



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:50 PM EDT

PDB ID : 5W23  
Title : Crystal Structure of RSV F in complex with 5C4 Fab  
Authors : Battles, M.B.; McLellan, J.S.  
Deposited on : 2017-06-05  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtrriage (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

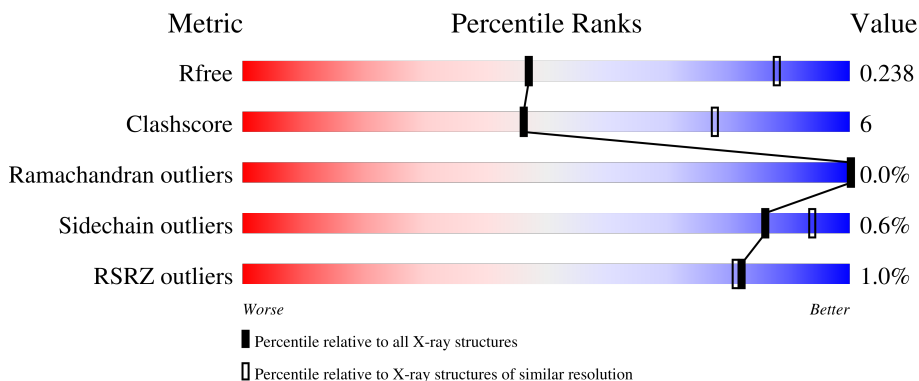
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



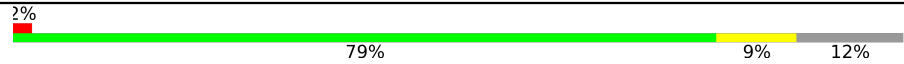



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	568	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">65%      14%      21%</p>
1	B	568	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">64%      15%      21%</p>
1	C	568	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">64%      15%      21%</p>
2	H	249	<div style="display: flex; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">82%      6%      12%</p>
2	I	249	<div style="display: flex; align-items: center;"> <div style="width: 77%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">77%      10%      12%</p>

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Mol	Chain	Length	Quality of chain
2	J	249	 2% 79% 9% 12%
3	L	241	 76% 14% 10%
3	M	241	 74% 15% 11%
3	N	241	 76% 12% 11%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20312 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
			Total	C	N	O	S			
1	A	446	3451	2178	570	682	21	0	0	0
1	B	448	3468	2189	572	686	21	0	0	0
1	C	449	3477	2194	574	688	21	0	0	0

