wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Jul 25, 2017 – 11:20 AM EDT

PDB ID	:	5VN3
EMDB ID:	:	EMD-8713
Title	:	Cryo-EM model of B41 SOSIP.664 in complex with soluble CD4 (D1-D2) and fragment antigen binding variable domain of 17b
Authors	:	Ozorowski, G.; Pallesen, J.; Ward, A.B.
Deposited on	:	unknown
Resolution	:	3.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

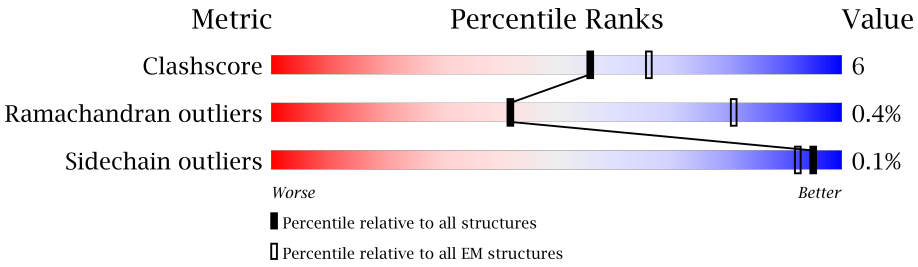
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	L	214	42% 9% 49%
1	N	214	42% 10% 49%
1	O	214	42% 9% 49%
2	A	153	83% 6% 11%
2	B	153	86% • 11%
2	D	153	86% • 11%
3	G	516	63% 12% 25%
3	I	516	63% 12% 25%
3	J	516	63% 12% 25%

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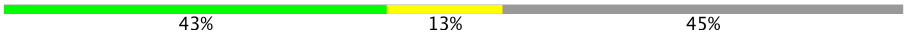
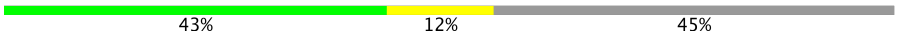
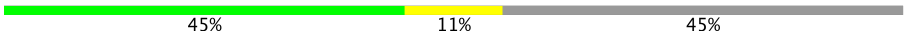
Mol	Chain	Length	Quality of chain
4	C	185	
4	E	185	
4	F	185	
5	H	229	
5	K	229	
5	M	229	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23727 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 17b Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	110	Total	C	N	O	S	0	0
			849	531	148	168	2		
1	N	110	Total	C	N	O	S	0	0
			849	531	148	168	2		
1	O	110	Total	C	N	O	S	0	0
			849	531	148	168	2		

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	136	Total	C	N	O	S	0	0
			1090	695	184	203	8		
2	B	136	Total	C	N	O	S	0	0
			1090	695	184	203	8		
2	D	136	Total	C	N	O	S	0	0
			1090	695	184	203	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	engineered mutation	UNP B3UEZ6
A	605	CYS	THR	engineered mutation	UNP B3UEZ6
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6
D	559	PRO	ILE	engineered mutation	UNP B3UEZ6
D	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	389	Total	C	N	O	S	0	0
			3050	1913	541	572	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	389	Total	C	N	O	S	0	0
			3050	1913	541	572	24		
3	J	389	Total	C	N	O	S	0	0
			3050	1913	541	572	24		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	MET	-	initiating methionine	UNP B3UES2
G	-3	ASP	-	expression tag	UNP B3UES2
G	-2	ALA	-	expression tag	UNP B3UES2
G	-1	MET	-	expression tag	UNP B3UES2
G	0	LYS	-	expression tag	UNP B3UES2
G	1	ARG	-	expression tag	UNP B3UES2
G	2	GLY	-	expression tag	UNP B3UES2
G	3	LEU	-	expression tag	UNP B3UES2
G	4	CYS	-	expression tag	UNP B3UES2
G	5	CYS	-	expression tag	UNP B3UES2
G	6	VAL	-	expression tag	UNP B3UES2
G	7	LEU	-	expression tag	UNP B3UES2
G	8	LEU	-	expression tag	UNP B3UES2
G	9	LEU	-	expression tag	UNP B3UES2
G	10	CYS	-	expression tag	UNP B3UES2
G	11	GLY	-	expression tag	UNP B3UES2
G	12	ALA	-	expression tag	UNP B3UES2
G	13	VAL	-	expression tag	UNP B3UES2
G	14	PHE	-	expression tag	UNP B3UES2
G	15	VAL	-	expression tag	UNP B3UES2
G	16	SER	-	expression tag	UNP B3UES2
G	17	PRO	-	expression tag	UNP B3UES2
G	18	SER	-	expression tag	UNP B3UES2
G	19	GLN	-	expression tag	UNP B3UES2
G	20	GLU	-	expression tag	UNP B3UES2
G	21	ILE	-	expression tag	UNP B3UES2
G	22	HIS	-	expression tag	UNP B3UES2
G	23	ALA	-	expression tag	UNP B3UES2
G	24	ARG	-	expression tag	UNP B3UES2
G	25	PHE	-	expression tag	UNP B3UES2
G	26	ARG	-	expression tag	UNP B3UES2
G	27	ARG	-	expression tag	UNP B3UES2
G	28	GLY	-	expression tag	UNP B3UES2
G	29	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	30	ARG	-	expression tag	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2
I	-4	MET	-	initiating methionine	UNP B3UES2
I	-3	ASP	-	expression tag	UNP B3UES2
I	-2	ALA	-	expression tag	UNP B3UES2
I	-1	MET	-	expression tag	UNP B3UES2
I	0	LYS	-	expression tag	UNP B3UES2
I	1	ARG	-	expression tag	UNP B3UES2
I	2	GLY	-	expression tag	UNP B3UES2
I	3	LEU	-	expression tag	UNP B3UES2
I	4	CYS	-	expression tag	UNP B3UES2
I	5	CYS	-	expression tag	UNP B3UES2
I	6	VAL	-	expression tag	UNP B3UES2
I	7	LEU	-	expression tag	UNP B3UES2
I	8	LEU	-	expression tag	UNP B3UES2
I	9	LEU	-	expression tag	UNP B3UES2
I	10	CYS	-	expression tag	UNP B3UES2
I	11	GLY	-	expression tag	UNP B3UES2
I	12	ALA	-	expression tag	UNP B3UES2
I	13	VAL	-	expression tag	UNP B3UES2
I	14	PHE	-	expression tag	UNP B3UES2
I	15	VAL	-	expression tag	UNP B3UES2
I	16	SER	-	expression tag	UNP B3UES2
I	17	PRO	-	expression tag	UNP B3UES2
I	18	SER	-	expression tag	UNP B3UES2
I	19	GLN	-	expression tag	UNP B3UES2
I	20	GLU	-	expression tag	UNP B3UES2
I	21	ILE	-	expression tag	UNP B3UES2
I	22	HIS	-	expression tag	UNP B3UES2
I	23	ALA	-	expression tag	UNP B3UES2
I	24	ARG	-	expression tag	UNP B3UES2
I	25	PHE	-	expression tag	UNP B3UES2
I	26	ARG	-	expression tag	UNP B3UES2
I	27	ARG	-	expression tag	UNP B3UES2
I	28	GLY	-	expression tag	UNP B3UES2
I	29	ALA	-	expression tag	UNP B3UES2
I	30	ARG	-	expression tag	UNP B3UES2
I	501	CYS	ALA	engineered mutation	UNP B3UES2
J	-4	MET	-	initiating methionine	UNP B3UES2
J	-3	ASP	-	expression tag	UNP B3UES2
J	-2	ALA	-	expression tag	UNP B3UES2
J	-1	MET	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	LYS	-	expression tag	UNP B3UES2
J	1	ARG	-	expression tag	UNP B3UES2
J	2	GLY	-	expression tag	UNP B3UES2
J	3	LEU	-	expression tag	UNP B3UES2
J	4	CYS	-	expression tag	UNP B3UES2
J	5	CYS	-	expression tag	UNP B3UES2
J	6	VAL	-	expression tag	UNP B3UES2
J	7	LEU	-	expression tag	UNP B3UES2
J	8	LEU	-	expression tag	UNP B3UES2
J	9	LEU	-	expression tag	UNP B3UES2
J	10	CYS	-	expression tag	UNP B3UES2
J	11	GLY	-	expression tag	UNP B3UES2
J	12	ALA	-	expression tag	UNP B3UES2
J	13	VAL	-	expression tag	UNP B3UES2
J	14	PHE	-	expression tag	UNP B3UES2
J	15	VAL	-	expression tag	UNP B3UES2
J	16	SER	-	expression tag	UNP B3UES2
J	17	PRO	-	expression tag	UNP B3UES2
J	18	SER	-	expression tag	UNP B3UES2
J	19	GLN	-	expression tag	UNP B3UES2
J	20	GLU	-	expression tag	UNP B3UES2
J	21	ILE	-	expression tag	UNP B3UES2
J	22	HIS	-	expression tag	UNP B3UES2
J	23	ALA	-	expression tag	UNP B3UES2
J	24	ARG	-	expression tag	UNP B3UES2
J	25	PHE	-	expression tag	UNP B3UES2
J	26	ARG	-	expression tag	UNP B3UES2
J	27	ARG	-	expression tag	UNP B3UES2
J	28	GLY	-	expression tag	UNP B3UES2
J	29	ALA	-	expression tag	UNP B3UES2
J	30	ARG	-	expression tag	UNP B3UES2
J	501	CYS	ALA	engineered mutation	UNP B3UES2

