SER:HA	2.24	0.73
2:H:59:TYR:HE2	2:H:69:LEU:HD13	1.52	0.72
1:N:354:TYR:CE2	1:N:420:ALA:HB1	2.24	0.72
1:N:188:THR:HG23	1:N:189:ARG:N	2.05	0.72
2:H:10:GLU:HG3	2:H:18:VAL:HG21	1.72	0.71
3:L:49:TYR:O	3:L:53:ASN:HB2	1.92	0.69
3:L:21:ILE:HG23	3:L:73:LEU:HB3	1.74	0.69
1:N:379:VAL:O	1:N:382:ALA:HB2	1.92	0.69
2:H:18:VAL:HG12	2:H:82(C):LEU:HD21	1.75	0.68
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.76	0.67
1:N:277:GLU:HB3	1:N:350:LYS:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:188:THR:HG22	1:N:207:TYR:CZ	2.31	0.66
1:N:177:GLY:HA2	1:N:195:SER:HB3	1.76	0.66
2:H:19:ARG:HG2	2:H:81:GLN:HB2	1.77	0.66
1:N:315:GLN:HG2	1:N:316:TYR:H	1.59	0.66
1:N:274:HIS:HB3	1:N:293:ASP:OD1	1.95	0.66
1:N:141:ARG:HH22	1:N:467:PHE:HA	1.60	0.65
1:N:336:LYS:HE2	1:N:339:ASP:HB2	1.79	0.65
3:L:39:ASN:HD21	3:L:45:LYS:CD	2.10	0.65
1:N:328:PRO:HG3	1:N:343:GLY:HA3	1.80	0.64
3:L:86:TYR:O	3:L:101:GLY:HA2	1.97	0.64
1:N:354:TYR:CZ	1:N:420:ALA:HB1	2.33	0.64
1:N:188:THR:HG23	1:N:189:ARG:H	1.61	0.63
1:N:297:GLY:N	1:N:340:PRO:HB3	2.13	0.63
5:N:475(G):MAN:O6	5:N:475(G):MAN:C1	2.46	0.62
3:L:15:LEU:HD21	3:L:80:GLN:HG3	1.80	0.62
1:N:321:VAL:O	1:N:321:VAL:HG12	1.99	0.62
2:H:30:THR:HA	2:H:52(A):PRO:HB2	1.82	0.62
1:N:355:LEU:HD22	1:N:383:LEU:HB2	1.82	0.61
1:N:138:THR:HG21	1:N:145:SER:N	2.16	0.61
1:N:159:ILE:HD12	1:N:161:TRP:CZ3	2.36	0.60
3:L:6:GLN:HG3	3:L:21:ILE:HD11	1.83	0.60
3:L:18:ARG:HH11	3:L:18:ARG:HG2	1.65	0.60
1:N:288:THR:HG23	1:N:304:ARG:HG2	1.82	0.60
1:N:138:THR:HG22	1:N:139:THR:O	2.01	0.59
4:N:471(C):BMA:O6	5:N:475(G):MAN:O5	2.20	0.59
1:N:158:LEU:HD12	1:N:159:ILE:N	2.17	0.59
1:N:318:CYS:O	1:N:386:ASP:HA	2.03	0.59
1:N:158:LEU:HD22	1:N:180:SER:OG	2.03	0.58
1:N:157:ALA:HB1	1:N:173:VAL:HG13	1.86	0.58
1:N:231:VAL:HB	1:N:287:ILE:HG12	1.85	0.58
1:N:224:ARG:NH2	1:N:244:GLY:O	2.37	0.58
1:N:168:THR:HG23	1:N:169(A):TYR:H	1.68	0.58
1:N:316:TYR:OH	1:N:340:PRO:HG3	2.03	0.58
1:N:245:SER:OG	1:N:248:GLY:N	2.37	0.57
1:N:408:GLY:HA3	1:N:423:TYR:CE1	2.40	0.57
1:N:411:MET:HG2	1:N:420:ALA:HA	1.87	0.56
1:N:203:ALA:HB3	1:N:215:ILE:HB	1.87	0.56
2:H:39:GLN:HB2	2:H:45:LEU:CD2	2.35	0.56
1:N:321:VAL:HG21	1:N:390:PRO:HD3	1.86	0.56
2:H:94:ARG:O	2:H:100(E):PHE:HA	2.06	0.56
1:N:329:ASN:HB3	3:L:32:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:355:LEU:HA	1:N:360:THR:HG23	1.88	0.55
4:N:471(C):BMA:O6	5:N:475(G):MAN:C1	2.55	0.55
1:N:177:GLY:HA3	1:N:194:ILE:O	2.07	0.55
1:N:124:CYS:HA	1:N:129:CYS:HA	1.89	0.55
