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

Jul 25, 2017 – 10:45 AM EDT

PDB ID	:	5VN8
EMDB ID:	:	EMD-8717
Title	:	Cryo-EM model of B41 SOSIP.664 in complex with fragment antigen binding variable domain of b12
Authors	:	Ozorowski, G.; Pallesen, J.; Ward, A.B.; Cottrell, C.A.
Deposited on	:	unknown
Resolution	:	3.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation 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.

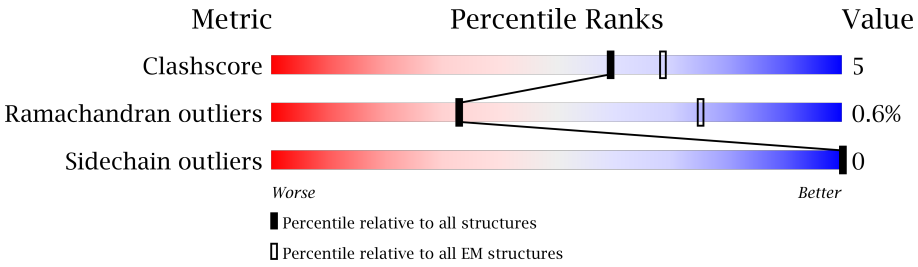
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 3.60 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	D	516	69% 15% 16%
1	E	516	68% 16% 16%
1	G	516	69% 15% 16%
2	A	153	86% 5% 9%
2	B	153	86% 5% 9%
2	C	153	86% 5% 9%
3	F	230	46% 9% 45%
3	H	230	47% 8% 45%
3	I	230	45% 10% 45%

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Mol	Chain	Length	Quality of chain
4	J	215	42% 7% 50%
4	K	215	41% 9% 50%
4	L	215	41% 9% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20589 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	435	Total	C	N	O	S	0	0
			3393	2119	600	649	25		
1	D	435	Total	C	N	O	S	0	0
			3393	2119	600	649	25		
1	E	435	Total	C	N	O	S	0	0
			3393	2119	600	649	25		

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

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

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

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	139	Total	C	N	O	S	0	0
			1104	705	186	205	8		
2	B	139	Total	C	N	O	S	0	0
			1104	705	186	205	8		
2	C	139	Total	C	N	O	S	0	0
			1104	705	186	205	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
C	559	PRO	ILE	engineered mutation	UNP B3UEZ6
C	605	CYS	THR	engineered mutation	UNP B3UEZ6

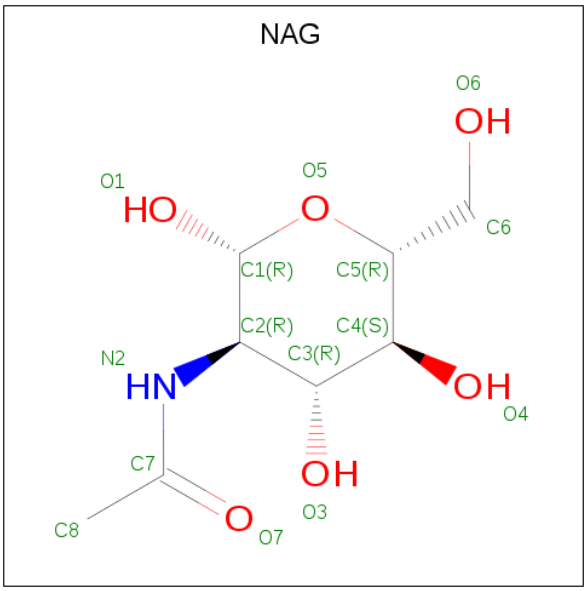
- Molecule 3 is a protein called b12 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	127	Total	C	N	O	S	0	0
			1013	642	175	191	5		
3	F	127	Total	C	N	O	S	0	0
			1013	642	175	191	5		
3	I	127	Total	C	N	O	S	0	0
			1013	642	175	191	5		

- Molecule 4 is a protein called b12 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	108	Total	C	N	O	S	0	0
			836	520	154	160	2		
4	J	108	Total	C	N	O	S	0	0
			836	520	154	160	2		
4	K	108	Total	C	N	O	S	0	0
			836	520	154	160	2		

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



Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	

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Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	G	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	

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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	

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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	D	1	Total	C	N	O	0
			406	232	29	145	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			56	32	4	20	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	E	1	Total	C	N	O	0
			406	232	29	145	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	C	1	Total	C	N	O	0
			56	32	4	20	

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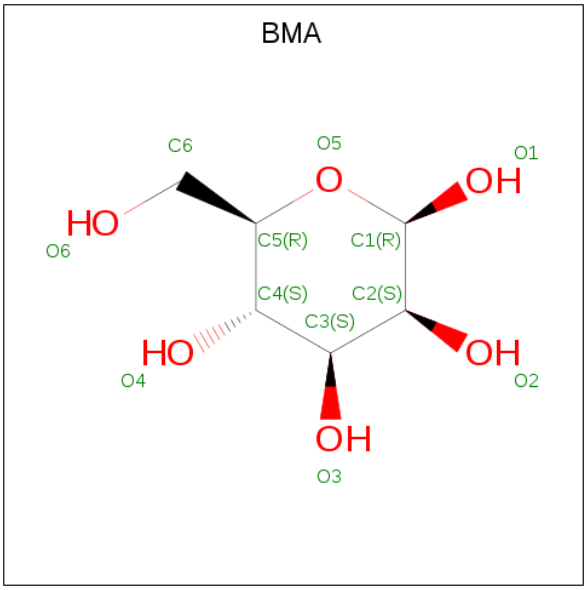
Mol	Chain	Residues	Atoms	AltConf
5	C	1	Total C N O 56 32 4 20	0

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



Mol	Chain	Residues	Atoms	AltConf
6	G	1	Total C O 44 24 20	0
6	G	1	Total C O 44 24 20	0
6	G	1	Total C O 44 24 20	0
6	G	1	Total C O 44 24 20	0
6	D	1	Total C O 44 24 20	0
6	D	1	Total C O 44 24 20	0
6	D	1	Total C O 44 24 20	0
6	D	1	Total C O 44 24 20	0
6	E	1	Total C O 44 24 20	0
6	E	1	Total C O 44 24 20	0

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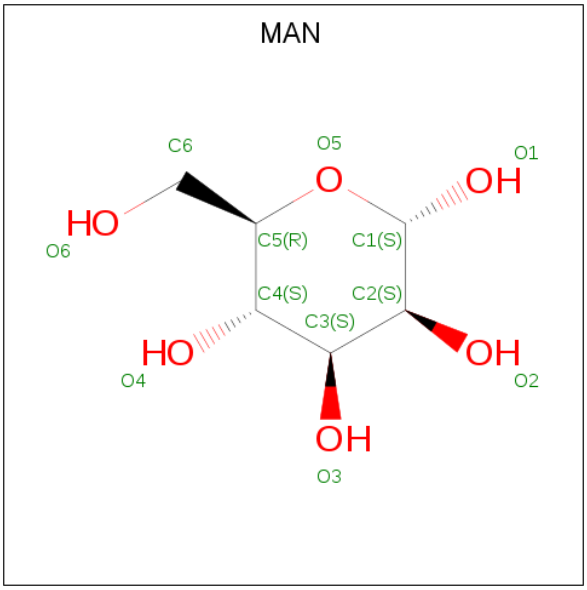
Mol	Chain	Residues	Atoms			AltConf
6	E	1	Total	C	O	0
			44	24	20	
6	E	1	Total	C	O	0
			44	24	20	

