



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:32 AM EDT

PDB ID : 7M0I
Title : Crystal structure of a human metapneumovirus subtype B2 trimeric fusion protein
Authors : Huang, J.; Mousa, J.J.
Deposited on : 2021-03-11
Resolution : 2.81 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

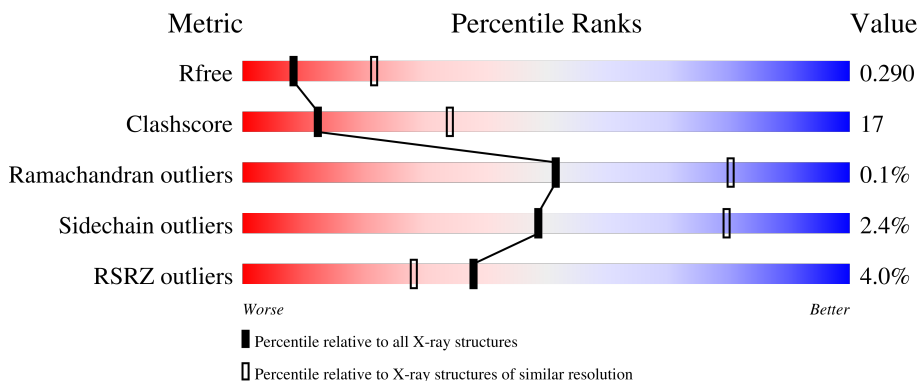
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	89	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">54% 25% 21%</p>
1	C	89	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">47% 31% 21%</p>
1	E	89	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">56% 21% 21%</p>
1	G	89	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">55% 20% 21%</p>
1	I	89	<div style="display: flex; align-items: center;"> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">58% 20% 21%</p>

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Mol	Chain	Length	Quality of chain
1	K	89	
2	B	431	
2	D	431	
2	F	431	
2	H	431	
2	J	431	
2	L	431	

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
3	NAG	G	201	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19556 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 F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	70	544	341	84	117	2	0	0	0
1	I	70	544	341	84	117	2	0	0	0
1	K	70	536	335	82	117	2	0	0	0
1	A	70	540	338	83	117	2	0	0	0
1	C	70	544	341	84	117	2	0	0	0
1	E	70	544	341	84	117	2	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	19	LEU	-	expression tag	UNP C6F474
G	20	LYS	-	expression tag	UNP C6F474
G	21	GLU	-	expression tag	UNP C6F474
G	22	SER	-	expression tag	UNP C6F474
G	102	LYS	-	expression tag	UNP C6F474
G	103	LYS	-	expression tag	UNP C6F474
G	104	ARG	-	expression tag	UNP C6F474
G	105	LYS	-	expression tag	UNP C6F474
G	106	ARG	-	expression tag	UNP C6F474
G	107	ARG	-	expression tag	UNP C6F474
I	19	LEU	-	expression tag	UNP C6F474
I	20	LYS	-	expression tag	UNP C6F474
I	21	GLU	-	expression tag	UNP C6F474
I	22	SER	-	expression tag	UNP C6F474
I	102	LYS	-	expression tag	UNP C6F474
I	103	LYS	-	expression tag	UNP C6F474
I	104	ARG	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
I	105	LYS	-	expression tag	UNP C6F474
I	106	ARG	-	expression tag	UNP C6F474
I	107	ARG	-	expression tag	UNP C6F474
K	19	LEU	-	expression tag	UNP C6F474
K	20	LYS	-	expression tag	UNP C6F474
K	21	GLU	-	expression tag	UNP C6F474
K	22	SER	-	expression tag	UNP C6F474
K	102	LYS	-	expression tag	UNP C6F474
K	103	LYS	-	expression tag	UNP C6F474
K	104	ARG	-	expression tag	UNP C6F474
K	105	LYS	-	expression tag	UNP C6F474
K	106	ARG	-	expression tag	UNP C6F474
K	107	ARG	-	expression tag	UNP C6F474
A	19	LEU	-	expression tag	UNP C6F474
A	20	LYS	-	expression tag	UNP C6F474
A	21	GLU	-	expression tag	UNP C6F474
A	22	SER	-	expression tag	UNP C6F474
A	102	LYS	-	expression tag	UNP C6F474
A	103	LYS	-	expression tag	UNP C6F474
A	104	ARG	-	expression tag	UNP C6F474
A	105	LYS	-	expression tag	UNP C6F474
A	106	ARG	-	expression tag	UNP C6F474
A	107	ARG	-	expression tag	UNP C6F474
C	19	LEU	-	expression tag	UNP C6F474
C	20	LYS	-	expression tag	UNP C6F474
C	21	GLU	-	expression tag	UNP C6F474
C	22	SER	-	expression tag	UNP C6F474
C	102	LYS	-	expression tag	UNP C6F474
C	103	LYS	-	expression tag	UNP C6F474
C	104	ARG	-	expression tag	UNP C6F474
C	105	LYS	-	expression tag	UNP C6F474
C	106	ARG	-	expression tag	UNP C6F474
C	107	ARG	-	expression tag	UNP C6F474
E	19	LEU	-	expression tag	UNP C6F474
E	20	LYS	-	expression tag	UNP C6F474
E	21	GLU	-	expression tag	UNP C6F474
E	22	SER	-	expression tag	UNP C6F474
E	102	LYS	-	expression tag	UNP C6F474
E	103	LYS	-	expression tag	UNP C6F474
E	104	ARG	-	expression tag	UNP C6F474
E	105	LYS	-	expression tag	UNP C6F474
E	106	ARG	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	ARG	-	expression tag	UNP C6F474

