



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:59 pm BST

PDB ID : 4HTT  
Title : Crystal Structure of Twin Arginine Translocase Receptor- TatC in DDM  
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Deposited on : 2012-11-01  
Resolution : 6.80 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	:	2.11
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)	:	2.11

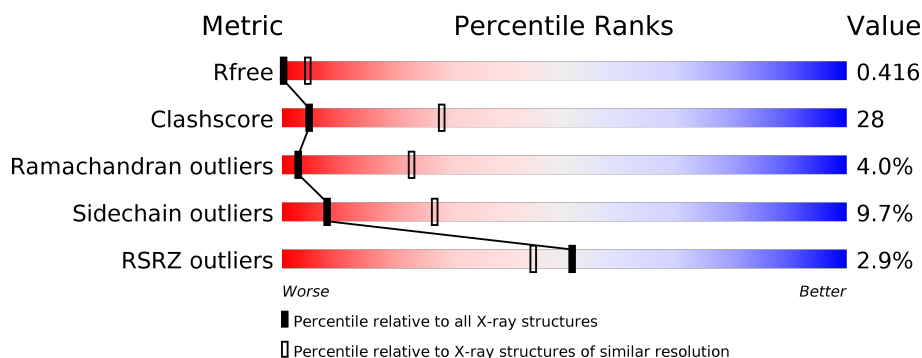
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.80 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	1003 (9.70-3.90)
Clashscore	141614	1067 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	418	<div> <div>2%</div> <div>24%</div> <div>26%</div> <div>46%</div> </div>
1	B	418	<div> <div>%</div> <div>23%</div> <div>26%</div> <div>46%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3608 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 Sec-independent protein translocase protein TatC, Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	16	0	0
			1804	1248	263	289	4			
1	B	225	Total	C	N	O	S	16	0	0
			1804	1248	263	289	4			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP O67305
A	0	GLY	-	EXPRESSION TAG	UNP O67305
A	236	GLU	-	EXPRESSION TAG	UNP P00720
A	237	ILE	-	EXPRESSION TAG	UNP P00720
A	238	GLY	-	EXPRESSION TAG	UNP P00720
A	239	SER	-	EXPRESSION TAG	UNP P00720
A	240	GLY	-	EXPRESSION TAG	UNP P00720
A	241	ALA	-	EXPRESSION TAG	UNP P00720
A	242	SER	-	EXPRESSION TAG	UNP P00720
A	296	THR	CYS	CONFLICT	UNP P00720
A	339	ALA	CYS	CONFLICT	UNP P00720
A	407	GLU	-	EXPRESSION TAG	UNP P00720
A	408	LEU	-	EXPRESSION TAG	UNP P00720
A	409	TYR	-	EXPRESSION TAG	UNP P00720
A	410	LYS	-	EXPRESSION TAG	UNP P00720
A	411	HIS	-	EXPRESSION TAG	UNP P00720
A	412	HIS	-	EXPRESSION TAG	UNP P00720
A	413	HIS	-	EXPRESSION TAG	UNP P00720
A	414	HIS	-	EXPRESSION TAG	UNP P00720
B	-1	MET	-	EXPRESSION TAG	UNP O67305
B	0	GLY	-	EXPRESSION TAG	UNP O67305
B	236	GLU	-	EXPRESSION TAG	UNP P00720
B	237	ILE	-	EXPRESSION TAG	UNP P00720
B	238	GLY	-	EXPRESSION TAG	UNP P00720
B	239	SER	-	EXPRESSION TAG	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	GLY	-	EXPRESSION TAG	UNP P00720
B	241	ALA	-	EXPRESSION TAG	UNP P00720
B	242	SER	-	EXPRESSION TAG	UNP P00720
B	296	THR	CYS	CONFLICT	UNP P00720
B	339	ALA	CYS	CONFLICT	UNP P00720
B	407	GLU	-	EXPRESSION TAG	UNP P00720
B	408	LEU	-	EXPRESSION TAG	UNP P00720
B	409	TYR	-	EXPRESSION TAG	UNP P00720
B	410	LYS	-	EXPRESSION TAG	UNP P00720
B	411	HIS	-	EXPRESSION TAG	UNP P00720
B	412	HIS	-	EXPRESSION TAG	UNP P00720
B	413	HIS	-	EXPRESSION TAG	UNP P00720
B	414	HIS	-	EXPRESSION TAG	UNP P00720

