



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 09:50 PM EDT

PDB ID : 3D2U  
Title : Structure of UL18, a Peptide-Binding Viral MHC Mimic, Bound to a Host Inhibitory Receptor  
Authors : Yang, Z.; Bjorkman, P.J.  
Deposited on : unknown  
Resolution : 2.21 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

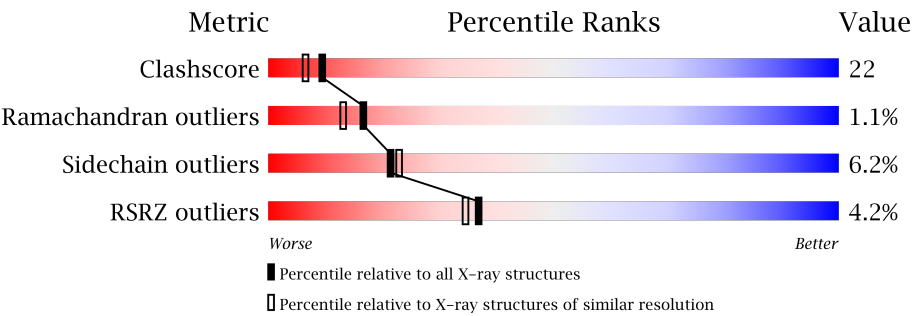
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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	281	<div><div>3%</div><div>64%</div><div>29%</div><div>5%</div><div>.</div></div>
1	E	281	<div><div>4%</div><div>69%</div><div>26%</div><div>.</div><div>.</div></div>
2	B	99	<div><div>2%</div><div>74%</div><div>26%</div></div>
2	F	99	<div><div>85%</div><div>12%</div><div>.</div></div>
3	D	198	<div><div>9%</div><div>60%</div><div>27%</div><div>.</div><div>.</div><div>8%</div></div>
3	H	198	<div><div>2%</div><div>71%</div><div>20%</div><div>.</div><div>7%</div></div>
4	C	9	<div><div>33%</div><div>56%</div><div>33%</div><div>11%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	9	

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
5	NAG	A	810	-	-	X	-
5	NAG	A	811	-	-	X	-
5	NAG	A	831	-	-	X	X
5	NAG	E	831	-	-	X	-
6	MAN	A	812	-	-	X	-
7	BMA	A	813	-	-	X	-
8	FUC	A	814	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9681 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 UL18 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	4	0	0
			2227	1412	372	434	9			
1	E	279	Total	C	N	O	S	8	0	0
			2209	1402	368	430	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	147	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	186	PRO	THR	VARIANT	UNP Q4A1U8
A	220	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	259	SER	CYS	ENGINEERED	UNP Q4A1U8
E	36	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	147	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	186	PRO	THR	VARIANT	UNP Q4A1U8
E	220	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	259	SER	CYS	ENGINEERED	UNP Q4A1U8

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			825	525	139	158	3			
2	F	99	Total	C	N	O	S	0	0	0
			825	525	139	158	3			

- Molecule 3 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	182	Total	C	N	O	S	0	0	0
			1418	904	238	270	6			
3	H	185	Total	C	N	O	S	4	0	0
			1443	920	243	274	6			

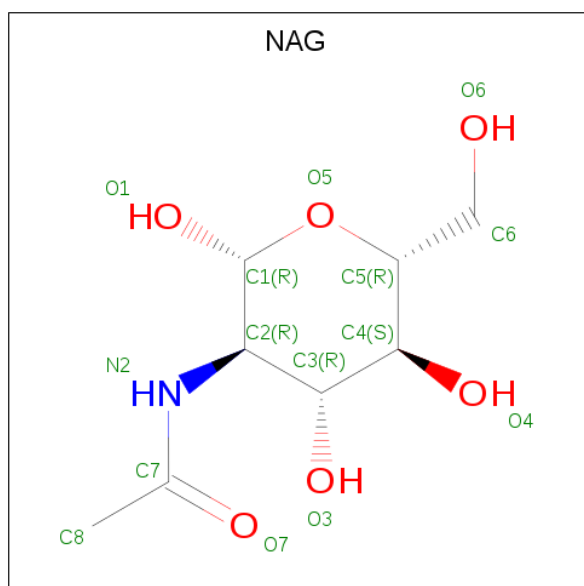
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	45	PRO	LEU	VARIANT	UNP Q8NHL6
D	119	THR	ILE	VARIANT	UNP Q8NHL6
D	132	ILE	SER	VARIANT	UNP Q8NHL6
H	45	PRO	LEU	VARIANT	UNP Q8NHL6
H	119	THR	ILE	VARIANT	UNP Q8NHL6
H	132	ILE	SER	VARIANT	UNP Q8NHL6

- Molecule 4 is a protein called Actin.

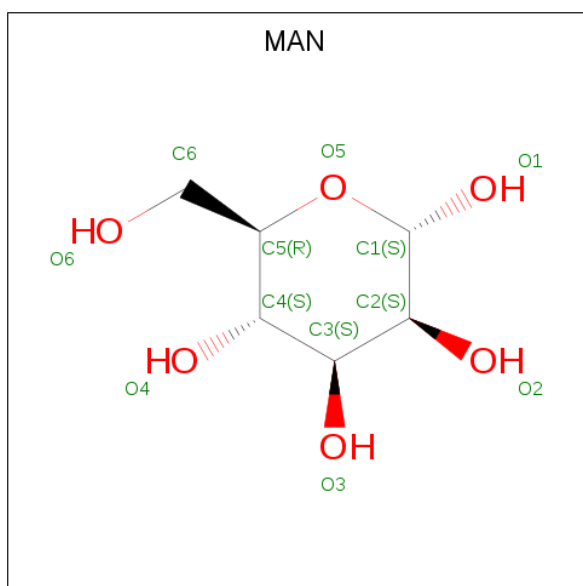
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	0	0	0
			71	47	14	10			
4	C	9	Total	C	N	O	0	0	0
			71	47	14	10			

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



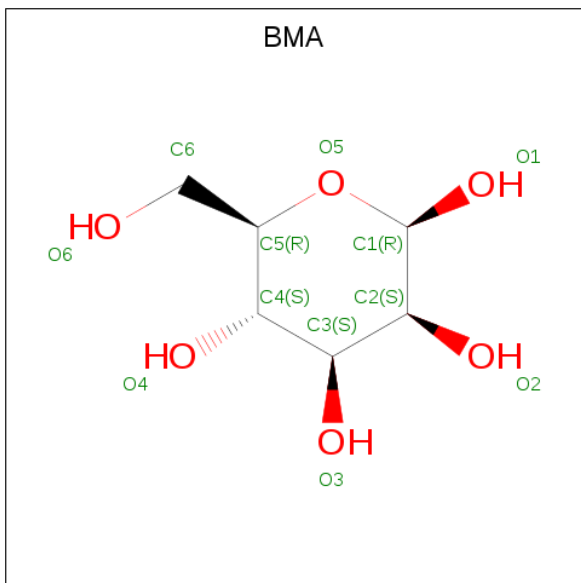
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		

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



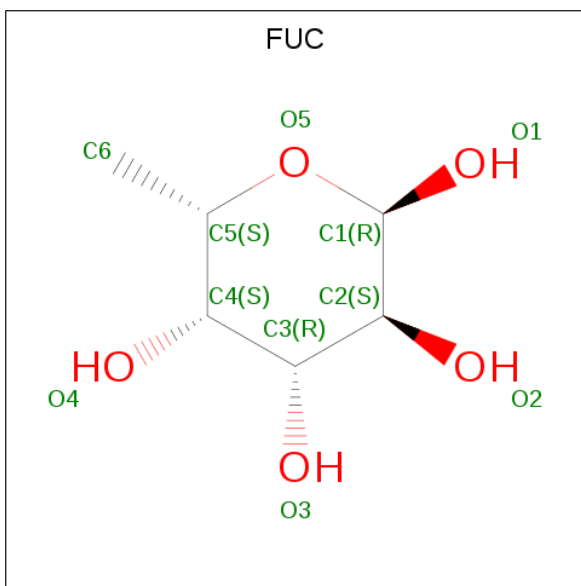
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



