



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 02:19 PM BST

PDB ID : 3TCX  
Title : Structure of Engineered Single Domain ICAM-1 D1 with High-Affinity aL 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 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.

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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) : 1.13  
EDS : 2.13  
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) : 2.13

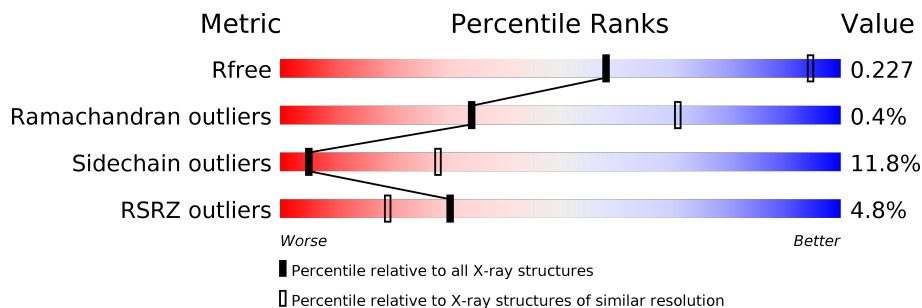
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 on 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	79% 19%
1	C	85	82% 18%
1	E	85	4% 82% 18%
1	G	85	75% 22%
1	I	85	82% 18%
1	K	85	82% 16%
1	M	85	82% 18%

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Mol	Chain	Length	Quality of chain
1	O	85	80% 20%
1	Q	85	81% 19%
1	S	85	82% 16%
1	U	85	81% 19%
1	W	85	81% 19%
1	Y	85	82% 18%
1	a	85	2% 82% 18%
2	B	180	1% 92% 8%
2	D	180	3% 92% 8%
2	F	180	7% 92% 8%
2	H	180	8% 93% 7%
2	J	180	5% 93% 7%
2	L	180	2% 91% 9%
2	N	180	8% 92% 8%
2	P	180	8% 93% 7%
2	R	180	8% 92% 8%
2	T	180	5% 92% 8%
2	V	180	5% 92% 8%
2	X	180	92% 7%
2	Z	180	15% 93% 7%
2	b	180	22% 93% 7%

## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	85	641	404	106	125	6	0	0	0
1	C	85	641	404	106	125	6	0	0	0
1	E	85	641	404	106	125	6	0	0	0
1	G	85	641	404	106	125	6	0	0	0
1	I	85	641	404	106	125	6	0	0	0
1	K	85	641	404	106	125	6	0	0	0
1	M	85	641	404	106	125	6	0	0	0
1	O	85	641	404	106	125	6	0	0	0
1	Q	85	641	404	106	125	6	0	0	0
1	S	85	641	404	106	125	6	0	0	0
1	U	85	641	404	106	125	6	0	0	0
1	W	85	641	404	106	125	6	0	0	0
1	Y	85	641	404	106	125	6	0	0	0
1	a	85	641	404	106	125	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
			Total	C	N	O	S			
2	N	180	1453	940	230	278	5	0	0	0
2	P	180	1453	940	230	278	5	0	0	0
2	R	180	1453	940	230	278	5	0	0	0
2	T	180	1453	940	230	278	5	0	0	0
2	V	180	1453	940	230	278	5	0	0	0
2	X	180	1453	940	230	278	5	0	0	0
2	Z	180	1453	940	230	278	5	0	0	0
2	b	180	1453	940	230	278	5	0	0	0

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	P	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0
3	Z	1	Total Mg 1 1	0	0
3	T	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0
3	X	1	Total Mg 1 1	0	0

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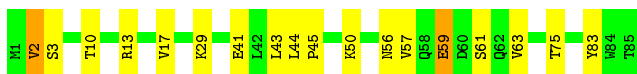
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	R	1	Total 1	Mg 1	0	0
3	L	1	Total 1	Mg 1	0	0
3	b	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

### 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

Chain A:  79% 19%




- Molecule 1: Intercellular adhesion molecule 1

Chain C:  82% 18%



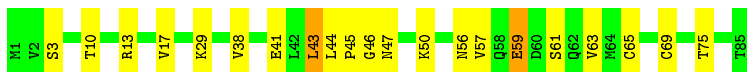
- Molecule 1: Intercellular adhesion molecule 1

Chain E:  4% 82% 18%




- Molecule 1: Intercellular adhesion molecule 1

Chain G:  75% 22%




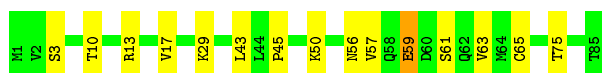
- Molecule 1: Intercellular adhesion molecule 1

Chain I:  82% 18%

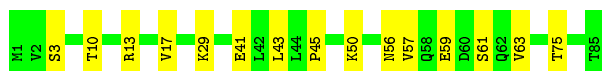
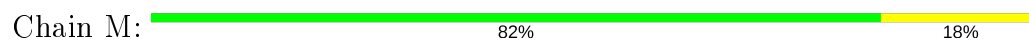