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:

24% 26% 46%

GLU	G227	M148	P78
LEU	K228	Y149	V79
ASP	L229	I150	I80
LYS	ALA	S151	L81
THR	HIS	F152	Y82
GLY	ARG	V153	Q83
VAL	LYS	L154	F84
ALA	ARG	V157	W85
ARG	LYS	V160	R86
ASN	THR	F162	R87
THR	ASN	G163	L88
ASN	GLY	S164	E89
VAL	SER	A165	P90
LEU	THR	F166	A91
THR	ALA	E167	L92
ARG	ALA	M168	Y93
MET	ASP	P169	S94
LYS	ASP	I170	R95
GLU	GLU	L171	E96
ALA	PHE	I172	K97
GLY	LEU	I173	R98
LYS	LEU	I174	A99
ARG	THR	L175	F100
TRP	ASP	A176	I101
ASP	GLU	R177	P102
GLU	ASN	K178	L103
ALA	ILE	L179	L104
ALA	ASP	R180	S107
VAL	VAL	F181	I108
ASN	ASP	L182	L109
LEU	GLY	I183	L110
ALA	ALA	V184	F111
LYS	VAL	V185	F117
SER	GLY	L186	L117
ARG	ILE	G187	I121
TRP	LEU	A188	V122
TRP	LEU	R189	L123
ASN	ARG	F190	P48
GLN	ALA	L191	E49
ASN	ALA	I192	L52
THR	LYS	V193	I53
PRO	ARG	L194	S56
ASN	GLY	V197	P67
ARG	ILE	L198	T58
ALA	LYS	G199	I63
LYS	ASP	A200	L64
VAL	THR	L201	I67
THR	GLY	L202	V71
LYS	LEU	A203	G72
PRO	TYR	P204	I74
VAL	THR	D205	I75
TYR	ILE	Q209	V76
ARG	ASP	V210	G77
VAL	SER	L211	F78
LEU	SER	W212	I79
ASP	HIS	A213	I79
ALA	LEU	I214	I63
VAL	THR	P215	L64
ARG	VAL	L216	I67
GLY	ARG	L217	V71
THR	SER	L218	G72
ALA	ALA	E221	F73
TRP	ASP	L222	I74
ASP	ILE	A223	I75
ALA	ALA	S224	V76
TYR	TYR	M225	G77
LYS	MET	L226	
ASN	VAL	P227	
LEU	PHE	L228	

