



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:23 AM BST

PDB ID : 5N0A  
Title : Crystal structure of A259C covalently linked dengue 2 virus envelope glycoprotein dimer in complex with the Fab fragment of the broadly neutralizing human antibody EDE2 A11  
Authors : Vaney, M.C.; Rouvinski, A.; Guardado-Calvo, P.; Sharma, A.; Rey, F.A.  
Deposited on : 2017-02-02  
Resolution : 3.90 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

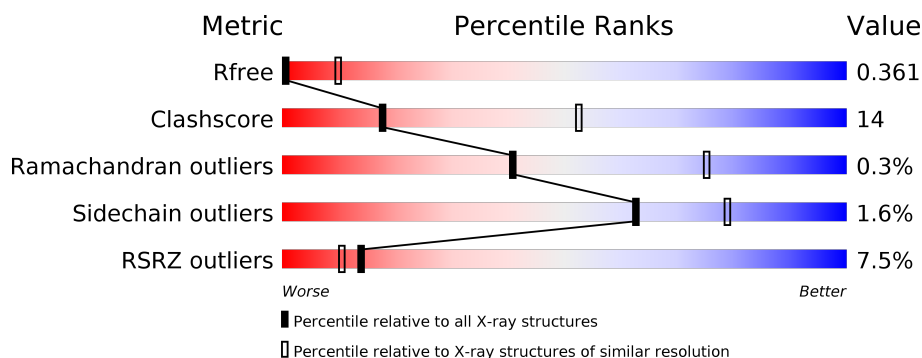
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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.



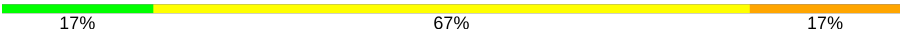
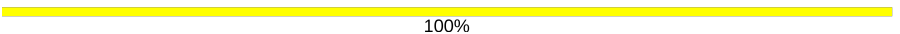
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 respectively. 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	430	<div> <div>10%</div> <div>63%</div> <div>22%</div> <div>13%</div> </div>
1	B	430	<div> <div>3%</div> <div>64%</div> <div>23%</div> <div>12%</div> </div>
2	H	283	<div> <div>6%</div> <div>41%</div> <div>5%</div> <div>54%</div> </div>
2	I	283	<div> <div>4%</div> <div>39%</div> <div>6%</div> <div>54%</div> </div>
3	L	218	<div> <div>2%</div> <div>47%</div> <div>50%</div> </div>
3	M	218	<div> <div>2%</div> <div>45%</div> <div>6%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	C	6	 17% 67% 17%
4	D	6	 100%

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	MAN	C	4	-	-	-	X
4	MAN	D	4	-	-	-	X
4	FUC	D	6	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9683 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 Envelope Glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2914	1842	497	551	24			
1	B	379	Total	C	N	O	S	0	0	0
			2943	1859	501	558	25			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	LYS	MET	conflict	UNP Q68Y26
A	259	CYS	ALA	engineered mutation	UNP Q68Y26
A	396	LEU	-	expression tag	UNP Q68Y26
A	397	VAL	-	expression tag	UNP Q68Y26
A	398	PRO	-	expression tag	UNP Q68Y26
A	399	ARG	-	expression tag	UNP Q68Y26
A	400	GLY	-	expression tag	UNP Q68Y26
A	401	SER	-	expression tag	UNP Q68Y26
A	402	SER	-	expression tag	UNP Q68Y26
A	403	ALA	-	expression tag	UNP Q68Y26
A	404	TRP	-	expression tag	UNP Q68Y26
A	405	SER	-	expression tag	UNP Q68Y26
A	406	HIS	-	expression tag	UNP Q68Y26
A	407	PRO	-	expression tag	UNP Q68Y26
A	408	GLN	-	expression tag	UNP Q68Y26
A	409	PHE	-	expression tag	UNP Q68Y26
A	410	GLU	-	expression tag	UNP Q68Y26
A	411	LYS	-	expression tag	UNP Q68Y26
A	412	GLY	-	expression tag	UNP Q68Y26
A	413	GLY	-	expression tag	UNP Q68Y26
A	414	SER	-	expression tag	UNP Q68Y26
A	415	GLY	-	expression tag	UNP Q68Y26
A	416	GLY	-	expression tag	UNP Q68Y26
A	417	GLY	-	expression tag	UNP Q68Y26
A	418	SER	-	expression tag	UNP Q68Y26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	GLY	-	expression tag	UNP Q68Y26
A	420	GLY	-	expression tag	UNP Q68Y26
A	421	SER	-	expression tag	UNP Q68Y26
A	422	ALA	-	expression tag	UNP Q68Y26
A	423	TRP	-	expression tag	UNP Q68Y26
A	424	SER	-	expression tag	UNP Q68Y26
A	425	HIS	-	expression tag	UNP Q68Y26
A	426	PRO	-	expression tag	UNP Q68Y26
A	427	GLN	-	expression tag	UNP Q68Y26
A	428	PHE	-	expression tag	UNP Q68Y26
A	429	GLU	-	expression tag	UNP Q68Y26
A	430	LYS	-	expression tag	UNP Q68Y26
B	118	LYS	MET	conflict	UNP Q68Y26
B	259	CYS	ALA	engineered mutation	UNP Q68Y26
B	396	LEU	-	expression tag	UNP Q68Y26
B	397	VAL	-	expression tag	UNP Q68Y26
B	398	PRO	-	expression tag	UNP Q68Y26
B	399	ARG	-	expression tag	UNP Q68Y26
B	400	GLY	-	expression tag	UNP Q68Y26
B	401	SER	-	expression tag	UNP Q68Y26
B	402	SER	-	expression tag	UNP Q68Y26
B	403	ALA	-	expression tag	UNP Q68Y26
B	404	TRP	-	expression tag	UNP Q68Y26
B	405	SER	-	expression tag	UNP Q68Y26
B	406	HIS	-	expression tag	UNP Q68Y26
B	407	PRO	-	expression tag	UNP Q68Y26
B	408	GLN	-	expression tag	UNP Q68Y26
B	409	PHE	-	expression tag	UNP Q68Y26
B	410	GLU	-	expression tag	UNP Q68Y26
B	411	LYS	-	expression tag	UNP Q68Y26
B	412	GLY	-	expression tag	UNP Q68Y26
B	413	GLY	-	expression tag	UNP Q68Y26
B	414	SER	-	expression tag	UNP Q68Y26
B	415	GLY	-	expression tag	UNP Q68Y26
B	416	GLY	-	expression tag	UNP Q68Y26
B	417	GLY	-	expression tag	UNP Q68Y26
B	418	SER	-	expression tag	UNP Q68Y26
B	419	GLY	-	expression tag	UNP Q68Y26
B	420	GLY	-	expression tag	UNP Q68Y26
B	421	SER	-	expression tag	UNP Q68Y26
B	422	ALA	-	expression tag	UNP Q68Y26
B	423	TRP	-	expression tag	UNP Q68Y26