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

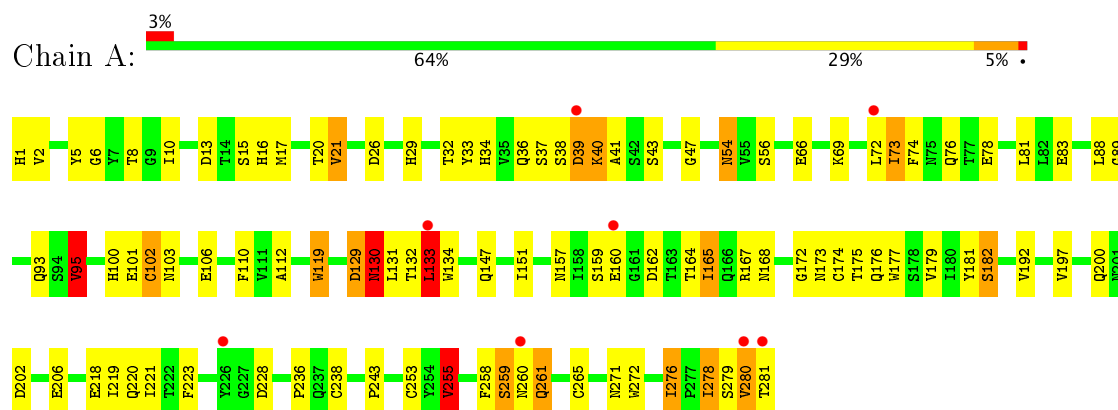
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	90	Total	O	0	0
			90	90		
9	B	48	Total	O	0	0
			48	48		
9	D	46	Total	O	0	0
			46	46		
9	E	62	Total	O	0	0
			62	62		
9	F	58	Total	O	0	0
			58	58		
9	H	58	Total	O	0	0
			58	58		

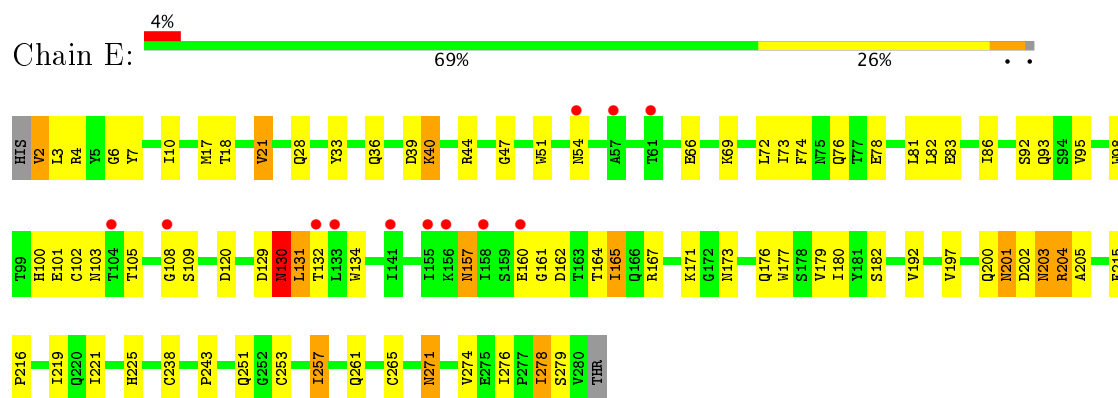
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

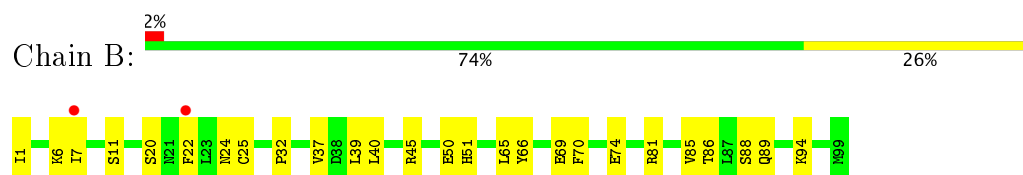
#### • Molecule 1: UL18 protein



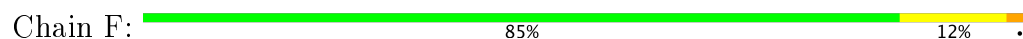
#### • Molecule 1: UL18 protein



#### • Molecule 2: Beta-2-microglobulin

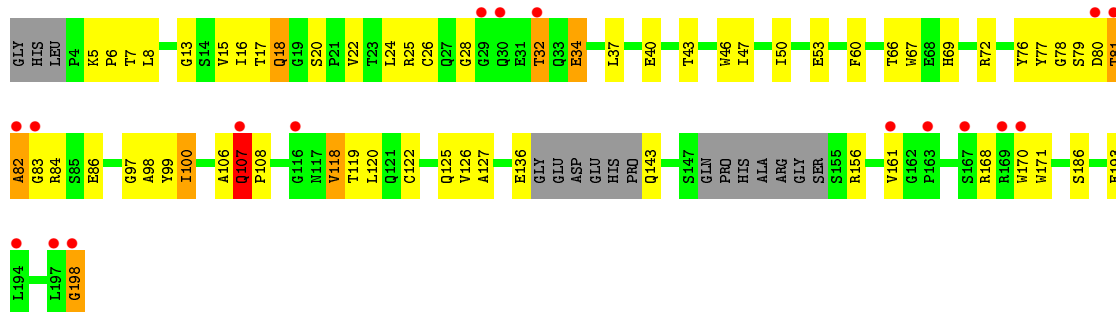


#### • Molecule 2: Beta-2-microglobulin

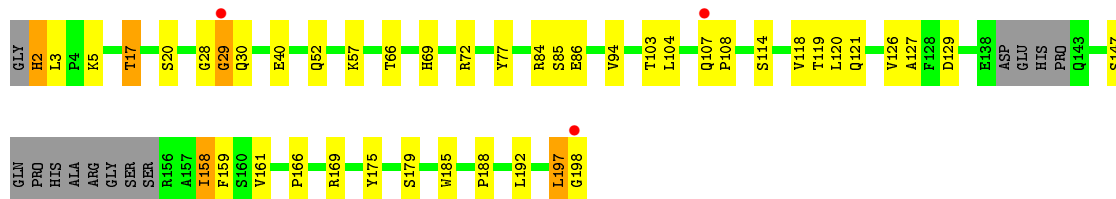




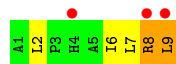
- Molecule 3: Leukocyte immunoglobulin-like receptor subfamily B member 1



