Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:55 pm BST

PDB ID	:	4HZU
Title	:	Structure of a bacterial energy-coupling factor transporter
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Deposited on	:	2012-11-15
Resolution	:	3.53 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 following versions of software and data (see references ⓘ) were used in the production of this report:

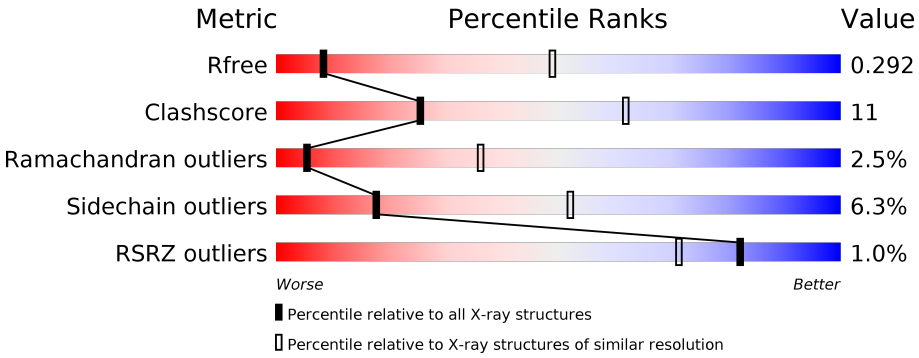
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.53 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 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 <=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	B	290	73% 24% •
2	A	279	2% 61% 32% • • •
3	T	266	64% 23% • 10%
4	S	166	% 73% 22% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7437 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 Energy-coupling factor transporter ATP-binding protein EcfA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	284	2217	1399	389	418	11	0	0	0

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	273	2096	1316	362	411	7	0	0	0

- Molecule 3 is a protein called Energy-coupling factor transporter transmembrane protein EcfT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	T	240	1917	1272	318	315	12	0	0	0

- Molecule 4 is a protein called Predicted membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	S	164	1207	801	197	201	8	0	0	0

3 Residue-property plots (i)

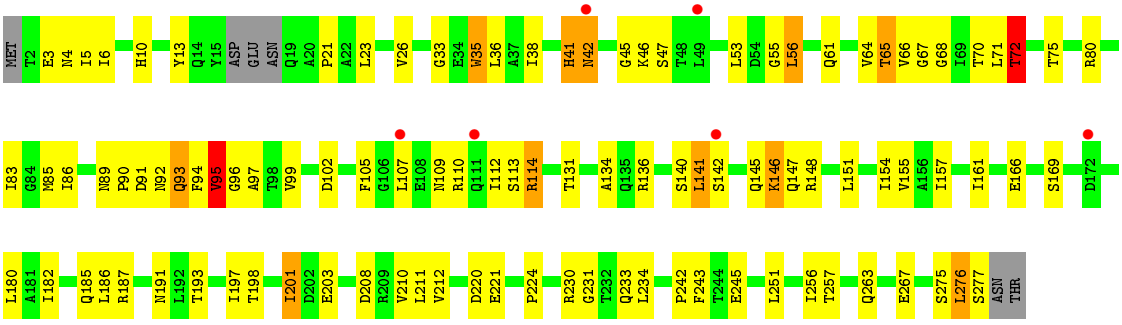
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA 1

Chain B:

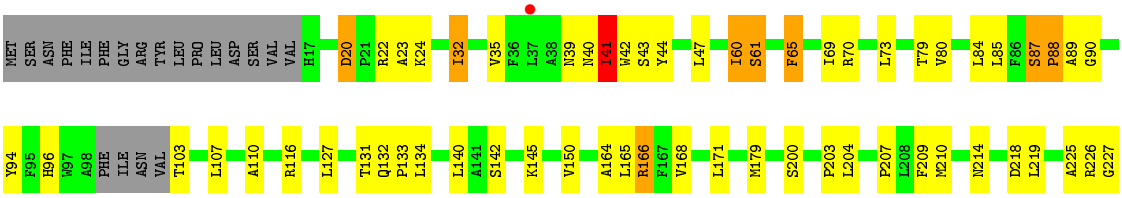
- Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA 2

Chain A:



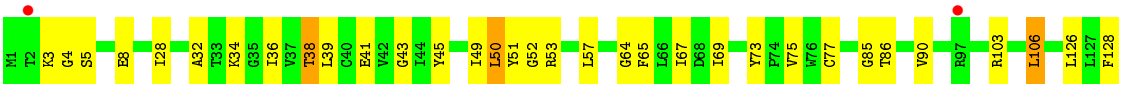
- Molecule 3: Energy-coupling factor transporter transmembrane protein EcfT

