



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:23 PM GMT

PDB ID : 5EVM
Title : Crystal Structure of Nipah Virus Fusion Glycoprotein in the Prefusion State
Authors : Xu, K.; Nikolov, D.B.
Deposited on : 2015-11-20
Resolution : 3.37 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

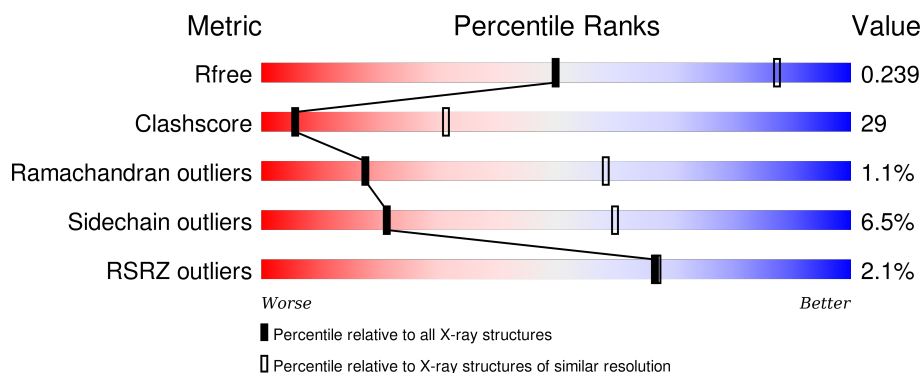
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



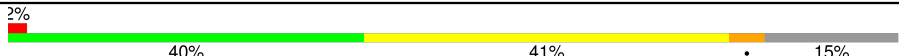
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	529	<div> <div>2%</div> <div>45% 38% 14%</div> </div>
1	B	529	<div> <div>2%</div> <div>44% 39% 14%</div> </div>
1	C	529	<div> <div>2%</div> <div>41% 41% 15%</div> </div>
1	D	529	<div> <div>2%</div> <div>43% 40% 14%</div> </div>
1	E	529	<div> <div>2%</div> <div>43% 39% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	529	

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
5	MLI	A	611	-	-	-	X
5	MLI	B	612	-	-	-	X
5	MLI	C	610	-	-	-	X
5	MLI	D	612	-	-	-	X
5	MLI	E	610	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21612 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3482	2204	571	687	20			
1	B	456	Total	C	N	O	S	0	0	0
			3478	2202	571	685	20			
1	C	450	Total	C	N	O	S	0	0	0
			3439	2178	562	679	20			
1	D	456	Total	C	N	O	S	0	0	0
			3482	2204	571	687	20			
1	E	456	Total	C	N	O	S	0	0	0
			3482	2204	571	687	20			
1	F	450	Total	C	N	O	S	0	0	0
			3439	2178	562	679	20			