- Molecule 1: Intercellular adhesion molecule 1

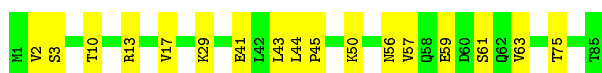
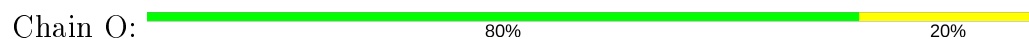
Chain K:  82% 16%



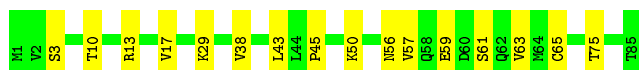
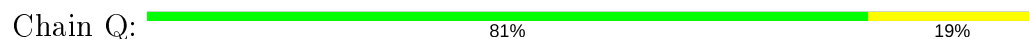
- Molecule 1: Intercellular adhesion molecule 1



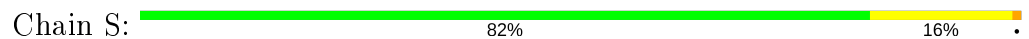
- Molecule 1: Intercellular adhesion molecule 1



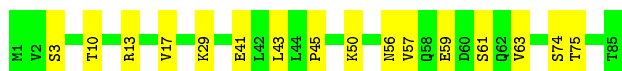
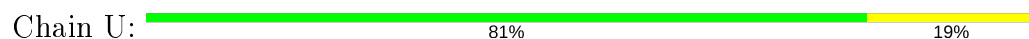
- Molecule 1: Intercellular adhesion molecule 1



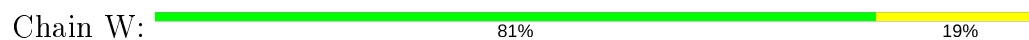
- Molecule 1: Intercellular adhesion molecule 1



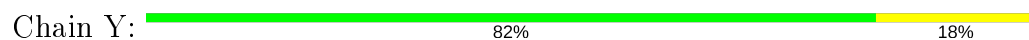
- Molecule 1: Intercellular adhesion molecule 1



- Molecule 1: Intercellular adhesion molecule 1

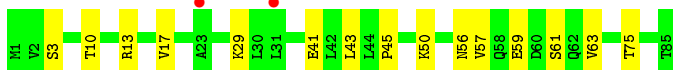
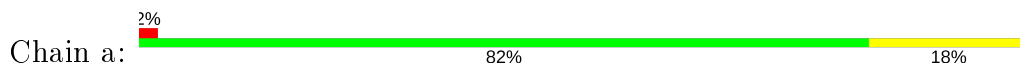


- Molecule 1: Intercellular adhesion molecule 1





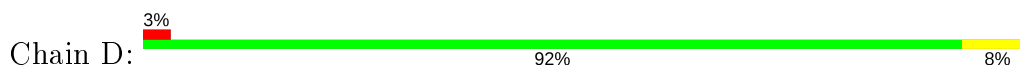
- Molecule 1: Intercellular adhesion molecule 1



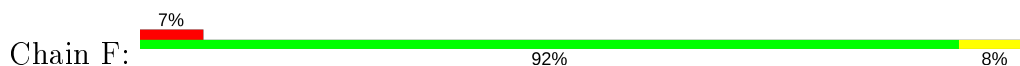
- Molecule 2: Integrin alpha-L



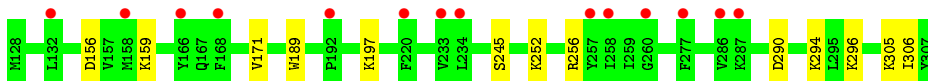
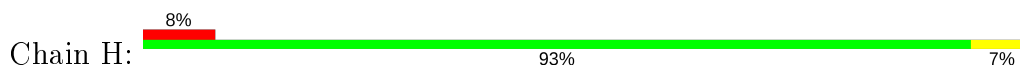
- Molecule 2: Integrin alpha-L