- Molecule 2 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	352	Total	C	N	O	S	0	0	0
			2677	1674	462	522	19			
2	J	352	Total	C	N	O	S	0	0	0
			2663	1664	458	522	19			
2	L	352	Total	C	N	O	S	0	0	0
			2677	1674	462	522	19			
2	B	351	Total	C	N	O	S	0	0	0
			2666	1667	460	520	19			
2	D	352	Total	C	N	O	S	0	0	0
			2668	1664	463	522	19			
2	F	351	Total	C	N	O	S	0	0	0
			2676	1673	464	520	19			

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	490	SER	-	expression tag	UNP C6F474
H	491	GLY	-	expression tag	UNP C6F474
H	492	ARG	-	expression tag	UNP C6F474
H	493	GLU	-	expression tag	UNP C6F474
H	494	ASN	-	expression tag	UNP C6F474
H	495	LEU	-	expression tag	UNP C6F474
H	496	TYR	-	expression tag	UNP C6F474
H	497	PHE	-	expression tag	UNP C6F474
H	498	GLN	-	expression tag	UNP C6F474
H	499	GLY	-	expression tag	UNP C6F474
H	500	GLY	-	expression tag	UNP C6F474
H	501	GLY	-	expression tag	UNP C6F474
H	502	GLY	-	expression tag	UNP C6F474
H	503	GLY	-	expression tag	UNP C6F474
H	504	SER	-	expression tag	UNP C6F474
H	505	GLY	-	expression tag	UNP C6F474
H	506	TYR	-	expression tag	UNP C6F474
H	507	ILE	-	expression tag	UNP C6F474
H	508	PRO	-	expression tag	UNP C6F474
H	509	GLU	-	expression tag	UNP C6F474
H	510	ALA	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
H	511	PRO	-	expression tag	UNP C6F474
H	512	ARG	-	expression tag	UNP C6F474
H	513	ASP	-	expression tag	UNP C6F474
H	514	GLN	-	expression tag	UNP C6F474
H	515	ALA	-	expression tag	UNP C6F474
H	516	TYR	-	expression tag	UNP C6F474
H	517	VAL	-	expression tag	UNP C6F474
H	518	ARG	-	expression tag	UNP C6F474
H	519	LYS	-	expression tag	UNP C6F474
H	520	ASP	-	expression tag	UNP C6F474
H	521	GLY	-	expression tag	UNP C6F474
H	522	GLU	-	expression tag	UNP C6F474
H	523	TRP	-	expression tag	UNP C6F474
H	524	VAL	-	expression tag	UNP C6F474
H	525	LEU	-	expression tag	UNP C6F474
H	526	LEU	-	expression tag	UNP C6F474
H	527	SER	-	expression tag	UNP C6F474
H	528	THR	-	expression tag	UNP C6F474
H	529	PHE	-	expression tag	UNP C6F474
H	530	LEU	-	expression tag	UNP C6F474
H	531	GLY	-	expression tag	UNP C6F474
H	532	GLY	-	expression tag	UNP C6F474
H	533	THR	-	expression tag	UNP C6F474
H	534	GLU	-	expression tag	UNP C6F474
H	535	GLY	-	expression tag	UNP C6F474
H	536	ARG	-	expression tag	UNP C6F474
H	537	HIS	-	expression tag	UNP C6F474
H	538	HIS	-	expression tag	UNP C6F474
H	539	HIS	-	expression tag	UNP C6F474
H	540	HIS	-	expression tag	UNP C6F474
H	541	HIS	-	expression tag	UNP C6F474
H	542	HIS	-	expression tag	UNP C6F474
J	490	SER	-	expression tag	UNP C6F474
J	491	GLY	-	expression tag	UNP C6F474
J	492	ARG	-	expression tag	UNP C6F474
J	493	GLU	-	expression tag	UNP C6F474
J	494	ASN	-	expression tag	UNP C6F474
J	495	LEU	-	expression tag	UNP C6F474
J	496	TYR	-	expression tag	UNP C6F474
J	497	PHE	-	expression tag	UNP C6F474
J	498	GLN	-	expression tag	UNP C6F474
J	499	GLY	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
J	500	GLY	-	expression tag	UNP C6F474
J	501	GLY	-	expression tag	UNP C6F474
J	502	GLY	-	expression tag	UNP C6F474
J	503	GLY	-	expression tag	UNP C6F474
J	504	SER	-	expression tag	UNP C6F474
J	505	GLY	-	expression tag	UNP C6F474
J	506	TYR	-	expression tag	UNP C6F474
J	507	ILE	-	expression tag	UNP C6F474
J	508	PRO	-	expression tag	UNP C6F474
J	509	GLU	-	expression tag	UNP C6F474
J	510	ALA	-	expression tag	UNP C6F474
J	511	PRO	-	expression tag	UNP C6F474
J	512	ARG	-	expression tag	UNP C6F474
J	513	ASP	-	expression tag	UNP C6F474
J	514	GLN	-	expression tag	UNP C6F474
J	515	ALA	-	expression tag	UNP C6F474
J	516	TYR	-	expression tag	UNP C6F474
J	517	VAL	-	expression tag	UNP C6F474
J	518	ARG	-	expression tag	UNP C6F474
J	519	LYS	-	expression tag	UNP C6F474
J	520	ASP	-	expression tag	UNP C6F474
J	521	GLY	-	expression tag	UNP C6F474
J	522	GLU	-	expression tag	UNP C6F474
J	523	TRP	-	expression tag	UNP C6F474
J	524	VAL	-	expression tag	UNP C6F474
J	525	LEU	-	expression tag	UNP C6F474
J	526	LEU	-	expression tag	UNP C6F474
J	527	SER	-	expression tag	UNP C6F474
J	528	THR	-	expression tag	UNP C6F474
J	529	PHE	-	expression tag	UNP C6F474
J	530	LEU	-	expression tag	UNP C6F474
J	531	GLY	-	expression tag	UNP C6F474
J	532	GLY	-	expression tag	UNP C6F474
J	533	THR	-	expression tag	UNP C6F474
J	534	GLU	-	expression tag	UNP C6F474
J	535	GLY	-	expression tag	UNP C6F474
J	536	ARG	-	expression tag	UNP C6F474
J	537	HIS	-	expression tag	UNP C6F474
J	538	HIS	-	expression tag	UNP C6F474
J	539	HIS	-	expression tag	UNP C6F474
J	540	HIS	-	expression tag	UNP C6F474
J	541	HIS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
J	542	HIS	-	expression tag	UNP C6F474
L	490	SER	-	expression tag	UNP C6F474
L	491	GLY	-	expression tag	UNP C6F474
L	492	ARG	-	expression tag	UNP C6F474
L	493	GLU	-	expression tag	UNP C6F474
L	494	ASN	-	expression tag	UNP C6F474
L	495	LEU	-	expression tag	UNP C6F474
L	496	TYR	-	expression tag	UNP C6F474
L	497	PHE	-	expression tag	UNP C6F474
L	498	GLN	-	expression tag	UNP C6F474
L	499	GLY	-	expression tag	UNP C6F474
L	500	GLY	-	expression tag	UNP C6F474
L	501	GLY	-	expression tag	UNP C6F474
L	502	GLY	-	expression tag	UNP C6F474
L	503	GLY	-	expression tag	UNP C6F474
L	504	SER	-	expression tag	UNP C6F474
L	505	GLY	-	expression tag	UNP C6F474
L	506	TYR	-	expression tag	UNP C6F474
L	507	ILE	-	expression tag	UNP C6F474
L	508	PRO	-	expression tag	UNP C6F474
L	509	GLU	-	expression tag	UNP C6F474
L	510	ALA	-	expression tag	UNP C6F474
L	511	PRO	-	expression tag	UNP C6F474
L	512	ARG	-	expression tag	UNP C6F474
L	513	ASP	-	expression tag	UNP C6F474
L	514	GLN	-	expression tag	UNP C6F474
