



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:03 PM GMT

PDB ID : 5ESV  
Title : Crystal Structure of Broadly Neutralizing Antibody CH03, Isolated from Donor CH0219, in Complex with Scaffolded Trimeric HIV-1 Env V1V2 Domain from the Clade C Superinfecting Strain of Donor CAP256.  
Authors : Gorman, J.; Yang, M.; Kwong, P.D.  
Deposited on : 2015-11-17  
Resolution : 3.10 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

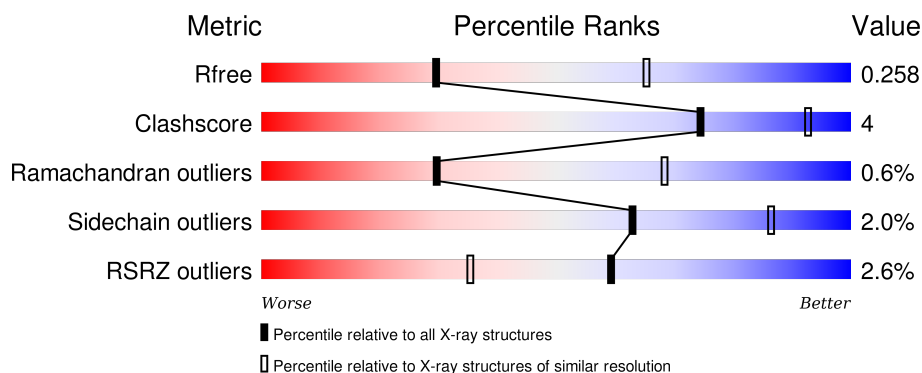
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	244	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	244	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>6%</div> </div> </div>
1	H	244	<div> <div></div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
2	B	215	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
2	D	215	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	L	215	
3	E	211	
3	F	211	
3	G	211	

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
4	NAG	E	402	-	-	-	X
4	NAG	F	401	-	-	-	X
4	NAG	F	407	X	-	-	-
4	NAG	G	403	-	-	-	X
6	MAN	E	413	-	-	-	X
6	MAN	E	414	-	-	-	X
6	MAN	G	407	-	-	-	X
6	MAN	G	413	-	-	-	X
7	ZN	E	422	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29608 atoms, of which 14564 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 CH03 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	0	0
			3429	1102	1684	300	336	7			
1	C	230	Total	C	H	N	O	S	0	0	0
			3412	1099	1673	297	336	7			
1	H	229	Total	C	H	N	O	S	0	0	0
			3415	1098	1677	299	334	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP S6BGE0
A	220	LEU	-	expression tag	UNP S6BGE0
A	221	GLU	-	expression tag	UNP S6BGE0
A	222	VAL	-	expression tag	UNP S6BGE0
A	223	LEU	-	expression tag	UNP S6BGE0
A	224	PHE	-	expression tag	UNP S6BGE0
C	219	GLY	-	expression tag	UNP S6BGE0
C	220	LEU	-	expression tag	UNP S6BGE0
C	221	GLU	-	expression tag	UNP S6BGE0
C	222	VAL	-	expression tag	UNP S6BGE0
C	223	LEU	-	expression tag	UNP S6BGE0
C	224	PHE	-	expression tag	UNP S6BGE0
H	219	GLY	-	expression tag	UNP S6BGE0
H	220	LEU	-	expression tag	UNP S6BGE0
H	221	GLU	-	expression tag	UNP S6BGE0
H	222	VAL	-	expression tag	UNP S6BGE0
H	223	LEU	-	expression tag	UNP S6BGE0
H	224	PHE	-	expression tag	UNP S6BGE0

- Molecule 2 is a protein called CH03 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	213	Total	C	H	N	O	S	0	0	0
			3241	1033	1598	283	323	4			
2	D	214	Total	C	H	N	O	S	0	0	0
			3256	1038	1604	284	326	4			
2	L	214	Total	C	H	N	O	S	0	0	0
			3256	1038	1604	284	326	4			

- Molecule 3 is a protein called 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	176	Total	C	H	N	O	S	0	0	0
			2673	833	1335	239	259	7			
3	F	179	Total	C	H	N	O	S	0	0	0
			2726	861	1356	242	260	7			
3	G	187	Total	C	H	N	O	S	0	0	0
			2831	887	1411	251	275	7			

There are 60 discrepancies between the modelled and reference sequences:

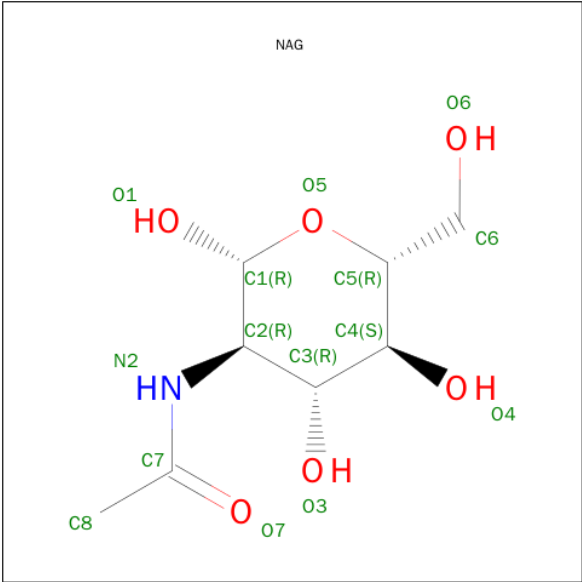
Chain	Residue	Modelled	Actual	Comment	Reference
E	111	SER	-	expression tag	UNP P44815
E	112	LEU	-	expression tag	UNP P44815
E	125	GLY	-	linker	UNP P44815
E	198	GLY	-	linker	UNP W6ICC0
E	199	GLY	-	linker	UNP W6ICC0
E	200	SER	-	linker	UNP W6ICC0
E	201	GLY	-	linker	UNP W6ICC0
E	?	-	ASP	deletion	UNP P44815
E	?	-	THR	deletion	UNP P44815
E	?	-	ASP	deletion	UNP P44815
E	?	-	MET	deletion	UNP P44815
E	?	-	GLN	deletion	UNP P44815
E	?	-	TYR	deletion	UNP P44815
E	323	GLY	-	expression tag	UNP P44815
E	324	LEU	-	expression tag	UNP P44815
E	325	GLU	-	expression tag	UNP P44815
E	326	VAL	-	expression tag	UNP P44815
E	327	LEU	-	expression tag	UNP P44815
E	328	PHE	-	expression tag	UNP P44815
E	329	GLN	-	expression tag	UNP P44815
F	111	SER	-	expression tag	UNP P44815
F	112	LEU	-	expression tag	UNP P44815

