



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:53 AM UTC

PDB ID : 4HTT / pdb_00004htt
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

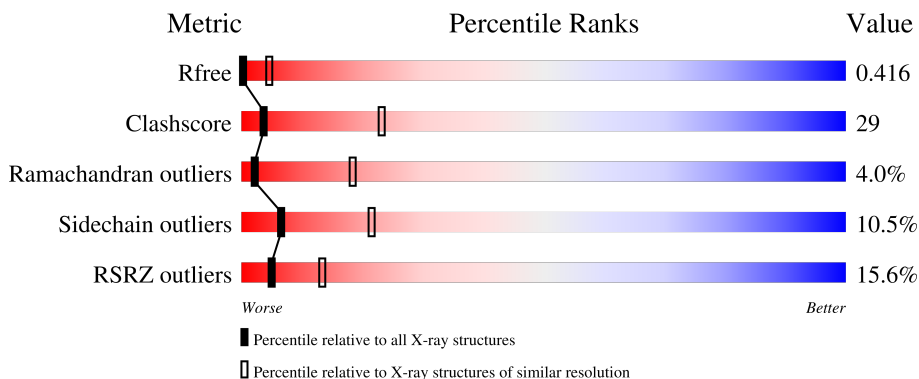
1 Overall quality at a glance

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}	180053	1165 (9.50-4.00)
Clashscore	190562	1006 (9.50-4.04)
Ramachandran outliers	187476	1052 (9.50-4.00)
Sidechain outliers	187428	1015 (9.50-4.00)
RSRZ outliers	180081	1158 (9.50-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	418	

2 Entry composition i

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
			Total	C	N	O	S			
1	A	225	1804	1248	263	289	4	16	0	0
1	B	225	1804	1248	263	289	4	16	0	0

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

V146	V151	V152	V153	L154	K155	L156	V157	V158	A159	F160	G161	I162	A163	F164	E166	M166	P167	I168	I179	F180	F181	L184	A185	S186	F187	R188	K189	Y190	F191	I192	V193	I194	V197	I198	G199	A200	F201	I202	A203	P204	D205	V206	Q209	V210	L211	M212	A213	I214	P215	L216	L217																					
E221	I222	S223	I224	F225	L226	G227	K228	L229	ALA	THR	THR	ARG	ARG	LYS	LYS	GLU	THR	ILE	GLY	SER	ILE	GLY	ALA	SER	LYS	MET	ASN	ASN	ILE	ILE	ILE	PHE	GLU	LYS	TRP	LEU	PHE	LEU	ASN	GLN	ASP	ILE	ASP	GLY	THR	TYR	ILE	TYR	LYS	ASP	THR	THR	GLY	TYR	TYR	LYS	THR	THR	ILE	GLY	ILE	GLY	HIS	L211	M212	LEU	A213	THR	THR	LYS	SER	PRO
SER	LEU	ASN	ALA	ALA	LYS	SER	GLU	LEU	ASP	LYS	ALA	THR	ILE	GLY	ARG	ALA	ARG	GLY	THR	THR	ASN	GLY	VAL	ILE	THR	ARG	MET	LYS	LEU	GLN	ALA	GLY	TRP	LEU	PHE	LEU	ASN	GLN	ASP	ILE	ASP	GLY	THR	TYR	ILE	TYR	LYS	ASP	THR	THR	GLY	TYR	LYS	THR	THR	ILE	GLY	HIS	L211	M212	LEU	A213	THR	THR	LYS	SER	PRO					
ALA	LEU	ILE	ASN	MET	VAL	PHE	GLN	MET	GLY	GLU	THR	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	THR	ASN	SER	LEU	ARG	MET	LEU	GLN	GLN	LYS	ARG	TRP	ASP	GLU	ALA	ALA	VAL	ASN	ALA	LYS	SER	ARG	TRP	TYR	ASN	GLN	THR	PRO	ASN	ARG	ALA	LYS	ARG	VAL	ILE	THR	THR	PHE	ARG	THR	GLY	THR	ALA										
TRP	ASP	ALA	TYR	ASN	LEU	GLU	LEU	TYR	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	THR	ASN	SER	LEU	ARG	MET	LEU	GLN	GLN	LYS	ARG	TRP	ASP	GLU	ALA	ALA	VAL	ASN	ALA	LYS	SER	ARG	TRP	TYR	ASN	GLN	THR	PRO	ASN	ARG	ALA	LYS	ARG	VAL	ILE	THR	THR	PHE	ARG	THR	GLY	THR	ALA										

4 Data and refinement statistics i

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.01Å 142.01Å 251.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 6.80 30.00 – 6.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-6.80) 93.5 (30.00-6.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.344 , 0.418 0.348 , 0.416	Depositor DCC
R_{free} test set	99 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 761.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	3608	wwPDB-VP
Average B, all atoms (Å ²)	474.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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](#)