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



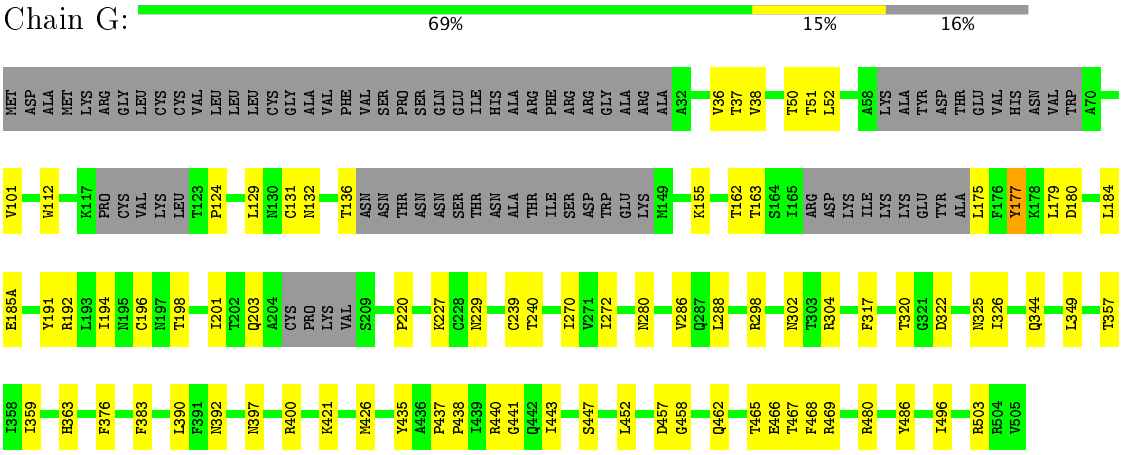
Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	C	O	0
			11	6	5	
7	D	1	Total	C	O	0
			11	6	5	
7	E	1	Total	C	O	0
			11	6	5	

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.

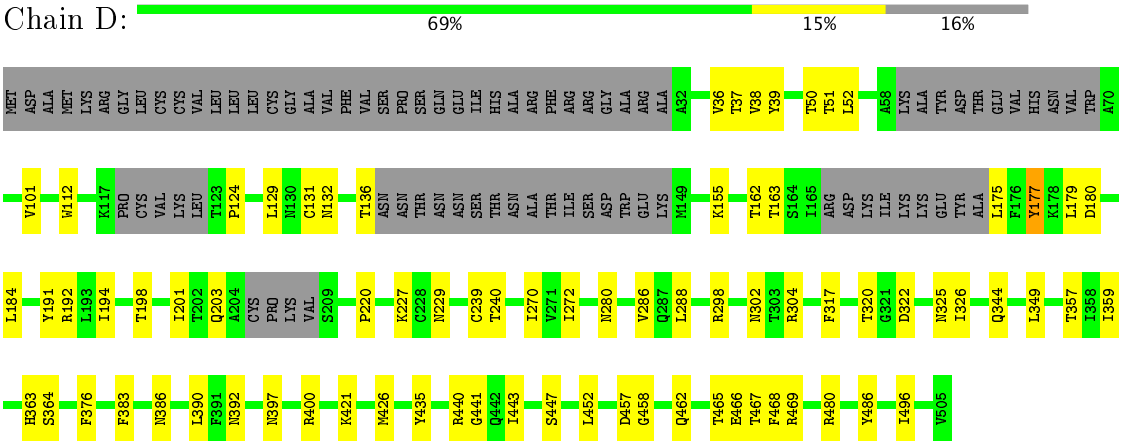
- Molecule 1: Envelope glycoprotein gp160

Chain G:



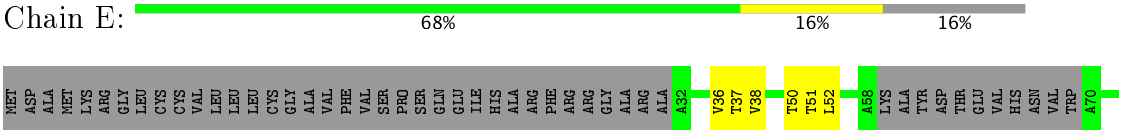
- Molecule 1: Envelope glycoprotein gp160

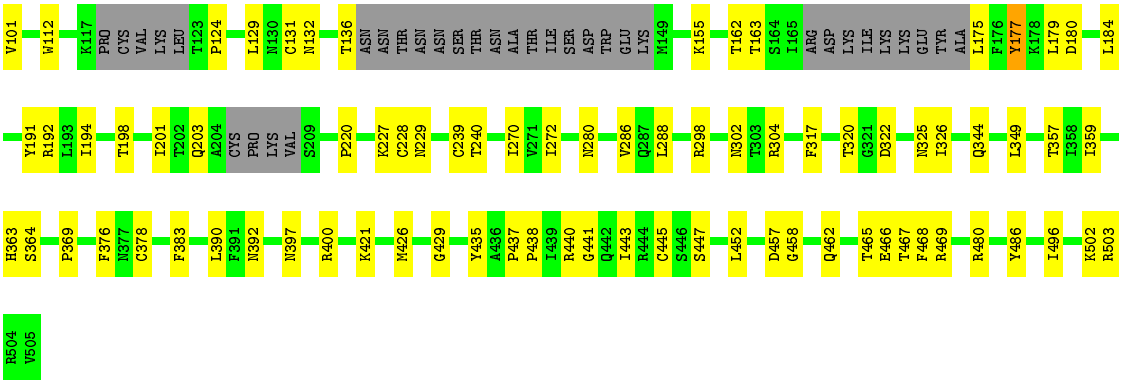
Chain D:



- Molecule 1: Envelope glycoprotein gp160

Chain E:



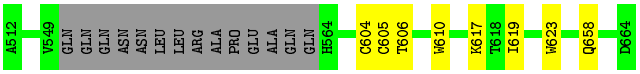


- Molecule 2: Envelope glycoprotein gp160

Chain A:

- Molecule 2: Envelope glycoprotein gp160

Chain B:

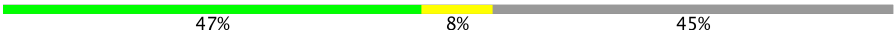


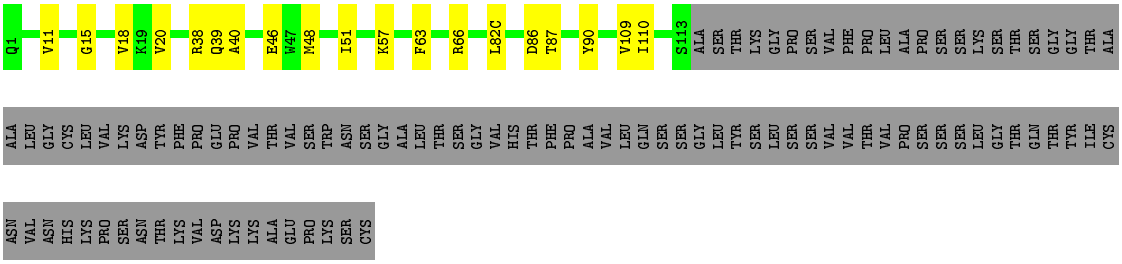
- Molecule 2: Envelope glycoprotein gp160

Chain C:

- Molecule 3: b12 Fab heavy chain

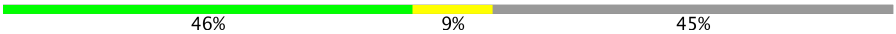
Chain H:

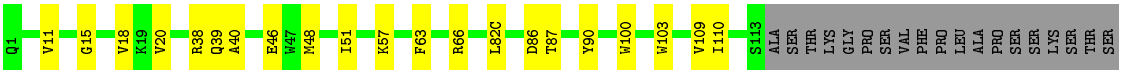


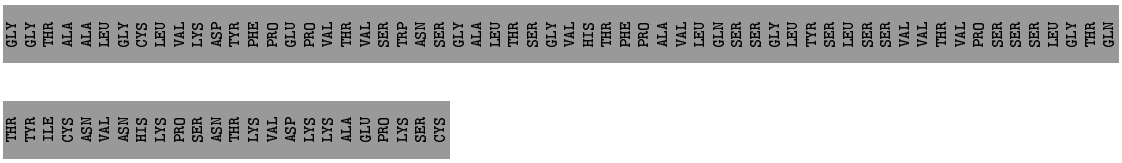


- Molecule 3: b12 Fab heavy chain

Chain F:

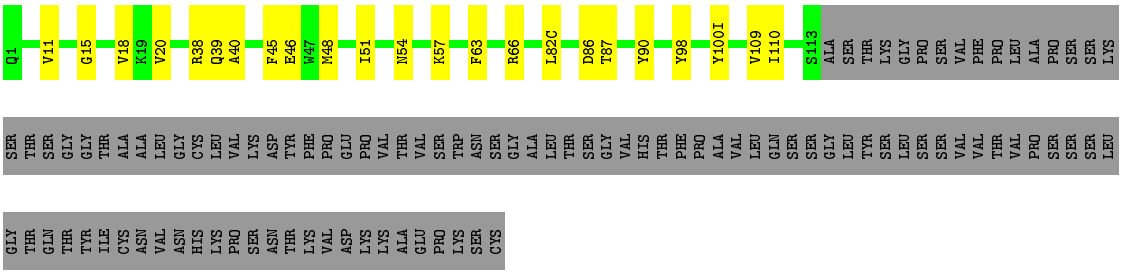






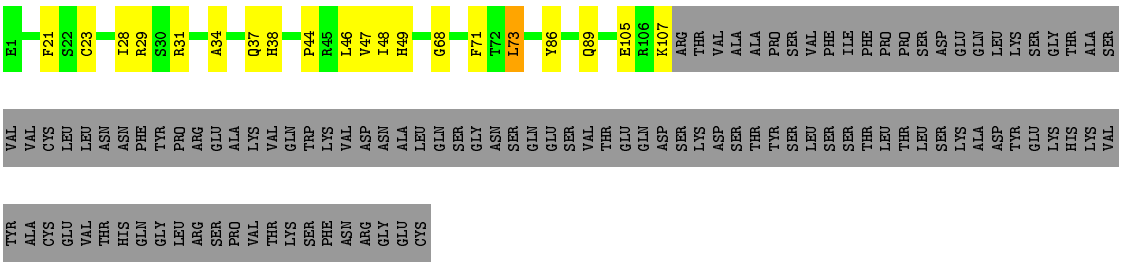
- Molecule 3: b12 Fab heavy chain

Chain I:



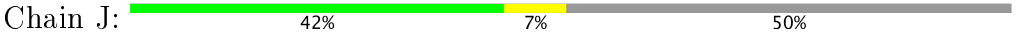
- Molecule 4: b12 Fab light chain

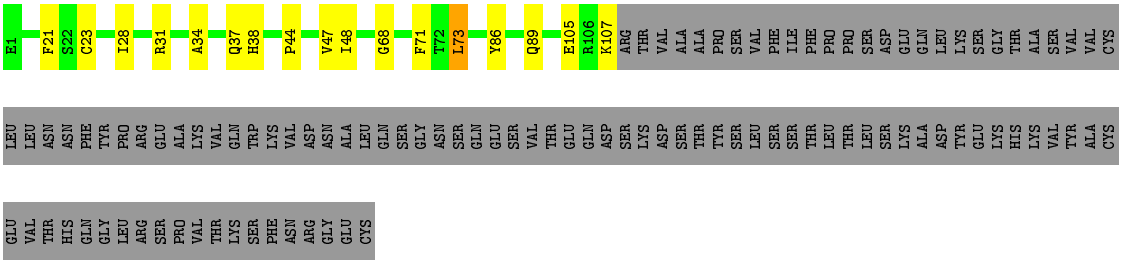
Chain L:



- Molecule 4: b12 Fab light chain

Chain J:





- Molecule 4: b12 Fab light chain

Chain K:

SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS

VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU ARG SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	88071	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	D	0.36	0/3459	0.65	1/4700 (0.0%)
1	E	0.36	0/3459	0.65	1/4700 (0.0%)
1	G	0.36	0/3459	0.65	1/4700 (0.0%)
2	A	0.35	0/1124	0.57	0/1523
2	B	0.35	0/1124	0.57	0/1523
2	C	0.35	0/1124	0.57	0/1523
3	F	0.33	0/1042	0.58	0/1416
3	H	0.33	0/1042	0.58	0/1416
3	I	0.32	0/1042	0.58	0/1416
4	J	0.31	0/855	0.60	1/1155 (0.1%)
4	K	0.31	0/855	0.60	1/1155 (0.1%)
4	L	0.31	0/855	0.60	1/1155 (0.1%)
All	All	0.34	0/19440	0.62	6/26382 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	73	LEU	CA-CB-CG	5.33	127.56	115.30
4	K	73	LEU	CA-CB-CG	5.32	127.54	115.30
4	L	73	LEU	CA-CB-CG	5.30	127.50	115.30
1	E	390	LEU	C-N-CA	5.04	134.31	121.70
1	D	390	LEU	C-N-CA	5.04	134.31	121.70
1	G	390	LEU	C-N-CA	5.01	134.22	121.70

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	D	3393	0	3290	49	0
1	E	3393	0	3290	54	0
1	G	3393	0	3290	50	0
2	A	1104	0	1092	5	0
2	B	1104	0	1092	6	0
2	C	1104	0	1092	5	0
3	F	1013	0	955	12	0
3	H	1013	0	955	10	0
3	I	1013	0	955	14	0
4	J	836	0	815	11	0
4	K	836	0	815	13	0
4	L	836	0	815	12	0
5	A	56	0	50	0	0
5	B	56	0	50	0	0
5	C	56	0	50	0	0
5	D	406	0	361	4	0
5	E	406	0	361	4	0
5	G	406	0	361	5	0
6	D	44	0	39	0	0
6	E	44	0	39	0	0
6	G	44	0	39	0	0
7	D	11	0	10	0	0
7	E	11	0	10	0	0
7	G	11	0	10	0	0
All	All	20589	0	19836	221	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 5.