- Molecule 3: Leukocyte immunoglobulin-like receptor subfamily B member 1



- Molecule 4: Actin



- Molecule 4: Actin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.37Å 98.11Å 172.15Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	47.46 – 2.21 47.46 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.46-2.21) 94.2 (47.46-2.21)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.259 0.236 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	A	0.48	0/2289	0.83	8/3120 (0.3%)
1	E	0.45	0/2270	0.76	3/3095 (0.1%)
2	B	0.43	0/848	0.74	0/1148
2	F	0.49	0/848	0.74	0/1148
3	D	0.45	0/1458	0.83	1/1988 (0.1%)
3	H	0.42	0/1484	0.80	1/2024 (0.0%)
4	C	0.49	0/72	1.01	0/96
4	G	0.46	0/72	0.88	0/96
All	All	0.46	0/9341	0.80	13/12715 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	30	GLN	N-CA-C	-10.30	83.19	111.00
3	D	198	GLY	N-CA-C	-6.80	96.09	113.10
1	A	174	CYS	CA-CB-SG	-6.66	102.02	114.00
1	A	255	VAL	CB-CA-C	-6.46	99.12	111.40
1	A	102	CYS	CA-CB-SG	6.35	125.43	114.00
1	A	192	VAL	N-CA-C	-6.28	94.06	111.00
1	A	47	GLY	N-CA-C	-5.93	98.28	113.10
1	A	95	VAL	CB-CA-C	-5.76	100.46	111.40
1	A	261	GLN	N-CA-C	5.66	126.27	111.00
1	E	271	ASN	N-CA-C	-5.59	95.89	111.00
1	E	192	VAL	N-CA-C	-5.46	96.25	111.00
1	E	47	GLY	N-CA-C	-5.34	99.76	113.10
1	A	133	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2227	0	2080	131	0
1	E	2209	0	2063	106	0
2	B	825	0	783	17	0
2	F	825	0	783	19	0
3	D	1418	0	1365	56	0
3	H	1443	0	1386	42	0
4	C	71	0	83	6	0
4	G	71	0	83	9	0
5	A	105	0	105	53	0
5	E	90	0	90	24	0
6	A	12	0	12	13	0
7	A	12	0	12	8	0
8	A	11	0	12	6	0
9	A	90	0	0	1	0
9	B	48	0	0	3	0
9	D	46	0	0	2	0
9	E	62	0	0	3	0
9	F	58	0	0	0	0
9	H	58	0	0	3	0
All	All	9681	0	8857	396	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 (396) 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:A:831:NAG:O4	5:A:832:NAG:H1	1.33	1.26
5:A:811:NAG:O4	6:A:812:MAN:H1	1.14	1.25
1:A:271:ASN:HD21	5:A:891:NAG:C1	1.51	1.21
1:E:164:THR:HG22	1:E:167:ARG:NH2	1.63	1.14
5:A:831:NAG:O4	5:A:832:NAG:C1	1.95	1.14
3:D:107:GLN:HA	3:D:107:GLN:HE21	0.97	1.11
6:A:812:MAN:C3	7:A:813:BMA:H1	1.81	1.10
3:D:100:ILE:HD11	3:D:126:VAL:HG21	1.29	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:LYS:HB3	3:H:86:GLU:HG3	1.35	1.08
1:A:40:LYS:HE3	1:A:74:PHE:CE2	1.91	1.05
1:A:260:ASN:HB3	1:A:261:GLN:HE21	1.21	1.05
3:D:107:GLN:HA	3:D:107:GLN:NE2	1.65	1.05
6:A:812:MAN:O3	7:A:813:BMA:H1	1.57	1.03
5:A:811:NAG:O4	6:A:812:MAN:C1	2.07	1.03
5:E:831:NAG:O4	5:E:832:NAG:O1	1.77	1.01
1:E:39:ASP:O	1:E:40:LYS:HB2	1.56	1.01
1:A:89:GLY:O	1:A:119:TRP:HZ3	1.45	0.99
1:A:157:ASN:OD1	5:A:861:NAG:H1	1.63	0.99
1:A:157:ASN:CG	5:A:861:NAG:H1	1.81	0.99
5:A:811:NAG:C4	6:A:812:MAN:H1	1.93	0.99
1:E:271:ASN:ND2	5:E:891:NAG:H1	1.78	0.97
1:E:17:MET:HE2	1:E:78:GLU:HA	1.49	0.95
5:A:811:NAG:HO4	6:A:812:MAN:H1	1.29	0.95
1:E:164:THR:HG22	1:E:167:ARG:HH22	1.27	0.95
1:A:173:ASN:ND2	5:A:871:NAG:H1	1.82	0.95
1:E:271:ASN:HD21	5:E:891:NAG:H1	1.32	0.92
1:A:271:ASN:HD21	5:A:891:NAG:H1	1.33	0.92
1:A:173:ASN:HD21	5:A:871:NAG:H1	1.33	0.91
2:F:1:ILE:HD13	2:F:2:GLN:N	1.86	0.90
1:E:157:ASN:ND2	5:E:861:NAG:H1	1.86	0.90
5:E:831:NAG:O4	5:E:832:NAG:C1	2.18	0.90
1:E:40:LYS:HE3	1:E:74:PHE:CE2	2.08	0.89
1:A:271:ASN:ND2	5:A:891:NAG:C1	2.36	0.89
1:A:40:LYS:HE3	1:A:74:PHE:HE2	1.38	0.89
5:A:831:NAG:HO4	5:A:832:NAG:C1	1.80	0.88
1:A:164:THR:HG22	1:A:167:ARG:HH12	1.37	0.88
1:A:265:CYS:HB2	1:A:278:ILE:HD12	1.54	0.87
1:E:265:CYS:HB2	1:E:278:ILE:HD12	1.55	0.87
1:A:89:GLY:O	1:A:119:TRP:CZ3	2.27	0.87
1:A:130:ASN:HD22	1:A:130:ASN:H	1.23	0.86
3:D:107:GLN:HE21	3:D:107:GLN:CA	1.85	0.85
1:E:271:ASN:ND2	5:E:891:NAG:C1	2.40	0.85
1:E:173:ASN:HD21	5:E:871:NAG:C1	1.89	0.85
1:E:82:LEU:O	1:E:86:ILE:HD13	1.76	0.84
1:A:173:ASN:ND2	5:A:871:NAG:C1	2.41	0.84
1:E:176:GLN:O	1:E:179:VAL:HG22	1.79	0.83
3:D:100:ILE:HD11	3:D:126:VAL:CG2	2.09	0.82
3:H:17:THR:HG22	3:H:20:SER:OG	1.80	0.81
5:E:831:NAG:O4	5:E:832:NAG:O5	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:812:MAN:C3	7:A:813:BMA:C1	2.58	0.80
1:A:103:ASN:CG	5:A:831:NAG:O1	2.19	0.80
1:E:17:MET:CE	1:E:78:GLU:HA	2.12	0.80
6:A:812:MAN:H3	7:A:813:BMA:C1	2.12	0.79
2:F:36:GLU:HG3	2:F:83:ASN:HB3	1.64	0.79
5:A:810:NAG:O4	5:A:811:NAG:C1	2.30	0.79
1:E:173:ASN:ND2	5:E:871:NAG:O1	2.14	0.79
1:A:271:ASN:ND2	5:A:891:NAG:H1	1.98	0.78
3:D:79:SER:N	3:D:83:GLY:O	2.16	0.78
1:E:202:ASP:OD2	3:H:84:ARG:NH1	2.18	0.77
1:E:129:ASP:C	1:E:131:LEU:H	1.89	0.76
3:H:66:THR:H	3:H:69:HIS:HD2	1.30	0.76
3:H:29:GLY:HA2	3:H:77:TYR:CE2	2.21	0.76
1:A:69:LYS:HE3	4:C:2:LEU:HB2	1.66	0.76
3:D:66:THR:H	3:D:69:HIS:HD2	1.33	0.76
1:A:260:ASN:CB	1:A:261:GLN:HE21	1.97	0.75
1:E:103:ASN:ND2	5:E:831:NAG:C1	2.49	0.75
6:A:812:MAN:H3	7:A:813:BMA:H1	1.65	0.75
1:E:160:GLU:O	1:E:164:THR:HG23	1.87	0.75
3:H:119:THR:HG22	3:H:158:ILE:HD12	1.69	0.75
1:A:17:MET:HE2	1:A:78:GLU:HA	1.67	0.74