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Chain	Residue	Modelled	Actual	Comment	Reference
F	125	GLY	-	linker	UNP P44815
F	198	GLY	-	linker	UNP W6ICC0
F	199	GLY	-	linker	UNP W6ICC0
F	200	SER	-	linker	UNP W6ICC0
F	201	GLY	-	linker	UNP W6ICC0
F	?	-	ASP	deletion	UNP P44815
F	?	-	THR	deletion	UNP P44815
F	?	-	ASP	deletion	UNP P44815
F	?	-	MET	deletion	UNP P44815
F	?	-	GLN	deletion	UNP P44815
F	?	-	TYR	deletion	UNP P44815
F	323	GLY	-	expression tag	UNP P44815
F	324	LEU	-	expression tag	UNP P44815
F	325	GLU	-	expression tag	UNP P44815
F	326	VAL	-	expression tag	UNP P44815
F	327	LEU	-	expression tag	UNP P44815
F	328	PHE	-	expression tag	UNP P44815
F	329	GLN	-	expression tag	UNP P44815
G	111	SER	-	expression tag	UNP P44815
G	112	LEU	-	expression tag	UNP P44815
G	125	GLY	-	linker	UNP P44815
G	198	GLY	-	linker	UNP W6ICC0
G	199	GLY	-	linker	UNP W6ICC0
G	200	SER	-	linker	UNP W6ICC0
G	201	GLY	-	linker	UNP W6ICC0
G	?	-	ASP	deletion	UNP P44815
G	?	-	THR	deletion	UNP P44815
G	?	-	ASP	deletion	UNP P44815
G	?	-	MET	deletion	UNP P44815
G	?	-	GLN	deletion	UNP P44815
G	?	-	TYR	deletion	UNP P44815
G	323	GLY	-	expression tag	UNP P44815
G	324	LEU	-	expression tag	UNP P44815
G	325	GLU	-	expression tag	UNP P44815
G	326	VAL	-	expression tag	UNP P44815
G	327	LEU	-	expression tag	UNP P44815
G	328	PHE	-	expression tag	UNP P44815
G	329	GLN	-	expression tag	UNP P44815

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



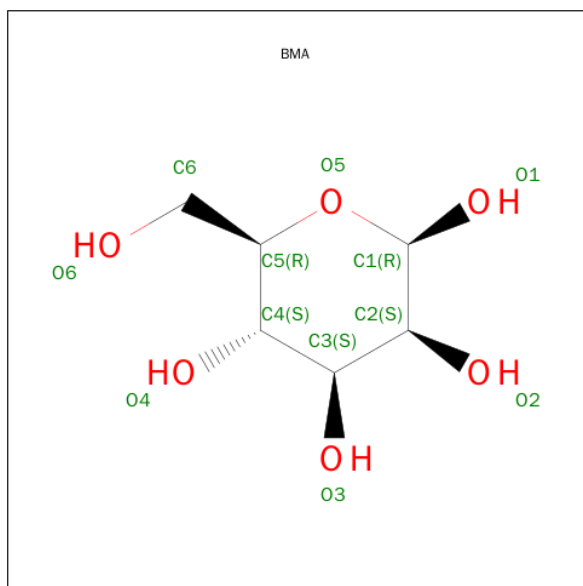
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	E	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	E	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	F	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	G	1	Total	C	H	N	O	0	0
			26	8	12	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			19	6	8	5		
5	E	1	Total	C	H	O	0	0
			17	6	6	5		

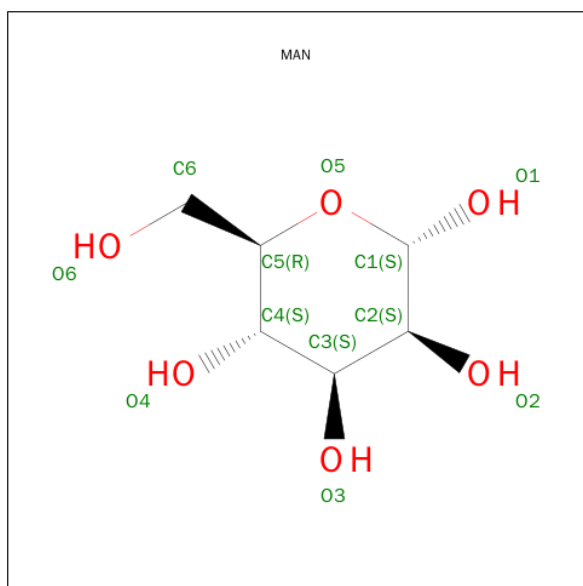
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			19	6	8	5		
5	F	1	Total	C	H	O	0	0
			21	6	10	5		
5	F	1	Total	C	H	O	0	0
			20	6	9	5		
5	F	1	Total	C	H	O	0	0
			19	6	8	5		
5	F	1	Total	C	H	O	0	0
			19	6	8	5		
5	G	1	Total	C	H	O	0	0
			19	6	8	5		
5	G	1	Total	C	H	O	0	0
			19	6	8	5		
5	G	1	Total	C	H	O	0	0
			19	6	8	5		

- Molecule 6 is 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
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	O	0	0
			19	6	8	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			19	6	8	5		
6	E	1	Total	C	H	O	0	0
			21	6	10	5		
6	E	1	Total	C	H	O	0	0
			20	6	9	5		
6	F	1	Total	C	H	O	0	0
			21	6	10	5		
6	F	1	Total	C	H	O	0	0
			19	6	8	5		
6	F	1	Total	C	H	O	0	0
			21	6	10	5		
6	F	1	Total	C	H	O	0	0
			20	6	9	5		
6	F	1	Total	C	H	O	0	0
			21	6	10	5		
6	F	1	Total	C	H	O	0	0
			19	6	8	5		
6	F	1	Total	C	H	O	0	0
			21	6	10	5		
6	F	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			20	6	9	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			19	6	8	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			19	6	8	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		
6	G	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Zn	0	0
			1	1		
7	F	1	Total	Zn	0	0
			1	1		
7	E	1	Total	Zn	0	0
			1	1		

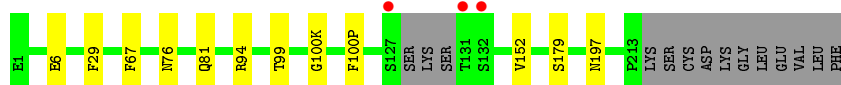
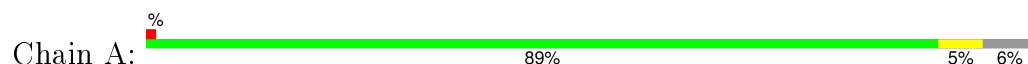
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	H	2	Total	O	0	0
			2	2		

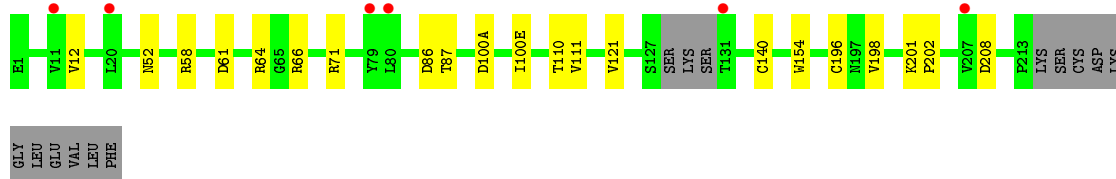
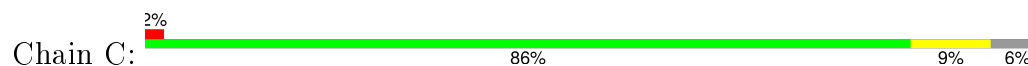
### 3 Residue-property plots [i](#)

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

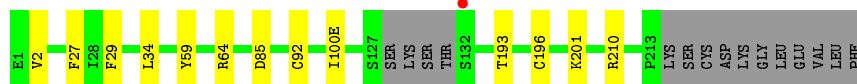
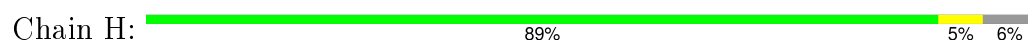
- Molecule 1: CH03 Heavy Chain



