Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:49 PM GMT

PDB ID	:	3V15
Title	:	Crystal structure of the Fe(II)/alpha-ketoglutarate dependent taurine dioxygenase from Pseudomonas putida KT2440
Authors	:	Knauer, S.H.; Dobbek, H.
Deposited on	:	2011-12-09
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

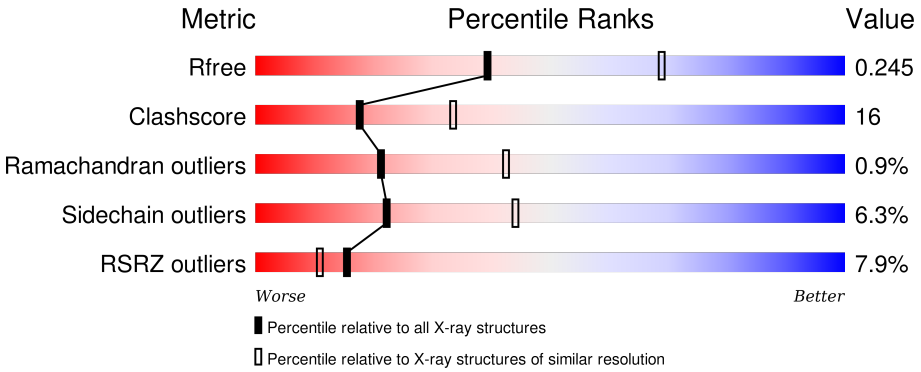
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	A	277	10% 69% 27%
1	B	277	8% 78% 18%
1	C	277	5% 77% 22%
1	D	277	9% 66% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9048 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 Alpha-ketoglutarate-dependent taurine dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2188	1388	395	403	2			
1	C	276	Total	C	N	O	S	0	0	0
			2194	1391	396	405	2			
1	B	275	Total	C	N	O	S	0	0	0
			2188	1388	395	403	2			
1	D	276	Total	C	N	O	S	0	0	0
			2194	1391	396	405	2			

- Molecule 2 is water.

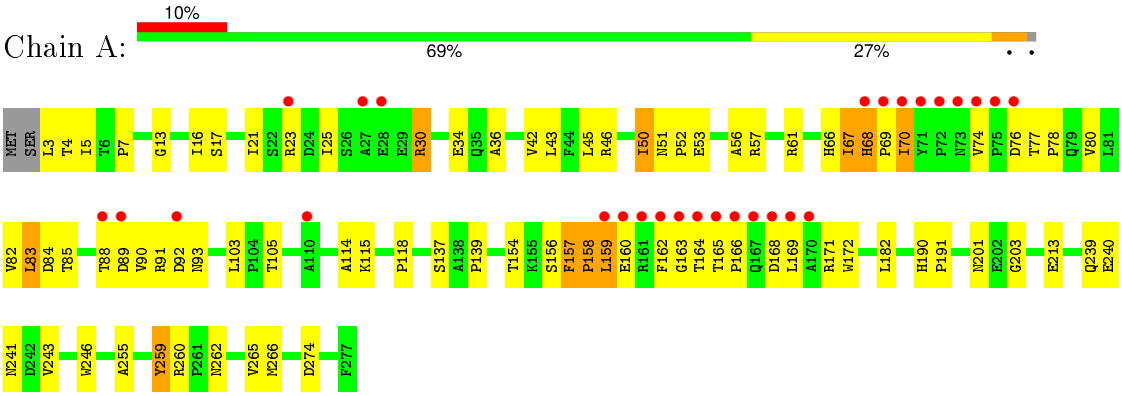
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	C	97	Total	O	0	0
			97	97		
2	B	81	Total	O	0	0
			81	81		
2	D	55	Total	O	0	0
			55	55		

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 errors 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.

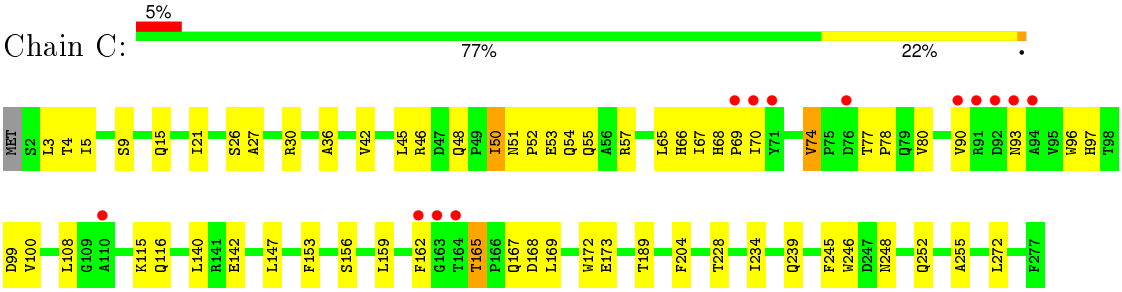
- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain A:



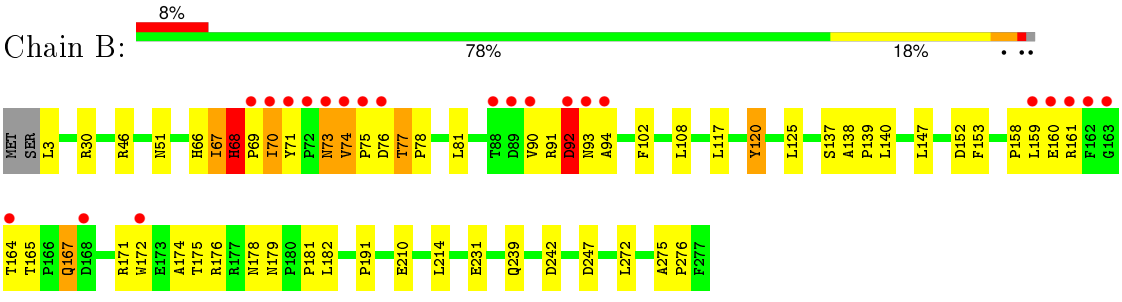
- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain C:



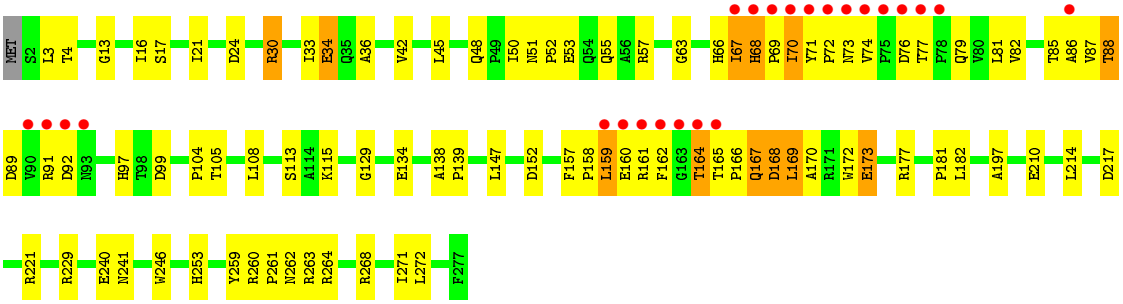
- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain B:



- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain D:


MET S2 L3 T4 G13 I16 S17 I21 D24 R30 I33 E34 Q35 A36 V42 L45 Q48 P49 I50 N51 P52 E53 Q54 Q55 A56 R57 G63 H66 I67 H68 P69 I70 Y71 P72 N73 V74 P75 D76 T77 P78 Q79 V80 L81 V82 T85 A86 V87 T88
D89 V90 R91 D92 N93 H97 T98 D99 P104 T105 L108 S113 A114 K115 G129 E134 A138 P139 L147 D152 F157 P158 L159 E160 R161 F162 G163 T164 T165 P166 Q167 D168 L169 A170 R171 W172 E173 R177 P181 L182 A197 E210 L214 D217
R221 R229 E240 N241 W246 H253 Y259 R260 P261 N262 R263 R264 R268 I271 L272 F277

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.89Å 101.85Å 162.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.78 – 2.60 29.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.78-2.60) 99.8 (29.39-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.183 , 0.254 0.171 , 0.245	Depositor DCC
R_{free} test set	2200 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 44029 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9048	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/2248	0.59	0/3074
1	B	0.40	0/2248	0.58	0/3074
1	C	0.40	0/2254	0.56	0/3082
1	D	0.40	0/2254	0.58	0/3082
All	All	0.40	0/9004	0.58	0/12312

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	68	HIS	Peptide
1	D	97	HIS	Peptide

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	2188	0	2136	90	0
1	B	2188	0	2136	58	0
1	C	2194	0	2141	46	0
1	D	2194	0	2141	85	0
2	A	51	0	0	2	0
2	B	81	0	0	4	1
2	C	97	0	0	3	0
2	D	55	0	0	7	1
All	All	9048	0	8554	275	1

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 16.