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Chain	Residue	Modelled	Actual	Comment	Reference
B	424	SER	-	expression tag	UNP Q68Y26
B	425	HIS	-	expression tag	UNP Q68Y26
B	426	PRO	-	expression tag	UNP Q68Y26
B	427	GLN	-	expression tag	UNP Q68Y26
B	428	PHE	-	expression tag	UNP Q68Y26
B	429	GLU	-	expression tag	UNP Q68Y26
B	430	LYS	-	expression tag	UNP Q68Y26

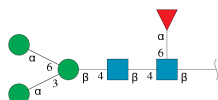
- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	131	Total	C	N	O	S	0	0	0
			1032	652	178	197	5			
2	I	131	Total	C	N	O	S	0	0	0
			1032	652	178	197	5			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	110	Total	C	N	O	S	0	0	0
			810	502	137	167	4			
3	M	110	Total	C	N	O	S	0	0	0
			810	502	137	167	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

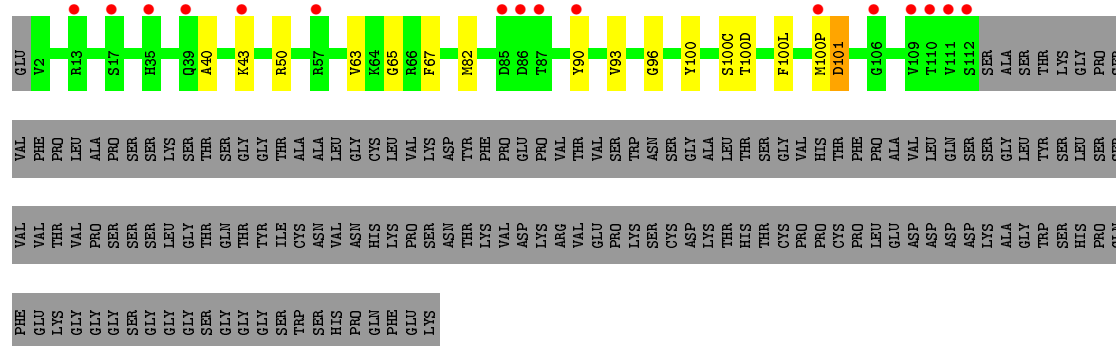
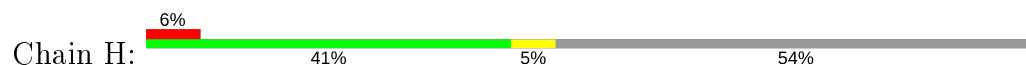
Chain A:

10% 63% 22% 13%

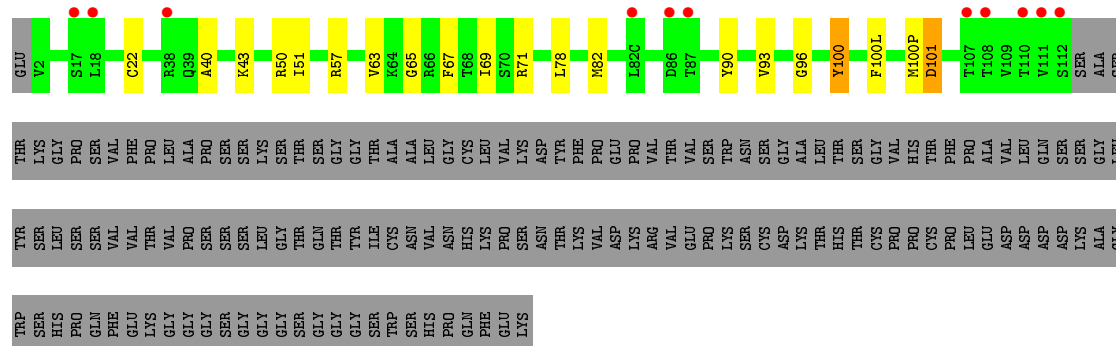
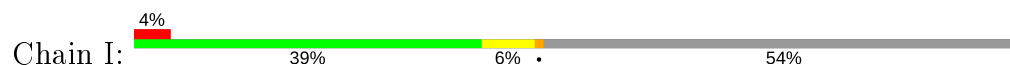
[illegible]

SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS

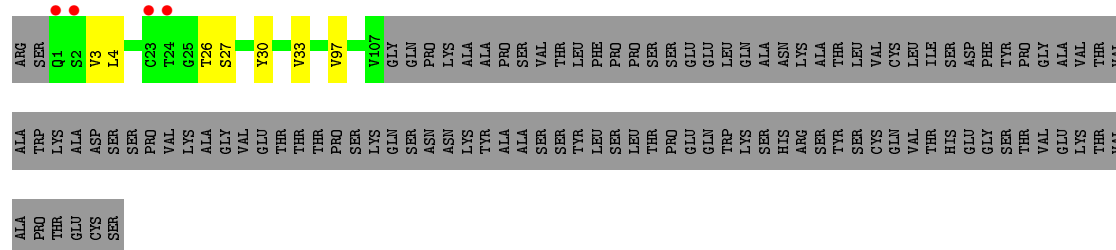
• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN



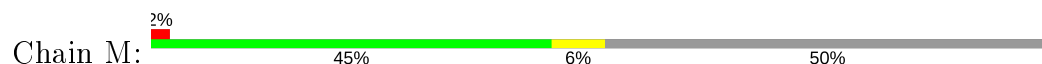
• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN



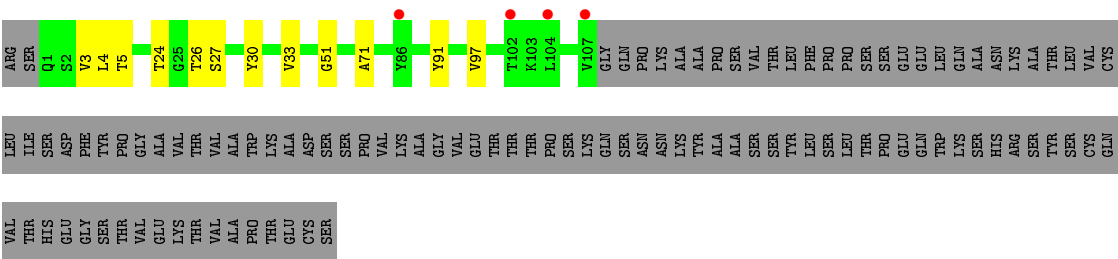
• Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11



• Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11







● Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.77Å 182.30Å 208.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.90 49.40 – 3.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-3.90) 90.7 (49.40-3.90)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	0.32	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.285 , 0.300 0.325 , 0.361	Depositor DCC
$R_{free}$ test set	955 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	1.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 110.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/2972	0.70	2/4014 (0.0%)
1	B	0.37	0/2998	0.68	0/4047
2	H	0.34	0/1060	0.66	1/1439 (0.1%)
2	I	0.35	0/1060	0.65	1/1439 (0.1%)
3	L	0.36	0/825	0.66	0/1122
3	M	0.36	0/825	0.64	0/1122
All	All	0.36	0/9740	0.67	4/13183 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLY	C-N-CA	5.36	135.09	121.70
2	I	101	ASP	CB-CG-OD2	5.23	123.01	118.30
2	H	101	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	203	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2914	0	2907	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2943	0	2943	103	0
2	H	1032	0	963	12	0
2	I	1032	0	963	41	0
3	L	810	0	798	5	0
3	M	810	0	798	11	0
4	C	71	0	61	1	0
4	D	71	0	61	2	0
All	All	9683	0	9494	260	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 14.