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	engineered mutation	UNP Q9IH63
A	305	ASP	ASN	engineered mutation	UNP Q9IH63
A	532	LYS	-	expression tag	UNP Q9IH63
A	533	LEU	-	expression tag	UNP Q9IH63
A	534	MET	-	expression tag	UNP Q9IH63
A	535	LYS	-	expression tag	UNP Q9IH63
A	536	GLN	-	expression tag	UNP Q9IH63
A	537	ILE	-	expression tag	UNP Q9IH63
A	538	GLU	-	expression tag	UNP Q9IH63
A	539	ASP	-	expression tag	UNP Q9IH63
A	540	LYS	-	expression tag	UNP Q9IH63
A	541	ILE	-	expression tag	UNP Q9IH63
A	542	GLU	-	expression tag	UNP Q9IH63
A	543	GLU	-	expression tag	UNP Q9IH63
A	544	ILE	-	expression tag	UNP Q9IH63
A	545	LEU	-	expression tag	UNP Q9IH63
A	546	SER	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
A	547	LYS	-	expression tag	UNP Q9IH63
A	548	ILE	-	expression tag	UNP Q9IH63
A	549	TYR	-	expression tag	UNP Q9IH63
A	550	HIS	-	expression tag	UNP Q9IH63
A	551	ILE	-	expression tag	UNP Q9IH63
A	552	GLU	-	expression tag	UNP Q9IH63
A	553	ASN	-	expression tag	UNP Q9IH63
A	554	GLU	-	expression tag	UNP Q9IH63
A	555	ILE	-	expression tag	UNP Q9IH63
A	556	ALA	-	expression tag	UNP Q9IH63
A	557	ARG	-	expression tag	UNP Q9IH63
A	558	ILE	-	expression tag	UNP Q9IH63
A	559	LYS	-	expression tag	UNP Q9IH63
A	560	LYS	-	expression tag	UNP Q9IH63
A	561	LEU	-	expression tag	UNP Q9IH63
A	562	ILE	-	expression tag	UNP Q9IH63
A	563	GLY	-	expression tag	UNP Q9IH63
A	564	GLU	-	expression tag	UNP Q9IH63
A	565	ALA	-	expression tag	UNP Q9IH63
A	566	PRO	-	expression tag	UNP Q9IH63
A	567	GLY	-	expression tag	UNP Q9IH63
A	568	GLY	-	expression tag	UNP Q9IH63
A	569	ILE	-	expression tag	UNP Q9IH63
A	570	GLU	-	expression tag	UNP Q9IH63
A	571	GLY	-	expression tag	UNP Q9IH63
A	572	ARG	-	expression tag	UNP Q9IH63
B	67	ASP	ASN	engineered mutation	UNP Q9IH63
B	305	ASP	ASN	engineered mutation	UNP Q9IH63
B	489	LYS	-	expression tag	UNP Q9IH63
B	490	LEU	-	expression tag	UNP Q9IH63
B	491	MET	-	expression tag	UNP Q9IH63
B	492	LYS	-	expression tag	UNP Q9IH63
B	493	GLN	-	expression tag	UNP Q9IH63
B	494	ILE	-	expression tag	UNP Q9IH63
B	495	GLU	-	expression tag	UNP Q9IH63
B	496	ASP	-	expression tag	UNP Q9IH63
B	497	LYS	-	expression tag	UNP Q9IH63
B	498	ILE	-	expression tag	UNP Q9IH63
B	499	GLU	-	expression tag	UNP Q9IH63
B	500	GLU	-	expression tag	UNP Q9IH63
B	501	ILE	-	expression tag	UNP Q9IH63
B	502	LEU	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	SER	-	expression tag	UNP Q9IH63
B	504	LYS	-	expression tag	UNP Q9IH63
B	505	ILE	-	expression tag	UNP Q9IH63
B	506	TYR	-	expression tag	UNP Q9IH63
B	507	HIS	-	expression tag	UNP Q9IH63
B	508	ILE	-	expression tag	UNP Q9IH63
B	509	GLU	-	expression tag	UNP Q9IH63
B	510	ASN	-	expression tag	UNP Q9IH63
B	511	GLU	-	expression tag	UNP Q9IH63
B	512	ILE	-	expression tag	UNP Q9IH63
B	513	ALA	-	expression tag	UNP Q9IH63
B	514	ARG	-	expression tag	UNP Q9IH63
B	515	ILE	-	expression tag	UNP Q9IH63
B	516	LYS	-	expression tag	UNP Q9IH63
B	517	LYS	-	expression tag	UNP Q9IH63
B	518	LEU	-	expression tag	UNP Q9IH63
B	519	ILE	-	expression tag	UNP Q9IH63
B	520	GLY	-	expression tag	UNP Q9IH63
B	521	GLU	-	expression tag	UNP Q9IH63
B	522	ALA	-	expression tag	UNP Q9IH63
B	523	PRO	-	expression tag	UNP Q9IH63
B	524	GLY	-	expression tag	UNP Q9IH63
B	525	GLY	-	expression tag	UNP Q9IH63
B	526	ILE	-	expression tag	UNP Q9IH63
B	527	GLU	-	expression tag	UNP Q9IH63
B	528	GLY	-	expression tag	UNP Q9IH63
B	529	ARG	-	expression tag	UNP Q9IH63
C	67	ASP	ASN	engineered mutation	UNP Q9IH63
C	305	ASP	ASN	engineered mutation	UNP Q9IH63
C	489	LYS	-	expression tag	UNP Q9IH63
C	490	LEU	-	expression tag	UNP Q9IH63
C	491	MET	-	expression tag	UNP Q9IH63
C	492	LYS	-	expression tag	UNP Q9IH63
C	493	GLN	-	expression tag	UNP Q9IH63
C	494	ILE	-	expression tag	UNP Q9IH63
C	495	GLU	-	expression tag	UNP Q9IH63
C	496	ASP	-	expression tag	UNP Q9IH63
C	497	LYS	-	expression tag	UNP Q9IH63
C	498	ILE	-	expression tag	UNP Q9IH63
C	499	GLU	-	expression tag	UNP Q9IH63
C	500	GLU	-	expression tag	UNP Q9IH63
C	501	ILE	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	502	LEU	-	expression tag	UNP Q9IH63
C	503	SER	-	expression tag	UNP Q9IH63
C	504	LYS	-	expression tag	UNP Q9IH63
C	505	ILE	-	expression tag	UNP Q9IH63
C	506	TYR	-	expression tag	UNP Q9IH63
C	507	HIS	-	expression tag	UNP Q9IH63
C	508	ILE	-	expression tag	UNP Q9IH63
C	509	GLU	-	expression tag	UNP Q9IH63
C	510	ASN	-	expression tag	UNP Q9IH63
C	511	GLU	-	expression tag	UNP Q9IH63
C	512	ILE	-	expression tag	UNP Q9IH63
C	513	ALA	-	expression tag	UNP Q9IH63
C	514	ARG	-	expression tag	UNP Q9IH63
C	515	ILE	-	expression tag	UNP Q9IH63
C	516	LYS	-	expression tag	UNP Q9IH63
C	517	LYS	-	expression tag	UNP Q9IH63
C	518	LEU	-	expression tag	UNP Q9IH63
C	519	ILE	-	expression tag	UNP Q9IH63
C	520	GLY	-	expression tag	UNP Q9IH63
C	521	GLU	-	expression tag	UNP Q9IH63
C	522	ALA	-	expression tag	UNP Q9IH63
C	523	PRO	-	expression tag	UNP Q9IH63
C	524	GLY	-	expression tag	UNP Q9IH63
C	525	GLY	-	expression tag	UNP Q9IH63
C	526	ILE	-	expression tag	UNP Q9IH63
C	527	GLU	-	expression tag	UNP Q9IH63
C	528	GLY	-	expression tag	UNP Q9IH63
C	529	ARG	-	expression tag	UNP Q9IH63
D	67	ASP	ASN	engineered mutation	UNP Q9IH63
D	305	ASP	ASN	engineered mutation	UNP Q9IH63
D	489	LYS	-	expression tag	UNP Q9IH63
D	490	LEU	-	expression tag	UNP Q9IH63
D	491	MET	-	expression tag	UNP Q9IH63
D	492	LYS	-	expression tag	UNP Q9IH63
D	493	GLN	-	expression tag	UNP Q9IH63
D	494	ILE	-	expression tag	UNP Q9IH63
D	495	GLU	-	expression tag	UNP Q9IH63
D	496	ASP	-	expression tag	UNP Q9IH63
D	497	LYS	-	expression tag	UNP Q9IH63
D	498	ILE	-	expression tag	UNP Q9IH63
D	499	GLU	-	expression tag	UNP Q9IH63
D	500	GLU	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
D	501	ILE	-	expression tag	UNP Q9IH63
D	502	LEU	-	expression tag	UNP Q9IH63
D	503	SER	-	expression tag	UNP Q9IH63
D	504	LYS	-	expression tag	UNP Q9IH63
D	505	ILE	-	expression tag	UNP Q9IH63
D	506	TYR	-	expression tag	UNP Q9IH63
D	507	HIS	-	expression tag	UNP Q9IH63
D	508	ILE	-	expression tag	UNP Q9IH63
D	509	GLU	-	expression tag	UNP Q9IH63
D	510	ASN	-	expression tag	UNP Q9IH63
D	511	GLU	-	expression tag	UNP Q9IH63
D	512	ILE	-	expression tag	UNP Q9IH63
D	513	ALA	-	expression tag	UNP Q9IH63
D	514	ARG	-	expression tag	UNP Q9IH63
D	515	ILE	-	expression tag	UNP Q9IH63
D	516	LYS	-	expression tag	UNP Q9IH63
D	517	LYS	-	expression tag	UNP Q9IH63
D	518	LEU	-	expression tag	UNP Q9IH63
D	519	ILE	-	expression tag	UNP Q9IH63
D	520	GLY	-	expression tag	UNP Q9IH63
D	521	GLU	-	expression tag	UNP Q9IH63
D	522	ALA	-	expression tag	UNP Q9IH63
D	523	PRO	-	expression tag	UNP Q9IH63
D	524	GLY	-	expression tag	UNP Q9IH63
D	525	GLY	-	expression tag	UNP Q9IH63
D	526	ILE	-	expression tag	UNP Q9IH63
D	527	GLU	-	expression tag	UNP Q9IH63
D	528	GLY	-	expression tag	UNP Q9IH63
D	529	ARG	-	expression tag	UNP Q9IH63
E	67	ASP	ASN	engineered mutation	UNP Q9IH63
E	305	ASP	ASN	engineered mutation	UNP Q9IH63
E	489	LYS	-	expression tag	UNP Q9IH63
E	490	LEU	-	expression tag	UNP Q9IH63
E	491	MET	-	expression tag	UNP Q9IH63
E	492	LYS	-	expression tag	UNP Q9IH63
E	493	GLN	-	expression tag	UNP Q9IH63
E	494	ILE	-	expression tag	UNP Q9IH63
E	495	GLU	-	expression tag	UNP Q9IH63
E	496	ASP	-	expression tag	UNP Q9IH63
E	497	LYS	-	expression tag	UNP Q9IH63
E	498	ILE	-	expression tag	UNP Q9IH63
E	499	GLU	-	expression tag	UNP Q9IH63