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	0.31	0/1853	0.83	5/2522 (0.2%)
1	B	0.31	0/1853	0.83	4/2522 (0.2%)
All	All	0.31	0/3706	0.83	9/5044 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	THR	CA-C-N	-7.01	111.08	119.84
1	B	141	THR	C-N-CA	-7.01	111.08	119.84
1	A	141	THR	CA-C-N	-6.96	111.15	119.84
1	A	141	THR	C-N-CA	-6.96	111.15	119.84
1	B	98	ARG	N-CA-C	-5.49	106.58	113.28
1	A	98	ARG	N-CA-C	-5.44	106.65	113.28
1	A	140	ALA	N-CA-C	5.35	116.30	107.20
1	B	140	ALA	N-CA-C	5.33	116.25	107.20
1	A	101	ILE	CB-CA-C	-5.01	108.94	113.70

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	108	0
1	B	1804	0	1946	114	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3608	0	3892	217	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 29.

All (217) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:98:ARG:HG3	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:A:91:ALA:C	1:A:92:LEU:HD12	2.28	0.59
1:B:52:LEU:HD23	1:B:144:LEU:HD12	1.85	0.58
1:B:98:ARG:O	1:B:98:ARG:HG3	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
1:B:216:LEU:H	1:B:216:LEU:HD12	1.69	0.57
1:A:185:ALA:O	1:A:188:ARG:HD2	2.03	0.57
1:B:202:ILE:HD11	1:B:212:MET:HE1	1.86	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:91:ALA:C	1:B:92:LEU:HD12	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:45:LYS:HA	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:N	1:A:143:TYR:HD1	2.08	0.51
1:B:143:TYR:N	1:B:143:TYR:CD1	2.77	0.51
1:A:162:ILE:O	1:A:165:GLU:HB2	2.11	0.51
1:B:89:GLU:HA	1:B:90:PRO:C	2.35	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:89:GLU:HA	1:A:90:PRO:C	2.35	0.50
1:A:77:SER:N	1:A:78:PRO:CD	2.74	0.50
1:A:142:PRO:HD2	1:A:143:TYR:HE1	1.76	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:A:200:ALA:HB1	1:B:189:LYS:HD2	1.94	0.50
1:B:143:TYR:N	1:B:143:TYR:HD1	2.09	0.50
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:123:LEU:N	1:B:124:PRO:HD2	2.26	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:13:ARG:HD2	1:B:87:PHE:CD1	2.48	0.48
1:B:77:SER:OG	1:B:78:PRO:HD3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:141:THR:C	1:A:143:TYR:H	2.22	0.47
1:B:160:PHE:CE1	1:B:212:MET:HB2	2.50	0.47
1:B:189:LYS:HA	1:B:192:ILE:HD12	1.96	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:A:160:PHE:CE1	1:A:212:MET:HB2	2.49	0.47
1:A:202:ILE:HD11	1:A:212:MET:HE1	1.97	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:121:ILE:O	1:A:124:PRO:HG2	2.15	0.47
1:B:141:THR:C	1:B:143:TYR:H	2.23	0.47
1:A:200:ALA:HB2	1:A:209:GLN:OE1	2.14	0.47
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:90:PRO:O	1:B:91:ALA:C	2.58	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:16:ILE:HG21	1:B:83:GLN:NE2	2.30	0.46
1:B:142:PRO:HD2	1:B:143:TYR:HE1	1.80	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: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:A:90:PRO:O	1:A:91:ALA:C	2.59	0.45
1:B:77:SER:CA	1:B:80:ILE:HD12	2.43	0.45
1:A:213:ALA:O	1:A:214:ILE:C	2.60	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:205:ASP:CG	1:B:206:VAL:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:CG2	1:B:150:ILE:HG21	2.44	0.45
1:B:141:THR:OG1	1:B:142:PRO:CD	2.64	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:B:202:ILE:HD11	1:B:212:MET:CE	2.46	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:85:TRP:C	1:A:87:PHE:H	2.27	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:B:52:LEU:HD22	1:B:146:VAL:HA	1.99	0.43
1:B:193:VAL:O	1:B:197:VAL:N	2.51	0.43
1:B:56:SER:HB3	1:B:57:PRO:HD2	2.01	0.42
1:B:179:ILE:HG21	1:B:184:LEU:HD21	2.01	0.42
1:A:149:TYR:O	1:A:152:PHE:HB3	2.19	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:85:TRP:C	1:B:87:PHE:H	2.28	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:85:TRP:CE3	1:A:85:TRP:HA	2.55	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:88:ILE:C	1:B:91:ALA:HB3	2.45	0.42
1:B:82:TYR:CE1	1:B:100:PHE:HZ	2.37	0.42
1:B:82:TYR:HD1	1:B:104:LEU:HD13	1.83	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: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:164:PHE:C	1:A:167:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:70:ALA:O	1:B:73:PHE:HB3	2.21	0.41
1:B:73:PHE:CE1	1:B:80:ILE:HD13	2.56	0.41
1:B:110:LEU:HD13	1:B:168:ILE:CG1	2.51	0.41
1:B:158:VAL:O	1:B:159:ALA:C	2.64	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:205:ASP:OD1	1:A:205:ASP:C	2.63	0.40
1:B:29:PHE:C	1:B:29:PHE:CD1	2.99	0.40
1:B:7:LEU:HB2	1:B:11:ARG:NH2	2.35	0.40
1:B:85:TRP:CE3	1:B:85:TRP:HA	2.57	0.40
1:B:123:LEU:HD22	1:B:153:VAL:HG13	2.03	0.40
1:A:47:TYR:N	1:A:48:PRO:HD3	2.37	0.40
1:B:7:LEU:HD23	1:B:7:LEU:N	2.37	0.40
1:B:15:ILE:O	1:B:19:ILE:HB	2.21	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%)	2	18
1	B	223/418 (53%)	193 (86%)	21 (9%)	9 (4%)	2	18
All	All	446/836 (53%)	385 (86%)	43 (10%)	18 (4%)	2	18

