



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 09:59 AM EDT

PDB ID : 3TCX  
Title : Structure of Engineered Single Domain ICAM-1 D1 with High-Affinity  $\alpha$ L Integrin I Domain of Native C-Terminal Helix Conformation  
Authors : Kang, S.; Kim, C.U.; Gu, X.; Owens, R.M.; van Rijn, S.J.; Boonyaleepun, V.; Mao, Y.; Springer, T.A.; Jin, M.M.  
Deposited on : 2011-08-09  
Resolution : 3.60 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](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
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

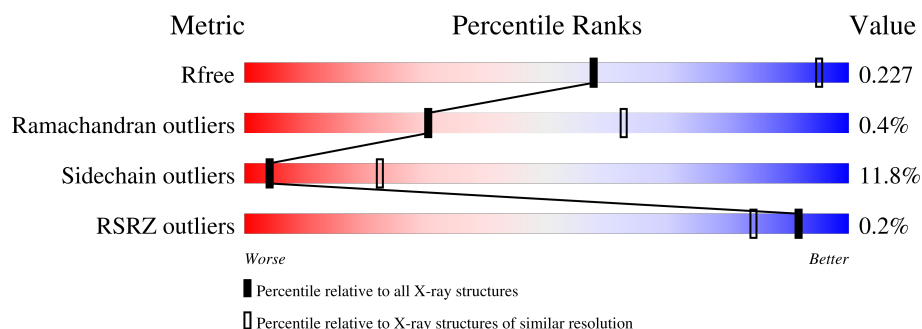
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1563 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