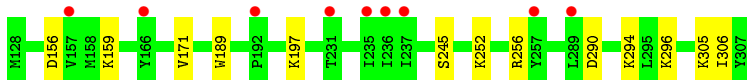
- Molecule 2: Integrin alpha-L



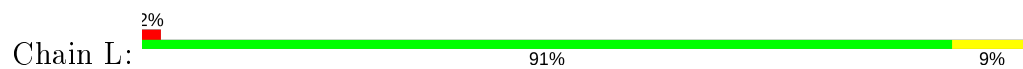
- Molecule 2: Integrin alpha-L



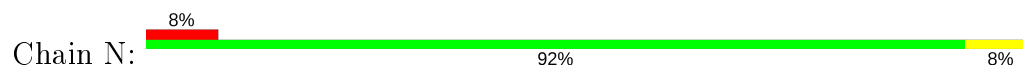
- Molecule 2: Integrin alpha-L



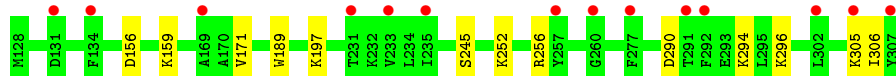
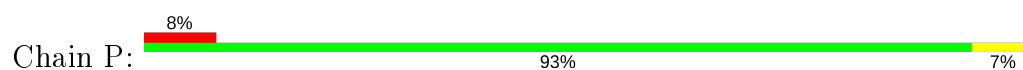
- Molecule 2: Integrin alpha-L



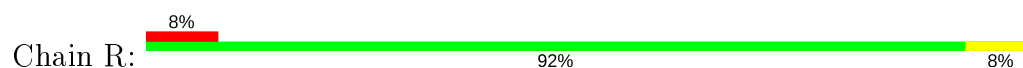
- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



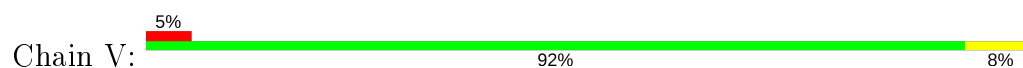
- Molecule 2: Integrin alpha-L



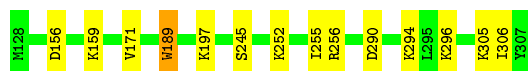
- Molecule 2: Integrin alpha-L



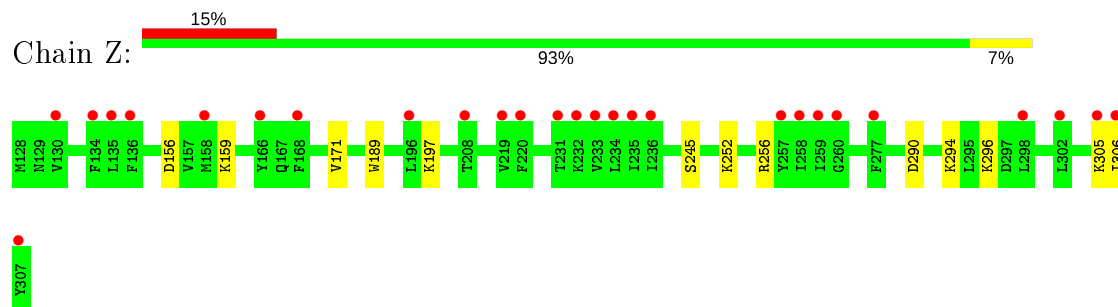
- Molecule 2: Integrin alpha-L



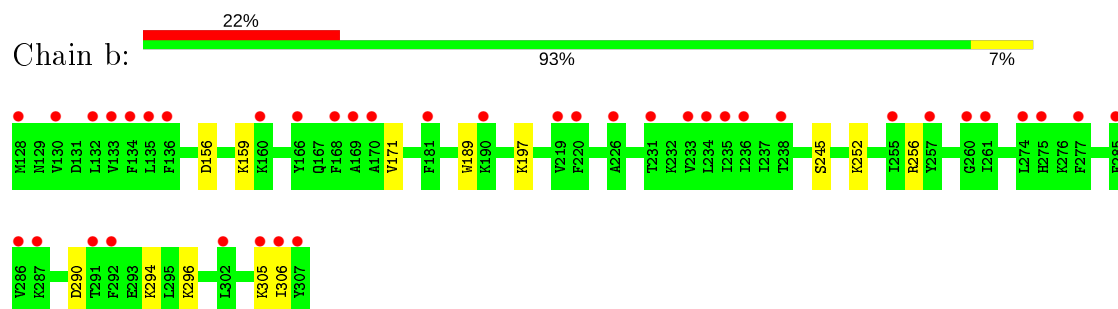
- Molecule 2: Integrin alpha-L



- 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) 95.9 (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)	Xtrriage
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 (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.2	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 105.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	165.0	wwPDB-VP

Xtrriage'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

All (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
1	S	59	GLU	CG-CD	5.52	1.60	1.51
1	Q	65	CYS	CB-SG	-5.42	1.73	1.81
1	G	69	CYS	CB-SG	-5.29	1.73	1.81
1	G	59	GLU	CG-CD	5.29	1.59	1.51
2	V	189	TRP	CB-CG	5.21	1.59	1.50

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 [i](#)

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%)	13	51
1	C	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	E	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	51
1	G	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	I	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	51
1	K	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	51
1	M	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	O	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	Q	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	S	83/85 (98%)	76 (92%)	6 (7%)	1 (1%)	13	51
1	U	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	51
1	W	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	Y	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	51
1	a	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	51
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%)	25	64
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%)	25	64
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%)	34	71