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
1	B	167	PRO
1	A	147	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/356 (55%)	174 (89%)	21 (11%)	6	21
1	B	195/356 (55%)	175 (90%)	20 (10%)	7	23
All	All	390/712 (55%)	349 (90%)	41 (10%)	6	21

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	SER
1	A	19	ILE
1	A	39	LEU
1	A	45	LYS
1	A	49	GLU
1	A	75	ILE
1	A	89	GLU
1	A	103	LEU
1	A	108	ILE
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
1	B	39	LEU
1	B	45	LYS
1	B	49	GLU
1	B	75	ILE
1	B	89	GLU
1	B	103	LEU
1	B	108	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	225/418 (53%)	0.86	42 (18%) 3 11	121, 471, 626, 717	4 (1%)
1	B	225/418 (53%)	0.91	28 (12%) 8 16	117, 472, 626, 717	4 (1%)
All	All	450/836 (53%)	0.88	70 (15%) 5 13	117, 472, 638, 717	8 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	PRO	15.1
1	B	59	GLU	13.2
1	B	141	THR	7.6
1	B	58	THR	7.6
1	B	61	LEU	7.4
1	B	101	ILE	7.2
1	A	181	PRO	7.0
1	A	125	LEU	5.7
1	A	129	PHE	5.6
1	A	6	HIS	5.3
1	A	15	ILE	5.2
1	A	201	ILE	5.2
1	A	130	LEU	5.0
1	A	226	LEU	4.9
1	A	101	ILE	4.8
1	A	188	ARG	4.7
1	A	189	LYS	4.6
1	A	184	LEU	4.4
1	B	62	PHE	4.3
1	B	112	MET	4.2
1	A	25	SER	4.1
1	A	185	ALA	4.1
1	A	74	ILE	3.8
1	B	190	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	112	MET	3.6
1	B	164	PHE	3.5
1	B	45	LYS	3.5
1	B	202	ILE	3.4
1	A	141	THR	3.3
1	B	41	GLU	3.3
1	B	73	PHE	3.3
1	A	174	GLN	3.2
1	B	105	LEU	3.2
1	A	134	GLY	3.2
1	A	224	ILE	3.1
1	B	181	PRO	3.1
1	A	75	ILE	3.1
1	B	74	ILE	3.1
1	A	35	VAL	3.1
1	A	93	TYR	3.0
1	B	163	ALA	3.0
1	A	223	SER	3.0
1	A	142	PRO	3.0
1	A	135	PHE	2.9
1	A	21	PHE	2.9
1	A	38	ILE	2.8
1	B	187	PHE	2.8
1	A	33	LYS	2.8
1	A	42	PRO	2.8
1	A	220	TYR	2.7
1	A	218	LEU	2.6
1	A	190	TYR	2.6
1	A	71	VAL	2.5
1	B	10	LEU	2.5
1	B	192	ILE	2.4
1	B	142	PRO	2.3
1	A	87	PHE	2.3
1	A	19	ILE	2.3
1	A	143	TYR	2.3
1	B	206	VAL	2.3
1	B	11	ARG	2.3
1	B	160	PHE	2.2
1	A	92	LEU	2.2
1	A	176	ALA	2.2
1	B	64	LEU	2.1
1	B	198	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	53	ILE	2.1
1	B	151	SER	2.0
1	A	196	PHE	2.0
1	A	54	THR	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 oligosaccharides 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.