1:N:404:SER:HA	1:N:426:LEU:HD23	1.87	0.55
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.42	0.54
1:N:386:ASP:OD1	1:N:387:LYS:HG3	2.07	0.54
2:H:12:VAL:HG22	2:H:13:LYS:N	2.22	0.54
1:N:119:GLU:HB2	1:N:134:LEU:HD23	1.88	0.54
1:N:430:ARG:HD3	1:N:434:ASP:HA	1.89	0.54
1:N:328:PRO:CG	1:N:343:GLY:HA3	2.37	0.54
1:N:120:PRO:HA	1:N:132:TYR:O	2.08	0.53
1:N:358:VAL:O	1:N:378:LYS:HE3	2.08	0.53
1:N:138:THR:HG22	1:N:139:THR:N	2.24	0.53
1:N:231:VAL:O	1:N:238:PRO:HD2	2.09	0.53
3:L:55:HIS:CD2	3:L:56:SER:H	2.26	0.53
3:L:4:LEU:HD22	3:L:23:CYS:SG	2.49	0.52
2:H:100(E):PHE:N	2:H:100(E):PHE:CD1	2.75	0.52
1:N:302:VAL:N	1:N:315:GLN:O	2.40	0.52
1:N:168:THR:HG22	1:N:170:ASN:N	2.18	0.52
2:H:89:VAL:HG22	2:H:108:THR:HG23	1.92	0.52
2:H:37:VAL:HG12	2:H:38:LYS:N	2.24	0.52
3:L:39:ASN:OD1	3:L:43:THR:HB	2.10	0.51
1:N:299:ASN:OD1	1:N:341:TYR:N	2.43	0.51
1:N:126:PRO:HD3	1:N:184:HIS:CE1	2.45	0.51
1:N:361:TRP:CE2	1:N:378:LYS:HB2	2.46	0.51
3:L:59:PRO:HB2	3:L:62:PHE:HD2	1.75	0.51
1:N:131:PHE:O	1:N:160:SER:HA	2.11	0.51
1:N:82:ARG:HB2	1:N:186:GLY:O	2.11	0.51
2:H:100(E):PHE:HD1	2:H:100(E):PHE:N	2.09	0.50
1:N:408:GLY:CA	1:N:423:TYR:CE1	2.94	0.50
2:H:2:VAL:HG13	2:H:27:TYR:CD1	2.45	0.50
1:N:224:ARG:NH1	1:N:276:GLU:OE2	2.45	0.50
1:N:379:VAL:HG12	1:N:388:SER:HB2	1.93	0.49
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.52	0.49
1:N:158:LEU:HG	1:N:174:GLU:HB2	1.94	0.49
1:N:336:LYS:CE	1:N:339:ASP:HB2	2.42	0.49
1:N:321:VAL:CG2	1:N:390:PRO:HD3	2.42	0.49
1:N:228:SER:HB2	1:N:350:LYS:NZ	2.27	0.49
1:N:149:ILE:HD11	1:N:431:PRO:HG3	1.94	0.49
2:H:33:ASN:HB2	2:H:95:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:188:THR:HG21	1:N:208:ASN:HB2	1.95	0.49
1:N:297:GLY:CA	1:N:340:PRO:HB3	2.43	0.49
1:N:122:VAL:CG2	1:N:423:TYR:HB3	2.42	0.49
1:N:110:GLU:HG2	1:N:141:ARG:NH1	2.28	0.48
3:L:10:SER:HA	3:L:103:ALA:O	2.13	0.48
1:N:188:THR:CG2	1:N:189:ARG:N	2.76	0.48
1:N:128:GLU:OE2	1:N:130:ARG:HD2	2.14	0.48
3:L:34:ASN:O	3:L:88:CYS:HA	2.13	0.48
1:N:221:ASN:HB3	1:N:244:GLY:HA2	1.95	0.48
3:L:55:HIS:HB3	3:L:58:VAL:HG21	1.96	0.48
1:N:97:TRP:HB2	1:N:446:MET:HE1	1.96	0.47
1:N:258:LYS:O	1:N:261:LYS:HG2	2.13	0.47
3:L:39:ASN:H	3:L:39:ASN:ND2	2.11	0.47
2:H:18:VAL:HG22	2:H:19:ARG:N	2.28	0.47
1:N:299:ASN:OD1	1:N:299:ASN:N	2.47	0.47
1:N:410:PHE:CE1	1:N:421:CYS:HB3	2.49	0.47
1:N:306:ASP:OD2	1:N:309:ALA:HB3	2.14	0.47
2:H:39:GLN:O	2:H:88:ALA:HB1	2.15	0.47
1:N:423:TYR:HA	1:N:445:SER:HA	1.96	0.47
1:N:219:ALA:HB3	1:N:243:ASP:OD1	2.15	0.47