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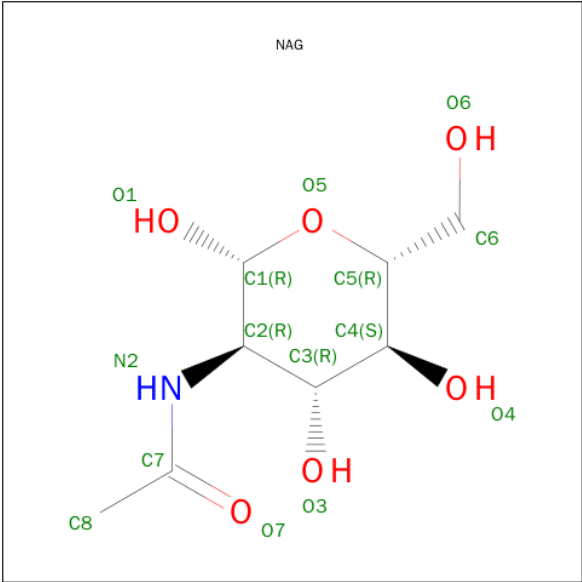
Chain	Residue	Modelled	Actual	Comment	Reference
E	500	GLU	-	expression tag	UNP Q9IH63
E	501	ILE	-	expression tag	UNP Q9IH63
E	502	LEU	-	expression tag	UNP Q9IH63
E	503	SER	-	expression tag	UNP Q9IH63
E	504	LYS	-	expression tag	UNP Q9IH63
E	505	ILE	-	expression tag	UNP Q9IH63
E	506	TYR	-	expression tag	UNP Q9IH63
E	507	HIS	-	expression tag	UNP Q9IH63
E	508	ILE	-	expression tag	UNP Q9IH63
E	509	GLU	-	expression tag	UNP Q9IH63
E	510	ASN	-	expression tag	UNP Q9IH63
E	511	GLU	-	expression tag	UNP Q9IH63
E	512	ILE	-	expression tag	UNP Q9IH63
E	513	ALA	-	expression tag	UNP Q9IH63
E	514	ARG	-	expression tag	UNP Q9IH63
E	515	ILE	-	expression tag	UNP Q9IH63
E	516	LYS	-	expression tag	UNP Q9IH63
E	517	LYS	-	expression tag	UNP Q9IH63
E	518	LEU	-	expression tag	UNP Q9IH63
E	519	ILE	-	expression tag	UNP Q9IH63
E	520	GLY	-	expression tag	UNP Q9IH63
E	521	GLU	-	expression tag	UNP Q9IH63
E	522	ALA	-	expression tag	UNP Q9IH63
E	523	PRO	-	expression tag	UNP Q9IH63
E	524	GLY	-	expression tag	UNP Q9IH63
E	525	GLY	-	expression tag	UNP Q9IH63
E	526	ILE	-	expression tag	UNP Q9IH63
E	527	GLU	-	expression tag	UNP Q9IH63
E	528	GLY	-	expression tag	UNP Q9IH63
E	529	ARG	-	expression tag	UNP Q9IH63
F	67	ASP	ASN	engineered mutation	UNP Q9IH63
F	305	ASP	ASN	engineered mutation	UNP Q9IH63
F	489	LYS	-	expression tag	UNP Q9IH63
F	490	LEU	-	expression tag	UNP Q9IH63
F	491	MET	-	expression tag	UNP Q9IH63
F	492	LYS	-	expression tag	UNP Q9IH63
F	493	GLN	-	expression tag	UNP Q9IH63
F	494	ILE	-	expression tag	UNP Q9IH63
F	495	GLU	-	expression tag	UNP Q9IH63
F	496	ASP	-	expression tag	UNP Q9IH63
F	497	LYS	-	expression tag	UNP Q9IH63
F	498	ILE	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
F	499	GLU	-	expression tag	UNP Q9IH63
F	500	GLU	-	expression tag	UNP Q9IH63
F	501	ILE	-	expression tag	UNP Q9IH63
F	502	LEU	-	expression tag	UNP Q9IH63
F	503	SER	-	expression tag	UNP Q9IH63
F	504	LYS	-	expression tag	UNP Q9IH63
F	505	ILE	-	expression tag	UNP Q9IH63
F	506	TYR	-	expression tag	UNP Q9IH63
F	507	HIS	-	expression tag	UNP Q9IH63
F	508	ILE	-	expression tag	UNP Q9IH63
F	509	GLU	-	expression tag	UNP Q9IH63
F	510	ASN	-	expression tag	UNP Q9IH63
F	511	GLU	-	expression tag	UNP Q9IH63
F	512	ILE	-	expression tag	UNP Q9IH63
F	513	ALA	-	expression tag	UNP Q9IH63
F	514	ARG	-	expression tag	UNP Q9IH63
F	515	ILE	-	expression tag	UNP Q9IH63
F	516	LYS	-	expression tag	UNP Q9IH63
F	517	LYS	-	expression tag	UNP Q9IH63
F	518	LEU	-	expression tag	UNP Q9IH63
F	519	ILE	-	expression tag	UNP Q9IH63
F	520	GLY	-	expression tag	UNP Q9IH63
F	521	GLU	-	expression tag	UNP Q9IH63
F	522	ALA	-	expression tag	UNP Q9IH63
F	523	PRO	-	expression tag	UNP Q9IH63
F	524	GLY	-	expression tag	UNP Q9IH63
F	525	GLY	-	expression tag	UNP Q9IH63
F	526	ILE	-	expression tag	UNP Q9IH63
F	527	GLU	-	expression tag	UNP Q9IH63
F	528	GLY	-	expression tag	UNP Q9IH63
F	529	ARG	-	expression tag	UNP Q9IH63

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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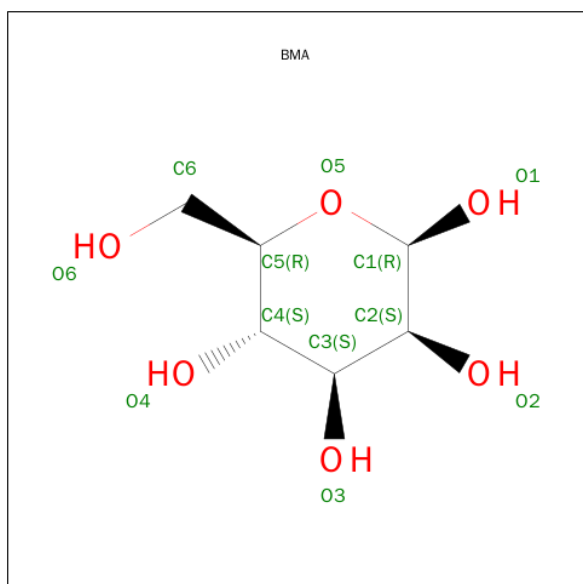
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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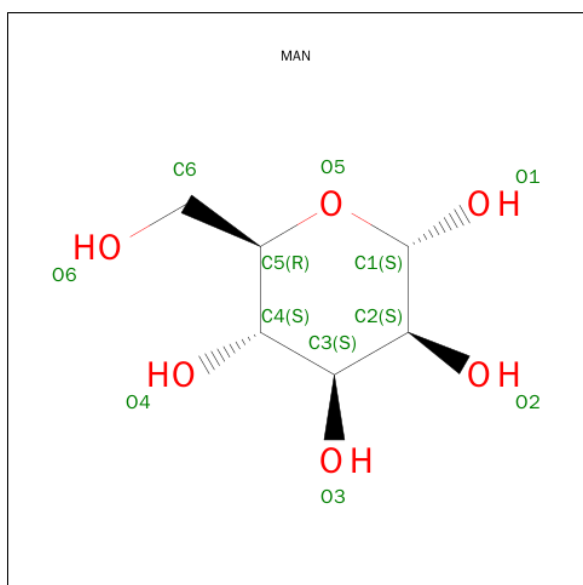
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