All (221) 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:15:GLY:H	3:I:82(C):LEU:HB2	1.58	0.69
3:H:15:GLY:H	3:H:82(C):LEU:HB2	1.58	0.69
3:F:15:GLY:H	3:F:82(C):LEU:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:GLY:H	3:I:54:ASN:HA	1.61	0.66
4:J:105:GLU:HG3	4:J:107:LYS:H	1.63	0.63
4:K:105:GLU:HG3	4:K:107:LYS:H	1.63	0.62
4:L:105:GLU:HG3	4:L:107:LYS:H	1.63	0.62
1:G:112:TRP:NE1	1:G:426:MET:SD	2.73	0.61
1:E:112:TRP:NE1	1:E:426:MET:SD	2.73	0.61
1:G:298:ARG:HE	1:G:443:ILE:HD12	1.66	0.61
1:D:112:TRP:NE1	1:D:426:MET:SD	2.73	0.60
2:C:604:CYS:SG	2:C:605:CYS:N	2.75	0.60
2:B:604:CYS:SG	2:B:605:CYS:N	2.75	0.60
1:E:298:ARG:HE	1:E:443:ILE:HD12	1.66	0.60
4:K:38:HIS:HD2	4:K:44:PRO:HG3	1.65	0.60
1:G:36:VAL:HG22	2:A:610:TRP:HE3	1.66	0.60
4:J:38:HIS:HD2	4:J:44:PRO:HG3	1.66	0.60
4:L:38:HIS:HD2	4:L:44:PRO:HG3	1.65	0.60
2:A:604:CYS:SG	2:A:605:CYS:N	2.75	0.59
1:D:304:ARG:HA	1:D:320:THR:HG22	1.84	0.59
1:D:304:ARG:HE	1:D:440:ARG:HH11	1.50	0.59
1:G:304:ARG:HE	1:G:440:ARG:HH11	1.50	0.59
1:D:298:ARG:HE	1:D:443:ILE:HD12	1.66	0.59
1:D:203:GLN:HE22	1:D:317:PHE:HA	1.68	0.59
1:E:304:ARG:HA	1:E:320:THR:HG22	1.84	0.58
1:G:304:ARG:HA	1:G:320:THR:HG22	1.84	0.58
1:G:192:ARG:NH1	5:G:603:NAG:O6	2.37	0.58
1:E:203:GLN:HE22	1:E:317:PHE:HA	1.68	0.58
1:G:203:GLN:HE22	1:G:317:PHE:HA	1.68	0.58
1:D:229:ASN:ND2	5:D:607:NAG:O6	2.37	0.57
1:D:37:THR:HG22	2:B:605:CYS:HA	1.87	0.57
1:E:304:ARG:HE	1:E:440:ARG:HH11	1.50	0.57
1:D:363:HIS:O	1:D:469:ARG:NH1	2.38	0.57
1:G:363:HIS:O	1:G:469:ARG:NH1	2.38	0.56
1:G:229:ASN:ND2	5:G:607:NAG:O6	2.38	0.56
1:E:192:ARG:NH1	5:E:603:NAG:O6	2.39	0.56
1:E:363:HIS:O	1:E:469:ARG:NH1	2.38	0.56
1:E:229:ASN:ND2	5:E:607:NAG:O6	2.39	0.56
1:G:503:ARG:HD2	2:A:653:GLN:HE22	1.72	0.56
1:D:177:TYR:OH	1:D:302:ASN:ND2	2.40	0.55
1:E:131:CYS:SG	1:E:132:ASN:N	2.80	0.55
1:G:131:CYS:SG	1:G:132:ASN:N	2.80	0.54
1:G:177:TYR:OH	1:G:302:ASN:ND2	2.40	0.54
1:E:184:LEU:HD11	1:E:192:ARG:HE	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:HG22	2:C:610:TRP:HE3	1.73	0.54
1:E:177:TYR:OH	1:E:302:ASN:ND2	2.40	0.54
1:G:36:VAL:O	2:A:606:THR:OG1	2.26	0.54
1:G:184:LEU:HD11	1:G:192:ARG:HE	1.73	0.53
1:D:192:ARG:NH1	5:D:603:NAG:O6	2.41	0.53
1:D:400:ARG:HB3	5:D:621:NAG:H61	1.90	0.53
1:D:184:LEU:HD11	1:D:192:ARG:HE	1.73	0.53
2:B:658:GLN:HE22	1:E:502:LYS:H	1.56	0.53
3:I:100(I):TYR:HB2	4:K:49:HIS:CE1	2.43	0.53
1:E:36:VAL:O	2:C:606:THR:OG1	2.25	0.53
1:D:36:VAL:HG22	2:B:610:TRP:HE3	1.73	0.52
1:E:38:VAL:HG12	1:E:496:ILE:HG22	1.91	0.52
1:D:38:VAL:HG12	1:D:496:ILE:HG22	1.91	0.52
1:G:198:THR:HB	1:G:201:ILE:HD11	1.92	0.52
1:D:131:CYS:SG	1:D:132:ASN:N	2.80	0.52
1:E:322:ASP:O	1:E:325:ASN:ND2	2.40	0.52
4:K:23:CYS:HB3	4:K:71:PHE:HB2	1.92	0.52
3:F:66:ARG:NH2	3:F:86:ASP:OD2	2.43	0.52
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.43	0.52
1:E:198:THR:HB	1:E:201:ILE:HD11	1.91	0.51
3:I:66:ARG:NH2	3:I:86:ASP:OD2	2.43	0.51
4:J:23:CYS:HB3	4:J:71:PHE:HB2	1.92	0.51
1:G:376:PHE:HB2	1:G:383:PHE:HB2	1.93	0.51
1:G:286:VAL:HB	1:G:452:LEU:HB2	1.92	0.51
1:E:376:PHE:HB2	1:E:383:PHE:HB2	1.93	0.51
3:F:87:THR:HG23	3:F:110:ILE:HA	1.92	0.51
1:G:38:VAL:HG12	1:G:496:ILE:HG22	1.91	0.51
1:G:175:LEU:N	1:G:320:THR:O	2.44	0.51
1:E:37:THR:HG22	2:C:605:CYS:HA	1.92	0.51
1:E:400:ARG:HB3	5:E:621:NAG:H61	1.92	0.51
1:E:357:THR:HG23	1:E:397:ASN:HA	1.93	0.51
1:D:357:THR:HG23	1:D:397:ASN:HA	1.93	0.51
1:E:175:LEU:N	1:E:320:THR:O	2.43	0.51
1:G:280:ASN:HD22	1:G:458:GLY:HA3	1.76	0.51
1:D:280:ASN:HD22	1:D:458:GLY:HA3	1.76	0.50
1:E:280:ASN:HD22	1:E:458:GLY:HA3	1.76	0.50
1:D:198:THR:HB	1:D:201:ILE:HD11	1.91	0.50
4:J:28:ILE:HG22	4:J:31:ARG:H	1.76	0.50
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.92	0.50
1:D:175:LEU:N	1:D:320:THR:O	2.43	0.50
1:G:196:CYS:SG	5:G:603:NAG:O6	2.66	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:23:CYS:HB3	4:L:71:PHE:HB2	1.92	0.50
1:G:322:ASP:O	1:G:325:ASN:ND2	2.40	0.50
3:I:87:THR:HG23	3:I:110:ILE:HA	1.92	0.50
1:D:322:ASP:O	1:D:325:ASN:ND2	2.40	0.50
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.92	0.49
1:D:376:PHE:HB2	1:D:383:PHE:HB2	1.93	0.49
1:G:357:THR:HG23	1:G:397:ASN:HA	1.93	0.49
3:H:87:THR:HG23	3:H:110:ILE:HA	1.92	0.49
1:G:400:ARG:HB3	5:G:621:NAG:H61	1.95	0.49
4:L:28:ILE:HG22	4:L:31:ARG:H	1.76	0.49
4:K:28:ILE:HG22	4:K:31:ARG:H	1.76	0.48
1:E:179:LEU:HB2	1:E:421:LYS:HG2	1.95	0.48
1:D:179:LEU:HB2	1:D:421:LYS:HG2	1.96	0.48
1:G:179:LEU:HB2	1:G:421:LYS:HG2	1.96	0.48
1:G:203:GLN:HG3	1:G:435:TYR:HB3	1.95	0.48
4:K:47:VAL:HG12	4:K:48:ILE:HG23	1.95	0.48
1:E:203:GLN:HG3	1:E:435:TYR:HB3	1.96	0.47
3:F:39:GLN:NE2	3:F:40:ALA:O	2.48	0.47
3:F:103:TRP:CD1	4:J:44:PRO:HB2	2.49	0.47
1:D:203:GLN:HG3	1:D:435:TYR:HB3	1.95	0.47
1:G:52:LEU:HD23	1:G:220:PRO:HD3	1.96	0.47
3:I:39:GLN:NE2	3:I:40:ALA:O	2.48	0.47
4:K:34:ALA:HB3	4:K:89:GLN:HG3	1.97	0.47
3:H:39:GLN:NE2	3:H:40:ALA:O	2.48	0.47
4:J:34:ALA:HB3	4:J:89:GLN:HG3	1.97	0.47
1:D:447:SER:HB3	5:D:610:NAG:HN2	1.80	0.47
1:G:37:THR:HG22	2:A:605:CYS:HA	1.96	0.47
1:D:52:LEU:HD23	1:D:220:PRO:HD3	1.96	0.47
4:J:47:VAL:HG12	4:J:48:ILE:HG23	1.95	0.46
1:E:503:ARG:HD2	2:C:653:GLN:HE22	1.81	0.46
1:E:52:LEU:HD23	1:E:220:PRO:HD3	1.96	0.46
4:L:47:VAL:HG12	4:L:48:ILE:HG23	1.95	0.46