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	379	VAL	ILE	conflict	UNP P03420
A	447	VAL	MET	conflict	UNP P03420
A	514	SER	-	expression tag	UNP P03420
A	515	ALA	-	expression tag	UNP P03420
A	516	ILE	-	expression tag	UNP P03420
A	517	GLY	-	expression tag	UNP P03420
A	518	GLY	-	expression tag	UNP P03420
A	519	TYR	-	expression tag	UNP P03420
A	520	ILE	-	expression tag	UNP P03420
A	521	PRO	-	expression tag	UNP P03420
A	522	GLU	-	expression tag	UNP P03420
A	523	ALA	-	expression tag	UNP P03420
A	524	PRO	-	expression tag	UNP P03420
A	525	ARG	-	expression tag	UNP P03420
A	526	ASP	-	expression tag	UNP P03420
A	527	GLY	-	expression tag	UNP P03420
A	528	GLN	-	expression tag	UNP P03420
A	529	ALA	-	expression tag	UNP P03420
A	530	TYR	-	expression tag	UNP P03420
A	531	VAL	-	expression tag	UNP P03420
A	532	ARG	-	expression tag	UNP P03420
A	533	LYS	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	534	ASP	-	expression tag	UNP P03420
A	535	GLY	-	expression tag	UNP P03420
A	536	GLU	-	expression tag	UNP P03420
A	537	TRP	-	expression tag	UNP P03420
A	538	VAL	-	expression tag	UNP P03420
A	539	LEU	-	expression tag	UNP P03420
A	540	LEU	-	expression tag	UNP P03420
A	541	SER	-	expression tag	UNP P03420
A	542	THR	-	expression tag	UNP P03420
A	543	PHE	-	expression tag	UNP P03420
A	544	LEU	-	expression tag	UNP P03420
A	545	GLY	-	expression tag	UNP P03420
A	546	GLY	-	expression tag	UNP P03420
A	547	LEU	-	expression tag	UNP P03420
A	548	VAL	-	expression tag	UNP P03420
A	549	PRO	-	expression tag	UNP P03420
A	550	ARG	-	expression tag	UNP P03420
A	551	GLY	-	expression tag	UNP P03420
A	552	SER	-	expression tag	UNP P03420
A	553	HIS	-	expression tag	UNP P03420
A	554	HIS	-	expression tag	UNP P03420
A	555	HIS	-	expression tag	UNP P03420
A	556	HIS	-	expression tag	UNP P03420
A	557	HIS	-	expression tag	UNP P03420
A	558	HIS	-	expression tag	UNP P03420
A	559	SER	-	expression tag	UNP P03420
A	560	ALA	-	expression tag	UNP P03420
A	561	TRP	-	expression tag	UNP P03420
A	562	SER	-	expression tag	UNP P03420
A	563	HIS	-	expression tag	UNP P03420
A	564	PRO	-	expression tag	UNP P03420
A	565	GLN	-	expression tag	UNP P03420
A	566	PHE	-	expression tag	UNP P03420
A	567	GLU	-	expression tag	UNP P03420
A	568	LYS	-	expression tag	UNP P03420
B	102	ALA	PRO	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420
B	514	SER	-	expression tag	UNP P03420
B	515	ALA	-	expression tag	UNP P03420
B	516	ILE	-	expression tag	UNP P03420
B	517	GLY	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	518	GLY	-	expression tag	UNP P03420
B	519	TYR	-	expression tag	UNP P03420
B	520	ILE	-	expression tag	UNP P03420
B	521	PRO	-	expression tag	UNP P03420
B	522	GLU	-	expression tag	UNP P03420
B	523	ALA	-	expression tag	UNP P03420
B	524	PRO	-	expression tag	UNP P03420
B	525	ARG	-	expression tag	UNP P03420
B	526	ASP	-	expression tag	UNP P03420
B	527	GLY	-	expression tag	UNP P03420
B	528	GLN	-	expression tag	UNP P03420
B	529	ALA	-	expression tag	UNP P03420
B	530	TYR	-	expression tag	UNP P03420
B	531	VAL	-	expression tag	UNP P03420
B	532	ARG	-	expression tag	UNP P03420
B	533	LYS	-	expression tag	UNP P03420
B	534	ASP	-	expression tag	UNP P03420
B	535	GLY	-	expression tag	UNP P03420
B	536	GLU	-	expression tag	UNP P03420
B	537	TRP	-	expression tag	UNP P03420
B	538	VAL	-	expression tag	UNP P03420
B	539	LEU	-	expression tag	UNP P03420
B	540	LEU	-	expression tag	UNP P03420
B	541	SER	-	expression tag	UNP P03420
B	542	THR	-	expression tag	UNP P03420
B	543	PHE	-	expression tag	UNP P03420
B	544	LEU	-	expression tag	UNP P03420
B	545	GLY	-	expression tag	UNP P03420
B	546	GLY	-	expression tag	UNP P03420
B	547	LEU	-	expression tag	UNP P03420
B	548	VAL	-	expression tag	UNP P03420
B	549	PRO	-	expression tag	UNP P03420
B	550	ARG	-	expression tag	UNP P03420
B	551	GLY	-	expression tag	UNP P03420
B	552	SER	-	expression tag	UNP P03420
B	553	HIS	-	expression tag	UNP P03420
B	554	HIS	-	expression tag	UNP P03420
B	555	HIS	-	expression tag	UNP P03420
B	556	HIS	-	expression tag	UNP P03420
B	557	HIS	-	expression tag	UNP P03420
B	558	HIS	-	expression tag	UNP P03420
B	559	SER	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	560	ALA	-	expression tag	UNP P03420
B	561	TRP	-	expression tag	UNP P03420
B	562	SER	-	expression tag	UNP P03420
B	563	HIS	-	expression tag	UNP P03420
B	564	PRO	-	expression tag	UNP P03420
B	565	GLN	-	expression tag	UNP P03420
B	566	PHE	-	expression tag	UNP P03420
B	567	GLU	-	expression tag	UNP P03420
B	568	LYS	-	expression tag	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
C	379	VAL	ILE	conflict	UNP P03420
C	447	VAL	MET	conflict	UNP P03420
C	514	SER	-	expression tag	UNP P03420
C	515	ALA	-	expression tag	UNP P03420
C	516	ILE	-	expression tag	UNP P03420
C	517	GLY	-	expression tag	UNP P03420
C	518	GLY	-	expression tag	UNP P03420
C	519	TYR	-	expression tag	UNP P03420
C	520	ILE	-	expression tag	UNP P03420
C	521	PRO	-	expression tag	UNP P03420
C	522	GLU	-	expression tag	UNP P03420
C	523	ALA	-	expression tag	UNP P03420
C	524	PRO	-	expression tag	UNP P03420
C	525	ARG	-	expression tag	UNP P03420
C	526	ASP	-	expression tag	UNP P03420
C	527	GLY	-	expression tag	UNP P03420
C	528	GLN	-	expression tag	UNP P03420
C	529	ALA	-	expression tag	UNP P03420
C	530	TYR	-	expression tag	UNP P03420
C	531	VAL	-	expression tag	UNP P03420
C	532	ARG	-	expression tag	UNP P03420
C	533	LYS	-	expression tag	UNP P03420
C	534	ASP	-	expression tag	UNP P03420
C	535	GLY	-	expression tag	UNP P03420
C	536	GLU	-	expression tag	UNP P03420
C	537	TRP	-	expression tag	UNP P03420
C	538	VAL	-	expression tag	UNP P03420
C	539	LEU	-	expression tag	UNP P03420
C	540	LEU	-	expression tag	UNP P03420
C	541	SER	-	expression tag	UNP P03420
C	542	THR	-	expression tag	UNP P03420
C	543	PHE	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
C	544	LEU	-	expression tag	UNP P03420
C	545	GLY	-	expression tag	UNP P03420
C	546	GLY	-	expression tag	UNP P03420
C	547	LEU	-	expression tag	UNP P03420
C	548	VAL	-	expression tag	UNP P03420
C	549	PRO	-	expression tag	UNP P03420
C	550	ARG	-	expression tag	UNP P03420
C	551	GLY	-	expression tag	UNP P03420
C	552	SER	-	expression tag	UNP P03420
C	553	HIS	-	expression tag	UNP P03420
C	554	HIS	-	expression tag	UNP P03420
C	555	HIS	-	expression tag	UNP P03420
C	556	HIS	-	expression tag	UNP P03420
C	557	HIS	-	expression tag	UNP P03420
C	558	HIS	-	expression tag	UNP P03420
C	559	SER	-	expression tag	UNP P03420
C	560	ALA	-	expression tag	UNP P03420
C	561	TRP	-	expression tag	UNP P03420
C	562	SER	-	expression tag	UNP P03420
C	563	HIS	-	expression tag	UNP P03420
C	564	PRO	-	expression tag	UNP P03420
C	565	GLN	-	expression tag	UNP P03420
C	566	PHE	-	expression tag	UNP P03420
C	567	GLU	-	expression tag	UNP P03420
C	568	LYS	-	expression tag	UNP P03420

- Molecule 2 is a protein called 5C4 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1638	1039	268	325	6			
2	I	219	Total	C	N	O	S	0	0	0
			1638	1039	268	325	6			
2	J	219	Total	C	N	O	S	0	0	0
			1638	1039	268	325	6			

- Molecule 3 is a protein called 5C4 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1670	1040	280	345	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	215	Total	C	N	O	S	0	0	0
			1662	1036	278	343	5			
3	N	215	Total	C	N	O	S	0	0	0
			1662	1036	278	343	5			