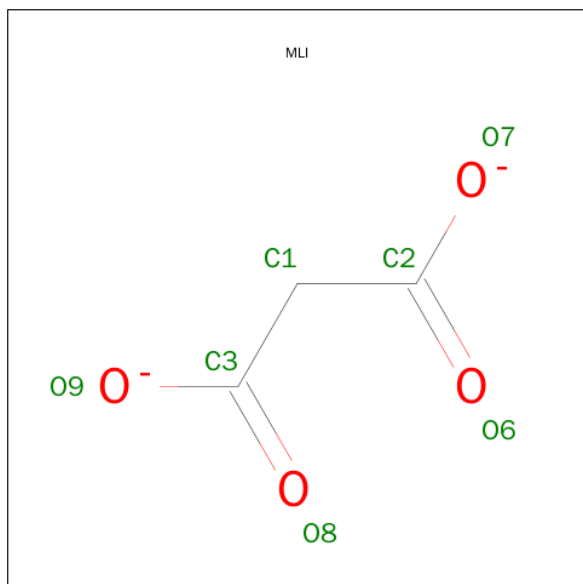
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4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

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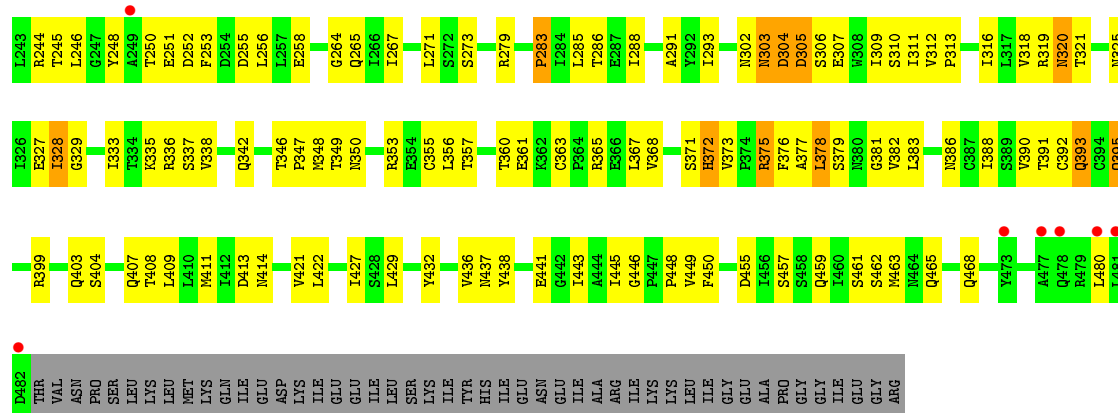
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			11	6	5		

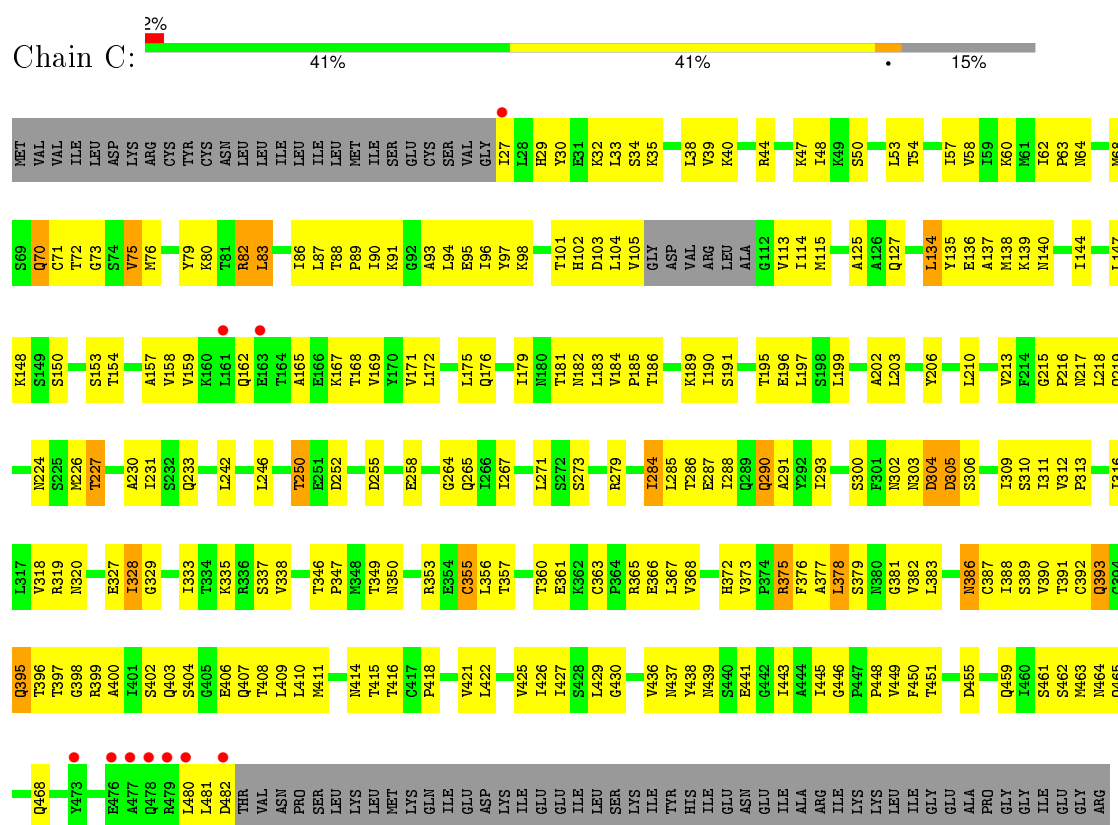
- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



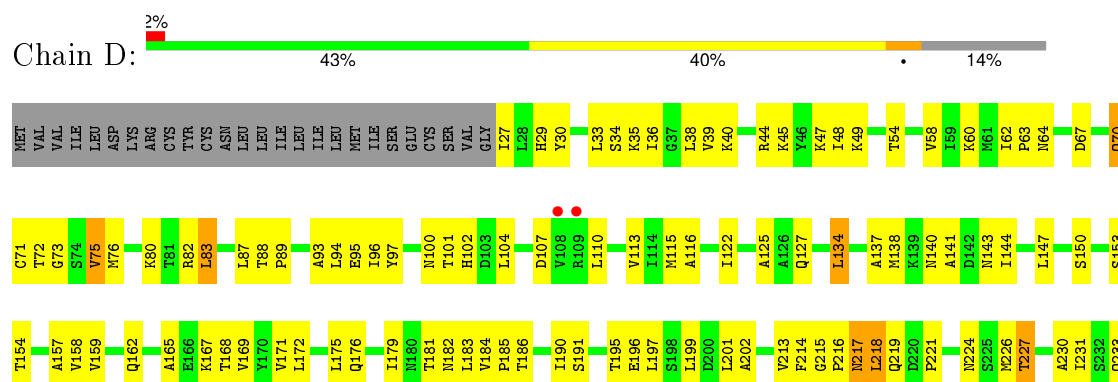
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	B	1	Total	C	O	0	0
			7	3	4		
5	C	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		
5	F	1	Total	C	O	0	0
			7	3	4		