- Chain B:
- 
- 23% 26% 46%
- | Residue | Category |
|---------|----------|
| I150    | Green    |
| S151    | Green    |
| F152    | Green    |
| V153    | Green    |
| L154    | Green    |
| K155    | Green    |
| L156    | Green    |
| V157    | Green    |
| F160    | Green    |
| G161    | Green    |
| I162    | Green    |
| A163    | Green    |
| F164    | Green    |
| E165    | Green    |
| M166    | Green    |
| P167    | Green    |
| I168    | Green    |
| I179    | Green    |
| L184    | Green    |
| A185    | Green    |
| R188    | Green    |
| K189    | Green    |
| Y190    | Green    |
| F191    | Green    |
| I192    | Green    |
| V193    | Green    |
| I194    | Green    |
| V197    | Green    |
| I198    | Green    |
| G199    | Green    |
| A200    | Green    |
| I201    | Green    |
| A202    | Green    |
| A203    | Green    |
| P204    | Green    |
| D205    | Green    |
| V206    | Green    |
| Q209    | Green    |
| V210    | Green    |
| L211    | Green    |
| M212    | Green    |
| A213    | Green    |
| I214    | Green    |
| P215    | Green    |
| L216    | Green    |
| L217    | Green    |
| E221    | Green    |
| I222    | Green    |
| S223    | Green    |
| I224    | Green    |
| F225    | Green    |
| L226    | Green    |
| C227    | Green    |
| S77     | Yellow   |
| V78     | Yellow   |
| P79     | Yellow   |
| I80     | Yellow   |
| I81     | Yellow   |
| Y82     | Yellow   |
| Q83     | Yellow   |
| F84     | Yellow   |
| W85     | Yellow   |
| R86     | Yellow   |
| F87     | Yellow   |
| I88     | Yellow   |
| E89     | Yellow   |
| P90     | Yellow   |
| A91     | Yellow   |
| L92     | Yellow   |
| Y93     | Yellow   |
| S94     | Yellow   |
| H95     | Yellow   |
| R98     | Yellow   |
| A99     | Yellow   |
| F100    | Yellow   |
| I101    | Yellow   |
| P102    | Yellow   |
| L103    | Yellow   |
| L104    | Yellow   |
| I108    | Yellow   |
| L109    | Yellow   |
| L110    | Yellow   |
| F111    | Yellow   |
| F117    | Yellow   |
| I121    | Yellow   |
| V122    | Yellow   |
| L123    | Yellow   |
| P124    | Yellow   |
| L125    | Yellow   |
| L130    | Yellow   |
| L131    | Yellow   |
| G134    | Yellow   |
| F135    | Yellow   |
| T136    | Yellow   |
| Q137    | Yellow   |
| L138    | Yellow   |
| L139    | Yellow   |
| A140    | Yellow   |
| T141    | Yellow   |
| P142    | Yellow   |
| Y143    | Yellow   |
| S144    | Yellow   |
| L144    | Yellow   |
| V146    | Yellow   |
| D147    | Yellow   |
| W148    | Yellow   |
| Y149    | Yellow   |
| A150    | Yellow   |
| G151    | Yellow   |
| F152    | Yellow   |
| P153    | Yellow   |
| L154    | Yellow   |
| R155    | Yellow   |
| L156    | Yellow   |
| T157    | Yellow   |
| E158    | Yellow   |
| A159    | Yellow   |
| G160    | Yellow   |
| V161    | Yellow   |
| F162    | Yellow   |
| P163    | Yellow   |
| L164    | Yellow   |
| L165    | Yellow   |
| R166    | Yellow   |
| I167    | Yellow   |
| S168    | Yellow   |
| L169    | Yellow   |
| A170    | Yellow   |
| G171    | Yellow   |
| V172    | Yellow   |
| F173    | Yellow   |
| I174    | Yellow   |
| W175    | Yellow   |
| F176    | Yellow   |
| I177    | Yellow   |
| MET     | Grey     |
| GLY     | Grey     |
| MET     | Grey     |
| PRO     | Grey     |
| LEU     | Grey     |
| THR     | Grey     |
| ES      | Grey     |
| H6      | Grey     |
| L7      | Grey     |
| R8      | Grey     |
| E9      | Grey     |
| L10     | Grey     |
| R11     | Grey     |
| Y12     | Grey     |
| R13     | Grey     |
| L14     | Grey     |
| I15     | Grey     |
| I16     | Grey     |
| S17     | Grey     |
| I18     | Grey     |
| I19     | Grey     |
| A20     | Grey     |
| F21     | Grey     |
| L22     | Grey     |
| L23     | Grey     |
| A32     | Grey     |
| V35     | Grey     |
| L39     | Grey     |
| K40     | Grey     |
| E41     | Grey     |
| P42     | Grey     |
| K45     | Grey     |
| E49     | Grey     |
| L52     | Grey     |
| I53     | Grey     |
| S56     | Grey     |
| P57     | Grey     |
| T58     | Grey     |
| L63     | Grey     |
| L64     | Grey     |
| L65     | Grey     |
| R66     | Grey     |
| I67     | Grey     |
| S68     | Grey     |
| L69     | Grey     |
| A70     | Grey     |
| G71     | Grey     |
| V72     | Grey     |
| F73     | Grey     |
| I74     | Grey     |
| W75     | Grey     |
| I76     | Grey     |

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.01Å 142.01Å 251.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 6.80 39.25 – 6.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-6.80) 95.0 (39.25-6.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 6.64Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.344 , 0.418 0.348 , 0.416	Depositor DCC
$R_{free}$ test set	99 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	409.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 398.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	3608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	474.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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

### 5.1 Standard geometry

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	0.28	0/1853	0.49	0/2522
1	B	0.28	0/1853	0.49	0/2522
All	All	0.28	0/3706	0.49	0/5044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1804	0	1946	104	0
1	B	1804	0	1946	108	2
All	All	3608	0	3892	207	2

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 28.