1:N:364:ARG:HH11	1:N:377:LEU:HD11	1.79	0.46
1:N:302:VAL:O	1:N:314:SER:HA	2.15	0.46
1:N:114:VAL:O	1:N:139:THR:HA	2.15	0.46
2:H:91:TYR:OH	3:L:38:GLN:NE2	2.49	0.46
3:L:21:ILE:HD12	3:L:22:SER:N	2.31	0.46
1:N:410:PHE:CE1	1:N:421:CYS:CB	2.99	0.46
1:N:324:ASP:O	1:N:327:ARG:HD3	2.16	0.46
3:L:19:VAL:O	3:L:74:THR:HA	2.16	0.46
3:L:55:HIS:CG	3:L:56:SER:N	2.83	0.46
1:N:254:ILE:HD13	1:N:312:HIS:CE1	2.50	0.46
2:H:31:ASN:O	2:H:98:SER:HB2	2.16	0.45
1:N:290:THR:HG23	1:N:317:ILE:HD11	1.97	0.45
1:N:268:LEU:HD22	1:N:269:ALA:N	2.31	0.45
1:N:100:TYR:HB3	1:N:445:SER:O	2.16	0.45
2:H:38:LYS:HD3	2:H:63:PHE:CE2	2.50	0.45
2:H:47:TRP:O	2:H:60:ASN:HB2	2.16	0.45
3:L:39:ASN:N	3:L:39:ASN:ND2	2.63	0.45
1:N:364:ARG:HD3	1:N:377:LEU:HD11	1.99	0.45
1:N:116:VAL:HG11	1:N:148:THR:HG21	1.99	0.45
3:L:18:ARG:NH1	3:L:18:ARG:HG2	2.31	0.44
2:H:59:TYR:CE2	2:H:69:LEU:HD13	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:188:THR:CG2	1:N:207:TYR:CZ	2.99	0.44
1:N:396:THR:C	1:N:397:ILE:HD12	2.37	0.44
1:N:275:ILE:HD13	1:N:301:PRO:CG	2.47	0.44
2:H:85:GLU:N	2:H:85:GLU:CD	2.71	0.44
3:L:45:LYS:HB3	3:L:45:LYS:HE3	1.57	0.44
2:H:18:VAL:CG2	2:H:19:ARG:N	2.80	0.44
1:N:266:GLU:HA	1:N:267:PRO:HD2	1.75	0.44
1:N:174:GLU:HA	1:N:174:GLU:OE1	2.18	0.44
1:N:463:LYS:HD2	1:N:463:LYS:N	2.33	0.44
2:H:36:TRP:CZ3	2:H:92:CYS:HB3	2.53	0.44
2:H:48:ILE:HG23	2:H:63:PHE:CB	2.47	0.44
1:N:411:MET:CG	1:N:420:ALA:HA	2.48	0.44
3:L:47:LEU:HD23	3:L:58:VAL:HG13	2.00	0.44
1:N:179:SER:HB3	1:N:194:ILE:HB	1.99	0.43
1:N:227:GLU:O	1:N:350:LYS:HE2	2.18	0.43
3:L:54:LEU:HA	3:L:54:LEU:HD12	1.75	0.43
2:H:54:ASN:OD1	2:H:56:ASP:HB2	2.17	0.43
1:N:152:ARG:HG2	1:N:178:TRP:HB2	2.00	0.43
1:N:329:ASN:HB3	3:L:32:TYR:OH	2.18	0.43
2:H:101:ASP:O	2:H:102:TYR:CD1	2.71	0.43
1:N:158:LEU:C	1:N:158:LEU:HD12	2.39	0.43
3:L:59:PRO:HB2	3:L:62:PHE:CD2	2.53	0.43
2:H:23:LYS:HG3	2:H:77:THR:HG22	1.99	0.43
1:N:194:ILE:HA	1:N:202:SER:O	2.19	0.43
1:N:149:ILE:HD12	1:N:430:ARG:HB3	2.00	0.43
1:N:227:GLU:OE1	1:N:227:GLU:HA	2.19	0.43
1:N:228:SER:HB2	1:N:350:LYS:CE	2.49	0.43
2:H:37:VAL:HG13	2:H:46:GLU:O	2.19	0.43
1:N:261:LYS:HB3	1:N:261:LYS:HE3	1.83	0.43
3:L:20:THR:HA	3:L:73:LEU:O	2.19	0.42
1:N:400:ASN:ND2	2:H:99:TYR:CG	2.87	0.42
1:N:110:GLU:HA	1:N:467:PHE:CE1	2.54	0.42
1:N:177:GLY:HA2	1:N:195:SER:CB	2.44	0.42
1:N:194:ILE:HG21	1:N:223:LEU:O	2.20	0.42
1:N:263:LEU:HD12	1:N:310:MET:CE	2.48	0.42
2:H:2:VAL:HG13	2:H:27:TYR:HD1	1.83	0.42
1:N:325:ASN:ND2	1:N:367:SER:O	2.52	0.42