All (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
1	K	45	PRO
1	M	45	PRO
1	O	45	PRO
1	Q	45	PRO
1	S	45	PRO
1	U	45	PRO
1	W	45	PRO
1	Y	45	PRO
1	a	45	PRO
2	L	205	LEU
2	F	205	LEU

### 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	76/76 (100%)	60 (79%)	16 (21%)	1	7
1	C	76/76 (100%)	63 (83%)	13 (17%)	2	13
1	E	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	G	76/76 (100%)	61 (80%)	15 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	K	76/76 (100%)	63 (83%)	13 (17%)	2	13
1	M	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	O	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	Q	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	S	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	U	76/76 (100%)	61 (80%)	15 (20%)	1	8
1	W	76/76 (100%)	61 (80%)	15 (20%)	1	8
1	Y	76/76 (100%)	62 (82%)	14 (18%)	1	10
1	a	76/76 (100%)	62 (82%)	14 (18%)	1	10
2	B	161/161 (100%)	147 (91%)	14 (9%)	10	41
2	D	161/161 (100%)	146 (91%)	15 (9%)	9	38
2	F	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	H	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	J	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	L	161/161 (100%)	146 (91%)	15 (9%)	9	38
2	N	161/161 (100%)	147 (91%)	14 (9%)	10	41
2	P	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	R	161/161 (100%)	146 (91%)	15 (9%)	9	38
2	T	161/161 (100%)	147 (91%)	14 (9%)	10	41
2	V	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	X	161/161 (100%)	147 (91%)	14 (9%)	10	41
2	Z	161/161 (100%)	148 (92%)	13 (8%)	11	43
2	b	161/161 (100%)	148 (92%)	13 (8%)	11	43
All	All	3318/3318 (100%)	2927 (88%)	391 (12%)	5	28