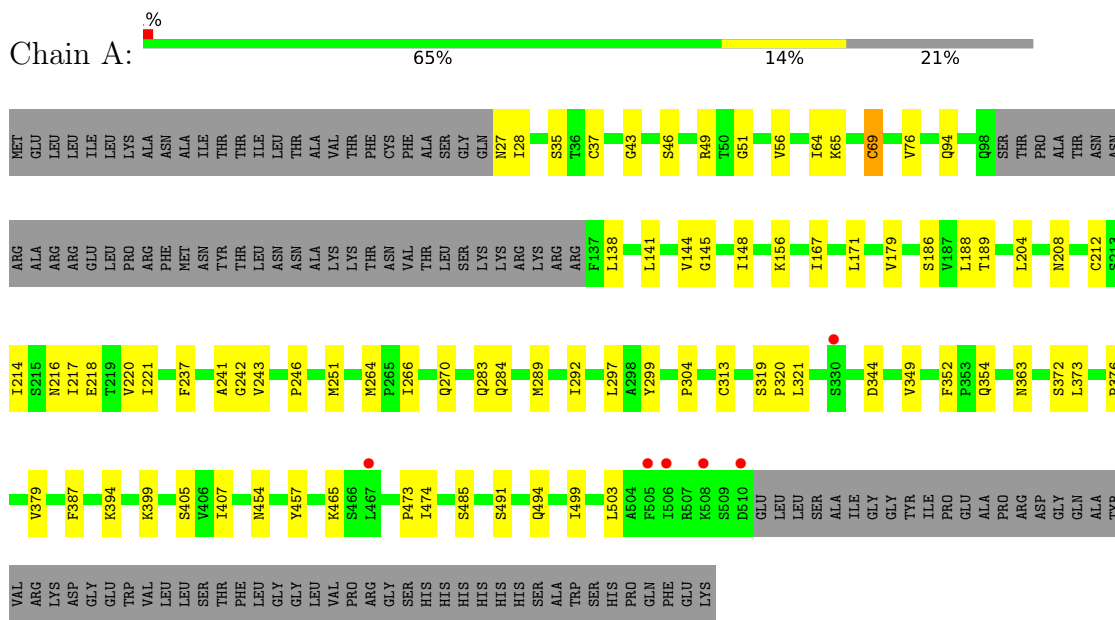
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	J	2	Total	Zn	0	0
			2	2		
4	N	1	Total	Zn	0	0
			1	1		

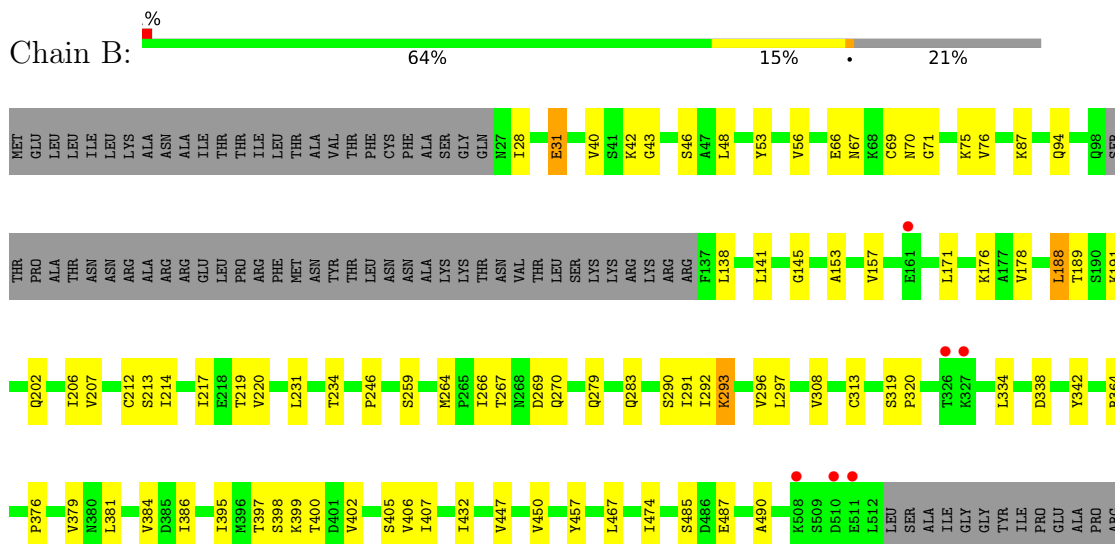
### 3 Residue-property plots [i](#)

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 F0

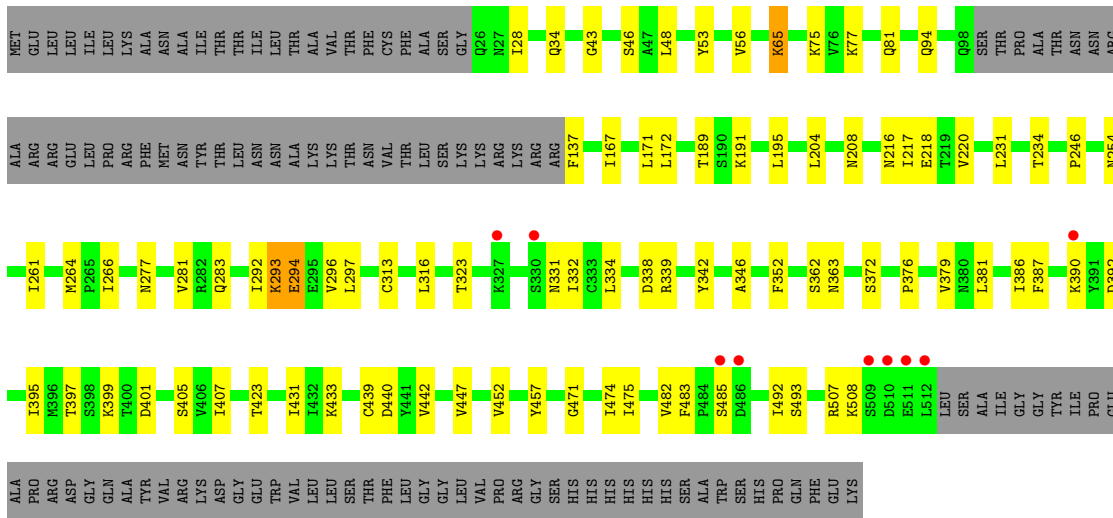


- Molecule 1: Fusion glycoprotein F0

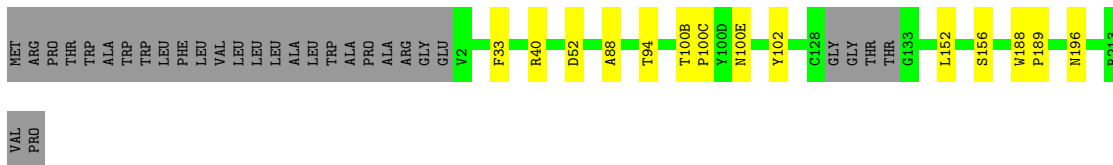
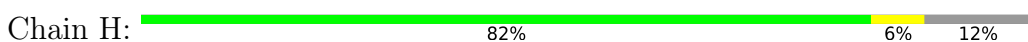


