



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:17 PM GMT

PDB ID : 4HTT  
Title : Crystal Structure of Twin Arginine Translocase Receptor- TatC in DDM  
Authors : Ramasamy, S.; Suloway, C.J.M.; Clemons Jr., W.M.  
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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

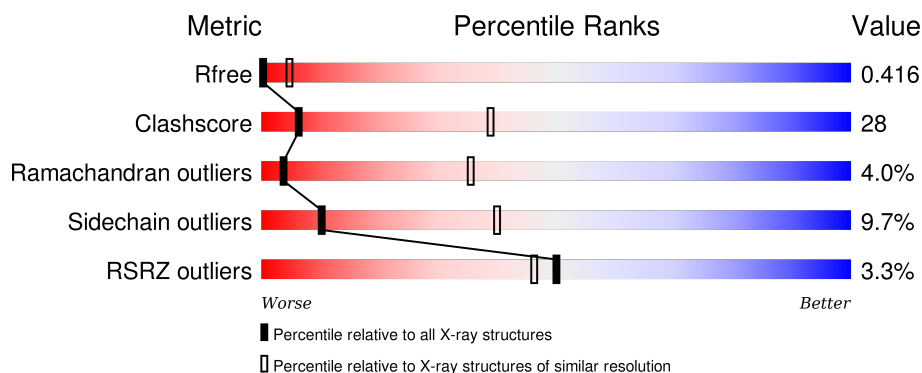
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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	
1	B	418	

## 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



K228	LEU	MET	LEU
I229	ASP	GLY	ASP
	LYS	GLU	LYS
	ALA	THR	ALA
	ILE	GLY	ILE
	ARG	VAL	ARG
	LYS	HIS	LYS
	LYS	ALA	LYS
	GLU	GLY	GLU
	ILE	PHE	ILE
	GLY	THR	GLY
	SER	ASN	SER
	VAL	ASN	VAL
	ILE	LEU	ILE
	ALA	ARG	ALA
	SER	MET	SER
	MET	LEU	MET
	ASN	GLN	ASN
	ILE	LYS	ILE
	PHE	ARG	PHE
	GLU	TRP	GLU
	MET	ASP	MET
	LEU	GLU	LEU
	ASP	ALA	ASP
	GLY	VAL	GLY
	ILE	ASN	ILE
	LYS	VAL	LYS
	ARG	SER	ARG
	GLY	ARG	GLY
	ILE	ILE	ILE
	LYS	TYR	LYS
	ASP	ASN	ASP
	THR	GLN	THR
	GLU	THR	GLU
	GLY	PRO	GLY
	TYR	ASN	TYR
	LEU	ARG	LEU
	LYS	ALA	LYS
	VAL	LYS	VAL
	THR	ARG	THR
	ILE	VAL	ILE
	ASP	THR	ASP
	LYS	THR	LYS
	THR	PHE	THR
	ILE	THR	ILE
	GLY	THR	GLY
	ARG	THR	ARG
	VAL	ARG	VAL
	ALA	ALA	ALA
	LEU	TRP	LEU
	ASN	ASP	ASN
	ILE	ALA	ILE
	TYR	TYR	TYR
	LYS	LYS	LYS
	ASN	ASN	ASN
	LEU	LEU	LEU
	PHE	PHE	PHE
	GLN	GLN	GLN