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	85	<div> <div></div> <div>79%19%</div> <div></div> </div>
1	C	85	<div> <div>82%18%</div> </div>
1	E	85	<div> <div>82%18%</div> </div>
1	G	85	<div> <div>75%22%</div> <div></div> </div>
1	I	85	<div> <div>82%18%</div> </div>
1	K	85	<div> <div>82%16%</div> <div></div> </div>
1	M	85	<div> <div>82%18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	85	<div> <div></div> <div>%</div> <div>80%</div> <div>20%</div> </div>
1	Q	85	<div> <div></div> <div>%</div> <div>81%</div> <div>19%</div> </div>
1	S	85	<div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	U	85	<div> <div></div> <div>%</div> <div>81%</div> <div>19%</div> </div>
1	W	85	<div> <div></div> <div>%</div> <div>81%</div> <div>19%</div> </div>
1	Y	85	<div> <div></div> <div>82%</div> <div>18%</div> </div>
1	a	85	<div> <div></div> <div>82%</div> <div>18%</div> </div>
2	B	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	D	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	F	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	H	180	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	J	180	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	L	180	<div> <div></div> <div>%</div> <div>91%</div> <div>9%</div> </div>
2	N	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	P	180	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	R	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	T	180	<div> <div></div> <div>92%</div> <div>8%</div> </div>
2	V	180	<div> <div></div> <div>%</div> <div>92%</div> <div>8%</div> <div>.</div> </div>
2	X	180	<div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div>
2	Z	180	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	b	180	<div> <div></div> <div>93%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29330 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 Intercellular adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	C	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	E	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	G	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	I	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	K	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	M	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	O	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	Q	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	S	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	U	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	W	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	Y	85	Total 641	C 404	N 106	O 125	S 6	0	0	0
1	a	85	Total 641	C 404	N 106	O 125	S 6	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	THR	engineered mutation	UNP P05362
A	10	THR	ILE	engineered mutation	UNP P05362
A	23	ALA	THR	engineered mutation	UNP P05362
A	38	VAL	PRO	engineered mutation	UNP P05362
A	63	VAL	PRO	engineered mutation	UNP P05362
A	67	ALA	SER	engineered mutation	UNP P05362
A	78	ALA	THR	engineered mutation	UNP P05362
C	1	MET	-	expression tag	UNP P05362
C	2	VAL	THR	engineered mutation	UNP P05362
C	10	THR	ILE	engineered mutation	UNP P05362
C	23	ALA	THR	engineered mutation	UNP P05362
C	38	VAL	PRO	engineered mutation	UNP P05362
C	63	VAL	PRO	engineered mutation	UNP P05362
C	67	ALA	SER	engineered mutation	UNP P05362
C	78	ALA	THR	engineered mutation	UNP P05362
E	1	MET	-	expression tag	UNP P05362
E	2	VAL	THR	engineered mutation	UNP P05362
E	10	THR	ILE	engineered mutation	UNP P05362
E	23	ALA	THR	engineered mutation	UNP P05362
E	38	VAL	PRO	engineered mutation	UNP P05362
E	63	VAL	PRO	engineered mutation	UNP P05362
E	67	ALA	SER	engineered mutation	UNP P05362
E	78	ALA	THR	engineered mutation	UNP P05362
G	1	MET	-	expression tag	UNP P05362
G	2	VAL	THR	engineered mutation	UNP P05362
G	10	THR	ILE	engineered mutation	UNP P05362
G	23	ALA	THR	engineered mutation	UNP P05362
G	38	VAL	PRO	engineered mutation	UNP P05362
G	63	VAL	PRO	engineered mutation	UNP P05362
G	67	ALA	SER	engineered mutation	UNP P05362
G	78	ALA	THR	engineered mutation	UNP P05362
I	1	MET	-	expression tag	UNP P05362
I	2	VAL	THR	engineered mutation	UNP P05362
I	10	THR	ILE	engineered mutation	UNP P05362
I	23	ALA	THR	engineered mutation	UNP P05362
I	38	VAL	PRO	engineered mutation	UNP P05362
I	63	VAL	PRO	engineered mutation	UNP P05362
I	67	ALA	SER	engineered mutation	UNP P05362
I	78	ALA	THR	engineered mutation	UNP P05362
K	1	MET	-	expression tag	UNP P05362
K	2	VAL	THR	engineered mutation	UNP P05362
K	10	THR	ILE	engineered mutation	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
K	23	ALA	THR	engineered mutation	UNP P05362
K	38	VAL	PRO	engineered mutation	UNP P05362
K	63	VAL	PRO	engineered mutation	UNP P05362
K	67	ALA	SER	engineered mutation	UNP P05362
K	78	ALA	THR	engineered mutation	UNP P05362
M	1	MET	-	expression tag	UNP P05362
M	2	VAL	THR	engineered mutation	UNP P05362
M	10	THR	ILE	engineered mutation	UNP P05362
M	23	ALA	THR	engineered mutation	UNP P05362
M	38	VAL	PRO	engineered mutation	UNP P05362
M	63	VAL	PRO	engineered mutation	UNP P05362
M	67	ALA	SER	engineered mutation	UNP P05362
M	78	ALA	THR	engineered mutation	UNP P05362
O	1	MET	-	expression tag	UNP P05362
O	2	VAL	THR	engineered mutation	UNP P05362
O	10	THR	ILE	engineered mutation	UNP P05362
O	23	ALA	THR	engineered mutation	UNP P05362
O	38	VAL	PRO	engineered mutation	UNP P05362
O	63	VAL	PRO	engineered mutation	UNP P05362
O	67	ALA	SER	engineered mutation	UNP P05362
O	78	ALA	THR	engineered mutation	UNP P05362
Q	1	MET	-	expression tag	UNP P05362
Q	2	VAL	THR	engineered mutation	UNP P05362
Q	10	THR	ILE	engineered mutation	UNP P05362
Q	23	ALA	THR	engineered mutation	UNP P05362
Q	38	VAL	PRO	engineered mutation	UNP P05362
Q	63	VAL	PRO	engineered mutation	UNP P05362
Q	67	ALA	SER	engineered mutation	UNP P05362
Q	78	ALA	THR	engineered mutation	UNP P05362
S	1	MET	-	expression tag	UNP P05362
S	2	VAL	THR	engineered mutation	UNP P05362
S	10	THR	ILE	engineered mutation	UNP P05362
S	23	ALA	THR	engineered mutation	UNP P05362
S	38	VAL	PRO	engineered mutation	UNP P05362
S	63	VAL	PRO	engineered mutation	UNP P05362
S	67	ALA	SER	engineered mutation	UNP P05362
S	78	ALA	THR	engineered mutation	UNP P05362
U	1	MET	-	expression tag	UNP P05362
U	2	VAL	THR	engineered mutation	UNP P05362
U	10	THR	ILE	engineered mutation	UNP P05362
U	23	ALA	THR	engineered mutation	UNP P05362
U	38	VAL	PRO	engineered mutation	UNP P05362