L	515	ALA	-	expression tag	UNP C6F474
L	516	TYR	-	expression tag	UNP C6F474
L	517	VAL	-	expression tag	UNP C6F474
L	518	ARG	-	expression tag	UNP C6F474
L	519	LYS	-	expression tag	UNP C6F474
L	520	ASP	-	expression tag	UNP C6F474
L	521	GLY	-	expression tag	UNP C6F474
L	522	GLU	-	expression tag	UNP C6F474
L	523	TRP	-	expression tag	UNP C6F474
L	524	VAL	-	expression tag	UNP C6F474
L	525	LEU	-	expression tag	UNP C6F474
L	526	LEU	-	expression tag	UNP C6F474
L	527	SER	-	expression tag	UNP C6F474
L	528	THR	-	expression tag	UNP C6F474
L	529	PHE	-	expression tag	UNP C6F474
L	530	LEU	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
L	531	GLY	-	expression tag	UNP C6F474
L	532	GLY	-	expression tag	UNP C6F474
L	533	THR	-	expression tag	UNP C6F474
L	534	GLU	-	expression tag	UNP C6F474
L	535	GLY	-	expression tag	UNP C6F474
L	536	ARG	-	expression tag	UNP C6F474
L	537	HIS	-	expression tag	UNP C6F474
L	538	HIS	-	expression tag	UNP C6F474
L	539	HIS	-	expression tag	UNP C6F474
L	540	HIS	-	expression tag	UNP C6F474
L	541	HIS	-	expression tag	UNP C6F474
L	542	HIS	-	expression tag	UNP C6F474
B	490	SER	-	expression tag	UNP C6F474
B	491	GLY	-	expression tag	UNP C6F474
B	492	ARG	-	expression tag	UNP C6F474
B	493	GLU	-	expression tag	UNP C6F474
B	494	ASN	-	expression tag	UNP C6F474
B	495	LEU	-	expression tag	UNP C6F474
B	496	TYR	-	expression tag	UNP C6F474
B	497	PHE	-	expression tag	UNP C6F474
B	498	GLN	-	expression tag	UNP C6F474
B	499	GLY	-	expression tag	UNP C6F474
B	500	GLY	-	expression tag	UNP C6F474
B	501	GLY	-	expression tag	UNP C6F474
B	502	GLY	-	expression tag	UNP C6F474
B	503	GLY	-	expression tag	UNP C6F474
B	504	SER	-	expression tag	UNP C6F474
B	505	GLY	-	expression tag	UNP C6F474
B	506	TYR	-	expression tag	UNP C6F474
B	507	ILE	-	expression tag	UNP C6F474
B	508	PRO	-	expression tag	UNP C6F474
B	509	GLU	-	expression tag	UNP C6F474
B	510	ALA	-	expression tag	UNP C6F474
B	511	PRO	-	expression tag	UNP C6F474
B	512	ARG	-	expression tag	UNP C6F474
B	513	ASP	-	expression tag	UNP C6F474
B	514	GLN	-	expression tag	UNP C6F474
B	515	ALA	-	expression tag	UNP C6F474
B	516	TYR	-	expression tag	UNP C6F474
B	517	VAL	-	expression tag	UNP C6F474
B	518	ARG	-	expression tag	UNP C6F474
B	519	LYS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	ASP	-	expression tag	UNP C6F474
B	521	GLY	-	expression tag	UNP C6F474
B	522	GLU	-	expression tag	UNP C6F474
B	523	TRP	-	expression tag	UNP C6F474
B	524	VAL	-	expression tag	UNP C6F474
B	525	LEU	-	expression tag	UNP C6F474
B	526	LEU	-	expression tag	UNP C6F474
B	527	SER	-	expression tag	UNP C6F474
B	528	THR	-	expression tag	UNP C6F474
B	529	PHE	-	expression tag	UNP C6F474
B	530	LEU	-	expression tag	UNP C6F474
B	531	GLY	-	expression tag	UNP C6F474
B	532	GLY	-	expression tag	UNP C6F474
B	533	THR	-	expression tag	UNP C6F474
B	534	GLU	-	expression tag	UNP C6F474
B	535	GLY	-	expression tag	UNP C6F474
B	536	ARG	-	expression tag	UNP C6F474
B	537	HIS	-	expression tag	UNP C6F474
B	538	HIS	-	expression tag	UNP C6F474
B	539	HIS	-	expression tag	UNP C6F474
B	540	HIS	-	expression tag	UNP C6F474
B	541	HIS	-	expression tag	UNP C6F474
B	542	HIS	-	expression tag	UNP C6F474
D	490	SER	-	expression tag	UNP C6F474
D	491	GLY	-	expression tag	UNP C6F474
D	492	ARG	-	expression tag	UNP C6F474
D	493	GLU	-	expression tag	UNP C6F474
D	494	ASN	-	expression tag	UNP C6F474
D	495	LEU	-	expression tag	UNP C6F474
D	496	TYR	-	expression tag	UNP C6F474
D	497	PHE	-	expression tag	UNP C6F474
D	498	GLN	-	expression tag	UNP C6F474
D	499	GLY	-	expression tag	UNP C6F474
D	500	GLY	-	expression tag	UNP C6F474
D	501	GLY	-	expression tag	UNP C6F474
D	502	GLY	-	expression tag	UNP C6F474
D	503	GLY	-	expression tag	UNP C6F474
D	504	SER	-	expression tag	UNP C6F474
D	505	GLY	-	expression tag	UNP C6F474
D	506	TYR	-	expression tag	UNP C6F474
D	507	ILE	-	expression tag	UNP C6F474
D	508	PRO	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
D	509	GLU	-	expression tag	UNP C6F474
D	510	ALA	-	expression tag	UNP C6F474
D	511	PRO	-	expression tag	UNP C6F474
D	512	ARG	-	expression tag	UNP C6F474
D	513	ASP	-	expression tag	UNP C6F474
D	514	GLN	-	expression tag	UNP C6F474
D	515	ALA	-	expression tag	UNP C6F474
D	516	TYR	-	expression tag	UNP C6F474
D	517	VAL	-	expression tag	UNP C6F474
D	518	ARG	-	expression tag	UNP C6F474
D	519	LYS	-	expression tag	UNP C6F474
D	520	ASP	-	expression tag	UNP C6F474
D	521	GLY	-	expression tag	UNP C6F474
D	522	GLU	-	expression tag	UNP C6F474
D	523	TRP	-	expression tag	UNP C6F474
D	524	VAL	-	expression tag	UNP C6F474
D	525	LEU	-	expression tag	UNP C6F474
D	526	LEU	-	expression tag	UNP C6F474
D	527	SER	-	expression tag	UNP C6F474
D	528	THR	-	expression tag	UNP C6F474
D	529	PHE	-	expression tag	UNP C6F474
D	530	LEU	-	expression tag	UNP C6F474
D	531	GLY	-	expression tag	UNP C6F474
D	532	GLY	-	expression tag	UNP C6F474
D	533	THR	-	expression tag	UNP C6F474
D	534	GLU	-	expression tag	UNP C6F474
D	535	GLY	-	expression tag	UNP C6F474
D	536	ARG	-	expression tag	UNP C6F474
D	537	HIS	-	expression tag	UNP C6F474
D	538	HIS	-	expression tag	UNP C6F474
D	539	HIS	-	expression tag	UNP C6F474
D	540	HIS	-	expression tag	UNP C6F474
D	541	HIS	-	expression tag	UNP C6F474
D	542	HIS	-	expression tag	UNP C6F474
F	490	SER	-	expression tag	UNP C6F474
F	491	GLY	-	expression tag	UNP C6F474
F	492	ARG	-	expression tag	UNP C6F474
F	493	GLU	-	expression tag	UNP C6F474
F	494	ASN	-	expression tag	UNP C6F474
F	495	LEU	-	expression tag	UNP C6F474
F	496	TYR	-	expression tag	UNP C6F474
F	497	PHE	-	expression tag	UNP C6F474