All (260) 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:B:46:ILE:HD12	1:B:140:VAL:CG2	1.28	1.56
1:B:46:ILE:CD1	1:B:140:VAL:CG2	1.85	1.51
2:I:50:ARG:NH1	2:I:100(L):PHE:HE2	1.28	1.31
1:B:46:ILE:CD1	1:B:140:VAL:HG21	1.52	1.24
2:I:67:PHE:CE1	2:I:82:MET:HB3	1.72	1.22
2:I:50:ARG:NH1	2:I:100(L):PHE:CE2	2.06	1.19
1:A:191:LEU:HD23	1:A:196:MET:HE2	1.30	1.14
1:A:219:PRO:HD3	1:A:237:LEU:HD13	1.13	1.11
1:A:219:PRO:CD	1:A:237:LEU:HD13	1.79	1.10
1:B:312:ILE:HG12	1:B:322:ILE:HG12	1.32	1.10
1:A:41:LEU:HD13	1:A:141:ILE:HD11	1.35	1.08
1:A:312:ILE:HG12	1:A:322:ILE:HG12	1.34	1.08
2:I:67:PHE:HE1	2:I:82:MET:HB3	0.90	1.06
1:B:41:LEU:HD13	1:B:141:ILE:HD11	1.35	1.04
1:A:219:PRO:HD3	1:A:237:LEU:CD1	1.89	1.02
1:A:191:LEU:HD23	1:A:196:MET:CE	1.90	1.01
1:B:46:ILE:HD13	1:B:140:VAL:HG21	1.41	1.00
1:B:46:ILE:HD11	1:B:140:VAL:CG2	1.97	0.95
2:I:67:PHE:HE1	2:I:82:MET:CB	1.79	0.95
1:A:191:LEU:CD2	1:A:196:MET:CE	2.47	0.91
1:B:46:ILE:CD1	1:B:140:VAL:HG23	1.70	0.90
1:A:255:SER:OG	1:B:255:SER:CB	2.20	0.89
1:B:46:ILE:CD1	1:B:140:VAL:CB	2.50	0.89
1:B:46:ILE:HD11	1:B:140:VAL:CB	2.02	0.89
1:B:46:ILE:HD11	1:B:140:VAL:HB	1.56	0.88
1:A:169:SER:HB2	1:A:185:CYS:O	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HB2	1:B:185:CYS:O	1.75	0.87
2:I:67:PHE:CE1	2:I:82:MET:CB	2.55	0.86
2:I:51:ILE:HD11	2:I:78:LEU:CD1	2.06	0.85
1:B:208:VAL:HG11	1:B:212:TRP:CE3	2.11	0.85
1:A:82:LEU:HB3	1:A:84:GLU:OE1	1.78	0.84
1:A:255:SER:OG	1:B:255:SER:HB3	1.77	0.84
1:B:82:LEU:HB3	1:B:84:GLU:OE1	1.77	0.83
3:M:5:THR:HG23	3:M:24:THR:HG23	1.60	0.83
1:B:302:CYS:N	1:B:333:CYS:SG	2.51	0.83
1:B:256:GLN:HA	1:B:259:CYS:SG	2.20	0.82
2:I:67:PHE:CE1	2:I:82:MET:CE	2.63	0.81
1:A:256:GLN:HA	1:A:259:CYS:SG	2.19	0.81
1:B:162:ILE:HD12	1:B:173:ALA:HB2	1.62	0.80
2:I:51:ILE:HG22	2:I:57:ARG:HG2	1.63	0.80
2:I:67:PHE:CZ	2:I:82:MET:HE2	2.17	0.79
2:I:63:VAL:HG22	2:I:67:PHE:HD2	1.46	0.79
2:I:67:PHE:CE1	2:I:82:MET:HE2	2.17	0.79
1:A:191:LEU:CD2	1:A:196:MET:HE1	2.12	0.77
1:B:46:ILE:HD12	1:B:140:VAL:HG23	0.76	0.75
1:B:99:ARG:NH1	1:B:103:ASN:OD1	2.19	0.75
1:B:46:ILE:HD11	1:B:140:VAL:HG21	1.64	0.73
1:A:255:SER:OG	1:B:255:SER:HB2	1.87	0.73
2:I:51:ILE:HG23	2:I:69:ILE:CG2	2.19	0.72
3:L:4:LEU:HD13	3:L:97:VAL:HG13	1.72	0.72
2:H:63:VAL:HG11	2:H:67:PHE:HB2	1.72	0.72
1:A:133:GLU:HB3	1:A:167:GLN:HG2	1.71	0.72
1:B:162:ILE:HD11	1:B:171:THR:CG2	2.20	0.72
3:M:4:LEU:HD13	3:M:97:VAL:HG13	1.72	0.72
1:A:191:LEU:HD21	1:A:196:MET:HE1	1.72	0.71
2:I:50:ARG:NH1	2:I:100(L):PHE:CZ	2.57	0.71
2:I:63:VAL:HG22	2:I:67:PHE:CD2	2.25	0.71
1:B:133:GLU:HB3	1:B:167:GLN:HG2	1.72	0.70
2:I:51:ILE:CG2	2:I:69:ILE:HG23	2.24	0.67
3:L:30:TYR:HA	3:L:33:VAL:HG23	1.77	0.67
1:B:46:ILE:HD12	1:B:140:VAL:CB	2.18	0.67
1:A:51:LYS:O	1:A:53:PRO:HD3	1.95	0.67
1:A:34:MET:HG2	1:A:40:THR:HG22	1.77	0.66
2:I:67:PHE:CZ	2:I:82:MET:CE	2.79	0.66
1:B:34:MET:HG2	1:B:40:THR:HG22	1.78	0.65
1:B:64:LYS:HB3	1:B:122:LYS:HD2	1.79	0.65
1:B:51:LYS:O	1:B:53:PRO:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:CYS:HB3	1:B:283:LEU:HD22	1.77	0.65
2:I:63:VAL:CG2	2:I:67:PHE:HD2	2.09	0.65
2:H:63:VAL:CG1	2:H:67:PHE:HB2	2.27	0.65
1:A:191:LEU:HD21	1:A:196:MET:CE	2.26	0.65