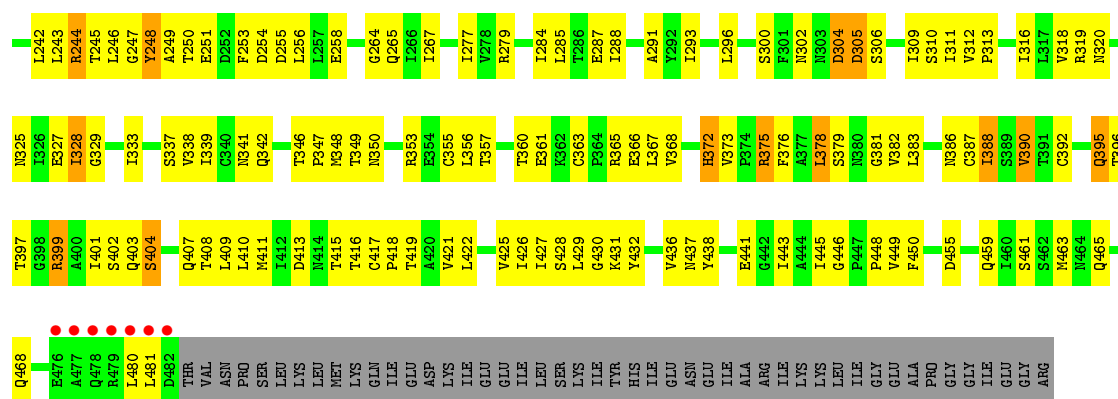


• Molecule 1: Fusion glycoprotein F0

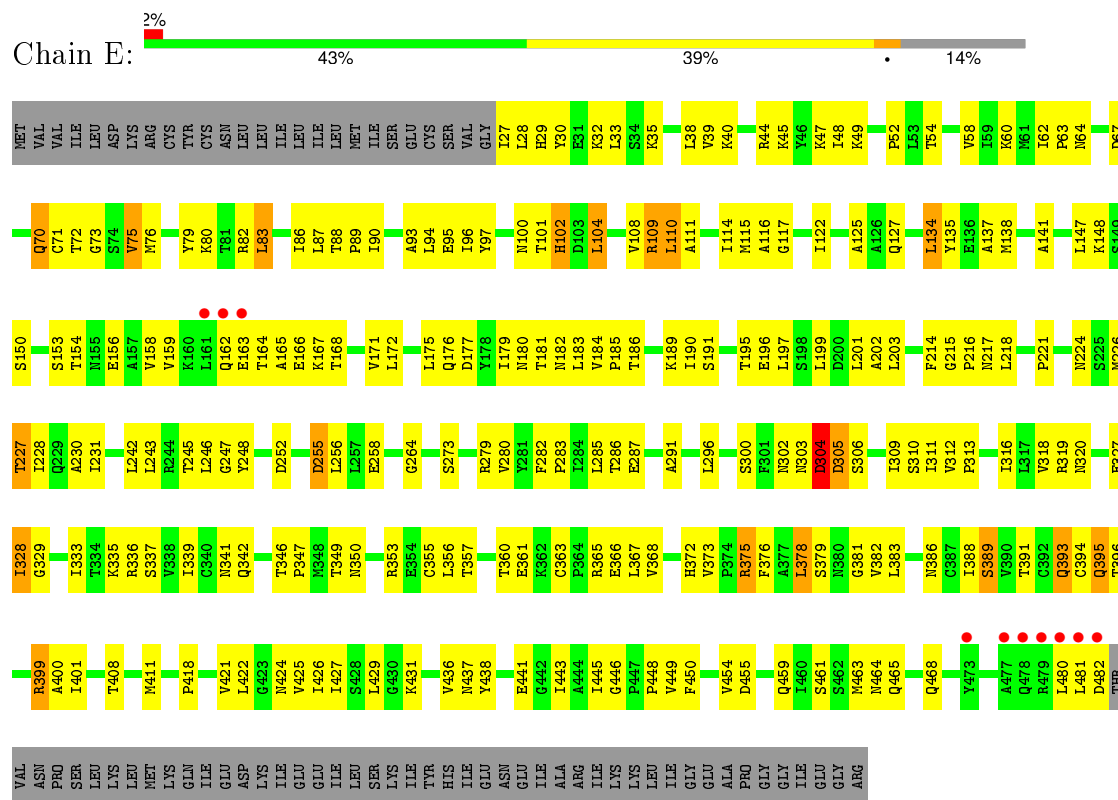


• Molecule 1: Fusion glycoprotein F0

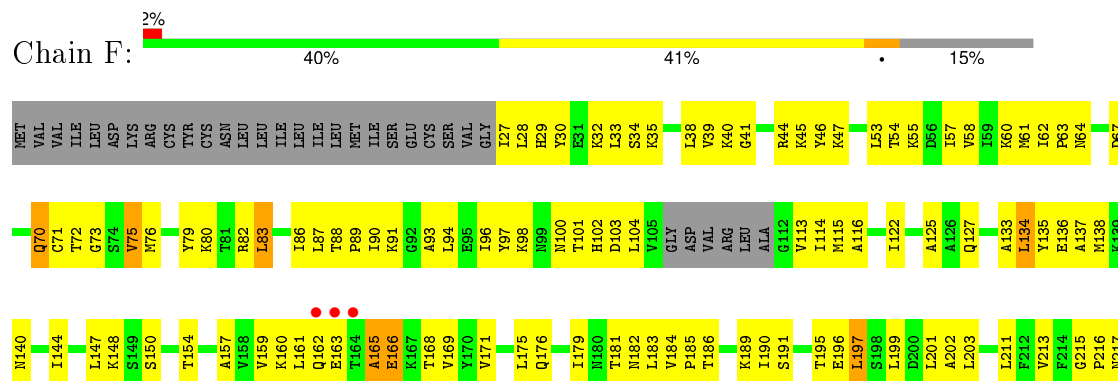




• Molecule 1: Fusion glycoprotein F0



• Molecule 1: Fusion glycoprotein F0



GLY	M463	T388	I316	L218
ARG	N464	S389	L317	Q219
	Q465	V390	V318	
	Q468	T391	R319	N224
	Y472	C392	N320	S225
	Y473	Q393		N226
	A477	C394	N325	T227
	Q478	Q395	I326	A230
	R479	T396	E327	I231
	L480	T397	I328	
	L481	G398	G329	
	D482	R399		L242
	THR	Q403	L332	
	VAL	S404	I333	L246
	ASN	G405	T334	G247
	PRO	E406	K335	Y248
	SER	Q407	R336	A249
	LEU	T408	S337	T250
	LYS	L409	V338	E251
	LEU	L410	I339	D252
	MET	M411	C340	F253
	LYS	I412	N341	D254
	LYS	D413	Q342	D255
	GLN	N414		
	ILE	T415	T346	E258
	GLU	T416	P347	
	ASP	C417	M348	G264
	LYS	P418	T349	Q265
	ILE	T419	N350	I266
	GLU	A420		I267
	GLU	V421	R353	
	ILE	L422	E354	L271
			C355	S272
		V425	L356	S273
		I426	T357	
		I427		R279
		S428	T360	
		L429	E361	P283
			R362	
		V436	C363	
		N437		T286
		Y438	E366	E287
		E441	I367	I288
		G442	V368	Q289
		I443		I290
		A444		A291
		I445	H372	
		G446	V373	I292
		V449	P374	I293
		F450	R375	
		D455	F376	N302
			A377	N303
			L378	D304
			S379	D305
			N380	S306
			G381	
			V382	I309
			L383	S310
				I311
				V312
				P313
				C387