3:D:81:THR:O	3:D:82:ALA:HB2	1.87	0.74
1:E:129:ASP:O	1:E:131:LEU:N	2.19	0.74
1:E:130:ASN:O	1:E:132:THR:HG23	1.87	0.74
1:A:40:LYS:CE	1:A:74:PHE:CD2	2.70	0.74
1:E:157:ASN:ND2	5:E:861:NAG:C1	2.50	0.73
1:A:176:GLN:O	1:A:179:VAL:HG22	1.87	0.73
1:A:40:LYS:HE3	1:A:74:PHE:CD2	2.23	0.73
3:D:28:GLY:O	3:D:32:THR:HG21	1.88	0.73
2:B:85:VAL:HG23	9:B:105:HOH:O	1.88	0.73
1:A:13:ASP:HB2	1:A:16:HIS:HB2	1.71	0.73
1:A:40:LYS:HE2	1:A:74:PHE:HD2	1.54	0.72
1:E:167:ARG:HG2	1:E:171:LYS:HE2	1.71	0.72
1:E:4:ARG:HB2	1:E:101:GLU:HG2	1.69	0.72
1:A:39:ASP:O	1:A:40:LYS:HB2	1.88	0.72
1:A:88:LEU:HD21	1:A:151:ILE:HD11	1.71	0.72
1:E:157:ASN:HD21	5:E:861:NAG:H1	1.55	0.72
3:D:13:GLY:O	3:D:16:ILE:HD11	1.89	0.71
6:A:812:MAN:O3	7:A:813:BMA:C1	2.37	0.71
5:A:810:NAG:H62	8:A:814:FUC:H2	1.70	0.71
4:C:6:ILE:H	4:C:6:ILE:HD12	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:CG	5:A:810:NAG:H1	2.11	0.71
1:E:83:GLU:HB3	9:E:912:HOH:O	1.90	0.71
1:A:20:THR:HG22	1:A:34:HIS:ND1	2.05	0.71
1:A:103:ASN:OD1	5:A:831:NAG:O1	2.07	0.70
1:A:197:VAL:HG11	1:A:279:SER:HB3	1.73	0.70
5:E:832:NAG:O1	5:E:832:NAG:C7	2.39	0.70
3:D:15:VAL:C	3:D:16:ILE:HD12	2.13	0.70
1:E:173:ASN:ND2	5:E:871:NAG:C1	2.55	0.70
1:E:202:ASP:OD1	3:H:84:ARG:NH1	2.24	0.69
1:A:130:ASN:N	1:A:130:ASN:HD22	1.90	0.69
1:A:276:ILE:H	1:A:276:ILE:HD13	1.58	0.69
6:A:812:MAN:H3	7:A:813:BMA:O1	1.93	0.68
3:H:166:PRO:HG3	3:H:198:GLY:O	1.94	0.68
3:H:147:SER:HB3	3:H:159:PHE:CE2	2.28	0.67
1:A:265:CYS:HB3	1:A:276:ILE:HD11	1.76	0.67
1:A:134:TRP:CZ2	4:C:7:LEU:HD11	2.30	0.66
1:A:17:MET:HE3	1:A:81:LEU:HB2	1.76	0.66
1:E:202:ASP:CG	3:H:84:ARG:NH1	2.49	0.66
1:E:98:TRP:HE1	4:G:6:ILE:HD13	1.61	0.65
3:D:125:GLN:HG2	9:D:213:HOH:O	1.95	0.65
1:A:76:GLN:NE2	4:C:8:ARG:HA	2.12	0.65
3:D:50:ILE:HD13	3:D:60:PHE:HD2	1.60	0.65
3:H:119:THR:CG2	3:H:158:ILE:HD12	2.27	0.65
3:D:28:GLY:O	3:D:32:THR:CG2	2.45	0.65
1:E:204:ARG:HG3	9:E:930:HOH:O	1.97	0.64
1:E:17:MET:HE1	1:E:78:GLU:O	1.98	0.64
5:A:810:NAG:C6	8:A:814:FUC:H2	2.27	0.64
1:E:108:GLY:HA3	1:E:179:VAL:HG12	1.80	0.64
1:E:6:GLY:O	1:E:21:VAL:HA	1.97	0.63
1:A:17:MET:HE1	1:A:78:GLU:O	1.98	0.63
3:D:100:ILE:HD13	3:D:100:ILE:N	2.14	0.63
2:F:1:ILE:HD13	2:F:2:GLN:H	1.58	0.63
1:A:1:HIS:HD2	1:A:26:ASP:OD2	1.81	0.63
1:E:40:LYS:HE3	1:E:74:PHE:CD2	2.33	0.63
1:E:7:TYR:OH	1:E:100:HIS:HE1	1.81	0.62
3:D:66:THR:H	3:D:69:HIS:CD2	2.17	0.62
1:E:17:MET:HE3	1:E:81:LEU:HB2	1.81	0.62
1:A:69:LYS:O	1:A:73:ILE:HD13	2.00	0.62
1:E:164:THR:CG2	1:E:167:ARG:HH22	2.07	0.62
1:A:40:LYS:HE2	1:A:74:PHE:CD2	2.33	0.62
1:E:161:GLY:O	1:E:165:ILE:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LYS:HE3	1:E:74:PHE:HE2	1.62	0.62
1:E:103:ASN:CG	5:E:831:NAG:O1	2.39	0.62
1:A:258:PHE:C	1:A:260:ASN:H	2.00	0.61
5:A:810:NAG:O4	5:A:811:NAG:H1	2.00	0.61
1:E:130:ASN:N	1:E:130:ASN:HD22	1.98	0.61
3:D:46:TRP:CZ3	3:D:50:ILE:HD11	2.35	0.61
2:F:36:GLU:CG	2:F:83:ASN:HB3	2.30	0.61
1:E:66:GLU:OE1	1:E:66:GLU:HA	2.01	0.61
3:H:66:THR:H	3:H:69:HIS:CD2	2.15	0.60
1:E:173:ASN:HD21	5:E:871:NAG:H1	1.64	0.60
1:E:73:ILE:HG12	4:G:6:ILE:HG13	1.83	0.60
1:E:103:ASN:ND2	5:E:831:NAG:O5	2.35	0.60
3:H:114:SER:HB2	3:H:197:LEU:O	2.01	0.60
3:D:107:GLN:HB3	3:D:108:PRO:CD	2.32	0.60
3:D:50:ILE:HD13	3:D:60:PHE:CD2	2.36	0.60
1:A:112:ALA:HB1	5:A:831:NAG:O7	2.01	0.60
1:E:17:MET:CE	1:E:81:LEU:HB2	2.32	0.60
1:A:76:GLN:HE21	4:C:8:ARG:HA	1.67	0.60
5:A:810:NAG:H62	8:A:814:FUC:C2	2.32	0.60
1:E:76:GLN:NE2	4:G:8:ARG:HA	2.17	0.59
1:A:8:THR:HG22	1:A:10:ILE:HD11	1.84	0.59
1:A:54:ASN:CG	5:A:810:NAG:C1	2.70	0.59
1:E:164:THR:HG22	1:E:167:ARG:HH21	1.60	0.59
3:H:114:SER:OG	3:H:166:PRO:HD3	2.03	0.59
1:A:54:ASN:N	1:A:54:ASN:HD22	2.00	0.59
1:A:221:ILE:HD12	1:A:221:ILE:N	2.18	0.59
1:A:10:ILE:N	1:A:10:ILE:HD12	2.17	0.59
2:F:7:ILE:HD12	2:F:7:ILE:N	2.18	0.58
2:B:81:ARG:HD2	9:B:107:HOH:O	2.02	0.58
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.39	0.58
1:A:129:ASP:O	1:A:131:LEU:HG	2.04	0.58
3:D:81:THR:O	3:D:82:ALA:CB	2.50	0.58
1:E:18:THR:HG22	1:E:36:GLN:HG2	1.86	0.58
1:E:66:GLU:OE1	1:E:69:LYS:HE2	2.04	0.58
1:A:112:ALA:CB	5:A:831:NAG:O7	2.52	0.58
1:A:265:CYS:O	1:A:276:ILE:HD13	2.04	0.58
2:F:1:ILE:CD1	3:H:127:ALA:N	2.67	0.57
2:B:20:SER:OG	2:B:69:GLU:OE2	2.23	0.57
2:B:7:ILE:N	2:B:7:ILE:HD12	2.20	0.57
5:A:831:NAG:O1	5:A:831:NAG:H82	2.04	0.57
4:G:6:ILE:HG22	4:G:7:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:ILE:CD1	2:F:2:GLN:O	2.52	0.57
1:E:130:ASN:H	1:E:130:ASN:HD22	1.53	0.57
1:E:54:ASN:ND2	5:E:810:NAG:O1	2.37	0.57
1:E:203:ASN:H	1:E:203:ASN:HD22	1.52	0.57
1:A:54:ASN:N	1:A:54:ASN:ND2	2.53	0.57
1:A:160:GLU:O	1:A:164:THR:HG23	2.05	0.56
1:A:17:MET:CE	1:A:81:LEU:HB2	2.35	0.56
1:E:131:LEU:HB2	1:E:167:ARG:HD3	1.86	0.56
1:E:164:THR:CG2	1:E:167:ARG:NH2	2.55	0.56
3:H:40:GLU:OE2	3:H:72:ARG:HD3	2.06	0.56
1:E:103:ASN:CG	5:E:831:NAG:C1	2.74	0.56
1:E:167:ARG:CG	1:E:171:LYS:HE2	2.35	0.56