- Molecule 1: CH03 Heavy Chain



- Molecule 1: CH03 Heavy Chain

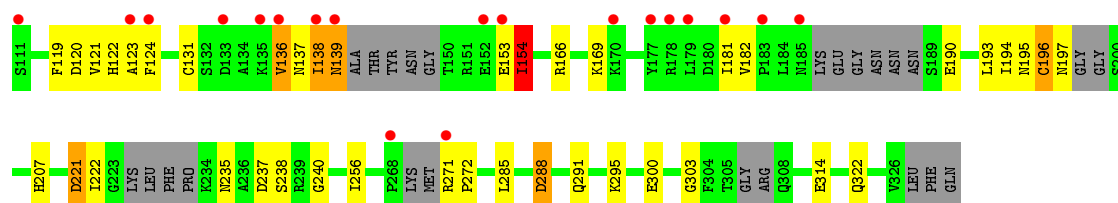


- Molecule 2: CH03 Light Chain



- Molecule 2: CH03 Light Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.69Å 98.21Å 170.63Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	41.99 – 3.10 41.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.99-3.10) 99.1 (41.99-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX (dev_2247: ???)	Depositor
R, $R_{free}$	0.208 , 0.259 0.207 , 0.258	Depositor DCC
$R_{free}$ test set	2004 reflections (4.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 44635 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	29608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.28	0/1789	0.48	0/2435
1	C	0.27	0/1783	0.46	0/2428
1	H	0.29	0/1782	0.48	0/2425
2	B	0.29	0/1682	0.47	0/2283
2	D	0.26	0/1691	0.46	0/2295
2	L	0.28	0/1691	0.46	0/2295
3	E	0.26	0/1346	0.47	0/1809
3	F	0.27	0/1381	0.48	0/1855
3	G	0.30	0/1430	0.53	0/1922
All	All	0.28	0/14575	0.48	0/19747

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
3	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	195	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	1684	1684	6	0
1	C	1739	1673	1673	11	0
1	H	1738	1677	1677	5	0
2	B	1643	1598	1598	8	0
2	D	1652	1604	1604	10	0
2	L	1652	1604	1604	8	0
3	E	1338	1335	1332	7	0
3	F	1370	1356	1373	21	0
3	G	1420	1411	1408	25	0
4	E	112	97	97	3	0
4	F	112	95	96	5	0
4	G	98	84	85	6	0
5	E	33	22	24	4	0
5	F	44	35	36	0	0
5	G	33	24	24	3	0
6	E	110	95	96	7	0
6	F	88	75	76	5	0
6	G	110	95	96	2	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
8	A	2	0	0	0	0
8	H	2	0	0	0	0
All	All	15044	14564	14583	119	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 4.