Chain T:



- Molecule 4: Predicted membrane protein

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.97Å 148.69Å 154.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 3.53 48.68 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.69-3.53) 96.8 (48.68-3.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.241 , 0.292 0.241 , 0.292	Depositor DCC
R_{free} test set	1157 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	134.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 72.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7437	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	B	0.22	0/2262	0.40	0/3071
2	A	0.22	0/2129	0.41	0/2895
3	T	0.24	0/1964	0.46	0/2662
4	S	0.24	0/1232	0.52	0/1681
All	All	0.23	0/7587	0.44	0/10309

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	B	2217	0	2195	43	0
2	A	2096	0	2094	67	0
3	T	1917	0	1995	47	0
4	S	1207	0	1311	24	0
All	All	7437	0	7595	160	0

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 11.

All (160) 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)
4:S:36:ILE:HG23	4:S:143:GLN:HG3	1.61	0.82
4:S:38:THR:HG22	4:S:41:GLU:HB3	1.64	0.78
2:A:230:ARG:HG2	2:A:233:GLN:HB2	1.71	0.73
4:S:28:ILE:HB	4:S:36:ILE:HB	1.72	0.71
3:T:35:VAL:O	3:T:116:ARG:NH1	2.24	0.70
2:A:36:LEU:HD11	2:A:211:LEU:HD13	1.75	0.68
3:T:32:ILE:HG23	4:S:75:VAL:HG12	1.76	0.68
3:T:88:PRO:HA	3:T:103:THR:HG22	1.75	0.67
2:A:212:VAL:HB	2:A:220:ASP:HB3	1.77	0.67
4:S:5:SER:HB3	4:S:8:GLU:HB3	1.75	0.67
3:T:39:ASN:O	3:T:43:SER:OG	2.15	0.65
2:A:166:GLU:HB3	2:A:169:SER:HB2	1.79	0.64
1:B:285:ARG:NH1	2:A:277:SER:OG	2.32	0.63
1:B:89:MET:HG2	1:B:168:VAL:HB	1.79	0.63
2:A:80:ARG:HD3	3:T:225:ALA:HA	1.79	0.63
4:S:128:PHE:HB3	4:S:129:GLY:HA3	1.80	0.62
2:A:33:GLY:O	2:A:187:ARG:NH1	2.33	0.62
1:B:54:ASN:ND2	1:B:89:MET:SD	2.74	0.61
1:B:55:ALA:HB1	1:B:80:LEU:HD13	1.83	0.60
2:A:93:GLN:NE2	2:A:147:GLN:OE1	2.34	0.60
2:A:64:VAL:HB	2:A:71:LEU:HD12	1.83	0.60
2:A:90:PRO:HB2	2:A:146:LYS:HB2	1.84	0.59
2:A:220:ASP:OD1	2:A:221:GLU:N	2.36	0.58
1:B:216:VAL:HB	1:B:233:VAL:HG21	1.86	0.57
1:B:64:ILE:HB	1:B:71:ILE:HB	1.87	0.56
3:T:87:SER:H	3:T:88:PRO:HD3	1.69	0.56
2:A:35:TRP:HB3	2:A:208:ASP:H	1.71	0.56
2:A:97:ALA:HB1	3:T:134:LEU:HD11	1.87	0.56
2:A:151:LEU:HD23	2:A:182:ILE:HD11	1.88	0.56
2:A:94:PHE:O	2:A:96:GLY:N	2.33	0.56
2:A:3:GLU:OE1	2:A:193:THR:OG1	2.21	0.56
3:T:226:ARG:HG3	3:T:227:GLY:H	1.71	0.55
2:A:23:LEU:HD22	2:A:26:VAL:HG21	1.88	0.55
3:T:84:LEU:O	3:T:88:PRO:HD3	2.05	0.55
2:A:91:ASP:OD2	2:A:146:LYS:NZ	2.40	0.55
3:T:210:MET:O	3:T:214:ASN:ND2	2.37	0.55
2:A:136:ARG:HE	2:A:141:LEU:HD22	1.72	0.54