1:A:103:ASN:ND2	5:A:831:NAG:O5	2.39	0.56
1:A:236:PRO:HA	1:A:255:VAL:HG13	1.86	0.56
1:E:131:LEU:HD12	1:E:167:ARG:HG3	1.88	0.55
1:A:130:ASN:N	1:A:130:ASN:ND2	2.53	0.55
3:D:6:PRO:HG3	3:D:76:TYR:HA	1.88	0.55
1:A:197:VAL:CG1	1:A:279:SER:HB3	2.35	0.55
1:E:28:GLN:NE2	1:E:51:TRP:HE1	2.05	0.55
5:A:810:NAG:O6	8:A:814:FUC:C1	2.55	0.55
2:B:86:THR:O	3:D:100:ILE:HD12	2.07	0.55
1:A:54:ASN:ND2	5:A:810:NAG:H1	2.22	0.54
1:E:129:ASP:C	1:E:131:LEU:N	2.60	0.54
5:A:811:NAG:C4	6:A:812:MAN:C1	2.77	0.54
3:D:67:TRP:CH2	3:D:98:ALA:HB2	2.42	0.54
1:E:215:PHE:CD1	1:E:216:PRO:HA	2.42	0.54
1:A:10:ILE:HG13	1:A:95:VAL:CG1	2.37	0.54
1:A:130:ASN:H	1:A:130:ASN:ND2	1.99	0.54
1:E:205:ALA:O	1:E:257:ILE:HD13	2.08	0.54
1:A:271:ASN:ND2	5:A:891:NAG:O5	2.38	0.54
1:A:202:ASP:CG	3:D:84:ARG:HH21	2.10	0.54
1:E:2:VAL:HG12	1:E:103:ASN:ND2	2.23	0.54
1:E:265:CYS:HB2	1:E:278:ILE:CD1	2.34	0.54
1:E:10:ILE:HD13	1:E:95:VAL:HB	1.89	0.54
3:D:16:ILE:N	3:D:16:ILE:HD12	2.23	0.53
1:E:271:ASN:HD21	5:E:891:NAG:C1	2.08	0.53
1:A:223:PHE:CE1	1:A:255:VAL:HG22	2.44	0.53
1:E:197:VAL:HG11	1:E:279:SER:HB3	1.90	0.53
1:A:258:PHE:C	1:A:260:ASN:N	2.62	0.53
1:A:54:ASN:HB3	5:A:810:NAG:O1	2.08	0.53
1:A:36:GLN:O	1:A:39:ASP:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:ND2	5:A:810:NAG:C1	2.72	0.53
1:E:157:ASN:O	1:E:157:ASN:ND2	2.42	0.53
1:A:5:TYR:HB2	1:A:100:HIS:CE1	2.43	0.53
3:D:171:TRP:CD1	3:D:193:GLU:HG2	2.44	0.53
3:H:121:GLN:HB2	3:H:158:ILE:HD11	1.91	0.53
3:H:28:GLY:O	3:H:29:GLY:O	2.26	0.53
1:E:10:ILE:HD12	1:E:93:GLN:NE2	2.24	0.52
1:A:133:LEU:HG	1:A:133:LEU:O	2.09	0.52
1:A:13:ASP:HB3	1:A:15:SER:H	1.74	0.52
1:A:157:ASN:ND2	5:A:861:NAG:H1	2.24	0.52
1:A:83:GLU:HB3	9:A:960:HOH:O	2.09	0.52
1:E:221:ILE:N	1:E:221:ILE:HD12	2.25	0.52
3:D:18:GLN:HG3	3:D:67:TRP:CZ2	2.44	0.52
1:A:173:ASN:CG	5:A:871:NAG:O1	2.49	0.51
1:A:276:ILE:N	1:A:276:ILE:HD13	2.24	0.51
5:E:891:NAG:H1	5:E:891:NAG:H82	1.92	0.51
1:A:164:THR:HG22	1:A:167:ARG:NH1	2.18	0.51
5:A:810:NAG:C4	5:A:811:NAG:HO1	2.17	0.51
1:A:10:ILE:HG13	1:A:95:VAL:HG12	1.93	0.51
3:D:100:ILE:HD13	3:D:100:ILE:H	1.75	0.51
1:E:276:ILE:CD1	1:E:278:ILE:HG13	2.41	0.51
1:E:105:THR:HG1	1:E:109:SER:HG	1.59	0.50
3:H:52:GLN:NE2	9:H:240:HOH:O	2.44	0.50
1:E:40:LYS:CE	1:E:74:PHE:CD2	2.94	0.50
1:A:41:ALA:C	1:A:43:SER:H	2.15	0.50
3:D:99:TYR:H	3:D:186:SER:HA	1.76	0.50
1:E:54:ASN:CG	5:E:810:NAG:O1	2.50	0.49
3:H:57:LYS:NZ	9:H:252:HOH:O	2.41	0.49
3:D:122:CYS:O	3:D:156:ARG:HA	2.11	0.49
2:F:1:ILE:HD11	3:H:127:ALA:N	2.26	0.49
3:D:7:THR:O	3:D:26:CYS:HA	2.12	0.49
1:A:54:ASN:H	1:A:54:ASN:ND2	2.11	0.49
3:D:13:GLY:O	3:D:16:ILE:CD1	2.61	0.49
2:F:1:ILE:HD13	2:F:2:GLN:O	2.12	0.49
3:H:119:THR:HG22	3:H:158:ILE:CD1	2.40	0.49
2:B:94:LYS:HE3	9:B:101:HOH:O	2.12	0.49
1:A:236:PRO:CA	1:A:255:VAL:HG13	2.43	0.49
1:A:73:ILE:N	1:A:73:ILE:CD1	2.76	0.49
5:A:810:NAG:O6	5:A:810:NAG:O4	2.29	0.49
1:A:93:GLN:HB2	2:B:32:PRO:HB3	1.95	0.49
1:E:197:VAL:CG1	1:E:279:SER:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:TYR:OH	1:E:100:HIS:CE1	2.64	0.49
3:H:29:GLY:CA	3:H:77:TYR:CE2	2.96	0.49
1:A:272:TRP:NE1	1:E:274:VAL:HG21	2.28	0.49
1:E:17:MET:HE3	1:E:81:LEU:CB	2.41	0.49
1:E:92:SER:OG	2:F:31:HIS:CD2	2.66	0.49
1:A:101:GLU:OE2	5:A:831:NAG:H1	2.13	0.48
1:A:157:ASN:CG	1:A:157:ASN:O	2.51	0.48
3:D:106:ALA:HA	3:D:120:LEU:HD23	1.95	0.48
3:H:147:SER:HB3	3:H:159:PHE:CZ	2.47	0.48
2:B:11:SER:HA	2:B:22:PHE:O	2.14	0.48
1:A:39:ASP:O	1:A:40:LYS:CB	2.54	0.48
1:E:134:TRP:CZ2	4:G:7:LEU:HD11	2.49	0.48
1:A:159:SER:OG	1:A:162:ASP:HB2	2.13	0.48
1:E:173:ASN:O	1:E:177:TRP:HD1	1.97	0.48
1:A:40:LYS:CE	1:A:74:PHE:CE2	2.77	0.48
1:A:265:CYS:HB3	1:A:276:ILE:CD1	2.44	0.47
1:E:276:ILE:O	1:E:276:ILE:HD12	2.14	0.47
1:A:132:THR:HG22	1:A:167:ARG:HH21	1.78	0.47
1:A:218:GLU:HA	1:A:218:GLU:OE1	2.14	0.47
1:A:165:ILE:O	1:A:165:ILE:HD12	2.15	0.47
1:A:281:THR:O	1:A:281:THR:HG22	2.14	0.47
3:H:2:HIS:HA	9:H:217:HOH:O	2.14	0.47
1:A:157:ASN:OD1	5:A:861:NAG:N2	2.47	0.47
3:D:100:ILE:H	3:D:100:ILE:CD1	2.27	0.47
1:A:37:SER:OG	1:A:78:GLU:OE1	2.28	0.47
3:H:158:ILE:HA	3:H:158:ILE:HD13	1.63	0.47
1:A:223:PHE:CD1	1:A:255:VAL:HG22	2.49	0.47
3:D:16:ILE:HG12	3:D:22:VAL:HB	1.97	0.47
1:A:265:CYS:CB	1:A:278:ILE:HD12	2.37	0.47
1:E:39:ASP:HB3	1:E:40:LYS:H	1.59	0.47
3:H:120:LEU:O	3:H:158:ILE:HD13	2.15	0.47
1:A:21:VAL:HG13	1:A:33:TYR:HB3	1.97	0.46
5:A:810:NAG:O6	8:A:814:FUC:O1	2.28	0.46
1:E:225:HIS:HE1	1:E:261:GLN:OE1	1.97	0.46
1:A:40:LYS:O	1:A:43:SER:HB3	2.15	0.46
1:A:41:ALA:C	1:A:43:SER:N	2.69	0.46
5:A:810:NAG:C4	5:A:811:NAG:O1	2.62	0.46
2:F:1:ILE:HD12	3:H:127:ALA:N	2.30	0.46
1:E:203:ASN:HD22	1:E:203:ASN:N	2.10	0.46
3:D:168:ARG:O	3:D:170:TRP:CD1	2.68	0.46
1:A:220:GLN:C	1:A:221:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:ILE:CD1	3:D:100:ILE:N	2.78	0.46
3:H:5:LYS:HB3	3:H:86:GLU:CG	2.26	0.46
3:H:175:TYR:CZ	3:H:188:PRO:HB3	2.51	0.46