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
4	E	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
4	F	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		

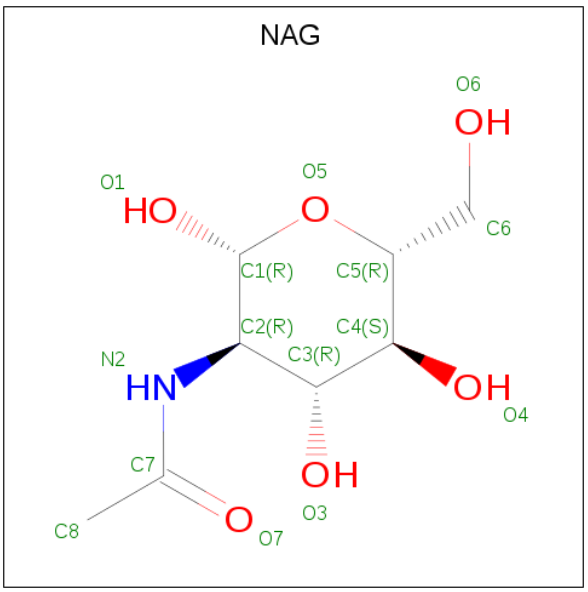
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	184	ASN	-	expression tag	UNP P01730
C	185	THR	-	expression tag	UNP P01730
E	184	ASN	-	expression tag	UNP P01730
E	185	THR	-	expression tag	UNP P01730
F	184	ASN	-	expression tag	UNP P01730
F	185	THR	-	expression tag	UNP P01730

- Molecule 5 is a protein called 17b Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	127	Total	C	N	O	S	0	0
			987	623	169	192	3		
5	K	127	Total	C	N	O	S	0	0
			987	623	169	192	3		
5	M	127	Total	C	N	O	S	0	0
			987	623	169	192	3		

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



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	

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Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 56	C 32	N 4	O 20	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0
6	G	1	Total 364	C 208	N 26	O 130	0

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Mol	Chain	Residues	Atoms				AltConf
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	G	1	Total	C	N	O	0
			364	208	26	130	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	

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Mol	Chain	Residues	Atoms				AltConf
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	I	1	Total	C	N	O	0
			364	208	26	130	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	

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Mol	Chain	Residues	Atoms				AltConf
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	

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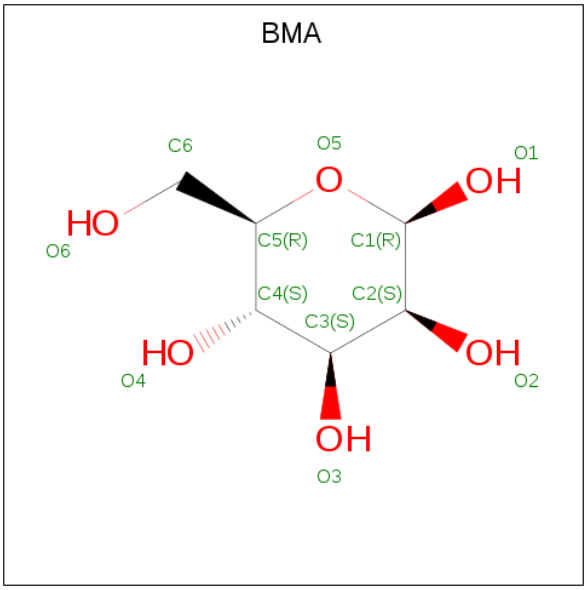
Mol	Chain	Residues	Atoms				AltConf
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	
6	J	1	Total	C	N	O	0
			364	208	26	130	

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



Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	G	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	

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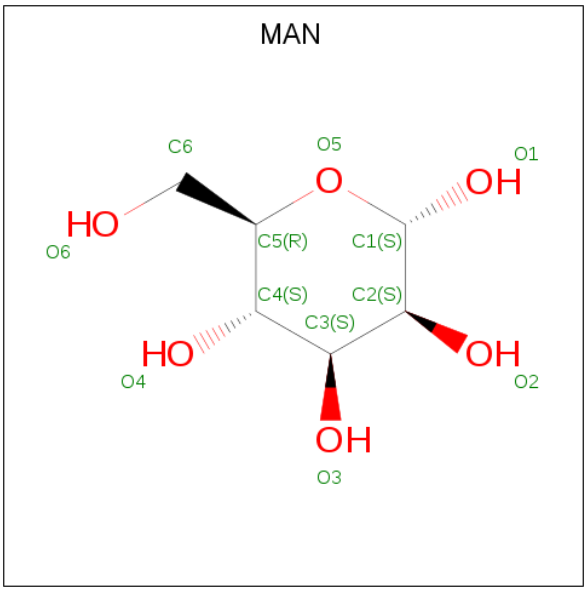
Mol	Chain	Residues	Atoms			AltConf
7	I	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	
7	I	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	
7	J	1	Total	C	O	0
			77	42	35	