1:G:357:THR:HB	1:G:465:THR:HG22	1.97	0.46
1:G:447:SER:HB3	5:G:610:NAG:HN2	1.81	0.46
1:E:447:SER:HB3	5:E:610:NAG:HN2	1.81	0.46
1:G:185(A):GLU:HB2	4:L:29:ARG:HB2	1.97	0.46
1:G:298:ARG:NH2	1:G:441:GLY:O	2.50	0.45
1:D:298:ARG:NH2	1:D:441:GLY:O	2.50	0.45
1:E:298:ARG:NH2	1:E:441:GLY:O	2.50	0.45
4:K:31:ARG:HE	4:K:68:GLY:H	1.64	0.45
1:E:357:THR:HB	1:E:465:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:34:ALA:HB3	4:L:89:GLN:HG3	1.97	0.45
4:K:21:PHE:HD2	4:K:73:LEU:HB2	1.82	0.45
4:L:37:GLN:HG3	4:L:86:TYR:HE1	1.82	0.45
1:D:357:THR:HB	1:D:465:THR:HG22	1.98	0.45
4:L:31:ARG:HE	4:L:68:GLY:H	1.64	0.45
1:G:457:ASP:OD2	1:G:469:ARG:NE	2.47	0.44
3:H:18:VAL:HG11	3:H:109:VAL:HG11	1.99	0.44
4:J:31:ARG:HE	4:J:68:GLY:H	1.64	0.44
3:I:18:VAL:HG11	3:I:109:VAL:HG11	1.99	0.44
4:J:21:PHE:HD2	4:J:73:LEU:HB2	1.82	0.44
4:L:21:PHE:HD2	4:L:73:LEU:HB2	1.82	0.44
4:J:37:GLN:HG3	4:J:86:TYR:HE1	1.82	0.44
4:K:34:ALA:H	4:K:89:GLN:HB2	1.82	0.44
4:J:34:ALA:H	4:J:89:GLN:HB2	1.83	0.44
1:D:462:GLN:NE2	1:D:466:GLU:OE2	2.51	0.44
1:E:378:CYS:HB3	1:E:445:CYS:HB3	1.85	0.44
1:D:239:CYS:SG	1:D:240:THR:N	2.91	0.44
1:E:136:THR:HB	1:E:326:ILE:HD13	2.00	0.44
1:G:101:VAL:HG21	1:G:480:ARG:HG2	2.00	0.44
1:E:101:VAL:HG21	1:E:480:ARG:HG2	2.00	0.44
1:G:239:CYS:SG	1:G:240:THR:N	2.91	0.44
3:H:51:ILE:HG13	3:H:57:LYS:HG2	1.99	0.44
3:F:18:VAL:HG11	3:F:109:VAL:HG11	1.99	0.44
1:D:136:THR:HB	1:D:326:ILE:HD13	2.00	0.43
1:D:36:VAL:O	2:B:606:THR:OG1	2.32	0.43
1:D:457:ASP:OD2	1:D:469:ARG:NE	2.47	0.43
4:K:37:GLN:HG3	4:K:86:TYR:HE1	1.82	0.43
1:E:462:GLN:NE2	1:E:466:GLU:OE2	2.51	0.43
3:F:51:ILE:HG13	3:F:57:LYS:HG2	2.00	0.43
1:G:462:GLN:NE2	1:G:466:GLU:OE2	2.51	0.43
4:L:34:ALA:H	4:L:89:GLN:HB2	1.82	0.43
1:E:180:ASP:HA	1:E:194:ILE:HB	2.01	0.43
1:G:227:LYS:HA	1:G:486:TYR:HB3	2.01	0.43
3:I:51:ILE:HG13	3:I:57:LYS:HG2	2.00	0.43
1:E:239:CYS:SG	1:E:240:THR:N	2.91	0.43
1:E:457:ASP:HB2	1:E:467:THR:HG23	2.01	0.43
1:G:136:THR:HB	1:G:326:ILE:HD13	2.00	0.43
1:D:227:LYS:HA	1:D:486:TYR:HB3	2.01	0.43
3:F:20:VAL:HG21	3:F:90:TYR:HD2	1.84	0.43
3:F:48:MET:HG2	3:F:63:PHE:HE2	1.83	0.43
3:H:48:MET:HG2	3:H:63:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.99	0.42
1:D:180:ASP:HA	1:D:194:ILE:HB	2.01	0.42
1:D:457:ASP:HB2	1:D:467:THR:HG23	2.01	0.42
1:E:270:ILE:HD12	1:E:344:GLN:HB2	2.01	0.42
3:I:20:VAL:HG21	3:I:90:TYR:HD2	1.84	0.42
1:D:162:THR:OG1	1:D:163:THR:N	2.53	0.42
1:D:270:ILE:HD12	1:D:344:GLN:HB2	2.01	0.42
1:G:270:ILE:HD12	1:G:344:GLN:HB2	2.02	0.42
3:H:20:VAL:HG21	3:H:90:TYR:HD2	1.84	0.42
1:E:227:LYS:HA	1:E:486:TYR:HB3	2.01	0.42
1:D:386:ASN:HB2	3:F:100:TRP:CZ3	2.55	0.42
1:E:50:THR:OG1	1:E:51:THR:N	2.53	0.42
3:I:45:PHE:HB2	4:K:98:PHE:CG	2.54	0.42
1:D:349:LEU:HD13	1:D:468:PHE:HE2	1.85	0.42
1:E:272:ILE:HG22	1:E:286:VAL:HG22	2.02	0.42
1:E:369:PRO:HG3	3:I:98:TYR:CE1	2.55	0.42
1:G:270:ILE:HG12	1:G:288:LEU:HA	2.01	0.42
1:D:270:ILE:HG12	1:D:288:LEU:HA	2.01	0.41
1:E:270:ILE:HG12	1:E:288:LEU:HA	2.01	0.41
1:G:349:LEU:HD13	1:G:468:PHE:HE2	1.85	0.41
1:D:155:LYS:HG2	1:D:191:TYR:HE2	1.85	0.41
1:E:363:HIS:ND1	1:E:364:SER:O	2.53	0.41
1:E:359:ILE:HD12	1:E:465:THR:HB	2.02	0.41
1:G:162:THR:OG1	1:G:163:THR:N	2.53	0.41
3:I:38:ARG:HB3	3:I:46:GLU:HG3	2.02	0.41
1:E:162:THR:OG1	1:E:163:THR:N	2.53	0.41
3:I:48:MET:HG2	3:I:63:PHE:HE2	1.83	0.41
1:D:363:HIS:ND1	1:D:364:SER:O	2.53	0.41
1:E:457:ASP:OD2	1:E:469:ARG:NE	2.47	0.41
1:G:180:ASP:HA	1:G:194:ILE:HB	2.01	0.41
1:G:50:THR:OG1	1:G:51:THR:N	2.53	0.41
1:E:349:LEU:HD13	1:E:468:PHE:HE2	1.85	0.41
1:D:272:ILE:HG22	1:D:286:VAL:HG22	2.02	0.41
1:G:359:ILE:HD12	1:G:465:THR:HB	2.02	0.41
4:K:46:LEU:HD21	4:K:49:HIS:HB2	2.03	0.41
3:F:38:ARG:HB3	3:F:46:GLU:HG3	2.02	0.41
1:G:457:ASP:HB2	1:G:467:THR:HG23	2.01	0.41
3:I:11:VAL:HG22	3:I:110:ILE:HB	2.03	0.41
1:D:39:TYR:HH	2:B:623:TRP:HH2	1.68	0.41
1:D:359:ILE:HD12	1:D:465:THR:HB	2.02	0.41
1:D:50:THR:OG1	1:D:51:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:PRO:HA	1:E:438:PRO:HD3	1.94	0.41
1:G:155:LYS:HG2	1:G:191:TYR:HE2	1.86	0.41
3:H:11:VAL:HG22	3:H:110:ILE:HB	2.03	0.41
1:E:129:LEU:HB2	1:E:191:TYR:HB2	2.03	0.40
1:E:228:CYS:SG	1:E:229:ASN:N	2.94	0.40
1:G:129:LEU:HB2	1:G:191:TYR:HB2	2.03	0.40
1:G:272:ILE:HG22	1:G:286:VAL:HG22	2.02	0.40
3:H:38:ARG:HB3	3:H:46:GLU:HG3	2.02	0.40
3:F:11:VAL:HG22	3:F:110:ILE:HB	2.03	0.40
1:G:437:PRO:HA	1:G:438:PRO:HD3	1.94	0.40
1:D:129:LEU:HB2	1:D:191:TYR:HB2	2.03	0.40
1:E:155:LYS:HG2	1:E:191:TYR:HE2	1.85	0.40
4:L:46:LEU:HD21	4:L:49:HIS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	D	423/516 (82%)	360 (85%)	60 (14%)	3 (1%)	25	68
1	E	423/516 (82%)	360 (85%)	60 (14%)	3 (1%)	25	68
1	G	423/516 (82%)	360 (85%)	60 (14%)	3 (1%)	25	68
2	A	135/153 (88%)	125 (93%)	8 (6%)	2 (2%)	12	55
2	B	135/153 (88%)	125 (93%)	8 (6%)	2 (2%)	12	55
2	C	135/153 (88%)	125 (93%)	8 (6%)	2 (2%)	12	55
3	F	125/230 (54%)	108 (86%)	17 (14%)	0	100	100
3	H	125/230 (54%)	108 (86%)	17 (14%)	0	100	100
3	I	125/230 (54%)	108 (86%)	17 (14%)	0	100	100
4	J	106/215 (49%)	93 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	106/215 (49%)	93 (88%)	13 (12%)	0	100	100
4	L	106/215 (49%)	93 (88%)	13 (12%)	0	100	100
All	All	2367/3342 (71%)	2058 (87%)	294 (12%)	15 (1%)	33	70