1:E:76:GLN:HE22	4:G:8:ARG:HB3	1.80	0.45
3:D:107:GLN:HB2	3:D:119:THR:O	2.16	0.45
3:D:198:GLY:HA2	9:D:215:HOH:O	2.16	0.45
1:E:10:ILE:HD13	1:E:95:VAL:CG2	2.46	0.45
3:H:107:GLN:HB3	3:H:119:THR:HB	1.98	0.45
5:A:810:NAG:H62	8:A:814:FUC:O3	2.17	0.45
3:D:80:ASP:O	3:D:82:ALA:N	2.49	0.45
1:A:73:ILE:HD13	1:A:73:ILE:N	2.32	0.45
3:D:40:GLU:OE2	3:D:72:ARG:HD3	2.17	0.45
2:F:95:TRP:CZ3	2:F:97:ARG:HG2	2.52	0.45
3:H:129:ASP:N	3:H:129:ASP:OD1	2.49	0.45
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.99	0.45
2:F:10:TYR:CD1	2:F:10:TYR:N	2.84	0.45
1:A:6:GLY:O	1:A:21:VAL:HA	2.17	0.45
5:A:831:NAG:O1	5:A:831:NAG:C7	2.64	0.45
1:E:103:ASN:ND2	5:E:831:NAG:O1	2.49	0.45
1:A:8:THR:HG22	1:A:10:ILE:CD1	2.46	0.44
3:H:118:VAL:HG22	3:H:119:THR:N	2.32	0.44
1:A:1:HIS:CE1	1:A:182:SER:OG	2.70	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.44
5:A:810:NAG:C4	5:A:811:NAG:C1	2.96	0.44
2:B:51:HIS:HA	2:B:65:LEU:O	2.17	0.44
2:F:1:ILE:HD12	3:H:127:ALA:HB2	1.99	0.44
3:D:8:LEU:HA	3:D:25:ARG:O	2.18	0.44
1:A:157:ASN:CG	5:A:861:NAG:C1	2.71	0.44
1:A:200:GLN:HE22	1:A:259:SER:HB2	1.83	0.44
2:F:1:ILE:HD11	3:H:126:VAL:C	2.38	0.44
1:A:17:MET:CE	1:A:78:GLU:HA	2.42	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.43
1:E:201:ASN:HD22	1:E:201:ASN:C	2.21	0.43
1:A:13:ASP:HB2	1:A:16:HIS:CB	2.45	0.43
1:A:173:ASN:CG	5:A:871:NAG:C1	2.87	0.43
1:A:54:ASN:OD1	5:A:810:NAG:H1	2.18	0.43
3:D:34:GLU:HB2	3:D:78:GLY:H	1.83	0.43
3:H:121:GLN:HA	3:H:158:ILE:HD13	1.99	0.43
1:A:29:HIS:CE1	1:A:32:THR:OG1	2.72	0.43
3:D:50:ILE:HD13	3:D:60:PHE:HB3	1.99	0.43
1:A:260:ASN:HB3	1:A:261:GLN:NE2	2.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:SER:OG	3:D:97:GLY:O	2.27	0.43
1:E:21:VAL:HG21	4:G:2:LEU:HD21	2.01	0.43
1:E:2:VAL:HA	1:E:102:CYS:O	2.19	0.43
2:F:1:ILE:HD12	2:F:2:GLN:O	2.19	0.43
3:H:175:TYR:CE2	3:H:188:PRO:HB3	2.54	0.43
5:A:810:NAG:O4	5:A:811:NAG:O1	1.88	0.43
1:E:219:ILE:HG23	1:E:221:ILE:HD11	2.00	0.43
2:B:6:LYS:C	2:B:7:ILE:HD12	2.39	0.43
3:D:118:VAL:HG13	3:D:161:VAL:HB	1.99	0.43
3:D:17:THR:CG2	3:D:20:SER:OG	2.66	0.43
2:F:25:CYS:HB2	2:F:39:LEU:HD21	2.01	0.43
1:A:168:ASN:O	1:A:172:GLY:N	2.52	0.43
4:G:6:ILE:CG2	4:G:7:LEU:N	2.81	0.43
1:E:86:ILE:HD12	1:E:86:ILE:N	2.34	0.42
1:A:238:CYS:HA	1:A:253:CYS:HA	2.00	0.42
1:A:129:ASP:O	1:A:131:LEU:N	2.52	0.42
6:A:812:MAN:C2	7:A:813:BMA:H1	2.45	0.42
1:A:147:GLN:O	1:A:151:ILE:HG12	2.19	0.42
1:A:173:ASN:OD1	5:A:871:NAG:H82	2.20	0.42
3:H:104:LEU:HG	3:H:192:LEU:HD22	2.00	0.42
3:D:34:GLU:O	3:D:77:TYR:HA	2.19	0.42
1:E:179:VAL:HG23	1:E:180:ILE:N	2.35	0.42
1:A:202:ASP:OD1	3:D:84:ARG:NH2	2.43	0.42
5:A:831:NAG:O4	5:A:832:NAG:O1	2.34	0.42
1:E:251:GLN:HA	9:E:895:HOH:O	2.20	0.42
1:A:206:GLU:HB2	3:D:43:THR:HG21	2.01	0.42
2:B:50:GLU:HA	2:B:50:GLU:OE1	2.20	0.42
3:D:50:ILE:CD1	3:D:60:PHE:HB3	2.50	0.42
1:E:92:SER:HB3	1:E:120:ASP:OD1	2.20	0.42
1:E:219:ILE:HG23	1:E:221:ILE:CD1	2.50	0.42
1:A:66:GLU:OE1	1:A:69:LYS:HE2	2.20	0.41
2:B:1:ILE:HG12	3:D:127:ALA:HB2	2.01	0.41
3:D:47:ILE:O	3:D:50:ILE:HD12	2.20	0.41
3:H:129:ASP:OD2	3:H:179:SER:CB	2.68	0.41
3:D:78:GLY:CA	3:D:83:GLY:O	2.68	0.41
1:E:21:VAL:HG13	1:E:33:TYR:HB3	2.01	0.41
1:A:157:ASN:O	1:A:157:ASN:OD1	2.38	0.41
3:D:5:LYS:HB3	3:D:86:GLU:HB3	2.02	0.41
3:H:3:LEU:HB2	3:H:85:SER:HA	2.02	0.41
1:E:238:CYS:HA	1:E:253:CYS:HA	2.02	0.41
1:A:177:TRP:HB3	1:A:181:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HB	2:B:66:TYR:CZ	2.56	0.41
1:A:73:ILE:HA	4:C:6:ILE:HG12	2.03	0.41
3:H:77:TYR:CZ	3:H:85:SER:HB3	2.55	0.41
1:A:110:PHE:HB2	1:A:175:THR:HG21	2.03	0.41
1:A:280:VAL:O	1:A:281:THR:HB	2.20	0.41
1:A:177:TRP:O	1:A:181:TYR:CD2	2.74	0.41
3:D:24:LEU:HD12	3:D:37:LEU:HD21	2.03	0.41
1:E:103:ASN:ND2	5:E:831:NAG:H1	2.35	0.41
1:A:219:ILE:HG23	1:A:221:ILE:CD1	2.51	0.41
1:A:200:GLN:HE22	1:A:259:SER:CB	2.34	0.41
1:E:86:ILE:N	1:E:86:ILE:CD1	2.84	0.40
1:E:44:ARG:HG3	1:E:44:ARG:HH11	1.85	0.40
5:A:831:NAG:O1	5:A:831:NAG:C8	2.69	0.40
1:E:160:GLU:N	1:E:160:GLU:OE1	2.41	0.40
1:E:162:ASP:O	1:E:165:ILE:HG23	2.21	0.40
1:E:205:ALA:C	1:E:257:ILE:HD13	2.41	0.40
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.03	0.40
3:H:94:VAL:HG11	3:H:185:TRP:CD2	2.56	0.40
4:G:9:LEU:HD12	4:G:9:LEU:O	2.22	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	A	279/281 (99%)	263 (94%)	13 (5%)	3 (1%)	17	13
1	E	277/281 (99%)	253 (91%)	20 (7%)	4 (1%)	13	9
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	D	176/198 (89%)	166 (94%)	7 (4%)	3 (2%)	11	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	179/198 (90%)	174 (97%)	3 (2%)	2 (1%)	17	13
4	C	7/9 (78%)	7 (100%)	0	0	100	100
4	G	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1119/1174 (95%)	1061 (95%)	46 (4%)	12 (1%)	17	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
3	D	82	ALA
1	E	130	ASN
3	D	81	THR
1	E	40	LYS
3	H	29	GLY
3	D	107	GLN
1	E	157	ASN
1	A	129	ASP
1	A	130	ASN
1	E	131	LEU
3	H	108	PRO

