



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2016 – 06:41 AM EDT

PDB ID : 5KZC  
Title : Crystal structure of an HIV-1 gp120 engineered outer domain with a Man9 glycan at position N276, in complex with broadly neutralizing antibody VRC01  
Authors : Julien, J.-P.; Jardine, J.G.; Diwanji, D.; Schief, W.R.; Wilson, I.A.  
Deposited on : 2016-07-24  
Resolution : 3.25 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-20027939  
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-20027939

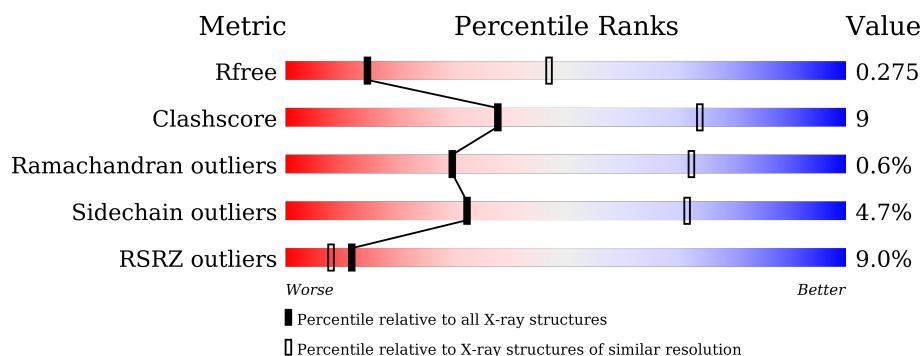
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	B	224	<div> <div>18%</div> <div>63% 30% . .</div> </div>
1	E	224	<div> <div>3%</div> <div>72% 21% . .</div> </div>
1	H	224	<div> <div>4%</div> <div>76% 17% . .</div> </div>
2	A	182	<div> <div>8%</div> <div>68% 25% . 7%</div> </div>
2	C	182	<div> <div>%</div> <div>76% 16% . 7%</div> </div>
2	F	182	<div> <div>11%</div> <div>59% 24% . 14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	210	
3	G	210	
3	L	210	

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	C	211	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13849 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 VRC01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1644	1041	285	308	10			
1	B	214	Total	C	N	O	S	0	0	0
			1644	1041	285	308	10			
1	E	214	Total	C	N	O	S	0	0	0
			1644	1041	285	308	10			

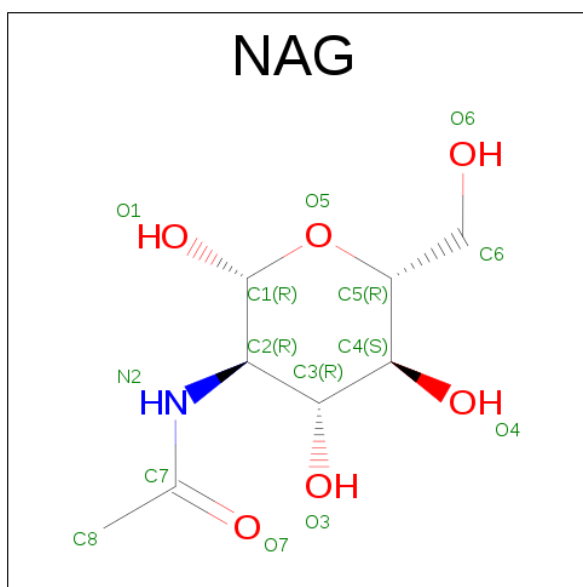
- Molecule 2 is a protein called Engineered outer domain of gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	170	Total	C	N	O	S	0	0	0
			1277	799	225	244	9			
2	C	170	Total	C	N	O	S	0	0	0
			1277	799	224	245	9			
2	F	156	Total	C	N	O	S	0	0	0
			1185	747	205	225	8			

- Molecule 3 is a protein called VRC01 Fab light chain.

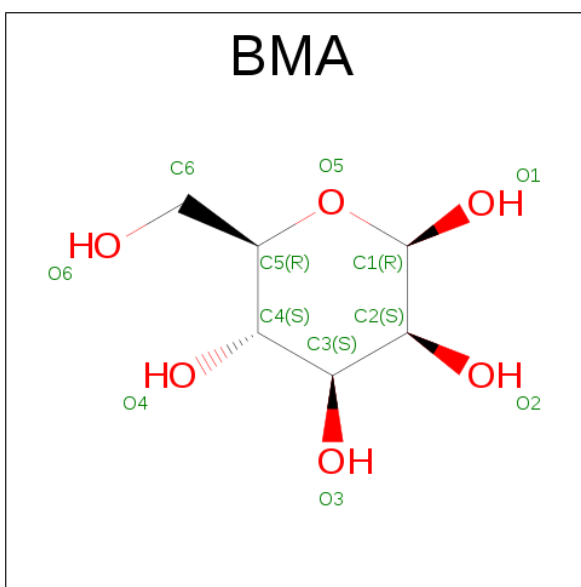
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	206	Total	C	N	O	S	0	0	0
			1603	1007	275	317	4			
3	D	209	Total	C	N	O	S	0	0	0
			1623	1017	278	323	5			
3	G	206	Total	C	N	O	S	0	0	0
			1603	1007	275	317	4			

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



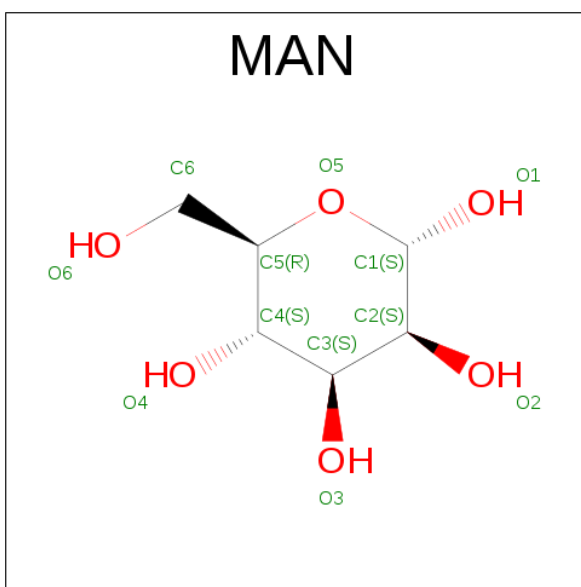
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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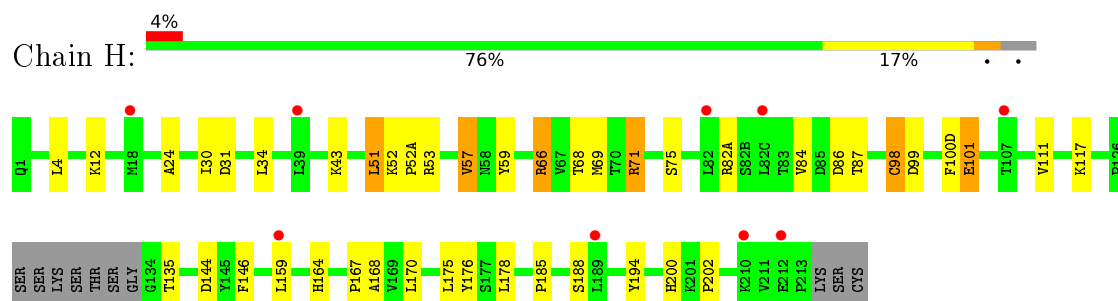
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C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