ASP GLY GLN ALA ALA TYR VAL TYR ARG LYS ASP ASP GLY GIU TRP VAL LEU LEU THR SER SER PHE PHE LEU LEU LEU GLY GLY VAL VAL ARG PRO PRO ARG GLY SER HIS HIS HIS HIS HIS SER SER TRP TRP HIS HIS PRO PHE GLN GLU LYS

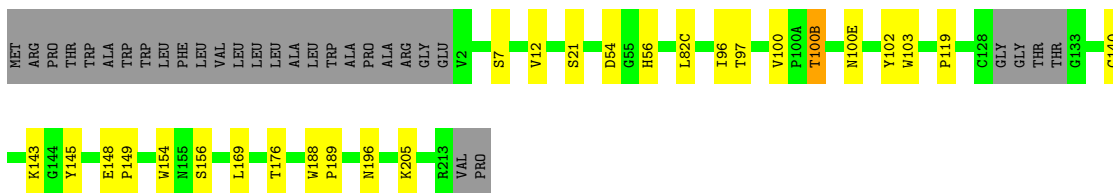
Molecule 1: Fusion glycoprotein F0



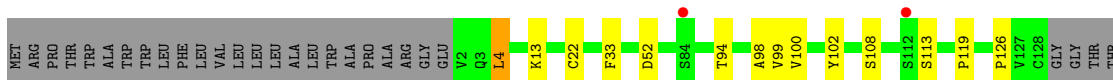
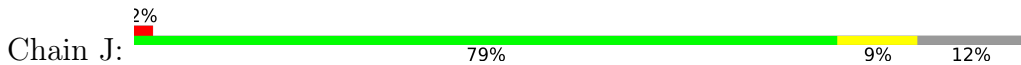
Molecule 2: 5C4 Fab heavy chain

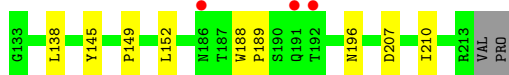


Molecule 2: 5C4 Fab heavy chain



Molecule 2: 5C4 Fab heavy chain





- Molecule 3: 5C4 Fab light chain

Chain L: 76% 14% 10%



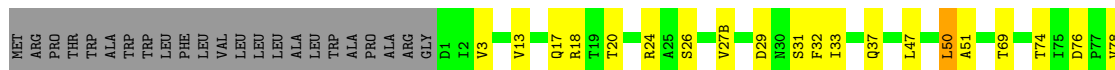
- Molecule 3: 5C4 Fab light chain

Chain M: 74% 15% 11%



- Molecule 3: 5C4 Fab light chain

Chain N: 76% 12% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.36Å 183.36Å 275.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.06 – 3.40 34.06 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.06-3.40) 98.9 (34.06-3.40)	Depositor EDS
$R_{merge}$	0.38	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 3.39Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.198 , 0.239 0.197 , 0.238	Depositor DCC
$R_{free}$ test set	3270 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.220	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

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

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	0.41	1/3500 (0.0%)	0.62	0/4741
1	B	0.44	2/3517 (0.1%)	0.63	2/4764 (0.0%)
1	C	0.38	0/3526	0.63	1/4776 (0.0%)
2	H	0.40	0/1680	0.61	0/2303
2	I	0.38	0/1680	0.61	0/2303
2	J	0.34	0/1680	0.60	0/2303
3	L	0.38	0/1708	0.62	0/2323
3	M	0.41	0/1700	0.63	2/2312 (0.1%)
3	N	0.42	0/1700	0.68	1/2312 (0.0%)
All	All	0.40	3/20691 (0.0%)	0.63	6/28137 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	GLU	CB-CG	8.31	1.68	1.52
1	A	69	CYS	CB-SG	-5.90	1.72	1.81
1	B	31	GLU	CG-CD	5.33	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	LEU	CA-CB-CG	6.88	131.12	115.30
1	B	31	GLU	OE1-CD-OE2	-6.34	115.69	123.30
3	M	50	LEU	CA-CB-CG	-5.66	102.29	115.30
3	M	50	LEU	C-N-CA	-5.38	108.25	121.70
1	C	172	LEU	CA-CB-CG	5.16	127.17	115.30
3	N	50	LEU	CA-CB-CG	-5.02	103.75	115.30

