



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:45 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

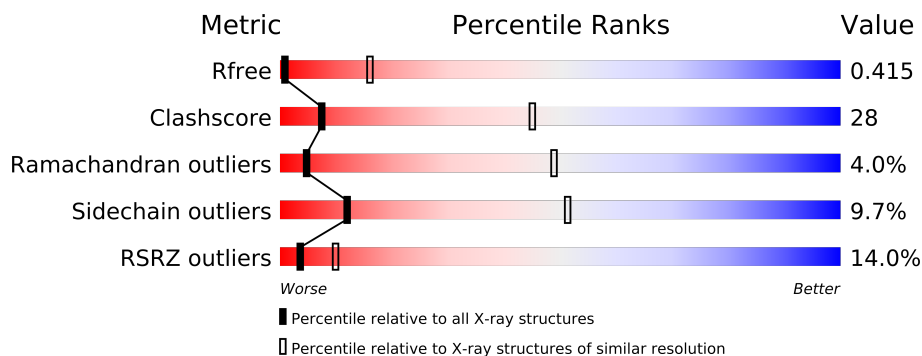
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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

Continued on next page...

Continued from previous page...

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

[illegible]

4 Data and refinement statistics

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 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
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 6.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.344 , 0.418 0.348 , 0.415	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	409.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 694.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 2281 reflections	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	3608	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (207) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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
1:B:216:LEU:HD12	1:B:216:LEU:H	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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.

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
--------	--------	-------------	----------

Atom-1	Atom-2	Distance(Å)	Clash(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

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	223/418 (53%)	192 (86%)	22 (10%)	9 (4%)	5	49
1	B	223/418 (53%)	193 (86%)	21 (9%)	9 (4%)	5	49
All	All	446/836 (53%)	385 (86%)	43 (10%)	18 (4%)	5	49

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 ⓘ

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%)	12	51
1	B	195/356 (55%)	176 (90%)	19 (10%)	12	51
All	All	390/712 (55%)	352 (90%)	38 (10%)	12	51

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 chains 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 ⓘ

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	35 (15%) 3 9	212, 472, 626, 717	4 (1%)
1	B	225/418 (53%)	0.63	28 (12%) 5 12	211, 472, 626, 717	4 (1%)
All	All	450/836 (53%)	0.75	63 (14%) 3 10	211, 472, 638, 717	8 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	THR	10.1
1	A	134	GLY	9.8
1	A	133	LEU	7.6
1	A	137	GLN	7.5
1	A	135	PHE	7.0
1	A	138	LEU	6.7
1	A	141	THR	6.4
1	A	132	GLY	6.3
1	A	139	LEU	6.1
1	A	140	ALA	6.0
1	A	142	PRO	5.8
1	A	131	LEU	5.0
1	A	49	GLU	4.7
1	A	47	TYR	4.7
1	B	134	GLY	4.6
1	B	135	PHE	4.6
1	A	50	VAL	4.0
1	A	143	TYR	3.9
1	B	132	GLY	3.8
1	A	51	GLU	3.8
1	B	136	THR	3.6
1	B	57	PRO	3.5
1	B	12	TYR	3.5
1	B	144	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	62	PHE	3.2
1	A	129	PHE	3.2
1	B	30	TYR	3.1
1	B	59	GLU	3.1
1	B	98	ARG	3.0
1	A	130	LEU	2.9
1	A	127	LEU	2.8
1	B	10	LEU	2.7
1	B	131	LEU	2.7
1	B	48	PRO	2.6
1	B	133	LEU	2.6
1	B	148	MET	2.6
1	A	176	ALA	2.5
1	B	228	LYS	2.5
1	B	229	LEU	2.5
1	A	228	LYS	2.5
1	B	145	SER	2.4
1	B	58	THR	2.4
1	A	128	LYS	2.4
1	A	36	PHE	2.4
1	B	6	HIS	2.3
1	A	33	LYS	2.3
1	B	31	PHE	2.3
1	A	7	LEU	2.3
1	A	97	LYS	2.2
1	A	43	ILE	2.2
1	A	6	HIS	2.2
1	A	225	PHE	2.2
1	B	11	ARG	2.2
1	B	28	ALA	2.1
1	A	178	VAL	2.1
1	B	45	LYS	2.1
1	A	226	LEU	2.1
1	A	93	TYR	2.1
1	A	52	LEU	2.1
1	B	9	GLU	2.1
1	A	229	LEU	2.0
1	B	143	TYR	2.0
1	B	139	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.