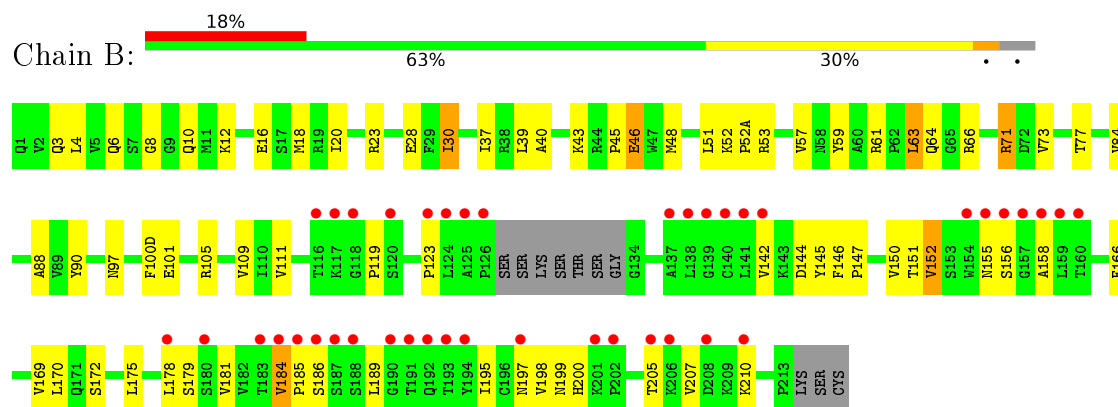
### 3 Residue-property plots

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

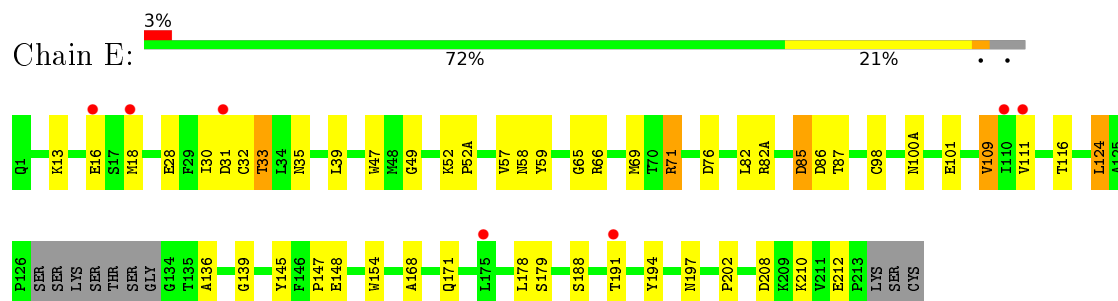
- Molecule 1: VRC01 Fab heavy chain



- Molecule 1: VRC01 Fab heavy chain

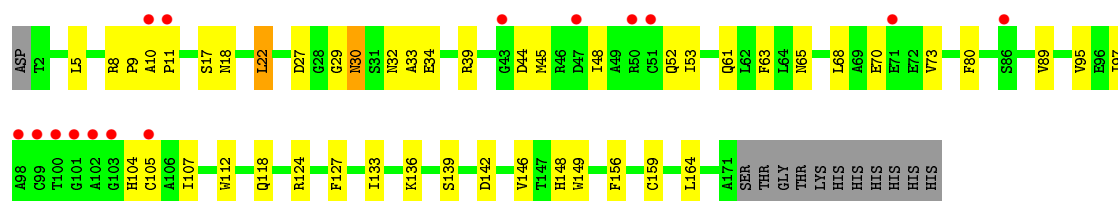


- Molecule 1: VRC01 Fab heavy chain

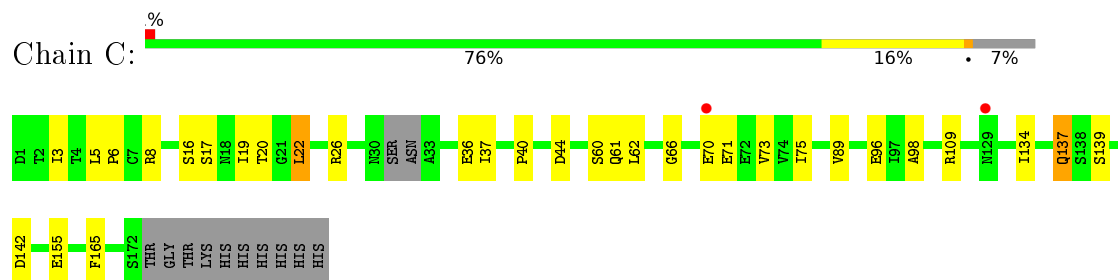


- Molecule 2: Engineered outer domain of gp120

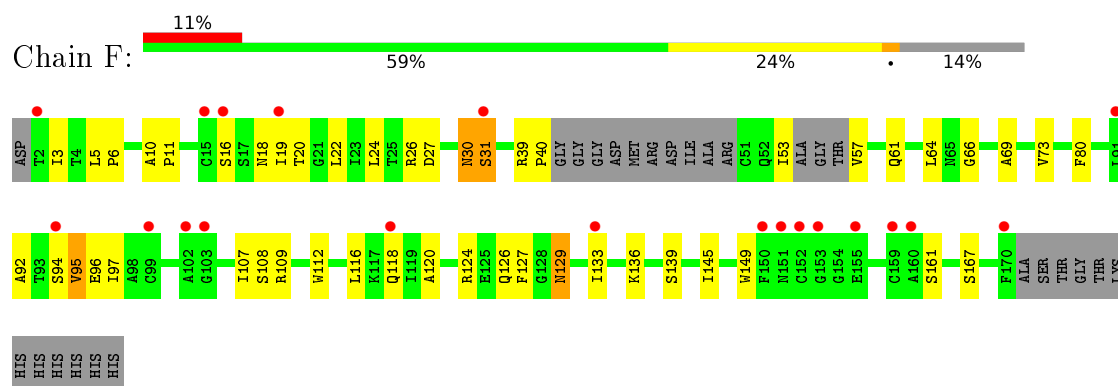




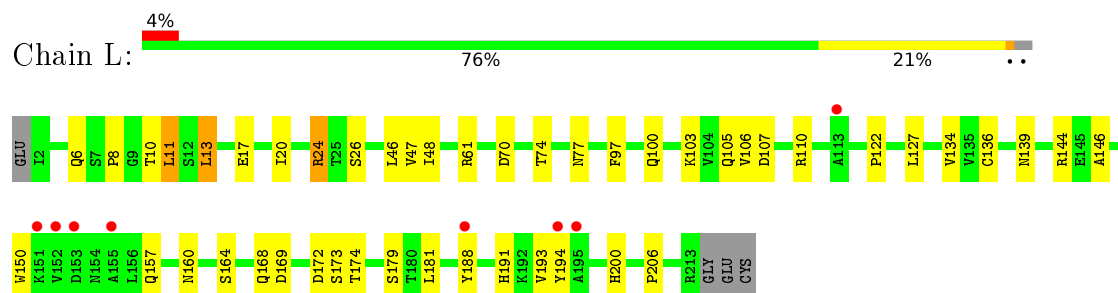
• Molecule 2: Engineered outer domain of gp120