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	3451	0	3494	56	0
1	B	3468	0	3511	59	1
1	C	3477	0	3519	63	0
2	H	1638	0	1605	8	0
2	I	1638	0	1605	18	0
2	J	1638	0	1605	16	0
3	L	1670	0	1592	18	1
3	M	1662	0	1586	22	0
3	N	1662	0	1586	18	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	N	1	0	0	0	0
All	All	20312	0	20103	255	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (255) 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:66:GLU:HG2	1:B:87:LYS:NZ	1.81	0.94
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.50	0.94
1:C:407:ILE:HD11	1:C:457:TYR:HB3	1.53	0.89
3:N:187:GLU:HA	3:N:211:ARG:HH12	1.35	0.88
1:C:334:LEU:HD11	1:C:395:ILE:HD12	1.59	0.85
1:B:407:ILE:HD11	1:B:457:TYR:HB3	1.59	0.84
1:B:66:GLU:HG2	1:B:87:LYS:HZ1	1.44	0.82
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.65	0.79
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.67	0.76
1:B:28:ILE:HA	1:B:43:GLY:HA3	1.69	0.74
2:I:100(B):THR:HG23	2:I:100(E):ASN:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:LEU:HD21	2:J:22:CYS:SG	2.30	0.72
3:M:31:SER:HB2	3:M:51:ALA:HB2	1.71	0.71
1:C:171:LEU:HD23	1:C:191:LYS:HB2	1.73	0.71
1:B:334:LEU:HD11	1:B:395:ILE:HD12	1.74	0.70
1:B:376:PRO:O	1:B:379:VAL:HG23	1.93	0.68
3:M:27(C):ASP:OD2	3:M:68:ARG:HA	1.93	0.68
1:B:75:LYS:HG2	1:C:218:GLU:HG2	1.75	0.66
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.77	0.66
1:C:34:GLN:NE2	1:C:471:GLY:O	2.28	0.66
1:A:289:MET:HE3	1:A:297:LEU:HD11	1.78	0.66
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.77	0.66
3:N:195:GLU:HG2	3:N:206:VAL:HG22	1.78	0.66
1:C:56:VAL:HB	1:C:189:THR:HG22	1.78	0.65
3:N:185:GLU:HA	3:N:188:ARG:HD3	1.78	0.65
1:B:67:ASN:OD1	1:B:69:CYS:HB3	1.97	0.65
1:B:171:LEU:O	1:B:191:LYS:NZ	2.21	0.65
1:B:31:GLU:OE2	1:B:42:LYS:HE2	1.97	0.65
1:C:442:VAL:HG21	1:C:447:VAL:HG21	1.80	0.64
3:N:13:VAL:HG11	3:N:78:VAL:HG21	1.77	0.64
1:B:399:LYS:HG3	1:B:485:SER:HB2	1.79	0.64
2:I:54:ASP:OD2	2:I:56:HIS:NE2	2.31	0.63
3:N:31:SER:HB2	3:N:51:ALA:HB2	1.81	0.63
3:N:187:GLU:HA	3:N:211:ARG:NH1	2.12	0.63
1:A:292:ILE:HG22	1:A:297:LEU:HA	1.81	0.62
1:C:323:THR:OG1	1:C:331:ASN:OD1	2.11	0.61
1:A:218:GLU:OE2	1:C:75:LYS:HE3	2.01	0.61
1:A:221:ILE:HD12	1:C:217:ILE:HD11	1.83	0.60
1:A:69:CYS:SG	1:A:76:VAL:HG13	2.42	0.60
1:C:332:ILE:HG23	1:C:475:ILE:HD11	1.82	0.60
1:A:394:LYS:NZ	1:B:400:THR:HG21	2.17	0.60
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.83	0.60
1:B:267:THR:HG22	1:B:269:ASP:H	1.67	0.59
3:M:145:ASN:HB3	3:M:197:THR:HB	1.84	0.59
2:J:196:ASN:ND2	2:J:207:ASP:OD1	2.36	0.58
1:A:344:ASP:HA	1:A:349:VAL:HA	1.84	0.58
1:B:217:ILE:O	1:B:220:VAL:HG12	2.04	0.58
3:L:83:ALA:HB2	3:L:106:ILE:HG12	1.84	0.58
1:B:75:LYS:CG	1:C:218:GLU:HG2	2.34	0.58
1:C:507:ARG:HH22	1:C:508:LYS:HE3	1.70	0.57
1:C:217:ILE:O	1:C:220:VAL:HG12	2.04	0.57
1:A:394:LYS:HZ3	1:B:400:THR:CG2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:175:MET:HG2	3:M:176:SER:N	2.19	0.57
3:N:187:GLU:CA	3:N:211:ARG:HH12	2.14	0.57
3:L:16:GLY:HA2	3:L:77:PRO:HB2	1.86	0.57
3:N:113:PRO:HG2	3:N:205:ILE:HD12	1.86	0.57
1:A:405:SER:HB3	1:A:457:TYR:CE2	2.40	0.56
1:C:423:THR:HG21	1:C:431:ILE:HG12	1.87	0.56
1:A:373:LEU:HD13	1:B:402:VAL:HG11	1.87	0.56
1:C:171:LEU:HD11	1:C:189:THR:OG1	2.05	0.56
1:C:405:SER:HB2	1:C:452:VAL:HG21	1.88	0.56
3:N:33:ILE:O	3:N:50:LEU:O	2.24	0.56
1:B:56:VAL:HB	1:B:189:THR:HG22	1.88	0.55
3:M:155:ARG:HD3	3:M:179:LEU:HD11	1.89	0.55
1:A:148:ILE:HD13	1:A:243:VAL:HG11	1.89	0.55
1:B:214:ILE:HG21	1:B:219:THR:HB	1.87	0.55
1:C:405:SER:HB3	1:C:457:TYR:CE2	2.42	0.55
3:N:145:ASN:HB3	3:N:197:THR:HB	1.89	0.55
1:B:76:VAL:HG22	1:B:213:SER:HA	1.89	0.54
3:M:33:ILE:O	3:M:50:LEU:O	2.25	0.54
1:B:153:ALA:O	1:B:157:VAL:HG23	2.07	0.54
3:L:147:LYS:HD3	3:L:154:GLU:OE2	2.07	0.54
1:A:212:CYS:HB2	2:J:99:VAL:HG11	1.89	0.54
1:C:167:ILE:HD12	1:C:189:THR:HG21	1.88	0.54
1:A:376:PRO:O	1:A:379:VAL:HG23	2.07	0.54
1:B:266:ILE:HD12	1:B:270:GLN:HB3	1.90	0.53
3:N:3:VAL:H	3:N:26:SER:HB3	1.73	0.53
1:C:28:ILE:HA	1:C:43:GLY:HA3	1.89	0.53
3:L:31:SER:HB2	3:L:51:ALA:HB2	1.89	0.53
2:I:188:TRP:CG	2:I:189:PRO:HA	2.44	0.53
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.90	0.53
2:J:13:LYS:NZ	2:J:113:SER:O	2.41	0.53
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.44	0.53
1:C:387:PHE:HE2	1:C:474:ILE:HD12	1.73	0.53
1:C:376:PRO:O	1:C:379:VAL:HG23	2.09	0.52
1:B:292:ILE:HG22	1:B:297:LEU:HA	1.91	0.52
1:C:433:LYS:NZ	1:C:440:ASP:OD2	2.40	0.52
3:L:33:ILE:O	3:L:50:LEU:O	2.28	0.52
1:A:217:ILE:O	1:A:220:VAL:HG12	2.10	0.52
1:A:28:ILE:HD11	1:A:363:ASN:HB3	1.92	0.52
3:M:13:VAL:HG11	3:M:78:VAL:HG21	1.92	0.52
1:A:217:ILE:HG23	1:C:217:ILE:HD12	1.91	0.51
1:C:387:PHE:CE2	1:C:474:ILE:HD12	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:32:PHE:HB2	3:N:92:ASN:HB2	1.92	0.51
1:C:399:LYS:HG3	1:C:485:SER:HB2	1.91	0.51
1:A:204:LEU:HD22	2:J:100:VAL:HG11	1.92	0.51
1:A:65:LYS:NZ	2:J:52:ASP:OD1	2.27	0.51
1:A:387:PHE:CE2	1:A:474:ILE:HD12	2.45	0.51
1:C:77:LYS:O	1:C:81:GLN:HB2	2.11	0.51
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.91	0.51
1:B:178:VAL:HG12	1:B:188:LEU:HD12	1.92	0.51
1:A:64:ILE:HG22	1:A:65:LYS:O	2.11	0.51
1:A:28:ILE:HA	1:A:43:GLY:HA3	1.91	0.50
1:C:204:LEU:O	1:C:208:ASN:ND2	2.43	0.50
1:A:241:ALA:HA	1:B:279:GLN:HG3	1.93	0.50
1:A:491:SER:H	1:A:494:GLN:HB2	1.76	0.50
2:I:12:VAL:HG11	2:I:82(C):LEU:HD22	1.93	0.50
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.94	0.50
1:B:46:SER:HB3	1:B:313:CYS:SG	2.52	0.50
3:L:29:ASP:OD1	3:L:29:ASP:O	2.29	0.50
3:M:184:ASP:O	3:M:188:ARG:HG3	2.11	0.50
1:B:138:LEU:HB3	1:B:141:LEU:HD12	1.93	0.50
2:H:188:TRP:CG	2:H:189:PRO:HA	2.47	0.49
1:C:216:ASN:HB3	1:C:218:GLU:OE1	2.12	0.49
1:B:207:VAL:HG13	1:B:212:CYS:HA	1.94	0.49
1:B:319:SER:OG	1:B:320:PRO:HD2	2.13	0.49
1:B:70:ASN:OD1	1:B:71:GLY:N	2.46	0.49
2:I:196:ASN:HB3	2:I:205:LYS:NZ	2.27	0.49
1:B:386:ILE:HG21	1:B:474:ILE:HD12	1.95	0.48
2:I:169:LEU:HD11	3:M:162:SER:HB2	1.95	0.48
1:C:264:MET:HE3	1:C:266:ILE:HD13	1.95	0.48