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	355.75Å 355.75Å 168.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.16 – 3.37 43.16 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.16-3.37) 99.4 (43.16-3.37)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.213 , 0.220 0.240 , 0.239	Depositor DCC
R_{free} test set	5593 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	102.8	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.0	EDS
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 112116 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21612	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, NAG, BMA, 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	0.44	0/3531	0.86	14/4800 (0.3%)
1	B	0.45	0/3527	0.83	10/4795 (0.2%)
1	C	0.45	0/3487	0.82	16/4739 (0.3%)
1	D	0.44	0/3531	0.80	13/4800 (0.3%)
1	E	0.44	0/3531	0.83	18/4800 (0.4%)
1	F	0.44	0/3487	0.94	18/4739 (0.4%)
All	All	0.44	0/21094	0.85	89/28673 (0.3%)

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	375	ARG	NE-CZ-NH1	-19.59	110.51	120.30
1	F	375	ARG	NE-CZ-NH2	18.42	129.51	120.30
1	A	353	ARG	NE-CZ-NH1	17.50	129.05	120.30
1	A	353	ARG	NE-CZ-NH2	-17.08	111.76	120.30
1	B	353	ARG	NE-CZ-NH1	16.66	128.63	120.30

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	3482	0	3510	203	0
1	B	3478	0	3506	221	0
1	C	3439	0	3463	238	0
1	D	3482	0	3510	232	0
1	E	3482	0	3510	219	0
1	F	3439	0	3464	242	0
2	A	84	0	73	3	0
2	B	84	0	72	7	0
2	C	84	0	74	5	0
2	D	84	0	72	5	0
2	E	84	0	73	9	0
2	F	84	0	73	3	0
3	A	11	0	8	2	0
4	A	33	0	30	1	0
4	B	55	0	48	2	0
4	C	33	0	28	1	0
4	D	55	0	48	1	0
4	E	33	0	29	1	0
4	F	44	0	38	0	0
5	A	7	0	2	0	0
5	B	7	0	2	0	0
5	C	7	0	2	0	0
5	D	7	0	2	0	0
5	E	7	0	2	1	0
5	F	7	0	2	0	0
All	All	21612	0	21641	1259	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 29.

The worst 5 of 1259 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:258:GLU:HG3	1:C:216:PRO:HD2	1.28	1.11
1:A:360:THR:HG21	1:A:443:ILE:HD11	1.29	1.09
1:B:468:GLN:HE21	2:B:607:NAG:H62	1.13	1.08
1:C:360:THR:HG21	1:C:443:ILE:HD11	1.35	1.08
1:A:437:ASN:O	1:A:441:GLU:HG2	1.53	1.07

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	454/529 (86%)	398 (88%)	52 (12%)	4 (1%)	21	63
1	B	454/529 (86%)	396 (87%)	53 (12%)	5 (1%)	17	58
1	C	446/529 (84%)	384 (86%)	57 (13%)	5 (1%)	17	58
1	D	454/529 (86%)	390 (86%)	60 (13%)	4 (1%)	21	63
1	E	454/529 (86%)	392 (86%)	58 (13%)	4 (1%)	21	63
1	F	446/529 (84%)	379 (85%)	59 (13%)	8 (2%)	11	47
All	All	2708/3174 (85%)	2339 (86%)	339 (12%)	30 (1%)	17	58

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	166	GLU
1	F	398	GLY
1	A	381	GLY
1	B	320	ASN
1	C	320	ASN

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	397/471 (84%)	371 (94%)	26 (6%)	21	60
1	B	396/471 (84%)	372 (94%)	24 (6%)	23	62
1	C	393/471 (83%)	369 (94%)	24 (6%)	23	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	397/471 (84%)	367 (92%)	30 (8%)	16	53
1	E	397/471 (84%)	371 (94%)	26 (6%)	21	60
1	F	393/471 (83%)	369 (94%)	24 (6%)	23	62
All	All	2373/2826 (84%)	2219 (94%)	154 (6%)	21	60

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	386	ASN
1	D	248	TYR
1	F	283	PRO
1	C	393	GLN
1	D	102	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	386	ASN
1	D	162	GLN
1	F	176	GLN
1	C	393	GLN
1	D	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

66 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$
2	NAG	A	601	1,2	14,14,15	0.68	0	15,19,21	0.83	1 (6%)
2	NAG	A	602	3,2	14,14,15	0.50	0	15,19,21	0.71	0
3	BMA	A	603	2,4	11,11,12	1.36	2 (18%)	15,15,17	1.58	2 (13%)
4	MAN	A	604	3	11,11,12	0.89	0	15,15,17	0.97	2 (13%)
4	MAN	A	605	3	11,11,12	0.94	1 (9%)	15,15,17	0.99	1 (6%)
2	NAG	A	606	1,2	14,14,15	0.86	0	15,19,21	1.17	2 (13%)
2	NAG	A	607	2	14,14,15	1.06	1 (7%)	15,19,21	0.81	0
2	NAG	A	608	1,2	14,14,15	0.69	0	15,19,21	0.81	0
2	NAG	A	609	2,4	14,14,15	0.73	0	15,19,21	0.86	0
4	MAN	A	610	2	11,11,12	0.87	0	15,15,17	1.24	3 (20%)
5	MLI	A	611	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	B	601	1,2	14,14,15	0.68	0	15,19,21	0.74	0
2	NAG	B	602	2,4	14,14,15	0.96	0	15,19,21	1.05	1 (6%)
4	MAN	B	603	2	11,11,12	1.02	1 (9%)	15,15,17	1.29	2 (13%)
2	NAG	B	604	1,2	14,14,15	0.74	0	15,19,21	0.89	1 (6%)
2	NAG	B	605	2,4	14,14,15	0.85	0	15,19,21	0.86	1 (6%)
4	MAN	B	606	2	11,11,12	0.92	1 (9%)	15,15,17	0.75	1 (6%)
2	NAG	B	607	1,2	14,14,15	0.60	0	15,19,21	0.88	1 (6%)
2	NAG	B	608	2,4	14,14,15	0.71	0	15,19,21	0.78	0
4	MAN	B	609	2,4	11,11,12	1.05	1 (9%)	15,15,17	1.72	3 (20%)
4	MAN	B	610	4	11,11,12	0.65	0	15,15,17	0.81	1 (6%)
4	MAN	B	611	4	11,11,12	0.71	0	15,15,17	0.76	1 (6%)
5	MLI	B	612	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	C	601	1,2	14,14,15	0.69	0	15,19,21	1.61	3 (20%)
2	NAG	C	602	2,4	14,14,15	0.74	0	15,19,21	1.39	3 (20%)
4	MAN	C	603	2,4	11,11,12	1.06	1 (9%)	15,15,17	0.59	0
4	MAN	C	604	4	11,11,12	0.61	0	15,15,17	0.64	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	C	605	4	11,11,12	0.73	0	15,15,17	0.78	1 (6%)
2	NAG	C	606	1,2	14,14,15	0.64	0	15,19,21	0.81	0
2	NAG	C	607	2	14,14,15	0.86	0	15,19,21	0.84	1 (6%)
2	NAG	C	608	1,2	14,14,15	0.77	0	15,19,21	1.24	2 (13%)
2	NAG	C	609	2	14,14,15	0.88	1 (7%)	15,19,21	0.61	0
5	MLI	C	610	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	D	601	1,2	14,14,15	0.71	1 (7%)	15,19,21	0.90	0
2	NAG	D	602	2,4	14,14,15	0.75	0	15,19,21	1.02	1 (6%)
4	MAN	D	603	2,4	11,11,12	0.80	0	15,15,17	0.73	1 (6%)
4	MAN	D	604	4	11,11,12	0.74	0	15,15,17	0.85	1 (6%)
2	NAG	D	605	1,2	14,14,15	0.57	0	15,19,21	0.67	0
2	NAG	D	606	2,4	14,14,15	0.82	0	15,19,21	1.06	2 (13%)
4	MAN	D	607	2,4	11,11,12	0.90	0	15,15,17	0.98	2 (13%)
4	MAN	D	608	4	11,11,12	0.84	0	15,15,17	0.74	1 (6%)
2	NAG	D	609	1,2	14,14,15	0.65	0	15,19,21	0.90	1 (6%)
2	NAG	D	610	2,4	14,14,15	0.71	0	15,19,21	0.77	0
4	MAN	D	611	2	11,11,12	1.16	1 (9%)	15,15,17	1.02	1 (6%)
5	MLI	D	612	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	E	601	1,2	14,14,15	0.67	0	15,19,21	1.00	1 (6%)
2	NAG	E	602	2,4	14,14,15	0.72	0	15,19,21	1.04	1 (6%)
4	MAN	E	603	2	11,11,12	0.90	0	15,15,17	0.84	1 (6%)
2	NAG	E	604	1,2	14,14,15	0.54	0	15,19,21	0.60	0
2	NAG	E	605	2,4	14,14,15	0.57	0	15,19,21	0.90	0
4	MAN	E	606	2,4	11,11,12	1.18	1 (9%)	15,15,17	0.94	2 (13%)
4	MAN	E	607	4	11,11,12	0.78	0	15,15,17	1.23	2 (13%)
2	NAG	E	608	1,2	14,14,15	0.76	0	15,19,21	0.73	1 (6%)
2	NAG	E	609	2	14,14,15	0.91	1 (7%)	15,19,21	0.62	0
5	MLI	E	610	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	F	601	1,2	14,14,15	0.83	0	15,19,21	0.94	2 (13%)
2	NAG	F	602	2	14,14,15	0.72	0	15,19,21	0.73	0
2	NAG	F	603	1,2	14,14,15	0.51	0	15,19,21	0.73	0
2	NAG	F	604	2,4	14,14,15	0.67	0	15,19,21	0.99	2 (13%)
4	MAN	F	605	2	11,11,12	0.85	0	15,15,17	0.85	1 (6%)
2	NAG	F	606	1,2	14,14,15	0.60	0	15,19,21	0.89	1 (6%)
2	NAG	F	607	2,4	14,14,15	0.70	0	15,19,21	0.76	1 (6%)
4	MAN	F	608	2,4	11,11,12	1.19	1 (9%)	15,15,17	0.56	0
4	MAN	F	609	4	11,11,12	0.83	0	15,15,17	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	F	610	4	11,11,12	0.92	1 (9%)	15,15,17	0.72	1 (6%)
5	MLI	F	611	-	0,6,6	0.00	-	0,7,7	0.00	-