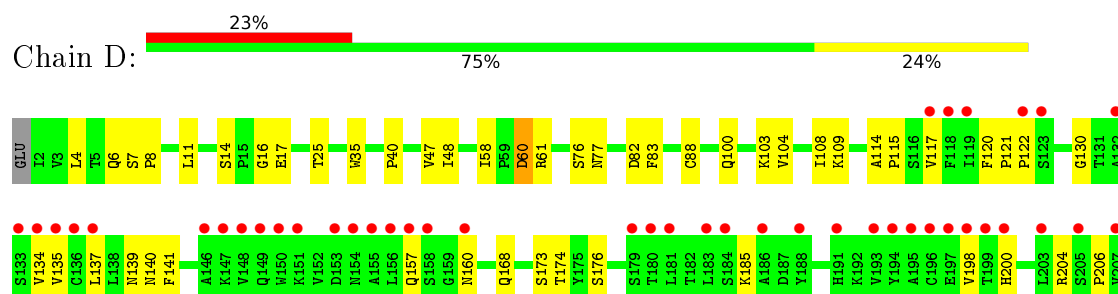
• Molecule 2: Engineered outer domain of gp120

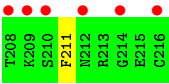


• Molecule 3: VRC01 Fab light chain

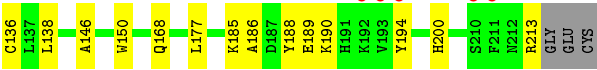
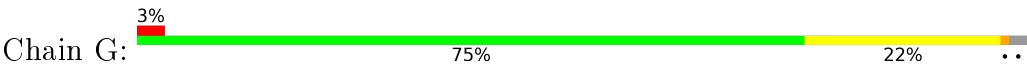


• Molecule 3: VRC01 Fab light chain





● Molecule 3: VRC01 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.51Å 113.51Å 412.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.94 – 3.25 39.94 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.94-3.25) 100.0 (39.94-3.25)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.223 , 0.274 0.223 , 0.275	Depositor DCC
$R_{free}$ test set	2179 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 79.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.29	0/1688	0.51	0/2299
1	E	0.28	0/1688	0.48	0/2299
1	H	0.26	0/1688	0.48	0/2299
2	A	0.26	0/1303	0.43	0/1767
2	C	0.28	0/1302	0.46	0/1764
2	F	0.25	0/1209	0.45	0/1639
3	D	0.28	0/1660	0.45	0/2253
3	G	0.27	0/1640	0.42	0/2228
3	L	0.27	0/1640	0.46	0/2228
All	All	0.27	0/13818	0.46	0/18776