All (207) 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:A:189:LYS:HB3	1:B:206:VAL:HG22	1.48	0.96
1:A:214:ILE:HA	1:A:217:LEU:HD12	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HG23	1:A:142:PRO:HD2	1.56	0.87
1:B:141:THR:HG23	1:B:142:PRO:HD2	1.59	0.85
1:A:164:PHE:O	1:A:167:PRO:HD2	1.80	0.81
1:B:214:ILE:HA	1:B:217:LEU:HD12	1.63	0.80
1:A:77:SER:HA	1:A:80:ILE:HD12	1.63	0.80
1:B:164:PHE:O	1:B:167:PRO:HD2	1.82	0.78
1:B:77:SER:HA	1:B:80:ILE:HD12	1.67	0.76
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.67	0.75
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.67	0.74
1:B:5:GLU:HG2	1:B:8:ARG:HH12	1.54	0.73
1:A:189:LYS:HB2	1:B:209:GLN:HE22	1.54	0.72
1:A:5:GLU:HG2	1:A:8:ARG:HH12	1.54	0.72
1:A:154:LEU:O	1:A:157:VAL:HG12	1.90	0.72
1:B:20:ALA:HA	1:B:23:ILE:HD12	1.73	0.70
1:A:221:GLU:O	1:A:224:ILE:HG13	1.92	0.70
1:B:90:PRO:HB3	1:B:95:HIS:HA	1.75	0.69
1:B:154:LEU:O	1:B:157:VAL:HG12	1.93	0.68
1:B:63:ILE:HG23	1:B:150:ILE:HG21	1.76	0.67
1:A:63:ILE:HG23	1:A:150:ILE:HG21	1.77	0.66
1:A:90:PRO:HB3	1:A:95:HIS:HA	1.77	0.66
1:B:221:GLU:O	1:B:224:ILE:HG13	1.96	0.65
1:A:20:ALA:HA	1:A:23:ILE:HD12	1.79	0.65
1:A:74:ILE:HA	1:A:111:PHE:HE2	1.62	0.64
1:A:67:ILE:HG12	1:A:154:LEU:HD11	1.78	0.64
1:A:52:LEU:HD23	1:A:144:LEU:HD12	1.80	0.64
1:A:141:THR:HG23	1:A:142:PRO:CD	2.27	0.63
1:B:185:ALA:O	1:B:188:ARG:HD2	1.99	0.62
1:B:141:THR:OG1	1:B:142:PRO:HD3	1.99	0.61
1:A:216:LEU:HD12	1:A:216:LEU:H	1.66	0.61
1:A:141:THR:OG1	1:A:142:PRO:HD3	2.01	0.60
1:B:74:ILE:HA	1:B:111:PHE:HE2	1.65	0.60
1:A:117:PHE:HA	1:A:121:ILE:HD13	1.84	0.60
1:B:141:THR:HG23	1:B:142:PRO:CD	2.30	0.60
1:A:98:ARG:HG3	1:A:98:ARG:O	2.01	0.60
1:A:213:ALA:HA	1:A:216:LEU:HD13	1.83	0.59
1:B:32:ALA:HB1	1:B:64:LEU:HG	1.84	0.59
1:B:125:LEU:HG	1:B:211:LEU:HD21	1.85	0.59
1:B:52:LEU:HD23	1:B:144:LEU:HD12	1.85	0.58
1:B:98:ARG:HG3	1:B:98:ARG:O	2.04	0.58
1:A:32:ALA:HB1	1:A:64:LEU:HG	1.86	0.58
1:B:144:LEU:HD13	1:B:145:SER:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD12	1:B:216:LEU:H	1.69	0.57
1:A:185:ALA:O	1:A:188:ARG:HD2	2.03	0.57
1:B:204:PRO:HG2	1:B:205:ASP:H	1.69	0.57
1:A:101:ILE:N	1:A:102:PRO:HD2	2.19	0.57
1:B:213:ALA:HA	1:B:216:LEU:HD13	1.87	0.57
1:B:41:GLU:HB3	1:B:42:PRO:HD3	1.87	0.57