All (119) 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)
6:F:411:MAN:O2	6:F:413:MAN:H2	1.65	0.97
2:B:108:ARG:NH1	2:B:109:THR:O	2.08	0.86
1:C:52:ASN:O	1:C:71:ARG:NH2	2.21	0.72
3:G:288:ASP:OD1	3:G:288:ASP:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:117:HIS:O	3:G:295:LYS:NZ	2.27	0.68
3:F:192:ARG:NH2	3:F:196:CYS:SG	2.68	0.67
3:E:260:ASP:OD1	3:E:293:ASN:ND2	2.30	0.64
6:F:411:MAN:C2	6:F:413:MAN:H2	2.28	0.63
2:D:6:GLN:O	2:D:100:GLN:NE2	2.33	0.62
3:F:124:PHE:HB2	3:F:125:GLY:CA	2.30	0.61
2:D:92:GLY:O	5:G:410:BMA:O4	2.18	0.61
2:L:161:GLU:OE1	2:L:161:GLU:N	2.33	0.60
3:G:221:ASP:OD1	3:G:221:ASP:N	2.34	0.60
2:L:105:GLU:OE2	2:L:173:TYR:OH	2.18	0.59
4:G:403:NAG:O7	4:G:403:NAG:O3	2.17	0.58
4:G:402:NAG:H83	4:G:402:NAG:H3	1.85	0.58
4:F:405:NAG:O3	4:F:405:NAG:O7	2.18	0.58
3:F:124:PHE:HB2	3:F:125:GLY:HA2	1.85	0.58
3:G:120:ASP:OD2	3:G:122:HIS:ND1	2.36	0.58
2:B:54:ARG:NH1	2:B:62:PHE:O	2.32	0.57
2:D:1:GLU:OE2	6:F:419:MAN:O6	2.19	0.56
4:G:403:NAG:C3	4:G:403:NAG:O7	2.54	0.55
1:H:193:THR:HG23	1:H:210:ARG:NH1	2.21	0.55
3:G:237:ASP:O	3:G:240:GLY:N	2.40	0.55
3:F:124:PHE:CB	3:F:125:GLY:CA	2.85	0.54
6:G:412:MAN:O3	6:G:412:MAN:O5	2.21	0.54
6:E:414:MAN:HO2	2:L:27(A):SER:HG	1.54	0.54
2:L:167:ASP:OD1	2:L:168:SER:N	2.41	0.53
1:C:61:ASP:OD1	1:C:64:ARG:NH2	2.41	0.53
3:E:273:HIS:O	3:E:274:ILE:CG1	2.56	0.53
4:F:405:NAG:HO6	6:F:417:MAN:HO6	0.54	0.53
4:F:401:NAG:O3	4:F:401:NAG:O7	2.21	0.53
4:E:401:NAG:O3	4:E:401:NAG:O7	2.26	0.53
3:G:138:ILE:N	3:G:139:ASN:HA	2.25	0.52
3:F:126:CYS:SG	3:F:192:ARG:NH2	2.83	0.52
3:F:278:ARG:NE	3:F:292:VAL:O	2.38	0.51
3:F:190:GLU:OE1	3:F:190:GLU:N	2.44	0.51
6:G:406:MAN:O2	6:G:407:MAN:C1	2.59	0.51
5:E:410:BMA:C6	6:E:412:MAN:O2	2.59	0.50
2:L:153:ALA:O	2:L:155:GLN:NE2	2.44	0.50
3:G:153:GLU:HA	3:G:154:ILE:CB	2.43	0.49
1:A:99:THR:OG1	4:E:416:NAG:H81	2.12	0.49
2:L:21:LEU:HD22	2:L:102:THR:HG21	1.93	0.49
4:F:407:NAG:H3	4:F:407:NAG:O7	2.11	0.49
5:E:410:BMA:H61	6:E:412:MAN:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:153:GLU:HA	3:G:154:ILE:HG22	1.93	0.49
1:H:59:TYR:O	1:H:64:ARG:NH2	2.45	0.49
1:C:100(A):ASP:OD2	1:C:100(E):ILE:HG12	2.13	0.48
3:G:123:ALA:O	3:G:124:PHE:HB2	2.13	0.48
3:E:210:THR:HG22	3:E:242:LEU:HA	1.93	0.48
3:F:226:PHE:HB2	3:F:227:PRO:HD3	1.94	0.48
3:G:271:ARG:N	3:G:272:PRO:CD	2.77	0.48
3:E:211:ASP:O	3:G:295:LYS:NZ	2.47	0.47
2:B:151:ASP:OD2	2:B:189:HIS:ND1	2.47	0.47
3:G:153:GLU:HA	3:G:154:ILE:HB	1.96	0.47
3:F:225:LEU:O	3:F:226:PHE:HB2	2.14	0.47
3:F:124:PHE:HD2	3:F:311:ILE:HG22	1.79	0.47
3:G:122:HIS:CE1	3:G:207:HIS:ND1	2.83	0.47
6:E:412:MAN:H4	6:E:413:MAN:H2	1.96	0.46
1:A:6:GLU:N	1:A:6:GLU:OE1	2.45	0.46
2:L:128:GLY:HA2	2:L:183:LYS:NZ	2.31	0.46
3:F:124:PHE:CD1	3:F:125:GLY:HA3	2.51	0.46
1:C:58:ARG:NH1	2:D:94:SER:OG	2.42	0.46
2:D:21:LEU:HD23	2:D:102:THR:HB	1.98	0.46
2:D:168:SER:O	1:H:201:LYS:NZ	2.42	0.46
1:C:121:VAL:HG11	1:C:198:VAL:HG11	1.98	0.45
1:C:196:CYS:O	1:C:208:ASP:HA	2.16	0.45
1:A:152:VAL:HA	1:A:197:ASN:O	2.15	0.45
3:G:120:ASP:OD2	3:G:122:HIS:CE1	2.69	0.45
2:D:151:ASP:OD2	2:D:189:HIS:HB3	2.16	0.45
4:G:415:NAG:O3	5:G:416:BMA:O5	2.28	0.45
1:H:29:PHE:CZ	1:H:34:LEU:HD11	2.52	0.45
1:A:29:PHE:CD2	1:A:76:ASN:HA	2.52	0.45
6:E:419:MAN:H2	6:E:421:MAN:O2	2.16	0.45
1:C:66:ARG:NH1	1:C:86:ASP:OD2	2.37	0.44
3:F:124:PHE:HD2	3:F:311:ILE:CG2	2.30	0.44
3:G:196:CYS:O	3:G:197:ASN:C	2.56	0.44
4:G:403:NAG:O3	5:G:404:BMA:H2	2.18	0.44
3:F:124:PHE:HD1	3:F:125:GLY:HA3	1.82	0.44
2:B:61:ARG:NH2	2:B:82:ASP:OD2	2.44	0.44
6:F:411:MAN:C2	6:F:413:MAN:C2	2.94	0.44
3:G:288:ASP:OD1	3:G:291:GLN:NE2	2.51	0.43
6:E:412:MAN:H4	6:E:413:MAN:C2	2.48	0.43
3:G:166:ARG:O	3:G:169:LYS:NZ	2.50	0.43
2:B:150:VAL:HG12	2:B:192:TYR:CD1	2.54	0.43
1:H:2:VAL:HG23	1:H:27:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:TYR:O	2:D:192:TYR:OH	2.36	0.43
3:G:256:ILE:HG13	3:G:285:LEU:HB3	2.00	0.43
3:G:190:GLU:OE2	4:G:402:NAG:H81	2.18	0.43
4:F:401:NAG:C3	4:F:401:NAG:O7	2.66	0.43
3:G:181:ILE:HG22	3:G:193:LEU:HA	2.01	0.43
3:F:124:PHE:CZ	3:F:309:GLU:HG3	2.54	0.42
1:C:154:TRP:CH2	1:C:196:CYS:SG	3.12	0.42
3:F:124:PHE:HD1	3:F:125:GLY:N	2.18	0.42
3:G:153:GLU:HA	3:G:154:ILE:CG2	2.49	0.42
1:A:67:PHE:HA	1:A:81:GLN:O	2.19	0.42
1:C:12:VAL:O	1:C:111:VAL:HA	2.19	0.42
2:B:170:ASP:O	2:B:171:SER:HB2	2.19	0.42
3:F:114:ARG:NE	3:F:216:ALA:O	2.43	0.42
3:G:137:ASN:HB2	3:G:139:ASN:HB2	2.02	0.42
1:C:201:LYS:N	1:C:202:PRO:CD	2.82	0.42
3:G:322:GLN:N	3:G:322:GLN:OE1	2.41	0.42
5:E:410:BMA:H62	6:E:412:MAN:H2	1.70	0.41
3:G:119:PHE:HD1	3:G:314:GLU:HG2	1.85	0.41
2:D:82:ASP:O	2:D:86:TYR:OH	2.31	0.41
2:B:189:HIS:O	2:B:211:ARG:HD3	2.20	0.41
1:C:87:THR:HG23	1:C:110:THR:HA	2.03	0.41
2:D:123:GLU:N	2:D:123:GLU:OE1	2.40	0.41
4:E:404:NAG:C6	5:E:405:BMA:C1	2.99	0.41
1:A:94:ARG:O	1:A:100(P):PHE:HA	2.20	0.41
2:L:125:LEU:O	2:L:183:LYS:HD3	2.21	0.41
3:F:193:LEU:HD13	3:F:194:ILE:H	1.86	0.41
3:F:129:LEU:HB3	3:F:157:CYS:HB3	2.03	0.41
3:E:274:ILE:HG13	3:E:275:ASP:N	2.36	0.41
3:G:153:GLU:HG3	3:G:154:ILE:O	2.21	0.40
3:F:239:ARG:NH2	3:F:283:GLU:OE2	2.54	0.40
2:B:6:GLN:O	2:B:100:GLN:NE2	2.54	0.40
3:F:308:GLN:HG2	3:F:309:GLU:H	1.87	0.40
3:E:291:GLN:HA	3:F:114:ARG:HH22	1.87	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	A	226/244 (93%)	212 (94%)	13 (6%)	1 (0%)	39	75
1	C	226/244 (93%)	209 (92%)	17 (8%)	0	100	100
1	H	225/244 (92%)	212 (94%)	13 (6%)	0	100	100
2	B	211/215 (98%)	200 (95%)	11 (5%)	0	100	100
2	D	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
2	L	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	34	72
3	E	162/211 (77%)	151 (93%)	9 (6%)	2 (1%)	16	52
3	F	165/211 (78%)	149 (90%)	14 (8%)	2 (1%)	16	52
3	G	173/211 (82%)	153 (88%)	16 (9%)	4 (2%)	8	35
All	All	1812/2010 (90%)	1690 (93%)	112 (6%)	10 (1%)	30	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	124	PHE
3	F	226	PHE
3	E	274	ILE
3	E	258	ASN
3	G	154	ILE
1	A	100(K)	GLY
3	G	196	CYS
3	G	136	VAL
3	G	303	GLY
2	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	A	191/204 (94%)	190 (100%)	1 (0%)	92	96
1	C	190/204 (93%)	189 (100%)	1 (0%)	92	96
1	H	190/204 (93%)	186 (98%)	4 (2%)	61	86
2	B	182/184 (99%)	181 (100%)	1 (0%)	92	96
2	D	183/184 (100%)	182 (100%)	1 (0%)	92	96
2	L	183/184 (100%)	182 (100%)	1 (0%)	92	96
3	E	141/170 (83%)	139 (99%)	2 (1%)	74	90
3	F	144/170 (85%)	138 (96%)	6 (4%)	36	73
3	G	149/170 (88%)	135 (91%)	14 (9%)	11	39
All	All	1553/1674 (93%)	1522 (98%)	31 (2%)	63	86

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	SER
2	B	43	SER
1	C	140	CYS
2	D	33	PHE
3	E	130	ASN
3	E	274	ILE
3	F	126	CYS
3	F	133	ASP
3	F	139	ASN
3	F	193	LEU
3	F	196	CYS
3	F	300	GLU
3	G	121	VAL
3	G	131	CYS
3	G	136	VAL
3	G	138	ILE
3	G	139	ASN
3	G	154	ILE
3	G	182	VAL
3	G	194	ILE
3	G	221	ASP
3	G	222	ILE
3	G	235	ASN