## 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	Depositor
R, $R_{free}$	0.344 , 0.418 0.348 , 0.416	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
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 , 398.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 2281 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:B:141:THR:HG23	1:B:142:PRO:CD	2.30	0.60
1:A:117:PHE:HA	1:A:121:ILE:HD13	1.84	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:B:144:LEU:HD13	1:B:145:SER:H	1.69	0.58
1:A:32:ALA:HB1	1:A:64:LEU:HG	1.86	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:B:144:LEU:HD13	1:B:145:SER:N	2.20	0.56
1:A:18:ILE:O	1:A:21:PHE:HB3	2.05	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:B:226:LEU:O	1:B:228:LYS:N	2.38	0.54
1:A:204:PRO:HG2	1:A:205:ASP:H	1.71	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:B:67:ILE:HG12	1:B:154:LEU:HD11	1.91	0.53
1:A:108:ILE:HG22	1:A:109:LEU:N	2.23	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:B:77:SER:N	1:B:78:PRO:CD	2.75	0.50
1:A:52:LEU:HB3	1:A:146:VAL:HG12	1.93	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:67:ILE:CG1	1:B:154:LEU:HD11	2.42	0.49
1:B:35:VAL:O	1:B:39:LEU:HD22	2.13	0.49
1:B:123:LEU:N	1:B:124:PRO:HD2	2.26	0.49
1:B:142:PRO:HD2	1:B:143:TYR:CE1	2.47	0.49
1:B:11:ARG:O	1:B:15:ILE:HG12	2.12	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:189:LYS:CB	1:B:206:VAL:HG22	2.32	0.49
1:A:85:TRP:CE3	1:A:88:ILE:HD11	2.48	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: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:39:LEU:HD13	1:A:39:LEU:N	2.30	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:B:202:ILE:HD11	1:B:212:MET:SD	2.55	0.46
1:A:82:TYR:HD1	1:A:104:LEU:HD13	1.80	0.46
1:B:52:LEU:CD2	1:B:144:LEU:HD12	2.45	0.46
1:B:142:PRO:HD2	1:B:143:TYR:HE1	1.80	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:16:ILE:HG21	1:B:83:GLN:NE2	2.30	0.46
1:B:191:PHE:O	1:B:194:ILE:HB	2.16	0.46
1:A:193:VAL:O	1:A:197:VAL:N	2.49	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:179:ILE:HG21	1:A:184:LEU:HD21	1.98	0.46
1:A:11:ARG:O	1:A:15:ILE:HG12	2.15	0.46
1:A:89:GLU:HA	1:A:90:PRO:C	2.35	0.46
1:A:16:ILE:HG21	1:A:83:GLN:NE2	2.31	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: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:149:TYR:O	1:A:152:PHE:HB3	2.19	0.42
1:A:218:LEU:O	1:A:221:GLU:HB2	2.20	0.42
1:B:191:PHE:CD2	1:B:217:LEU:HD23	2.54	0.42
1:A:202:ILE:HD11	1:A:212:MET:SD	2.59	0.42
1:A:85:TRP:HA	1:A:85:TRP:CE3	2.55	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:B:65:ILE:HA	1:B:68:SER:OG	2.20	0.42
1:B:90:PRO:O	1:B:91:ALA:C	2.58	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: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:B:35:VAL:HG11	1:B:71:VAL:HG21	2.02	0.41
1:B:222:ILE:O	1:B:225:PHE:HB3	2.20	0.41
1:A:81:LEU:HD13	1:A:107:SER:HB2	2.03	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:B:73:PHE:CE1	1:B:80:ILE:HD13	2.56	0.41
1:B:70:ALA:O	1:B:73:PHE:HB3	2.21	0.41
1:A:7:LEU:HB2	1:A:11:ARG:NH2	2.35	0.41
1:A:19:ILE:CG2	1:A:20:ALA:N	2.84	0.41
1:B:45:LYS:HE3	1:B:45:LYS:HA	2.02	0.41
1:B:110:LEU:HD13	1:B:168:ILE:CG1	2.51	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:B:7:LEU:HB2	1:B:11:ARG:NH2	2.35	0.40
1:A:90:PRO:O	1:A:91:ALA:C	2.59	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: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
1:A:47:TYR:N	1:A:48:PRO:HD3	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%)	4	35
1	B	223/418 (53%)	193 (86%)	21 (9%)	9 (4%)	4	35
All	All	446/836 (53%)	385 (86%)	43 (10%)	18 (4%)	4	35

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%)	10	40
1	B	195/356 (55%)	176 (90%)	19 (10%)	10	40
All	All	390/712 (55%)	352 (90%)	38 (10%)	10	40

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%)	-0.11	9 (4%)	42	40	212, 472, 626, 717	4 (1%)
1	B	225/418 (53%)	-0.19	6 (2%)	58	54	211, 472, 626, 717	4 (1%)
All	All	450/836 (53%)	-0.15	15 (3%)	50	46	211, 472, 638, 717	8 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	4.0
1	B	145	SER	3.7
1	A	134	GLY	3.7
1	B	52	LEU	3.3
1	A	135	PHE	2.5
1	B	144	LEU	2.5
1	B	134	GLY	2.4
1	A	142	PRO	2.3
1	B	135	PHE	2.3
1	A	132	GLY	2.3
1	A	94	SER	2.3
1	A	141	THR	2.2
1	A	136	THR	2.2
1	B	136	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.