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	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
1	H	99	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1644	0	1611	45	0
1	E	1644	0	1611	34	0
1	H	1644	0	1611	34	0
2	A	1277	0	1239	29	0
2	C	1277	0	1239	15	0
2	F	1185	0	1151	27	0
3	D	1623	0	1566	32	0
3	G	1603	0	1552	23	0
3	L	1603	0	1552	27	0
4	A	56	0	50	1	0
4	C	56	0	50	1	0
4	F	28	0	24	0	0
5	A	11	0	8	0	0
5	C	11	0	8	0	0
5	F	11	0	8	0	0
6	A	66	0	56	0	0
6	C	66	0	56	0	0
6	F	44	0	38	0	0
All	All	13849	0	13430	252	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 9.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52(A):PRO:O	1:E:71:ARG:NH2	2.04	0.90
3:L:110:ARG:HD2	3:L:173:SER:HB2	1.56	0.87
3:L:188:TYR:O	3:L:194:TYR:OH	1.96	0.83
3:D:47:VAL:HG12	3:D:48:ILE:HG12	1.63	0.81
1:E:32:CYS:HB3	1:E:98:CYS:HB3	1.68	0.75
1:E:87:THR:HG22	1:E:111:VAL:H	1.53	0.73
3:D:157:GLN:HB3	3:D:160:ASN:HD21	1.56	0.70
1:B:181:VAL:HG21	3:D:137:LEU:HD11	1.71	0.70
3:G:47:VAL:HG12	3:G:48:ILE:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:47:VAL:HG12	3:L:48:ILE:HG12	1.74	0.69
1:B:12:LYS:HZ3	1:B:18:MET:HA	1.57	0.69
3:D:120:PHE:HB2	3:D:135:VAL:HG22	1.76	0.68
2:A:22:LEU:HD12	2:A:89:VAL:HB	1.74	0.68
1:H:51:LEU:HD23	1:H:57:VAL:HG23	1.75	0.68
2:A:95:VAL:HG12	2:A:107:ILE:HD11	1.76	0.68
2:A:52:GLN:HE22	2:C:137:GLN:H	1.40	0.68
2:F:20:THR:HG21	2:F:66:GLY:H	1.59	0.68
3:L:24:ARG:NH1	3:L:70:ASP:OD1	2.27	0.67
2:F:107:ILE:HD12	2:F:108:SER:H	1.59	0.67
1:H:59:TYR:HE1	1:H:69:MET:HG2	1.60	0.67
1:H:68:THR:OG1	1:H:82(A):ARG:NH2	2.29	0.66
3:G:188:TYR:O	3:G:194:TYR:OH	2.14	0.66
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.28	0.66
2:C:20:THR:HG21	2:C:66:GLY:H	1.60	0.65
1:B:144:ASP:HB3	1:B:175:LEU:HD13	1.77	0.65
1:B:51:LEU:HD23	1:B:57:VAL:HG22	1.77	0.65
3:L:6:GLN:O	3:L:100:GLN:NE2	2.30	0.64
2:F:19:ILE:HB	2:F:95:VAL:HG23	1.79	0.64
1:H:101:GLU:HG2	3:L:46:LEU:HD23	1.78	0.64
3:G:18:THR:HB	3:G:76:SER:HA	1.80	0.63
1:H:52(A):PRO:O	1:H:71:ARG:NH1	2.32	0.62
1:E:145:TYR:OH	1:E:148:GLU:OE1	2.16	0.62
1:E:30:ILE:HA	1:E:52(A):PRO:HB2	1.82	0.62
1:B:61:ARG:HA	1:B:64:GLN:HG2	1.82	0.61
3:G:122:PRO:HD3	3:G:134:VAL:HG22	1.81	0.61
1:B:142:VAL:HB	1:B:178:LEU:HG	1.82	0.61
3:D:61:ARG:NH1	3:D:82:ASP:OD2	2.35	0.60
2:A:80:PHE:HB3	2:A:127:PHE:HE1	1.67	0.60
1:H:51:LEU:HD11	1:H:71:ARG:HB3	1.84	0.60
3:D:4:LEU:HD22	3:D:25:THR:HG22	1.84	0.59
2:A:97:ILE:HA	2:A:107:ILE:HD13	1.85	0.59
3:D:122:PRO:HD3	3:D:134:VAL:HG22	1.83	0.59
3:D:168:GLN:HE21	3:D:173:SER:HB3	1.68	0.59
2:C:3:ILE:HG13	2:C:109:ARG:HB2	1.85	0.59
1:E:85:ASP:OD1	1:E:85:ASP:N	2.27	0.58
2:A:22:LEU:CD1	2:A:89:VAL:HB	2.33	0.58
1:B:48:MET:HG2	1:B:63:LEU:HD21	1.85	0.58
1:H:87:THR:HG22	1:H:111:VAL:H	1.68	0.58
1:B:90:TYR:HE1	1:B:109:VAL:HG22	1.69	0.58
1:B:51:LEU:HD11	1:B:71:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:60:ASP:OD1	3:D:60:ASP:N	2.31	0.57
3:L:103:LYS:NZ	3:L:105:GLN:OE1	2.36	0.57
3:L:107:ASP:OD1	3:L:168:GLN:NE2	2.37	0.57
3:D:139:ASN:O	3:D:176:SER:OG	2.23	0.57
3:L:61:ARG:NH1	3:L:77:ASN:O	2.38	0.57
1:B:166:PHE:HD2	1:B:179:SER:HB2	1.69	0.56
1:B:57:VAL:HG11	1:B:59:TYR:CZ	2.40	0.56
2:F:112:TRP:CZ3	2:F:116:LEU:HD22	2.40	0.56
2:F:3:ILE:HG13	2:F:109:ARG:HB2	1.86	0.56
3:L:122:PRO:HD3	3:L:134:VAL:HG22	1.87	0.56
1:B:152:VAL:HG12	1:B:198:VAL:HG22	1.88	0.56
2:A:80:PHE:HB3	2:A:127:PHE:CE1	2.40	0.56
1:E:28:GLU:HB3	1:E:31:ASP:HB2	1.88	0.56
1:B:186:SER:HA	1:B:189:LEU:HD13	1.88	0.55
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.88	0.55
1:H:71:ARG:NH2	2:A:142:ASP:OD1	2.40	0.55
3:D:83:PHE:HA	3:D:104:VAL:HG23	1.88	0.55
3:D:141:PHE:HB2	3:D:200:HIS:CE1	2.40	0.55
3:G:108:ILE:HB	3:G:168:GLN:HE22	1.71	0.55
2:A:148:HIS:HD2	2:A:159:CYS:HB2	1.72	0.55
1:H:164:HIS:HD2	3:L:139:ASN:HD21	1.55	0.54
2:F:129:ASN:N	2:F:129:ASN:OD1	2.40	0.54
1:H:12:LYS:O	1:H:111:VAL:HA	2.07	0.54
1:B:155:ASN:HB2	1:B:158:ALA:HB3	1.89	0.54
3:D:17:GLU:OE1	3:D:109:LYS:NZ	2.39	0.54
1:B:12:LYS:O	1:B:111:VAL:HA	2.08	0.53
1:H:4:LEU:HD23	1:H:24:ALA:HB2	1.90	0.53
1:H:51:LEU:HD22	1:H:52:LYS:N	2.23	0.53
3:G:110:ARG:NH1	3:G:111:THR:O	2.41	0.53
3:G:38:GLN:HB3	3:G:85:VAL:HG13	1.91	0.53
2:A:149:TRP:HE1	2:A:156:PHE:HB3	1.74	0.53
2:F:18:ASN:HB3	2:F:94:SER:HB3	1.91	0.53