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			66	36	30	
8	G	1	Total	C	O	0
			66	36	30	
8	G	1	Total	C	O	0
			66	36	30	
8	G	1	Total	C	O	0
			66	36	30	
8	G	1	Total	C	O	0
			66	36	30	
8	G	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	I	1	Total	C	O	0
			66	36	30	
8	J	1	Total	C	O	0
			66	36	30	
8	J	1	Total	C	O	0
			66	36	30	

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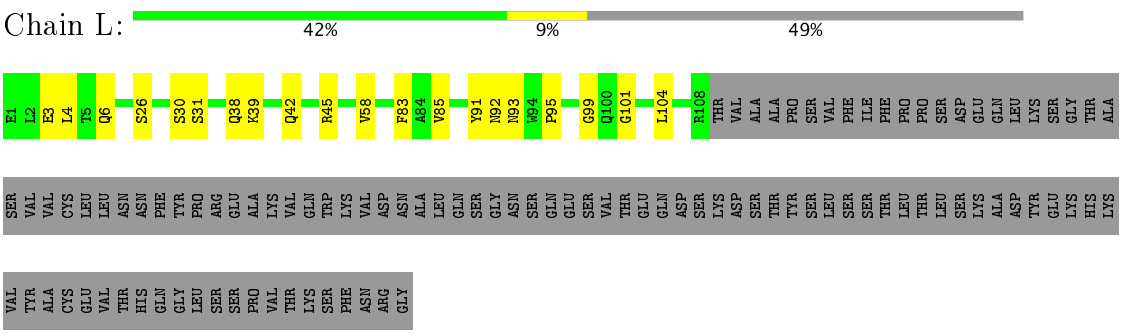
Mol	Chain	Residues	Atoms			AltConf
8	J	1	Total	C	O	0
			66	36	30	
8	J	1	Total	C	O	0
			66	36	30	
8	J	1	Total	C	O	0
			66	36	30	
8	J	1	Total	C	O	0
			66	36	30	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

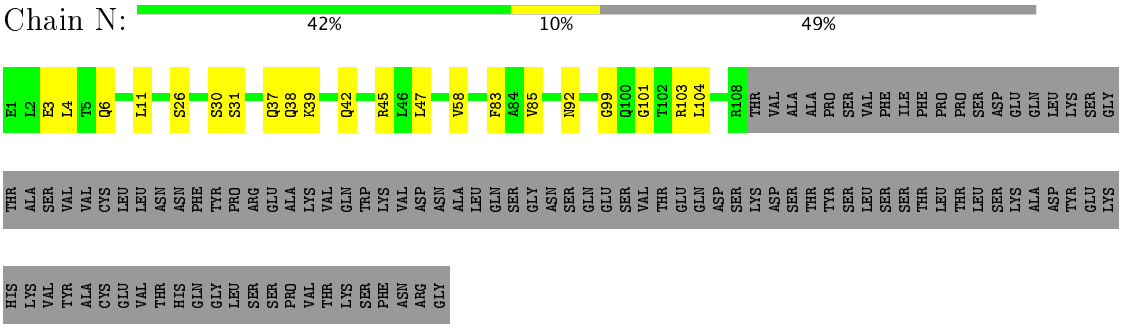
- Molecule 1: 17b Fab light chain

Chain L:



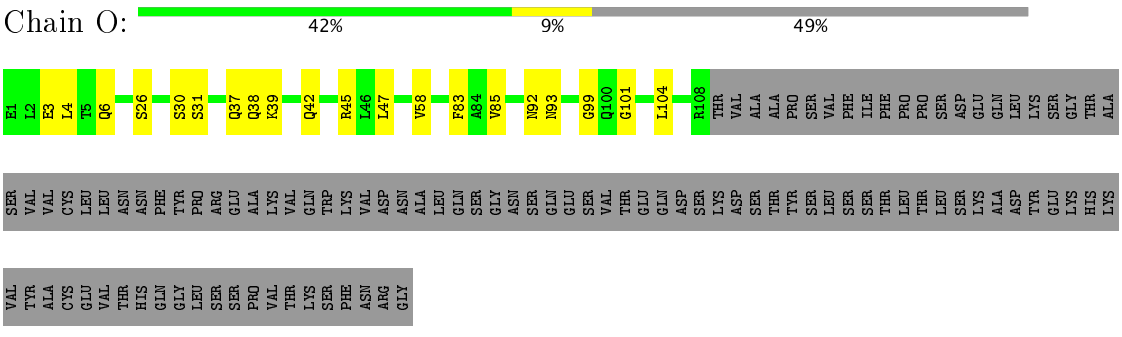
- Molecule 1: 17b Fab light chain

Chain N:



- Molecule 1: 17b Fab light chain

Chain O:



- Molecule 2: Envelope glycoprotein gp160

Chain A:

• Molecule 2: Envelope glycoprotein gp160

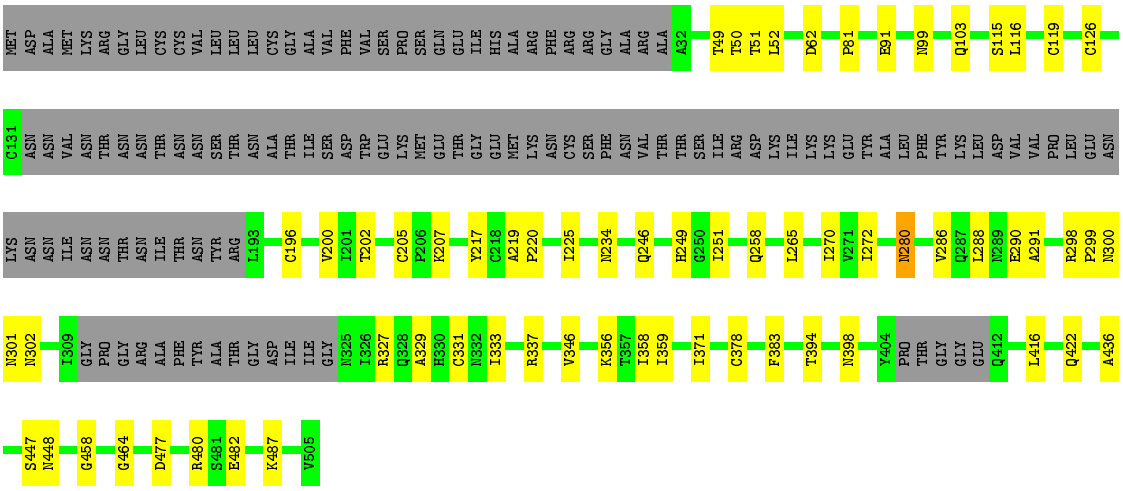
Chain B:

• Molecule 2: Envelope glycoprotein gp160

Chain D:

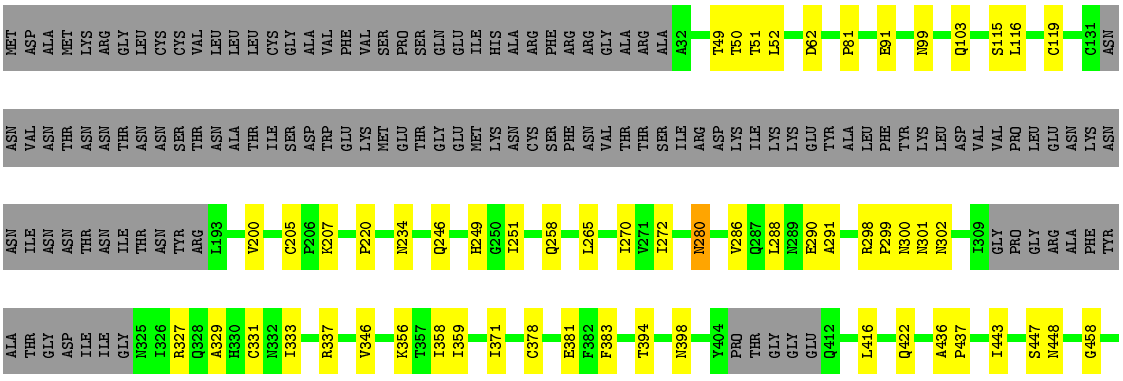
• Molecule 3: Envelope glycoprotein gp160

Chain G:



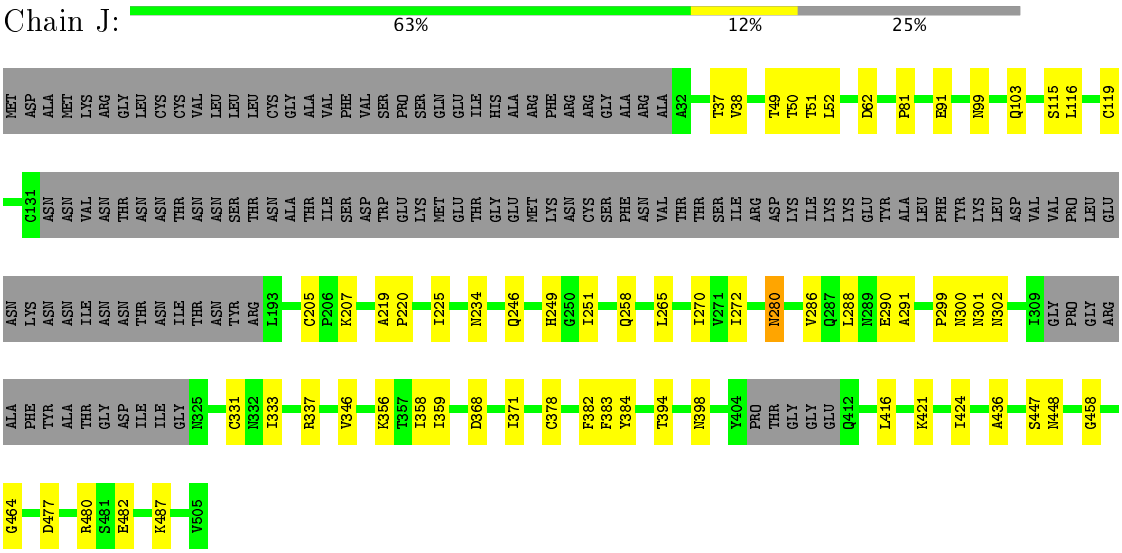
• Molecule 3: Envelope glycoprotein gp160

Chain I:



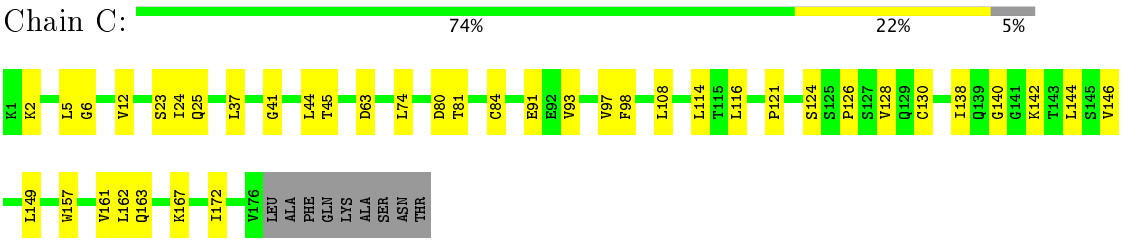
• Molecule 3: Envelope glycoprotein gp160

Chain J:



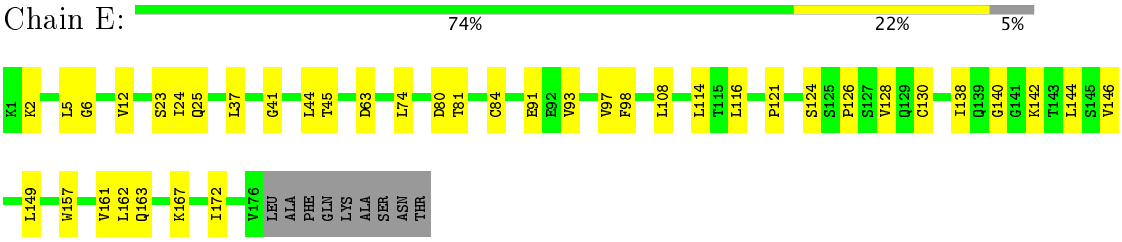
• Molecule 4: T-cell surface glycoprotein CD4

Chain C:



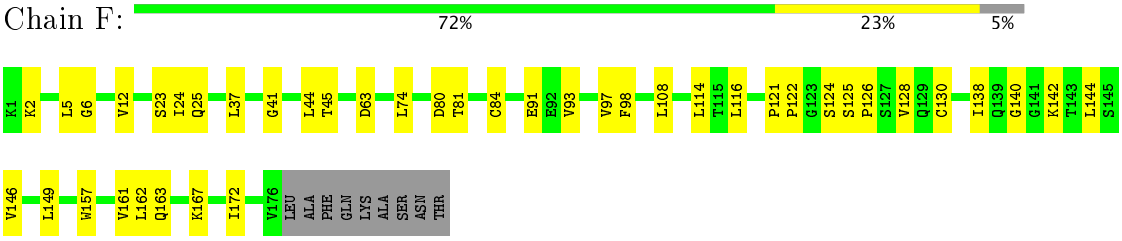
• Molecule 4: T-cell surface glycoprotein CD4

Chain E:



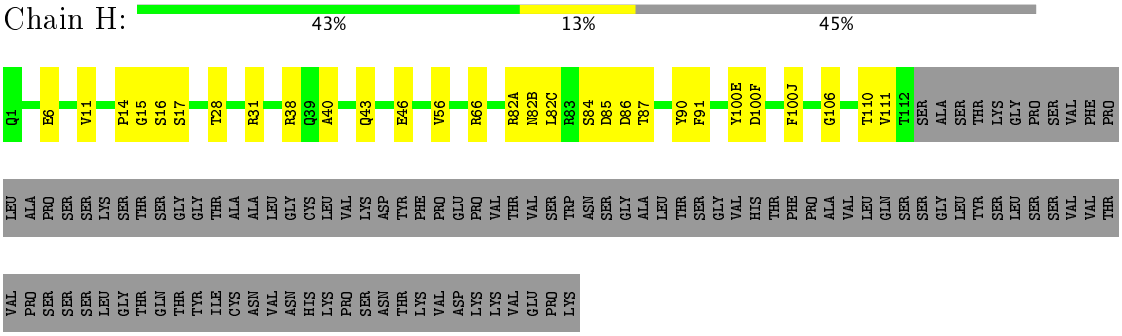
• Molecule 4: T-cell surface glycoprotein CD4

Chain F:



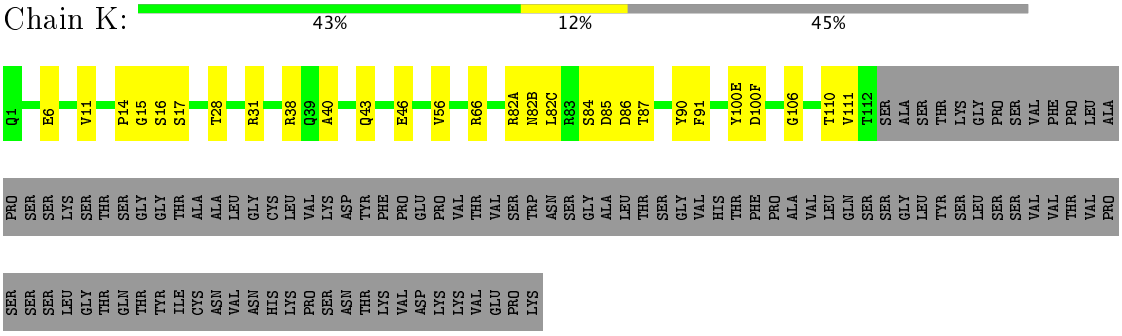
- Molecule 5: 17b Fab heavy chain

Chain H:



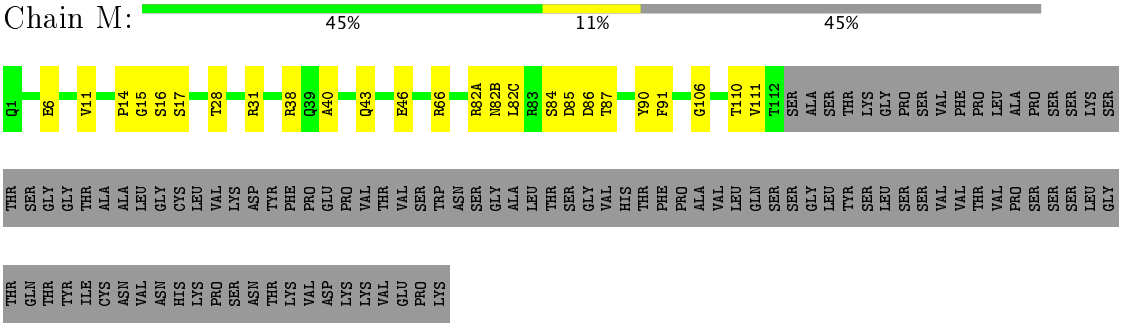
- Molecule 5: 17b Fab heavy chain

Chain K:



- Molecule 5: 17b Fab heavy chain

Chain M:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	46855	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	38168	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	L	0.40	0/869	0.63	0/1181
1	N	0.40	0/869	0.63	0/1181
1	O	0.40	0/869	0.63	0/1181
2	A	0.53	0/1110	0.57	0/1503
2	B	0.53	0/1110	0.57	0/1503
2	D	0.53	0/1110	0.57	0/1503
3	G	0.52	0/3115	0.68	0/4236
3	I	0.52	0/3115	0.68	0/4236
3	J	0.52	0/3115	0.68	0/4236
4	C	0.34	0/1389	0.60	0/1873
4	E	0.34	0/1389	0.60	0/1873
4	F	0.34	0/1389	0.60	0/1873
5	H	0.45	0/1008	0.64	0/1368
5	K	0.45	0/1008	0.64	0/1368
5	M	0.45	0/1008	0.64	0/1368
All	All	0.47	0/22473	0.64	0/30483

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	849	0	819	16	0
1	N	849	0	819	12	0
1	O	849	0	819	13	0
2	A	1090	0	1074	5	0
2	B	1090	0	1074	2	0
2	D	1090	0	1074	4	0
3	G	3050	0	2977	38	0
3	I	3050	0	2977	36	0
3	J	3050	0	2977	36	0
4	C	1370	0	1398	23	0
4	E	1370	0	1398	23	0
4	F	1370	0	1398	26	0
5	H	987	0	958	22	0
5	K	987	0	958	20	0
5	M	987	0	958	17	0
6	A	56	0	52	0	0
6	B	56	0	52	0	0
6	D	56	0	52	0	0
6	G	364	0	315	2	0
6	I	364	0	318	1	0
6	J	364	0	318	1	0
7	G	77	0	66	0	0
7	I	77	0	66	0	0
7	J	77	0	66	0	0
8	G	66	0	58	0	0
8	I	66	0	58	0	0
8	J	66	0	58	0	0
All	All	23727	0	23157	279	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 6.

The worst 5 of 279 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:52:LEU:H	3:I:103:GLN:HE22	1.34	0.75
3:J:52:LEU:H	3:J:103:GLN:HE22	1.35	0.75
3:G:52:LEU:H	3:G:103:GLN:HE22	1.35	0.75
5:M:6:GLU:HG3	5:M:106:GLY:H	1.59	0.67
5:K:6:GLU:HG3	5:K:106:GLY:H	1.59	0.67

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	L	108/214 (50%)	91 (84%)	17 (16%)	0	100	100
1	N	108/214 (50%)	91 (84%)	17 (16%)	0	100	100
1	O	108/214 (50%)	91 (84%)	17 (16%)	0	100	100
2	A	132/153 (86%)	127 (96%)	5 (4%)	0	100	100
2	B	132/153 (86%)	127 (96%)	5 (4%)	0	100	100
2	D	132/153 (86%)	127 (96%)	5 (4%)	0	100	100
3	G	381/516 (74%)	335 (88%)	42 (11%)	4 (1%)	18	62
3	I	381/516 (74%)	335 (88%)	42 (11%)	4 (1%)	18	62
3	J	381/516 (74%)	335 (88%)	42 (11%)	4 (1%)	18	62
4	C	174/185 (94%)	148 (85%)	26 (15%)	0	100	100
4	E	174/185 (94%)	148 (85%)	26 (15%)	0	100	100
4	F	174/185 (94%)	148 (85%)	26 (15%)	0	100	100
5	H	125/229 (55%)	116 (93%)	9 (7%)	0	100	100
5	K	125/229 (55%)	116 (93%)	9 (7%)	0	100	100
5	M	125/229 (55%)	116 (93%)	9 (7%)	0	100	100
All	All	2760/3891 (71%)	2451 (89%)	297 (11%)	12 (0%)	42	77