2:A:109:ASN:HB2	3:T:228:TYR:HA	1.89	0.53
2:A:210:VAL:HG23	2:A:224:PRO:HG3	1.89	0.53
1:B:38:ILE:HB	1:B:202:VAL:HG13	1.90	0.53
3:T:40:ASN:HA	3:T:41:ILE:HB	1.91	0.53
2:A:102:ASP:O	3:T:226:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:41:HIS:CD2	2:A:42:ASN:H	2.26	0.53
2:A:6:ILE:HG12	2:A:64:VAL:HG13	1.91	0.53
3:T:79:THR:HA	4:S:131:PRO:HG2	1.90	0.53
2:A:141:LEU:HB2	2:A:142:SER:HB2	1.90	0.52
3:T:85:LEU:O	3:T:90:GLY:HA3	2.09	0.52
1:B:132:VAL:HG11	1:B:157:ALA:HB2	1.91	0.52
1:B:112:LYS:HA	1:B:116:MET:HB3	1.92	0.52
1:B:3:ILE:HB	1:B:30:VAL:HB	1.91	0.52
3:T:80:VAL:HG13	3:T:110:ALA:HB1	1.92	0.52
2:A:251:LEU:HD22	2:A:256:ILE:HD12	1.92	0.51
4:S:126:LEU:N	4:S:128:PHE:O	2.43	0.51
1:B:152:ARG:NH1	1:B:172:PRO:O	2.41	0.51
2:A:70:THR:O	2:A:75:THR:OG1	2.22	0.51
3:T:24:LYS:HD2	3:T:131:THR:HG22	1.93	0.51
2:A:71:LEU:HD22	2:A:72:THR:HG23	1.92	0.51
3:T:35:VAL:HG13	3:T:116:ARG:HD2	1.92	0.50
1:B:132:VAL:O	1:B:134:LEU:N	2.44	0.50
3:T:209:PHE:HZ	4:S:43:GLY:HA2	1.77	0.50
2:A:102:ASP:OD1	3:T:226:ARG:NH2	2.44	0.50
2:A:5:ILE:HB	2:A:65:THR:HG23	1.94	0.50
1:B:12:TYR:O	1:B:20:HIS:N	2.45	0.49
4:S:52:GLY:H	4:S:53:ARG:HB2	1.77	0.49
1:B:170:ASP:HA	1:B:202:VAL:HG23	1.93	0.49
1:B:279:ALA:HA	2:A:256:ILE:HD11	1.94	0.49
3:T:231:SER:C	3:T:233:HIS:H	2.15	0.49
2:A:38:ILE:HB	2:A:197:ILE:HG13	1.95	0.48
2:A:166:GLU:HA	2:A:198:THR:HG22	1.94	0.48
1:B:166:VAL:HG22	1:B:198:THR:HB	1.95	0.48
1:B:285:ARG:HD2	2:A:276:LEU:HB2	1.96	0.48
4:S:51:TYR:HB2	4:S:52:GLY:O	2.13	0.48
1:B:50:ILE:HG23	1:B:168:VAL:HG11	1.94	0.48
2:A:56:LEU:HD23	2:A:56:LEU:H	1.79	0.47
1:B:96:ASN:O	3:T:207:PRO:HB3	2.14	0.47
1:B:146:LEU:HD23	1:B:150:GLN:HB3	1.96	0.47
4:S:103:ARG:HA	4:S:106:LEU:HB2	1.96	0.47
2:A:182:ILE:HA	2:A:185:GLN:HG2	1.97	0.47
2:A:201:ILE:HD11	2:A:242:PRO:HG3	1.96	0.47
3:T:87:SER:H	3:T:88:PRO:CD	2.28	0.47
2:A:4:ASN:HD21	2:A:161:ILE:HD13	1.80	0.47
1:B:82:PRO:O	1:B:85:GLN:HG3	2.14	0.47
2:A:95:VAL:HG12	3:T:219:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:HA	1:B:13:GLN:HA	1.63	0.46
3:T:44:TYR:OH	3:T:116:ARG:NH2	2.48	0.46
2:A:276:LEU:HD12	2:A:277:SER:H	1.80	0.46
3:T:40:ASN:HB3	3:T:42:TRP:N	2.29	0.46
1:B:262:LEU:HD21	2:A:276:LEU:HD13	1.96	0.46
2:A:92:ASN:HD22	3:T:218:ASP:HB2	1.81	0.45
1:B:104:ARG:HB2	1:B:139:ALA:HB1	1.97	0.45
4:S:51:TYR:N	4:S:52:GLY:HA2	2.30	0.45
3:T:40:ASN:HB3	3:T:42:TRP:H	1.81	0.45
1:B:63:THR:HG22	1:B:72:THR:HG22	1.98	0.45
4:S:45:TYR:O	4:S:49:ILE:HG13	2.16	0.45
4:S:64:GLY:HA2	4:S:67:ILE:HD12	1.98	0.45
2:A:151:LEU:HD12	2:A:154:ILE:HD11	2.00	0.44
3:T:179:MET:HG3	3:T:204:LEU:HD13	1.99	0.44
2:A:109:ASN:ND2	3:T:228:TYR:HD2	2.16	0.44
2:A:71:LEU:HA	2:A:72:THR:HA	1.86	0.44