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Mol	Chain	Res	Type
3	G	238	SER
3	G	288	ASP
3	G	300	GLU
1	H	85	ASP
1	H	92	CYS
1	H	100(E)	ILE
1	H	196	CYS
2	L	195	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	122	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 3 are monoatomic - leaving 61 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
4	NAG	E	401	3,4	14,14,15	0.56	0	15,19,21	0.56	0
4	NAG	E	402	4	14,14,15	0.49	0	15,19,21	0.99	1 (6%)
4	NAG	E	403	3,4	14,14,15	0.56	0	15,19,21	0.49	0
4	NAG	E	404	5,4	14,14,15	0.30	0	15,19,21	0.98	1 (6%)
5	BMA	E	405	4,6	11,11,12	1.46	2 (18%)	15,15,17	1.94	4 (26%)
6	MAN	E	406	5	11,11,12	0.85	0	15,15,17	1.61	3 (20%)
6	MAN	E	407	5	11,11,12	0.89	0	15,15,17	0.91	2 (13%)
4	NAG	E	408	3,4	14,14,15	0.42	0	15,19,21	0.26	0
4	NAG	E	409	5,4	14,14,15	0.70	1 (7%)	15,19,21	0.70	0
5	BMA	E	410	4,6	11,11,12	1.56	1 (9%)	15,15,17	1.06	0
6	MAN	E	411	5	11,11,12	0.85	1 (9%)	15,15,17	1.08	1 (6%)
6	MAN	E	412	5,6	11,11,12	2.22	3 (27%)	15,15,17	2.28	6 (40%)
6	MAN	E	413	6	11,11,12	1.54	2 (18%)	15,15,17	1.59	3 (20%)
6	MAN	E	414	6	11,11,12	1.11	1 (9%)	15,15,17	2.01	4 (26%)
4	NAG	E	415	3,4	14,14,15	0.43	0	15,19,21	0.32	0
4	NAG	E	416	5,4	14,14,15	0.65	0	15,19,21	0.47	0
5	BMA	E	417	4,6	11,11,12	0.76	1 (9%)	15,15,17	1.04	0
6	MAN	E	418	5	11,11,12	1.13	1 (9%)	15,15,17	0.79	0
6	MAN	E	419	5,6	11,11,12	1.66	2 (18%)	15,15,17	1.49	4 (26%)
6	MAN	E	420	6	11,11,12	0.98	1 (9%)	15,15,17	0.98	2 (13%)
6	MAN	E	421	6	11,11,12	1.22	0	15,15,17	1.39	1 (6%)
4	NAG	F	401	3,4	14,14,15	0.98	1 (7%)	15,19,21	0.79	1 (6%)
4	NAG	F	402	5,4	14,14,15	0.81	1 (7%)	15,19,21	1.17	1 (6%)
5	BMA	F	403	4	11,11,12	0.99	0	15,15,17	0.98	0
4	NAG	F	404	3,4	14,14,15	0.35	0	15,19,21	0.36	0
4	NAG	F	405	5,4	14,14,15	0.25	0	15,19,21	0.81	1 (6%)
5	BMA	F	406	4	11,11,12	1.60	2 (18%)	15,15,17	1.75	4 (26%)
4	NAG	F	407	3,4	14,14,15	1.78	2 (14%)	15,19,21	1.29	3 (20%)
4	NAG	F	408	5,4	14,14,15	0.40	0	15,19,21	0.54	0
5	BMA	F	409	4,6	11,11,12	0.92	1 (9%)	15,15,17	0.79	1 (6%)
6	MAN	F	410	5	11,11,12	0.75	1 (9%)	15,15,17	1.09	1 (6%)
6	MAN	F	411	5,6	11,11,12	1.24	1 (9%)	15,15,17	2.03	4 (26%)
6	MAN	F	412	6	11,11,12	1.18	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	F	413	6	11,11,12	1.14	2 (18%)	15,15,17	1.90	1 (6%)
4	NAG	F	414	3,4	14,14,15	0.25	0	15,19,21	0.58	0
4	NAG	F	415	5,4	14,14,15	0.24	0	15,19,21	0.54	0
5	BMA	F	416	4,6	11,11,12	1.11	2 (18%)	15,15,17	1.56	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	F	417	5	11,11,12	0.85	0	15,15,17	2.20	3 (20%)
6	MAN	F	418	5,6	11,11,12	1.05	1 (9%)	15,15,17	1.57	3 (20%)
6	MAN	F	419	6	11,11,12	0.88	1 (9%)	15,15,17	1.18	2 (13%)
6	MAN	F	420	6	11,11,12	1.12	1 (9%)	15,15,17	1.04	1 (6%)
4	NAG	G	401	3	14,14,15	0.65	1 (7%)	15,19,21	0.40	0
4	NAG	G	402	3,4	14,14,15	0.62	0	15,19,21	1.34	2 (13%)
4	NAG	G	403	5,4	14,14,15	0.41	0	15,19,21	1.03	2 (13%)
5	BMA	G	404	4,6	11,11,12	1.19	1 (9%)	15,15,17	1.34	3 (20%)
6	MAN	G	405	5	11,11,12	1.23	2 (18%)	15,15,17	1.58	4 (26%)
6	MAN	G	406	5,6	11,11,12	1.01	1 (9%)	15,15,17	1.25	2 (13%)
6	MAN	G	407	6	11,11,12	1.51	3 (27%)	15,15,17	1.47	4 (26%)
4	NAG	G	408	3,4	14,14,15	0.29	0	15,19,21	0.42	0
4	NAG	G	409	5,4	14,14,15	0.38	0	15,19,21	0.45	0
5	BMA	G	410	4,6	11,11,12	0.71	0	15,15,17	1.16	2 (13%)
6	MAN	G	411	5	11,11,12	1.21	1 (9%)	15,15,17	1.27	3 (20%)
6	MAN	G	412	5,6	11,11,12	0.99	1 (9%)	15,15,17	1.65	1 (6%)
6	MAN	G	413	6	11,11,12	1.28	3 (27%)	15,15,17	2.09	6 (40%)
4	NAG	G	414	3,4	14,14,15	0.28	0	15,19,21	0.31	0
4	NAG	G	415	5,4	14,14,15	0.48	0	15,19,21	0.26	0
5	BMA	G	416	4,6	11,11,12	0.82	1 (9%)	15,15,17	1.22	2 (13%)
6	MAN	G	417	5	11,11,12	0.87	1 (9%)	15,15,17	2.35	2 (13%)
6	MAN	G	418	5,6	11,11,12	1.23	2 (18%)	15,15,17	0.94	1 (6%)
6	MAN	G	419	6	11,11,12	0.89	1 (9%)	15,15,17	1.39	4 (26%)
6	MAN	G	420	6	11,11,12	0.94	0	15,15,17	1.50	2 (13%)