1:A:184:LEU:HD12	1:A:224:ILE:HG22	1.86	0.57
1:B:101:ILE:N	1:B:102:PRO:HD2	2.20	0.57
1:A:41:GLU:HB3	1:A:42:PRO:HD3	1.87	0.56
1:A:18:ILE:O	1:A:21:PHE:HB3	2.05	0.56
1:B:144:LEU:HD13	1:B:145:SER:N	2.20	0.56
1:A:14:LEU:O	1:A:18:ILE:HG12	2.06	0.56
1:A:125:LEU:HG	1:A:211:LEU:HD21	1.88	0.56
1:B:14:LEU:O	1:B:18:ILE:HG12	2.05	0.55
1:A:144:LEU:HD13	1:A:145:SER:N	2.21	0.55
1:B:184:LEU:HD12	1:B:224:ILE:HG22	1.88	0.55
1:A:226:LEU:O	1:A:228:LYS:N	2.39	0.55
1:A:204:PRO:HG2	1:A:205:ASP:H	1.71	0.54
1:B:226:LEU:O	1:B:228:LYS:N	2.38	0.54
1:B:18:ILE:O	1:B:21:PHE:HB3	2.06	0.54
1:A:67:ILE:CG1	1:A:154:LEU:HD11	2.37	0.54
1:B:130:LEU:HB3	1:B:131:LEU:HD23	1.88	0.54
1:A:53:ILE:O	1:A:146:VAL:HG22	2.08	0.54
1:A:91:ALA:C	1:A:92:LEU:HD12	2.28	0.54
1:A:130:LEU:HB3	1:A:131:LEU:HD23	1.90	0.54
1:A:108:ILE:HG22	1:A:109:LEU:N	2.23	0.53
1:B:67:ILE:HG12	1:B:154:LEU:HD11	1.91	0.53
1:A:166:MET:HB2	1:A:167:PRO:HD3	1.90	0.53
1:B:108:ILE:HG22	1:B:109:LEU:N	2.22	0.53
1:A:143:TYR:N	1:A:143:TYR:CD1	2.77	0.53
1:A:142:PRO:HD2	1:A:143:TYR:CE1	2.44	0.53
1:A:52:LEU:HB3	1:A:146:VAL:CG1	2.39	0.53
1:A:144:LEU:HD13	1:A:145:SER:H	1.74	0.53
1:B:52:LEU:HB3	1:B:146:VAL:CG1	2.39	0.52
1:A:45:LYS:HA	1:A:45:LYS:HE3	1.91	0.52
1:A:71:VAL:HA	1:A:74:ILE:HG12	1.91	0.52
1:B:166:MET:HB2	1:B:167:PRO:HD3	1.91	0.52
1:A:13:ARG:HD2	1:A:87:PHE:HD1	1.75	0.52
1:B:162:ILE:O	1:B:165:GLU:HB2	2.10	0.52
1:A:143:TYR:HD1	1:A:143:TYR:N	2.08	0.51
1:B:143:TYR:CD1	1:B:143:TYR:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ALA:C	1:B:92:LEU:HD12	2.30	0.51
1:A:162:ILE:O	1:A:165:GLU:HB2	2.11	0.51
1:B:117:PHE:HA	1:B:121:ILE:HD13	1.93	0.51
1:B:13:ARG:HD2	1:B:87:PHE:HB2	1.92	0.51
1:A:52:LEU:CD2	1:A:144:LEU:HD12	2.41	0.50
1:A:142:PRO:HD2	1:A:143:TYR:HE1	1.76	0.50
1:A:77:SER:N	1:A:78:PRO:CD	2.74	0.50
1:A:123:LEU:N	1:A:124:PRO:HD2	2.27	0.50
1:B:53:ILE:O	1:B:146:VAL:HG22	2.11	0.50
1:A:52:LEU:HB3	1:A:146:VAL:HG12	1.93	0.50
1:B:77:SER:N	1:B:78:PRO:CD	2.75	0.50
1:B:143:TYR:HD1	1:B:143:TYR:N	2.09	0.50
1:A:200:ALA:HB1	1:B:189:LYS:HD2	1.94	0.50
1:B:123:LEU:N	1:B:124:PRO:HD2	2.26	0.49
1:B:35:VAL:O	1:B:39:LEU:HD22	2.13	0.49
1:B:67:ILE:CG1	1:B:154:LEU:HD11	2.42	0.49
1:B:11:ARG:O	1:B:15:ILE:HG12	2.12	0.49