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	301	ASN
3	I	301	ASN
3	J	301	ASN
3	G	299	PRO
3	I	299	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	L	91/184 (50%)	91 (100%)	0	100 100
1	N	91/184 (50%)	91 (100%)	0	100 100
1	O	91/184 (50%)	91 (100%)	0	100 100
2	A	117/130 (90%)	117 (100%)	0	100 100
2	B	117/130 (90%)	117 (100%)	0	100 100
2	D	117/130 (90%)	117 (100%)	0	100 100
3	G	344/453 (76%)	344 (100%)	0	100 100
3	I	344/453 (76%)	344 (100%)	0	100 100
3	J	344/453 (76%)	344 (100%)	0	100 100
4	C	160/167 (96%)	159 (99%)	1 (1%)	89 95
4	E	160/167 (96%)	159 (99%)	1 (1%)	89 95
4	F	160/167 (96%)	159 (99%)	1 (1%)	89 95
5	H	105/193 (54%)	105 (100%)	0	100 100
5	K	105/193 (54%)	105 (100%)	0	100 100
5	M	105/193 (54%)	105 (100%)	0	100 100
All	All	2451/3381 (72%)	2448 (100%)	3 (0%)	95 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	24	ILE
4	E	24	ILE
4	F	24	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	103	GLN

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Mol	Chain	Res	Type
3	I	422	GLN
3	J	398	ASN
2	B	656	ASN
3	J	422	GLN

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)