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Chain	Residue	Modelled	Actual	Comment	Reference
U	63	VAL	PRO	engineered mutation	UNP P05362
U	67	ALA	SER	engineered mutation	UNP P05362
U	78	ALA	THR	engineered mutation	UNP P05362
W	1	MET	-	expression tag	UNP P05362
W	2	VAL	THR	engineered mutation	UNP P05362
W	10	THR	ILE	engineered mutation	UNP P05362
W	23	ALA	THR	engineered mutation	UNP P05362
W	38	VAL	PRO	engineered mutation	UNP P05362
W	63	VAL	PRO	engineered mutation	UNP P05362
W	67	ALA	SER	engineered mutation	UNP P05362
W	78	ALA	THR	engineered mutation	UNP P05362
Y	1	MET	-	expression tag	UNP P05362
Y	2	VAL	THR	engineered mutation	UNP P05362
Y	10	THR	ILE	engineered mutation	UNP P05362
Y	23	ALA	THR	engineered mutation	UNP P05362
Y	38	VAL	PRO	engineered mutation	UNP P05362
Y	63	VAL	PRO	engineered mutation	UNP P05362
Y	67	ALA	SER	engineered mutation	UNP P05362
Y	78	ALA	THR	engineered mutation	UNP P05362
a	1	MET	-	expression tag	UNP P05362
a	2	VAL	THR	engineered mutation	UNP P05362
a	10	THR	ILE	engineered mutation	UNP P05362
a	23	ALA	THR	engineered mutation	UNP P05362
a	38	VAL	PRO	engineered mutation	UNP P05362
a	63	VAL	PRO	engineered mutation	UNP P05362
a	67	ALA	SER	engineered mutation	UNP P05362
a	78	ALA	THR	engineered mutation	UNP P05362

- Molecule 2 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	D	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	F	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	H	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	J	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	L	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	P	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	R	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	T	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	V	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	X	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	Z	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			
2	b	180	Total	C	N	O	S	0	0	0
			1453	940	230	278	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	MET	-	expression tag	UNP P20701
B	189	TRP	ARG	SEE REMARK 999	UNP P20701
B	265	SER	PHE	engineered mutation	UNP P20701
D	128	MET	-	expression tag	UNP P20701
D	189	TRP	ARG	SEE REMARK 999	UNP P20701
D	265	SER	PHE	engineered mutation	UNP P20701
F	128	MET	-	expression tag	UNP P20701
F	189	TRP	ARG	SEE REMARK 999	UNP P20701
F	265	SER	PHE	engineered mutation	UNP P20701
H	128	MET	-	expression tag	UNP P20701
H	189	TRP	ARG	SEE REMARK 999	UNP P20701
H	265	SER	PHE	engineered mutation	UNP P20701
J	128	MET	-	expression tag	UNP P20701
J	189	TRP	ARG	SEE REMARK 999	UNP P20701
J	265	SER	PHE	engineered mutation	UNP P20701
L	128	MET	-	expression tag	UNP P20701
L	189	TRP	ARG	SEE REMARK 999	UNP P20701
L	265	SER	PHE	engineered mutation	UNP P20701
N	128	MET	-	expression tag	UNP P20701
N	189	TRP	ARG	SEE REMARK 999	UNP P20701
N	265	SER	PHE	engineered mutation	UNP P20701
P	128	MET	-	expression tag	UNP P20701
P	189	TRP	ARG	SEE REMARK 999	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
P	265	SER	PHE	engineered mutation	UNP P20701
R	128	MET	-	expression tag	UNP P20701
R	189	TRP	ARG	SEE REMARK 999	UNP P20701
R	265	SER	PHE	engineered mutation	UNP P20701
T	128	MET	-	expression tag	UNP P20701
T	189	TRP	ARG	SEE REMARK 999	UNP P20701
T	265	SER	PHE	engineered mutation	UNP P20701
V	128	MET	-	expression tag	UNP P20701
V	189	TRP	ARG	SEE REMARK 999	UNP P20701
V	265	SER	PHE	engineered mutation	UNP P20701
X	128	MET	-	expression tag	UNP P20701
X	189	TRP	ARG	SEE REMARK 999	UNP P20701
X	265	SER	PHE	engineered mutation	UNP P20701
Z	128	MET	-	expression tag	UNP P20701
Z	189	TRP	ARG	SEE REMARK 999	UNP P20701
Z	265	SER	PHE	engineered mutation	UNP P20701
b	128	MET	-	expression tag	UNP P20701
b	189	TRP	ARG	SEE REMARK 999	UNP P20701
b	265	SER	PHE	engineered mutation	UNP P20701