### 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	242/244 (99%)	219 (90%)	23 (10%)	10	9
1	E	240/244 (98%)	226 (94%)	14 (6%)	23	26
2	B	93/94 (99%)	90 (97%)	3 (3%)	44	55
2	F	93/94 (99%)	90 (97%)	3 (3%)	44	55
3	D	156/171 (91%)	147 (94%)	9 (6%)	23	26
3	H	158/171 (92%)	151 (96%)	7 (4%)	33	39
4	C	7/7 (100%)	6 (86%)	1 (14%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	996/1032 (96%)	934 (94%)	62 (6%)	21	23

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

Mol	Chain	Res	Type
1	A	2	VAL
1	A	21	VAL
1	A	38	SER
1	A	39	ASP
1	A	54	ASN
1	A	56	SER
1	A	72	LEU
1	A	73	ILE
1	A	95	VAL
1	A	102	CYS
1	A	106	GLU
1	A	119	TRP
1	A	130	ASN
1	A	133	LEU
1	A	165	ILE
1	A	182	SER
1	A	228	ASP
1	A	243	PRO
1	A	255	VAL
1	A	259	SER
1	A	276	ILE
1	A	278	ILE
1	A	280	VAL
2	B	70	PHE
2	B	74	GLU
2	B	89	GLN
3	D	18	GLN
3	D	32	THR
3	D	34	GLU
3	D	53	GLU
3	D	100	ILE
3	D	107	GLN
3	D	118	VAL
3	D	136	GLU
3	D	143	GLN
1	E	2	VAL

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Mol	Chain	Res	Type
1	E	3	LEU
1	E	21	VAL
1	E	72	LEU
1	E	130	ASN
1	E	165	ILE
1	E	182	SER
1	E	200	GLN
1	E	201	ASN
1	E	203	ASN
1	E	204	ARG
1	E	243	PRO
1	E	257	ILE
1	E	278	ILE
2	F	1	ILE
2	F	70	PHE
2	F	83	ASN
3	H	2	HIS
3	H	17	THR
3	H	103	THR
3	H	158	ILE
3	H	161	VAL
3	H	169	ARG
3	H	197	LEU
4	G	8	ARG
4	G	9	LEU
4	C	6	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	29	HIS
1	A	54	ASN
1	A	76	GLN
1	A	220	GLN
1	A	225	HIS
1	A	261	GLN
1	A	271	ASN
2	B	2	GLN
2	B	31	HIS
2	B	89	GLN
3	D	18	GLN

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Mol	Chain	Res	Type
3	D	69	HIS
3	D	107	GLN
3	D	143	GLN
3	D	146	ASN
3	D	180	ASN
1	E	28	GLN
1	E	54	ASN
1	E	76	GLN
1	E	100	HIS
1	E	103	ASN
1	E	157	ASN
1	E	173	ASN
1	E	185	GLN
1	E	200	GLN
1	E	201	ASN
1	E	203	ASN
1	E	225	HIS
1	E	271	ASN
2	F	31	HIS
2	F	83	ASN
3	H	69	HIS
3	H	117	ASN
3	H	180	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	810	-	15,15,15	0.67	0	21,21,21	1.14	2 (9%)
5	NAG	A	811	-	15,15,15	0.65	0	21,21,21	1.38	2 (9%)
6	MAN	A	812	-	12,12,12	0.37	0	17,17,17	1.01	1 (5%)
7	BMA	A	813	-	12,12,12	0.46	0	17,17,17	0.55	0
8	FUC	A	814	-	11,11,11	0.60	0	15,16,16	1.29	2 (13%)
5	NAG	A	831	-	15,15,15	0.86	0	21,21,21	1.61	2 (9%)
5	NAG	A	832	-	15,15,15	0.72	0	21,21,21	1.99	3 (14%)
5	NAG	A	861	-	15,15,15	0.86	1 (6%)	21,21,21	2.00	3 (14%)
5	NAG	A	871	-	15,15,15	0.36	0	21,21,21	1.25	4 (19%)
5	NAG	A	891	-	15,15,15	0.69	0	21,21,21	1.58	3 (14%)
5	NAG	E	810	-	15,15,15	0.46	0	21,21,21	0.69	0
5	NAG	E	831	-	15,15,15	0.94	1 (6%)	21,21,21	1.43	2 (9%)
5	NAG	E	832	-	15,15,15	0.79	1 (6%)	21,21,21	0.89	1 (4%)
5	NAG	E	861	-	15,15,15	0.73	1 (6%)	21,21,21	0.90	1 (4%)
5	NAG	E	871	-	15,15,15	0.47	0	21,21,21	1.06	2 (9%)
5	NAG	E	891	-	15,15,15	0.52	0	21,21,21	0.92	1 (4%)