1:N:355:LEU:HD23	1:N:360:THR:CG2	2.50	0.42
2:H:96:GLY:N	2:H:100(D):GLY:O	2.51	0.42
1:N:397:ILE:N	1:N:397:ILE:HD12	2.34	0.42
2:H:1:GLN:O	2:H:26:GLY:HA3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:SER:O	2:H:77:THR:HG23	2.20	0.41
3:L:58:VAL:HA	3:L:59:PRO:HD3	1.80	0.41
1:N:422:PHE:CZ	1:N:446:MET:HB2	2.54	0.41
3:L:25:ALA:HB2	3:L:29:ILE:HD13	2.02	0.41
2:H:12:VAL:CG2	2:H:13:LYS:N	2.83	0.41
1:N:444:VAL:HG21	1:N:458:TRP:CB	2.51	0.41
1:N:320:PRO:HD2	1:N:388:SER:O	2.20	0.41
2:H:23:LYS:HA	2:H:77:THR:HG22	2.02	0.41
1:N:217:THR:OG1	1:N:220:ARG:HA	2.21	0.41
3:L:49:TYR:CE1	3:L:53:ASN:HB3	2.56	0.41
3:L:55:HIS:HB3	3:L:58:VAL:CG2	2.50	0.41
1:N:320:PRO:O	1:N:331:PRO:HD2	2.20	0.41
1:N:180:SER:HB2	1:N:192:ILE:O	2.21	0.41
1:N:147:GLY:O	1:N:149:ILE:N	2.54	0.41
3:L:2:ILE:HA	3:L:26:SER:OG	2.21	0.41
1:N:291:CYS:O	1:N:300:ARG:HD3	2.21	0.41
1:N:218:TRP:CE2	1:N:253:ARG:HD2	2.56	0.41
1:N:275:ILE:HD13	1:N:301:PRO:HG3	2.03	0.40
2:H:96:GLY:HA3	2:H:100(C):GLY:O	2.22	0.40
1:N:257:PHE:CE1	1:N:262:ILE:HG12	2.56	0.40
1:N:289:CYS:O	1:N:302:VAL:HA	2.21	0.40
1:N:444:VAL:HG21	1:N:458:TRP:HB2	2.04	0.40
1:N:135:SER:HB2	1:N:159:ILE:HG12	2.02	0.40
1:N:263:LEU:HD12	1:N:310:MET:HE2	2.02	0.40
1:N:231:VAL:HG11	1:N:282:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	386/388 (100%)	354 (92%)	29 (8%)	3 (1%)	24 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	118/120 (98%)	104 (88%)	13 (11%)	1 (1%)	24	41
3	L	102/104 (98%)	92 (90%)	8 (8%)	2 (2%)	9	15
All	All	606/612 (99%)	550 (91%)	50 (8%)	6 (1%)	19	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	148	THR
3	L	28	ASP
1	N	295	TRP
1	N	222	ILE
2	H	16	ALA
3	L	68	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	N	341/341 (100%)	311 (91%)	30 (9%)	12	23
2	H	98/98 (100%)	86 (88%)	12 (12%)	6	11
3	L	91/91 (100%)	81 (89%)	10 (11%)	8	14
All	All	530/530 (100%)	478 (90%)	52 (10%)	10	19

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	89	LYS
1	N	99	ILE
1	N	112	SER
1	N	141	ARG
1	N	154	GLN
1	N	158	LEU
1	N	168	THR
1	N	200	ASN

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Mol	Chain	Res	Type
1	N	202	SER
1	N	209	ARG
1	N	217	THR
1	N	224	ARG
1	N	230	CYS
1	N	240	VAL
1	N	258	LYS
1	N	261	LYS
1	N	268	LEU
1	N	283	GLU
1	N	292	ARG
1	N	298	SER
1	N	308	VAL
1	N	332	THR
1	N	333	VAL
1	N	364	ARG
1	N	367	SER
1	N	395	GLN
1	N	414	GLU
1	N	416	GLU
1	N	464	ILE
1	N	468	LEU
2	H	30	THR
2	H	40	SER
2	H	50	ILE
2	H	69	LEU
2	H	74	SER
2	H	80	MET
2	H	82(C)	LEU