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0
3	P	1	Total Mg 1 1	0	0
3	R	1	Total Mg 1 1	0	0
3	T	1	Total Mg 1 1	0	0

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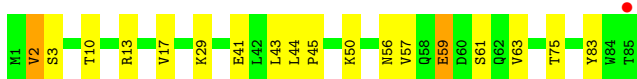
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	1	Total 1	Mg 1	0	0
3	X	1	Total 1	Mg 1	0	0
3	Z	1	Total 1	Mg 1	0	0
3	b	1	Total 1	Mg 1	0	0

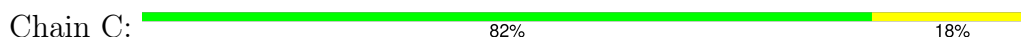
### 3 Residue-property plots [i](#)

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: Intercellular adhesion molecule 1



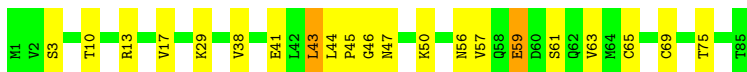
- Molecule 1: Intercellular adhesion molecule 1



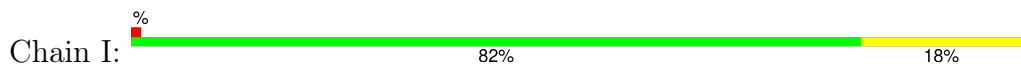
- Molecule 1: Intercellular adhesion molecule 1



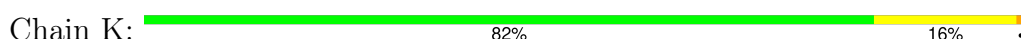
- Molecule 1: Intercellular adhesion molecule 1



- Molecule 1: Intercellular adhesion molecule 1



- Molecule 1: Intercellular adhesion molecule 1







- Molecule 1: Intercellular adhesion molecule 1

Chain a: 82% 18%



- Molecule 2: Integrin alpha-L

Chain B: 92% 8%



- Molecule 2: Integrin alpha-L

Chain D: 92% 8%



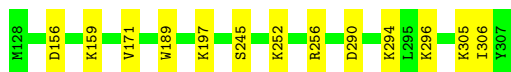
- Molecule 2: Integrin alpha-L

Chain F: 92% 8%



- Molecule 2: Integrin alpha-L

Chain H: 93% 7%



- Molecule 2: Integrin alpha-L

Chain J: 93% 7%



- Molecule 2: Integrin alpha-L

Chain L: 91% 9%



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



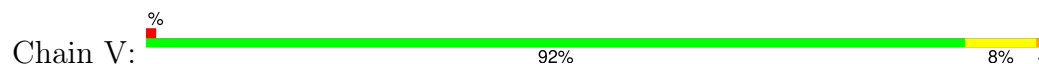
- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L





● Molecule 2: Integrin alpha-L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.04Å 166.33Å 299.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.60 49.54 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.54-3.60) 96.0 (49.54-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.13 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.218 , 0.234 0.210 , 0.227	Depositor DCC
$R_{free}$ test set	2984 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 127.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% 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: MG