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
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	604	3	-	0/2/19/22	0/1/1/1
4	MAN	A	605	3	-	0/2/19/22	0/1/1/1
2	NAG	A	606	1,2	-	1/6/23/26	0/1/1/1
2	NAG	A	607	2	-	0/6/23/26	0/1/1/1
2	NAG	A	608	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	609	2,4	-	0/6/23/26	0/1/1/1
4	MAN	A	610	2	-	0/2/19/22	0/1/1/1
5	MLI	A	611	-	-	0/0/4/4	0/0/0/0
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	2,4	-	0/6/23/26	0/1/1/1
4	MAN	B	603	2	-	0/2/19/22	0/1/1/1
2	NAG	B	604	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	605	2,4	-	0/6/23/26	0/1/1/1
4	MAN	B	606	2	-	0/2/19/22	0/1/1/1
2	NAG	B	607	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	608	2,4	-	0/6/23/26	0/1/1/1
4	MAN	B	609	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	610	4	-	0/2/19/22	0/1/1/1
4	MAN	B	611	4	-	0/2/19/22	0/1/1/1
5	MLI	B	612	-	-	0/0/4/4	0/0/0/0
2	NAG	C	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	602	2,4	-	0/6/23/26	0/1/1/1
4	MAN	C	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	604	4	-	0/2/19/22	0/1/1/1
4	MAN	C	605	4	-	0/2/19/22	1/1/1/1
2	NAG	C	606	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	607	2	-	2/6/23/26	0/1/1/1
2	NAG	C	608	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	609	2	-	0/6/23/26	0/1/1/1
5	MLI	C	610	-	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	602	2,4	-	0/6/23/26	0/1/1/1
4	MAN	D	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	604	4	-	0/2/19/22	0/1/1/1
2	NAG	D	605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	606	2,4	-	0/6/23/26	0/1/1/1
4	MAN	D	607	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	608	4	-	0/2/19/22	0/1/1/1
2	NAG	D	609	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	610	2,4	-	2/6/23/26	0/1/1/1
4	MAN	D	611	2	-	0/2/19/22	0/1/1/1
5	MLI	D	612	-	-	0/0/4/4	0/0/0/0
2	NAG	E	601	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	602	2,4	-	0/6/23/26	0/1/1/1
4	MAN	E	603	2	-	0/2/19/22	1/1/1/1
2	NAG	E	604	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	605	2,4	-	0/6/23/26	0/1/1/1
4	MAN	E	606	2,4	-	0/2/19/22	0/1/1/1
4	MAN	E	607	4	-	0/2/19/22	0/1/1/1
2	NAG	E	608	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	609	2	-	0/6/23/26	0/1/1/1
5	MLI	E	610	-	-	0/0/4/4	0/0/0/0
2	NAG	F	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	602	2	-	0/6/23/26	0/1/1/1
2	NAG	F	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	604	2,4	-	1/6/23/26	0/1/1/1
4	MAN	F	605	2	-	0/2/19/22	0/1/1/1
2	NAG	F	606	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	607	2,4	-	0/6/23/26	0/1/1/1
4	MAN	F	608	2,4	-	0/2/19/22	0/1/1/1
4	MAN	F	609	4	-	0/2/19/22	0/1/1/1
4	MAN	F	610	4	-	0/2/19/22	0/1/1/1
5	MLI	F	611	-	-	0/0/4/4	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	606	MAN	C2-C3	2.08	1.55	1.52
3	A	603	BMA	O2-C2	2.14	1.48	1.43
4	B	603	MAN	C2-C3	2.15	1.55	1.52
4	B	609	MAN	C4-C5	2.18	1.57	1.53
4	F	610	MAN	C2-C3	2.20	1.55	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	NAG	C4-C3-C2	-3.96	105.20	111.34
2	D	606	NAG	C2-N2-C7	-2.84	119.41	123.11
2	A	606	NAG	C2-N2-C7	-2.76	119.52	123.11
2	B	604	NAG	C2-N2-C7	-2.69	119.61	123.11
2	D	609	NAG	C2-N2-C7	-2.57	119.76	123.11

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	610	NAG	C8-C7-N2-C2
2	A	606	NAG	O7-C7-N2-C2
2	C	607	NAG	C8-C7-N2-C2
2	C	608	NAG	C8-C7-N2-C2
2	F	604	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	605	MAN	C1-C2-C3-C4-C5-O5
4	E	603	MAN	C1-C2-C3-C4-C5-O5