2	H	100	ARG
2	H	100(E)	PHE
2	H	105	GLN
2	H	108	THR
2	H	110	THR
3	L	11	LEU
3	L	19	VAL
3	L	21	ILE
3	L	24	ARG
3	L	33	LEU
3	L	39	ASN
3	L	45	LYS
3	L	69	THR

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Mol	Chain	Res	Type
3	L	73	LEU
3	L	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	338	ASN
1	N	345	ASN
2	H	31	ASN
2	H	39	GLN
2	H	76	ASN
3	L	38	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 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	NAG	N	469(A)	1,4	14,14,15	1.52	3 (21%)	15,19,21	2.61	5 (33%)
4	NAG	N	470(B)	4	14,14,15	1.46	3 (21%)	15,19,21	1.71	3 (20%)
4	BMA	N	471(C)	4	11,11,12	2.50	3 (27%)	14,15,17	1.74	3 (21%)
4	MAN	N	472(D)	4	11,11,12	2.60	5 (45%)	14,15,17	1.42	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	N	473(E)	4	11,11,12	1.71	3 (27%)	14,15,17	2.33	4 (28%)
4	MAN	N	474(F)	4	11,11,12	1.44	2 (18%)	14,15,17	2.04	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	N	469(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	470(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	N	471(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	472(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	473(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	474(F)	4	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	472(D)	MAN	C2-C3	-6.12	1.44	1.52
4	N	471(C)	BMA	O3-C3	-5.65	1.29	1.43
4	N	471(C)	BMA	C2-C3	-3.36	1.47	1.52
4	N	474(F)	MAN	C1-C2	-3.26	1.44	1.52
4	N	472(D)	MAN	O3-C3	-3.24	1.35	1.43
4	N	470(B)	NAG	O5-C1	-2.56	1.39	1.43
4	N	473(E)	MAN	C2-C3	-2.30	1.49	1.52
4	N	472(D)	MAN	C4-C5	-2.17	1.48	1.53
4	N	474(F)	MAN	C4-C5	-2.14	1.48	1.53
4	N	469(A)	NAG	C1-C2	-2.07	1.49	1.52
4	N	470(B)	NAG	C4-C3	2.05	1.57	1.52
4	N	473(E)	MAN	O5-C1	2.13	1.47	1.43
4	N	469(A)	NAG	O4-C4	2.35	1.48	1.43
4	N	472(D)	MAN	C1-C2	2.63	1.58	1.52
4	N	472(D)	MAN	O5-C5	2.84	1.49	1.43
4	N	470(B)	NAG	O5-C5	3.01	1.50	1.43
4	N	469(A)	NAG	C4-C5	3.45	1.60	1.53
4	N	473(E)	MAN	C4-C3	3.52	1.61	1.52
4	N	471(C)	BMA	O5-C5	4.88	1.54	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	469(A)	NAG	C8-C7-N2	-5.93	104.75	116.11
4	N	469(A)	NAG	C3-C2-N2	-3.86	101.31	110.56
4	N	470(B)	NAG	O3-C3-C2	-3.84	101.50	109.11
4	N	471(C)	BMA	C6-C5-C4	-3.60	104.14	113.02
4	N	473(E)	MAN	C3-C4-C5	-2.88	105.19	110.20
4	N	472(D)	MAN	O2-C2-C1	-2.87	103.45	109.21
4	N	470(B)	NAG	C1-O5-C5	-2.78	108.72	112.25
4	N	474(F)	MAN	C2-C3-C4	-2.50	106.80	111.04
4	N	471(C)	BMA	O3-C3-C2	-2.27	105.90	110.00