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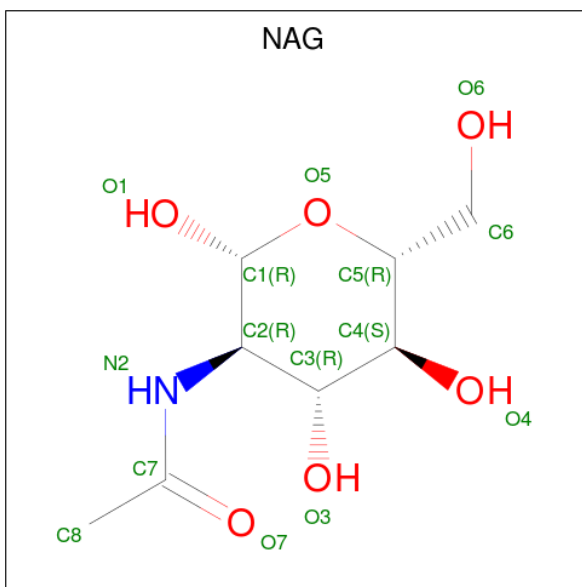
Chain	Residue	Modelled	Actual	Comment	Reference
F	498	GLN	-	expression tag	UNP C6F474
F	499	GLY	-	expression tag	UNP C6F474
F	500	GLY	-	expression tag	UNP C6F474
F	501	GLY	-	expression tag	UNP C6F474
F	502	GLY	-	expression tag	UNP C6F474
F	503	GLY	-	expression tag	UNP C6F474
F	504	SER	-	expression tag	UNP C6F474
F	505	GLY	-	expression tag	UNP C6F474
F	506	TYR	-	expression tag	UNP C6F474
F	507	ILE	-	expression tag	UNP C6F474
F	508	PRO	-	expression tag	UNP C6F474
F	509	GLU	-	expression tag	UNP C6F474
F	510	ALA	-	expression tag	UNP C6F474
F	511	PRO	-	expression tag	UNP C6F474
F	512	ARG	-	expression tag	UNP C6F474
F	513	ASP	-	expression tag	UNP C6F474
F	514	GLN	-	expression tag	UNP C6F474
F	515	ALA	-	expression tag	UNP C6F474
F	516	TYR	-	expression tag	UNP C6F474
F	517	VAL	-	expression tag	UNP C6F474
F	518	ARG	-	expression tag	UNP C6F474
F	519	LYS	-	expression tag	UNP C6F474
F	520	ASP	-	expression tag	UNP C6F474
F	521	GLY	-	expression tag	UNP C6F474
F	522	GLU	-	expression tag	UNP C6F474
F	523	TRP	-	expression tag	UNP C6F474
F	524	VAL	-	expression tag	UNP C6F474
F	525	LEU	-	expression tag	UNP C6F474
F	526	LEU	-	expression tag	UNP C6F474
F	527	SER	-	expression tag	UNP C6F474
F	528	THR	-	expression tag	UNP C6F474
F	529	PHE	-	expression tag	UNP C6F474
F	530	LEU	-	expression tag	UNP C6F474
F	531	GLY	-	expression tag	UNP C6F474
F	532	GLY	-	expression tag	UNP C6F474
F	533	THR	-	expression tag	UNP C6F474
F	534	GLU	-	expression tag	UNP C6F474
F	535	GLY	-	expression tag	UNP C6F474
F	536	ARG	-	expression tag	UNP C6F474
F	537	HIS	-	expression tag	UNP C6F474
F	538	HIS	-	expression tag	UNP C6F474
F	539	HIS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
F	540	HIS	-	expression tag	UNP C6F474
F	541	HIS	-	expression tag	UNP C6F474
F	542	HIS	-	expression tag	UNP C6F474