1:B:308:ILE:HD11	1:B:387:LEU:HD13	1.79	0.65
1:A:315:THR:HG23	1:A:317:HIS:H	1.61	0.64
1:B:315:THR:HG23	1:B:317:HIS:H	1.62	0.63
1:B:253:LEU:HG	1:B:253:LEU:O	1.97	0.63
1:A:207:LEU:HG	1:A:270:ILE:HD11	1.81	0.63
1:A:253:LEU:O	1:A:253:LEU:HG	1.98	0.63
1:B:392:PHE:CD1	1:B:392:PHE:O	2.52	0.62
2:I:51:ILE:HG23	2:I:69:ILE:HG21	1.80	0.62
1:B:46:ILE:CD1	1:B:140:VAL:HB	2.22	0.62
2:H:96:GLY:HA3	2:H:101:ASP:OD2	1.99	0.62
2:I:96:GLY:HA3	2:I:101:ASP:OD2	1.99	0.62
2:I:67:PHE:CE1	2:I:82:MET:HE3	2.34	0.62
1:A:392:PHE:O	1:A:392:PHE:CD1	2.52	0.62
2:H:50:ARG:HH12	2:H:100(L):PHE:HE2	1.48	0.61
2:I:51:ILE:HD11	2:I:78:LEU:HD12	1.82	0.61
2:I:51:ILE:HG23	2:I:69:ILE:HG23	1.83	0.61
3:M:33:VAL:HG11	3:M:71:ALA:HB1	1.82	0.60
1:B:207:LEU:CD2	1:B:279:PHE:HZ	2.14	0.60
3:M:3:VAL:HB	3:M:26:THR:HG22	1.84	0.60
2:I:51:ILE:HG12	2:I:69:ILE:CD1	2.32	0.60
1:A:277:LEU:HB3	1:A:279:PHE:CE2	2.37	0.59
3:L:3:VAL:HB	3:L:26:THR:HG22	1.84	0.59
3:L:4:LEU:CD1	3:L:97:VAL:HG13	2.33	0.59
1:A:337:PHE:CD1	1:A:380:VAL:HG22	2.38	0.59
1:A:48:THR:CG2	1:A:279:PHE:CD2	2.85	0.59
2:H:50:ARG:NH1	2:H:100(L):PHE:CE2	2.71	0.59
1:A:46:ILE:HG13	1:A:140:VAL:CG2	2.33	0.58
2:H:50:ARG:NH1	2:H:100(L):PHE:HE2	2.01	0.58
3:M:4:LEU:CD1	3:M:97:VAL:HG13	2.33	0.58
1:A:230:ASN:HD22	1:A:230:ASN:H	1.51	0.58
3:L:26:THR:HG23	3:L:27:SER:H	1.69	0.58
3:M:26:THR:HG23	3:M:27:SER:H	1.69	0.57
1:A:219:PRO:CG	1:A:237:LEU:HD13	2.34	0.57
1:A:241:LYS:HD3	1:B:271:GLN:HE22	1.70	0.57
1:B:99:ARG:HA	1:B:103:ASN:HD21	1.70	0.56
1:A:239:THR:HB	1:A:251:VAL:HG13	1.88	0.56
1:A:48:THR:CG2	1:A:279:PHE:HD2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:33:VAL:HG11	3:M:71:ALA:CB	2.36	0.56
1:A:33:THR:CG2	1:A:43:PHE:HE1	2.19	0.56
1:A:306:PHE:O	1:A:387:LEU:HD11	2.06	0.56
1:B:219:PRO:HD3	1:B:237:LEU:HD13	1.88	0.56
3:M:30:TYR:O	3:M:33:VAL:HG12	2.06	0.56
1:A:230:ASN:HD22	1:A:230:ASN:N	2.03	0.55
1:A:294:LEU:HD12	1:A:297:MET:CE	2.37	0.55
1:A:64:LYS:HB2	1:A:122:LYS:HD2	1.87	0.54
1:B:339:ILE:HG22	1:B:339:ILE:O	2.07	0.54
1:B:33:THR:CG2	1:B:43:PHE:HE1	2.20	0.54
1:B:91:ILE:HD13	1:B:238:VAL:CB	2.37	0.54
1:B:289:MET:HG2	1:B:292:LEU:HD12	1.90	0.54
1:A:339:ILE:HG22	1:A:339:ILE:O	2.07	0.54
2:H:100(C):SER:HB3	4:D:1:NAG:HN2	1.73	0.54
1:A:289:MET:HG2	1:A:292:LEU:HD12	1.89	0.54
1:B:239:THR:HB	1:B:251:VAL:HG13	1.89	0.54
1:B:43:PHE:CE2	1:B:141:ILE:HD12	2.43	0.54
1:B:65:LEU:HG	1:B:252:VAL:HG12	1.90	0.54
2:H:93:VAL:HG11	2:H:100(P):MET:HB3	1.90	0.53
1:A:99:ARG:NH1	1:A:105:CYS:SG	2.82	0.53
1:A:43:PHE:CE2	1:A:141:ILE:HD12	2.43	0.53
1:B:141:ILE:HG23	1:B:175:LEU:HD21	1.90	0.53
2:I:50:ARG:HH12	2:I:100(L):PHE:HE2	0.61	0.53
2:I:93:VAL:HG11	2:I:100(P):MET:HB3	1.90	0.53
1:A:296:GLY:C	1:A:298:SER:H	2.12	0.53
3:M:33:VAL:CG1	3:M:51:GLY:HA2	2.39	0.53
1:A:141:ILE:HG23	1:A:175:LEU:HD21	1.90	0.52
1:A:74:CYS:HB2	1:A:77:GLN:HG3	1.91	0.52
1:A:65:LEU:HG	1:A:252:VAL:HG12	1.90	0.52
2:I:67:PHE:HD1	2:I:82:MET:HA	1.75	0.52
1:B:296:GLY:C	1:B:298:SER:H	2.13	0.52
1:B:74:CYS:HB2	1:B:77:GLN:HG3	1.92	0.52
2:I:100(L):PHE:CD2	3:M:91:TYR:OH	2.59	0.52
1:A:48:THR:HG22	1:A:279:PHE:CD2	2.45	0.52
1:A:258:GLY:HA3	1:B:256:GLN:OE1	2.10	0.51
1:A:207:LEU:HG	1:A:270:ILE:CD1	2.40	0.51