All (275) 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:68:HIS:HB3	1:A:69:PRO:HA	1.29	1.11
1:D:68:HIS:CE1	1:D:81:LEU:HD11	1.92	1.03
1:B:68:HIS:HB3	1:B:69:PRO:HD3	1.44	0.99
1:A:274:ASP:OD1	2:A:289:HOH:O	1.87	0.92
1:D:167:GLN:O	2:D:321:HOH:O	1.89	0.89
1:D:53:GLU:O	1:D:57:ARG:HG3	1.75	0.87
1:A:114:ALA:HA	1:A:266:MET:HG2	1.57	0.86
1:B:74:VAL:HG12	1:B:75:PRO:HD2	1.57	0.85
1:A:68:HIS:HB3	1:A:69:PRO:CA	2.08	0.84
1:A:16:ILE:HD11	1:A:43:LEU:HD13	1.60	0.83
1:A:157:PHE:H	1:A:158:PRO:HD2	1.45	0.82
1:A:42:VAL:HG23	1:A:246:TRP:HB3	1.62	0.80
1:C:189:THR:O	2:C:278:HOH:O	2.01	0.79
1:A:93:ASN:HB3	1:A:255:ALA:HB3	1.63	0.79
1:D:157:PHE:CE2	1:D:159:LEU:HB2	2.18	0.79
1:D:68:HIS:HE1	1:D:81:LEU:HD11	1.46	0.77
1:A:16:ILE:HB	1:A:45:LEU:HD21	1.66	0.77
1:C:93:ASN:HB3	1:C:255:ALA:HB3	1.64	0.77
1:A:46:ARG:NH2	1:A:239:GLN:HB3	2.01	0.75
1:B:91:ARG:HG2	1:B:92:ASP:H	1.51	0.75
1:D:79:GLN:O	2:D:286:HOH:O	2.06	0.73
1:A:70:ILE:O	1:A:70:ILE:HG22	1.86	0.73
1:A:162:PHE:HD2	1:A:169:LEU:HD21	1.55	0.71
1:B:3:LEU:N	2:B:318:HOH:O	2.23	0.70
1:D:55:GLN:OE1	2:D:283:HOH:O	2.09	0.70
1:A:45:LEU:HB2	1:A:243:VAL:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:H	1:D:161:ARG:HH22	1.39	0.69
1:D:89:ASP:OD2	1:D:164:THR:HG21	1.93	0.69
1:D:68:HIS:N	1:D:68:HIS:ND1	2.41	0.68
1:B:159:LEU:HG	1:B:172:TRP:CH2	2.29	0.68
1:D:24:ASP:CG	1:D:57:ARG:HH22	1.96	0.68
1:B:71:TYR:HB3	1:B:81:LEU:HD11	1.76	0.67
1:A:213:GLU:H	1:D:161:ARG:NH2	1.92	0.67
1:D:74:VAL:HG22	1:D:77:THR:O	1.95	0.67
1:A:52:PRO:HB3	1:A:74:VAL:HG21	1.76	0.67
1:D:66:HIS:ND1	1:D:272:LEU:HD21	2.10	0.67
1:D:81:LEU:HD12	1:D:81:LEU:N	2.11	0.66
1:A:46:ARG:HH21	1:A:239:GLN:HB3	1.59	0.66
1:B:68:HIS:HB3	1:B:69:PRO:CD	2.20	0.65
1:B:158:PRO:HG2	1:B:161:ARG:HD3	1.78	0.65
1:A:265:VAL:O	1:A:266:MET:HG3	1.97	0.65
1:D:214:LEU:O	2:D:281:HOH:O	2.15	0.65
1:C:252:GLN:OE1	2:C:318:HOH:O	2.14	0.65
1:B:172:TRP:CH2	1:B:176:ARG:HD3	2.32	0.64
1:A:66:HIS:NE2	1:A:69:PRO:HB3	2.11	0.64
1:D:88:THR:HG22	1:D:89:ASP:H	1.62	0.64
1:B:92:ASP:C	1:B:94:ALA:H	2.00	0.64
1:A:74:VAL:HG13	1:A:82:VAL:CG2	2.27	0.64
1:A:154:THR:O	1:A:158:PRO:HD3	1.97	0.64
1:A:67:ILE:HG22	1:A:78:PRO:HB2	1.78	0.64
1:A:51:ASN:OD1	1:A:53:GLU:HB3	1.98	0.64
1:B:191:PRO:HG3	2:B:319:HOH:O	1.96	0.64
1:B:179:ASN:O	2:B:329:HOH:O	2.15	0.64
1:A:159:LEU:HD11	1:A:169:LEU:HD22	1.81	0.63
1:A:74:VAL:HG23	1:A:77:THR:O	1.99	0.62
1:A:21:ILE:HD13	1:A:45:LEU:HD12	1.82	0.62
1:C:93:ASN:HB3	1:C:255:ALA:CB	2.29	0.62
1:C:3:LEU:C	1:C:3:LEU:HD23	2.20	0.62
1:D:157:PHE:CZ	1:D:159:LEU:HB2	2.35	0.62
1:B:167:GLN:HG3	1:B:167:GLN:O	1.99	0.61
1:D:104:PRO:CA	1:D:182:LEU:HD11	2.30	0.61
1:A:259:TYR:HD2	1:A:259:TYR:H	1.49	0.61
1:D:168:ASP:O	1:D:168:ASP:CG	2.39	0.61
1:D:104:PRO:HA	1:D:182:LEU:HD11	1.83	0.60
1:B:159:LEU:HD12	1:B:159:LEU:H	1.66	0.60
1:A:105:THR:HG23	1:A:105:THR:O	2.01	0.60
1:C:51:ASN:OD1	1:C:54:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:O	1:A:160:GLU:HG3	2.03	0.59