1:B:142:PRO:HD2	1:B:143:TYR:CE1	2.47	0.49
1:A:13:ARG:HD2	1:A:87:PHE:HB2	1.93	0.49
1:A:13:ARG:HD2	1:A:87:PHE:CD1	2.47	0.49
1:A:85:TRP:CE3	1:A:88:ILE:HD11	2.48	0.49
1:A:189:LYS:CB	1:B:206:VAL:HG22	2.32	0.49
1:A:77:SER:CA	1:A:80:ILE:HD12	2.38	0.48
1:B:77:SER:OG	1:B:78:PRO:HD3	2.12	0.48
1:B:13:ARG:HD2	1:B:87:PHE:CD1	2.48	0.48
1:B:121:ILE:O	1:B:124:PRO:HG2	2.13	0.48
1:B:189:LYS:HE3	1:B:190:TYR:CE2	2.48	0.48
1:A:13:ARG:NH2	1:A:86:ARG:HG2	2.28	0.48
1:A:191:PHE:O	1:A:194:ILE:HB	2.14	0.48
1:A:35:VAL:O	1:A:39:LEU:HD22	2.14	0.47
1:B:13:ARG:HD2	1:B:87:PHE:HD1	1.78	0.47
1:B:189:LYS:HA	1:B:192:ILE:HD12	1.96	0.47
1:B:160:PHE:CE1	1:B:212:MET:HB2	2.50	0.47
1:B:200:ALA:HB2	1:B:209:GLN:OE1	2.14	0.47
1:A:39:LEU:HD13	1:A:39:LEU:N	2.30	0.47
1:B:19:ILE:O	1:B:23:ILE:HG13	2.14	0.47
1:B:222:ILE:O	1:B:226:LEU:HD13	2.15	0.47
1:A:160:PHE:CE1	1:A:212:MET:HB2	2.49	0.47
1:B:89:GLU:HA	1:B:90:PRO:C	2.35	0.47
1:A:121:ILE:O	1:A:124:PRO:HG2	2.15	0.47
1:A:200:ALA:HB2	1:A:209:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HA	1:A:111:PHE:CE2	2.47	0.46
1:A:82:TYR:HD1	1:A:104:LEU:HD13	1.80	0.46
1:B:202:ILE:HD11	1:B:212:MET:SD	2.55	0.46
1:B:52:LEU:CD2	1:B:144:LEU:HD12	2.45	0.46
1:A:85:TRP:CZ3	1:A:88:ILE:HD11	2.50	0.46
1:A:88:ILE:HD12	1:A:89:GLU:HB3	1.97	0.46
1:B:142:PRO:HD2	1:B:143:TYR:HE1	1.80	0.46
1:B:16:ILE:HG21	1:B:83:GLN:NE2	2.30	0.46
1:A:193:VAL:O	1:A:197:VAL:N	2.49	0.46
1:B:191:PHE:O	1:B:194:ILE:HB	2.16	0.46
1:B:71:VAL:HA	1:B:74:ILE:HG12	1.98	0.46
1:A:82:TYR:CE1	1:A:100:PHE:HZ	2.33	0.46
1:A:11:ARG:O	1:A:15:ILE:HG12	2.15	0.46
1:A:179:ILE:HG21	1:A:184:LEU:HD21	1.98	0.46
1:A:16:ILE:HG21	1:A:83:GLN:NE2	2.31	0.46
1:A:89:GLU:HA	1:A:90:PRO:C	2.35	0.46
1:B:85:TRP:CE3	1:B:88:ILE:HD11	2.51	0.46
1:A:77:SER:OG	1:A:78:PRO:HD3	2.15	0.46
1:B:74:ILE:HA	1:B:111:PHE:CE2	2.48	0.45
1:B:13:ARG:NH2	1:B:86:ARG:HG2	2.31	0.45
1:B:202:ILE:HD11	1:B:212:MET:CE	2.46	0.45
1:B:77:SER:CA	1:B:80:ILE:HD12	2.43	0.45
1:B:199:GLY:O	1:B:203:ALA:HB3	2.16	0.45
1:B:85:TRP:CZ3	1:B:88:ILE:HD11	2.51	0.45
1:B:141:THR:OG1	1:B:142:PRO:CD	2.64	0.45
1:B:63:ILE:CG2	1:B:150:ILE:HG21	2.44	0.45
1:A:19:ILE:O	1:A:23:ILE:HG13	2.17	0.44
1:B:67:ILE:HG12	1:B:154:LEU:HD21	1.98	0.44
1:A:214:ILE:CA	1:A:217:LEU:HD12	2.37	0.44