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	G	1	Total 14	C 8	N 1	O 5	0	0
3	H	1	Total 14	C 8	N 1	O 5	0	0
3	H	1	Total 14	C 8	N 1	O 5	0	0
3	I	1	Total 14	C 8	N 1	O 5	0	0
3	J	1	Total 14	C 8	N 1	O 5	0	0
3	J	1	Total 14	C 8	N 1	O 5	0	0
3	K	1	Total 14	C 8	N 1	O 5	0	0
3	L	1	Total 14	C 8	N 1	O 5	0	0
3	L	1	Total 14	C 8	N 1	O 5	0	0

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

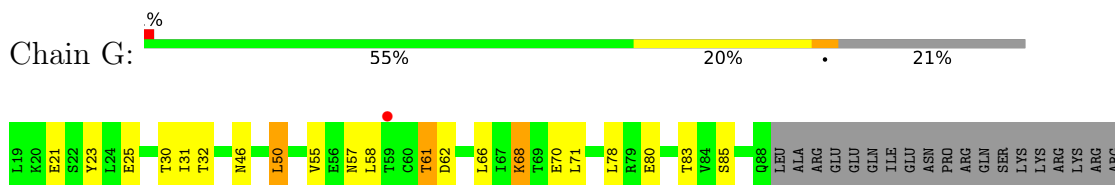
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		
4	I	2	Total	O	0	0
			2	2		
4	J	4	Total	O	0	0
			4	4		
4	L	6	Total	O	0	0
			6	6		
4	B	5	Total	O	0	0
			5	5		
4	C	2	Total	O	0	0
			2	2		
4	D	4	Total	O	0	0
			4	4		
4	F	1	Total	O	0	0
			1	1		

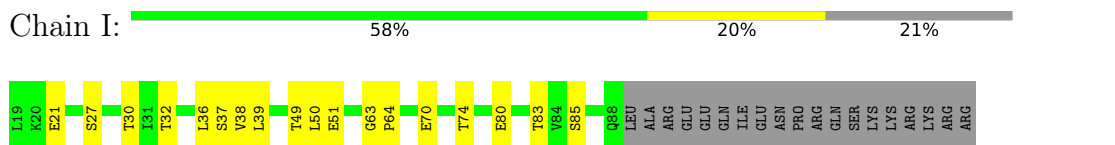
3 Residue-property plots [i](#)