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	E	401	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	402	4	-	0/6/23/26	0/1/1/1
4	NAG	E	403	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	404	5,4	-	0/6/23/26	0/1/1/1
5	BMA	E	405	4,6	-	0/2/19/22	0/1/1/1
6	MAN	E	406	5	-	0/2/19/22	1/1/1/1
6	MAN	E	407	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	408	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	409	5,4	-	0/6/23/26	0/1/1/1
5	BMA	E	410	4,6	-	0/2/19/22	0/1/1/1
6	MAN	E	411	5	-	0/2/19/22	0/1/1/1
6	MAN	E	412	5,6	-	0/2/19/22	0/1/1/1
6	MAN	E	413	6	-	0/2/19/22	0/1/1/1
6	MAN	E	414	6	-	0/2/19/22	0/1/1/1
4	NAG	E	415	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	416	5,4	-	0/6/23/26	0/1/1/1
5	BMA	E	417	4,6	-	0/2/19/22	0/1/1/1
6	MAN	E	418	5	-	0/2/19/22	0/1/1/1
6	MAN	E	419	5,6	-	0/2/19/22	0/1/1/1
6	MAN	E	420	6	-	0/2/19/22	0/1/1/1
6	MAN	E	421	6	-	0/2/19/22	1/1/1/1
4	NAG	F	401	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	402	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	403	4	-	0/2/19/22	0/1/1/1
4	NAG	F	404	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	405	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	406	4	-	0/2/19/22	0/1/1/1
4	NAG	F	407	3,4	1/1/6/7	0/6/23/26	0/1/1/1
4	NAG	F	408	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	409	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	410	5	-	0/2/19/22	0/1/1/1
6	MAN	F	411	5,6	-	0/2/19/22	0/1/1/1
6	MAN	F	412	6	-	0/2/19/22	0/1/1/1
6	MAN	F	413	6	-	0/2/19/22	0/1/1/1
4	NAG	F	414	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	415	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	416	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	417	5	-	0/2/19/22	0/1/1/1
6	MAN	F	418	5,6	-	0/2/19/22	0/1/1/1
6	MAN	F	419	6	-	0/2/19/22	1/1/1/1
6	MAN	F	420	6	-	0/2/19/22	0/1/1/1
4	NAG	G	401	3	-	0/6/23/26	0/1/1/1
4	NAG	G	402	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	403	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	404	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	405	5	-	0/2/19/22	0/1/1/1
6	MAN	G	406	5,6	-	0/2/19/22	1/1/1/1
6	MAN	G	407	6	-	0/2/19/22	0/1/1/1
4	NAG	G	408	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	409	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	410	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	411	5	-	0/2/19/22	0/1/1/1
6	MAN	G	412	5,6	-	0/2/19/22	1/1/1/1
6	MAN	G	413	6	-	0/2/19/22	0/1/1/1
4	NAG	G	414	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	415	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	416	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	417	5	-	0/2/19/22	0/1/1/1
6	MAN	G	418	5,6	-	0/2/19/22	0/1/1/1
6	MAN	G	419	6	-	0/2/19/22	0/1/1/1
6	MAN	G	420	6	-	0/2/19/22	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	407	NAG	O5-C1	-5.56	1.34	1.43
5	E	410	BMA	O5-C1	-4.46	1.36	1.43
6	E	412	MAN	C2-C3	-3.76	1.47	1.52
6	E	419	MAN	O5-C1	-3.57	1.37	1.43
4	F	407	NAG	C1-C2	-3.47	1.47	1.52
6	G	411	MAN	O5-C1	-3.13	1.38	1.43
6	F	412	MAN	O5-C1	-3.12	1.38	1.43
6	G	407	MAN	O5-C1	-2.94	1.38	1.43
6	E	420	MAN	O5-C1	-2.91	1.39	1.43
6	E	413	MAN	C2-C3	-2.86	1.48	1.52
6	E	412	MAN	O5-C1	-2.77	1.39	1.43
6	E	418	MAN	O5-C1	-2.63	1.39	1.43
6	G	412	MAN	C2-C3	-2.62	1.49	1.52
6	F	420	MAN	O5-C1	-2.61	1.39	1.43
6	E	411	MAN	O5-C1	-2.55	1.39	1.43
6	G	418	MAN	O5-C1	-2.47	1.39	1.43
5	G	416	BMA	O5-C1	-2.41	1.39	1.43
4	E	409	NAG	O5-C1	-2.36	1.39	1.43
6	G	405	MAN	O5-C1	-2.29	1.40	1.43
5	F	416	BMA	O5-C1	-2.28	1.40	1.43
6	G	413	MAN	O5-C1	-2.18	1.40	1.43
4	G	401	NAG	O5-C1	-2.15	1.40	1.43
5	F	409	BMA	O5-C1	-2.07	1.40	1.43
6	F	410	MAN	O5-C1	-2.05	1.40	1.43
5	E	417	BMA	O5-C1	-2.04	1.40	1.43
6	G	413	MAN	C1-C2	2.01	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	418	MAN	C4-C5	2.05	1.57	1.53
6	G	419	MAN	C2-C3	2.05	1.55	1.52
5	F	416	BMA	C4-C5	2.06	1.57	1.53
6	F	419	MAN	O5-C5	2.15	1.48	1.43
6	G	417	MAN	O5-C5	2.24	1.48	1.43
6	F	418	MAN	C2-C3	2.29	1.55	1.52
6	F	413	MAN	C4-C5	2.30	1.58	1.53
6	G	405	MAN	C4-C5	2.32	1.58	1.53
6	G	406	MAN	C2-C3	2.35	1.55	1.52
6	E	414	MAN	C1-C2	2.36	1.58	1.52
6	F	413	MAN	O5-C5	2.37	1.48	1.43
6	E	419	MAN	C2-C3	2.39	1.55	1.52
6	G	407	MAN	C4-C3	2.43	1.58	1.52
5	E	405	BMA	C4-C3	2.51	1.59	1.52
5	G	404	BMA	C1-C2	2.60	1.58	1.52
4	F	402	NAG	O5-C1	2.61	1.48	1.43
6	G	413	MAN	C2-C3	2.64	1.56	1.52
4	F	401	NAG	C1-C2	2.84	1.56	1.52
6	F	411	MAN	O3-C3	2.85	1.49	1.43
6	G	407	MAN	C2-C3	2.95	1.56	1.52
5	F	406	BMA	C1-C2	3.03	1.59	1.52
6	E	413	MAN	O5-C5	3.21	1.50	1.43