1:B:100:GLU:HG2	1:B:105:GLN:HB2	1.98	0.44
1:B:192:HIS:HA	1:B:197:LEU:HB3	1.99	0.44
3:T:60:ILE:HA	3:T:61:SER:CB	2.47	0.44
3:T:65:PHE:O	3:T:69:ILE:HG13	2.17	0.44
2:A:105:PHE:CE2	3:T:228:TYR:HB3	2.53	0.44
1:B:35:TYR:CD1	1:B:213:ALA:HA	2.53	0.44
3:T:20:ASP:HB2	3:T:22:ARG:N	2.33	0.44
4:S:65:PHE:CD1	4:S:77:CYS:HB2	2.53	0.44
1:B:192:HIS:HB2	1:B:199:ILE:HD12	1.99	0.44
4:S:38:THR:HB	4:S:143:GLN:HG2	1.99	0.44
1:B:246:ASP:OD1	1:B:247:VAL:N	2.51	0.43
1:B:99:PHE:HB3	3:T:207:PRO:HG3	2.00	0.43
1:B:86:HIS:HE1	1:B:165:LYS:HD2	1.83	0.43
4:S:57:LEU:HB2	4:S:85:GLY:O	2.17	0.43
1:B:95:GLU:OE2	1:B:152:ARG:NE	2.42	0.43
4:S:3:LYS:H	4:S:4:GLY:HA2	1.83	0.43
3:T:142:SER:HA	3:T:145:LYS:HE2	2.01	0.43
3:T:231:SER:OG	3:T:232:GLU:N	2.52	0.43
2:A:142:SER:HB3	2:A:145:GLN:HB2	1.99	0.43
1:B:268:PRO:HG3	1:B:277:TYR:HD2	1.84	0.43
1:B:41:HIS:HE2	1:B:244:GLN:HB2	1.84	0.43
3:T:23:ALA:HB1	3:T:250:TRP:CD1	2.54	0.43
2:A:145:GLN:HG2	2:A:148:ARG:NH2	2.34	0.43
2:A:55:GLY:HA3	2:A:80:ARG:HH21	1.84	0.43
1:B:104:ARG:NH1	1:B:126:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:112:ILE:HA	2:A:113:SER:HA	1.77	0.42
1:B:260:ARG:HB2	1:B:261:GLY:HA2	2.00	0.42
3:T:166:ARG:C	3:T:166:ARG:HE	2.22	0.42
3:T:233:HIS:HA	3:T:234:ARG:HA	1.84	0.42
2:A:180:LEU:HD11	2:A:203:GLU:HG3	2.00	0.42
1:B:107:ILE:HG23	1:B:158:GLY:HA2	2.01	0.42
3:T:89:ALA:HB3	3:T:94:TYR:CZ	2.54	0.42
4:S:65:PHE:CZ	4:S:69:ILE:HD11	2.54	0.42
2:A:99:VAL:HB	2:A:134:ALA:HA	2.00	0.42
2:A:10:HIS:HB2	2:A:61:GLN:HB2	2.00	0.42
3:T:132:GLN:HA	3:T:133:PRO:HD3	1.90	0.42
3:T:200:SER:O	3:T:203:PRO:HD2	2.19	0.42
2:A:231:GLY:O	2:A:234:LEU:HB2	2.20	0.42
2:A:45:GLY:O	2:A:47:SER:N	2.53	0.42
1:B:250:ALA:HA	2:A:243:PHE:CZ	2.54	0.42
3:T:226:ARG:HG3	3:T:227:GLY:N	2.34	0.42
2:A:263:GLN:HB3	2:A:267:GLU:HB2	2.02	0.42
2:A:94:PHE:HB3	3:T:166:ARG:NH1	2.35	0.42
2:A:110:ARG:HH22	3:T:227:GLY:HA2	1.84	0.42
4:S:86:THR:O	4:S:90:VAL:HG23	2.20	0.42
2:A:71:LEU:HB3	2:A:72:THR:OG1	2.20	0.41
2:A:113:SER:HA	2:A:114:ARG:HH11	1.85	0.41
1:B:41:HIS:NE2	1:B:244:GLN:HB2	2.35	0.41
3:T:164:ALA:O	3:T:168:VAL:HG23	2.20	0.41
1:B:5:PHE:HB2	1:B:28:LEU:HG	2.03	0.41
4:S:163:PRO:HB2	4:S:164:ASP:H	1.74	0.41
1:B:11:THR:HB	1:B:21:THR:HG22	2.03	0.41
2:A:35:TRP:HB3	2:A:208:ASP:N	2.33	0.41
4:S:50:LEU:HD22	4:S:162:LYS:HD2	2.02	0.40
4:S:52:GLY:HA3	4:S:53:ARG:HA	1.88	0.40
2:A:86:ILE:HD11	2:A:151:LEU:HD13	2.03	0.40
2:A:67:GLY:HA2	2:A:68:GLY:HA2	1.50	0.40
2:A:107:LEU:HD23	2:A:157:ILE:HD13	2.03	0.40
1:B:55:ALA:HB2	1:B:83:LEU:HD23	2.03	0.40
2:A:110:ARG:NH1	2:A:157:ILE:HD12	2.37	0.40
2:A:66:VAL:HG21	2:A:83:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