1:C:90:VAL:O	1:C:90:VAL:HG12	2.02	0.59
1:D:89:ASP:CG	1:D:164:THR:HG21	2.23	0.59
1:C:42:VAL:HG23	1:C:246:TRP:HB3	1.85	0.59
1:C:169:LEU:O	1:C:173:GLU:HG3	2.02	0.59
1:D:152:ASP:OD1	1:D:181:PRO:HG3	2.03	0.59
1:D:72:PRO:HG2	1:D:82:VAL:O	2.02	0.59
1:A:162:PHE:CD2	1:A:169:LEU:HD11	2.38	0.59
1:A:16:ILE:HB	1:A:45:LEU:CD2	2.33	0.58
1:B:152:ASP:OD2	1:B:181:PRO:HG3	2.04	0.58
1:D:85:THR:HB	1:D:264:ARG:H	1.68	0.58
1:A:16:ILE:CB	1:A:45:LEU:HD21	2.34	0.58
1:D:138:ALA:HB3	1:D:139:PRO:HD3	1.84	0.58
1:A:157:PHE:C	1:A:159:LEU:H	2.07	0.58
1:B:92:ASP:C	1:B:94:ALA:N	2.57	0.57
1:D:30:ARG:NH2	1:D:34:GLU:OE2	2.33	0.57
1:C:93:ASN:HA	1:C:97:HIS:CE1	2.39	0.57
1:D:260:ARG:HG3	1:D:261:PRO:HA	1.86	0.57
1:A:154:THR:O	1:A:158:PRO:CD	2.52	0.57
1:A:159:LEU:HD21	1:A:169:LEU:HD22	1.87	0.57
1:A:68:HIS:ND1	1:A:70:ILE:HD12	2.19	0.57
1:A:70:ILE:O	1:A:70:ILE:CG2	2.53	0.57
1:A:157:PHE:N	1:A:158:PRO:HD2	2.12	0.57
1:C:74:VAL:HG13	1:C:77:THR:O	2.05	0.57
1:B:137:SER:HB3	1:B:139:PRO:HD2	1.86	0.57
1:A:3:LEU:HD11	1:A:16:ILE:HG23	1.87	0.56
1:C:162:PHE:CD2	1:C:172:TRP:HD1	2.23	0.56
1:A:163:GLY:HA2	1:A:164:THR:C	2.27	0.55
1:D:87:VAL:HG12	1:D:88:THR:N	2.22	0.55
1:D:34:GLU:HG2	2:D:320:HOH:O	2.06	0.55
1:C:99:ASP:OD2	2:C:292:HOH:O	2.18	0.55
1:C:51:ASN:HB2	1:C:52:PRO:HD2	1.90	0.54
1:C:5:ILE:HD13	1:C:36:ALA:HB2	1.88	0.54
1:D:86:ALA:HB2	1:D:263:ARG:HD2	1.90	0.54
1:D:53:GLU:H	1:D:53:GLU:CD	2.11	0.53
1:A:159:LEU:HG	1:A:169:LEU:HD13	1.90	0.53
1:D:70:ILE:O	1:D:71:TYR:HB2	2.09	0.53
1:A:50:ILE:O	1:A:115:LYS:NZ	2.31	0.53
1:A:159:LEU:HG	1:A:162:PHE:HB3	1.91	0.53
1:A:69:PRO:O	1:A:70:ILE:HB	2.08	0.53
1:D:77:THR:HG23	1:D:79:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:CD1	1:A:30:ARG:HB2	2.38	0.52
1:B:68:HIS:HA	1:B:73:ASN:ND2	2.25	0.52
1:C:156:SER:HB2	1:C:204:PHE:CE1	2.45	0.52
1:C:45:LEU:N	1:C:45:LEU:HD12	2.25	0.52
1:A:16:ILE:O	1:A:45:LEU:CD2	2.57	0.51
1:C:159:LEU:HG	1:C:172:TRP:CH2	2.46	0.51
1:C:52:PRO:HB3	1:C:74:VAL:HG11	1.92	0.51
1:A:89:ASP:OD2	1:A:91:ARG:HG2	2.11	0.51
1:D:16:ILE:HB	1:D:45:LEU:HD11	1.93	0.51
1:B:108:LEU:HD23	1:B:108:LEU:C	2.31	0.51
1:A:162:PHE:HE2	1:A:168:ASP:OD2	1.94	0.50
1:D:166:PRO:O	1:D:169:LEU:HD23	2.10	0.50
1:D:173:GLU:HB3	1:D:177:ARG:HH12	1.76	0.50
1:C:67:ILE:O	1:C:69:PRO:HD3	2.11	0.50
1:D:259:TYR:O	1:D:262:ASN:HB2	2.12	0.49
1:B:91:ARG:HG2	1:B:92:ASP:N	2.24	0.49
1:C:26:SER:O	1:C:27:ALA:C	2.51	0.49
1:A:13:GLY:HA2	1:A:42:VAL:O	2.12	0.49
1:B:159:LEU:HG	1:B:172:TRP:CZ2	2.47	0.49
1:A:61:ARG:NH2	2:A:327:HOH:O	2.07	0.49
1:B:66:HIS:HB2	1:B:272:LEU:HD21	1.94	0.49
1:D:21:ILE:HG12	1:D:48:GLN:HG2	1.93	0.49
1:B:67:ILE:HG13	1:B:68:HIS:N	2.27	0.48
1:A:157:PHE:CB	1:A:172:TRP:HE1	2.26	0.48
1:D:165:THR:HG21	1:D:169:LEU:HB3	1.94	0.48
1:D:217:ASP:O	1:D:221:ARG:HG3	2.13	0.48
1:B:125:LEU:N	1:B:125:LEU:HD12	2.28	0.48
1:D:16:ILE:HB	1:D:45:LEU:CD1	2.43	0.48
1:C:165:THR:HG23	1:C:168:ASP:OD2	2.14	0.48