3:L:145:ASN:HB3	3:L:197:THR:HB	1.95	0.48
1:B:40:VAL:HG12	1:B:42:LYS:HG3	1.94	0.48
1:A:145:GLY:HA2	1:B:407:ILE:HD12	1.94	0.48
1:A:138:LEU:HB3	1:A:141:LEU:HD12	1.96	0.48
1:A:387:PHE:HE2	1:A:474:ILE:HD12	1.79	0.48
1:B:176:LYS:NZ	1:B:259:SER:OG	2.46	0.48
2:I:97:THR:HG21	3:M:55:GLU:OE2	2.14	0.48
2:J:188:TRP:CG	2:J:189:PRO:HA	2.49	0.48
1:C:53:TYR:CE2	1:C:264:MET:HG2	2.48	0.48
2:I:54:ASP:OD2	2:I:56:HIS:CE1	2.67	0.48
3:L:150:ILE:HD12	3:L:155:ARG:HD2	1.96	0.47
3:L:151:ASP:OD2	3:L:189:HIS:ND1	2.47	0.47
1:A:399:LYS:HG3	1:A:485:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LEU:HA	1:B:384:VAL:HG22	1.95	0.47
1:B:405:SER:HB3	1:B:457:TYR:CE2	2.49	0.47
2:H:100(B):THR:HG22	2:H:100(C):PRO:HD2	1.95	0.47
1:B:67:ASN:HB2	2:I:100:VAL:HG22	1.94	0.47
1:C:423:THR:HG23	1:C:431:ILE:HG23	1.95	0.47
1:A:37:CYS:HB2	1:A:321:LEU:HD13	1.95	0.47
1:A:289:MET:CE	1:A:297:LEU:HD11	2.44	0.47
1:C:46:SER:HB3	1:C:313:CYS:SG	2.54	0.47
1:B:202:GLN:O	1:B:206:ILE:HG13	2.14	0.47
2:J:4:LEU:HB2	2:J:102:TYR:CE1	2.50	0.47
1:A:46:SER:HB3	1:A:313:CYS:SG	2.55	0.46
1:A:56:VAL:HB	1:A:189:THR:HG22	1.97	0.46
1:A:454:ASN:HD21	1:C:346:ALA:HB3	1.80	0.46
1:B:48:LEU:HB2	1:B:308:VAL:HB	1.97	0.46
1:B:145:GLY:HA2	1:C:407:ILE:HD12	1.96	0.46
1:B:487:GLU:HB3	1:B:490:ALA:HB2	1.97	0.46
3:L:151:ASP:HA	3:L:191:SER:HB3	1.96	0.46
3:M:186:TYR:O	3:M:192:TYR:OH	2.31	0.46
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.98	0.46
1:C:342:TYR:CE2	1:C:379:VAL:HG11	2.51	0.46
2:I:156:SER:H	2:I:196:ASN:ND2	2.14	0.46
3:M:195:GLU:HG2	3:M:206:VAL:HG22	1.97	0.46
1:C:137:PHE:HE1	1:C:339:ARG:CZ	2.28	0.46
1:A:179:VAL:O	1:A:186:SER:HA	2.15	0.46
1:B:94:GLN:HA	1:B:292:ILE:HD11	1.97	0.46
1:C:316:LEU:HD23	1:C:338:ASP:O	2.16	0.46
2:H:152:LEU:HA	2:H:196:ASN:O	2.17	0.45
3:M:65:SER:OG	3:M:72:THR:HB	2.15	0.45
1:C:46:SER:HB2	1:C:48:LEU:CD1	2.47	0.45
2:I:103:TRP:CE3	3:M:44:PRO:HD2	2.52	0.45
2:J:126:PRO:HD3	2:J:138:LEU:CD2	2.46	0.45
3:N:18:ARG:HB2	3:N:76:ASP:HB2	1.99	0.45
1:A:156:LYS:HA	1:A:156:LYS:HD3	1.74	0.45
1:B:398:SER:HA	1:B:485:SER:O	2.17	0.45
1:C:386:ILE:HG12	1:C:492:ILE:CD1	2.47	0.45
1:B:66:GLU:HG2	1:B:87:LYS:HZ2	1.75	0.45
1:C:264:MET:HB2	1:C:264:MET:HE2	1.79	0.45
1:C:401:ASP:OD1	1:C:401:ASP:O	2.35	0.45
2:I:96:ILE:HD11	2:I:102:TYR:CD2	2.52	0.45
1:A:266:ILE:HD12	1:A:270:GLN:HB3	1.98	0.45
1:C:381:LEU:HD11	1:C:390:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:SER:HB3	2:I:21:SER:OG	2.17	0.45
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.98	0.44
1:C:332:ILE:HD12	1:C:399:LYS:HG2	1.99	0.44
1:A:319:SER:OG	1:A:320:PRO:HD2	2.17	0.44
3:L:34:HIS:O	3:L:88:CYS:HA	2.18	0.44
1:B:450:VAL:CG1	1:B:457:TYR:HB2	2.47	0.44
1:A:237:PHE:CD1	1:A:242:GLY:HA2	2.53	0.44
1:A:394:LYS:HZ1	1:B:400:THR:HG21	1.82	0.44
1:A:144:VAL:HB	1:B:406:VAL:HG13	2.00	0.44
1:A:251:MET:HG3	1:A:299:TYR:CE2	2.53	0.44
1:C:334:LEU:HD12	1:C:397:THR:HG22	1.99	0.43
2:H:40:ARG:HG2	2:H:88:ALA:HB2	2.01	0.43
3:L:13:VAL:HG11	3:L:78:VAL:HG21	1.99	0.43
1:A:284:GLN:HB2	1:A:304:PRO:HG3	2.00	0.43
3:N:27(B):VAL:HG21	3:N:33:ILE:HG12	2.00	0.43
1:A:264:MET:HB2	1:A:264:MET:HE2	1.67	0.43
1:B:290:SER:OG	1:B:291:ILE:N	2.52	0.43
3:M:151:ASP:HA	3:M:191:SER:HB3	2.01	0.43
2:J:108:SER:HB3	2:J:149:PRO:HD3	2.00	0.43
1:C:231:LEU:O	1:C:234:THR:HG22	2.18	0.43
3:M:50:LEU:HD23	3:M:50:LEU:HA	1.73	0.43
2:I:143:LYS:HG3	2:I:176:THR:OG1	2.18	0.43
2:J:33:PHE:O	2:J:94:THR:HG22	2.19	0.43
3:L:24:ARG:HA	3:L:69:THR:O	2.20	0.42
3:N:24:ARG:HA	3:N:69:THR:O	2.19	0.42
1:A:27:ASN:HB3	1:A:28:ILE:HD12	2.01	0.42
1:C:292:ILE:HG22	1:C:297:LEU:HB2	2.01	0.42
2:J:138:LEU:HD22	2:J:210:ILE:HG21	2.00	0.42
1:A:35:SER:O	1:A:474:ILE:HG12	2.18	0.42
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.20	0.42
2:H:100(B):THR:HB	2:H:100(E):ASN:HB2	2.01	0.42
1:A:94:GLN:HA	1:A:292:ILE:HD11	2.01	0.42
1:C:386:ILE:HG12	1:C:492:ILE:HD11	2.00	0.42
1:C:442:VAL:CG2	1:C:447:VAL:HG21	2.46	0.42
3:M:76:ASP:HA	3:M:77:PRO:HA	1.86	0.42
1:A:167:ILE:HD12	1:A:189:THR:HG21	2.02	0.42
1:B:66:GLU:CG	1:B:87:LYS:HZ1	2.23	0.42
1:C:362:SER:OG	1:C:363:ASN:N	2.51	0.42
1:A:465:LYS:HD2	1:A:465:LYS:HA	1.94	0.42
2:H:156:SER:HA	2:H:196:ASN:HD22	1.85	0.42
3:L:48:ILE:HD13	3:L:54:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:OD1	2:J:98:ALA:HB1	2.20	0.42
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.55	0.42
1:C:292:ILE:HA	1:C:296:VAL:O	2.20	0.41
2:I:140:CYS:HB2	2:I:154:TRP:CH2	2.55	0.41
1:C:94:GLN:HG3	1:C:292:ILE:HD11	2.00	0.41
3:M:48:ILE:HD13	3:M:54:LEU:HA	2.02	0.41
2:J:119:PRO:CB	2:J:145:TYR:HB3	2.48	0.41
1:B:264:MET:HB2	1:B:264:MET:HE2	1.80	0.41
2:I:148:GLU:HB3	2:I:149:PRO:HA	2.02	0.41
1:B:53:TYR:OH	1:B:188:LEU:HD13	2.21	0.41
2:J:152:LEU:HA	2:J:196:ASN:O	2.20	0.41
1:C:261:ILE:HA	1:C:264:MET:HE2	2.02	0.41
1:C:292:ILE:HG21	1:C:292:ILE:HD13	1.82	0.41
1:C:482:VAL:HG12	1:C:482:VAL:O	2.21	0.41
3:M:149:LYS:HA	3:M:153:SER:O	2.20	0.41
1:B:231:LEU:O	1:B:234:THR:HG22	2.20	0.41
1:A:204:LEU:O	1:A:208:ASN:ND2	2.53	0.41
1:A:321:LEU:HD11	1:A:473:PRO:HB3	2.02	0.41
1:A:499:ILE:O	1:A:503:LEU:N	2.46	0.41
1:B:334:LEU:HD12	1:B:397:THR:HG22	2.03	0.41
1:A:214:ILE:CD1	1:A:217:ILE:HA	2.51	0.41
1:B:56:VAL:O	1:B:189:THR:HA	2.21	0.41
1:B:292:ILE:HA	1:B:296:VAL:O	2.21	0.41
1:B:293:LYS:HB3	1:B:293:LYS:HE2	1.79	0.41
2:H:33:PHE:O	2:H:94:THR:HG22	2.21	0.41
3:L:39:LYS:HG2	3:L:84:ALA:HB2	2.02	0.41
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.91	0.40
1:C:392:ASP:OD2	1:C:493:SER:OG	2.27	0.40
3:M:18:ARG:HB3	3:M:76:ASP:CG	2.41	0.40
1:C:277:ASN:O	1:C:281:VAL:HG23	2.21	0.40
1:C:397:THR:HB	1:C:483:PHE:HE1	1.87	0.40
1:C:65:LYS:NZ	2:H:52:ASP:OD1	2.54	0.40
2:I:54:ASP:OD2	2:I:56:HIS:CD2	2.75	0.40
3:N:13:VAL:HG13	3:N:17:GLN:OE1	2.21	0.40
1:C:293:LYS:C	1:C:294:GLU:HG2	2.42	0.40
3:M:175:MET:HE2	3:M:175:MET:HB3	1.84	0.40
1:A:49:ARG:HH12	1:A:51:GLY:HA2	1.87	0.40
3:L:32:PHE:O	3:L:90:GLN:HA	2.21	0.40
3:N:20:THR:HG22	3:N:74:THR:OG1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:OE2	3:L:189:HIS:ND1[7_657]	2.12	0.08