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	B	282/290 (97%)	262 (93%)	17 (6%)	3 (1%)	14 54
2	A	269/279 (96%)	243 (90%)	16 (6%)	10 (4%)	3 28
3	T	234/266 (88%)	201 (86%)	27 (12%)	6 (3%)	5 35
4	S	162/166 (98%)	142 (88%)	15 (9%)	5 (3%)	4 32
All	All	947/1001 (95%)	848 (90%)	75 (8%)	24 (2%)	5 36

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	GLY
2	A	21	PRO
2	A	95	VAL
3	T	41	ILE
3	T	87	SER
4	S	162	LYS
2	A	41	HIS
2	A	46	LYS
3	T	88	PRO
4	S	50	LEU
2	A	72	THR
2	A	93	GLN
2	A	140	SER
4	S	32	ALA
4	S	163	PRO
2	A	275	SER
3	T	60	ILE
2	A	89	ASN
2	A	191	ASN
3	T	231	SER
4	S	161	LEU
3	T	262	ILE

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Mol	Chain	Res	Type
1	B	196	GLY
1	B	115	GLY

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	B	233/237 (98%)	230 (99%)	3 (1%)	69 87
2	A	228/234 (97%)	209 (92%)	19 (8%)	11 41
3	T	205/230 (89%)	184 (90%)	21 (10%)	7 34
4	S	131/133 (98%)	124 (95%)	7 (5%)	22 57
All	All	797/834 (96%)	747 (94%)	50 (6%)	18 52

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	129	LEU
1	B	184	MET
1	B	202	VAL
2	A	13	TYR
2	A	35	TRP
2	A	42	ASN
2	A	53	LEU
2	A	56	LEU
2	A	65	THR
2	A	72	THR
2	A	85	MET
2	A	95	VAL
2	A	114	ARG
2	A	131	THR
2	A	141	LEU
2	A	146	LYS
2	A	155	VAL
2	A	186	LEU
2	A	201	ILE

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Mol	Chain	Res	Type
2	A	245	GLU
2	A	257	THR
2	A	276	LEU
3	T	20	ASP
3	T	32	ILE
3	T	41	ILE
3	T	47	LEU
3	T	61	SER
3	T	65	PHE
3	T	70	ARG
3	T	73	LEU
3	T	96	HIS
3	T	107	LEU
3	T	127	LEU
3	T	140	LEU
3	T	150	VAL
3	T	165	LEU
3	T	166	ARG
3	T	171	LEU
3	T	250	TRP
3	T	251	LEU
3	T	263	PHE
3	T	264	ARG
3	T	265	HIS
4	S	34	LYS
4	S	38	THR
4	S	39	LEU
4	S	73	TYR
4	S	106	LEU
4	S	130	TRP
4	S	144	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	93	GLN
2	A	147	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

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, 95^{th} 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	B	284/290 (97%)	-0.20	1 (0%)	92	87	67, 116, 172, 233	0
2	A	273/279 (97%)	-0.08	6 (2%)	62	48	86, 139, 196, 257	0
3	T	240/266 (90%)	-0.19	1 (0%)	92	87	92, 168, 219, 259	0
4	S	164/166 (98%)	-0.21	2 (1%)	79	67	90, 139, 200, 253	0
All	All	961/1001 (96%)	-0.17	10 (1%)	82	71	67, 136, 206, 259	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	111	GLN	4.6
4	S	97	ARG	4.4
1	B	220	HIS	3.4
3	T	37	LEU	3.1
2	A	172	ASP	2.7
4	S	2	THR	2.5
2	A	142	SER	2.2
2	A	49	LEU	2.1
2	A	107	LEU	2.1
2	A	42	ASN	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.