3:L:191:HIS:O	3:L:193:VAL:N	2.40	0.52
1:H:164:HIS:CD2	3:L:139:ASN:HD21	2.27	0.52
2:C:75:ILE:HG22	2:C:89:VAL:HG22	1.90	0.52
2:A:112:TRP:CZ2	2:A:164:LEU:HG	2.43	0.52
1:B:145:TYR:CZ	1:B:150:VAL:HG23	2.45	0.52
3:D:8:PRO:HD2	3:D:11:LEU:HD11	1.92	0.52
2:F:61:GLN:NE2	2:F:145:ILE:O	2.33	0.51
1:H:167:PRO:HG2	3:L:164:SER:HB2	1.92	0.51
2:A:61:GLN:NE2	2:A:146:VAL:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:ARG:HD3	2:F:127:PHE:HE2	1.76	0.51
1:B:151:THR:HB	1:B:199:ASN:HB2	1.93	0.51
2:C:70:GLU:CD	2:C:70:GLU:H	2.13	0.51
1:E:18:MET:SD	1:E:109:VAL:HG11	2.50	0.51
3:G:4:LEU:HD22	3:G:25:THR:HG22	1.93	0.51
1:B:119:PRO:HD2	1:B:205:THR:HB	1.93	0.51
3:D:130:GLY:O	3:D:185:LYS:N	2.44	0.51
1:B:84:VAL:HA	1:B:111:VAL:HG22	1.93	0.50
3:G:189:GLU:HA	3:G:213:ARG:HD3	1.92	0.50
1:E:59:TYR:HE1	1:E:69:MET:HG2	1.77	0.50
2:A:5:LEU:HB2	2:A:105:CYS:HB2	1.94	0.50
2:F:97:ILE:HG22	2:F:107:ILE:HB	1.94	0.50
2:C:22:LEU:HD12	2:C:89:VAL:HB	1.93	0.49
2:A:73:VAL:HG11	2:A:118:GLN:HB3	1.94	0.49
3:L:146:ALA:HB2	3:L:200:HIS:HD2	1.76	0.49
1:E:124:LEU:HB2	1:E:139:GLY:C	2.32	0.49
1:H:188:SER:OG	1:H:194:TYR:OH	2.16	0.49
1:B:52(A):PRO:O	1:B:71:ARG:NH2	2.45	0.49
1:B:150:VAL:HG11	1:B:152:VAL:HG13	1.95	0.49
1:E:71:ARG:HG3	1:E:71:ARG:HH21	1.77	0.49
3:G:2:ILE:HB	3:G:26:SER:HB2	1.95	0.49
3:D:204:ARG:O	3:D:204:ARG:NH1	2.46	0.48
2:F:69:ALA:HB3	2:F:92:ALA:HB2	1.95	0.48
3:G:33:LEU:HD13	3:G:71:TYR:CD1	2.48	0.48
1:H:185:PRO:HG2	1:H:188:SER:HB2	1.94	0.48
2:C:37:ILE:HD13	2:C:134:ILE:HB	1.96	0.48
1:H:84:VAL:HA	1:H:111:VAL:HG23	1.95	0.48
2:A:30:ASN:HB3	3:L:97:PHE:CZ	2.48	0.48
2:A:17:SER:OG	2:A:65:ASN:OD1	2.32	0.48
3:D:108:ILE:HB	3:D:168:GLN:HE22	1.79	0.48
1:B:184:VAL:HG22	1:B:185:PRO:HD2	1.95	0.47
1:E:116:THR:HG22	1:E:147:PRO:HD3	1.96	0.47
1:E:59:TYR:CE1	1:E:69:MET:HG2	2.49	0.47
1:E:66:ARG:HD2	1:E:82:LEU:HD11	1.97	0.47
1:B:195:ILE:HG22	1:B:210:LYS:HA	1.97	0.47
1:B:30:ILE:HA	1:B:52(A):PRO:HB2	1.97	0.47
1:E:58:ASN:ND2	2:F:26:ARG:O	2.40	0.47
2:A:124:ARG:HG3	2:A:133:ILE:HD11	1.97	0.47
2:A:32:ASN:O	2:A:34:GLU:N	2.40	0.47
2:C:40:PRO:HG3	2:C:165:PHE:CD2	2.50	0.46
1:B:23:ARG:HA	1:B:77:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:61:ARG:HH12	3:D:82:ASP:CG	2.19	0.46
3:D:35:TRP:CZ3	3:D:88:CYS:HB3	2.51	0.46
1:B:39:LEU:HD22	1:B:45:PRO:HB3	1.98	0.46
2:A:29:GLY:HA3	2:A:30:ASN:HA	1.72	0.46
1:B:10:GLN:NE2	1:B:20:ILE:HG22	2.30	0.46
1:E:47:TRP:CZ2	1:E:49:GLY:HA2	2.50	0.46
3:G:136:CYS:HB2	3:G:150:TRP:CH2	2.50	0.46
1:E:35:ASN:ND2	1:E:100(A):ASN:OD1	2.45	0.46
1:E:66:ARG:NH1	1:E:86:ASP:OD2	2.48	0.46
2:F:120:ALA:HA	2:F:133:ILE:HD12	1.97	0.46
2:A:30:ASN:HD22	2:A:30:ASN:H	1.62	0.46
1:H:51:LEU:HD22	1:H:51:LEU:C	2.36	0.46
3:L:150:TRP:CE2	3:L:181:LEU:HB2	2.51	0.46
2:A:17:SER:HA	4:A:210:NAG:H83	1.97	0.46
1:E:168:ALA:HA	1:E:178:LEU:HB3	1.97	0.46
2:F:57:VAL:HG11	2:F:64:LEU:HB2	1.98	0.46
1:E:139:GLY:HA2	1:E:154:TRP:CH2	2.51	0.45
1:E:194:TYR:H	1:E:210:LYS:HZ3	1.64	0.45
2:F:73:VAL:HG11	2:F:118:GLN:HB3	1.97	0.45
1:B:40:ALA:HB2	1:B:88:ALA:HB2	1.99	0.45
3:G:39:ARG:HH12	3:G:45:ARG:HH11	1.64	0.45
2:A:48:ILE:HG23	2:A:63:PHE:HE1	1.82	0.45
3:D:6:GLN:O	3:D:100:GLN:NE2	2.50	0.45
3:D:141:PHE:HB2	3:D:200:HIS:HE1	1.82	0.45
1:B:205:THR:HG22	1:B:207:VAL:HG23	1.98	0.45
2:F:39:ARG:NH2	2:F:136:LYS:HD3	2.31	0.45
3:G:24:ARG:NE	3:G:70:ASP:OD1	2.49	0.45
3:G:89:GLN:HG2	3:G:90:GLN:N	2.31	0.45
3:L:136:CYS:HB2	3:L:150:TRP:CZ2	2.52	0.45
1:B:146:PHE:HA	1:B:147:PRO:HA	1.72	0.45
2:C:17:SER:OG	4:C:211:NAG:O7	2.28	0.45
3:D:121:PRO:HB3	3:D:211:PHE:CE2	2.52	0.45
1:E:197:ASN:ND2	1:E:208:ASP:OD1	2.48	0.45
2:F:126:GLN:HG3	2:F:127:PHE:CD1	2.53	0.44
3:G:146:ALA:HB2	3:G:200:HIS:HD2	1.82	0.44
3:L:10:THR:OG1	3:L:144:ARG:NH1	2.50	0.44
2:A:39:ARG:NH2	2:A:136:LYS:HD3	2.33	0.44
1:B:40:ALA:HB3	1:B:43:LYS:HE3	1.99	0.44
1:E:33:THR:HG23	1:E:52:LYS:HG2	2.00	0.44
1:E:171:GLN:HG2	1:E:171:GLN:H	1.62	0.44
2:F:120:ALA:O	2:F:124:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:GLN:HE22	3:G:133:SER:HB2	1.82	0.44
3:G:138:LEU:HB2	3:G:177:LEU:HB3	1.99	0.44
1:H:30:ILE:HA	1:H:52(A):PRO:HB2	1.97	0.44
3:L:169:ASP:O	3:L:173:SER:N	2.40	0.44
2:C:16:SER:OG	2:C:98:ALA:HA	2.17	0.44
2:A:17:SER:OG	2:A:18:ASN:N	2.50	0.44
1:E:147:PRO:HD2	1:E:202:PRO:HB2	2.00	0.44