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	392	ASN
1	D	392	ASN
1	E	392	ASN
1	G	177	TYR
2	A	619	ILE
1	D	177	TYR
2	B	619	ILE
1	E	177	TYR
2	C	619	ILE
2	A	617	LYS
2	B	617	LYS
2	C	617	LYS
1	G	124	PRO
1	D	124	PRO
1	E	124	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	D	382/453 (84%)	382 (100%)	0	100	100
1	E	382/453 (84%)	382 (100%)	0	100	100
1	G	382/453 (84%)	382 (100%)	0	100	100
2	A	118/130 (91%)	118 (100%)	0	100	100
2	B	118/130 (91%)	118 (100%)	0	100	100
2	C	118/130 (91%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	107/195 (55%)	107 (100%)	0	100	100
3	H	107/195 (55%)	107 (100%)	0	100	100
3	I	107/195 (55%)	107 (100%)	0	100	100
4	J	91/187 (49%)	91 (100%)	0	100	100
4	K	91/187 (49%)	91 (100%)	0	100	100
4	L	91/187 (49%)	91 (100%)	0	100	100
All	All	2094/2895 (72%)	2094 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	103	GLN
1	G	203	GLN
1	G	229	ASN
1	G	302	ASN
2	A	564	HIS
2	A	653	GLN
2	A	658	GLN
4	L	38	HIS
1	D	103	GLN
1	D	203	GLN
1	D	229	ASN
1	D	302	ASN
1	D	417	GLN
2	B	564	HIS
2	B	658	GLN
4	J	38	HIS
1	E	103	GLN
1	E	203	GLN
1	E	229	ASN
1	E	302	ASN
2	C	564	HIS
4	K	49	HIS