All (391) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	SER
1	A	10	THR
1	A	13	ARG
1	A	17	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	29	LYS
1	A	41	GLU
1	A	43	LEU
1	A	50	LYS
1	A	56	ASN
1	A	57	VAL
1	A	59	GLU
1	A	61	SER
1	A	63	VAL
1	A	75	THR
1	A	83	TYR
2	B	156	ASP
2	B	159	LYS
2	B	171	VAL
2	B	189	TRP
2	B	197	LYS
2	B	245	SER
2	B	252	LYS
2	B	255	ILE
2	B	256	ARG
2	B	290	ASP
2	B	294	LYS
2	B	296	LYS
2	B	305	LYS
2	B	306	ILE
1	C	3	SER
1	C	10	THR
1	C	13	ARG
1	C	17	VAL
1	C	29	LYS
1	C	43	LEU
1	C	50	LYS
1	C	56	ASN
1	C	57	VAL
1	C	59	GLU
1	C	61	SER
1	C	63	VAL
1	C	75	THR
2	D	156	ASP
2	D	159	LYS
2	D	171	VAL
2	D	176	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	189	TRP
2	D	197	LYS
2	D	212	ILE
2	D	245	SER
2	D	252	LYS
2	D	256	ARG
2	D	290	ASP
2	D	294	LYS
2	D	296	LYS
2	D	305	LYS
2	D	306	ILE
1	E	3	SER
1	E	10	THR
1	E	13	ARG
1	E	17	VAL
1	E	29	LYS
1	E	41	GLU
1	E	43	LEU
1	E	50	LYS
1	E	56	ASN
1	E	57	VAL
1	E	59	GLU
1	E	61	SER
1	E	63	VAL
1	E	75	THR
2	F	156	ASP
2	F	159	LYS
2	F	171	VAL
2	F	189	TRP
2	F	197	LYS
2	F	245	SER
2	F	252	LYS
2	F	256	ARG
2	F	290	ASP
2	F	294	LYS
2	F	296	LYS
2	F	305	LYS
2	F	306	ILE
1	G	3	SER
1	G	10	THR
1	G	13	ARG
1	G	17	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	29	LYS
1	G	38	VAL
1	G	41	GLU
1	G	43	LEU
1	G	50	LYS
1	G	56	ASN
1	G	57	VAL
1	G	59	GLU
1	G	61	SER
1	G	63	VAL
1	G	75	THR
2	H	156	ASP
2	H	159	LYS
2	H	171	VAL
2	H	189	TRP
2	H	197	LYS
2	H	245	SER
2	H	252	LYS
2	H	256	ARG
2	H	290	ASP
2	H	294	LYS
2	H	296	LYS
2	H	305	LYS
2	H	306	ILE
1	I	3	SER
1	I	10	THR
1	I	13	ARG
1	I	17	VAL
1	I	29	LYS
1	I	41	GLU
1	I	43	LEU
1	I	50	LYS
1	I	56	ASN
1	I	57	VAL
1	I	59	GLU
1	I	61	SER
1	I	63	VAL
1	I	75	THR
2	J	156	ASP
2	J	159	LYS
2	J	171	VAL
2	J	189	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	197	LYS
2	J	245	SER
2	J	252	LYS
2	J	256	ARG
2	J	290	ASP
2	J	294	LYS
2	J	296	LYS
2	J	305	LYS
2	J	306	ILE
1	K	3	SER
1	K	10	THR
1	K	13	ARG
1	K	17	VAL
1	K	29	LYS
1	K	43	LEU
1	K	50	LYS
1	K	56	ASN
1	K	57	VAL
1	K	59	GLU
1	K	61	SER
1	K	63	VAL
1	K	75	THR
2	L	156	ASP
2	L	159	LYS
2	L	171	VAL
2	L	189	TRP
2	L	197	LYS
2	L	212	ILE
2	L	245	SER
2	L	252	LYS
2	L	255	ILE
2	L	256	ARG
2	L	290	ASP
2	L	294	LYS
2	L	296	LYS
2	L	305	LYS
2	L	306	ILE
1	M	3	SER
1	M	10	THR
1	M	13	ARG
1	M	17	VAL
1	M	29	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	41	GLU
1	M	43	LEU
1	M	50	LYS
1	M	56	ASN
1	M	57	VAL
1	M	59	GLU
1	M	61	SER
1	M	63	VAL
1	M	75	THR
2	N	156	ASP
2	N	159	LYS
2	N	171	VAL
2	N	189	TRP
2	N	197	LYS
2	N	212	ILE
2	N	245	SER
2	N	252	LYS
2	N	256	ARG
2	N	290	ASP
2	N	294	LYS
2	N	296	LYS
2	N	305	LYS
2	N	306	ILE
1	O	3	SER
1	O	10	THR
1	O	13	ARG
1	O	17	VAL
1	O	29	LYS
1	O	41	GLU
1	O	43	LEU
1	O	50	LYS
1	O	56	ASN
1	O	57	VAL
1	O	59	GLU
1	O	61	SER
1	O	63	VAL
1	O	75	THR
2	P	156	ASP
2	P	159	LYS
2	P	171	VAL
2	P	189	TRP
2	P	197	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	245	SER
2	P	252	LYS
2	P	256	ARG
2	P	290	ASP
2	P	294	LYS
2	P	296	LYS
2	P	305	LYS
2	P	306	ILE
1	Q	3	SER
1	Q	10	THR
1	Q	13	ARG
1	Q	17	VAL
1	Q	29	LYS
1	Q	38	VAL
1	Q	43	LEU
1	Q	50	LYS
1	Q	56	ASN
1	Q	57	VAL
1	Q	59	GLU
1	Q	61	SER
1	Q	63	VAL
1	Q	75	THR
2	R	156	ASP
2	R	159	LYS
2	R	165	SER
2	R	171	VAL
2	R	189	TRP
2	R	197	LYS
2	R	212	ILE
2	R	245	SER
2	R	252	LYS
2	R	256	ARG
2	R	290	ASP
2	R	294	LYS
2	R	296	LYS
2	R	305	LYS
2	R	306	ILE
1	S	3	SER
1	S	10	THR
1	S	13	ARG
1	S	17	VAL
1	S	29	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	S	41	GLU
1	S	43	LEU
1	S	50	LYS
1	S	56	ASN
1	S	57	VAL
1	S	59	GLU
1	S	61	SER
1	S	63	VAL
1	S	75	THR
2	T	156	ASP
2	T	159	LYS
2	T	171	VAL
2	T	189	TRP
2	T	197	LYS
2	T	212	ILE
2	T	245	SER
2	T	252	LYS
2	T	256	ARG
2	T	290	ASP
2	T	294	LYS
2	T	296	LYS
2	T	305	LYS
2	T	306	ILE
1	U	3	SER
1	U	10	THR
1	U	13	ARG
1	U	17	VAL
1	U	29	LYS
1	U	41	GLU
1	U	43	LEU
1	U	50	LYS
1	U	56	ASN
1	U	57	VAL
1	U	59	GLU
1	U	61	SER
1	U	63	VAL
1	U	74	SER
1	U	75	THR
2	V	156	ASP
2	V	159	LYS
2	V	171	VAL
2	V	189	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	V	197	LYS
2	V	245	SER
2	V	252	LYS
2	V	256	ARG
2	V	290	ASP
2	V	294	LYS
2	V	296	LYS
2	V	305	LYS
2	V	306	ILE
1	W	3	SER
1	W	10	THR
1	W	13	ARG
1	W	17	VAL
1	W	29	LYS
1	W	30	LEU
1	W	41	GLU
1	W	43	LEU
1	W	50	LYS
1	W	56	ASN
1	W	57	VAL
1	W	59	GLU
1	W	61	SER
1	W	63	VAL
1	W	75	THR
2	X	156	ASP
2	X	159	LYS
2	X	171	VAL
2	X	189	TRP
2	X	197	LYS
2	X	245	SER
2	X	252	LYS
2	X	255	ILE
2	X	256	ARG
2	X	290	ASP
2	X	294	LYS
2	X	296	LYS
2	X	305	LYS
2	X	306	ILE
1	Y	3	SER
1	Y	10	THR
1	Y	13	ARG
1	Y	17	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	29	LYS
1	Y	41	GLU
1	Y	43	LEU
1	Y	50	LYS
1	Y	56	ASN
1	Y	57	VAL
1	Y	59	GLU
1	Y	61	SER
1	Y	63	VAL
1	Y	75	THR
2	Z	156	ASP
2	Z	159	LYS
2	Z	171	VAL
2	Z	189	TRP
2	Z	197	LYS
2	Z	245	SER
2	Z	252	LYS
2	Z	256	ARG
2	Z	290	ASP
2	Z	294	LYS
2	Z	296	LYS
2	Z	305	LYS
2	Z	306	ILE
1	a	3	SER
1	a	10	THR
1	a	13	ARG
1	a	17	VAL
1	a	29	LYS
1	a	41	GLU
1	a	43	LEU
1	a	50	LYS
1	a	56	ASN
1	a	57	VAL
1	a	59	GLU
1	a	61	SER
1	a	63	VAL
1	a	75	THR
2	b	156	ASP
2	b	159	LYS
2	b	171	VAL
2	b	189	TRP
2	b	197	LYS