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	A	810	-	-	0/6/26/26	0/1/1/1
5	NAG	A	811	-	-	0/6/26/26	0/1/1/1
6	MAN	A	812	-	-	0/2/22/22	0/1/1/1
7	BMA	A	813	-	-	0/2/22/22	0/1/1/1
8	FUC	A	814	-	-	0/0/20/20	0/1/1/1
5	NAG	A	831	-	-	0/6/26/26	0/1/1/1
5	NAG	A	832	-	-	0/6/26/26	0/1/1/1
5	NAG	A	861	-	-	0/6/26/26	0/1/1/1
5	NAG	A	871	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	891	-	-	0/6/26/26	0/1/1/1
5	NAG	E	810	-	-	0/6/26/26	0/1/1/1
5	NAG	E	831	-	-	0/6/26/26	0/1/1/1
5	NAG	E	832	-	-	0/6/26/26	0/1/1/1
5	NAG	E	861	-	-	0/6/26/26	0/1/1/1
5	NAG	E	871	-	-	0/6/26/26	0/1/1/1
5	NAG	E	891	-	-	2/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	832	NAG	C1-C2	-2.31	1.50	1.52
5	E	831	NAG	O4-C4	-2.20	1.37	1.43
5	E	861	NAG	C1-C2	2.20	1.55	1.52
5	A	861	NAG	C1-C2	2.78	1.56	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	831	NAG	C1-C2-C3	-5.95	102.43	110.54
5	A	831	NAG	O4-C4-C3	-3.18	103.44	110.36
5	E	831	NAG	C4-C3-C2	-2.95	105.95	110.33
5	A	810	NAG	C1-C2-N2	-2.71	107.58	110.73
5	E	832	NAG	C1-C2-C3	-2.34	107.35	110.54
5	A	832	NAG	C3-C4-C5	-2.16	106.41	110.22
5	A	871	NAG	C1-C2-N2	-2.10	108.29	110.73
5	A	871	NAG	C4-C3-C2	2.09	113.43	110.33
5	E	871	NAG	C1-C2-C3	2.18	113.52	110.54
5	E	861	NAG	O5-C1-C2	2.20	111.73	109.52
5	A	810	NAG	O5-C1-C2	2.26	111.79	109.52
5	E	871	NAG	C4-C3-C2	2.34	113.80	110.33
5	A	871	NAG	C1-C2-C3	2.34	113.74	110.54
5	E	891	NAG	O5-C1-C2	2.45	111.98	109.52
8	A	814	FUC	C6-C5-C4	2.49	117.50	113.07
5	A	891	NAG	C4-C3-C2	2.67	114.29	110.33
5	A	811	NAG	C1-C2-C3	2.68	114.20	110.54
6	A	812	MAN	C4-C3-C2	2.78	115.74	110.84
5	A	871	NAG	O5-C1-C2	3.24	112.78	109.52
5	A	832	NAG	C1-C2-C3	3.45	115.25	110.54
8	A	814	FUC	C3-C4-C5	3.45	115.10	109.68
5	A	861	NAG	C4-C3-C2	3.49	115.51	110.33
5	A	891	NAG	O5-C1-C2	3.92	113.45	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	811	NAG	O5-C1-C2	4.17	113.71	109.52
5	E	831	NAG	O5-C1-C2	4.24	113.78	109.52
5	A	891	NAG	C1-C2-C3	4.30	116.41	110.54
5	A	861	NAG	O5-C1-C2	5.51	115.06	109.52
5	A	861	NAG	C1-C2-C3	5.59	118.17	110.54
5	A	832	NAG	O5-C1-C2	7.08	116.63	109.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	891	NAG	O7-C7-N2-C2
5	E	891	NAG	C1-C2-N2-C7

There are no ring outliers.

16 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	810	NAG	19	0
5	A	811	NAG	11	0
6	A	812	MAN	13	0
7	A	813	BMA	8	0
8	A	814	FUC	6	0
5	A	831	NAG	13	0
5	A	832	NAG	4	0
5	A	861	NAG	5	0
5	A	871	NAG	6	0
5	A	891	NAG	5	0
5	E	810	NAG	2	0
5	E	831	NAG	9	0
5	E	832	NAG	4	0
5	E	861	NAG	3	0
5	E	871	NAG	4	0
5	E	891	NAG	5	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 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	281/281 (100%)	0.32	8 (2%) 53 51	29, 42, 55, 61	1 (0%)
1	E	279/281 (99%)	0.37	12 (4%) 36 34	26, 42, 57, 63	2 (0%)
2	B	99/99 (100%)	0.41	2 (2%) 65 63	28, 38, 51, 56	0
2	F	99/99 (100%)	0.41	0 100 100	22, 36, 49, 55	0
3	D	182/198 (91%)	0.57	17 (9%) 9 8	32, 45, 57, 65	0
3	H	185/198 (93%)	0.25	3 (1%) 72 70	23, 37, 52, 62	1 (0%)
4	C	9/9 (100%)	1.28	3 (33%) 0 0	45, 52, 58, 61	0
4	G	9/9 (100%)	1.75	3 (33%) 0 0	48, 54, 60, 63	0
All	All	1143/1174 (97%)	0.39	48 (4%) 37 34	22, 41, 56, 65	4 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	29	GLY	4.7
1	E	108	GLY	4.6
1	A	280	VAL	4.6
1	A	281	THR	4.1
1	E	133	LEU	4.0
4	G	4	HIS	3.8
3	D	167	SER	3.7
4	G	9	LEU	3.7
1	A	39	ASP	3.4
3	D	81	THR	3.3
3	D	30	GLN	3.2
4	C	8	ARG	3.2
1	A	226	TYR	3.1
3	D	163	PRO	3.1
3	D	198	GLY	3.0
3	D	82	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	116	GLY	2.9
4	G	8	ARG	2.9
3	D	107	GLN	2.9
4	C	4	HIS	2.9
3	D	29	GLY	2.8
1	E	61	THR	2.7
3	D	80	ASP	2.7
3	H	198	GLY	2.7
4	C	6	ILE	2.7
3	D	161	VAL	2.6
1	E	104	THR	2.6
3	H	107	GLN	2.5
3	D	197	LEU	2.5
1	E	54	ASN	2.5
3	D	170	TRP	2.5
1	A	260	ASN	2.4
2	B	7	ILE	2.3
3	D	83	GLY	2.3
1	E	158	ILE	2.3
1	E	57	ALA	2.2
3	D	169	ARG	2.2
1	E	141	ILE	2.2
1	E	155	ILE	2.2
1	A	133	LEU	2.2
3	D	194	LEU	2.1
1	E	156	LYS	2.1
1	E	132	THR	2.1
2	B	22	PHE	2.1
1	A	72	LEU	2.0
1	A	160	GLU	2.0
1	E	160	GLU	2.0
3	D	32	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	NAG	A	831	15/15	0.88	0.21	4.16	41,51,71,76	0
5	NAG	E	831	15/15	0.89	0.21	1.01	43,55,62,71	0
7	BMA	A	813	12/12	0.92	0.17	0.73	34,47,56,67	0
5	NAG	A	811	15/15	0.92	0.16	-	39,50,59,59	0
5	NAG	A	871	15/15	0.81	0.29	-	50,61,74,81	0
5	NAG	E	810	15/15	0.85	0.16	-	46,57,64,64	0
5	NAG	A	861	15/15	0.73	0.31	-	52,61,73,73	0
5	NAG	A	832	15/15	0.87	0.16	-	44,54,66,75	0
5	NAG	A	810	15/15	0.88	0.18	-	37,50,69,70	0
5	NAG	E	861	15/15	0.62	0.35	-	46,63,72,74	0
5	NAG	A	891	15/15	0.71	0.34	-	46,60,71,74	0
8	FUC	A	814	11/11	0.82	0.18	-	51,55,72,74	0
6	MAN	A	812	12/12	0.93	0.19	-	39,49,72,73	0
5	NAG	E	891	15/15	0.60	0.33	-	52,59,69,71	0
5	NAG	E	871	15/15	0.76	0.40	-	55,62,78,78	0
5	NAG	E	832	15/15	0.87	0.21	-	44,55,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.