5.3.3 RNA

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)

114 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	701	2	14,14,15	0.32	0	15,19,21	0.46	0
5	NAG	A	702	2	14,14,15	0.35	0	15,19,21	0.51	0
5	NAG	A	703	2	14,14,15	0.25	0	15,19,21	0.53	0
5	NAG	A	704	2	14,14,15	0.37	0	15,19,21	0.58	0
5	NAG	B	701	2	14,14,15	0.24	0	15,19,21	0.48	0
5	NAG	B	702	2	14,14,15	0.41	0	15,19,21	0.58	0
5	NAG	B	703	2	14,14,15	0.27	0	15,19,21	0.46	0
5	NAG	B	704	2	14,14,15	0.33	0	15,19,21	0.58	0
5	NAG	C	701	2	14,14,15	0.25	0	15,19,21	0.52	0
5	NAG	C	702	2	14,14,15	0.41	0	15,19,21	0.55	0
5	NAG	C	703	2	14,14,15	0.26	0	15,19,21	0.47	0
5	NAG	C	704	2	14,14,15	0.33	0	15,19,21	0.61	0
5	NAG	D	601	1	14,14,15	0.21	0	15,19,21	0.44	0
5	NAG	D	602	1	14,14,15	0.37	0	15,19,21	0.50	0
5	NAG	D	603	1,5	14,14,15	0.25	0	15,19,21	0.72	0
5	NAG	D	604	5	14,14,15	0.32	0	15,19,21	0.59	0
5	NAG	D	605	1,5	14,14,15	0.28	0	15,19,21	0.63	0
5	NAG	D	606	5	14,14,15	0.33	0	15,19,21	0.51	0
5	NAG	D	607	1,5	14,14,15	0.17	0	15,19,21	0.49	0
5	NAG	D	608	5,6	14,14,15	0.21	0	15,19,21	0.59	0
6	BMA	D	609	5	11,11,12	0.58	0	13,15,17	1.15	1 (7%)
5	NAG	D	610	1,5	14,14,15	0.18	0	15,19,21	0.66	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	D	611	5,6	14,14,15	0.22	0	15,19,21	0.59	0
6	BMA	D	612	5,7	11,11,12	0.70	0	13,15,17	0.88	0
7	MAN	D	613	6	11,11,12	0.79	0	13,15,17	1.38	2 (15%)
5	NAG	D	614	1,5	14,14,15	0.25	0	15,19,21	0.63	0
5	NAG	D	615	5	14,14,15	0.33	0	15,19,21	0.47	0
5	NAG	D	616	1,5	14,14,15	0.27	0	15,19,21	0.55	0
5	NAG	D	617	5	14,14,15	0.40	0	15,19,21	0.67	1 (6%)
5	NAG	D	618	1	14,14,15	0.39	0	15,19,21	0.54	0
5	NAG	D	619	1,5	14,14,15	0.22	0	15,19,21	0.58	0
5	NAG	D	620	5	14,14,15	0.44	0	15,19,21	0.48	0
5	NAG	D	621	1	14,14,15	0.29	0	15,19,21	0.99	1 (6%)
5	NAG	D	622	1	14,14,15	0.34	0	15,19,21	0.61	0
5	NAG	D	623	1,5	14,14,15	0.50	0	15,19,21	0.56	0
5	NAG	D	624	5,6	14,14,15	0.26	0	15,19,21	0.56	0
6	BMA	D	625	5	11,11,12	0.74	0	13,15,17	1.09	1 (7%)
5	NAG	D	626	1,5	14,14,15	0.77	1 (7%)	15,19,21	0.92	0
5	NAG	D	627	5,6	14,14,15	0.31	0	15,19,21	0.75	0
6	BMA	D	628	5	11,11,12	0.74	0	13,15,17	1.37	2 (15%)
5	NAG	D	629	1	14,14,15	0.41	0	15,19,21	0.66	1 (6%)
5	NAG	D	630	1	14,14,15	1.33	1 (7%)	15,19,21	1.58	1 (6%)
5	NAG	D	631	1,5	14,14,15	0.30	0	15,19,21	0.65	1 (6%)
5	NAG	D	632	5	14,14,15	0.25	0	15,19,21	0.62	0
5	NAG	D	633	1,5	14,14,15	0.20	0	15,19,21	0.69	1 (6%)
5	NAG	D	634	5	14,14,15	0.36	0	15,19,21	0.60	0
5	NAG	E	601	1	14,14,15	0.24	0	15,19,21	0.42	0
5	NAG	E	602	1	14,14,15	0.42	0	15,19,21	0.49	0
5	NAG	E	603	1,5	14,14,15	0.26	0	15,19,21	0.79	1 (6%)
5	NAG	E	604	5	14,14,15	0.32	0	15,19,21	0.64	0
5	NAG	E	605	1,5	14,14,15	0.22	0	15,19,21	0.59	0
5	NAG	E	606	5	14,14,15	0.32	0	15,19,21	0.50	0
5	NAG	E	607	1,5	14,14,15	0.27	0	15,19,21	0.62	0
5	NAG	E	608	5,6	14,14,15	0.20	0	15,19,21	0.63	0
6	BMA	E	609	5	11,11,12	0.58	0	13,15,17	1.11	1 (7%)
5	NAG	E	610	1,5	14,14,15	0.19	0	15,19,21	0.64	1 (6%)
5	NAG	E	611	5,6	14,14,15	0.23	0	15,19,21	0.63	0
6	BMA	E	612	5,7	11,11,12	0.71	0	13,15,17	0.91	0
7	MAN	E	613	6	11,11,12	0.79	0	13,15,17	1.36	2 (15%)
5	NAG	E	614	1,5	14,14,15	0.22	0	15,19,21	0.64	0
5	NAG	E	615	5	14,14,15	0.35	0	15,19,21	0.50	0
5	NAG	E	616	1,5	14,14,15	0.24	0	15,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	617	5	14,14,15	0.29	0	15,19,21	0.60	0
5	NAG	E	618	1	14,14,15	0.37	0	15,19,21	0.63	1 (6%)
5	NAG	E	619	1,5	14,14,15	0.28	0	15,19,21	0.51	0
5	NAG	E	620	5	14,14,15	0.45	0	15,19,21	0.49	0
5	NAG	E	621	1	14,14,15	0.31	0	15,19,21	0.89	1 (6%)
5	NAG	E	622	1	14,14,15	0.35	0	15,19,21	0.72	1 (6%)
5	NAG	E	623	1,5	14,14,15	0.39	0	15,19,21	0.64	0
5	NAG	E	624	5,6	14,14,15	0.36	0	15,19,21	0.53	0
6	BMA	E	625	5	11,11,12	0.81	0	13,15,17	1.02	1 (7%)
5	NAG	E	626	1,5	14,14,15	0.73	1 (7%)	15,19,21	0.93	0
5	NAG	E	627	5,6	14,14,15	0.23	0	15,19,21	0.66	0
6	BMA	E	628	5	11,11,12	0.81	0	13,15,17	1.40	2 (15%)
5	NAG	E	629	1	14,14,15	0.31	0	15,19,21	0.81	1 (6%)
5	NAG	E	630	1	14,14,15	1.28	1 (7%)	15,19,21	1.58	1 (6%)
5	NAG	E	631	1,5	14,14,15	0.25	0	15,19,21	0.71	1 (6%)
5	NAG	E	632	5	14,14,15	0.22	0	15,19,21	0.61	0
5	NAG	E	633	1,5	14,14,15	0.23	0	15,19,21	0.62	0
5	NAG	E	634	5	14,14,15	0.33	0	15,19,21	0.54	0
5	NAG	G	601	1	14,14,15	0.22	0	15,19,21	0.44	0
5	NAG	G	602	1	14,14,15	0.48	0	15,19,21	0.52	0
5	NAG	G	603	1,5	14,14,15	0.23	0	15,19,21	0.75	0
5	NAG	G	604	5	14,14,15	0.33	0	15,19,21	0.66	1 (6%)
5	NAG	G	605	1,5	14,14,15	0.24	0	15,19,21	0.63	0
5	NAG	G	606	5	14,14,15	0.33	0	15,19,21	0.49	0
5	NAG	G	607	1,5	14,14,15	0.21	0	15,19,21	0.58	0
5	NAG	G	608	5,6	14,14,15	0.21	0	15,19,21	0.61	0
6	BMA	G	609	5	11,11,12	0.62	0	13,15,17	1.11	1 (7%)
5	NAG	G	610	1,5	14,14,15	0.21	0	15,19,21	0.63	1 (6%)
5	NAG	G	611	5,6	14,14,15	0.22	0	15,19,21	0.62	0
6	BMA	G	612	5,7	11,11,12	0.70	0	13,15,17	0.90	0
7	MAN	G	613	6	11,11,12	0.78	0	13,15,17	1.36	2 (15%)
5	NAG	G	614	1,5	14,14,15	0.21	0	15,19,21	0.61	0
5	NAG	G	615	5	14,14,15	0.32	0	15,19,21	0.51	0
5	NAG	G	616	1,5	14,14,15	0.25	0	15,19,21	0.57	0
5	NAG	G	617	5	14,14,15	0.29	0	15,19,21	0.61	0
5	NAG	G	618	1	14,14,15	0.36	0	15,19,21	0.60	0
5	NAG	G	619	1,5	14,14,15	0.27	0	15,19,21	0.50	0
5	NAG	G	620	5	14,14,15	0.46	0	15,19,21	0.52	0
5	NAG	G	621	1	14,14,15	0.33	0	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	G	622	1	14,14,15	0.34	0	15,19,21	0.73	1 (6%)
5	NAG	G	623	1,5	14,14,15	0.41	0	15,19,21	0.63	0
5	NAG	G	624	5,6	14,14,15	0.33	0	15,19,21	0.51	0
6	BMA	G	625	5	11,11,12	0.80	0	13,15,17	1.02	1 (7%)
5	NAG	G	626	1,5	14,14,15	0.91	1 (7%)	15,19,21	0.98	1 (6%)
5	NAG	G	627	5,6	14,14,15	0.23	0	15,19,21	0.69	0
6	BMA	G	628	5	11,11,12	0.75	0	13,15,17	1.44	2 (15%)
5	NAG	G	629	1	14,14,15	0.33	0	15,19,21	0.81	1 (6%)
5	NAG	G	630	1	14,14,15	1.30	1 (7%)	15,19,21	1.62	1 (6%)
5	NAG	G	631	1,5	14,14,15	0.24	0	15,19,21	0.70	1 (6%)
5	NAG	G	632	5	14,14,15	0.22	0	15,19,21	0.61	0
5	NAG	G	633	1,5	14,14,15	0.22	0	15,19,21	0.66	0
5	NAG	G	634	5	14,14,15	0.33	0	15,19,21	0.55	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
5	NAG	A	701	2	-	0/6/23/26	0/1/1/1
5	NAG	A	702	2	-	0/6/23/26	0/1/1/1
5	NAG	A	703	2	-	0/6/23/26	0/1/1/1
5	NAG	A	704	2	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2	-	0/6/23/26	0/1/1/1
5	NAG	B	702	2	-	0/6/23/26	0/1/1/1
5	NAG	B	703	2	-	0/6/23/26	0/1/1/1
5	NAG	B	704	2	-	0/6/23/26	0/1/1/1
5	NAG	C	701	2	-	0/6/23/26	0/1/1/1
5	NAG	C	702	2	-	0/6/23/26	0/1/1/1
5	NAG	C	703	2	-	0/6/23/26	0/1/1/1
5	NAG	C	704	2	-	0/6/23/26	0/1/1/1
5	NAG	D	601	1	-	0/6/23/26	0/1/1/1
5	NAG	D	602	1	-	0/6/23/26	0/1/1/1
5	NAG	D	603	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	604	5	-	0/6/23/26	0/1/1/1
5	NAG	D	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	606	5	-	0/6/23/26	0/1/1/1