129 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	$\#\|Z\| > 2$
6	NAG	A	701	2	14,14,15	0.58	0	15,19,21	0.56	0
6	NAG	A	702	2	14,14,15	0.46	0	15,19,21	0.79	1 (6%)
6	NAG	A	703	2	14,14,15	0.73	0	15,19,21	0.70	1 (6%)
6	NAG	A	704	2	14,14,15	0.32	0	15,19,21	0.52	0
6	NAG	B	701	2	14,14,15	0.40	0	15,19,21	0.52	0
6	NAG	B	702	2	14,14,15	0.46	0	15,19,21	0.70	1 (6%)
6	NAG	B	703	2	14,14,15	0.51	0	15,19,21	0.70	1 (6%)
6	NAG	B	704	2	14,14,15	0.27	0	15,19,21	0.40	0
6	NAG	D	701	2	14,14,15	0.49	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	D	702	2	14,14,15	0.44	0	15,19,21	0.68	1 (6%)
6	NAG	D	703	2	14,14,15	0.60	0	15,19,21	0.71	1 (6%)
6	NAG	D	704	2	14,14,15	0.26	0	15,19,21	0.57	0
6	NAG	G	601	3	14,14,15	0.23	0	15,19,21	0.53	0
6	NAG	G	602	3,6	14,14,15	0.68	1 (7%)	15,19,21	0.66	0
6	NAG	G	603	6	14,14,15	0.26	0	15,19,21	0.80	1 (6%)
6	NAG	G	604	3,6	14,14,15	0.32	0	15,19,21	0.77	1 (6%)
6	NAG	G	605	7,6	14,14,15	0.24	0	15,19,21	0.51	0
7	BMA	G	606	6	11,11,12	0.82	0	13,15,17	1.08	1 (7%)
6	NAG	G	607	3,6	14,14,15	1.19	1 (7%)	15,19,21	0.61	0
6	NAG	G	608	7,6	14,14,15	0.23	0	15,19,21	0.59	0
7	BMA	G	609	8,6	11,11,12	0.66	0	13,15,17	1.02	1 (7%)
8	MAN	G	610	8,7	11,11,12	0.98	0	13,15,17	1.80	2 (15%)
8	MAN	G	611	8	11,11,12	0.80	0	13,15,17	1.59	2 (15%)
8	MAN	G	612	8	11,11,12	0.75	0	13,15,17	1.11	2 (15%)
8	MAN	G	613	7	11,11,12	1.05	2 (18%)	13,15,17	1.31	3 (23%)
6	NAG	G	614	3,6	14,14,15	1.02	1 (7%)	15,19,21	0.82	1 (6%)
6	NAG	G	615	7,6	14,14,15	0.20	0	15,19,21	0.80	1 (6%)
7	BMA	G	616	8,6	11,11,12	0.76	0	13,15,17	0.95	1 (7%)
8	MAN	G	617	7	11,11,12	0.98	1 (9%)	13,15,17	1.14	2 (15%)
6	NAG	G	618	3,6	14,14,15	0.35	0	15,19,21	0.55	0
6	NAG	G	619	6	14,14,15	0.32	0	15,19,21	0.64	0
6	NAG	G	620	3,6	14,14,15	0.17	0	15,19,21	0.70	1 (6%)
6	NAG	G	621	6	14,14,15	0.27	0	15,19,21	0.51	0
6	NAG	G	622	3	14,14,15	0.27	0	15,19,21	0.45	0
6	NAG	G	623	3	14,14,15	0.36	0	15,19,21	0.46	0
6	NAG	G	624	3,6	14,14,15	0.70	1 (7%)	15,19,21	0.82	1 (6%)
6	NAG	G	625	7,6	14,14,15	0.22	0	15,19,21	0.50	0
7	BMA	G	626	8,6	11,11,12	0.63	0	13,15,17	1.08	1 (7%)
8	MAN	G	627	7	11,11,12	1.00	1 (9%)	13,15,17	1.73	2 (15%)
6	NAG	G	628	3,6	14,14,15	0.26	0	15,19,21	0.51	0
6	NAG	G	629	7,6	14,14,15	0.22	0	15,19,21	0.58	0
7	BMA	G	630	6	11,11,12	0.77	0	13,15,17	0.92	1 (7%)
6	NAG	G	631	3	14,14,15	0.45	0	15,19,21	0.58	0
6	NAG	G	632	3,6	14,14,15	0.33	0	15,19,21	0.80	1 (6%)
6	NAG	G	633	7,6	14,14,15	0.26	0	15,19,21	0.79	1 (6%)
7	BMA	G	634	6	11,11,12	0.76	0	13,15,17	0.94	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	G	635	3,6	14,14,15	0.48	0	15,19,21	0.81	1 (6%)
6	NAG	G	636	6	14,14,15	0.29	0	15,19,21	0.57	0
6	NAG	G	637	3,6	14,14,15	0.27	0	15,19,21	0.53	0
6	NAG	G	638	7,6	14,14,15	0.41	0	15,19,21	0.55	0
7	BMA	G	639	6	11,11,12	0.65	0	13,15,17	0.87	0
6	NAG	I	601	3	14,14,15	0.31	0	15,19,21	0.48	0
6	NAG	I	602	3,6	14,14,15	0.72	1 (7%)	15,19,21	0.67	0
6	NAG	I	603	6	14,14,15	0.24	0	15,19,21	0.79	1 (6%)
6	NAG	I	604	3,6	14,14,15	0.30	0	15,19,21	0.77	1 (6%)
6	NAG	I	605	7,6	14,14,15	0.25	0	15,19,21	0.48	0
7	BMA	I	606	6	11,11,12	0.82	0	13,15,17	1.06	1 (7%)
6	NAG	I	607	3,6	14,14,15	0.24	0	15,19,21	0.89	1 (6%)
6	NAG	I	608	7,6	14,14,15	0.21	0	15,19,21	0.63	0
7	BMA	I	609	8,6	11,11,12	0.67	0	13,15,17	1.03	1 (7%)
8	MAN	I	610	8,7	11,11,12	0.98	0	13,15,17	1.81	2 (15%)
8	MAN	I	611	8	11,11,12	0.80	0	13,15,17	1.52	2 (15%)
8	MAN	I	612	8	11,11,12	0.78	0	13,15,17	1.08	2 (15%)
8	MAN	I	613	7	11,11,12	1.04	2 (18%)	13,15,17	1.36	3 (23%)
6	NAG	I	614	3,6	14,14,15	1.01	1 (7%)	15,19,21	0.78	1 (6%)
6	NAG	I	615	7,6	14,14,15	0.24	0	15,19,21	0.79	1 (6%)
7	BMA	I	616	8,6	11,11,12	0.72	0	13,15,17	0.97	1 (7%)
8	MAN	I	617	7	11,11,12	1.05	2 (18%)	13,15,17	1.14	2 (15%)
6	NAG	I	618	3,6	14,14,15	0.34	0	15,19,21	0.55	0
6	NAG	I	619	6	14,14,15	0.35	0	15,19,21	0.65	0
6	NAG	I	620	3,6	14,14,15	0.22	0	15,19,21	0.72	1 (6%)
6	NAG	I	621	6	14,14,15	0.29	0	15,19,21	0.55	0
6	NAG	I	622	3	14,14,15	0.22	0	15,19,21	0.46	0
6	NAG	I	623	3	14,14,15	0.30	0	15,19,21	0.49	0
6	NAG	I	624	3,6	14,14,15	0.77	1 (7%)	15,19,21	0.83	1 (6%)
6	NAG	I	625	7,6	14,14,15	0.19	0	15,19,21	0.50	0
7	BMA	I	626	8,6	11,11,12	0.56	0	13,15,17	1.21	3 (23%)
8	MAN	I	627	7	11,11,12	0.90	1 (9%)	13,15,17	1.65	2 (15%)
6	NAG	I	628	3,6	14,14,15	0.33	0	15,19,21	0.54	0
6	NAG	I	629	7,6	14,14,15	0.21	0	15,19,21	0.65	1 (6%)
7	BMA	I	630	6	11,11,12	0.79	0	13,15,17	0.93	1 (7%)
6	NAG	I	631	3	14,14,15	0.39	0	15,19,21	0.59	0
6	NAG	I	632	3,6	14,14,15	0.31	0	15,19,21	0.78	1 (6%)
6	NAG	I	633	7,6	14,14,15	0.26	0	15,19,21	0.75	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	I	634	6	11,11,12	0.77	0	13,15,17	1.01	1 (7%)
6	NAG	I	635	3,6	14,14,15	0.57	1 (7%)	15,19,21	0.74	1 (6%)
6	NAG	I	636	6	14,14,15	0.30	0	15,19,21	0.57	0
6	NAG	I	637	3,6	14,14,15	0.29	0	15,19,21	0.53	0
6	NAG	I	638	7,6	14,14,15	0.49	0	15,19,21	0.54	0
7	BMA	I	639	6	11,11,12	0.58	0	13,15,17	0.84	0
6	NAG	J	601	3	14,14,15	0.24	0	15,19,21	0.58	0
6	NAG	J	602	3,6	14,14,15	0.68	1 (7%)	15,19,21	0.64	0
6	NAG	J	603	6	14,14,15	0.22	0	15,19,21	0.77	1 (6%)
6	NAG	J	604	3,6	14,14,15	0.35	0	15,19,21	0.79	1 (6%)
6	NAG	J	605	7,6	14,14,15	0.21	0	15,19,21	0.52	0
7	BMA	J	606	6	11,11,12	0.82	0	13,15,17	1.01	1 (7%)
6	NAG	J	607	3,6	14,14,15	0.28	0	15,19,21	0.79	1 (6%)
6	NAG	J	608	7,6	14,14,15	0.23	0	15,19,21	0.61	0
7	BMA	J	609	8,6	11,11,12	0.68	0	13,15,17	1.10	1 (7%)
8	MAN	J	610	8,7	11,11,12	0.97	1 (9%)	13,15,17	1.82	2 (15%)
8	MAN	J	611	8	11,11,12	0.84	0	13,15,17	1.49	2 (15%)
8	MAN	J	612	8	11,11,12	0.74	0	13,15,17	1.15	2 (15%)
8	MAN	J	613	7	11,11,12	1.03	1 (9%)	13,15,17	1.41	3 (23%)
6	NAG	J	614	3,6	14,14,15	0.97	1 (7%)	15,19,21	0.83	1 (6%)
6	NAG	J	615	7,6	14,14,15	0.27	0	15,19,21	0.76	1 (6%)
7	BMA	J	616	8,6	11,11,12	0.75	0	13,15,17	0.96	1 (7%)
8	MAN	J	617	7	11,11,12	0.95	0	13,15,17	1.16	2 (15%)
6	NAG	J	618	3,6	14,14,15	0.34	0	15,19,21	0.57	0
6	NAG	J	619	6	14,14,15	0.32	0	15,19,21	0.66	1 (6%)
6	NAG	J	620	3,6	14,14,15	0.18	0	15,19,21	0.64	0
6	NAG	J	621	6	14,14,15	0.27	0	15,19,21	0.57	0
6	NAG	J	622	3	14,14,15	0.24	0	15,19,21	0.43	0
6	NAG	J	623	3	14,14,15	0.30	0	15,19,21	0.45	0
6	NAG	J	624	3,6	14,14,15	0.76	1 (7%)	15,19,21	0.82	1 (6%)
6	NAG	J	625	7,6	14,14,15	0.21	0	15,19,21	0.52	0
7	BMA	J	626	8,6	11,11,12	0.54	0	13,15,17	1.09	2 (15%)
8	MAN	J	627	7	11,11,12	1.08	1 (9%)	13,15,17	1.81	2 (15%)
6	NAG	J	628	3,6	14,14,15	0.25	0	15,19,21	0.48	0
6	NAG	J	629	7,6	14,14,15	0.21	0	15,19,21	0.60	0
7	BMA	J	630	6	11,11,12	0.79	0	13,15,17	0.92	1 (7%)
6	NAG	J	631	3	14,14,15	0.40	0	15,19,21	0.58	0
6	NAG	J	632	3,6	14,14,15	0.48	0	15,19,21	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	J	633	7,6	14,14,15	0.29	0	15,19,21	0.80	1 (6%)
7	BMA	J	634	6	11,11,12	0.75	0	13,15,17	0.95	1 (7%)
6	NAG	J	635	3,6	14,14,15	0.51	0	15,19,21	0.76	1 (6%)
6	NAG	J	636	6	14,14,15	0.28	0	15,19,21	0.57	0
6	NAG	J	637	3,6	14,14,15	0.29	0	15,19,21	0.52	0
6	NAG	J	638	7,6	14,14,15	0.44	0	15,19,21	0.51	0
7	BMA	J	639	6	11,11,12	0.60	0	13,15,17	0.85	0