3:D:11:LEU:HB2	3:D:104:VAL:HG12	2.00	0.44
1:E:57:VAL:O	2:F:139:SER:OG	2.28	0.44
1:H:146:PHE:HB2	1:H:175:LEU:HD22	2.00	0.44
2:F:24:LEU:HD23	2:F:40:PRO:HA	2.00	0.43
3:G:127:LEU:O	3:G:185:LYS:HD2	2.17	0.43
3:G:61:ARG:HH12	3:G:79:GLU:HB2	1.83	0.43
3:D:117:VAL:HG21	3:D:198:VAL:HG21	2.01	0.43
3:D:168:GLN:HE21	3:D:173:SER:CB	2.31	0.43
3:G:186:ALA:O	3:G:190:LYS:HG3	2.18	0.43
3:L:157:GLN:HB3	3:L:160:ASN:HD21	1.84	0.43
3:L:20:ILE:HG12	3:L:74:THR:HG22	2.00	0.43
1:B:3:GLN:O	1:B:4:LEU:HD23	2.18	0.43
1:E:87:THR:CG2	1:E:111:VAL:H	2.28	0.43
1:H:30:ILE:HD12	1:H:53:ARG:HE	1.84	0.43
1:E:188:SER:HB2	1:E:191:THR:HB	1.99	0.43
2:F:18:ASN:HA	2:F:96:GLU:HA	2.00	0.43
3:D:115:PRO:HA	3:D:140:ASN:O	2.19	0.43
1:E:136:ALA:HA	3:G:118:PHE:HE2	1.83	0.43
1:E:13:LYS:O	1:E:16:GLU:HG2	2.19	0.43
3:G:15:PRO:HD3	3:G:106:VAL:HG23	2.01	0.43
1:H:200:HIS:CD2	1:H:202:PRO:HD2	2.53	0.43
3:L:20:ILE:HG23	3:L:74:THR:HG22	2.01	0.43
1:B:119:PRO:HD3	1:B:200:HIS:CD2	2.53	0.43
1:B:30:ILE:HG22	1:B:73:VAL:HG13	2.00	0.43
3:L:136:CYS:HB3	3:L:179:SER:HB3	2.00	0.43
2:F:10:ALA:HA	2:F:11:PRO:HD3	1.72	0.42
2:F:5:LEU:HA	2:F:6:PRO:HD2	1.85	0.42
1:H:117:LYS:HD2	1:H:144:ASP:O	2.18	0.42
1:H:75:SER:HB3	1:E:76:ASP:OD2	2.19	0.42
2:A:5:LEU:O	2:A:104:HIS:HA	2.19	0.42
1:B:156:SER:N	1:B:197:ASN:OD1	2.52	0.42
1:B:71:ARG:NH1	2:C:142:ASP:OD1	2.53	0.42
1:H:170:LEU:HD13	1:H:176:TYR:CE1	2.54	0.42
2:F:96:GLU:O	2:F:107:ILE:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:VAL:HG11	1:H:59:TYR:CZ	2.54	0.42
1:H:57:VAL:HG12	2:A:139:SER:HB2	2.01	0.42
1:B:8:GLY:HA2	1:B:105:ARG:NH2	2.35	0.42
3:D:114:ALA:HA	3:D:115:PRO:HD3	1.88	0.42
3:D:16:GLY:O	3:D:77:ASN:HA	2.19	0.42
3:D:7:SER:HA	3:D:8:PRO:HA	1.79	0.42
1:H:52:LYS:HA	1:H:52(A):PRO:HD3	1.84	0.42
3:D:140:ASN:ND2	3:D:174:THR:OG1	2.34	0.42
2:F:30:ASN:O	2:F:31:SER:HB2	2.19	0.42
1:E:210:LYS:HE3	1:E:212:GLU:HG3	2.02	0.41
2:C:60:SER:O	2:C:62:LEU:N	2.46	0.41
2:F:16:SER:HB3	2:F:97:ILE:O	2.19	0.41
1:B:37:ILE:HG23	1:B:46:GLU:O	2.20	0.41
2:A:44:ASP:OD1	2:A:45:MET:N	2.49	0.41
2:A:8:ARG:HA	2:A:9:PRO:HA	1.83	0.41
1:B:52:LYS:HA	1:B:52(A):PRO:HD3	1.73	0.41
1:B:123:PRO:HB3	1:B:210:LYS:O	2.21	0.41
1:B:150:VAL:HG12	1:B:151:THR:N	2.36	0.41
2:C:19:ILE:HD13	2:C:62:LEU:HD13	2.02	0.41
3:D:204:ARG:HA	3:D:204:ARG:HD2	1.95	0.41
3:D:58:ILE:HA	3:D:58:ILE:HD13	1.91	0.41
2:F:80:PHE:HB3	2:F:127:PHE:CE1	2.56	0.41
3:L:8:PRO:HG2	3:L:11:LEU:HB2	2.03	0.41
3:L:13:LEU:HB2	3:L:17:GLU:OE2	2.20	0.41
1:B:146:PHE:HB2	1:B:175:LEU:CD2	2.51	0.41
1:E:65:GLY:O	1:E:82(A):ARG:NH2	2.54	0.41
1:H:43:LYS:HE3	1:H:43:LYS:HB2	1.93	0.41
1:H:87:THR:HG22	1:H:111:VAL:N	2.35	0.40
1:B:12:LYS:NZ	1:B:18:MET:HA	2.30	0.40
1:B:6:GLN:NE2	1:B:90:TYR:O	2.49	0.40
2:C:5:LEU:HA	2:C:6:PRO:HD3	1.90	0.40
1:H:12:LYS:HB2	1:H:111:VAL:HG12	2.02	0.40
1:H:31:ASP:HB3	1:H:98:CYS:SG	2.61	0.40
2:A:10:ALA:HA	2:A:11:PRO:HD3	1.83	0.40
1:B:57:VAL:HG11	1:B:59:TYR:CE1	2.55	0.40
2:C:26:ARG:HD2	2:C:36:GLU:OE1	2.22	0.40
3:L:127:LEU:HD23	3:L:127:LEU:HA	1.84	0.40
1:E:194:TYR:H	1:E:210:LYS:NZ	2.18	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	B	210/224 (94%)	195 (93%)	13 (6%)	2 (1%)	19	62
1	E	210/224 (94%)	199 (95%)	11 (5%)	0	100	100
1	H	210/224 (94%)	199 (95%)	10 (5%)	1 (0%)	34	75
2	A	168/182 (92%)	154 (92%)	12 (7%)	2 (1%)	16	58
2	C	166/182 (91%)	158 (95%)	7 (4%)	1 (1%)	30	72
2	F	150/182 (82%)	137 (91%)	11 (7%)	2 (1%)	15	56
3	D	207/210 (99%)	197 (95%)	8 (4%)	2 (1%)	19	62
3	G	204/210 (97%)	194 (95%)	10 (5%)	0	100	100
3	L	204/210 (97%)	193 (95%)	10 (5%)	1 (0%)	34	75
All	All	1729/1848 (94%)	1626 (94%)	92 (5%)	11 (1%)	30	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	SER
2	F	30	ASN
2	A	70	GLU
1	B	100(D)	PHE
2	A	33	ALA
1	H	100(D)	PHE
2	C	61	GLN
3	D	40	PRO
2	F	31	SER
3	L	206	PRO
3	D	206	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	B	183/193 (95%)	169 (92%)	14 (8%)	16	52
1	E	183/193 (95%)	175 (96%)	8 (4%)	35	73
1	H	183/193 (95%)	174 (95%)	9 (5%)	31	70
2	A	138/149 (93%)	133 (96%)	5 (4%)	42	77
2	C	138/149 (93%)	129 (94%)	9 (6%)	21	60
2	F	131/149 (88%)	123 (94%)	8 (6%)	23	63
3	D	181/182 (100%)	177 (98%)	4 (2%)	60	86
3	G	179/182 (98%)	173 (97%)	6 (3%)	44	79
3	L	179/182 (98%)	172 (96%)	7 (4%)	39	76
All	All	1495/1572 (95%)	1425 (95%)	70 (5%)	32	71