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Mol	Chain	Res	Type
2	b	245	SER
2	b	252	LYS
2	b	256	ARG
2	b	290	ASP
2	b	294	LYS
2	b	296	LYS
2	b	305	LYS
2	b	306	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
2	B	167	GLN
2	B	172	GLN
2	B	213	ASN
2	B	275	HIS
1	C	47	ASN
1	C	56	ASN
2	D	167	GLN
2	D	172	GLN
2	D	275	HIS
1	E	58	GLN
2	F	167	GLN
2	F	172	GLN
2	F	213	ASN
2	F	275	HIS
1	G	47	ASN
1	G	56	ASN
2	H	167	GLN
2	H	172	GLN
2	H	275	HIS
1	I	47	ASN
1	I	56	ASN
2	J	167	GLN
2	J	172	GLN
2	J	213	ASN
2	J	275	HIS
1	K	56	ASN
2	L	167	GLN
2	L	172	GLN
2	L	275	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	47	ASN
1	M	58	GLN
2	N	167	GLN
2	N	172	GLN
2	N	275	HIS
1	O	56	ASN
2	P	167	GLN
2	P	172	GLN
2	P	213	ASN
2	P	275	HIS
1	Q	56	ASN
2	R	167	GLN
2	R	172	GLN
2	R	275	HIS
1	S	47	ASN
1	S	56	ASN
2	T	167	GLN
2	T	172	GLN
2	T	213	ASN
2	T	275	HIS
1	U	56	ASN
2	V	167	GLN
2	V	172	GLN
2	V	213	ASN
2	V	275	HIS
1	W	56	ASN
2	X	167	GLN
2	X	172	GLN
2	X	213	ASN
2	X	275	HIS
1	Y	56	ASN
2	Z	167	GLN
2	Z	172	GLN
2	Z	275	HIS
1	a	47	ASN
1	a	58	GLN
2	b	167	GLN
2	b	172	GLN
2	b	275	HIS