### 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	442/568 (78%)	427 (97%)	15 (3%)	0	100	100
1	B	444/568 (78%)	423 (95%)	21 (5%)	0	100	100
1	C	445/568 (78%)	427 (96%)	18 (4%)	0	100	100
2	H	215/249 (86%)	214 (100%)	1 (0%)	0	100	100
2	I	215/249 (86%)	214 (100%)	1 (0%)	0	100	100
2	J	215/249 (86%)	214 (100%)	1 (0%)	0	100	100
3	L	214/241 (89%)	206 (96%)	8 (4%)	0	100	100
3	M	213/241 (88%)	208 (98%)	5 (2%)	0	100	100
3	N	213/241 (88%)	206 (97%)	6 (3%)	1 (0%)	29	61
All	All	2616/3174 (82%)	2539 (97%)	76 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	29	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	407/510 (80%)	403 (99%)	4 (1%)	76	88
1	B	409/510 (80%)	406 (99%)	3 (1%)	84	92
1	C	410/510 (80%)	405 (99%)	5 (1%)	71	85
2	H	187/210 (89%)	186 (100%)	1 (0%)	88	94
2	I	187/210 (89%)	186 (100%)	1 (0%)	88	94
2	J	187/210 (89%)	186 (100%)	1 (0%)	88	94
3	L	192/212 (91%)	192 (100%)	0	100	100
3	M	191/212 (90%)	191 (100%)	0	100	100
3	N	191/212 (90%)	191 (100%)	0	100	100
All	All	2361/2796 (84%)	2346 (99%)	15 (1%)	86	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	188	LEU
1	A	216	ASN
1	A	354	GLN
1	B	188	LEU
1	B	293	LYS
1	B	364	ARG
1	C	65	LYS
1	C	254	ASN
1	C	293	LYS
1	C	294	GLU
1	C	439	CYS
2	H	102	TYR
2	I	100(B)	THR
2	J	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	454	ASN
1	A	494	GLN
2	H	196	ASN
3	L	92	ASN
2	I	196	ASN