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	0.99	1/652 (0.2%)	0.93	1/887 (0.1%)
1	C	0.90	0/652	0.88	0/887
1	E	0.67	0/652	0.78	0/887
1	G	0.92	3/652 (0.5%)	0.84	0/887
1	I	0.71	0/652	0.80	0/887
1	K	0.96	2/652 (0.3%)	0.88	0/887
1	M	0.78	0/652	0.80	0/887
1	O	0.80	0/652	0.83	1/887 (0.1%)
1	Q	0.78	1/652 (0.2%)	0.77	0/887
1	S	0.79	1/652 (0.2%)	0.81	0/887
1	U	0.79	0/652	0.80	0/887
1	W	0.81	0/652	0.85	0/887
1	Y	0.66	0/652	0.76	0/887
1	a	0.71	0/652	0.76	0/887
2	B	0.65	0/1482	0.68	0/1994
2	D	0.58	0/1482	0.66	0/1994
2	F	0.47	0/1482	0.60	0/1994
2	H	0.50	0/1482	0.62	0/1994
2	J	0.50	0/1482	0.62	0/1994
2	L	0.72	0/1482	0.71	0/1994
2	N	0.50	0/1482	0.61	0/1994
2	P	0.50	0/1482	0.61	0/1994
2	R	0.51	0/1482	0.63	0/1994
2	T	0.52	0/1482	0.63	0/1994
2	V	0.59	1/1482 (0.1%)	0.64	0/1994
2	X	0.64	1/1482 (0.1%)	0.67	0/1994
2	Z	0.47	0/1482	0.60	0/1994
2	b	0.43	0/1482	0.59	0/1994
All	All	0.64	10/29876 (0.0%)	0.70	2/40334 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	O	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	65	CYS	CB-SG	-6.37	1.71	1.82
1	A	59	GLU	CG-CD	5.80	1.60	1.51
1	G	65	CYS	CB-SG	-5.78	1.72	1.81
2	X	189	TRP	CB-CG	5.74	1.60	1.50
1	K	59	GLU	CG-CD	5.54	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	VAL	CB-CA-C	-6.26	99.50	111.40
1	O	2	VAL	CB-CA-C	-5.15	101.62	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	LEU	Peptide
1	C	44	LEU	Peptide
1	G	44	LEU	Peptide
1	O	44	LEU	Peptide

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	C	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	E	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
1	G	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	I	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
1	K	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
1	M	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	O	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	Q	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	S	83/85 (98%)	76 (92%)	6 (7%)	1 (1%)	11	43
1	U	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
1	W	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	Y	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	11	43
1	a	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
2	B	178/180 (99%)	155 (87%)	23 (13%)	0	100	100
2	D	178/180 (99%)	157 (88%)	21 (12%)	0	100	100
2	F	178/180 (99%)	160 (90%)	17 (10%)	1 (1%)	22	55
2	H	178/180 (99%)	158 (89%)	20 (11%)	0	100	100
2	J	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
2	L	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	22	55
2	N	178/180 (99%)	161 (90%)	17 (10%)	0	100	100
2	P	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	R	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
2	T	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	V	178/180 (99%)	158 (89%)	20 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	178/180 (99%)	160 (90%)	18 (10%)	0	100	100
2	Z	178/180 (99%)	161 (90%)	17 (10%)	0	100	100
2	b	178/180 (99%)	159 (89%)	19 (11%)	0	100	100
All	All	3654/3710 (98%)	3311 (91%)	327 (9%)	16 (0%)	30	63

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	C	45	PRO
1	E	45	PRO
1	G	45	PRO
1	I	45	PRO

### 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	76/76 (100%)	60 (79%)	16 (21%)	1	6
1	C	76/76 (100%)	63 (83%)	13 (17%)	1	10
1	E	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	G	76/76 (100%)	61 (80%)	15 (20%)	1	7
1	I	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	K	76/76 (100%)	63 (83%)	13 (17%)	1	10
1	M	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	O	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	Q	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	S	76/76 (100%)	62 (82%)	14 (18%)	1	8
1	U	76/76 (100%)	61 (80%)	15 (20%)	1	7
1	W	76/76 (100%)	61 (80%)	15 (20%)	1	7
1	Y	76/76 (100%)	62 (82%)	14 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	76/76 (100%)	62 (82%)	14 (18%)	1	8
2	B	161/161 (100%)	147 (91%)	14 (9%)	8	33
2	D	161/161 (100%)	146 (91%)	15 (9%)	7	31
2	F	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	H	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	J	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	L	161/161 (100%)	146 (91%)	15 (9%)	7	31
2	N	161/161 (100%)	147 (91%)	14 (9%)	8	33
2	P	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	R	161/161 (100%)	146 (91%)	15 (9%)	7	31
2	T	161/161 (100%)	147 (91%)	14 (9%)	8	33
2	V	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	X	161/161 (100%)	147 (91%)	14 (9%)	8	33
2	Z	161/161 (100%)	148 (92%)	13 (8%)	9	35
2	b	161/161 (100%)	148 (92%)	13 (8%)	9	35
All	All	3318/3318 (100%)	2927 (88%)	391 (12%)	4	22