5	NAG	D	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	608	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	609	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	610	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	611	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	612	5,7	-	0/2/19/22	0/1/1/1
7	MAN	D	613	6	-	0/2/19/22	0/1/1/1
5	NAG	D	614	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	615	5	-	0/6/23/26	0/1/1/1
5	NAG	D	616	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	617	5	-	0/6/23/26	0/1/1/1
5	NAG	D	618	1	-	0/6/23/26	0/1/1/1
5	NAG	D	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	620	5	-	0/6/23/26	0/1/1/1
5	NAG	D	621	1	-	0/6/23/26	0/1/1/1
5	NAG	D	622	1	-	0/6/23/26	0/1/1/1
5	NAG	D	623	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	624	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	625	5	-	0/2/19/22	0/1/1/1
5	NAG	D	626	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	627	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	628	5	-	0/2/19/22	0/1/1/1
5	NAG	D	629	1	-	0/6/23/26	0/1/1/1
5	NAG	D	630	1	-	0/6/23/26	0/1/1/1
5	NAG	D	631	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	632	5	-	0/6/23/26	0/1/1/1
5	NAG	D	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	634	5	-	0/6/23/26	0/1/1/1
5	NAG	E	601	1	-	0/6/23/26	0/1/1/1
5	NAG	E	602	1	-	0/6/23/26	0/1/1/1
5	NAG	E	603	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	604	5	-	0/6/23/26	0/1/1/1
5	NAG	E	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	606	5	-	0/6/23/26	0/1/1/1
5	NAG	E	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	608	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	609	5	-	0/2/19/22	0/1/1/1
5	NAG	E	610	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	611	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	612	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	613	6	-	0/2/19/22	0/1/1/1
5	NAG	E	614	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	615	5	-	0/6/23/26	0/1/1/1
5	NAG	E	616	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	617	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	618	1	-	0/6/23/26	0/1/1/1
5	NAG	E	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	620	5	-	0/6/23/26	0/1/1/1
5	NAG	E	621	1	-	0/6/23/26	0/1/1/1
5	NAG	E	622	1	-	0/6/23/26	0/1/1/1
5	NAG	E	623	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	624	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	625	5	-	0/2/19/22	0/1/1/1
5	NAG	E	626	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	627	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	628	5	-	0/2/19/22	0/1/1/1
5	NAG	E	629	1	-	0/6/23/26	0/1/1/1
5	NAG	E	630	1	-	0/6/23/26	0/1/1/1
5	NAG	E	631	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	632	5	-	0/6/23/26	0/1/1/1
5	NAG	E	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	634	5	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1	-	0/6/23/26	0/1/1/1
5	NAG	G	602	1	-	0/6/23/26	0/1/1/1
5	NAG	G	603	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	604	5	-	0/6/23/26	0/1/1/1
5	NAG	G	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	606	5	-	0/6/23/26	0/1/1/1
5	NAG	G	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	608	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	609	5	-	0/2/19/22	0/1/1/1
5	NAG	G	610	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	611	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	612	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	613	6	-	0/2/19/22	0/1/1/1
5	NAG	G	614	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	615	5	-	0/6/23/26	0/1/1/1
5	NAG	G	616	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	617	5	-	0/6/23/26	0/1/1/1
5	NAG	G	618	1	-	0/6/23/26	0/1/1/1
5	NAG	G	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	620	5	-	0/6/23/26	0/1/1/1
5	NAG	G	621	1	-	0/6/23/26	0/1/1/1
5	NAG	G	622	1	-	0/6/23/26	0/1/1/1
5	NAG	G	623	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	624	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	625	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	626	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	627	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	628	5	-	0/2/19/22	0/1/1/1
5	NAG	G	629	1	-	0/6/23/26	0/1/1/1
5	NAG	G	630	1	-	0/6/23/26	0/1/1/1
5	NAG	G	631	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	632	5	-	0/6/23/26	0/1/1/1
5	NAG	G	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	634	5	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	626	NAG	O5-C1	-3.17	1.38	1.43
5	D	626	NAG	O5-C1	-2.71	1.39	1.43
5	E	626	NAG	O5-C1	-2.53	1.39	1.43
5	E	630	NAG	O5-C1	4.49	1.51	1.43
5	G	630	NAG	O5-C1	4.54	1.51	1.43
5	D	630	NAG	O5-C1	4.72	1.51	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	613	MAN	O2-C2-C3	-2.37	105.52	110.17
7	G	613	MAN	O2-C2-C3	-2.36	105.53	110.17
7	D	613	MAN	O2-C2-C3	-2.33	105.60	110.17
5	E	618	NAG	C1-O5-C5	2.01	114.93	112.17
6	E	625	BMA	C1-O5-C5	2.02	114.95	112.17
5	E	610	NAG	C1-O5-C5	2.02	114.95	112.17
5	G	610	NAG	C1-O5-C5	2.05	114.99	112.17
6	G	625	BMA	C1-O5-C5	2.07	115.02	112.17
5	D	631	NAG	C1-O5-C5	2.08	115.04	112.17
5	D	633	NAG	C1-O5-C5	2.10	115.06	112.17
5	D	629	NAG	C1-O5-C5	2.12	115.09	112.17
5	G	604	NAG	C1-O5-C5	2.12	115.09	112.17
5	E	603	NAG	C1-O5-C5	2.14	115.12	112.17
5	D	617	NAG	C1-O5-C5	2.16	115.15	112.17
5	D	610	NAG	C1-O5-C5	2.17	115.16	112.17
5	G	626	NAG	C3-C4-C5	2.26	114.20	110.22
6	E	628	BMA	C1-C2-C3	2.28	112.54	109.65
5	G	631	NAG	C1-O5-C5	2.28	115.31	112.17
6	G	628	BMA	C1-C2-C3	2.30	112.56	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	631	NAG	C1-O5-C5	2.30	115.34	112.17
6	D	628	BMA	C1-C2-C3	2.36	112.64	109.65
6	D	625	BMA	C1-O5-C5	2.37	115.44	112.17
5	E	621	NAG	C1-O5-C5	2.40	115.48	112.17
5	G	621	NAG	C1-O5-C5	2.43	115.52	112.17
5	E	622	NAG	C1-O5-C5	2.44	115.53	112.17
5	G	622	NAG	C1-O5-C5	2.48	115.58	112.17
5	D	621	NAG	C1-O5-C5	2.64	115.81	112.17
5	G	629	NAG	C1-O5-C5	2.68	115.86	112.17
5	E	629	NAG	C1-O5-C5	2.73	115.93	112.17
6	G	609	BMA	C1-O5-C5	2.97	116.26	112.17
6	D	628	BMA	C1-O5-C5	3.08	116.41	112.17
6	E	609	BMA	C1-O5-C5	3.08	116.41	112.17
6	D	609	BMA	C1-O5-C5	3.14	116.50	112.17
6	E	628	BMA	C1-O5-C5	3.36	116.79	112.17
6	G	628	BMA	C1-O5-C5	3.58	117.09	112.17
7	G	613	MAN	C1-O5-C5	3.85	117.47	112.17
7	E	613	MAN	C1-O5-C5	3.86	117.48	112.17
7	D	613	MAN	C1-O5-C5	3.97	117.63	112.17
5	E	630	NAG	C1-O5-C5	5.84	120.22	112.17
5	D	630	NAG	C1-O5-C5	5.92	120.32	112.17
5	G	630	NAG	C1-O5-C5	6.00	120.43	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	603	NAG	1	0
5	D	607	NAG	1	0
5	D	610	NAG	1	0
5	D	621	NAG	1	0
5	E	603	NAG	1	0
5	E	607	NAG	1	0
5	E	610	NAG	1	0
5	E	621	NAG	1	0
5	G	603	NAG	2	0
5	G	607	NAG	1	0
5	G	610	NAG	1	0
5	G	621	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.