### 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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	446/568 (78%)	-0.22	6 (1%) 77 76	26, 60, 104, 148	0
1	B	448/568 (78%)	-0.24	6 (1%) 77 76	38, 63, 102, 156	0
1	C	449/568 (79%)	-0.25	9 (2%) 65 64	33, 64, 109, 172	0
2	H	219/249 (87%)	-0.27	0 100 100	24, 59, 105, 122	0
2	I	219/249 (87%)	-0.33	0 100 100	31, 56, 87, 107	0
2	J	219/249 (87%)	-0.05	5 (2%) 60 59	28, 70, 105, 121	0
3	L	216/241 (89%)	-0.26	0 100 100	32, 64, 84, 95	0
3	M	215/241 (89%)	-0.30	0 100 100	29, 51, 75, 95	0
3	N	215/241 (89%)	-0.32	0 100 100	24, 50, 103, 122	0
All	All	2646/3174 (83%)	-0.25	26 (0%) 82 81	24, 60, 103, 172	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ASP	3.2
1	A	505	PHE	2.9
1	B	510	ASP	2.8
1	B	327	LYS	2.8
1	A	506	ILE	2.7
1	C	330	SER	2.7
2	J	191	GLN	2.7
1	C	510	ASP	2.7
1	C	390	LYS	2.6
1	B	326	THR	2.6
1	A	508	LYS	2.5
1	C	327	LYS	2.5
1	A	330	SER	2.4
1	B	161	GLU	2.4
1	A	467	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	112	SER	2.4
2	J	192	THR	2.4
1	C	509	SER	2.3
1	C	512	LEU	2.2
1	C	485	SER	2.2
1	B	511	GLU	2.2
1	C	511	GLU	2.2
1	B	508	LYS	2.2
1	C	486	ASP	2.1
2	J	186	ASN	2.1
2	J	84	SER	2.1

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ZN	B	601	1/1	0.79	0.26	120,120,120,120	0
4	ZN	A	601	1/1	0.85	0.18	106,106,106,106	0
4	ZN	C	601	1/1	0.92	0.26	116,116,116,116	0
4	ZN	I	301	1/1	0.92	0.15	103,103,103,103	0
4	ZN	H	301	1/1	0.94	0.19	112,112,112,112	0
4	ZN	J	302	1/1	0.95	0.11	106,106,106,106	0
4	ZN	J	301	1/1	0.97	0.13	88,88,88,88	0
4	ZN	N	301	1/1	0.97	0.05	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.