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

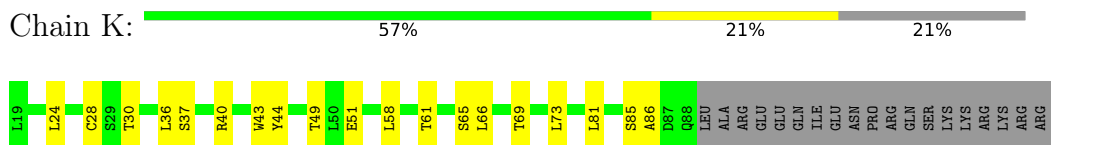
- Molecule 1: Fusion glycoprotein F2



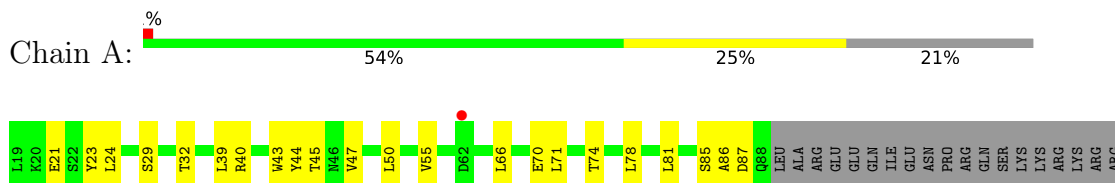
- Molecule 1: Fusion glycoprotein F2



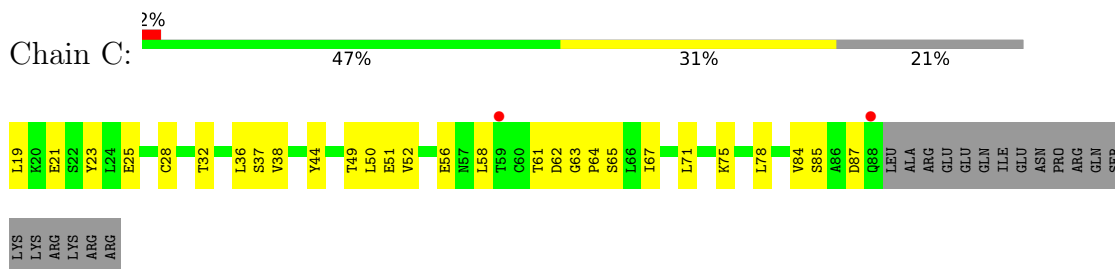
- Molecule 1: Fusion glycoprotein F2

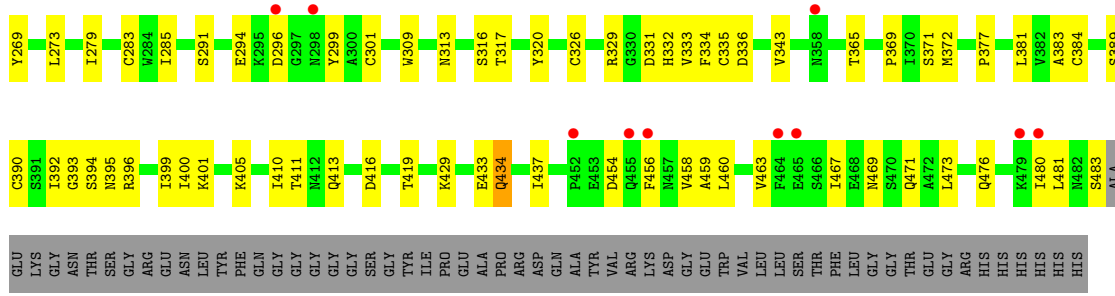


- Molecule 1: Fusion glycoprotein F2

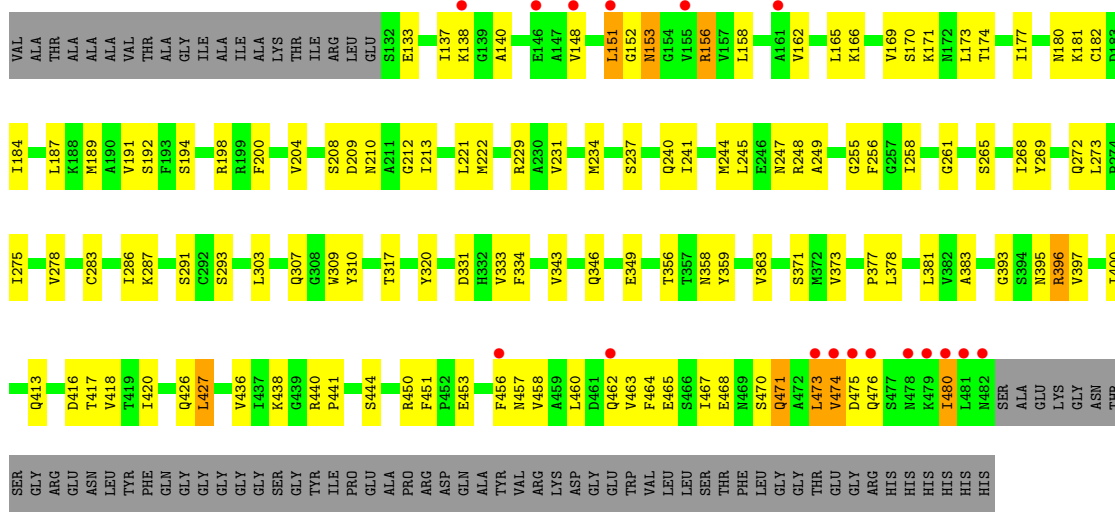


- Molecule 1: Fusion glycoprotein F2





• Molecule 2: Fusion glycoprotein F1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.53Å 128.10Å 431.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.81 49.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	75.5 (49.69-2.81) 75.6 (49.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.254 , 0.291 0.254 , 0.290	Depositor DCC
R_{free} test set	5880 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	19556	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.61	0/546	0.90	0/743
1	C	0.63	0/550	0.94	1/747 (0.1%)
1	E	0.62	0/550	0.87	1/747 (0.1%)
1	G	0.75	0/550	0.96	1/747 (0.1%)
1	I	0.61	0/550	0.94	0/747
1	K	0.56	0/542	0.89	2/739 (0.3%)
2	B	0.64	1/2708 (0.0%)	0.92	5/3672 (0.1%)
2	D	0.57	1/2709 (0.0%)	0.85	3/3674 (0.1%)
2	F	0.61	0/2718	0.96	8/3683 (0.2%)
2	H	0.69	3/2719 (0.1%)	0.97	8/3687 (0.2%)
2	J	0.62	0/2705	0.89	3/3671 (0.1%)
2	L	0.64	2/2719 (0.1%)	0.87	2/3687 (0.1%)
All	All	0.63	7/19566 (0.0%)	0.91	34/26544 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	384	CYS	CB-SG	-7.99	1.68	1.82
2	H	273	LEU	C-N	7.12	1.47	1.34
2	L	384	CYS	CB-SG	-6.41	1.71	1.82
2	L	397	VAL	C-O	-5.79	1.12	1.23
2	H	390	CYS	CB-SG	-5.73	1.72	1.81

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	350	CYS	CA-CB-SG	-11.83	92.71	114.00
2	H	361	CYS	CA-CB-SG	-10.86	94.46	114.00
2	L	384	CYS	CA-CB-SG	-9.47	96.95	114.00
2	J	350	CYS	CA-CB-SG	-9.30	97.25	114.00
2	J	361	CYS	CA-CB-SG	-8.51	98.69	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	540	0	525	25	0
1	C	544	0	536	28	0
1	E	544	0	536	24	0
1	G	544	0	536	23	0
1	I	544	0	536	20	0
1	K	536	0	514	22	0
2	B	2666	0	2638	130	0
2	D	2668	0	2636	134	0
2	F	2676	0	2660	131	0
2	H	2677	0	2649	128	0
2	J	2663	0	2616	109	0
2	L	2677	0	2649	103	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	28	0	26	0	0
3	E	14	0	13	0	0
3	F	28	0	26	0	0
3	G	14	0	13	2	0
3	H	28	0	26	0	0
3	I	14	0	13	0	0
3	J	28	0	26	0	0
3	K	14	0	13	0	0
3	L	28	0	26	1	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	4	0
4	I	2	0	0	0	0
4	J	4	0	0	0	0
4	L	6	0	0	0	0
All	All	19556	0	19265	656	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 17.

The worst 5 of 656 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)
2:H:350:CYS:SG	4:H:701:HOH:O	2.00	1.16
2:H:361:CYS:SG	4:H:701:HOH:O	2.08	1.09
2:F:393:GLY:C	2:F:417:THR:HG22	1.80	1.02