1:D:88:THR:HG22	1:D:89:ASP:N	2.28	0.48
1:D:72:PRO:O	1:D:81:LEU:HA	2.14	0.48
1:D:4:THR:O	1:D:16:ILE:HA	2.14	0.48
1:D:24:ASP:OD1	1:D:57:ARG:NH2	2.39	0.48
1:A:158:PRO:HA	1:A:172:TRP:CZ2	2.49	0.47
1:A:91:ARG:HD2	1:A:260:ARG:HH22	1.79	0.47
1:A:66:HIS:CD2	1:A:69:PRO:HB3	2.49	0.47
1:D:77:THR:HG23	1:D:79:GLN:CG	2.44	0.47
1:A:74:VAL:HG13	1:A:82:VAL:HG21	1.96	0.47
1:A:240:GLU:O	1:A:241:ASN:HB2	2.14	0.47
1:C:50:ILE:HG13	1:C:55:GLN:HB2	1.97	0.47
1:D:42:VAL:HG23	1:D:246:TRP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD23	1:D:108:LEU:C	2.35	0.47
1:A:137:SER:HB3	1:A:139:PRO:HD2	1.96	0.47
1:A:4:THR:HB	1:A:17:SER:OG	2.13	0.47
1:C:67:ILE:HG13	1:C:78:PRO:HB2	1.96	0.47
1:D:113:SER:OG	1:D:115:LYS:HE2	2.15	0.47
1:A:90:VAL:O	1:A:90:VAL:HG23	2.15	0.47
1:D:147:LEU:HD22	1:D:210:GLU:HB2	1.97	0.46
1:D:68:HIS:NE2	1:D:81:LEU:HD21	2.30	0.46
1:A:159:LEU:O	1:A:160:GLU:HB3	2.15	0.46
1:C:3:LEU:C	1:C:3:LEU:CD2	2.83	0.46
1:B:46:ARG:NH1	1:B:239:GLN:HG2	2.31	0.46
1:B:68:HIS:ND1	1:B:69:PRO:N	2.63	0.46
1:B:74:VAL:CG1	1:B:75:PRO:HD2	2.38	0.46
1:D:91:ARG:HD2	1:D:91:ARG:HA	1.75	0.46
1:D:51:ASN:HB2	1:D:52:PRO:HD2	1.96	0.46
1:C:93:ASN:CB	1:C:255:ALA:HB3	2.41	0.46
1:C:68:HIS:CE1	1:C:70:ILE:HG22	2.50	0.46
1:D:79:GLN:H	1:D:79:GLN:HG2	1.56	0.46
1:D:104:PRO:HG2	1:D:105:THR:HG22	1.98	0.46
1:B:182:LEU:HD12	1:B:182:LEU:C	2.36	0.46
1:A:160:GLU:CG	1:A:160:GLU:O	2.63	0.45
1:A:164:THR:O	1:A:165:THR:C	2.53	0.45
1:A:118:PRO:HG2	1:A:259:TYR:CD1	2.51	0.45
1:A:5:ILE:HD13	1:A:36:ALA:HB2	1.98	0.45
1:D:81:LEU:CD1	1:D:81:LEU:N	2.78	0.45
1:D:157:PHE:CZ	1:D:159:LEU:HG	2.51	0.45
1:B:247:ASP:OD2	2:B:328:HOH:O	2.21	0.45
1:D:81:LEU:H	1:D:81:LEU:HD12	1.82	0.45
1:B:167:GLN:O	1:B:171:ARG:HG3	2.16	0.45
1:A:7:PRO:HB2	1:B:120:TYR:CE1	2.52	0.45
1:D:71:TYR:HD2	1:D:81:LEU:HD23	1.81	0.45
1:D:3:LEU:C	1:D:3:LEU:HD23	2.37	0.45
1:C:15:GLN:NE2	1:C:46:ARG:HG3	2.31	0.45
1:A:23:ARG:HA	1:A:57:ARG:NH2	2.32	0.45
1:C:74:VAL:HG22	1:C:77:THR:H	1.82	0.45
1:B:102:PHE:O	1:B:182:LEU:HD21	2.17	0.45
1:A:159:LEU:HD13	1:A:159:LEU:HA	1.83	0.45
1:D:50:ILE:O	1:D:115:LYS:NZ	2.50	0.45
1:A:83:LEU:HD13	1:A:84:ASP:N	2.32	0.45
1:A:162:PHE:CZ	1:A:165:THR:HG21	2.52	0.44
1:C:30:ARG:C	1:C:30:ARG:HD3	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLU:O	1:C:57:ARG:HG3	2.16	0.44
1:A:165:THR:O	1:A:169:LEU:HD12	2.16	0.44
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.77	0.44
1:C:21:ILE:HG12	1:C:48:GLN:CG	2.48	0.44
1:C:46:ARG:NH2	1:C:239:GLN:HG3	2.32	0.44
1:C:67:ILE:O	1:C:67:ILE:HG23	2.17	0.44
1:B:120:TYR:CD2	1:B:120:TYR:N	2.86	0.44
1:B:67:ILE:HA	1:B:78:PRO:O	2.18	0.44
1:B:68:HIS:CB	1:B:69:PRO:CD	2.90	0.44
1:A:201:ASN:HD22	1:A:203:GLY:H	1.66	0.44
1:C:100:VAL:HG23	1:C:100:VAL:O	2.17	0.44
1:D:33:ILE:O	1:D:36:ALA:HB3	2.18	0.43
1:D:66:HIS:HB2	1:D:272:LEU:HG	2.00	0.43
1:D:68:HIS:CB	1:D:69:PRO:HD2	2.48	0.43
1:D:81:LEU:HD22	1:D:268:ARG:HH11	1.83	0.43
1:A:157:PHE:HB2	1:A:172:TRP:HE1	1.83	0.43