1:A:256:GLN:OE1	1:B:258:GLY:HA3	2.11	0.51
1:A:322:ILE:CD1	1:A:378:ILE:HG21	2.40	0.51
1:A:183:MET:HG2	1:A:185:CYS:SG	2.51	0.51
1:B:99:ARG:NH1	1:B:105:CYS:SG	2.84	0.51
1:A:192:ASP:O	1:A:196:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HD13	1:A:279:PHE:CE1	2.45	0.51
2:I:51:ILE:HD11	2:I:78:LEU:HD11	1.93	0.51
2:I:67:PHE:CD1	2:I:82:MET:CB	2.94	0.51
2:I:51:ILE:HD12	2:I:71:ARG:HD2	1.93	0.50
1:A:377:TYR:CD1	1:A:390:ASN:OD1	2.65	0.50
1:B:376:SER:OG	1:B:391:TRP:HB3	2.11	0.50
1:A:207:LEU:CG	1:A:270:ILE:HD11	2.42	0.50
1:B:133:GLU:HB3	1:B:167:GLN:CG	2.41	0.50
2:I:67:PHE:CE1	2:I:82:MET:CG	2.94	0.50
1:A:206:TRP:NE1	1:A:269:GLU:HG2	2.26	0.50
1:B:322:ILE:CD1	1:B:378:ILE:HG21	2.42	0.49
1:B:90:PHE:CE1	1:B:118:LYS:HB2	2.47	0.49
1:B:148:GLU:O	1:B:323:ARG:NH2	2.46	0.49
1:B:220:TRP:CZ2	1:B:232:ILE:HG21	2.47	0.49
1:B:34:MET:HG2	1:B:40:THR:CG2	2.43	0.49
1:B:91:ILE:HD13	1:B:238:VAL:HB	1.94	0.49
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.47	0.49
1:A:192:ASP:O	1:A:196:MET:CG	2.60	0.49
1:B:308:ILE:CD1	1:B:387:LEU:HD13	2.41	0.49
3:M:33:VAL:HG13	3:M:51:GLY:HA2	1.94	0.49
1:B:206:TRP:NE1	1:B:269:GLU:HG2	2.27	0.49
1:A:241:LYS:HD3	1:B:271:GLN:NE2	2.28	0.49
1:A:71:GLU:HB2	1:A:82:LEU:HD21	1.94	0.48
1:B:194:ASN:O	1:B:194:ASN:OD1	2.31	0.48
1:A:194:ASN:OD1	1:A:194:ASN:O	2.30	0.48
2:H:82:MET:HE1	2:H:90:TYR:CE2	2.48	0.48
1:A:312:ILE:HG12	1:A:322:ILE:CG1	2.25	0.48
1:A:46:ILE:HG13	1:A:140:VAL:HG23	1.95	0.48
1:B:136:GLU:HA	1:B:165:THR:HG22	1.95	0.48
1:B:207:LEU:HD21	1:B:279:PHE:HZ	1.78	0.48
1:A:136:GLU:HA	1:A:165:THR:HG22	1.96	0.47
1:A:230:ASN:H	1:A:230:ASN:ND2	2.12	0.47
1:B:71:GLU:HB2	1:B:82:LEU:HD21	1.95	0.47
2:I:67:PHE:CD1	2:I:82:MET:HA	2.49	0.47
1:B:132:PRO:HG3	1:B:193:PHE:HB2	1.96	0.47
1:B:312:ILE:HG12	1:B:322:ILE:CG1	2.23	0.47
1:A:34:MET:HG2	1:A:40:THR:CG2	2.42	0.47
1:A:103:ASN:OD1	2:H:100(D):THR:HG23	2.14	0.47
1:A:33:THR:HG22	1:A:43:PHE:HE1	1.79	0.47
2:I:67:PHE:CD1	2:I:82:MET:HB3	2.41	0.47
1:A:253:LEU:O	1:A:253:LEU:CG	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG11	1:B:212:TRP:CZ3	2.49	0.47
1:A:271:GLN:HE22	1:B:241:LYS:HD3	1.79	0.47
1:A:132:PRO:HG3	1:A:193:PHE:HB2	1.97	0.47
1:B:309:VAL:HB	1:B:323:ARG:HG2	1.96	0.47
1:B:207:LEU:HD22	1:B:279:PHE:HZ	1.79	0.46
1:A:137:TYR:HB2	1:A:164:ILE:HG13	1.97	0.46
1:B:64:LYS:HG2	1:B:120:THR:HB	1.98	0.46
1:A:125:MET:HB3	1:A:201:MET:HG3	1.98	0.46
1:B:207:LEU:HD21	1:B:279:PHE:CZ	2.51	0.46
1:A:226:THR:O	1:A:227:GLN:HB2	2.16	0.46
1:B:182:THR:HB	1:B:288:ARG:HB2	1.98	0.45
1:B:162:ILE:HD11	1:B:171:THR:HB	1.99	0.45
2:I:51:ILE:HG12	2:I:69:ILE:HD13	1.97	0.45
1:B:33:THR:HG22	1:B:43:PHE:HE1	1.80	0.45
1:A:133:GLU:HB3	1:A:167:GLN:CG	2.41	0.45
1:B:253:LEU:CG	1:B:253:LEU:O	2.63	0.45
1:A:207:LEU:CD1	1:A:270:ILE:HD11	2.47	0.45
1:A:132:PRO:O	1:A:135:LEU:HB2	2.16	0.45
1:B:207:LEU:CD1	1:B:270:ILE:HG13	2.47	0.45
1:A:270:ILE:HD13	1:A:279:PHE:HE1	1.83	0.44
1:A:20:TRP:HA	1:A:287:LEU:O	2.18	0.44
1:B:132:PRO:O	1:B:135:LEU:HB2	2.16	0.44
1:B:162:ILE:HD11	1:B:171:THR:HG22	1.94	0.44
1:B:137:TYR:HB2	1:B:164:ILE:HG13	1.98	0.44
1:B:20:TRP:HA	1:B:287:LEU:O	2.17	0.44
1:B:222:PRO:HD2	1:B:225:ASP:HB3	2.00	0.44