5	E	405	BMA	C2-C3	3.31	1.57	1.52
5	F	406	BMA	C2-C3	3.90	1.57	1.52
6	E	412	MAN	C4-C5	4.68	1.63	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	412	MAN	C1-C2-C3	-4.50	104.11	109.55
6	F	418	MAN	O3-C3-C4	-3.31	102.90	110.36
6	E	421	MAN	O2-C2-C3	-3.17	103.79	110.19
6	E	412	MAN	C1-C2-C3	-3.11	105.78	109.55
6	F	419	MAN	O2-C2-C3	-2.88	104.38	110.19
6	E	414	MAN	O2-C2-C3	-2.85	104.45	110.19
5	E	405	BMA	O5-C5-C4	-2.69	105.68	110.13
6	E	406	MAN	O2-C2-C3	-2.59	104.97	110.19
6	F	411	MAN	C1-C2-C3	-2.54	106.48	109.55
6	E	419	MAN	O2-C2-C3	-2.48	105.19	110.19
6	E	412	MAN	O2-C2-C3	-2.46	105.23	110.19
6	F	417	MAN	O2-C2-C3	-2.39	105.38	110.19
6	G	411	MAN	O2-C2-C3	-2.38	105.40	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	404	BMA	C3-C4-C5	-2.37	106.00	110.23
6	G	407	MAN	O2-C2-C3	-2.35	105.44	110.19
6	G	413	MAN	O2-C2-C3	-2.35	105.46	110.19
5	F	406	BMA	C1-O5-C5	-2.34	108.69	112.14
6	G	418	MAN	O2-C2-C3	-2.33	105.48	110.19
6	E	420	MAN	O2-C2-C3	-2.31	105.54	110.19
6	E	413	MAN	O2-C2-C3	-2.30	105.55	110.19
6	F	410	MAN	O2-C2-C3	-2.28	105.59	110.19
6	G	405	MAN	O2-C2-C3	-2.26	105.63	110.19
6	E	411	MAN	O2-C2-C3	-2.23	105.70	110.19
5	F	406	BMA	O5-C5-C4	-2.16	106.55	110.13
6	G	419	MAN	O2-C2-C3	-2.12	105.91	110.19
6	G	420	MAN	O2-C2-C3	-2.12	105.92	110.19
5	F	409	BMA	O2-C2-C3	-2.12	105.92	110.19
6	F	412	MAN	O2-C2-C3	-2.10	105.94	110.19
5	G	416	BMA	O2-C2-C3	-2.08	106.00	110.19
6	F	420	MAN	O2-C2-C3	-2.07	106.02	110.19
6	F	411	MAN	C3-C4-C5	-2.02	106.62	110.23
6	E	407	MAN	O2-C2-C3	-2.02	106.11	110.19
4	F	401	NAG	O5-C5-C4	-2.02	106.79	110.13
6	G	413	MAN	O5-C5-C4	-2.01	106.81	110.13
5	G	410	BMA	O2-C2-C3	-2.00	106.15	110.19
5	G	404	BMA	O5-C5-C6	2.01	111.64	107.34
6	G	411	MAN	O5-C1-C2	2.04	114.15	110.89
4	G	403	NAG	C1-O5-C5	2.06	115.17	112.14
4	F	407	NAG	C2-N2-C7	2.06	125.79	123.11
6	E	419	MAN	O3-C3-C2	2.14	113.93	110.01
5	F	416	BMA	C1-O5-C5	2.19	115.36	112.14
6	E	420	MAN	C1-O5-C5	2.19	115.36	112.14
6	F	419	MAN	C1-O5-C5	2.19	115.36	112.14
5	G	404	BMA	O3-C3-C2	2.20	114.03	110.01
6	G	419	MAN	O5-C1-C2	2.23	114.46	110.89
6	E	407	MAN	C1-O5-C5	2.23	115.42	112.14
6	G	405	MAN	C3-C4-C5	2.33	114.39	110.23
6	F	418	MAN	C2-C3-C4	2.33	115.12	111.05
6	G	407	MAN	C3-C4-C5	2.34	114.41	110.23
6	G	413	MAN	C1-O5-C5	2.36	115.61	112.14
5	F	406	BMA	C2-C3-C4	2.36	115.17	111.05
4	F	407	NAG	O5-C5-C4	2.36	114.05	110.13
6	G	405	MAN	O5-C5-C4	2.39	114.09	110.13
4	F	405	NAG	C1-O5-C5	2.46	115.75	112.14
6	E	419	MAN	C1-C2-C3	2.48	112.55	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	411	MAN	C1-C2-C3	2.49	112.57	109.55
6	E	419	MAN	C3-C4-C5	2.52	114.73	110.23
4	F	407	NAG	C3-C4-C5	2.53	114.74	110.23
4	G	402	NAG	O5-C5-C4	2.55	114.36	110.13
5	G	416	BMA	C1-O5-C5	2.58	115.94	112.14
4	G	403	NAG	C2-N2-C7	2.59	126.47	123.11
4	E	402	NAG	C1-O5-C5	2.59	115.94	112.14
6	E	413	MAN	O5-C1-C2	2.60	115.06	110.89
6	G	407	MAN	C1-C2-C3	2.67	112.79	109.55
6	G	413	MAN	C2-C3-C4	2.70	115.75	111.05
5	E	405	BMA	C2-C3-C4	2.72	115.80	111.05
6	E	406	MAN	O5-C1-C2	2.75	115.29	110.89
6	G	406	MAN	C1-O5-C5	2.76	116.20	112.14
5	G	410	BMA	C1-O5-C5	2.79	116.25	112.14
6	G	419	MAN	C1-C2-C3	2.80	112.94	109.55
6	G	419	MAN	C1-O5-C5	2.82	116.29	112.14
6	G	406	MAN	O3-C3-C2	2.95	115.40	110.01
6	E	412	MAN	O5-C5-C4	2.99	115.08	110.13
6	F	418	MAN	C3-C4-C5	3.09	115.74	110.23
5	E	405	BMA	O5-C1-C2	3.15	115.94	110.89
6	E	412	MAN	O2-C2-C1	3.18	115.59	109.23
6	G	407	MAN	C2-C3-C4	3.21	116.65	111.05
4	G	402	NAG	C2-N2-C7	3.24	127.31	123.11
6	E	414	MAN	O5-C1-C2	3.44	116.40	110.89
4	E	404	NAG	C1-O5-C5	3.46	117.23	112.14
5	F	416	BMA	C3-C4-C5	3.56	116.58	110.23
6	F	411	MAN	C1-O5-C5	3.57	117.39	112.14
6	G	413	MAN	O5-C1-C2	3.63	116.69	110.89
6	F	417	MAN	O5-C1-C2	3.65	116.73	110.89
6	G	405	MAN	C1-O5-C5	3.65	117.51	112.14
6	E	412	MAN	C3-C4-C5	3.69	116.81	110.23
4	F	402	NAG	C1-O5-C5	3.82	117.76	112.14
6	E	414	MAN	C1-O5-C5	3.92	117.91	112.14
6	G	417	MAN	O5-C1-C2	4.09	117.43	110.89
6	E	406	MAN	C1-O5-C5	4.16	118.25	112.14
6	E	413	MAN	C1-O5-C5	4.21	118.34	112.14
5	F	406	BMA	C1-C2-C3	4.31	114.78	109.55
6	G	420	MAN	C1-O5-C5	4.37	118.56	112.14
6	E	412	MAN	C1-O5-C5	4.43	118.65	112.14
6	E	414	MAN	C1-C2-C3	4.48	114.98	109.55
5	E	405	BMA	C1-C2-C3	4.59	115.11	109.55
6	G	413	MAN	C1-C2-C3	5.25	115.92	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	411	MAN	O3-C3-C2	5.50	120.09	110.01
6	F	413	MAN	C1-O5-C5	6.15	121.19	112.14
6	F	417	MAN	C1-O5-C5	6.64	121.90	112.14
6	G	417	MAN	C1-O5-C5	7.21	122.74	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	407	NAG	C1