2:J:138:LYS:HE3	2:L:481:LEU:HB3	1.45	0.98
2:H:350:CYS:O	2:H:354:ILE:HD12	1.66	0.95

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 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	68/89 (76%)	67 (98%)	1 (2%)	0	100	100
1	C	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	E	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	G	68/89 (76%)	66 (97%)	0	2 (3%)	4	15
1	I	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	K	68/89 (76%)	68 (100%)	0	0	100	100
2	B	349/431 (81%)	336 (96%)	13 (4%)	0	100	100
2	D	350/431 (81%)	334 (95%)	16 (5%)	0	100	100
2	F	349/431 (81%)	342 (98%)	7 (2%)	0	100	100
2	H	350/431 (81%)	338 (97%)	12 (3%)	0	100	100
2	J	350/431 (81%)	338 (97%)	12 (3%)	0	100	100
2	L	350/431 (81%)	339 (97%)	11 (3%)	0	100	100
All	All	2506/3120 (80%)	2426 (97%)	78 (3%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	61	THR
1	G	62	ASP

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 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	63/82 (77%)	63 (100%)	0	100	100
1	C	64/82 (78%)	62 (97%)	2 (3%)	40	72
1	E	64/82 (78%)	63 (98%)	1 (2%)	62	87
1	G	64/82 (78%)	63 (98%)	1 (2%)	62	87
1	I	64/82 (78%)	64 (100%)	0	100	100
1	K	62/82 (76%)	62 (100%)	0	100	100
2	B	297/357 (83%)	288 (97%)	9 (3%)	41	73
2	D	297/357 (83%)	289 (97%)	8 (3%)	44	77
2	F	299/357 (84%)	288 (96%)	11 (4%)	34	66
2	H	298/357 (84%)	292 (98%)	6 (2%)	55	83
2	J	295/357 (83%)	286 (97%)	9 (3%)	40	72
2	L	298/357 (84%)	293 (98%)	5 (2%)	60	86
All	All	2165/2634 (82%)	2113 (98%)	52 (2%)	49	80

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	471	GLN
2	D	166	LYS
2	F	473	LEU
2	B	477	SER
2	D	137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
3	NAG	J	602	2	14,14,15	0.50	0	17,19,21	0.75	1 (5%)
3	NAG	L	602	2	14,14,15	1.14	1 (7%)	17,19,21	1.36	1 (5%)
3	NAG	B	602	2	14,14,15	0.68	1 (7%)	17,19,21	1.17	1 (5%)
3	NAG	L	601	2	14,14,15	0.48	0	17,19,21	1.52	3 (17%)
3	NAG	K	201	1	14,14,15	0.72	0	17,19,21	0.59	0
3	NAG	J	601	2	14,14,15	1.07	1 (7%)	17,19,21	0.99	1 (5%)
3	NAG	E	201	1	14,14,15	1.47	2 (14%)	17,19,21	0.77	0
3	NAG	C	201	1	14,14,15	0.82	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	F	602	2	14,14,15	0.89	1 (7%)	17,19,21	0.72	1 (5%)
3	NAG	B	601	2	14,14,15	1.04	1 (7%)	17,19,21	0.71	1 (5%)
3	NAG	D	602	2	14,14,15	1.82	1 (7%)	17,19,21	1.68	1 (5%)
3	NAG	F	601	2	14,14,15	0.79	1 (7%)	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	201	1	14,14,15	0.97	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	G	201	1	14,14,15	1.44	2 (14%)	17,19,21	0.86	0
3	NAG	H	602	2	14,14,15	1.38	2 (14%)	17,19,21	0.62	0
3	NAG	I	201	1	14,14,15	1.47	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	D	601	2	14,14,15	0.73	1 (7%)	17,19,21	0.50	0
3	NAG	H	601	2	14,14,15	0.55	0	17,19,21	1.03	2 (11%)