2:I:100:TYR:CE1	4:C:2:NAG:H4	2.53	0.43
1:A:33:THR:HG21	1:A:43:PHE:HE1	1.83	0.43
1:A:146:GLY:O	1:A:365:VAL:HA	2.18	0.43
1:B:208:VAL:CG1	1:B:212:TRP:CE3	2.94	0.43
1:A:277:LEU:CB	1:A:279:PHE:CE2	3.01	0.43
1:A:65:LEU:HG	1:A:252:VAL:CG1	2.49	0.43
1:A:198:LEU:HD13	1:A:207:LEU:HD21	2.00	0.42
2:H:40:ALA:HB3	2:H:43:LYS:HD2	2.00	0.42
1:B:146:GLY:O	1:B:365:VAL:HA	2.19	0.42
1:B:7:SER:O	1:B:317:HIS:HE1	2.02	0.42
1:A:222:PRO:HD2	1:A:225:ASP:HB3	2.01	0.42
1:B:219:PRO:HA	1:B:232:ILE:O	2.19	0.42
1:B:65:LEU:HD12	1:B:252:VAL:HG13	2.01	0.42
2:I:40:ALA:HB3	2:I:43:LYS:HD2	2.00	0.42
1:B:207:LEU:HD13	1:B:270:ILE:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HG	1:B:252:VAL:CG1	2.49	0.42
1:A:219:PRO:HA	1:A:232:ILE:O	2.19	0.42
1:A:41:LEU:HD11	1:A:292:LEU:HD11	2.02	0.42
2:I:51:ILE:HG21	2:I:69:ILE:HG23	2.00	0.42
1:A:307:LYS:HZ3	1:A:307:LYS:HB3	1.84	0.42
1:B:208:VAL:HG12	1:B:209:HIS:N	2.35	0.42
1:B:87:ASP:HB3	1:B:90:PHE:HD2	1.83	0.42
1:A:308:ILE:O	1:A:308:ILE:HG23	2.20	0.42
1:A:66:THR:HG23	1:A:118:LYS:HB3	2.01	0.42
1:B:207:LEU:CD2	1:B:279:PHE:CZ	2.99	0.42
1:B:66:THR:HG23	1:B:118:LYS:HB3	2.02	0.42
1:B:307:LYS:HB3	1:B:307:LYS:HZ3	1.85	0.41
1:A:65:LEU:HD12	1:A:252:VAL:HG13	2.01	0.41
1:A:7:SER:O	1:A:317:HIS:HE1	2.02	0.41
1:B:170:THR:HA	1:B:183:MET:O	2.20	0.41
2:I:82:MET:HE1	2:I:90:TYR:CE2	2.54	0.41
1:A:219:PRO:CD	1:A:237:LEU:CD1	2.66	0.41
1:B:41:LEU:HD11	1:B:292:LEU:HD11	2.02	0.41
1:B:33:THR:HG21	1:B:43:PHE:HE1	1.84	0.41
1:A:40:THR:HG21	1:A:352:ILE:O	2.21	0.41
1:B:40:THR:HG21	1:B:352:ILE:O	2.20	0.41
1:A:201:MET:CE	1:A:260:MET:HB3	2.50	0.41
1:A:230:ASN:N	1:A:230:ASN:ND2	2.69	0.41
1:A:294:LEU:HD12	1:A:297:MET:HE3	2.03	0.41
2:I:67:PHE:CD1	2:I:82:MET:HG2	2.56	0.41
2:I:22:CYS:HB3	2:I:78:LEU:HB3	2.03	0.41
1:B:149:HIS:HB3	4:D:1:NAG:H2	2.03	0.41
1:A:379:ILE:HG13	1:A:388:LYS:HA	2.04	0.40
1:B:91:ILE:HD13	1:B:238:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/430 (85%)	346 (95%)	18 (5%)	1 (0%)	41	75
1	B	369/430 (86%)	351 (95%)	17 (5%)	1 (0%)	41	75
2	H	129/283 (46%)	124 (96%)	4 (3%)	1 (1%)	19	57
2	I	129/283 (46%)	124 (96%)	4 (3%)	1 (1%)	19	57
3	L	108/218 (50%)	104 (96%)	4 (4%)	0	100	100
3	M	108/218 (50%)	104 (96%)	4 (4%)	0	100	100
All	All	1208/1862 (65%)	1153 (95%)	51 (4%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	MET
1	B	297	MET
2	I	65	GLY
2	H	65	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	326/368 (89%)	319 (98%)	7 (2%)	53	73
1	B	330/368 (90%)	322 (98%)	8 (2%)	49	69
2	H	109/236 (46%)	108 (99%)	1 (1%)	78	87
2	I	109/236 (46%)	108 (99%)	1 (1%)	78	87
3	L	92/185 (50%)	92 (100%)	0	100	100
3	M	92/185 (50%)	92 (100%)	0	100	100
All	All	1058/1578 (67%)	1041 (98%)	17 (2%)	62	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	86	GLN
1	A	99	ARG
1	A	135	LEU
1	A	230	ASN
1	A	259	CYS
1	A	376	SER
1	B	1	MET
1	B	86	GLN
1	B	99	ARG
1	B	135	LEU
1	B	196	MET
1	B	259	CYS
1	B	279	PHE
1	B	333	CYS
2	H	100	TYR
2	I	100	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	194	ASN
1	A	230	ASN
1	A	271	GLN
1	B	134	ASN
1	B	194	ASN
1	B	271	GLN
1	B	386	GLN
3	L	37	GLN
3	M	37	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 ⓘ