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	406	MAN	C1-C2-C3-C4-C5-O5
6	F	419	MAN	C1-C2-C3-C4-C5-O5
6	E	421	MAN	C1-C2-C3-C4-C5-O5
6	G	406	MAN	C1-C2-C3-C4-C5-O5
6	G	412	MAN	C1-C2-C3-C4-C5-O5

26 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	NAG	1	0
4	E	404	NAG	1	0
5	E	405	BMA	1	0
5	E	410	BMA	3	0
6	E	412	MAN	5	0
6	E	413	MAN	2	0
6	E	414	MAN	1	0
4	E	416	NAG	1	0
6	E	419	MAN	1	0
6	E	421	MAN	1	0
4	F	401	NAG	2	0
4	F	405	NAG	2	0
4	F	407	NAG	1	0
6	F	411	MAN	3	0
6	F	413	MAN	3	0
6	F	417	MAN	1	0
6	F	419	MAN	1	0
4	G	402	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	403	NAG	3	0
5	G	404	BMA	1	0
6	G	406	MAN	1	0
6	G	407	MAN	1	0
5	G	410	BMA	1	0
6	G	412	MAN	1	0
4	G	415	NAG	1	0
5	G	416	BMA	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	230/244 (94%)	0.00	3 (1%) 79 62	31, 54, 92, 138	0
1	C	230/244 (94%)	0.38	6 (2%) 59 35	61, 97, 137, 157	0
1	H	229/244 (93%)	-0.03	1 (0%) 93 85	38, 61, 98, 117	0
2	B	213/215 (99%)	-0.01	2 (0%) 85 72	33, 59, 92, 123	0
2	D	214/215 (99%)	0.05	1 (0%) 91 83	54, 78, 109, 140	0
2	L	214/215 (99%)	0.09	4 (1%) 70 48	32, 61, 122, 158	0
3	E	176/211 (83%)	0.35	7 (3%) 42 20	38, 78, 134, 177	0
3	F	179/211 (84%)	0.27	6 (3%) 49 24	36, 86, 148, 171	0
3	G	187/211 (88%)	0.52	19 (10%) 9 3	39, 80, 150, 168	0
All	All	1872/2010 (93%)	0.17	49 (2%) 59 35	31, 71, 131, 177	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	111	SER	6.3
3	G	111	SER	6.1
3	F	202	GLY	6.0
3	G	268	PRO	5.9
3	E	136	VAL	4.2
1	A	131	THR	4.2
3	G	178	ARG	4.2
3	G	185	ASN	3.7
1	C	20	LEU	3.4
3	E	268	PRO	3.4
1	C	79	TYR	3.1
2	L	148	TRP	3.1
3	G	183	PRO	3.0
3	F	197	ASN	2.9
3	G	153	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	124	PHE	2.8
3	G	135	LYS	2.8
2	B	187	GLU	2.8
2	L	147	GLN	2.8
1	C	80	LEU	2.8
1	H	132	SER	2.7
3	G	138	ILE	2.7
1	A	127	SER	2.7
3	G	152	GLU	2.7
3	G	181	ILE	2.6
1	C	207	VAL	2.5
3	G	271	ARG	2.5
2	L	160	GLN	2.4
3	G	170	LYS	2.4
1	A	132	SER	2.4
3	G	177	TYR	2.4
3	G	136	VAL	2.3
3	E	154	ILE	2.3
1	C	131	THR	2.3
2	L	154	LEU	2.2
3	E	155	LYS	2.2
3	G	133	ASP	2.2
3	E	137	ASN	2.2
3	E	167	ASP	2.2
3	G	123	ALA	2.2
3	F	176	PHE	2.1
1	C	11	VAL	2.1
3	F	155	LYS	2.1
3	F	185	ASN	2.1
2	B	188	LYS	2.1
3	F	203	ASP	2.1
3	G	139	ASN	2.1
2	D	121	SER	2.1
3	G	179	LEU	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
6	MAN	G	407	11/12	0.81	0.38	13.55	121,127,151,152	0
4	NAG	G	403	14/15	0.79	0.34	7.37	107,115,136,138	0
4	NAG	E	402	14/15	0.77	0.48	5.49	101,109,130,133	0
6	MAN	E	413	11/12	0.64	0.47	3.19	112,119,142,144	0
7	ZN	E	422	1/1	0.77	0.47	3.05	216,216,216,216	1
4	NAG	F	401	14/15	0.75	0.51	2.99	127,136,159,163	0
6	MAN	E	414	11/12	0.70	0.29	2.83	103,108,128,129	0
6	MAN	G	413	11/12	0.59	0.39	2.73	121,125,149,152	0
4	NAG	F	405	14/15	0.70	0.39	1.81	128,133,160,160	0
4	NAG	G	401	14/15	0.69	0.36	1.35	104,114,137,137	0
6	MAN	E	418	11/12	0.87	0.22	1.28	56,67,80,82	0
5	BMA	F	409	11/12	0.91	0.23	1.11	48,55,68,68	0
4	NAG	E	401	14/15	0.84	0.37	1.05	94,110,133,133	0
4	NAG	F	402	14/15	0.70	0.37	0.96	120,138,162,166	0
4	NAG	E	404	14/15	0.76	0.29	0.68	94,108,126,130	0
4	NAG	E	403	14/15	0.91	0.26	0.43	76,83,98,100	0
6	MAN	E	420	11/12	0.95	0.28	0.39	70,79,91,96	0
4	NAG	G	402	14/15	0.82	0.26	0.29	87,94,111,113	0
6	MAN	E	419	11/12	0.93	0.24	-0.02	62,67,78,81	0
4	NAG	E	409	14/15	0.93	0.23	-0.16	79,98,116,116	0
6	MAN	E	411	11/12	0.96	0.22	-0.19	41,50,58,65	0
5	BMA	E	410	11/12	0.92	0.24	-0.20	60,75,89,91	0
4	NAG	G	408	14/15	0.81	0.32	-0.21	109,129,156,156	0
4	NAG	G	414	14/15	0.92	0.21	-0.50	50,60,72,72	0
4	NAG	F	414	14/15	0.91	0.22	-0.57	82,87,102,105	0
4	NAG	E	415	14/15	0.92	0.21	-0.57	45,56,66,66	0
4	NAG	G	409	14/15	0.90	0.21	-0.70	95,107,129,129	0
4	NAG	F	404	14/15	0.88	0.22	-0.91	109,119,139,143	0
4	NAG	F	415	14/15	0.89	0.20	-0.99	79,88,101,105	0
4	NAG	F	407	14/15	0.93	0.22	-1.00	68,84,95,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	416	14/15	0.94	0.19	-1.04	40,48,58,64	0
4	NAG	F	408	14/15	0.93	0.18	-1.04	55,67,80,80	0
6	MAN	G	411	11/12	0.93	0.19	-1.08	79,87,105,106	0
6	MAN	F	410	11/12	0.96	0.19	-1.10	34,42,51,54	0
5	BMA	G	410	11/12	0.93	0.20	-1.25	88,95,118,118	0
7	ZN	F	421	1/1	0.88	0.23	-1.26	67,67,67,67	1
4	NAG	E	408	14/15	0.93	0.17	-1.28	88,96,115,117	0
4	NAG	G	415	14/15	0.95	0.17	-1.40	49,59,69,71	0
5	BMA	G	404	11/12	0.78	0.26	-	121,126,152,154	0
6	MAN	G	419	11/12	0.78	0.24	-	86,93,110,113	0
6	MAN	F	420	11/12	0.77	0.30	-	130,136,163,167	0
6	MAN	G	405	11/12	0.55	0.49	-	132,135,162,165	0
5	BMA	E	417	11/12	0.97	0.20	-	43,49,63,63	0
6	MAN	F	413	11/12	0.72	0.25	-	92,103,124,125	0
5	BMA	F	406	11/12	0.65	0.30	-	113,121,145,146	0
6	MAN	E	412	11/12	0.64	0.25	-	95,104,125,125	0
6	MAN	E	421	11/12	0.77	0.35	-	68,80,96,98	0
6	MAN	G	412	11/12	0.76	0.22	-	107,114,137,137	0
6	MAN	G	418	11/12	0.92	0.18	-	77,82,98,99	0
6	MAN	G	406	11/12	0.80	0.29	-	121,126,150,151	0
5	BMA	F	403	11/12	0.62	0.45	-	134,137,163,164	0
6	MAN	E	406	11/12	0.41	0.72	-	127,132,158,162	0
6	MAN	E	407	11/12	0.78	0.32	-	107,112,133,134	0
6	MAN	F	417	11/12	0.76	0.27	-	121,130,156,157	0
6	MAN	G	420	11/12	0.87	0.24	-	93,101,122,123	0
6	MAN	F	418	11/12	0.89	0.19	-	108,121,146,146	0
6	MAN	F	411	11/12	0.91	0.19	-	70,87,107,107	0
5	BMA	F	416	11/12	0.89	0.20	-	96,104,122,126	0
5	BMA	G	416	11/12	0.93	0.20	-	61,71,82,86	0
6	MAN	F	419	11/12	0.68	0.24	-	124,127,151,153	0
6	MAN	F	412	11/12	0.74	0.32	-	101,107,128,130	0
5	BMA	E	405	11/12	0.47	0.37	-	113,122,147,148	0
7	ZN	G	421	1/1	0.92	0.32	-	109,109,109,109	1
6	MAN	G	417	11/12	0.83	0.19	-	87,97,115,118	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.