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	LEU
1	H	51	LEU
1	H	57	VAL
1	H	66	ARG
1	H	71	ARG
1	H	98	CYS
1	H	101	GLU
1	H	135	THR
1	H	159	LEU
2	A	22	LEU
2	A	27	ASP
2	A	30	ASN
2	A	53	ILE
2	A	68	LEU
3	L	11	LEU
3	L	13	LEU
3	L	24	ARG
3	L	26	SER

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Mol	Chain	Res	Type
3	L	106	VAL
3	L	172	ASP
3	L	174	THR
1	B	16	GLU
1	B	28	GLU
1	B	30	ILE
1	B	46	GLU
1	B	53	ARG
1	B	63	LEU
1	B	66	ARG
1	B	71	ARG
1	B	97	ASN
1	B	101	GLU
1	B	152	VAL
1	B	169	VAL
1	B	170	LEU
1	B	184	VAL
2	C	8	ARG
2	C	22	LEU
2	C	44	ASP
2	C	71	GLU
2	C	73	VAL
2	C	96	GLU
2	C	137	GLN
2	C	139	SER
2	C	155	GLU
3	D	14	SER
3	D	60	ASP
3	D	76	SER
3	D	103	LYS
1	E	33	THR
1	E	39	LEU
1	E	71	ARG
1	E	85	ASP
1	E	101	GLU
1	E	109	VAL
1	E	124	LEU
1	E	179	SER
2	F	22	LEU
2	F	27	ASP
2	F	53	ILE
2	F	95	VAL

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Mol	Chain	Res	Type
2	F	129	ASN
2	F	149	TRP
2	F	161	SER
2	F	167	SER
3	G	2	ILE
3	G	3	VAL
3	G	18	THR
3	G	73	LEU
3	G	74	THR
3	G	124	ASP

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

Mol	Chain	Res	Type
1	H	102	HIS
1	H	164	HIS
2	A	30	ASN
2	A	52	GLN
2	A	83	ASN
2	A	148	HIS
3	D	157	GLN
3	D	160	ASN
2	F	90	GLN
2	F	163	GLN
3	G	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