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	56	ASN
1	U	43	LEU
2	R	159	LYS
1	S	56	ASN
2	V	245	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	172	GLN
2	X	275	HIS
1	a	58	GLN
2	J	213	ASN
2	J	172	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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	85/85 (100%)	-0.75	1 (1%) 76 55	69, 88, 125, 143	0
1	C	85/85 (100%)	-0.70	0 100 100	71, 94, 134, 166	0
1	E	85/85 (100%)	-0.48	0 100 100	110, 139, 193, 230	0
1	G	85/85 (100%)	-0.65	0 100 100	79, 108, 166, 194	0
1	I	85/85 (100%)	-0.38	1 (1%) 76 55	96, 141, 228, 320	0
1	K	85/85 (100%)	-0.65	0 100 100	77, 100, 142, 171	0
1	M	85/85 (100%)	-0.65	1 (1%) 76 55	96, 116, 149, 163	0
1	O	85/85 (100%)	-0.65	1 (1%) 76 55	78, 109, 160, 182	0
1	Q	85/85 (100%)	-0.63	1 (1%) 76 55	90, 112, 161, 190	0
1	S	85/85 (100%)	-0.67	0 100 100	91, 109, 141, 168	0
1	U	85/85 (100%)	-0.65	1 (1%) 76 55	87, 106, 141, 166	0
1	W	85/85 (100%)	-0.64	1 (1%) 76 55	85, 104, 139, 169	0
1	Y	85/85 (100%)	-0.71	0 100 100	95, 122, 182, 209	0
1	a	85/85 (100%)	-0.60	0 100 100	99, 132, 216, 231	0
2	B	180/180 (100%)	-0.75	0 100 100	69, 124, 207, 256	0
2	D	180/180 (100%)	-0.73	0 100 100	78, 146, 229, 289	0
2	F	180/180 (100%)	-0.56	0 100 100	129, 220, 367, 441	0
2	H	180/180 (100%)	-0.72	0 100 100	108, 189, 288, 366	0
2	J	180/180 (100%)	-0.64	0 100 100	97, 182, 314, 409	0
2	L	180/180 (100%)	-0.66	1 (0%) 85 69	72, 115, 189, 225	0
2	N	180/180 (100%)	-0.75	0 100 100	111, 172, 255, 306	0
2	P	180/180 (100%)	-0.78	0 100 100	116, 190, 295, 377	0
2	R	180/180 (100%)	-0.69	0 100 100	104, 187, 297, 390	0
2	T	180/180 (100%)	-0.66	0 100 100	96, 170, 266, 336	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	V	180/180 (100%)	-0.64	1 (0%) 85 69	94, 150, 238, 293	0
2	X	180/180 (100%)	-0.71	0 100 100	85, 126, 195, 239	0
2	Z	180/180 (100%)	-0.73	0 100 100	122, 211, 329, 418	0
2	b	180/180 (100%)	-0.69	0 100 100	137, 258, 398, 507	0
All	All	3710/3710 (100%)	-0.67	9 (0%) 92 84	69, 146, 294, 507	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	85	THR	3.3
2	V	189	TRP	3.3
1	I	6	PRO	3.2
1	A	85	THR	2.6
1	Q	85	THR	2.5

## 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
3	MG	b	901	1/1	0.95	0.12	131,131,131,131	0
3	MG	R	901	1/1	0.96	0.12	88,88,88,88	0
3	MG	L	901	1/1	0.96	0.13	52,52,52,52	0
3	MG	T	901	1/1	0.97	0.08	84,84,84,84	0
3	MG	F	901	1/1	0.97	0.11	118,118,118,118	0
3	MG	V	901	1/1	0.98	0.09	77,77,77,77	0
3	MG	X	901	1/1	0.98	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	H	901	1/1	0.98	0.12	88,88,88,88	0
3	MG	D	901	1/1	0.99	0.07	62,62,62,62	0
3	MG	J	901	1/1	0.99	0.03	88,88,88,88	0
3	MG	B	901	1/1	0.99	0.09	51,51,51,51	0
3	MG	N	901	1/1	0.99	0.09	94,94,94,94	0
3	MG	Z	901	1/1	0.99	0.12	104,104,104,104	0
3	MG	P	901	1/1	0.99	0.13	97,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.