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
6	NAG	A	701	2	-	0/6/23/26	0/1/1/1
6	NAG	A	702	2	-	0/6/23/26	0/1/1/1
6	NAG	A	703	2	-	0/6/23/26	0/1/1/1
6	NAG	A	704	2	-	0/6/23/26	0/1/1/1
6	NAG	B	701	2	-	0/6/23/26	0/1/1/1
6	NAG	B	702	2	-	0/6/23/26	0/1/1/1
6	NAG	B	703	2	-	0/6/23/26	0/1/1/1
6	NAG	B	704	2	-	0/6/23/26	0/1/1/1
6	NAG	D	701	2	-	0/6/23/26	0/1/1/1
6	NAG	D	702	2	-	0/6/23/26	0/1/1/1
6	NAG	D	703	2	-	0/6/23/26	0/1/1/1
6	NAG	D	704	2	-	0/6/23/26	0/1/1/1
6	NAG	G	601	3	-	0/6/23/26	0/1/1/1
6	NAG	G	602	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	603	6	-	0/6/23/26	0/1/1/1
6	NAG	G	604	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	605	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	606	6	-	0/2/19/22	0/1/1/1
6	NAG	G	607	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	610	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	611	8	-	0/2/19/22	0/1/1/1
8	MAN	G	612	8	-	0/2/19/22	0/1/1/1
8	MAN	G	613	7	-	0/2/19/22	0/1/1/1
6	NAG	G	614	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	615	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	616	8,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	G	617	7	-	0/2/19/22	0/1/1/1
6	NAG	G	618	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	619	6	-	0/6/23/26	0/1/1/1
6	NAG	G	620	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	621	6	-	0/6/23/26	0/1/1/1
6	NAG	G	622	3	-	0/6/23/26	0/1/1/1
6	NAG	G	623	3	-	0/6/23/26	0/1/1/1
6	NAG	G	624	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	625	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	626	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	627	7	-	0/2/19/22	0/1/1/1
6	NAG	G	628	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	629	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	630	6	-	0/2/19/22	0/1/1/1
6	NAG	G	631	3	-	0/6/23/26	0/1/1/1
6	NAG	G	632	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	633	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	634	6	-	0/2/19/22	0/1/1/1
6	NAG	G	635	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	636	6	-	0/6/23/26	0/1/1/1
6	NAG	G	637	3,6	-	0/6/23/26	0/1/1/1
6	NAG	G	638	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	639	6	-	0/2/19/22	0/1/1/1
6	NAG	I	601	3	-	0/6/23/26	0/1/1/1
6	NAG	I	602	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	603	6	-	0/6/23/26	0/1/1/1
6	NAG	I	604	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	605	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	606	6	-	0/2/19/22	0/1/1/1
6	NAG	I	607	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	I	610	8,7	-	0/2/19/22	0/1/1/1
8	MAN	I	611	8	-	0/2/19/22	0/1/1/1
8	MAN	I	612	8	-	0/2/19/22	0/1/1/1
8	MAN	I	613	7	-	0/2/19/22	0/1/1/1
6	NAG	I	614	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	615	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	616	8,6	-	0/2/19/22	0/1/1/1
8	MAN	I	617	7	-	0/2/19/22	0/1/1/1
6	NAG	I	618	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	619	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	620	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	621	6	-	0/6/23/26	0/1/1/1
6	NAG	I	622	3	-	0/6/23/26	0/1/1/1
6	NAG	I	623	3	-	0/6/23/26	0/1/1/1
6	NAG	I	624	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	625	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	626	8,6	-	0/2/19/22	0/1/1/1
8	MAN	I	627	7	-	0/2/19/22	0/1/1/1
6	NAG	I	628	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	629	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	630	6	-	0/2/19/22	0/1/1/1
6	NAG	I	631	3	-	0/6/23/26	0/1/1/1
6	NAG	I	632	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	633	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	634	6	-	0/2/19/22	0/1/1/1
6	NAG	I	635	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	636	6	-	0/6/23/26	0/1/1/1
6	NAG	I	637	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	638	7,6	-	0/6/23/26	0/1/1/1
7	BMA	I	639	6	-	0/2/19/22	0/1/1/1
6	NAG	J	601	3	-	0/6/23/26	0/1/1/1
6	NAG	J	602	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	603	6	-	0/6/23/26	0/1/1/1
6	NAG	J	604	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	605	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	606	6	-	0/2/19/22	0/1/1/1
6	NAG	J	607	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	610	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	611	8	-	0/2/19/22	0/1/1/1
8	MAN	J	612	8	-	0/2/19/22	0/1/1/1
8	MAN	J	613	7	-	0/2/19/22	0/1/1/1
6	NAG	J	614	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	615	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	616	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	617	7	-	0/2/19/22	0/1/1/1
6	NAG	J	618	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	619	6	-	0/6/23/26	0/1/1/1
6	NAG	J	620	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	621	6	-	0/6/23/26	0/1/1/1
6	NAG	J	622	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	623	3	-	0/6/23/26	0/1/1/1
6	NAG	J	624	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	625	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	626	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	627	7	-	0/2/19/22	0/1/1/1
6	NAG	J	628	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	629	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	630	6	-	0/2/19/22	0/1/1/1
6	NAG	J	631	3	-	0/6/23/26	0/1/1/1
6	NAG	J	632	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	633	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	634	6	-	0/2/19/22	0/1/1/1
6	NAG	J	635	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	636	6	-	0/6/23/26	0/1/1/1
6	NAG	J	637	3,6	-	0/6/23/26	0/1/1/1
6	NAG	J	638	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	639	6	-	0/2/19/22	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	607	NAG	O5-C1	-4.29	1.36	1.43
6	G	614	NAG	O5-C1	-3.71	1.37	1.43
6	I	614	NAG	O5-C1	-3.65	1.37	1.43
6	J	614	NAG	O5-C1	-3.49	1.38	1.43
6	I	624	NAG	O5-C1	-2.80	1.39	1.43

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	611	MAN	O2-C2-C3	-4.46	101.41	110.17
8	I	611	MAN	O2-C2-C3	-4.35	101.64	110.17
8	J	611	MAN	O2-C2-C3	-4.28	101.78	110.17
8	I	610	MAN	O2-C2-C3	-3.76	102.80	110.17
8	J	610	MAN	O2-C2-C3	-3.68	102.95	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	607	NAG	1	0
6	G	608	NAG	1	0
6	G	631	NAG	1	0
6	I	631	NAG	1	0
6	J	631	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.