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
3	NAG	J	602	2	-	2/6/23/26	0/1/1/1
3	NAG	L	602	2	-	1/6/23/26	0/1/1/1
3	NAG	B	602	2	-	2/6/23/26	0/1/1/1
3	NAG	L	601	2	-	4/6/23/26	0/1/1/1
3	NAG	K	201	1	-	1/6/23/26	0/1/1/1
3	NAG	J	601	2	-	2/6/23/26	0/1/1/1
3	NAG	E	201	1	-	1/6/23/26	0/1/1/1
3	NAG	C	201	1	-	0/6/23/26	0/1/1/1
3	NAG	F	602	2	-	2/6/23/26	0/1/1/1
3	NAG	B	601	2	-	1/6/23/26	0/1/1/1
3	NAG	D	602	2	-	1/6/23/26	0/1/1/1
3	NAG	F	601	2	-	1/6/23/26	0/1/1/1
3	NAG	A	201	1	-	2/6/23/26	0/1/1/1
3	NAG	G	201	1	-	2/6/23/26	0/1/1/1
3	NAG	H	602	2	-	1/6/23/26	0/1/1/1
3	NAG	I	201	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	2	-	2/6/23/26	0/1/1/1
3	NAG	H	601	2	-	3/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NAG	O5-C1	6.64	1.54	1.43
3	I	201	NAG	O5-C1	5.34	1.52	1.43
3	E	201	NAG	O5-C1	4.96	1.51	1.43
3	G	201	NAG	O5-C1	4.52	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	602	NAG	O5-C1	4.09	1.50	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NAG	C1-O5-C5	6.47	120.96	112.19
3	L	602	NAG	C1-O5-C5	4.89	118.82	112.19
3	L	601	NAG	C2-N2-C7	4.40	129.17	122.90
3	B	602	NAG	C1-O5-C5	4.02	117.64	112.19
3	A	201	NAG	C1-O5-C5	-3.70	107.17	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	201	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	201	NAG	O5-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	601	NAG	1	0
3	G	201	NAG	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	70/89 (78%)	-0.06	1 (1%) 75 69	12, 27, 67, 96	0
1	C	70/89 (78%)	-0.06	2 (2%) 51 41	8, 31, 63, 75	0
1	E	70/89 (78%)	-0.12	1 (1%) 75 69	9, 28, 61, 75	0
1	G	70/89 (78%)	-0.17	1 (1%) 75 69	5, 25, 50, 62	0
1	I	70/89 (78%)	-0.22	0 100 100	7, 23, 47, 61	0
1	K	70/89 (78%)	-0.23	0 100 100	7, 22, 49, 65	0
2	B	351/431 (81%)	0.28	28 (7%) 12 7	10, 28, 109, 128	0
2	D	352/431 (81%)	0.18	22 (6%) 20 12	7, 29, 105, 126	0
2	F	351/431 (81%)	0.20	17 (4%) 30 21	8, 28, 106, 123	0
2	H	352/431 (81%)	0.10	14 (3%) 38 28	5, 26, 99, 114	0
2	J	352/431 (81%)	0.11	12 (3%) 45 35	6, 27, 101, 115	0
2	L	352/431 (81%)	0.03	3 (0%) 84 80	5, 30, 98, 111	0
All	All	2530/3120 (81%)	0.10	101 (3%) 38 28	5, 28, 102, 128	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	ALA	5.5
2	B	140	ALA	4.9
2	B	136	ALA	4.9
2	F	480	ILE	4.6
2	J	478	ASN	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
3	NAG	H	602	14/15	0.64	0.33	55,77,85,88	0
3	NAG	G	201	14/15	0.67	0.45	64,85,94,103	0
3	NAG	A	201	14/15	0.68	0.34	46,81,94,96	0
3	NAG	B	602	14/15	0.72	0.26	43,63,74,75	0
3	NAG	J	601	14/15	0.73	0.37	73,84,89,89	0
3	NAG	C	201	14/15	0.75	0.29	57,75,87,89	0
3	NAG	H	601	14/15	0.78	0.24	52,74,81,86	0
3	NAG	F	602	14/15	0.78	0.24	35,64,83,85	0
3	NAG	L	602	14/15	0.79	0.30	39,58,62,65	0
3	NAG	D	602	14/15	0.82	0.24	35,61,76,80	0
3	NAG	E	201	14/15	0.84	0.28	48,61,68,69	0
3	NAG	I	201	14/15	0.85	0.18	37,59,63,63	0
3	NAG	L	601	14/15	0.85	0.24	56,74,89,103	0
3	NAG	D	601	14/15	0.85	0.16	69,82,89,91	0
3	NAG	J	602	14/15	0.86	0.22	52,59,67,69	0
3	NAG	K	201	14/15	0.89	0.27	48,62,69,72	0
3	NAG	B	601	14/15	0.90	0.16	66,73,75,76	0
3	NAG	F	601	14/15	0.91	0.21	63,71,75,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.