1:B:9:GLU:HB3	1:B:87:PHE:HE1	1.82	0.44
1:A:199:GLY:O	1:A:203:ALA:HB3	2.18	0.44
1:A:73:PHE:CE1	1:A:80:ILE:HD13	2.52	0.44
1:A:210:VAL:O	1:A:214:ILE:HG12	2.18	0.44
1:B:149:TYR:O	1:B:152:PHE:HB3	2.18	0.43
1:A:141:THR:OG1	1:A:142:PRO:CD	2.66	0.43
1:B:39:LEU:N	1:B:39:LEU:HD13	2.33	0.43
1:A:189:LYS:CB	1:B:209:GLN:HE22	2.27	0.43
1:B:210:VAL:O	1:B:214:ILE:HG12	2.17	0.43
1:B:137:GLN:HE21	1:B:137:GLN:HB2	1.51	0.43
1:A:141:THR:C	1:A:143:TYR:H	2.22	0.43
1:B:52:LEU:HD22	1:B:146:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:O	1:B:197:VAL:N	2.51	0.43
1:B:179:ILE:HG21	1:B:184:LEU:HD21	2.01	0.42
1:B:56:SER:HB3	1:B:57:PRO:HD2	2.01	0.42
1:A:149:TYR:O	1:A:152:PHE:HB3	2.19	0.42
1:B:141:THR:C	1:B:143:TYR:H	2.23	0.42
1:B:52:LEU:HB3	1:B:146:VAL:HG12	2.01	0.42
1:A:218:LEU:O	1:A:221:GLU:HB2	2.20	0.42
1:A:202:ILE:HD11	1:A:212:MET:SD	2.59	0.42
1:B:191:PHE:CD2	1:B:217:LEU:HD23	2.54	0.42
1:A:15:ILE:O	1:A:19:ILE:HB	2.20	0.42
1:A:193:VAL:CG2	1:A:194:ILE:N	2.83	0.42
1:A:85:TRP:HA	1:A:85:TRP:CE3	2.55	0.42
1:B:65:ILE:HA	1:B:68:SER:OG	2.20	0.42
1:B:82:TYR:HD1	1:B:104:LEU:HD13	1.83	0.42
1:B:82:TYR:CE1	1:B:100:PHE:HZ	2.37	0.42
1:B:90:PRO:O	1:B:91:ALA:C	2.58	0.42
1:A:222:ILE:O	1:A:226:LEU:HD13	2.20	0.41
1:A:189:LYS:HE3	1:A:190:TYR:CE2	2.54	0.41
1:A:56:SER:HB3	1:A:57:PRO:HD2	2.01	0.41
1:A:81:LEU:HD13	1:A:107:SER:HB2	2.03	0.41
1:B:222:ILE:O	1:B:225:PHE:HB3	2.20	0.41
1:B:35:VAL:HG11	1:B:71:VAL:HG21	2.02	0.41
1:A:9:GLU:HB3	1:A:87:PHE:HE1	1.86	0.41
1:A:189:LYS:HA	1:A:192:ILE:HD12	2.02	0.41
1:B:122:VAL:HG12	1:B:156:LEU:HD21	2.03	0.41
1:A:7:LEU:HB2	1:A:11:ARG:NH2	2.35	0.41
1:B:45:LYS:HE3	1:B:45:LYS:HA	2.02	0.41
1:B:73:PHE:CE1	1:B:80:ILE:HD13	2.56	0.41
1:A:19:ILE:CG2	1:A:20:ALA:N	2.84	0.41
1:B:110:LEU:HD13	1:B:168:ILE:CG1	2.51	0.41
1:B:70:ALA:O	1:B:73:PHE:HB3	2.21	0.41
1:A:222:ILE:O	1:A:225:PHE:HB3	2.20	0.40
1:A:110:LEU:HD13	1:A:168:ILE:CG1	2.51	0.40
1:A:90:PRO:O	1:A:91:ALA:C	2.59	0.40
1:B:7:LEU:HB2	1:B:11:ARG:NH2	2.35	0.40
1:A:213:ALA:O	1:A:214:ILE:C	2.60	0.40
1:B:123:LEU:HD22	1:B:153:VAL:HG13	2.03	0.40
1:B:85:TRP:CE3	1:B:85:TRP:HA	2.57	0.40
1:A:47:TYR:N	1:A:48:PRO:HD3	2.37	0.40
1:B:15:ILE:O	1:B:19:ILE:HB	2.21	0.40
1:B:7:LEU:N	1:B:7:LEU:HD23	2.37	0.40