1:A:56:ALA:HB2	1:A:77:THR:HG21	2.00	0.43
1:A:91:ARG:CD	1:A:260:ARG:HH22	2.32	0.43
1:B:164:THR:O	1:B:164:THR:HG22	2.18	0.43
1:D:157:PHE:HB2	1:D:172:TRP:CZ2	2.54	0.43
1:D:166:PRO:C	1:D:168:ASP:N	2.71	0.43
1:C:42:VAL:HG11	1:C:234:ILE:HD11	2.01	0.43
1:C:96:TRP:CG	1:C:228:THR:HG21	2.54	0.43
1:A:159:LEU:HB3	1:A:162:PHE:H	1.83	0.43
1:C:165:THR:OG1	1:C:167:GLN:HB2	2.19	0.43
1:B:275:ALA:HA	1:B:276:PRO:HD3	1.75	0.43
1:B:160:GLU:N	1:B:160:GLU:CD	2.73	0.42
1:A:67:ILE:CG2	1:A:78:PRO:HB2	2.45	0.42
1:B:120:TYR:HD2	1:B:120:TYR:N	2.16	0.42
1:B:174:ALA:O	1:B:178:ASN:N	2.52	0.42
1:B:46:ARG:HD3	1:B:242:ASP:OD1	2.19	0.42
1:B:231:GLU:OE1	1:B:231:GLU:N	2.47	0.42
1:B:138:ALA:N	1:B:139:PRO:CD	2.82	0.42
1:A:25:ILE:HD12	1:A:61:ARG:NH1	2.35	0.42
1:B:67:ILE:HD12	1:B:78:PRO:HB2	2.01	0.42
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.49	0.42
1:A:157:PHE:C	1:A:159:LEU:N	2.73	0.42
1:A:93:ASN:HB3	1:A:255:ALA:CB	2.41	0.42
1:D:72:PRO:HB2	1:D:82:VAL:HB	2.01	0.42
1:D:72:PRO:CG	1:D:82:VAL:O	2.67	0.42
1:D:63:GLY:HA3	1:D:271:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD23	1:C:108:LEU:C	2.40	0.42
1:D:70:ILE:HG13	1:D:71:TYR:CD1	2.55	0.42
1:C:93:ASN:HA	1:C:97:HIS:HE1	1.81	0.42
1:B:69:PRO:CB	1:B:70:ILE:HA	2.50	0.41
1:B:3:LEU:C	1:B:3:LEU:HD13	2.40	0.41
1:D:168:ASP:C	1:D:170:ALA:H	2.23	0.41
1:D:67:ILE:HD12	1:D:67:ILE:H	1.86	0.41
1:A:190:HIS:HA	1:A:191:PRO:HD3	1.85	0.41
1:C:165:THR:CG2	1:C:168:ASP:OD2	2.69	0.41
1:B:175:THR:HA	1:B:178:ASN:HB2	2.01	0.41
1:A:162:PHE:CE2	1:A:168:ASP:OD2	2.73	0.41
1:D:104:PRO:N	1:D:182:LEU:HD11	2.36	0.41
1:A:259:TYR:O	1:A:262:ASN:HB2	2.20	0.41
1:B:117:LEU:HD12	1:B:239:GLN:HA	2.02	0.41
1:C:3:LEU:HD23	1:C:4:THR:N	2.36	0.41
1:D:4:THR:HG22	2:D:299:HOH:O	2.19	0.41
1:B:210:GLU:OE1	1:B:210:GLU:N	2.49	0.41
1:D:157:PHE:CZ	1:D:159:LEU:CG	3.03	0.41
1:D:13:GLY:HA2	1:D:42:VAL:O	2.20	0.41
1:C:66:HIS:HB2	1:C:272:LEU:HD21	2.02	0.41
1:A:91:ARG:HD2	1:A:260:ARG:NH2	2.35	0.41
1:C:140:LEU:HD12	1:C:140:LEU:HA	1.76	0.41
1:A:16:ILE:CD1	1:A:43:LEU:HD13	2.43	0.41
1:C:74:VAL:HG12	1:C:80:VAL:O	2.21	0.41
1:D:129:GLY:O	1:D:197:ALA:HA	2.21	0.41
1:A:66:HIS:CD2	1:A:68:HIS:H	2.39	0.41
1:B:69:PRO:HA	1:B:71:TYR:H	1.86	0.41
1:B:74:VAL:HB	1:B:77:THR:OG1	2.21	0.41
1:B:160:GLU:HB2	1:B:161:ARG:HH21	1.86	0.41
1:A:74:VAL:HG22	1:A:80:VAL:O	2.21	0.41
1:D:21:ILE:HG12	1:D:48:GLN:CG	2.50	0.41
1:A:7:PRO:HB2	1:B:120:TYR:CD1	2.55	0.41
1:C:108:LEU:O	1:C:248:ASN:N	2.52	0.41
1:D:99:ASP:OD2	1:D:253:HIS:HE1	2.04	0.41
1:D:70:ILE:HG13	1:D:71:TYR:N	2.35	0.41
1:B:51:ASN:C	1:B:51:ASN:OD1	2.60	0.41
1:D:240:GLU:O	1:D:241:ASN:HB2	2.21	0.41
1:B:174:ALA:O	1:B:178:ASN:HB2	2.21	0.40
1:B:46:ARG:CD	1:B:242:ASP:OD1	2.69	0.40
1:B:70:ILE:H	1:B:70:ILE:HG12	1.64	0.40
1:B:159:LEU:HB2	1:B:160:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG23	1:A:51:ASN:N	2.36	0.40
1:D:21:ILE:HD13	1:D:45:LEU:HD22	2.02	0.40
1:D:229:ARG:NH1	2:D:328:HOH:O	2.53	0.40