4	N	469(A)	NAG	C3-C4-C5	-2.18	106.40	110.20
4	N	472(D)	MAN	C6-C5-C4	2.14	118.29	113.02
4	N	473(E)	MAN	O4-C4-C3	2.21	115.31	110.34
4	N	473(E)	MAN	O6-C6-C5	2.35	119.10	111.33
4	N	470(B)	NAG	O4-C4-C3	3.00	117.09	110.34
4	N	469(A)	NAG	C2-N2-C7	3.27	127.23	123.04
4	N	471(C)	BMA	O5-C5-C6	3.34	114.57	107.35
4	N	469(A)	NAG	O7-C7-C8	5.06	131.35	122.06
4	N	473(E)	MAN	C1-O5-C5	6.51	120.51	112.25
4	N	474(F)	MAN	C1-O5-C5	6.64	120.68	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	471(C)	BMA	2	0

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	N	475(G)	-	11,11,12	2.44	5 (45%)	14,15,17	3.02	9 (64%)
6	NAG	N	476(A)	1	14,14,15	1.66	3 (21%)	15,19,21	1.44	3 (20%)
7	NDG	N	477(A)	1	14,14,15	2.95	6 (42%)	15,19,21	2.41	5 (33%)

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	MAN	N	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	N	476(A)	1	-	0/6/23/26	0/1/1/1
7	NDG	N	477(A)	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(G)	MAN	O5-C5	-3.11	1.36	1.43
5	N	475(G)	MAN	O4-C4	-2.85	1.36	1.43
7	N	477(A)	NDG	C3-C2	-2.10	1.47	1.52
5	N	475(G)	MAN	C6-C5	2.25	1.60	1.51
7	N	477(A)	NDG	C4-C5	2.83	1.59	1.53
7	N	477(A)	NDG	C4-C3	2.84	1.59	1.52
6	N	476(A)	NAG	C3-C2	2.98	1.59	1.52
6	N	476(A)	NAG	C4-C3	3.14	1.60	1.52
6	N	476(A)	NAG	C4-C5	3.35	1.60	1.53
5	N	475(G)	MAN	C1-C2	4.05	1.61	1.52
7	N	477(A)	NDG	C8-C7	4.54	1.59	1.50
5	N	475(G)	MAN	O5-C1	4.68	1.51	1.43
7	N	477(A)	NDG	O-C1	5.26	1.52	1.43
7	N	477(A)	NDG	C1-C2	6.99	1.62	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(G)	MAN	O4-C4-C3	-4.67	99.83	110.34
7	N	477(A)	NDG	C4-C3-C2	-4.26	104.61	111.23
7	N	477(A)	NDG	C3-C2-N2	-3.15	103.01	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	476(A)	NAG	C2-N2-C7	-2.84	119.39	123.04
7	N	477(A)	NDG	C2-N2-C7	-2.38	119.98	123.04
5	N	475(G)	MAN	O2-C2-C3	-2.35	105.40	110.12
5	N	475(G)	MAN	O4-C4-C5	-2.27	103.22	109.24
6	N	476(A)	NAG	O5-C5-C6	-2.27	102.44	107.35
6	N	476(A)	NAG	C4-C3-C2	-2.04	108.06	111.23
5	N	475(G)	MAN	C2-C3-C4	-2.02	107.61	111.04
5	N	475(G)	MAN	C1-O5-C5	-2.02	109.69	112.25
5	N	475(G)	MAN	O5-C1-C2	2.77	115.35	110.86
7	N	477(A)	NDG	O3-C3-C4	3.31	117.80	110.34
5	N	475(G)	MAN	C6-C5-C4	3.89	122.60	113.02
5	N	475(G)	MAN	O2-C2-C1	5.05	119.33	109.21
7	N	477(A)	NDG	C1-O-C5	5.52	119.26	112.25
5	N	475(G)	MAN	C3-C4-C5	5.90	120.48	110.20

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
5	N	475(G)	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.