### 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 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 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, 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%)	-0.18	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	69, 88, 125, 143	0
1	C	85/85 (100%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	71, 94, 134, 166	0
1	E	85/85 (100%)	0.03	3 (3%) <span style="border: 1px solid red; padding: 2px;">44</span> <span style="border: 1px solid red; padding: 2px;">29</span>	110, 139, 193, 230	0
1	G	85/85 (100%)	-0.16	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	79, 108, 166, 194	0
1	I	85/85 (100%)	0.01	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">66</span>	96, 141, 228, 320	0
1	K	85/85 (100%)	-0.29	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	77, 100, 142, 171	0
1	M	85/85 (100%)	-0.22	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	96, 116, 149, 163	0
1	O	85/85 (100%)	-0.20	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	78, 109, 160, 182	0
1	Q	85/85 (100%)	-0.20	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	90, 112, 161, 190	0
1	S	85/85 (100%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	91, 109, 141, 168	0
1	U	85/85 (100%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	87, 106, 141, 166	0
1	W	85/85 (100%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	85, 104, 139, 169	0
1	Y	85/85 (100%)	-0.13	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	95, 122, 182, 209	0
1	a	85/85 (100%)	-0.06	2 (2%) <span style="border: 1px solid red; padding: 2px;">59</span> <span style="border: 1px solid red; padding: 2px;">42</span>	99, 132, 216, 231	0
2	B	180/180 (100%)	-0.09	2 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">68</span>	69, 124, 207, 256	0
2	D	180/180 (100%)	-0.03	6 (3%) <span style="border: 1px solid red; padding: 2px;">46</span> <span style="border: 1px solid red; padding: 2px;">31</span>	78, 146, 229, 289	0
2	F	180/180 (100%)	0.29	13 (7%) <span style="border: 1px solid red; padding: 2px;">15</span> <span style="border: 1px solid red; padding: 2px;">9</span>	129, 220, 367, 441	0
2	H	180/180 (100%)	0.29	14 (7%) <span style="border: 1px solid red; padding: 2px;">13</span> <span style="border: 1px solid red; padding: 2px;">8</span>	108, 189, 288, 366	0
2	J	180/180 (100%)	0.19	9 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">18</span>	97, 182, 314, 409	0
2	L	180/180 (100%)	-0.07	3 (1%) <span style="border: 1px solid blue; padding: 2px;">70</span> <span style="border: 1px solid blue; padding: 2px;">55</span>	72, 115, 189, 225	0
2	N	180/180 (100%)	0.40	14 (7%) <span style="border: 1px solid red; padding: 2px;">13</span> <span style="border: 1px solid red; padding: 2px;">8</span>	111, 172, 255, 306	0
2	P	180/180 (100%)	0.35	14 (7%) <span style="border: 1px solid red; padding: 2px;">13</span> <span style="border: 1px solid red; padding: 2px;">8</span>	116, 190, 295, 377	0
2	R	180/180 (100%)	0.41	14 (7%) <span style="border: 1px solid red; padding: 2px;">13</span> <span style="border: 1px solid red; padding: 2px;">8</span>	104, 187, 297, 390	0
2	T	180/180 (100%)	0.05	9 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">18</span>	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%)	0.15	9 (5%) 28 18	94, 150, 238, 293	0
2	X	180/180 (100%)	-0.11	0 100 100	85, 126, 195, 239	0
2	Z	180/180 (100%)	0.61	27 (15%) 2 1	122, 211, 329, 418	0
2	b	180/180 (100%)	0.86	39 (21%) 0 0	137, 258, 398, 507	0
All	All	3710/3710 (100%)	0.11	179 (4%) 30 19	69, 146, 294, 507	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	307	TYR	10.9
2	N	307	TYR	7.3
2	Z	220	PHE	6.9
2	T	306	ILE	6.0