All (1) 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)
2:B:300:HOH:O	2:D:311:HOH:O[2_454]	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	273/277 (99%)	253 (93%)	15 (6%)	5 (2%)	11	21
1	B	273/277 (99%)	261 (96%)	10 (4%)	2 (1%)	26	51
1	C	274/277 (99%)	255 (93%)	18 (7%)	1 (0%)	39	65
1	D	274/277 (99%)	255 (93%)	17 (6%)	2 (1%)	26	51
All	All	1094/1108 (99%)	1024 (94%)	60 (6%)	10 (1%)	21	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	158	PRO
1	B	68	HIS
1	D	88	THR
1	A	166	PRO
1	A	70	ILE
1	A	157	PHE

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Mol	Chain	Res	Type
1	D	158	PRO
1	C	115	LYS
1	B	92	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	233/235 (99%)	219 (94%)	14 (6%)	24	47
1	B	233/235 (99%)	216 (93%)	17 (7%)	17	35
1	C	234/235 (100%)	224 (96%)	10 (4%)	35	64
1	D	234/235 (100%)	216 (92%)	18 (8%)	16	31
All	All	934/940 (99%)	875 (94%)	59 (6%)	22	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	34	GLU
1	A	50	ILE
1	A	67	ILE
1	A	76	ASP
1	A	83	LEU
1	A	85	THR
1	A	88	THR
1	A	92	ASP
1	A	156	SER
1	A	159	LEU
1	A	171	ARG
1	A	182	LEU
1	A	259	TYR
1	C	9	SER
1	C	50	ILE
1	C	65	LEU
1	C	74	VAL