29 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
2	A	602	NAG	2	0
3	A	603	BMA	2	0
4	A	605	MAN	1	0
2	A	608	NAG	1	0
2	B	601	NAG	1	0
2	B	602	NAG	1	0
2	B	607	NAG	4	0
2	B	608	NAG	3	0
4	B	609	MAN	2	0
2	C	601	NAG	1	0
2	C	602	NAG	1	0
4	C	605	MAN	1	0
2	C	606	NAG	2	0
2	C	608	NAG	1	0
2	D	601	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	NAG	4	0
2	D	605	NAG	1	0
4	D	607	MAN	1	0
4	D	608	MAN	1	0
2	E	601	NAG	2	0
2	E	604	NAG	2	0
2	E	605	NAG	5	0
4	E	606	MAN	1	0
4	E	607	MAN	1	0
5	E	610	MLI	1	0
2	F	603	NAG	2	0
2	F	604	NAG	2	0
2	F	606	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	456/529 (86%)	0.08	10 (2%) 65 65	63, 116, 150, 186	0
1	B	456/529 (86%)	0.02	9 (1%) 68 68	61, 116, 150, 186	0
1	C	450/529 (85%)	0.08	10 (2%) 65 65	65, 116, 152, 186	1 (0%)
1	D	456/529 (86%)	0.05	9 (1%) 68 68	65, 117, 152, 185	0
1	E	456/529 (86%)	0.05	10 (2%) 65 65	62, 116, 150, 186	0
1	F	450/529 (85%)	0.10	8 (1%) 71 71	70, 117, 155, 185	0
All	All	2724/3174 (85%)	0.06	56 (2%) 67 67	61, 116, 151, 186	1 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	ALA	5.0
1	F	482	ASP	4.8
1	B	482	ASP	4.5
1	C	479	ARG	4.3
1	A	523	LEU	4.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MLI	E	610	7/7	0.77	0.42	6.53	142,142,142,143	0
5	MLI	B	612	7/7	0.77	0.43	4.49	143,144,144,144	0
5	MLI	D	612	7/7	0.76	0.36	3.27	134,134,136,136	0
5	MLI	C	610	7/7	0.78	0.35	3.22	140,141,142,143	0
5	MLI	A	611	7/7	0.76	0.36	3.02	135,136,136,137	0
2	NAG	A	608	14/15	0.91	0.30	1.95	160,160,160,160	0
2	NAG	D	605	14/15	0.90	0.33	1.84	160,160,160,160	0
2	NAG	F	603	14/15	0.90	0.33	1.65	162,162,162,162	0
5	MLI	F	611	7/7	0.87	0.27	0.52	133,134,134,135	0
2	NAG	A	601	14/15	0.91	0.23	0.26	157,157,157,157	0
2	NAG	E	601	14/15	0.90	0.29	0.26	159,159,159,159	0
2	NAG	E	604	14/15	0.89	0.23	0.24	157,157,157,157	0
2	NAG	C	606	14/15	0.88	0.23	0.10	152,152,152,152	0
2	NAG	B	607	14/15	0.87	0.23	0.09	163,163,163,163	0
4	MAN	B	610	11/12	0.62	0.49	-	189,189,189,189	0
4	MAN	F	610	11/12	0.84	0.47	-	186,186,186,186	0
2	NAG	B	608	14/15	0.74	0.40	-	177,177,177,177	0
2	NAG	A	606	14/15	0.89	0.27	-	158,158,158,158	0
4	MAN	E	603	11/12	0.60	0.38	-	179,179,179,179	0
2	NAG	A	602	14/15	0.77	0.30	-	171,171,171,171	0
2	NAG	C	601	14/15	0.87	0.30	-	160,160,160,160	0
2	NAG	F	602	14/15	0.78	0.41	-	173,173,173,173	0
2	NAG	F	604	14/15	0.89	0.44	-	176,176,176,176	0
2	NAG	E	609	14/15	0.84	0.39	-	164,164,164,164	0
2	NAG	D	610	14/15	0.82	0.35	-	163,163,163,163	0
2	NAG	D	601	14/15	0.89	0.30	-	160,160,160,160	0
4	MAN	F	605	11/12	0.38	0.47	-	183,183,183,183	0
4	MAN	D	607	11/12	0.80	0.42	-	178,178,178,178	0
2	NAG	A	609	14/15	0.82	0.36	-	173,173,173,173	0
2	NAG	B	605	14/15	0.78	0.45	-	172,172,172,172	0
2	NAG	D	606	14/15	0.85	0.41	-	171,171,171,171	0
4	MAN	C	605	11/12	0.70	0.40	-	188,188,188,188	0
4	MAN	A	604	11/12	0.72	0.30	-	177,177,177,177	0
4	MAN	D	604	11/12	0.62	0.44	-	184,184,184,184	0
4	MAN	A	605	11/12	0.80	0.44	-	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	604	14/15	0.84	0.29	-	163,163,163,163	0
4	MAN	F	609	11/12	0.67	0.49	-	187,187,187,187	0
4	MAN	D	611	11/12	0.51	0.42	-	169,169,169,169	0
2	NAG	B	601	14/15	0.85	0.26	-	154,154,154,154	0
4	MAN	B	609	11/12	0.85	0.38	-	187,187,187,187	0
2	NAG	E	605	14/15	0.89	0.38	-	170,170,170,170	0
2	NAG	F	606	14/15	0.88	0.28	-	162,162,162,162	0
2	NAG	F	601	14/15	0.77	0.32	-	166,166,166,166	0
4	MAN	B	611	11/12	0.79	0.43	-	190,190,190,190	0
2	NAG	B	602	14/15	0.78	0.47	-	166,166,166,166	0
2	NAG	A	607	14/15	0.89	0.32	-	162,162,162,162	0
2	NAG	E	608	14/15	0.82	0.32	-	159,159,159,159	0
4	MAN	F	608	11/12	0.89	0.45	-	183,183,183,183	0
4	MAN	E	606	11/12	0.83	0.37	-	178,178,178,178	0
4	MAN	D	608	11/12	0.74	0.50	-	181,181,181,181	0
2	NAG	D	609	14/15	0.81	0.26	-	155,155,155,155	0
4	MAN	E	607	11/12	0.85	0.37	-	180,180,180,180	0
2	NAG	C	602	14/15	0.82	0.32	-	173,173,173,173	0
3	BMA	A	603	11/12	0.87	0.41	-	177,177,177,177	0
4	MAN	B	606	11/12	0.41	0.43	-	176,176,176,176	0
4	MAN	C	603	11/12	0.71	0.38	-	185,185,185,185	0
4	MAN	A	610	11/12	0.67	0.40	-	179,179,179,179	0
2	NAG	E	602	14/15	0.79	0.42	-	172,172,172,172	0
4	MAN	D	603	11/12	0.88	0.44	-	180,180,180,180	0
2	NAG	D	602	14/15	0.87	0.40	-	170,170,170,170	0
2	NAG	F	607	14/15	0.85	0.36	-	170,170,170,170	0
4	MAN	B	603	11/12	0.73	0.42	-	171,171,171,171	0
2	NAG	C	609	14/15	0.82	0.44	-	171,171,171,171	0
4	MAN	C	604	11/12	0.82	0.45	-	188,188,188,188	0
2	NAG	C	607	14/15	0.88	0.29	-	157,157,157,157	0
2	NAG	C	608	14/15	0.84	0.35	-	164,164,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.