2	T	307	TYR	6.0
2	F	289	LEU	5.8
2	b	307	TYR	5.6
2	b	260	GLY	5.2
2	b	305	LYS	5.1
2	b	292	PHE	5.0
2	b	257	TYR	4.9
2	F	305	LYS	4.8
1	I	85	THR	4.8
2	Z	257	TYR	4.7
2	b	277	PHE	4.6
2	Z	166	TYR	4.5
2	Z	259	ILE	4.4
2	b	231	THR	4.3
2	H	257	TYR	4.3
2	b	275	HIS	4.3
2	V	305	LYS	4.3
2	Z	307	TYR	4.3
2	Z	158	MET	4.2
2	Z	134	PHE	4.2
2	R	260	GLY	4.2
2	J	257	TYR	4.2
2	Z	235	ILE	3.9
2	b	190	LYS	3.9
2	H	220	PHE	3.8
2	b	168	PHE	3.8
2	Z	260	GLY	3.7
2	F	166	TYR	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Z	302	LEU	3.6
2	b	160	LYS	3.6
2	b	306	ILE	3.6
2	N	261	ILE	3.5
2	R	166	TYR	3.5
2	F	231	THR	3.5
2	b	166	TYR	3.5
2	b	220	PHE	3.4
2	b	234	LEU	3.4
2	H	258	ILE	3.4
2	J	231	THR	3.4
2	F	134	PHE	3.3
1	E	85	THR	3.3
2	b	291	THR	3.3
2	V	291	THR	3.3
2	H	233	VAL	3.3
2	H	260	GLY	3.3
2	Z	135	LEU	3.3
2	T	297	ASP	3.3
2	H	166	TYR	3.2
2	Z	231	THR	3.2
2	V	168	PHE	3.2
2	R	291	THR	3.2
2	b	235	ILE	3.2
2	V	289	LEU	3.2
2	b	236	ILE	3.2
2	P	307	TYR	3.2
2	b	302	LEU	3.2
2	V	292	PHE	3.1
2	L	289	LEU	3.1
2	N	237	ILE	3.1
2	H	168	PHE	3.1
2	Z	232	LYS	3.1
2	P	131	ASP	3.1
2	Z	168	PHE	3.1
2	N	233	VAL	3.1
2	b	286	VAL	3.0
2	b	219	VAL	3.0
2	F	306	ILE	3.0
2	J	289	LEU	3.0
2	N	260	GLY	3.0
2	b	134	PHE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	P	291	THR	3.0
2	Z	234	LEU	3.0
2	P	292	PHE	3.0
2	R	306	ILE	3.0
2	b	128	MET	2.9
2	b	135	LEU	2.9
2	V	257	TYR	2.9
2	R	168	PHE	2.9
2	P	235	ILE	2.8
2	b	287	LYS	2.8
2	b	233	VAL	2.8
1	a	23	ALA	2.8
2	H	234	LEU	2.8
2	N	257	TYR	2.7
2	N	134	PHE	2.7
2	Z	130	VAL	2.7
2	H	286	VAL	2.7
2	J	192	PRO	2.7
2	F	257	TYR	2.7
2	B	305	LYS	2.7
2	R	305	LYS	2.7
2	Z	298	LEU	2.7
2	N	259	ILE	2.6
2	R	130	VAL	2.6
2	H	277	PHE	2.6
2	T	220	PHE	2.6
2	P	277	PHE	2.6
2	P	169	ALA	2.6
2	T	289	LEU	2.6
2	R	227	ARG	2.6
2	P	233	VAL	2.6
2	Z	305	LYS	2.6
2	V	134	PHE	2.5
2	b	169	ALA	2.5
2	Z	277	PHE	2.5
2	R	189	TRP	2.5
2	F	170	ALA	2.5
2	H	192	PRO	2.4
2	P	134	PHE	2.4
2	N	131	ASP	2.4
2	T	168	PHE	2.4
2	Z	219	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	N	294	LYS	2.4
2	N	288	ILE	2.4
2	b	261	ILE	2.4
2	H	132	LEU	2.4
2	F	237	ILE	2.3
2	b	255	ILE	2.3
2	b	133	VAL	2.3
2	b	285	PHE	2.3
2	N	302	LEU	2.3
2	P	302	LEU	2.3
2	N	282	ALA	2.3
2	F	277	PHE	2.3
2	J	235	ILE	2.3
2	b	238	THR	2.3
2	J	237	ILE	2.3
2	Z	258	ILE	2.3
2	Z	233	VAL	2.3
2	b	132	LEU	2.3
2	P	260	GLY	2.3
2	b	136	PHE	2.3
2	J	157	VAL	2.3
2	R	295	LEU	2.2
2	V	298	LEU	2.2
2	b	130	VAL	2.2
2	P	231	THR	2.2
2	Z	136	PHE	2.2
2	D	233	VAL	2.2
2	N	298	LEU	2.2
2	B	307	TYR	2.2
2	P	257	TYR	2.2
2	D	307	TYR	2.2
2	R	277	PHE	2.2
2	H	158	MET	2.2
2	F	292	PHE	2.2
2	b	170	ALA	2.2
2	L	257	TYR	2.1
2	L	290	ASP	2.1
2	Z	236	ILE	2.1
1	a	31	LEU	2.1
2	R	132	LEU	2.1
2	F	298	LEU	2.1
2	T	135	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	T	303	GLN	2.1
2	D	164	THR	2.1
1	E	18	LEU	2.1
2	b	181	PHE	2.1
2	H	287	LYS	2.1
2	D	294	LYS	2.1
2	Z	208	THR	2.1
2	D	257	TYR	2.1
2	P	305	LYS	2.0
2	Z	306	ILE	2.0
2	F	286	VAL	2.0
2	V	294	LYS	2.0
2	b	226	ALA	2.0
2	J	166	TYR	2.0
2	D	168	PHE	2.0
2	Z	196	LEU	2.0
2	J	236	ILE	2.0
1	E	17	VAL	2.0
2	R	292	PHE	2.0
2	T	166	TYR	2.0
2	b	274	LEU	2.0

## 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	F	901	1/1	0.93	0.19	118,118,118,118	0
3	MG	b	901	1/1	0.94	0.20	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	V	901	1/1	0.98	0.11	77,77,77,77	0
3	MG	T	901	1/1	0.98	0.14	84,84,84,84	0
3	MG	X	901	1/1	0.98	0.17	65,65,65,65	0
3	MG	H	901	1/1	0.99	0.20	88,88,88,88	0
3	MG	L	901	1/1	0.99	0.24	52,52,52,52	0
3	MG	J	901	1/1	0.99	0.11	88,88,88,88	0
3	MG	P	901	1/1	0.99	0.20	97,97,97,97	0
3	MG	D	901	1/1	0.99	0.17	62,62,62,62	0
3	MG	N	901	1/1	0.99	0.16	94,94,94,94	0
3	MG	R	901	1/1	0.99	0.18	88,88,88,88	0
3	MG	Z	901	1/1	1.00	0.24	104,104,104,104	0
3	MG	B	901	1/1	1.00	0.17	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.