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Mol	Chain	Res	Type
1	C	116	GLN
1	C	142	GLU
1	C	147	LEU
1	C	153	PHE
1	C	165	THR
1	C	245	PHE
1	B	30	ARG
1	B	67	ILE
1	B	70	ILE
1	B	73	ASN
1	B	74	VAL
1	B	76	ASP
1	B	77	THR
1	B	90	VAL
1	B	92	ASP
1	B	93	ASN
1	B	120	TYR
1	B	140	LEU
1	B	147	LEU
1	B	153	PHE
1	B	165	THR
1	B	167	GLN
1	B	214	LEU
1	D	17	SER
1	D	30	ARG
1	D	34	GLU
1	D	67	ILE
1	D	68	HIS
1	D	70	ILE
1	D	73	ASN
1	D	76	ASP
1	D	92	ASP
1	D	134	GLU
1	D	159	LEU
1	D	160	GLU
1	D	162	PHE
1	D	164	THR
1	D	167	GLN
1	D	168	ASP
1	D	169	LEU
1	D	173	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	201	ASN
1	C	68	HIS
1	C	93	ASN
1	C	201	ASN
1	C	253	HIS
1	B	73	ASN
1	B	201	ASN
1	D	41	GLN
1	D	201	ASN

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	A	275/277 (99%)	0.25	28 (10%) 9 5	18, 47, 144, 231	0
1	B	275/277 (99%)	-0.14	22 (8%) 15 10	16, 34, 113, 223	0
1	C	276/277 (99%)	-0.20	13 (4%) 35 28	15, 34, 97, 186	0
1	D	276/277 (99%)	0.19	24 (8%) 13 8	19, 41, 146, 225	0
All	All	1102/1108 (99%)	0.02	87 (7%) 15 11	15, 38, 127, 231	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	PRO	12.4
1	D	74	VAL	11.3
1	B	75	PRO	11.0
1	A	163	GLY	10.6
1	D	75	PRO	10.6
1	A	69	PRO	10.6
1	A	162	PHE	10.5
1	D	72	PRO	8.7
1	D	162	PHE	8.6
1	D	68	HIS	8.6
1	B	70	ILE	8.4
1	D	93	ASN	8.2
1	A	70	ILE	8.1
1	A	164	THR	8.1
1	A	166	PRO	8.1
1	D	76	ASP	7.6
1	D	71	TYR	7.3
1	A	161	ARG	7.0
1	B	72	PRO	6.9
1	B	76	ASP	6.7
1	B	74	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	70	ILE	6.4
1	A	68	HIS	6.4
1	A	165	THR	6.2
1	B	71	TYR	6.1
1	A	71	TYR	5.9
1	C	71	TYR	5.6
1	D	73	ASN	5.6
1	D	159	LEU	5.5
1	A	160	GLU	5.2
1	A	167	GLN	5.1
1	D	77	THR	5.1
1	C	92	ASP	5.1
1	A	169	LEU	4.6
1	B	159	LEU	4.6
1	C	69	PRO	4.5
1	A	76	ASP	4.3
1	D	161	ARG	4.3
1	A	92	ASP	4.3
1	B	93	ASN	4.3
1	D	92	ASP	4.3
1	D	164	THR	4.3
1	D	91	ARG	4.2
1	C	164	THR	4.2
1	C	162	PHE	4.1
1	B	69	PRO	4.1
1	D	67	ILE	4.0
1	D	163	GLY	4.0
1	D	160	GLU	3.8
1	D	78	PRO	3.7
1	D	90	VAL	3.7
1	A	72	PRO	3.7
1	A	170	ALA	3.6
1	B	162	PHE	3.5
1	C	163	GLY	3.4
1	B	73	ASN	3.3
1	A	88	THR	3.3
1	B	90	VAL	3.3
1	B	163	GLY	3.2
1	A	159	LEU	3.2
1	A	89	ASP	3.1
1	B	164	THR	3.0
1	A	23	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	91	ARG	2.9
1	D	165	THR	2.7
1	C	90	VAL	2.7
1	D	86	ALA	2.6
1	A	75	PRO	2.6
1	B	92	ASP	2.5
1	C	70	ILE	2.5
1	A	27	ALA	2.5
1	B	94	ALA	2.4
1	A	168	ASP	2.4
1	B	89	ASP	2.4
1	B	172	TRP	2.4
1	B	88	THR	2.4
1	B	161	ARG	2.3
1	C	93	ASN	2.3
1	C	76	ASP	2.3
1	C	110	ALA	2.3
1	A	73	ASN	2.2
1	B	160	GLU	2.2
1	B	168	ASP	2.2
1	A	110	ALA	2.1
1	C	94	ALA	2.1
1	A	28	GLU	2.1
1	A	74	VAL	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.