12 monosaccharides 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	C	1	1,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	C	2	4	14,14,15	0.34	0	17,19,21	1.33	3 (17%)
4	BMA	C	3	4	11,11,12	0.40	0	15,15,17	1.12	1 (6%)
4	MAN	C	4	4	11,11,12	0.38	0	15,15,17	0.98	1 (6%)
4	MAN	C	5	4	11,11,12	0.36	0	15,15,17	0.89	1 (6%)
4	FUC	C	6	4	10,10,11	0.44	0	14,14,16	0.93	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	D	2	4	14,14,15	0.35	0	17,19,21	1.31	3 (17%)
4	BMA	D	3	4	11,11,12	0.36	0	15,15,17	1.16	1 (6%)
4	MAN	D	4	4	11,11,12	0.39	0	15,15,17	0.98	1 (6%)
4	MAN	D	5	4	11,11,12	0.37	0	15,15,17	0.84	1 (6%)
4	FUC	D	6	4	10,10,11	0.44	0	14,14,16	0.94	1 (7%)

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	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	1/1/1/1
4	MAN	C	4	4	-	1/2/19/22	1/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	FUC	C	6	4	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	D	4	4	-	1/2/19/22	1/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	FUC	D	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-O5-C5	3.92	117.51	112.19
4	C	3	BMA	C1-O5-C5	3.69	117.19	112.19
4	D	4	MAN	C1-O5-C5	3.52	116.96	112.19
4	C	4	MAN	C1-O5-C5	3.50	116.94	112.19
4	D	2	NAG	C1-O5-C5	3.47	116.89	112.19
4	C	2	NAG	C1-O5-C5	3.40	116.79	112.19
4	C	2	NAG	O5-C1-C2	3.38	116.62	111.29
4	D	2	NAG	O5-C1-C2	3.24	116.40	111.29
4	C	5	MAN	C1-O5-C5	2.94	116.18	112.19
4	D	5	MAN	C1-O5-C5	2.76	115.93	112.19
4	D	2	NAG	O4-C4-C5	2.15	114.64	109.30
4	C	2	NAG	O4-C4-C5	2.15	114.63	109.30
4	C	6	FUC	C1-O5-C5	2.15	117.64	112.78
4	D	6	FUC	C1-O5-C5	2.12	117.59	112.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	BMA	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C1-C2-C3-C4-C5-O5
4	D	3	BMA	C1-C2-C3-C4-C5-O5
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	D	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	C	2	NAG	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	373/430 (86%)	0.89	44 (11%) 4 4	81, 143, 236, 287	0
1	B	379/430 (88%)	0.58	14 (3%) 41 32	68, 142, 233, 287	0
2	H	131/283 (46%)	0.80	16 (12%) 4 4	89, 133, 218, 295	0
2	I	131/283 (46%)	0.72	11 (8%) 11 9	91, 130, 189, 229	0
3	L	110/218 (50%)	0.30	4 (3%) 42 33	83, 121, 163, 204	0
3	M	110/218 (50%)	0.38	4 (3%) 42 33	83, 128, 166, 235	0
All	All	1234/1862 (66%)	0.67	93 (7%) 14 10	68, 138, 218, 295	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	MET	5.6
1	A	20	TRP	4.4
1	A	28	GLY	4.3
1	A	334	LYS	4.0
1	A	50	ALA	4.0
1	B	190	GLY	3.7
1	A	300	SER	3.5
1	A	190	GLY	3.3
1	A	160	LYS	3.2
1	A	14	GLY	3.2
1	A	306	PHE	3.2
1	B	201	MET	3.2
2	H	111	VAL	3.1
1	A	337	PHE	3.1
1	A	388	LYS	3.1
2	H	87	THR	3.0
2	I	82(C)	LEU	3.0
1	A	335	ILE	3.0
1	A	191	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	289	MET	2.9
2	I	87	THR	2.9
1	A	183	MET	2.9
1	A	350	ARG	2.9
1	A	284	LYS	2.8
1	A	164	ILE	2.8
1	A	39	PRO	2.8
2	H	109	VAL	2.8
2	H	110	THR	2.8
1	A	280	THR	2.8
1	A	248	GLN	2.7
2	H	43	LYS	2.7
1	B	329	ASP	2.7
2	H	106	GLY	2.7
2	H	100(P)	MET	2.7
2	I	108	THR	2.6
1	A	43	PHE	2.6
3	L	1	GLN	2.6
1	B	184	GLU	2.5
1	B	264	LEU	2.5
1	A	182	THR	2.5
1	B	355	ASN	2.5
1	A	326	TYR	2.5
2	H	35	HIS	2.5
3	M	104	LEU	2.5
2	I	110	THR	2.5
1	B	21	VAL	2.5
3	M	107	VAL	2.5
1	A	380	VAL	2.4
2	I	86	ASP	2.4
1	A	279	PHE	2.4
2	I	18	LEU	2.4
2	I	107	THR	2.4
1	B	167	GLN	2.3
1	A	172	GLU	2.3
1	A	139	ILE	2.3
2	I	111	VAL	2.3
2	H	17	SER	2.3
1	B	168	SER	2.3
3	M	102	THR	2.3
3	M	86	TYR	2.3
1	A	90	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	141	ILE	2.3
2	H	112	SER	2.2
3	L	23	CYS	2.2
1	A	325	GLN	2.2
3	L	24	THR	2.2
1	A	21	VAL	2.2
1	A	308	ILE	2.2
1	A	295	LYS	2.2
1	A	264	LEU	2.2
2	H	90	TYR	2.2
2	H	13	ARG	2.2
1	A	292	LEU	2.1
2	I	17	SER	2.1
2	H	57	ARG	2.1
2	H	85	ASP	2.1
1	B	303	THR	2.1
1	A	162	ILE	2.1
1	A	338	GLU	2.1
1	A	23	ILE	2.1
1	A	379	ILE	2.1
2	H	39	GLN	2.1
3	L	2	SER	2.0
1	B	348	LEU	2.0
2	I	112	SER	2.0
1	A	322	ILE	2.0
2	I	38	ARG	2.0
1	B	172	GLU	2.0
1	B	223	GLY	2.0
1	B	349	GLY	2.0
1	A	189	THR	2.0
1	A	287	LEU	2.0
2	H	86	ASP	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](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUC	D	6	10/11	0.72	0.53	179,185,188,189	0
4	MAN	D	4	11/12	0.72	0.43	172,184,188,190	0
4	MAN	C	4	11/12	0.79	0.42	162,183,190,199	0
4	FUC	C	6	10/11	0.80	0.29	171,175,183,190	0
4	BMA	D	3	11/12	0.80	0.29	97,109,131,155	0
4	MAN	C	5	11/12	0.84	0.36	109,116,124,136	0
4	MAN	D	5	11/12	0.86	0.30	104,125,132,133	0
4	NAG	D	1	14/15	0.86	0.29	87,101,171,184	0
4	NAG	D	2	14/15	0.88	0.26	83,99,149,159	0
4	NAG	C	1	14/15	0.90	0.27	96,118,153,167	0
4	NAG	C	2	14/15	0.93	0.25	95,113,144,146	0
4	BMA	C	3	11/12	0.96	0.26	81,104,118,137	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.