29 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$
4	NAG	A	201	2,4	14,14,15	0.41	0	15,19,21	0.36	0
4	NAG	A	202	5,4	14,14,15	0.47	0	15,19,21	0.34	0
5	BMA	A	203	4,6	11,11,12	0.82	1 (9%)	15,15,17	1.14	1 (6%)
6	MAN	A	204	5,6	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
6	MAN	A	205	6	11,11,12	1.00	1 (9%)	15,15,17	0.87	1 (6%)
6	MAN	A	206	5,6	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
6	MAN	A	207	6	11,11,12	0.74	1 (9%)	15,15,17	1.08	1 (6%)
6	MAN	A	208	6	11,11,12	0.88	0	15,15,17	0.94	1 (6%)
6	MAN	A	209	6	11,11,12	1.11	1 (9%)	15,15,17	1.01	1 (6%)
4	NAG	A	210	2	14,14,15	0.22	0	15,19,21	0.45	0
4	NAG	A	211	2	14,14,15	0.32	0	15,19,21	0.53	0
4	NAG	C	201	2	14,14,15	0.46	0	15,19,21	0.42	0
4	NAG	C	202	2,4	14,14,15	0.16	0	15,19,21	0.48	0
4	NAG	C	203	5,4	14,14,15	0.49	0	15,19,21	0.38	0
5	BMA	C	204	4,6	11,11,12	0.71	0	15,15,17	1.04	1 (6%)
6	MAN	C	205	5,6	11,11,12	0.97	1 (9%)	15,15,17	1.08	1 (6%)
6	MAN	C	206	6	11,11,12	0.93	1 (9%)	15,15,17	1.20	3 (20%)
6	MAN	C	207	5,6	11,11,12	1.00	1 (9%)	15,15,17	1.22	1 (6%)
6	MAN	C	208	6	11,11,12	0.88	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	C	209	6	11,11,12	0.94	1 (9%)	15,15,17	0.95	1 (6%)
6	MAN	C	210	6	11,11,12	0.60	0	15,15,17	1.17	2 (13%)
4	NAG	C	211	2	14,14,15	0.24	0	15,19,21	0.61	0
4	NAG	F	201	2,4	14,14,15	0.21	0	15,19,21	0.45	0
4	NAG	F	202	5,4	14,14,15	0.24	0	15,19,21	0.41	0
5	BMA	F	203	4,6	11,11,12	0.92	1 (9%)	15,15,17	1.00	0
6	MAN	F	204	5	11,11,12	0.88	0	15,15,17	0.85	0
6	MAN	F	205	5,6	11,11,12	0.63	0	15,15,17	1.20	2 (13%)
6	MAN	F	206	6	11,11,12	0.68	0	15,15,17	0.98	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	F	207	6	11,11,12	0.86	0	15,15,17	1.09	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	A	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	A	202	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	203	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	204	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	205	6	-	0/2/19/22	0/1/1/1
6	MAN	A	206	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	207	6	-	0/2/19/22	0/1/1/1
6	MAN	A	208	6	-	0/2/19/22	0/1/1/1
6	MAN	A	209	6	-	0/2/19/22	0/1/1/1
4	NAG	A	210	2	-	0/6/23/26	0/1/1/1
4	NAG	A	211	2	-	0/6/23/26	0/1/1/1
4	NAG	C	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	202	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	203	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	204	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	205	5,6	-	0/2/19/22	0/1/1/1
6	MAN	C	206	6	-	0/2/19/22	0/1/1/1
6	MAN	C	207	5,6	-	0/2/19/22	0/1/1/1
6	MAN	C	208	6	-	0/2/19/22	0/1/1/1
6	MAN	C	209	6	-	0/2/19/22	0/1/1/1
6	MAN	C	210	6	-	0/2/19/22	0/1/1/1
4	NAG	C	211	2	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	202	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	203	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	204	5	-	0/2/19/22	0/1/1/1
6	MAN	F	205	5,6	-	0/2/19/22	0/1/1/1
6	MAN	F	206	6	-	0/2/19/22	0/1/1/1
6	MAN	F	207	6	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	209	MAN	O5-C1	-2.96	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	207	MAN	O5-C1	-2.81	1.39	1.43
6	A	205	MAN	O5-C1	-2.52	1.39	1.43
6	C	208	MAN	O5-C1	-2.44	1.39	1.43
6	C	209	MAN	O5-C1	-2.37	1.39	1.43
5	A	203	BMA	O5-C1	-2.34	1.39	1.43
5	F	203	BMA	O5-C1	-2.30	1.40	1.43
6	C	206	MAN	O5-C1	-2.05	1.40	1.43
6	C	205	MAN	O5-C1	-2.03	1.40	1.43
6	A	207	MAN	O5-C1	-2.00	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	207	MAN	O2-C2-C3	-2.76	104.62	110.19
6	A	206	MAN	O2-C2-C3	-2.66	104.82	110.19
6	C	208	MAN	O2-C2-C3	-2.60	104.95	110.19
6	F	205	MAN	O2-C2-C3	-2.58	104.99	110.19
6	A	207	MAN	O2-C2-C3	-2.44	105.27	110.19
6	C	210	MAN	O2-C2-C3	-2.31	105.54	110.19
6	C	206	MAN	O2-C2-C3	-2.24	105.67	110.19
6	C	206	MAN	C1-C2-C3	-2.24	106.84	109.55
6	F	206	MAN	O2-C2-C3	-2.21	105.73	110.19
6	C	209	MAN	O2-C2-C3	-2.17	105.81	110.19
6	A	205	MAN	O2-C2-C3	-2.08	105.99	110.19
6	A	204	MAN	O2-C2-C3	-2.08	106.00	110.19
6	A	209	MAN	C1-C2-C3	-2.02	107.10	109.55
6	F	207	MAN	O2-C2-C3	-2.01	106.14	110.19
6	A	208	MAN	O2-C2-C3	-2.00	106.15	110.19
6	F	206	MAN	C1-O5-C5	2.02	115.11	112.14
5	C	204	BMA	C1-O5-C5	2.02	115.12	112.14
6	F	207	MAN	C1-O5-C5	2.15	115.30	112.14
5	A	203	BMA	C1-O5-C5	2.28	115.49	112.14
6	A	204	MAN	C1-O5-C5	2.44	115.72	112.14
6	C	206	MAN	C1-O5-C5	2.57	115.91	112.14
6	C	205	MAN	C1-O5-C5	2.59	115.95	112.14
6	C	210	MAN	C1-O5-C5	2.66	116.05	112.14
6	A	206	MAN	C1-O5-C5	2.67	116.07	112.14
6	F	205	MAN	C1-O5-C5	2.75	116.19	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	210	NAG	1	0
4	C	211	NAG	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	B	214/224 (95%)	1.02	41 (19%) 2 1	51, 99, 238, 258	0
1	E	214/224 (95%)	0.30	7 (3%) 50 40	73, 116, 153, 166	0
1	H	214/224 (95%)	0.32	9 (4%) 40 30	69, 116, 155, 168	0
2	A	170/182 (93%)	0.64	15 (8%) 12 8	76, 131, 172, 213	0
2	C	170/182 (93%)	0.20	2 (1%) 81 72	54, 91, 135, 186	0
2	F	156/182 (85%)	0.81	20 (12%) 5 3	109, 162, 198, 207	0
3	D	209/210 (99%)	1.00	49 (23%) 1 1	46, 110, 243, 263	0
3	G	206/210 (98%)	0.16	7 (3%) 49 39	55, 95, 157, 188	0
3	L	206/210 (98%)	0.28	8 (3%) 43 33	58, 103, 167, 185	0
All	All	1759/1848 (95%)	0.52	158 (8%) 12 8	46, 115, 207, 263	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	13.6
1	B	126	PRO	11.6
3	D	195	ALA	11.2
1	B	159	LEU	9.0
1	B	158	ALA	7.7
1	B	125	ALA	7.1
1	B	193	THR	7.0
3	D	135	VAL	6.7
3	D	134	VAL	6.1
1	B	194	TYR	6.0
3	D	196	CYS	5.8
3	D	136	CYS	5.7
3	D	148	VAL	5.7
1	B	180	SER	5.4
3	D	147	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
3	D	153	ASP	5.2
1	B	157	GLY	5.1
3	D	157	GLN	5.0
1	B	192	GLN	4.8
3	D	154	ASN	4.7
1	B	191	THR	4.6
3	D	207	VAL	4.6
1	B	202	PRO	4.5
3	D	146	ALA	4.5
1	B	185	PRO	4.3
3	L	194	TYR	4.2
3	D	183	LEU	4.2
1	B	187	SER	4.1
3	D	133	SER	4.1
3	D	208	THR	4.0
2	A	99	CYS	4.0
2	F	159	CYS	3.9
3	D	203	LEU	3.9
3	D	214	GLY	3.8
3	D	181	LEU	3.8
3	D	198	VAL	3.8
1	B	141	LEU	3.7
2	F	19	ILE	3.7
3	D	216	CYS	3.7
1	B	178	LEU	3.7
3	D	186	ALA	3.6
2	A	102	ALA	3.6
2	F	160	ALA	3.6
3	D	194	TYR	3.6
1	B	186	SER	3.6
3	D	205	SER	3.6
1	B	208	ASP	3.5
1	B	137	ALA	3.5
1	E	18	MET	3.5
3	G	210	SER	3.5
3	D	150	TRP	3.4
3	D	180	THR	3.4
1	B	120	SER	3.3
3	L	113	ALA	3.2
1	B	183	THR	3.2
2	F	152	CYS	3.2
1	B	188	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	L	195	ALA	3.2
1	B	117	LYS	3.2
2	A	43	GLY	3.1
3	D	210	SER	3.1
1	H	18	MET	3.1
2	A	47	ASP	3.0
3	D	188	TYR	3.0
2	A	100	THR	3.0
1	H	212	GLU	3.0
3	D	117	VAL	3.0
3	D	151	LYS	2.9
1	H	189	LEU	2.9
3	D	200	HIS	2.9
1	H	82(C)	LEU	2.9
3	D	179	SER	2.9
2	A	71	GLU	2.8
1	E	191	THR	2.8
1	B	210	LYS	2.8
2	F	15	CYS	2.8
3	D	149	GLN	2.8
3	G	194	TYR	2.8
3	G	211	PHE	2.8
1	B	124	LEU	2.8
1	B	206	LYS	2.7
3	L	155	ALA	2.7
1	E	175	LEU	2.7
3	D	160	ASN	2.7
2	A	86	SER	2.7
3	G	133	SER	2.7
2	A	50	ARG	2.7
1	B	197	ASN	2.7
1	B	116	THR	2.7
3	D	209	LYS	2.7
3	L	188	TYR	2.7
3	D	155	ALA	2.7
3	L	151	LYS	2.7
1	B	155	ASN	2.6
2	F	150	PHE	2.6
1	B	184	VAL	2.6
3	L	152	VAL	2.6
1	H	159	LEU	2.6
3	D	118	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	156	SER	2.6
2	F	31	SER	2.6
1	B	139	GLY	2.6
2	F	118	GLN	2.6
1	E	31	ASP	2.5
3	D	184	SER	2.5
1	B	118	GLY	2.5
3	G	132	ALA	2.5
3	D	197	GLU	2.5
1	B	140	CYS	2.5
3	G	192	LYS	2.5
1	E	110	ILE	2.5
2	F	170	PHE	2.4
3	D	212	ASN	2.4
2	F	102	ALA	2.4
1	B	201	LYS	2.4
3	D	199	THR	2.4
1	B	123	PRO	2.4
1	B	154	TRP	2.4
3	D	119	ILE	2.4
2	A	11	PRO	2.4
1	H	82	LEU	2.4
2	A	98	ALA	2.4
2	F	2	THR	2.3
2	A	101	GLY	2.3
3	D	193	VAL	2.3
2	F	155	GLU	2.3
2	F	133	ILE	2.3
2	F	153	GLY	2.3
3	D	158	SER	2.3
2	F	103	GLY	2.3
1	B	142	VAL	2.2
2	F	91	LEU	2.2
2	A	103	GLY	2.2
2	F	94	SER	2.2
1	B	190	GLY	2.2
3	D	137	LEU	2.2
2	A	10	ALA	2.2
2	C	70	GLU	2.1
1	B	205	THR	2.1
2	A	51	CYS	2.1
2	F	99	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	151	ASN	2.1
2	C	129	ASN	2.1
3	L	153	ASP	2.1
1	E	111	VAL	2.1
3	G	193	VAL	2.1
1	H	107	THR	2.1
3	D	191	HIS	2.1
1	B	160	THR	2.0
2	A	105	CYS	2.0
3	D	123	SER	2.0
3	D	122	PRO	2.0
1	H	39	LEU	2.0
2	F	16	SER	2.0
3	D	132	ALA	2.0
3	D	156	LEU	2.0
1	E	16	GLU	2.0
1	H	210	LYS	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
4	NAG	C	211	14/15	0.84	0.28	2.09	86,115,119,125	0
4	NAG	A	210	14/15	0.82	0.39	1.79	122,143,163,167	0
4	NAG	C	201	14/15	0.67	0.25	0.27	102,113,121,121	0
4	NAG	C	202	14/15	0.93	0.21	-0.34	59,67,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	211	14/15	0.79	0.21	-0.64	113,124,128,132	0
4	NAG	F	201	14/15	0.93	0.16	-1.00	90,100,134,138	0
4	NAG	A	201	14/15	0.95	0.17	-1.26	50,68,88,99	0
6	MAN	F	206	11/12	0.91	0.14	-	121,127,139,143	0
6	MAN	C	205	11/12	0.92	0.17	-	94,119,127,128	0
6	MAN	C	210	11/12	0.92	0.20	-	65,69,88,91	0
6	MAN	F	207	11/12	0.81	0.24	-	117,121,142,147	0
5	BMA	C	204	11/12	0.94	0.15	-	73,88,95,113	0
6	MAN	C	209	11/12	0.92	0.18	-	83,111,119,120	0
6	MAN	C	207	11/12	0.96	0.14	-	58,60,68,71	0
6	MAN	C	208	11/12	0.95	0.15	-	75,86,105,110	0
6	MAN	A	208	11/12	0.80	0.31	-	126,136,147,151	0
4	NAG	A	202	14/15	0.96	0.17	-	78,83,86,90	0
5	BMA	A	203	11/12	0.93	0.17	-	74,89,102,110	0
6	MAN	A	204	11/12	0.89	0.27	-	97,108,121,128	0
6	MAN	A	209	11/12	0.94	0.16	-	82,97,107,109	0
6	MAN	A	207	11/12	0.90	0.20	-	109,122,127,138	0
4	NAG	F	202	14/15	0.95	0.21	-	93,109,116,117	0
6	MAN	A	206	11/12	0.96	0.18	-	77,93,104,106	0
6	MAN	C	206	11/12	0.84	0.28	-	141,147,160,161	0
4	NAG	C	203	14/15	0.96	0.17	-	69,75,88,93	0
6	MAN	A	205	11/12	0.81	0.17	-	102,132,137,138	0
6	MAN	F	204	11/12	0.76	0.27	-	125,131,136,139	0
5	BMA	F	203	11/12	0.89	0.20	-	110,116,126,133	0
6	MAN	F	205	11/12	0.94	0.12	-	96,104,110,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.