All (2) 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:95:HIS:NE2	1:B:95:HIS:NE2[8_775]	1.93	0.27
1:B:22:LEU:CD1	1:B:22:LEU:CD1[6_565]	2.13	0.07

## 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	223/418 (53%)	192 (86%)	22 (10%)	9 (4%)	3	23
1	B	223/418 (53%)	193 (86%)	21 (9%)	9 (4%)	3	23
All	All	446/836 (53%)	385 (86%)	43 (10%)	18 (4%)	3	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	141	THR
1	A	211	LEU
1	B	94	SER
1	B	141	THR
1	A	91	ALA
1	A	94	SER
1	B	58	THR
1	B	91	ALA
1	B	211	LEU
1	A	227	GLY
1	B	227	GLY
1	A	167	PRO
1	B	204	PRO
1	A	204	PRO
1	B	147	ASP

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Mol	Chain	Res	Type
1	B	167	PRO
1	A	147	ASP

### 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	195/356 (55%)	176 (90%)	19 (10%)	8	27
1	B	195/356 (55%)	176 (90%)	19 (10%)	8	27
All	All	390/712 (55%)	352 (90%)	38 (10%)	8	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	SER
1	A	39	LEU
1	A	45	LYS
1	A	49	GLU
1	A	75	ILE
1	A	89	GLU
1	A	98	ARG
1	A	110	LEU
1	A	131	LEU
1	A	137	GLN
1	A	138	LEU
1	A	139	LEU
1	A	141	THR
1	A	143	TYR
1	A	144	LEU
1	A	165	GLU
1	A	193	VAL
1	A	205	ASP
1	B	7	LEU
1	B	17	SER

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	45	LYS
1	B	49	GLU
1	B	75	ILE
1	B	89	GLU
1	B	98	ARG
1	B	110	LEU
1	B	131	LEU
1	B	137	GLN
1	B	138	LEU
1	B	139	LEU
1	B	141	THR
1	B	143	TYR
1	B	144	LEU
1	B	165	GLU
1	B	193	VAL
1	B	205	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	B	137	GLN
1	B	209	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	225/418 (53%)	-0.16	8 (3%)	42 38	212, 472, 626, 717	4 (1%)
1	B	225/418 (53%)	-0.23	5 (2%)	62 54	211, 472, 626, 717	4 (1%)
All	All	450/836 (53%)	-0.20	13 (2%)	51 44	211, 472, 638, 717	8 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	3.8
1	B	145	SER	3.6
1	A	134	GLY	3.4
1	B	52	LEU	3.0
1	A	135	PHE	2.4
1	B	144	LEU	2.3
1	A	142	PRO	2.3
1	B	134	GLY	2.2
1	A	94	SER	2.1
1	B	135	PHE	2.1
1	A	132	GLY	2.1
1	A	141	THR	2.1
1	A	97	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.